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Crown Ether Stereoisomerism: Implications in Metal Ion Extraction and Ionic Liquid Design

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CROWN ETHER STEREOISOMERISM: IMPLICATIONS IN METAL ION

EXTRACTION AND IONIC LIQUID DESIGN

By

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ABSTRACT

CROWN ETHER STEREOISOMERISM: IMPLICATIONS IN METAL ION EXTRACTION AND IONIC LIQUID DESIGN

by

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Since their discovery more than four decades ago, crown ethers (CEs) have been the subject of intense investigation in a number of fields. Although many of the structural features that govern the behavior of these compounds have been thoroughly explored, the effect of their stereochemistry has received relatively little attention.

In the present work, crown ether stereochemistry is shown to have important implications in both the design of ternary (*i.e.,* three-component) ionic liquids (TILs) and metal ion extraction. Specifically, as a first step toward the development of guidelines for the rational design of ternary ionic liquids employing crown ethers as the neutral extractant, a systematic examination of the effect of crown ether stereochemistry (employing dicyclohexano-18-crown-6 (DCH18C6) as a representative crown compound), along with ring size, the nature and number of donor atoms, and the presence of functional groups, on the thermal properties (*i.e.,* melting point or glass transition; decomposition or evaporation) of these compounds was carried out. Stereochemistry was found to have no appreciable impact on the onset temperature for mass loss. Rather, molecular weight and aromaticity were found to be more influential. Stereochemistry

was, however, found to significantly affect the melting point of a TIL prepared from it; while the metal-CE formation constant, which varies with stereoisomer was observed to determine the onset temperature for mass loss of the TIL.

To explore the implications of crown ether stereoisomerism in metal ion extraction, the formation constants for alkaline earth cation complexes with the isomers of DCH18C6 and selected stereoisomers of di-*tert*-butylcyclohexano-18-crown-6 (DtBuCH18C6) were measured. These values were found to vary inversely with the ligand strain (*i.e.,* reorganizational) energy for the isomer, as determined by molecular mechanics calculations. Using this relationship (along with additional identification methods), three isomers of DtBuCH18C6, which were separated by preparative LC, were definitively identified. Three additional isomers were partially identified.

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Chapter 1 : Introduction

1.1: History of Crown Ethers

Although macrocyclic polyethers were first described by Lüttringhaus in 1937 (*1*) what we now know as "crown ethers" were first reported by Pedersen nearly 50 years ago (*2*). In his work, Pedersen sought to prepare a series of bi- and multidentate phenolic ligands for use in examining the catalytic properties of the vanadyl group, VO. A by-product whose structure was ultimately determined to be dibenzo-18-crown-6 (Figure 1.1) was formed, however. Subsequent work with this compound and a number of related ones demonstrated that they are able to complex alkali and alkaline earth metal cations, an ability exhibited by a few other complexing agents (*2, 3*).
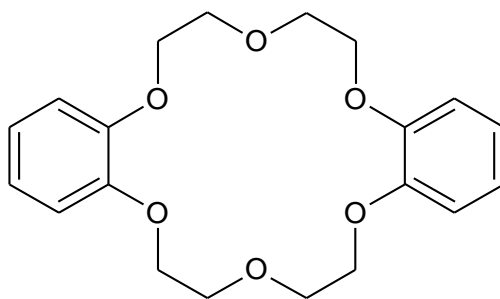
Figure 1.1: Dibenzo-18-crown-6 (DB18C6)

1.2: Complexation Ability of Crown Ethers

In the decades since these initial reports, crown ethers and their complexation properties have been thoroughly studied (*4-7*). As a result, it is now well known that the complexation ability of a crown ether is dependent on a number of factors, among them the crown ether ring size, the number and location of donor atoms, and the presence of functional groups in the crown ether. Changes in ring size can have a significant

influence on which ions are likely to form a stable complex with a given crown ether. Typically ions with an ionic radius close to the size of the crown ether ring have higher formation constants than ions that are either too large or too small to fully interact with the donor atoms present in the ring. There are exceptions to this rule, however. For example, although the ring size of 15-crown-5 is a better match for sodium, as can be seen from Figure 1.2, 18-crown-6 has a higher formation constant for sodium in methanol. Interestingly, as can be seen from Figure 1.3, 18-crown-6 actually has the highest formation constant for each of the cations examined, indicating that while cation-crown cavity size matching does influence complexation, other factors (*e.g.,* crown ether flexibility) also exert an impact on the formation constants observed (*8*).
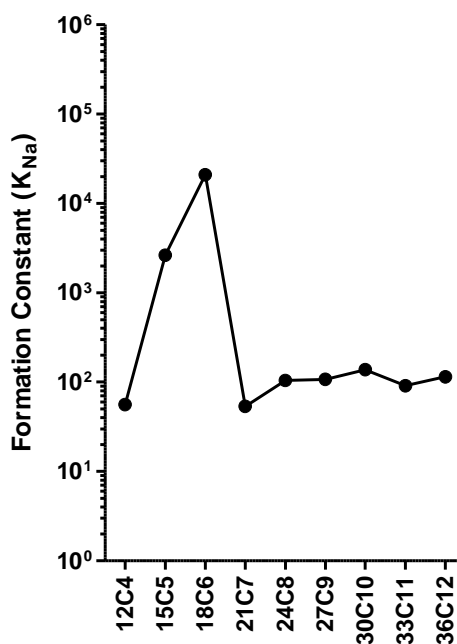
Figure 1.2: Relationship between Crown Ether Ring Size and the Formation Constants for Sodium (*9*)
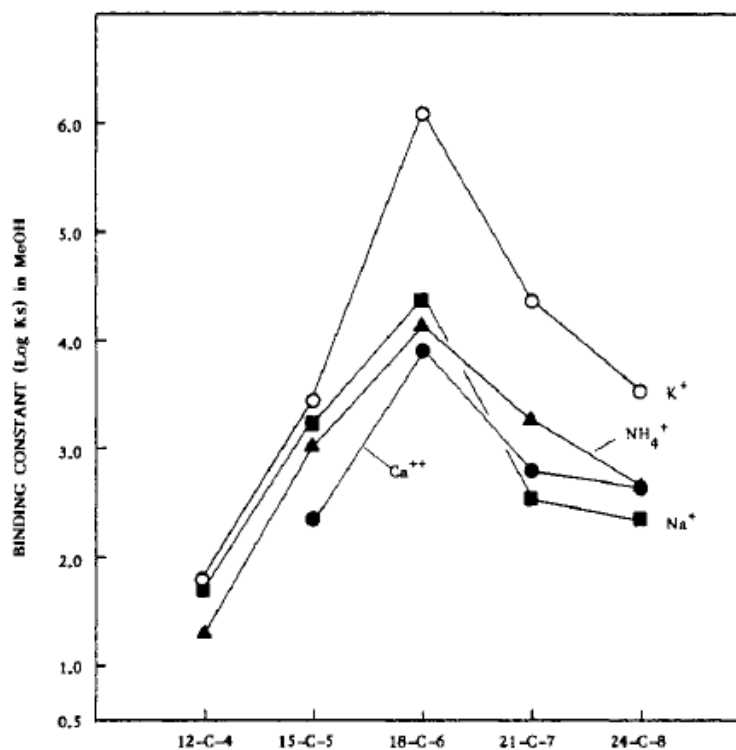
Figure 1.3: Cation Binding by Simple Crown Ethers (*8*)

Another factor that is known to influence the complexation ability of a crown ether is the identity and the location of donor atoms present in the ring. The only difference between the two crown ethers depicted in Figure 1.4 is the location of the sulfur atoms, but this subtle difference results in a more than two order of magnitude difference in the formation constants for most of the cations studied (*10*). The number and identity of functional groups on the crown ring can also influence the formation constants (*4-7*). For example, Izatt *et al.* (*11*) has shown the addition of a pyridine group to an 18-crown-6 ring substantially increases the formation constant for calcium and silver ions *versus* 18-crown-6. In addition, Zhang *et al.(12)* were able to enhance the

selectivity of diaza-18-crown-6 for potassium and barium ions by the addition of quinolone and substituted phenol groups.
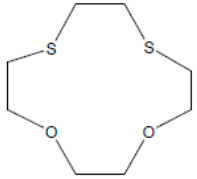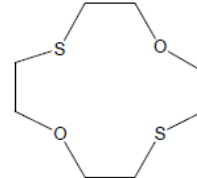
Thiocrown ethers	Cation	$LogK_{e(1:1)}$
	Na^+	5,201411
	K^+	3,668301
	Ca^{2+}	4,322273
	Zn^{2+}	3,61645
	Mg^{2+}	4,359118
	Ag^+	4,193181
	Fe^{2+}	4,805206
	Na^+	4,390158
	K^+	6,070913
	Ca^{2+}	6,125411
	Zn^{2+}	3,982648
	Mg^{2+}	5,055571
	Ag^+	3,812031
	Fe^{2+}	6,405304

Figure 1.4: Formation Constants for (top) 1,4-dithio-12-crown-4 and (bottom) 1,7-dithio-12- crown-4 in a 1:1 (dioxane:water) Mixture (Modified from (*10*))

1.3: Stereochemical Effects of Crown Ethers

In constrast to these structural modifications, whose effects on complex formation have been studied in depth, crown ether stereochemistry has garnered relatively little attention. The most well-known crown ether stereoisomer effects are those arising in dicyclohexano-18-crown-6 (DCH18C6), which can exist as five distinct isomers (Figures 1.5 and 1.6). Of these, the *cis-syn-cis* and *cis-anti-cis* forms, which are the major constituents of commercial preparation of DCH18C6, have been the most thoroughly investigated. It is now well established that these two isomers differ significantly in their metal ion complexation properties. For example, Lin *et al.* (*13*) have shown that better

fractionation of zinc isotopes occurs with the *cis-syn-cis* isomer than the *cis-anti-cis* isomer. Other work by Izatt *et al.* (*14*) using isothermal titration calorimetry (Table 1.1) has shown that the *cis-syn-cis* isomer is generally a better metal ion complexing agent than the *cis-anti-cis* form. Using ion-selective electrodes (Table 1.1), Frensdorff (*15*) has shown that the same trend holds for monovalent metal cations in methanol. Although some exceptions have been reported (*e.g.,* amino acid complexation (*16*)), for the most part, the *cis-syn-cis* form typically yields stronger complexes than does the *cis-anti-cis* form. Although the magnitude of the differences between the metal ion formation constants observed with the two forms of DCH18C6 clearly indicates that crown ether stereochemistry is an area worthy of further study, the difficulty in isolating or synthesizing individual crown ether stereoisomers has complicated such work. In fact, it was not until the development of new synthetic routes that allowed for the isomer-specific synthesis of the *trans-syn-trans*, *trans-anti-trans*, and *cis-trans* isomers that studies of DCH18C6 could be extended to all of its five forms (*17-19*). With these others isomers in hand, Hay *et al.* (*20*) were able to explain the relationship between the ligand strain energy of the various forms (as calculated by MM3) and formation constants with potassium ion. Similarly, Vogel (*21*) determined the effect of crown ether stereoisomerism on complex formation between all five DCH18C6 isomers and various alkali metals. Dietz *et al. (22)* were able to determine the effect of DCH18C6 stereoisomerism on the ability of the various isomers to form synergistic complexes in the extraction of alkaline earth metal ions by organophosphorus reagents. In all of these studies, it was concluded that the isomers differ significantly in their complex-forming

abilities, in some cases by as much as 1-2 orders of magnitude (Figure 1.7). In addition, the strength of metal ion complex formation was consistently found to follow the order: *cis-syn-cis* > *cis-anti-cis* > *cis-trans* > *trans-syn-trans* > *trans-anti-trans.* It was anticipated that the knowledge gained in the study of these isomers would facilitate studies of more complex families of stereoisomers, most notably the di-*tert*-butyl-substituted analogs of DCH18C6 (abbreviated DtBuCH18C6).

Table 1.1: Formation Constant Comparison between the Two Most Prominent Isomers of DCH18C6

	Log $K_{f\,in\,MeOH}$ (*15*)		Log $K_{f\,in\,Water}$ (*14*)	
	K^+	Cs^+	K^+	Cs^+
DCH18C6A	6.01	4.61	2.02	0.96
DCH18C6B	5.38	3.49	1.63	NM
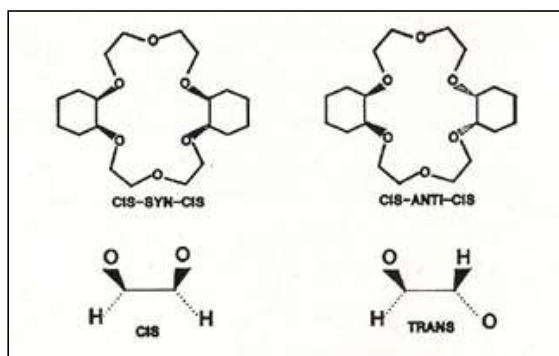
Figure 1.5: Stereochemistry of DCH18C6
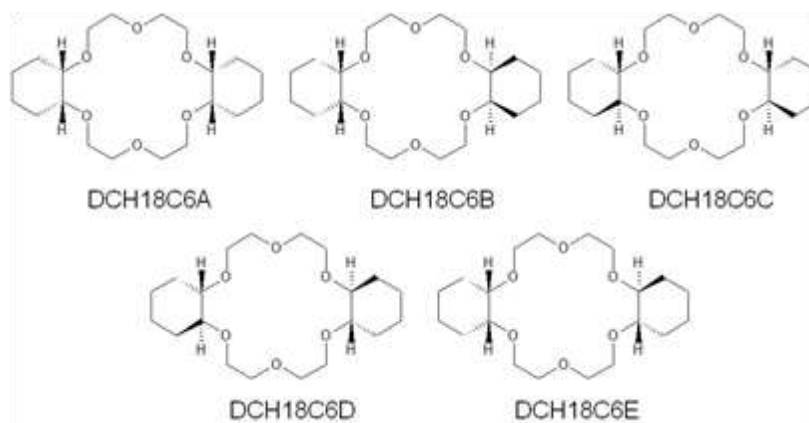
Figure 1.6: Stereoisomers of Dicyclohexano-18-crown-6 (DCH18C6)
Top Row: (left) *cis-syn-cis* (A); (middle) *cis-anti-cis* (B); (right) *trans-syn-trans* (C);
Bottom Row: (left) *trans-anti-trans* (D); (right) *cis-trans* (E)
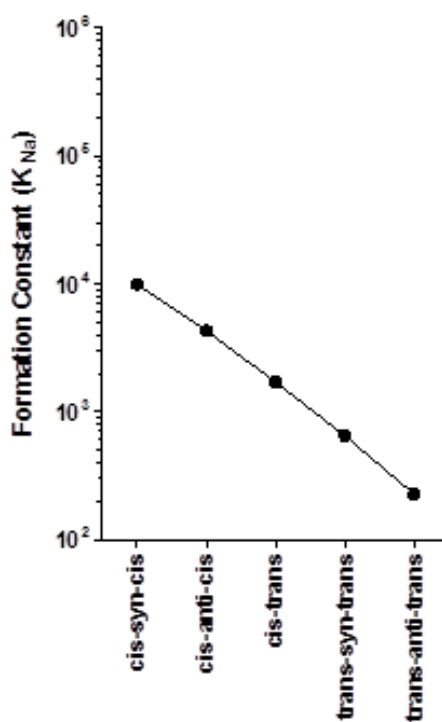
Figure 1.7: Formation Constants for the Family of DCH18C6 with Sodium (*21*)

This particular derivative of DCH18C6 is of interest because the addition of a *tert*-butyl group to each of the cyclohexano groups results in a substantial decrease in the water solubility of the crown ether. That is, although DCH18C6 forms strong complexes with strontium ion, it is too water soluble to permit its use in large-scale extraction processes. In contrast, the di-*tert*-butyl derivative has been successfully employed as the basis of an extraction chromatographic resin (*23*) for the separation and preconcentration of radiostrontium from biological and environmental samples and in the SREX process (*24*), which is used to remove radiostrontium from nuclear waste.

Unfortunately the addition of *tert*-butyl groups to DCH18C6 raises the number of possible isomers from five to forty (with the twelve *cis-cis* isomers expected to be predominant) (Figures 1.8, 1.9 and 1.10). This is the result of the harsh conditions necessary to hydrogenate the more sterically hindered di-*tert*-butylbenzo-18-crown-6 precursor *versus* the hydrogenation of dibenzo-18-crown-6. As was the case for DCH18C6, little research has been performed to date on these isomers. Molecular mechanics calculations by Hay *et al*. (*25, 26*) however, which indicate that the effect of variations in crown ether stereochemistry on the expected metal complexation and extraction ability is as great (or greater than) the effect observed upon changing the ring size of the crown ether (Figure 1.11), suggest that this is a promising area for investigation.
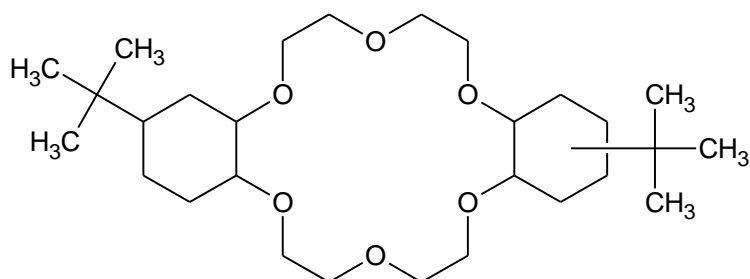
Figure 1.8: 4,4'(5')-di(*tert*-butylcyclohexano)-18-crown-6 (DtBuCH18C6)
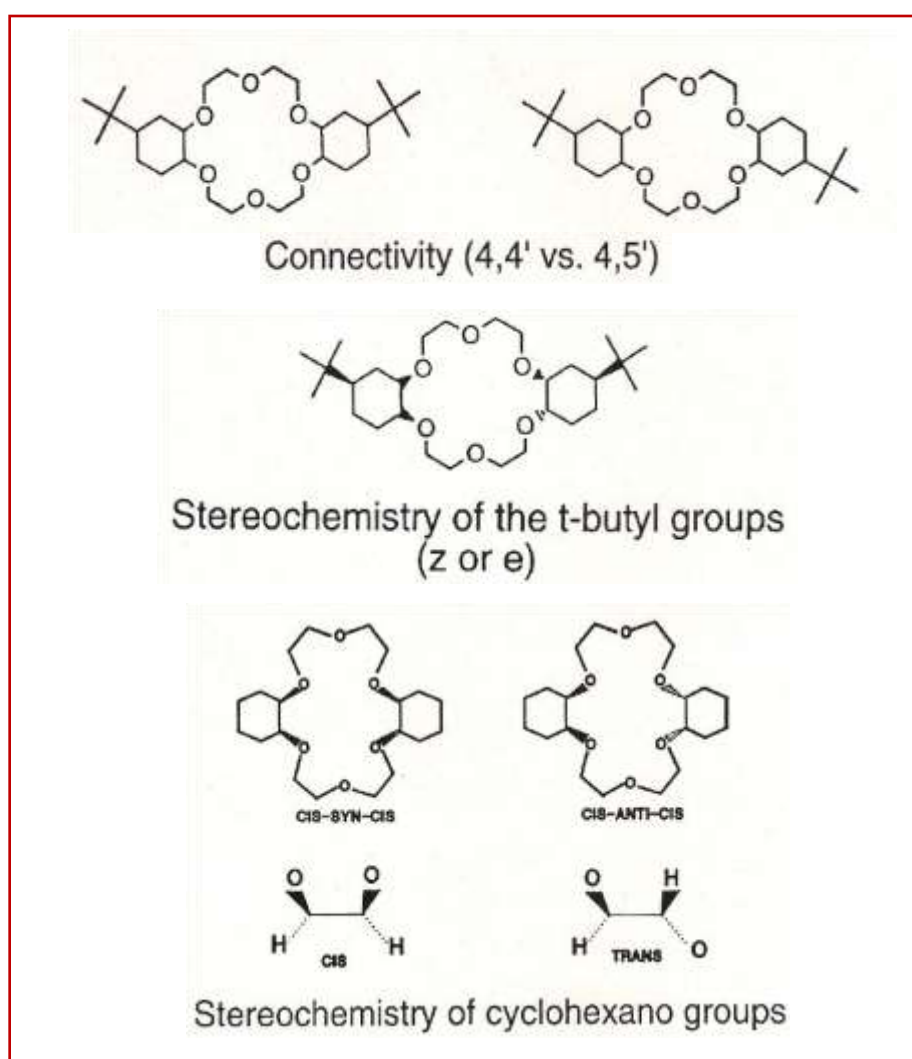
Figure 1.9: Stereochemistry of DtBuCH18C6

4(z),5'(z)-cis-syn-cis

4(z),5'(e)-cis-syn-cis

4(e),5'(e)-cis-syn-cis

4(z),5'(z)-cis-anti-cis

4(z),5'(e)-cis-anti-cis

4(e),5'(e)-cis-anti-cis

4(z),4'(z)-cis-syn-cis

4(z),4'(e)-cis-syn-cis

4(e),4'(e)-cis-syn-cis

4(z),4'(z)-cis-anti-cis

4(z),4'(e)-cis-anti-cis

4(e),4'(e)-cis-anti-cis
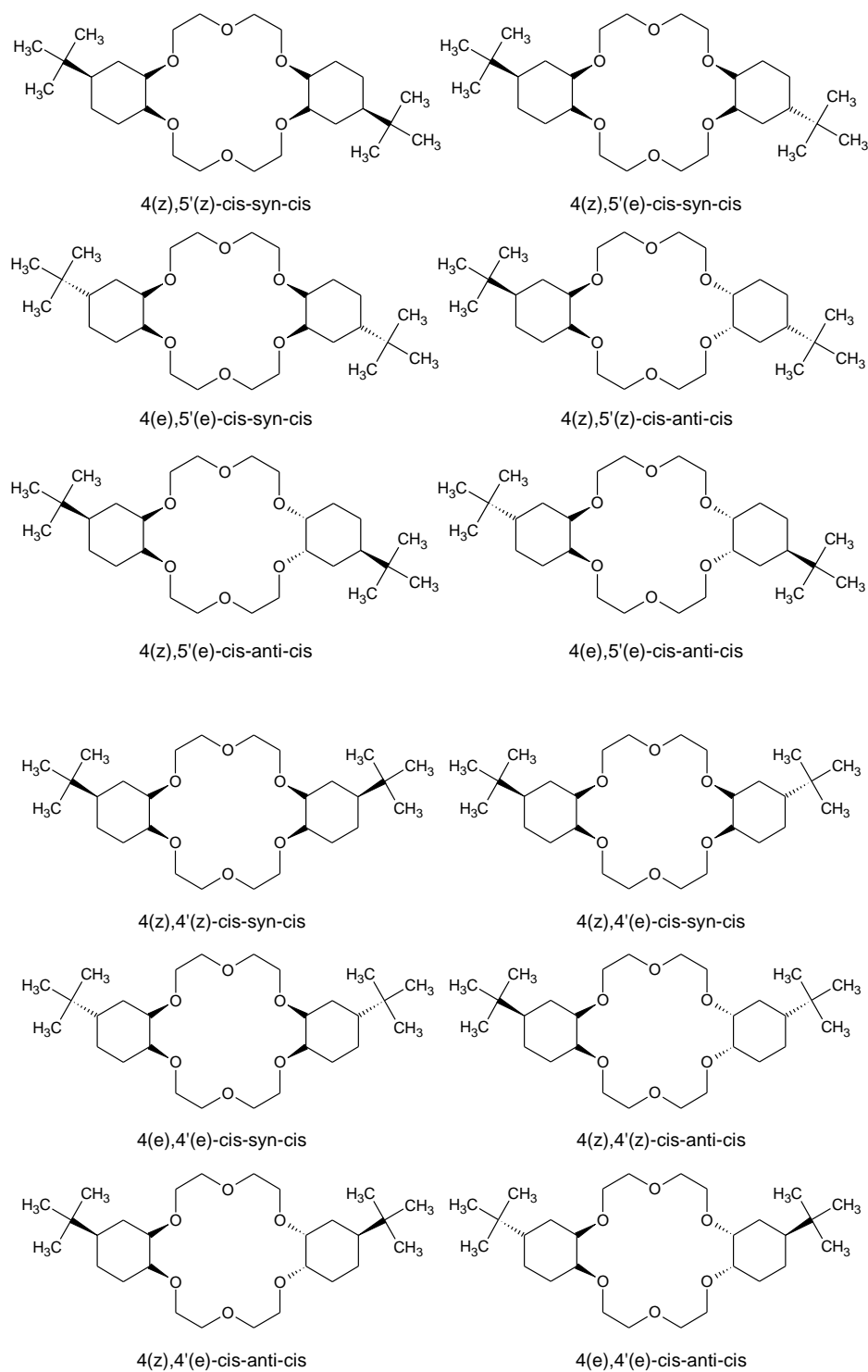
Figure 1.10: The *cis-cis* Isomers of DtBuCH18C6
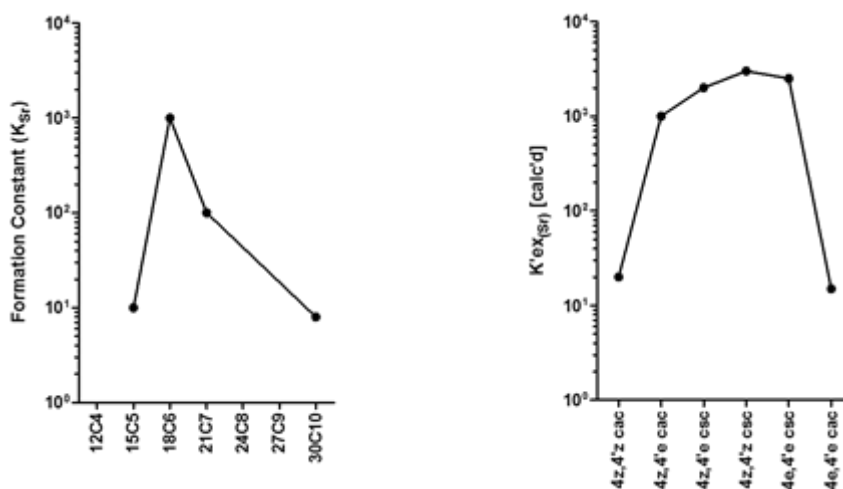
Figure 1.11: (left) The Effect of Ring Size on the Formation Constants of Strontium-Crown Ether Complexes, and (right) The Effect of Stereochemistry on the Conditional Extraction Constants for Strontium Extraction by DtBuCH18C6.

1.4: Ionic Liquids

Since their introduction in the early 1990's (*27*), ionic liquids (low-melting ionic salts) have been the subject of intense study, a result of their many unique properties (*e.g.,* facile tunability, high thermal stability, wide liquid range, high ionicity, and low volatility) (*28-34*). Almost without exception, the ILs examined to date have consisted of two components. Recently, however, the first examples of a new class of ionic liquids comprising three components have been synthesized (*35-40*). These new ionic liquids, termed "ternary" ionic liquids (TILs), are composed of a cation, a neutral complexing agent for that cation, and a number of different anions (Figure 1.12). Although similar in many respects to traditional (*i.e.,* two component) ionic liquids, the addition of a third

component greatly increases the potential tunability of the TILs. To date, nearly all of the published work in this area has involved the use of a crown ether as the neutral complexing agent. As was the case in the initial investigations of traditional ionic liquids, an examination of the relationship between the properties of the individual components and those of the resultant ionic liquids is essential to the development of guidelines for the rational design of new TILs (*28-30, 33, 41-50*). The ease with which the structural characteristics of a crown ether (*e.g.,* ring size, substitutions, and stereochemistry) provides significant opportunities to obtain insights into structure-property relationships in this unique new family of solvents.
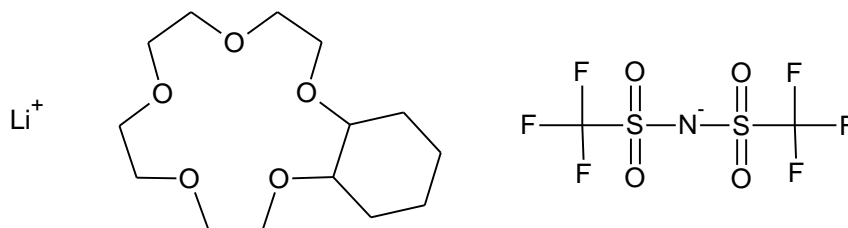
Figure 1.12: The First Crown Ether-Based Ternary Ionic Liquid (lithium cyclohexano-15-crown-5 *bis*(trifluoromethylsulfonyl)imide)

1.5: Overview of Chapters

In Chapter 2, the thermal properties (*e.g.,* onset temperature of mass loss, melting point, and glass transition) of a variety macrocyclic polyethers are explored as a first step toward their eventual use in the synthesis of ternary ionic liquids. The results are shown to lead to the identification of principles for the design of new TILs.

In Chapter 3, the formation of ternary ionic liquids incorporating macrocyclic polyethers is explored, with emphasis on the effect of crown ether stereochemistry on

TIL properties. This study, which was designed to provide information on the influence of the individual components of the TIL on its properties, has revealed a relationship between the thermal stability of a TIL and the formation constant, K_f, of the metal-crown ether complex.

In Chapter 4, isothermal titration calorimetry (ITC) studies of the complexation of various alkaline earth metal cations with four of the five isomers of DCH18C6 in methanol are described. The observed formation constants are shown to depend upon the ligand strain (*i.e.,* reorganizational) energy of the isomers, as determined by molecular mechanics calculations. In addition to being of fundamental interest, these results lay the groundwork for the application of this relationship in the identification of DtBuCH18C6 stereoisomers.

In Chapter 5, efforts to separate the stereoisomers of di-*tert*-butylcyclohexano-18-crown-6 present in a typical commercial batch of the material are described. Column chromatography and flash chromatography are shown to be ineffective for this separation. Preparative liquid chromatography utilizing an evaporative light scattering detector, in contrast, can provide satisfactory separation. Analysis of selected fractions using analytical-scale high performance liquid chromatography (to confirm the purity prior to further analysis to determine the identity of the individual di-*tert*-butylcyclohexano-18-crown-6 isomers) is described.

In Chapter 6, a number of different methods that result in the partial and/or complete identification of the various stereoisomers of di-*tert*-butylcyclohexano-18-

crown-6 are described. Of the methods explored (NMR, ITC or liquid-liquid extraction in combination with molecular mechanics, and X-ray crystallography), only x-ray crystallography can be used on a stand-alone basis to definitively identify a stereoisomer. In other cases, a combination of different techniques is required for identification.

Finally, in Chapter 7, the results of this research are summarized and recommendations for future work are provided.

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Chapter 2 : Investigations of the Thermal Properties of Macrocyclic Polyethers

2.1: Introduction

Since the introduction of the first air- and water-stable ionic liquids (ILs) more than two decades ago (*1*), there has been considerable interest in the application of these compounds in a variety of fields, a result of their many unique properties (*e.g.,* facile tunability, high thermal stability, wide liquid range, high ionicity, and low volatility (*2-7*)). To date, the vast majority of the ionic liquids prepared have consisted of two components: a bulky, typically asymmetric organic cation and any of a wide array of organic or inorganic anions. Recently however, a new class of ionic liquids has been described that consists of three components: a metal cation, a neutral complexing agent for that cation, and a conventional ionic liquid anion (*e.g.*, *bis*(trifluoromethylsulfonyl) imide, abbreviated Tf_2N^-) (*8-13*). These new ionic liquids, henceforth referred to as "ternary" ionic liquids (TILs), have been shown to act much like "traditional" binary (*i.e.*, two-component) ionic liquids. For example, conductivity measurements on these new TILs yield results comparable to those obtained for imidazolium-based ionic liquids (*8*). In addition, these ILs have been shown to dissolve a wide range of solutes, much like many traditional ionic liquids (*14*). One significant advantage of TILs over conventional ionic liquids is the added degree of tunability. That is, for a three-component system, the number of possible ionic liquids is far greater than for two-component systems. Despite this enormous range of possibilities, the investigations of TILs performed to date have focused almost exclusively on those employing a crown ether as the neutral complexing agent (*11-13*).

It seems self-evident that the properties of the constituents of an ionic liquid should influence those of the ionic liquids itself. Indeed, work by Gianellis (*15*) and Rickert (*16*) in which the characteristics of various ionic liquids incorporating a polyoxometallate anion were examined, showed (not unexpectedly) that the use of a more thermally stable IL cation yields an IL with greater thermal stability. This suggests that the thermal properties of a crown ether, in particular its volatility and/or propensity toward decomposition, should affect the characteristics of ILs prepared from it. Further support for this notion is found in recent results reported by Dai *et al*. (*17*) for a series of ILs comprising a hydrated alkali metal cation in combination with a bulky inorganic anion (*i.e*., $[La(TiW_{11}O_{39})_2]$). In this instance, the loss of the water(s) of hydration upon heating was found to convert the IL to an amorphous solid.

Despite the apparent importance of the thermal characteristics of crown ethers to the design of TILs incorporating these molecules, little information has been published concerning these properties. In fact, although crown ethers were first described in the 1960's (*18*), neither their stability (*i.e.*, the onset temperature of vaporization and/or decomposition) nor that of their complexes has been systematically investigated (*19-23*). Rather, the vast majority of published work on the thermal properties of these compounds has concerned their melting point and glass transition temperatures. In contrast, extensive investigation of the thermal stability of conventional ionic liquids have been performed (*5, 24*). As a result, the effect of cation and anion structure on their thermal stability is well known (*7*). For diakyl- and trialkyl- imidazolium ILs (*25, 26*) for example, the alkyl chain length of the cation has been shown to have little or no effect on the onset

temperature for decomposition of the IL. Replacement of the C-2 hydrogen with an alkyl group, however results in a significant increase in onset temperature. For ammonium-based ILs (*25*), the relationship between the alkyl chain length of the cation and the onset temperature of decomposition is parabolic, with the shortest and longest chain lengths exhibiting higher onset temperatures than are observed for intermediate chain lengths. As was the case for imidazolium ILs, for pyridinium ILs (*27*), the alkyl chain length of the IL cation has little effect on the onset temperature of the IL. For anions, regardless of the cation associated with it, the following generalized trend in thermal stability is seen: PF_6^- > BETI⁻ (*bis*(perfluoroethylsulfonyl)imide) > Tf_2N^- > BF_4^- > ME⁻ (*tris* (trifluoromethylsulfonyl)methide) ~ AsF_6^- > I⁻ ~ Br⁻~ Cl⁻ (*7*).

In this chapter, we describe the results of thermogravimetric and differential scanning calorimetry experiments on a wide range of crown ethers. This study has been undertaken to obtain an improved understanding of the thermal properties of crown ethers, to determine if these properties can be correlated with the molecular structure (*e.g.*, stereochemistry), and to identify promising candidates (*i.e.*, high onset temperature for vaporization or decomposition) for use as a neutral complexing agent in a new series of ternary ionic liquids.

2.2: Experimental

2.2.1: Materials

Figure 2.1 shows the nearly two dozen crown ethers examined in this study, along with the abbreviations used hereafter for each. The *cis-syn-cis* (DCH18C6A) and *cis-anti-*

cis (DCH18C6B) isomers of dicyclohexano-18-crown-6 isomers were purchased from Acros Organics (Geel, Belgium), while the *trans-syn-trans* (DCH18C6C), *trans-anti-trans* (DCH18C6D), and *cis-trans* (DCH18C6E) isomers were generously donated by Argonne National Laboratory (Argonne, IL, USA). The 24-crown-8 (24C8) was provided by Texas Tech University (Lubbock, TX. USA). The 12-crown-4 (12C4), benzo-15-crown-5 (B15C5), benzo-18-crown-6 (B18C6), cyclen (Cyclen), cyclohexano-15-crown-5 (mixed isomers) (CH15C5Mix), cyclohexano-18-crown-6 (mixed isomers) (CH18C6Mix), and dibenzo-18-crown-6 (DB18C6) were purchased from Acros Organics. The 1,4,7,10-tetrathiacyclododecane (12S4),1-aza-12-crown-4 (1A12C4), 1-aza-15-crown-5 (1A15C5), 1-aza-18-crown-6 (1A18C6), 15-crown-5 (15C5), and 18-crown-6 (18C6) were purchased from Sigma Aldrich (St. Louis, MO. USA). The 4-*tert*-butylbenzo-18-crown-6 (4tbB18C6), 4-*tert*-butylcyclohexano-18-crown-6 (4tbCH18C6), and dicyclohexano-18-crown-6 (a mixture of A and B isomers) (DCH18C6Mix) were purchased from Parish Chemical Company (Orem, UT. USA). All chemicals were used without further purification unless noted otherwise.

2.2.2: Instruments

TGA measurements were performed with a TA Instruments Q50 (New Castle, DE USA). All measurements were performed under a nitrogen atmosphere in a platinum pan. DSC measurements were performed with a TA Instruments Q20 (New Castle, DE USA). All measurements were performed in a nitrogen environment utilizing a Tzero Aluminum pan with a hermetically sealed lid. A TA Instruments Refrigerated Cooling System 90 (RCS90) was used to reach temperatures below 0°C.
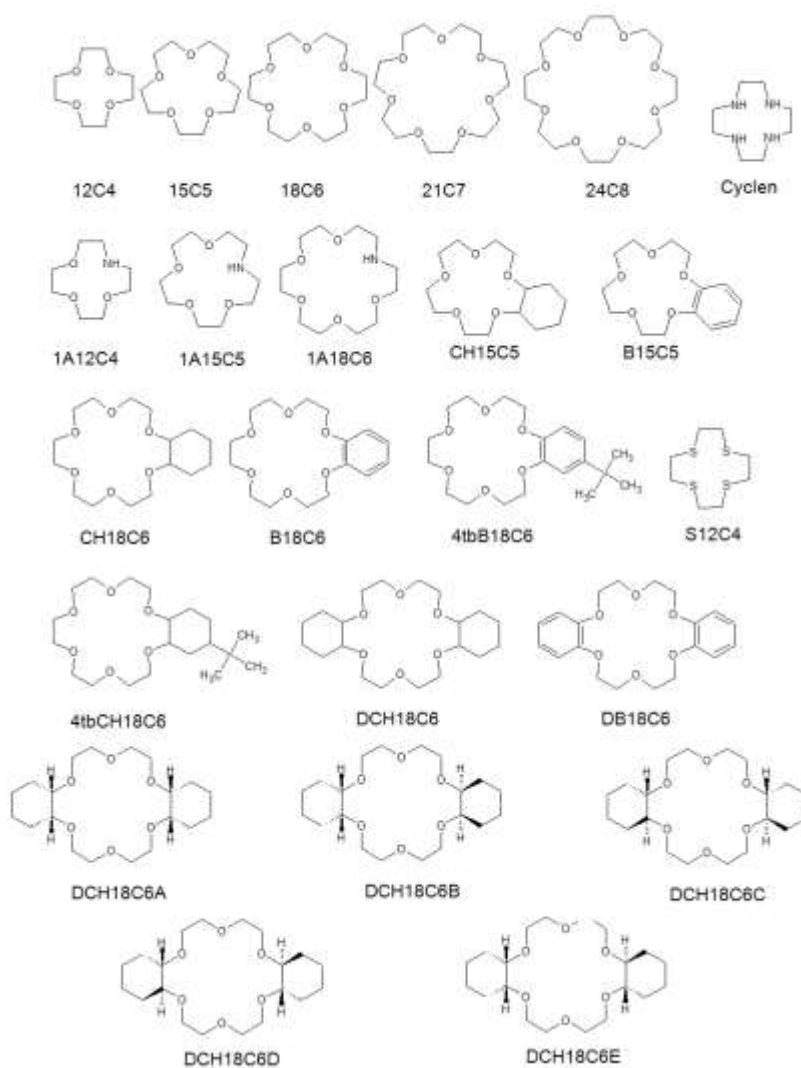
Figure 2.1: Crown Ethers Examined

2.2.3: Methods

2.2.3.1: Thermal Property Determination

In a typical set of experiments, TGA measurements were first performed to acquire information (*i.e.* onset temperature of decomposition or evaporation) needed in subsequent DSC measurements. In the TGA experiments, the sample (solid or liquid) was

placed in a tared platinum pan, the pan was loaded into the furnace, and the furnace was closed. All samples were then heated from room temperature to a final temperature of 1000°C using a 10°C/min temperature ramp. Sample data collection was halted if a mass of 0 mg was reached before 1000°C. Between analyses the furnace was air cooled for 8-10 minutes to ensure that the system had again reached room temperature. The mass of the sample taken, which was obtained from the instrument's micro-balance, was between 5.5 mg $\pm$ 0.5 mg for most samples. The onset temperature of mass loss (defined as the temperature corresponding to the intersection of an extrapolation of the initial plateau and of the steeply declining segment of the thermogram for each of the compounds) and the first derivative plot were obtained through TA Universal Analysis, a software program provided by the manufacturer of the system (Appendix A).

In a DSC experiment, the sample (solid or liquid) was placed into a tared Tzero aluminum pan and hermetically sealed using a die press provided with the system. The sample masses ranged from 1.0 to 6.0mg. To start the measurements, all samples were cooled to -75°C, held there for 5 minutes, and then ramped at a rate of 10°C/min to a temperature shown (by TGA) to result in no more than 1% mass loss for the main component of the sample (solvent and impurity peaks were neglected). The melting points and glass transitions were identified through TA Universal Analysis software (Appendix A).

2.3: Results

2.3.1: Decomposition or Evaporation?
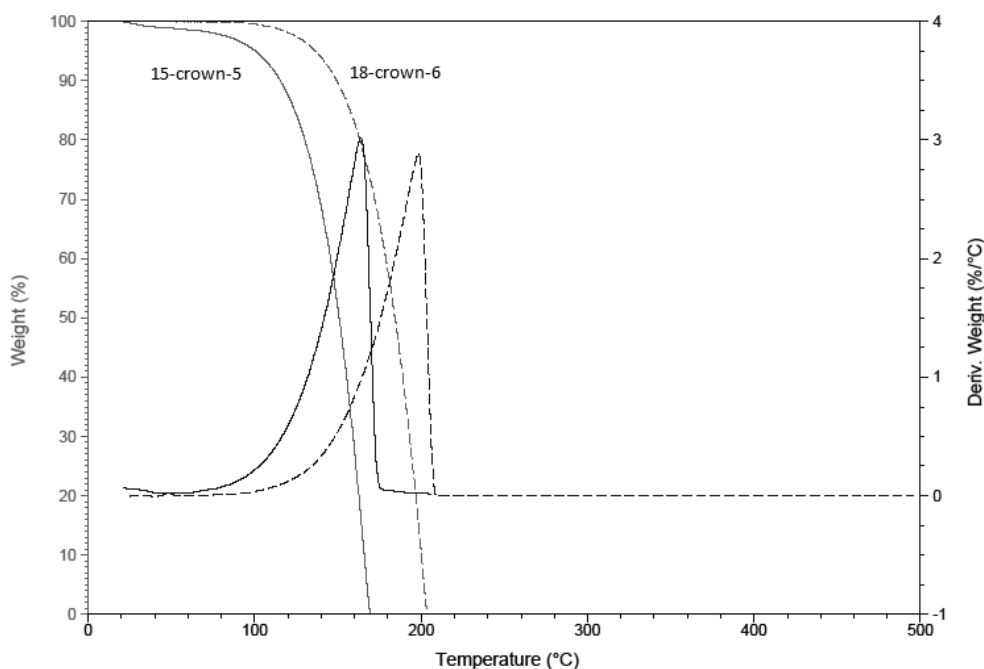
Figure 2.2: TGA Thermogram of 15-crown-5 and 18-crown-6 with first derivative peaks

When a sample is subjected to heating, the observed mass loss can, in principle, be the result of either decomposition or evaporation/sublimation. As shown in Figure 2.2, which shows the results of a thermogravimetric analysis of two crown ethers, it is not readily possible to distinguish between these processes. That is, 15-crown-5, which has been reported to evaporate when heated yields a thermogram essentially identical to that obtained for 18-crown-6, which has been reported to decompose (*23*). Our conclusion as to the underlying cause of mass loss observed upon heating the crown ethers was based on a consideration of the vaporization enthalpies for various crown ethers. As shown in

Figure 2.3 and Table 2.1, higher vaporization enthalpies are generally associated with higher onset temperatures for mass loss. Unfortunately, vaporization enthalpies are not available for all of the crown ethers used in our study. Nonetheless, the limited data available strongly suggest that evaporation/sublimation, rather than decomposition, is responsible for the mass loss observed upon heating the various crown ethers. It is important to note here that the distinction between the two processes, while interesting from a fundamental perspective, is not important in consideration of the behavior of the prospective ILs made from a crown ether. That is, IL stability requires that its components neither evaporate nor decompose over the temperature range of interest. In evaporation, the crown simply boils off and renders the ionic liquid useless. For example, Dai *et al. (17)* have recently shown for a series of ILs consisting of a hydrated alkali metal cation and a polyoxometallate anion that removal of water upon warming converts the IL to a mud-like substance exhibiting none of the properties of the original ionic liquid. In decomposition, the crown degrades into multiple components, again rendering the ionic liquid useless. For this reason, we have chosen to describe our results in terms of a temperature corresponding to the onset of mass loss, without regard to the details of the process by which mass loss occurs.
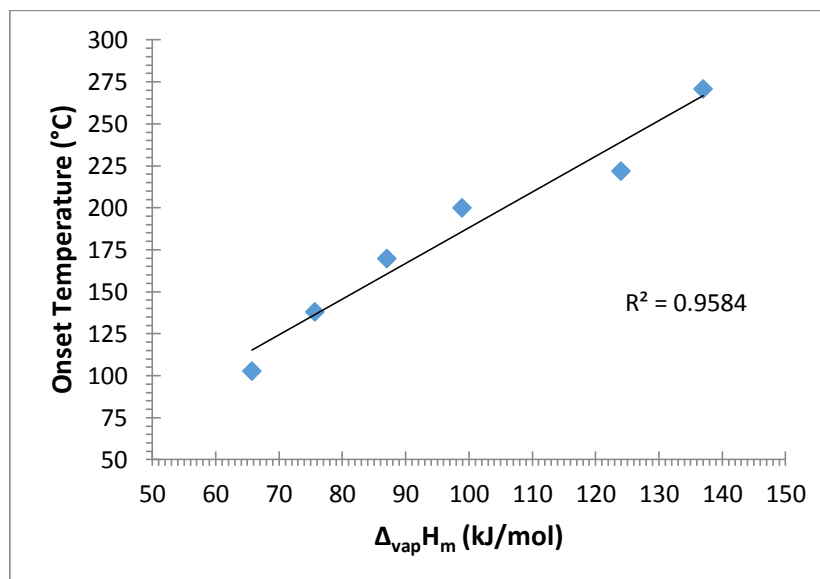
Figure 2.3: Plot of Onset Temperature for Mass Loss vs. the Enthalphy of Vaporization
for a Series of Crown Ethers

Table 2.1: Onset Temperature and Enthalpy of Vaporization Energies

	Onset (°C)	$\Delta_{vap}H_m$ (kJ/mol)(*28*)
dibenzo-18-crown-6	271	137
dicyclohexano-18-crown-6	222	124
benzo-15-crown-5	200	98.9
18-crown-6	170	87
15-crown-5	139	75.7
12-crown-4	103	65.7

2.3.2: Structural Properties of Crown Ethers Affecting the Temperature Corresponding to the Onset of Mass Loss

Of the various factors that have led to interest in crown ethers as metal ion complexing agents over the last four decades, their structural diversity is especially significant. Numerous crown ether structural characteristics are now known to influence the strength and selectivity of their metal ion binding, among them the nature, number and arrangement of binding atoms, as well as the type and amount of substituents appended to the macro ring (*29-31*). Efforts to evaluate these compounds as possible building blocks for new ionic liquids must therefore consider numerous parameters. Accordingly, in examining the thermal properties of these ligands, we have determined the effect of a variety of structural features on these properties. For simplification of the discussion, these compounds have been arranged into a series of groups according to ring size, the nature of macro ring heteroatoms, the type of substituents, or the stereochemistry of the molecules. In all, twenty-three materials comprising six distinct groups were studied. These are depicted in Figure 2.1.

2.3.3: Onset of Mass Loss for "Conventional" *vs.* 1-Aza Crown Ethers
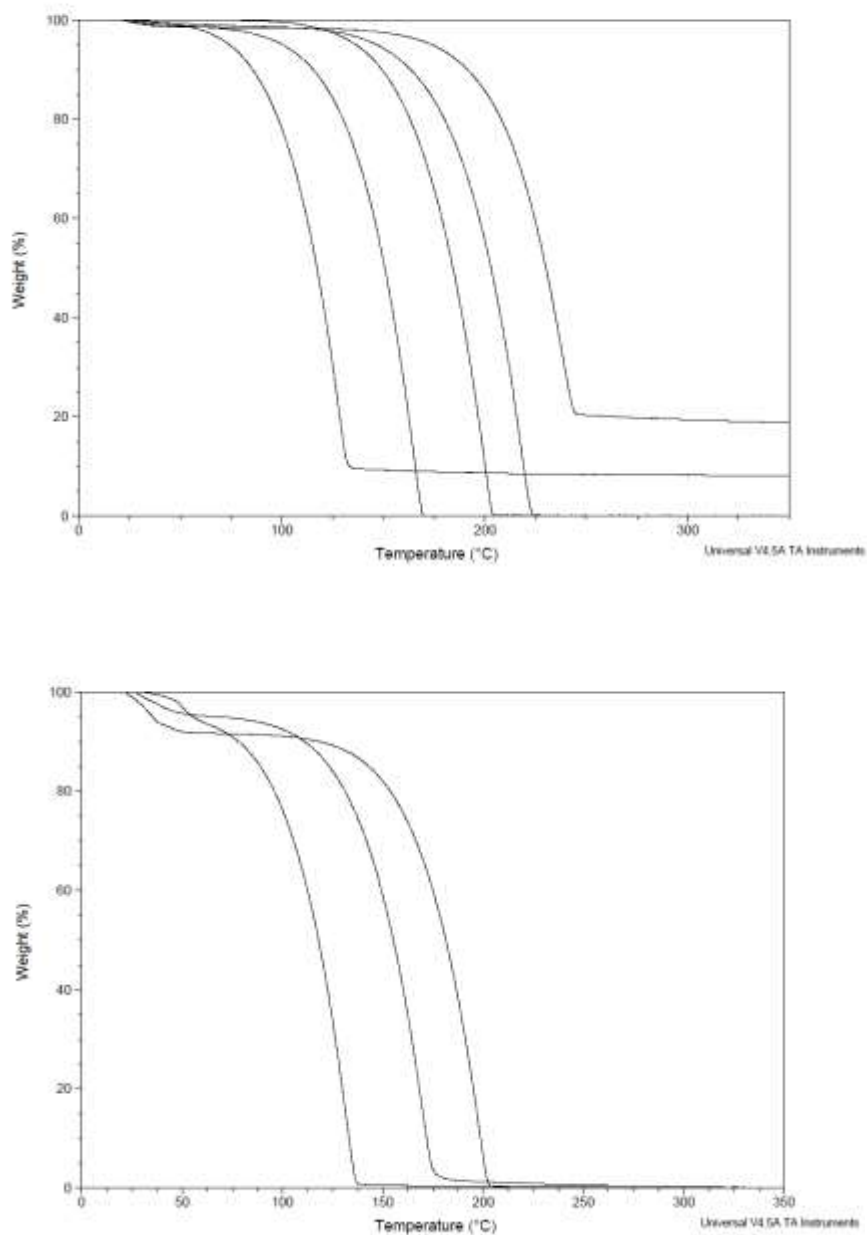
Figure 2.4: (top panel) TGA Thermograms of five "conventional" crown ethers (left to right: 12C4, 15C5, 18C6, 21C7, and 24C8) and (bottom panel) TGA Thermograms of three 1-aza crown ethers (left to right: 1A12C4, 1A15C5, and 1A18C6)

Figure 2.4 (top panel) depicts the thermograms obtained for the first group, a series of five "conventional" crown ethers, in which the only oxygen donor atoms are present, while Figure 2.4 (bottom panel) depicts the thermograms for mono-nitrogen substituted crown (1-aza) ethers. Table 2.2 lists the temperatures corresponding to the onset of mass loss for each crown ether. As can be seen, for the conventional crown ethers, rising molecular weight is accompanied by an increase in T_{onset}. Interestingly, a doubling of the molecular weight (from 176 g/mol for 12-crown-4 to 352 g/mol for 24-crown-8) results in a near doubling of the onset temperature. A similar increase in onset temperature with increasing molecular weight is also seen in the series of compounds incorporating a nitrogen heteroatom in place of one oxygen atom, indicating that here too thermal stability (*i.e.,* resistance to volatilization or decomposition) increases with molecular weight.

As already noted, little information concerning the thermal stability of these compounds has been published. Obviously some insight into the expected trends might be obtained by consideration of other families of organic compounds. Prior work concerning the relationship between thermal stability and molecular weight for other organic compounds has yielded conflicting results, however (*32*). For example, in an examination of the thermal degradation of poly(ethylene glycols) (PEGs) and poly (ethylene oxides) (PEOs) of different molecular weights, Vrandecic *et al.* (*33*) observed no significant change in thermal stability (as reflected in the temperature corresponding to 5% mass loss) with molecular weight. In contrast, and in agreement with the observations made here, Adam *et al.* (*34*) noted in a series of isothermal decomposition

measurements that the extent of weight loss by polycarbonates prepared from 2,2-bis(4-hydroxyphenyl)propane is greater for low molecular weight samples. In this case as well then, thermal stability is favored by increasing molecular weight. As we have already noted, however, it is likely that the observed mass losses are the result of evaporation of the crown ether, rather than its decomposition. Thus the relationship between the boiling point of a compound and its molecular weight is the issue, and here, the literature is consistent. That is, for a given family of molecules, the boiling point of a compound generally increases with increasing molecular weight. This trend is illustrated by the results shown for primary alcohols (*35*) and methyl and ethyl ethers (*36*) in Figure 2.5. That such a relationship is also observed for the two groups of crown ethers is yet another indication that the mass losses seen have their origins in evaporation, not decomposition.

Table 2.2: Thermal Properties of Crown Ethers

Abbrev	Name	Mol. Wt. (g/mol)	Melting Point / Glass Transition (°C)	Published (°C)	Onset (°C)
DCH18C6A	*cis-syn-cis*-dicyclohexano-18-crown-6	372.5	61.22	61-62(*37*)	224
DCH18C6B	*cis-anti-cis*-dicyclohexano-18-crown-6	372.5	69.95	69-70(*37*)	217
DCH18C6C	*trans-syn-trans*-dicyclohexano-18-crown-6	372.5	117.09	118-119(*37*)	221
DCH18C6D	*trans-anti-trans*-dicyclohexano-18-crown-6	372.5	62.40	77-80(*38*)	218
DCH18C6E	*cis-trans*-dicyclohexano-18-crown-6	372.5	-37.45		224
DCH18C6Mix	dicyclohexano-18-crown-6	372.5	52.29	40-60(*39*)	222
DB18C6	dibenzo-18-crown-6	360.4	163.61	164(*39*)	271
CH18C6 Mix	cyclohexano-18-crown-6 (mix of isomers)	318.41	-61.11 GT= -31.30	<26(*18*)	178*
CH15C5Mix	cyclohexano-15-crown-5 (mix of isomers)	274.35	-61.06	<26(*18*)	159*
S12C4	1,4,7,10-tetrathiacyclododecane	240.47	113.86 / 129.15	214-216(*40*)	217*
Cyclen	Cyclen	172.27	54.61 / 72.81	32-34(*41*) 114-116(*42*)	145
B18C6	benzo-18-crown-6	312.36	44.77	43-45(*43*)	222
B15C5	benzo-15-crown-5	268.31	81.92	78-81(*44*)	200
24C8	24-crown-8	352.42	18.22 / 20.70		210
21C7	21-crown-7	308.37	GT = -32.51		189
18C6	18-crown-6	264.32	34.56	36-38.5(*45*)	170
15C5	15-crown-5	220.26	-36.45		139
12C4	12-crown-4	176.21	14.87	16(*36*)	103
1A18C6	1-aza-18-crown-6	263.33	53.86	48-51(*46*)	170
1A15C5	1-aza-15-crown-5	219.28	C	27-30 (*47*)	142
1A12C4	1-aza-12-crown-4	175.23	57.97	57-59(*48*)	108
4tbCH18C6	4-t-butyl-cyclohexano-18-crown-6	374.51	-55.60%	<26(*18*)	225
4tbB18C6	4-t-butyl-benzo-18-crown-6	368.46	-38.82%	35-37(*18*)	210

* - Multiple Components Present, % - Appears Like a Hybrid of a Melting Point and Glass Transition,
C – Complex Thermal Event
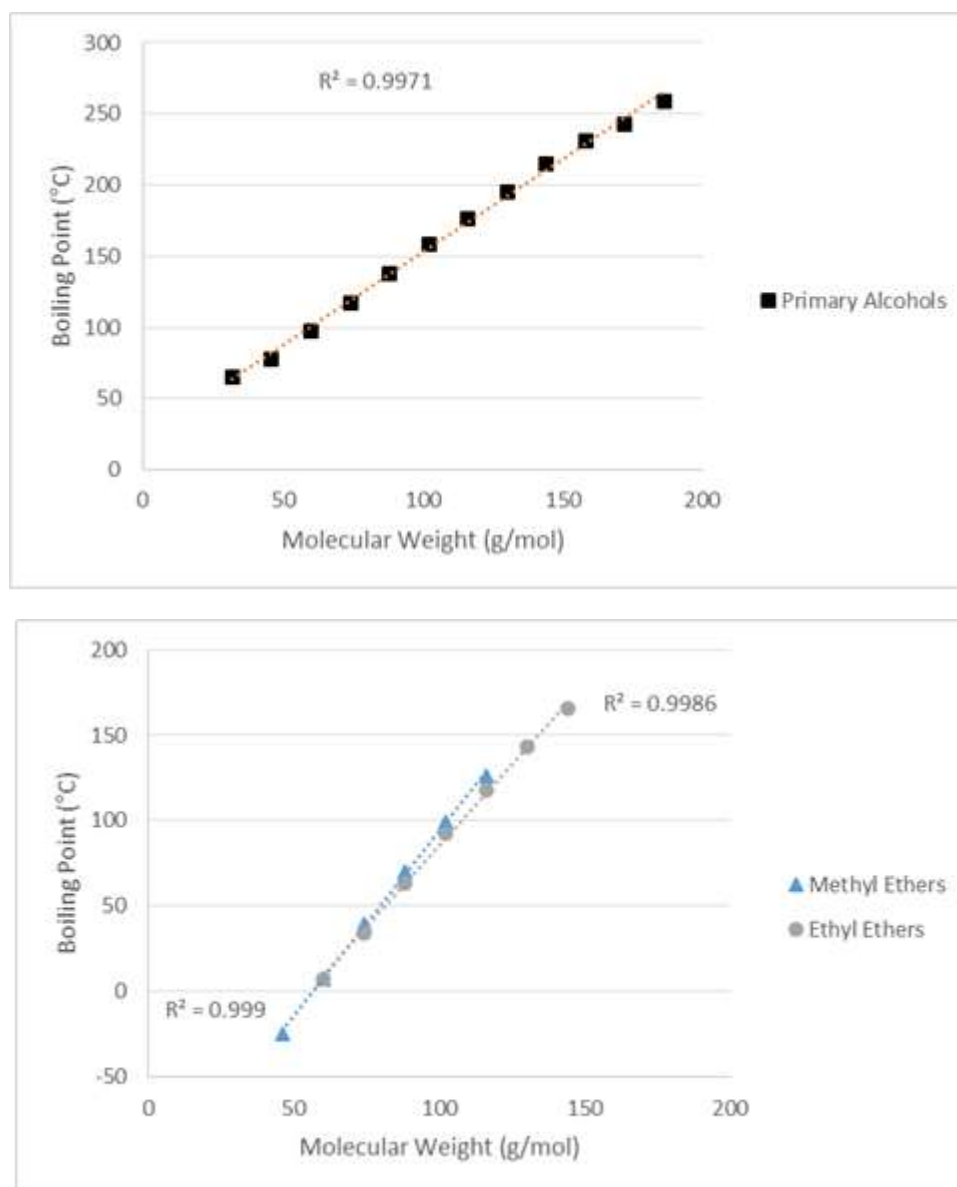
Figure 2.5: (top panel) Molecular Weight vs. Boiling Point for Primary Alcohols *(35)*;
(bottom panel) Molecular Weight vs. Boiling Point for Methyl and Ethyl Ethers *(36)*

2.3.4: Onset of Mass Loss for 12-crown-4 and its Nitrogen and Sulfur Analogs

Figure 2.6 depicts the thermograms obtained for three crown ethers differing only

in the nature of the heteroatom in the macro ring: 12-crown-4, cyclen (its nitrogen

analog), and 1,4,7,10-tetrathiacyclododecane (12S4), its sulfur analog. As can be seen from Table 2.2, while replacement of one of the oxygen atoms of 18-crown-6 with a nitrogen atom has essentially no effect on the onset temperature, replacement of all four of the oxygen atoms of 12-crown-4 with nitrogen atoms results in a significant (*ca.* 40°C) increase. An even more pronounced effect is seen upon substitution of sulfur atoms for all of the macro ring oxygens, which leads to a more than 100°C increase in the onset temperature.
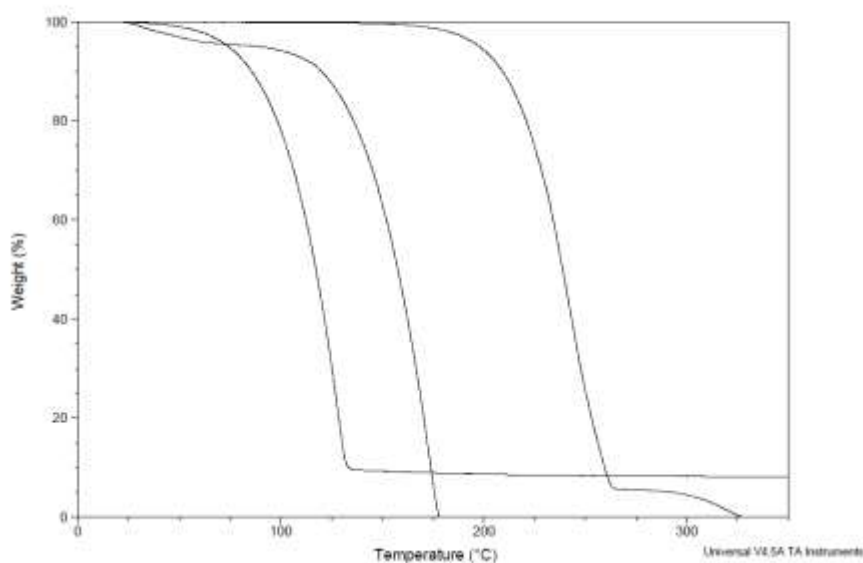
Figure 2.6: TGA Thermograms of 12-crown-4 (left), cylen (center), and 12S4 (right)

2.3.5: Onset of Mass Loss for the Stereoisomers of DCH18C6
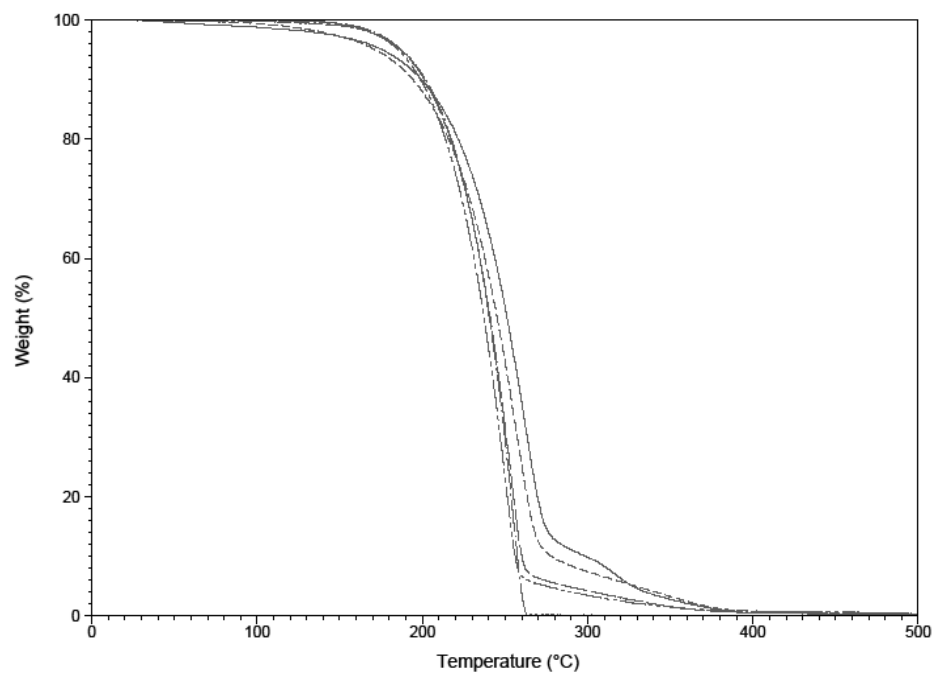
Figure 2.7: TGA Thermogram of the Five Isomers of DCH18C6
(left to right: Isomer B, D, C, A=E)

Figure 2.7 presents the thermograms of the five isomers of dicyclohexano-18-crown-6, which only differ in the stereochemistry of the hydrogens at the junction of the cyclohexano groups with the crown ether ring. Regardless of the stereochemical orientation of the isomer studied, all samples exhibited an onset of mass loss within a 7°C range (217-224°C).

2.3.6: Onset of Mass Loss for Aromatic and Aliphatic (cyclohexano- and *tert*-butyl) Substituted Crown Ethers

Figure 2.8 presents the thermogram obtained for the next set of compounds considered, whose study was undertaken in an attempt to determine the influence of aromatic *versus* aliphatic substitution on T_{onset}. As shown (and summarized in Table 2.1), while incorporation of a cyclohexano group into 18-crown-6 raises T_{onset} only slightly (from 170°C to 178°C), appending a single benzo group to the same molecule raises the onset temperature markedly (from 170°C to 222°C). Similarly, the onset of mass loss for cyclohexano-15-crown-5 begins at 159°C, only 20°C above the onset temperature for the unsubstituted 15-crown-5. Consistent with the results obtained for 18-crown-6, however, incorporation of a benzo group yields a much more pronounced rise in T_{onset}, in this case to 200°C. Thus, while the results for aliphatic substitution are consistent with those observed (see above) for the conventional crown ethers varying in ring size (and thus, molecular weight), the changes in T_{onset} that accompany aromatic substitution are greater than would be expected on the basis of the changes in molecular weight alone. This is also the case for molecules incorporating a pair of cyclohexano- or benzo- groups. For example, as already noted, dicyclohexano-18-crown-6 begins to lose mass at *ca.* 220°C (regardless of isomeric form). In contrast, dibenzo-18-crown-6 exhibits a T_{onset} of 271°C, significantly higher than that observed for either its mono-benzo analog, or any of the alphatic crown ethers considered. Interestingly, all of these results are consistent with those of a study of the thermal degradation of alkylimidazolium salts by Awad *et al.* (*49*), in which it was observed that as the alkyl chain length of the IL cation increased, the thermal degradation of the IL also increased. Thus higher aromatic content favors thermal

stability. Overall then, it appears that the balance between aromatic and aliphatic content is at least as influential in determining the thermal stability of a crown ether as is molecular weight. A further demonstration of this is found in the results shown in Table 1 for 4-*tert*-butylcyclohexano-18-crown-6 and its benzo analog. Addition of a *tert*-butyl-group to benzo-18-crown-6 actually reduces T_{onset} (from 225°C to 210°C), while as expected from molecular weight considerations, the same substitution raises the T_{onset} of the cyclohexano crown ether.
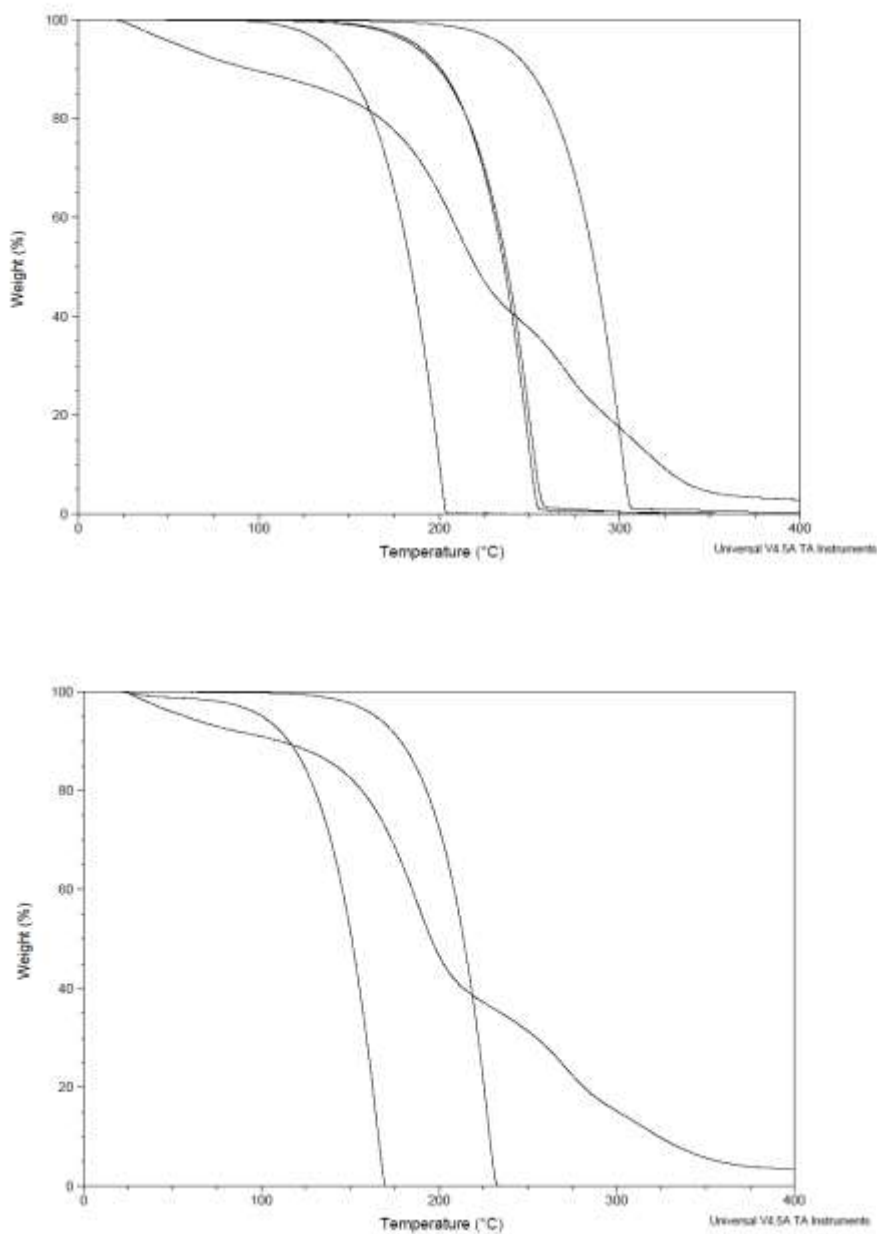
Figure 2.8: (top panel) TGA Thermograms of 18C6, CH18C6Mix, B18C6/DCH18C6, DB18C6; (bottom panel) TGA Thermograms of 15C5, CH15C5Mix, and B15C5

While perhaps not as influential as aromatic content in determining T_{onset}, molecular weight may actually be more useful in efforts to make quantitative estimates of crown ether thermal stability. That is, as can be seen from Figure 2.8 (top panel), which summarizes the data obtained for all of the aliphatic crown ethers in this work (with the exception of compounds incorporating only N or S heteroatoms), when the onset temperatures for mass loss are plotted versus molecular weight, all of the data fall upon a line of near-unit slope (on a log-log scale). To the best of our knowledge, such a correlation has not been observed previously for this family of complexing agents. That analogous results are obtained for other families of organic compounds (*e.g.* primary alcohols) lends further support to the notion that heating leads to evaporation of the crown ethers considered here.
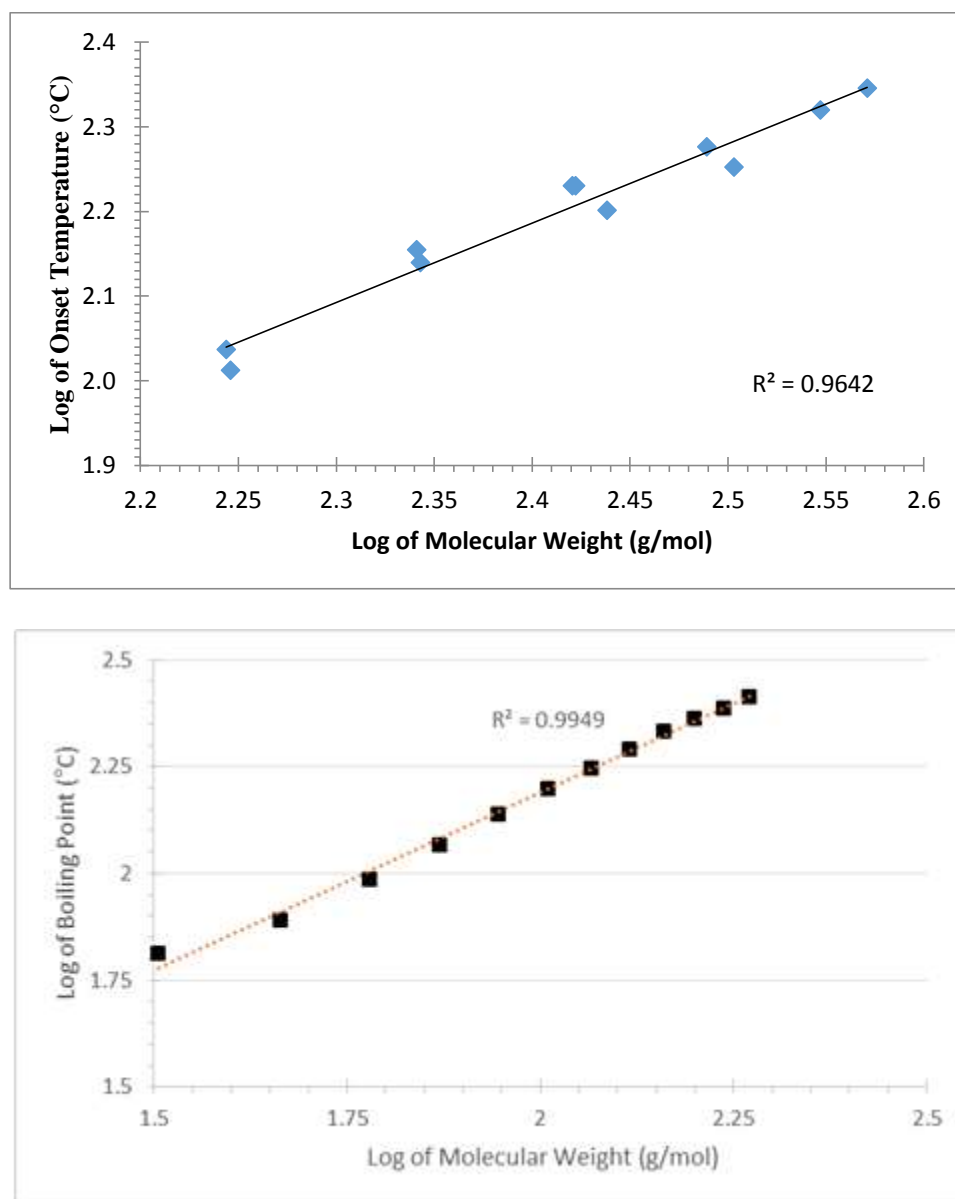
Figure 2.9: (top panel) Log-Log Plot of Molecular Weight vs. Onset Temperature of Mass Loss for Aliphatic Crown Ethers; (bottom panel) Log-Log Plot of Molecular Weight vs. Boiling Point of Primary Alcohols

2.3.7: Melting Point/ Glass Transitions

With few exceptions (*i.e.,* 1,4,7,10-tetrathiacyclododecane, cyclen, and 1-aza-15-crown-5), all melting points obtained match published results. Analysis of the DSC thermograms show that there is no obvious relationship between melting point and/or glass transition temperature of a crown ether and its ring size, substitution, donor atoms, or stereochemistry. This is not unexpected given that the melting point of a molecule is dependent on many different factors and thus cannot be attributed solely to the effects outline in the previous sections (*50, 51*). In fact, prior studies seeking to estimate the melting points of aliphatic crown ethers (*e.g.* to explain why 15-crown-5 has a lower melting point than either 12-crown-4 or 18-crown-6 (*51*)) indicate that an understanding of the packing of the crown ethers is necessary to rationalize the phase transitions of these molecules.

2.4: Conclusions

We have investigated the thermal properties of crown ethers that vary in ring size, substitution, nature of the donor atoms, and stereochemistry of the macrocycle. Through this survey and making the reasonable assumption that the thermal stability of a ternary IL incorporating a crown ether will increase with increasing T_{onset} for the crown itself, we have been able to identify several good candidates for preparation of crown-based ternary ionic liquids. In addition, we identified a relationship between the onset temperature of mass loss and molecular weight for many of the compounds. Not unexpectedly, we were unable to identify any trends in the phase transitions (melting point or glass transitions) observed. To obtain a better understanding of the factors dictating these phase transitions

for the crown ethers, packing studies must be performed (specifically focusing on the number of molecules of the crown ether present within a crystal (*52-54*) and calculated packing coefficients, which reflect the solvent accessible voids present (*55*)).

2.5: References

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Chapter 3 : Preparation and Characterization of Novel Ternary Ionic Liquids Incorporating Crown Ethers

3.1: Introduction

In the previous chapter, the thermal properties of a wide range of crown ethers were surveyed, thereby enabling the identification of suitable candidates for use as the neutral complexing agent in a series of new ternary ionic liquids (TILs). As already noted, these TILs, which comprise three components (*i.e.* a cation, a neutral complexing agent, and a traditional ionic liquid anion), are expected to behave in a manner similar to that of traditional ionic liquids while offering additional design flexibility (*1-5*). In addition to the possibility of providing a better understanding of the relationship between the thermal properties of a neutral complexing agent and those of ILs produced from it, crown ethers offer the opportunity to examine the effect of the stereochemistry of the complexing agent on the TIL properties. With this in mind, we have prepared and characterized a series of TILs incorporating the various stereoisomers of dicyclohexano-18-crown-6 (DCH18C6) depicted in Figure 3.1. For the sake of comparison, we have also prepared additional TILs from other crown compounds (15-crown-5, 18-crown-6, 21-crown-7, and benzo-18-crown-6). In an effort to understand the influence of the individual components comprising the ILs formed on their properties, we have also varied the nature of the IL anion employed.
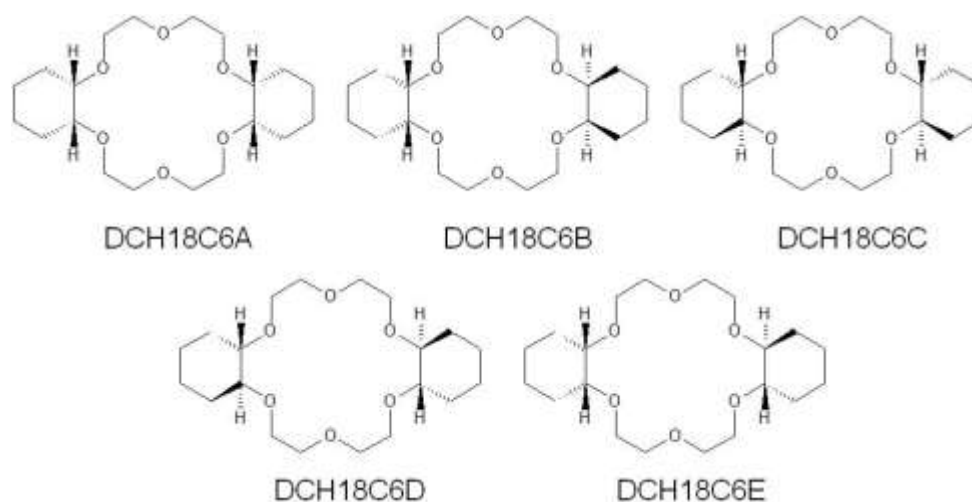
Figure 3.1: Stereoisomers of Dicyclohexano-18-crown-6 (DCH18C6)
Top Row: (left) *cis-syn-cis* (A); (middle) *cis-anti-cis* (B); (right) *trans-syn-trans* (C);
Bottom Row: (left) *trans-anti-trans* (D); (right) *cis-trans* (E)

3.2: Experimental

3.2.1: Materials

Cis-syn-cis (A) and *cis-anti-cis* (B) dicyclohexano-18-crown-6 were obtained from Acros Organics (Geel, Belgium). The other isomers were generously provided by Argonne National Laboratory (Argonne, IL, USA). 21-crown-7 was provided by Texas Tech University (Lubbock, TX, USA), while 15-crown-5, 18-crown-6, and benzo-18-crown-6 were obtained from Sigma-Aldrich (St Louis, MO, USA). Potassium *bis*(trifluromethylsulfonyl)imide (KTf$_2$N) was obtained from Wako Chemicals (Osaka, Japan). Deuterated chloroform and methylene chloride were obtained from Cambridge Isotope Laboratories (Tweksbury, MA, USA). HPLC grade methanol was purchased from Fisher Scientific (Waltham, MA, USA). All aqueous solutions were prepared using

deionized water with a specific resistance of $18M\Omega \cdot cm^{-1}$. All chemicals were used without additional purification unless noted otherwise.

3.2.2: Instruments

TGA measurements were performed with a TA Instruments Q50 (New Castle, DE, USA). All measurements were carried out under a nitrogen atmosphere using a platinum pan. DSC measurements were performed with a TA Instruments Q20 (New Castle, DE, USA) in a nitrogen environment utilizing a Tzero aluminum pan with a hermetically sealed lid. A TA Instruments (New Castle, DE, USA) RCS90 refrigerated cooling system was used to reach temperatures below 0°C.

3.2.3.1: Instrumental Methods

In a typical set of experiments, TGA measurements were first performed to acquire information (*i.e.,* the onset temperature of evaporation or decomposition) needed in subsequent DSC measurements. In the TGA experiments, the sample (solid or liquid) was placed in a tared platinum pan, the pan was loaded into the furnace, and the furnace was closed. All samples were then heated from room temperature to a final temperature of 1000°C using a 10°C/min temperature ramp. Sample data collection was halted if a mass of 0 mg was reached before 1000°C. Between analyses, the furnace was air cooled for 8-10 minutes to ensure that the system had again reached room temperature. The mass of the sample taken, which was obtained from the instrument's micro-balance, was in the range 3.5 ±0.5 mg for most samples. The onset temperature of mass loss (defined as the temperature corresponding to the intersection of the extrapolation of the initial plateau and of the steeply declining segment of the thermogram for each of the compounds) and

first derivative plot were obtained through TA Universal Analysis, a software program provided by the manufacturer of the system (Appendix A).

In a DSC experiment, the sample was placed into a tared Tzero aluminum pan and hermetically sealed using a die press provided with the system. The sample masses ranged from 1.0 to 6.0 mg. To start the measurements, all samples were cooled to -75°C, held there for 5 minutes, and then ramped at a rate of 10°C/min to a temperature shown (by TGA) to result in no more than 1% mass loss for the main component of the sample (solvent and impurity peaks were neglected). The melting points and glass transitions were identified through TA Universal Analysis software (Appendix A).

Elemental analyses (carbon, hydrogen, and nitrogen (CHN)) were carried out by Galbraith Laboratories (Knoxville, TN USA) employing a vanadium pentoxide catalyst to ensure total destruction of the *bis*(trifluormethylsulfonyl)imide group during combustion (*6*). NMR spectra were acquired on a Bruker DPX300 NMR spectrometer operating at 300.13 MHz for hydrogen, 75.47 MHz for carbon, and 288 MHz for fluorine. A z-gradient broadband (BBO) probe was utilized for all NMR experiments, and the spectra obtained were acquired using either deutrated chloroform or methylene chloride for all ^{1}H, ^{13}C, and ^{19}F experiments. Spectra of the ternary ionic liquids were compared with pure crown ether samples to verify the presence of the crown ether in the newly formed ionic liquid. Mass spectra were collected using a Thermo Surveyor MSQ with an electrospray (ESI) probe with a 3kV capillary and a 350°C probe temperature (with the help of Megan McCallum (UWM)) or a Shimadzu LCMS-2020 utilizing a DUIS-2020 dual ion source (both positive and negative electrospray ionization (ESI) and

atmospheric-pressure chemical ionization (APCI)) with the help of Dr. Zhiqiang (Mark) Wang (UWM).

Crystal structures were obtained by Dr. Sergey Lindeman (Marquette University, Milwaukee, WI, USA) using an Oxford SuperNova diffractometer using Mo (Kα) radiation at 100K (-173.15°C). Using Olex2, the structure was solved with the XS structure solution program using direct methods and refined with the XL refinement package using least square minimization (Appendix B).

3.2.2.2: Synthesis of potassium-crown ether-*bis*(trifluoromethylsulfonyl)imide Complexes

Potassium *cis-syn-cis*-dicyclohexano-18-crown-*6 bis*(trifluoromethylsulfonyl)imide [1]
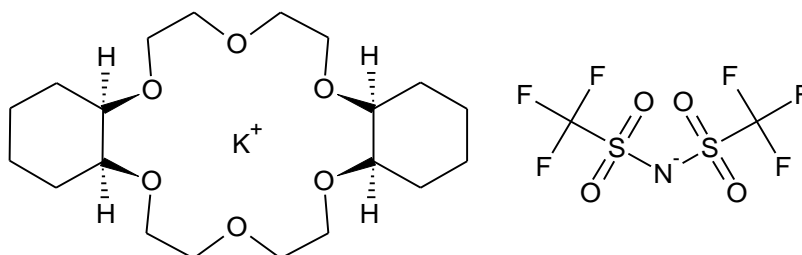
A solution (1 mL) containing at least a 10% mole excess of potassium *bis*(trifluoromethylsulfonyl)imide (92.8mg, 0.291mmol) in water was added to twice its volume of a solution of *cis-syn-cis*-dicyclohexano-18-crown-6 (98.0mg, 0.263mmol) in 1:1 (v/v) water-methanol. The mixture was then vortexed, followed by gentle stirring for 24 hours. During this time, the complex precipitated out as a white solid. This solid was washed twice with a 3:1 (v/v) water-methanol mixture to remove unreacted KTf_2N and then dried at 60°C for 8 hours under vacuum (25 in. Hg). Yield: 93.7%; mp: 100.35°C;

initial onset (3.632mg): 306°C; ^{1}H (CDCl$_3$): 1.29(4H), 1.58(8H), 1.89(4H), 3.50(12H), 3.76(8H); ^{13}C (CD$_2$Cl$_2$): DCH18C6A = 21.42, 25.97, 66.65, 70.47, 77.82 / Tf$_2$N$^-$ = 117.74, 122.00 (320Hz coupling); ^{19}F (CDCl$_3$): -78.9ppm ; CHN: C = 38.30% (expected: 38.20%), H = 5.28% (expected: 5.25%), N: 1.92% (expected: 2.03%); MS: 395 m/z (DCH18C6A-Na)$^+$, 411 m/z (DCH18C6A-K)$^+$, 280 m/z (Tf$_2$N)$^-$, 147 m/z (NSO$_2$CF$_3$)$^-$

Potassium *cis-anti-cis*-dicyclohexano-18-crown-6 *bis*(trifluoromethylsulfonyl)imide [2]
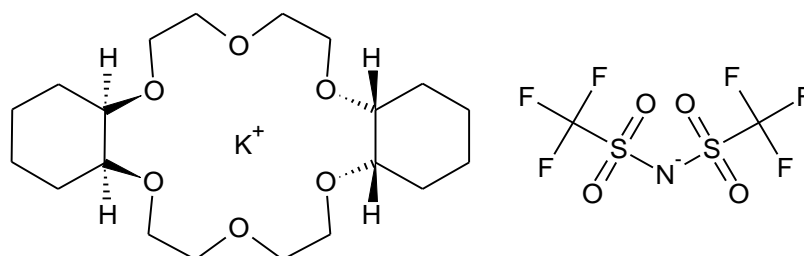
See the method for **[1]** for the synthesis (mass DCH18C6B: 92.1mg, 0.247mmol; mass KTf$_2$N: 87.2mg, 0.273mmol). Yield: 83.8%; mp: 159.60°C; initial onset (3.399mg): 291°C ; ^{1}H (CDCl$_3$): 1.25 (4H), 1.57 (8H), 1.93 (4H), 3.36 (4H), 3.61(12H), 3.85(4H); ^{13}C (CD$_2$Cl$_2$): DCH18C6B = 21.43, 25.43, 66.16, 70.40, 78.40 / Tf$_2$N$^-$ = Too weak to be seen; ^{19}F (CDCl$_3$): -79.0; CHN: C = 38.24% (expected: 38.20%), H = 5.27% (expected: 5.25%), N: 2.30% (expected: 2.03%); MS: 395m/z (DCH18C6B-Na)$^+$, 411m/z (DCH18C6B-K)$^+$, 280m/z (Tf$_2$N)$^-$, 147m/z (NSO$_2$CF$_3$)$^-$; The crystal structure of the complex is provided as Figure 3.11.

Potassium *trans-syn-trans*-dicyclohexano-18-crown-6 *bis*(trifluoromethylsulfonyl)imide [3]
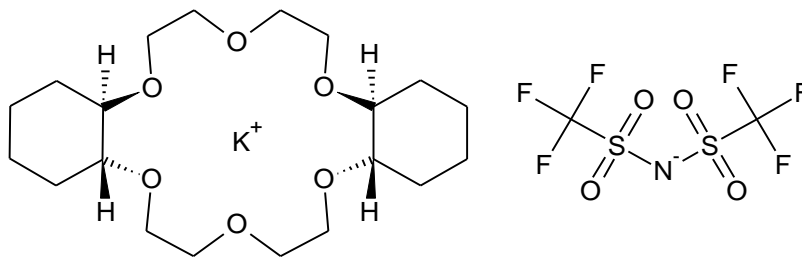
See the method for **[1]** for the synthesis (mass DCH18C6C: 46.1mg, 0.124mmol / mass KTf$_2$N:44.2mg, 0.138mmol).Yield: 54.8%; mp: 128.30°C; initial onset (3.562mg): 277°C; ^{1}H (CDCl$_3$): 1.11 (8H), 1.75 (4H), 2.20(4H), 3.29 (4H), 3.52 (8H), 3.73 (8H); ^{13}C (CD$_2$Cl$_2$): DCH18C6C = 23.89, 28.72, 65.61, 70.68, 80.32 / Tf$_2$N$^-$ = Too weak to be seen; ^{19}F (CDCl$_3$): -78.8ppm; CHN: C = 38.29% (expected: 38.20%), H = 5.26% (expected: 5.25%), N: 2.09% (expected: 2.03%); MS: 395m/z (DCH18C6C-Na)$^+$, 411m/z (DCH18C6C-K)$^+$, 280m/z (Tf$_2$N)$^-$, 147m/z (NSO$_2$CF$_3$)$^-$

Potassium *trans-anti-trans*-dicyclohexano-18-crown-6 *bis*(trifluoromethylsulfonyl)imide [4]
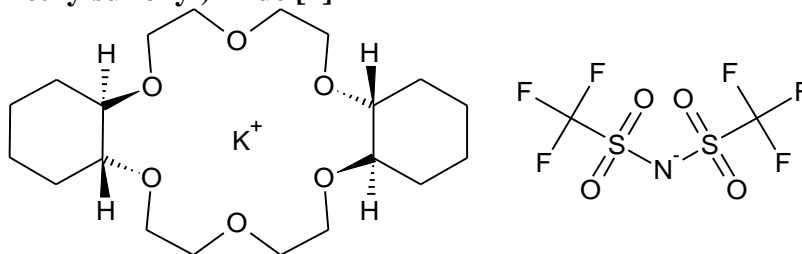
See the method for **[1]** for the synthesis (mass DCH18C6D: 94.0mg, 0.252mmol; mass KTf$_2$N: 88.6mg, 0.278mmol).Yield: 76.6%; mp: 70.4°C; initial onset (3.647mg): 274°C; ^{1}H (CD$_2$Cl$_2$): 1.16 (8H), 1.76 (4H), 2.19 (4H), 3.36 (4H), 3.56 (8H), 3.68 (8H); ^{13}C (CD$_2$Cl$_2$): DCH18C6D = 23.92, 28.80, 64.97, 70.15, 79.77 / Tf$_2$N$^-$ = Too weak to be seen; ^{19}F (CDCl$_3$): -78.9ppm; CHN: C = 38.34% (expected: 38.20%), H = 5.32% (expected:

5.25%), N: 1.91% (expected: 2.03%) ; MS: 395m/z (DCH18C6D-Na)[+], 411m/z (DCH18C6D-K)[+], 280m/z (Tf$_2$N)[-], 147m/z (NSO$_2$CF$_3$)[-]

Potassium *cis-trans*-dicyclohexano-18-crown-6 *bis*(trfluoromethylsulfonyl)imide [5]
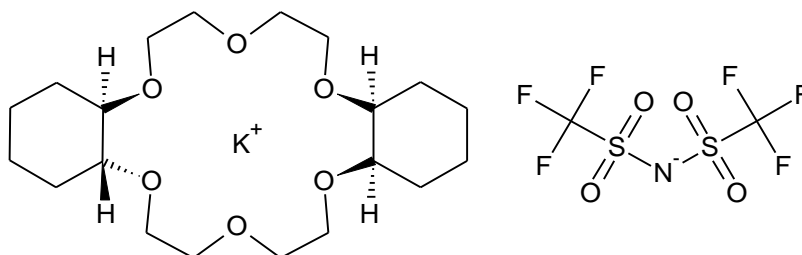
See the method for **[1]** for the synthesis (mass DCH18C6E: 93.3mg, 0.250mmol / mass KTf$_2$N:89.2mg, 0.279mmol) Yield: 84.3% mp: 77.36°C; initial onset (3.710mg): 294°C (three components present); ^{1}H (CDCl$_3$): 1.26(8H), 1.93 (6H), 2.50(2H), 3.85(20H); ^{13}C (CD$_2$Cl$_2$): DCH18C6E = 23.90, 25.40, 26.17, 28.67, 28.73, 64.61, 66.01, 66.11, 66.78, 70.21, 70.47, 70.59, 70.65, 79.80, 80.39 / Tf$_2$N[-] = Too weak to be seen; ^{19}F (CDCl$_3$): -78.9ppm; CHN: C = 38.39% (expected: 38.20%), H = 5.37% (expected: 5.25%), N: 1.90% (expected: 2.03%); MS: 395m/z (DCH18C6E-Na)[+], 411m/z (DCH18C6E-K)[+], 280m/z (Tf$_2$N)[-], 147m/z (NSO$_2$CF$_3$)[-]

Potassium 15-crown-5 *bis*(trifluoromethylsulfonyl)imide [6]
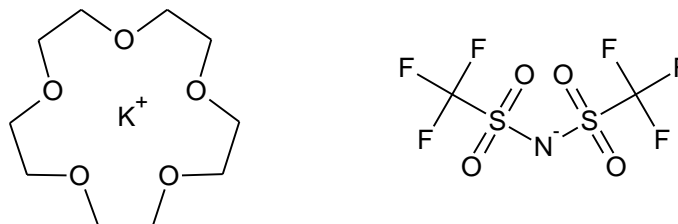
A solution (4 mL) containing a 10% mole excess of potassium *bis*(trifluoromethylsulfonyl)imide (653.1mg, 2.056mmol) dissolved in water was slowly added to 2 mL of a solution of 15-crown-5 (409.0mg, 1.857mmol) in water. The resultant mixture was vortexed, and then stirred for 24 hours. During this time, the complex precipitated out as a white solid. The solid was washed twice with water (4mL) and dried for at least 8 hours under vacuum (25 in. Hg). Yield: 51.5 %; mp: 79.9 / 94.2 °C; initial onset (3.972mg): 171°C (multiple components present); ^1H (CDCl$_3$): 3.65 ^{13}C (CDCl$_3$): 68.52; ^{19}F (CDCl$_3$): -78.79; CHN of K(15C5)$_2$Tf$_2$N: C = 34.91% (expected: 34.78%), H = 5.14% (expected: 5.31%), N: 1.80% (expected:1.84%); MS: 259m/z (15C5-K)$^+$, 480m/z ((15C5)$_2$-K)$^+$, 280m/z (Tf$_2$N)$^-$, 599m/z (K(Tf$_2$N)$_2$)$^-$

Potassium 18-crown-6 *bis*(trifluoromethylsulfonyl)imide [7]
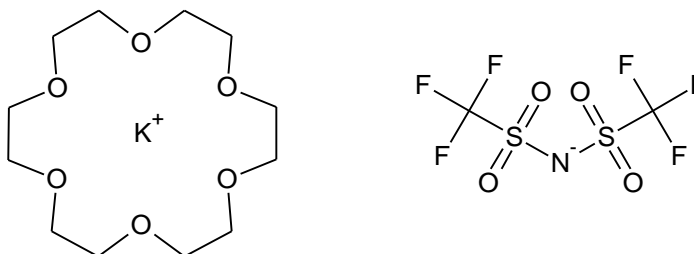
See the method for **[6]** for the synthesis (mass 18-crown-6: 181.2 mg, 0.686 mmol; mass KTf$_2$N: 252.2 mg, 0.790 mmol). The complex was obtained as a white precipitate. Yield:

72.6 %; mp: 164.00 °C; initial onset (4.1110mg): 269°C; ^{1}H (CDCl$_3$):3.63; ^{13}C (CDCl$_3$): 70.00; ^{19}F (CDCl$_3$): -79.01; CHN: C = 29.0% (expected: 28.8%), H = 4.11% (expected: 4.15%), N: 2.38% (expected: 2.40%); MS: 287m/z (18C6-Na)$^+$, 308m/z (18C6-K)$^+$, 280m/z (Tf$_2$N)$^-$, 599m/z (K(Tf$_2$N)$_2$)$^-$

Potassium 21-crown-7 *bis*(trifluoromethylsulfonyl)imide [8]
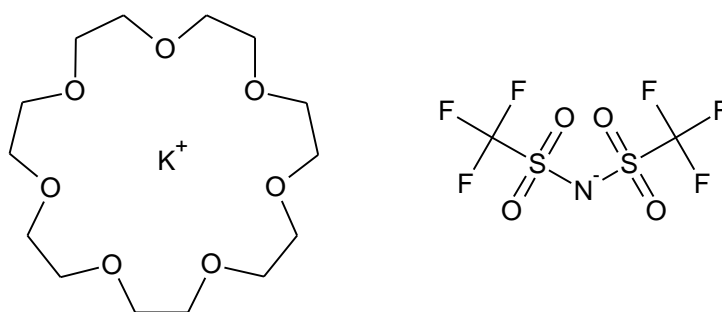
See the method for **[6]** for the synthesis (mass 21-crown-7: 240.0 mg, 0.778 mmol; mass KTf$_2$N: 277.5 mg, 0.869 mmol). The complex precipitated out as a clear gel. Yield: 37.6 %; mp: -49.90 (hybrid of mp/gt) / 96.30 °C; initial onset (3.9830mg): 260°C (multiple components present); ^{1}H (CD$_2$Cl$_2$): 3.68, 3.63; ^{13}C (CD$_2$Cl$_2$): 68.85, 70.03; ^{19}F (CD$_2$Cl$_2$): -79.54; CHN: C = 30.96% (expected: 30.62%), H = 4.52% (expected: 4.50%), N: 2.15% (expected: 2.32%); MS: 327m/z (21C7·H$_2$O)$^+$, 332m/z (21C7·Na)$^+$, 347m/z (21C7·K)$^+$, 280m/z (Tf$_2$N)$^-$, 599m/z (K(Tf$_2$N)$_2$)$^-$

Potassium benzo-18-crown-6 *bis*(trifluoromethylsulfonyl)imide [9]
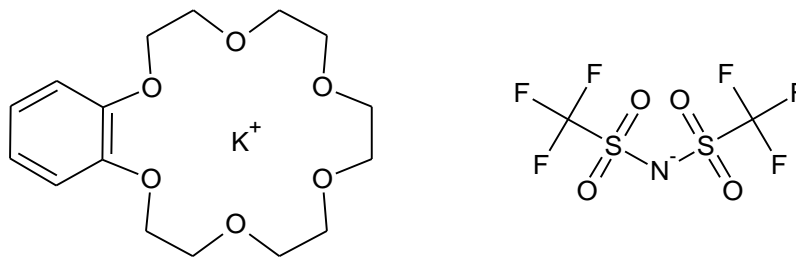
A solution (2 mL) containing a 10% molar (133.2 mg, 0.417 mmol) excess of potassium *bis*(trifluoromethylsulfonyl)imide in water was slowly added to a solution (2 mL) of benzo-18-crown-6 (118.5 mg, 0.379 mmol) dissolved in methanol. The resultant mixture was vortexed, and stirred for 24 hours during which the complex precipitated out as a yellowish-white solid. This solid was washed twice with an equal volume of water, then dried at 60-80C under vacuum (25 in. Hg) for at least 8 hours. Yield: NA% mp: 60.450 °C; initial onset (3.7060mg): 289°C; ^{1}H (CD$_2$Cl$_2$): 1.69, 3.66, 3.73, 3.87, 6.92; ^{13}C (CD$_2$Cl$_2$): 66.77, 68.89, 69.80, 69.93, 111.29, 121.28, 146.78; ^{19}C (CD$_2$Cl$_2$): -79.68; CHN: C = 35.80% (expected: 34.23%), H = 3.79% (expected: 3.83%), N: 1.96% (expected: 2.22%); MS: 330m/z (B18C6·H$_2$O)$^+$, 335m/z (B18C6·Na)$^+$, 351m/z (B18C6·K)$^+$, 280m/z (Tf$_2$N)$^-$, 599m/z (K(Tf$_2$N)$_2$)$^-$

Potassium *cis-anti-cis*-dicyclohexano-18-crown-6 bromide [10]
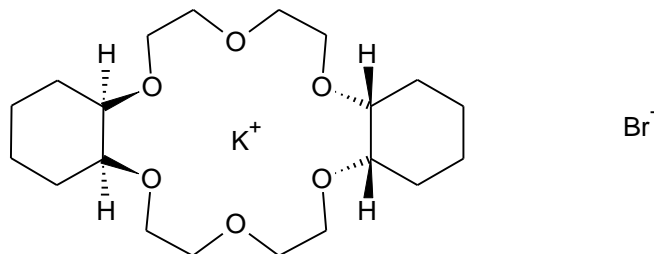
A solution (3mL) of potassium bromide (67.7mg, 0.569mmol) dissolved in water was slowly added to 3 mL of an equimolar solution of *cis-anti-cis*-dicyclohexano-18-crown-6 (212.0mg, 0.569mmol) in methanol. The resultant mixture was vortexed, and then stirred for 12 hours, during which the complex precipitated out as a white solid. The precipitate was dried at 80°C in a vacuum oven (25 in. Hg) for at least 12 hours. Yield: 100 % mp: 121.78 °C; initial onset (3.7810mg): 215°C (multiple components present); ^{1}H (CD$_2$Cl$_2$): 1.33, 1.60, 1.95, 3.55, 3.71 ^{13}C (CD$_2$Cl$_2$):21.54, 25.67, 66.40, 70.50, 78.36; CHN: C = 47.37% (expected: 48.87%), H = 7.26% (expected: 7.38%), N: <0.5% (expected:0%); MS: 395 m/z (DCH18C6B-Na$^+$), 411 m/z (DCH18C6B-K$^+$)

3.3: Results

3.3.1: Onset Temperature of Mass Loss for Potassium-Crown Ether-Anion Complexes

Figure 3.2 shows the TGA thermograms of potassium-DCH18C6-*bis*(trifluoromethylsulfonyl)imide complexes examined. In all cases, two significant mass losses are readily observed, along with a third much less prominent mass loss near 1000°C. The magnitude of the first mass loss, which is roughly 54% of the original mass

indicates that heating first causes the loss of the crown ether, then of the Tf_2N^- anion (*ca.* 40% of the original mass). Finally, in some cases, a further decrease in mass due to loss of potassium is observed (Figure 3.2). In the case of the ionic liquid formed between 15-crown-5 and KTf_2N, the observed mass losses are consistent with the presence of two molecules of the crown ether in the complex (Figure 3.3).
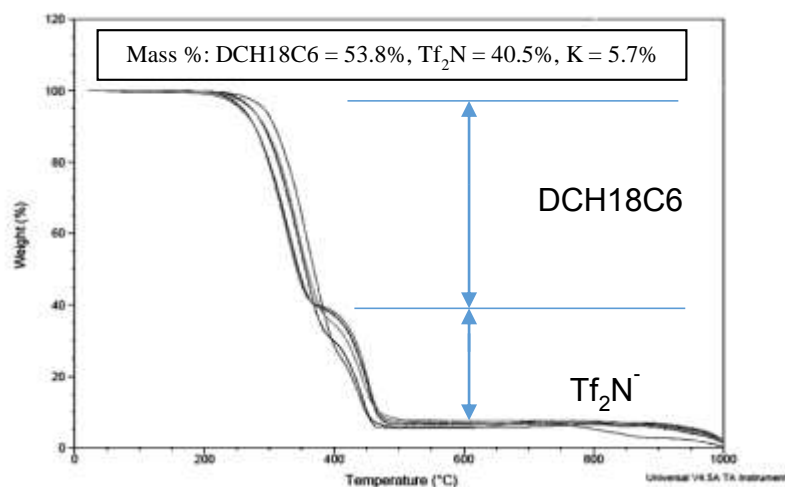
Figure 3.2: TGA Thermogram of KTf_2N-Complexes of DCH18C6
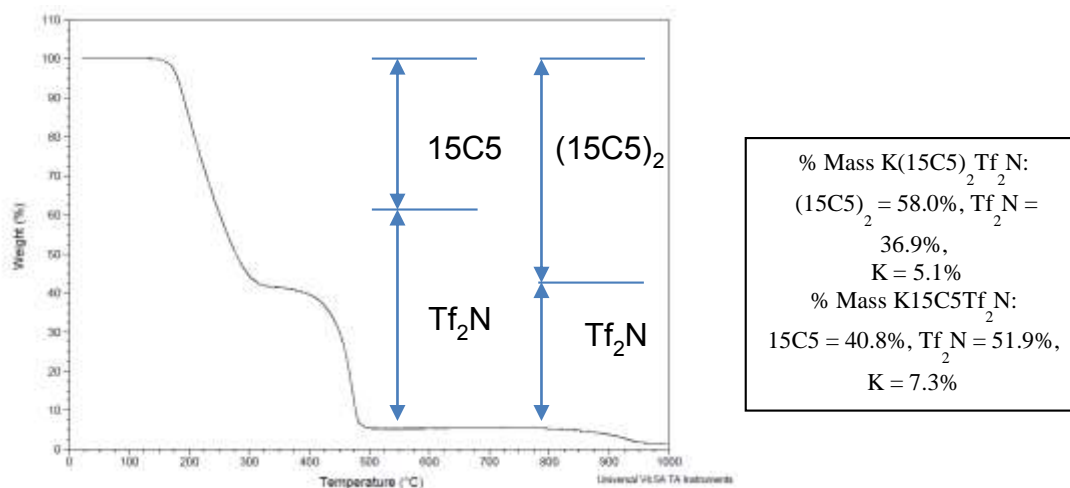
Figure 3.3: (left) TGA Thermogram of $K(15C5)_2Tf_2N$ and (right) % Mass Breakdown of $K(15C5)_2Tf_2N$ and $K15C5Tf_2N$

In most cases (with the exception of potassium *cis-anti-cis*-dicyclohexano-18-crown-6 bromide), it is apparent that the onset temperature of mass loss for the complex is at least 40°C higher than that of the uncomplexed crown ether, which indicates that complexation to potassium *bis*(trifluoromethylsulfonyl)imide improves the thermal stability of the crown ether (Figures 3.4 and 3.5). In contrast, the onset temperature for potassium *cis-anti-cis*-dicyclohexano-18-crown-6 bromide is similar to that that of the free crown ether (Figure 3.6). It is interesting to note that for conventional ionic liquids, for example those comprising an imidazolium cation in combination with a series of anions (Table 3.1), it is bromide anion which yields the ILs exhibiting the poorest thermal stability.
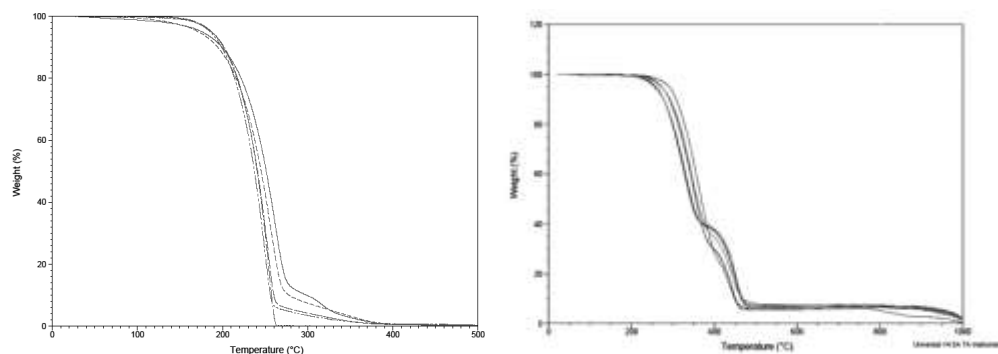
Figure 3.4: (left) Onset Temperatures for DCH18C6 Stereoisomers and (right) for their K$^+$Tf$_2$N$^-$ Complexes
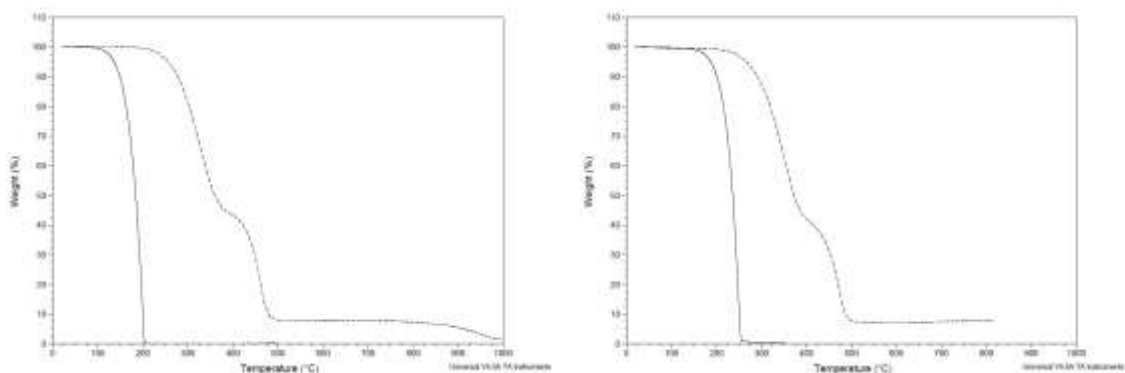
Figure 3.5: (left) TGA Thermogram of 18-crown-6 and its KTf2N complex and (right) of benzo-18-crown-6 KTf2N complex
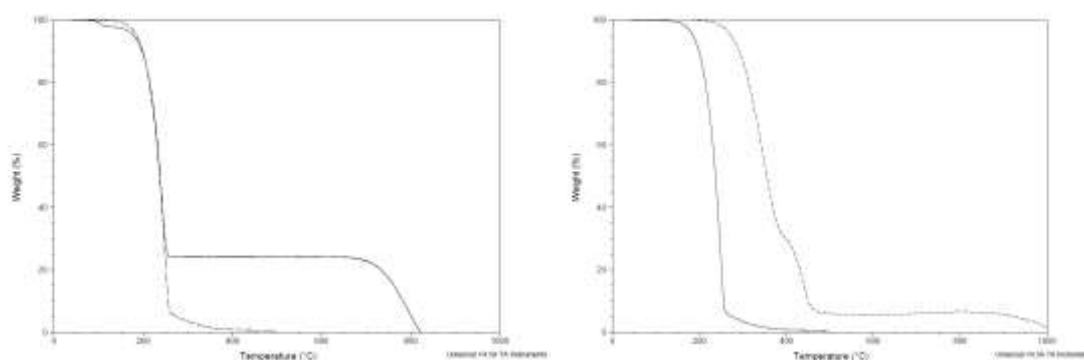
Figure 3.6: (left) TGA Thermogram of DCH18C6B and KDCH18C6BBr, and (right) TGA THermogram of DCH18C6 and KDCH18C6BTf$_2$N

Table 3.1: Onset Temperature of Mass Loss Variation with Anions for Imidazolium-Based Ionic Liquids (7)

The T_{onset} (°C) of [C$_n$mim][X]				
Anions (X)	[C$_2$mim][X]	[C$_4$mim][X]	[C$_6$mim][X]	[C$_8$mim][X]
Br	287	279	267	272
BF$_4$	NM	420	413	411
PF$_6$	NM	423	361	299
BETI	415	398	401	418
NTf$_2$	444	421	418	416

Careful examination of the TGA results obtained for the various KTf_2N-crown ether complexes and for the constituent crown ethers indicates that the increase in the temperature corresponding to the onset of mass loss (for the complexed crown ether *vs.* the free crown ether) is directly related to the formation constant of the K^+-crown ether complex. That is, higher formation constants are associated with larger increases in the onset temperatures of mass loss, as shown in Table 3.2 and Figure 3.7. Interestingly, if the data is plotted on a semi-log scale, a rougly linear relationship between the two parameters is observed. To the best of our knowledge, such a relationship has not been reported previously. Its significant to the design of thermally stable TILs is readily evident. That is, TIL thermal stability is favored by strong metal cation-complexing agent interactions.

Table 3.2: Data Regarding Formation Constants and Onset Temperatures for All KTf2N-crown ether Complexes

	Log K in MeOH	T_{Onset} for Crown Ether (°C)	T_{Onset} for Complex (°C)	Increase In Onset Temperature
18C6 *(8)*	6.09	170	270	100
DCH18C6A *(9)*	5.88	224	306	82
DCH18C6B *(9)*	5.33	217	291	74
B18C6 *(8)*	5.18	221	289	68
DCH18C6E *(9)*	4.53	224	294	70
21C7 *(8)*	4.22	189	260	71
DCH18C6C *(9)*	4.08	221	277	56
DCH18C6D *(9)*	3.10	218	274	56
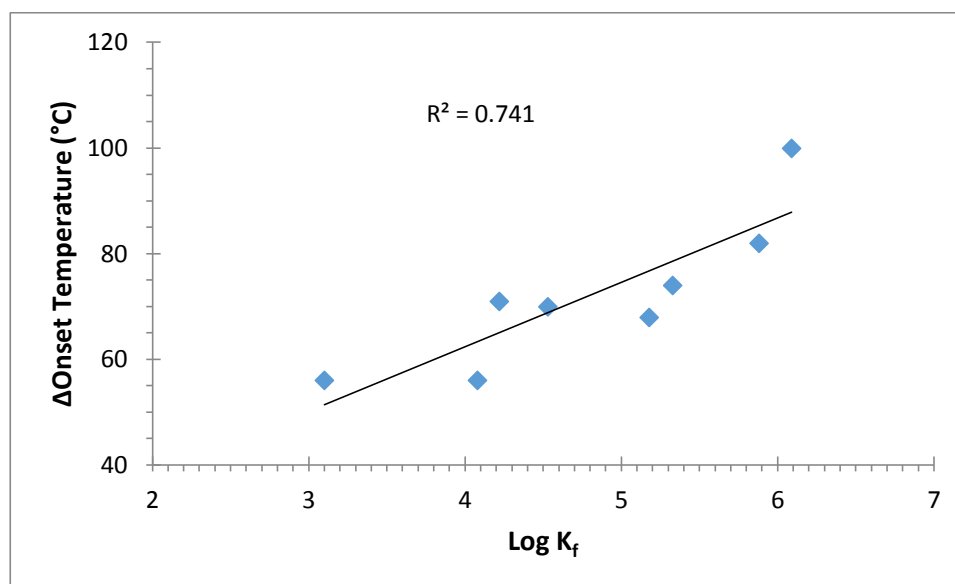
Figure 3.7: Relationship between the Formation Constants and Change in Onset
Temperatures for KTf2N-Crown Ether Complexes

Potassium complexes incorporating anions other than Tf_2N^- and Br^- were also
prepared, using a method for the preparation of 18-crown-6 complexes first published by
Song *et al. (4, 5)*. In most cases, a pure ionic liquid was not obtained when using
DCH18C6B, however, as demonstrated by DSC (which showed that the complex
contained significant amounts of unreacted starting material) (Figures 3.8) or CHN
analysis. Of twelve newly formed potassium salt complexes of DCH18C6 (Table 3.3)
only one was found to yield CHN results consistent with a pure compound (Table 3.4).
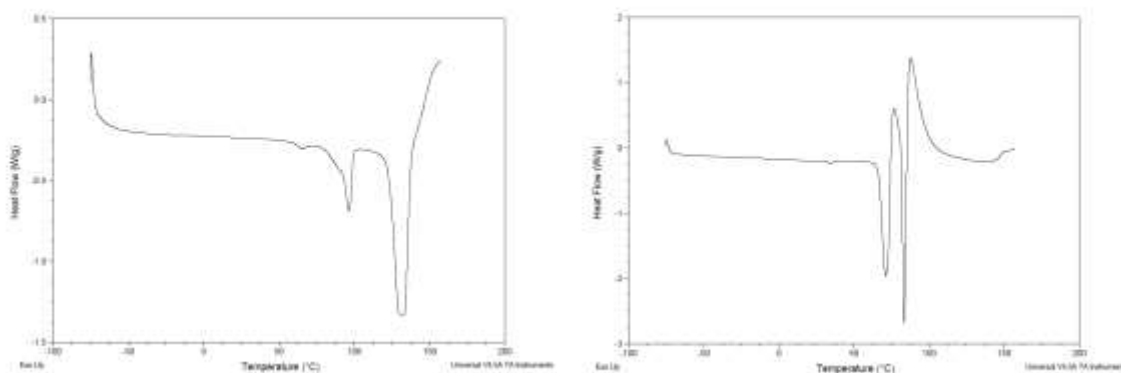
Figure 3.8: DSC Thermogram of (left) potassium DCH18C6B iodide and (right) potassium DHC18C6B hydroxide

Table 3.3: Potassium Salt Complexes of DCH18C6

Potassium Hydroxide	Potassium Acetate
Potassium Carbonate	Potassium Bicarbonate
Potassium Nitrate	Potassium Iodide
Potassium Hydrogen Phthalate	Potassium Bromide
Potassium Chloride	Monopotassium Phosphate
Dipotassium Phosphate	

Table 3.4: CHN Data for Potassium DCH18C6B Complexes

	Experimental			Theoretical		
	%C	%H	%N	%C	%H	%N
Potassium DCH18C6B Acetate	53.74	8.28	<0.5	56.14	8.35	0
Potassium DCH18C6B Bromide	47.37	7.26	<0.5	48.87	7.38	0
Potassium DCH18C6B Iodide	40.00	6.03	<0.5	44.61	6.74	0
Potasium DCH18C6B Phosphate Monobasic	27.94	4.81	<0.5	47.23	7.53	0

3.3.2: Stereoisomer Effects on the Melting Points of Ternary Ionic Liquids: Potassium dicyclohexano-18-crown-*6 bis*(trifluoromethylsulfonyl)imide Complexes

A complete picture of the relationship between the properties of TILs and crown ether stereochemistry requires that stereochemical effects on melting points also be considered. Here we describe our initial work in this area, in particular our studies of the thermal behavior of a variety of TILs prepared from DCH18C6 and alkali metal *bis*(trifluromethylsulfonyl)imides. Figure 3.9 shows the results of a differential scanning calorimetry (DSC) measurements on five $K^+DCH18C6Tf_2N^-$ complexes, while Table 3.5 summarizes the melting points and/or glass transitions obtained there from. Although some have suggested that ionic compounds with melting points as high as 200°C (*3-5*) be considered "ionic liquids", the most widely accepted definitions require a melting point of less than or equal to either 100°C (10) or 150°C (*11*). By the strictest standard, two of the five complexes would be classified as ionic liquids. Applying the more lenient 150°C cutoff would result in classification of four of the five complexes as ionic liquids (the potassium complex with isomer B being the exception). None of the complexes can be regarded as a room-temperature ionic liquid, as is readily evident from the data presented. For each complex, a single endothermic event is observed, consistent with an occurrence of a melting event for the complex. If the individual components were not interacting, the DSC would exhibit two separate melting points; one for the crown ether and the other for the potassium *bis*(trifluoromethylsulfonyl)imide (Figure 3.10)
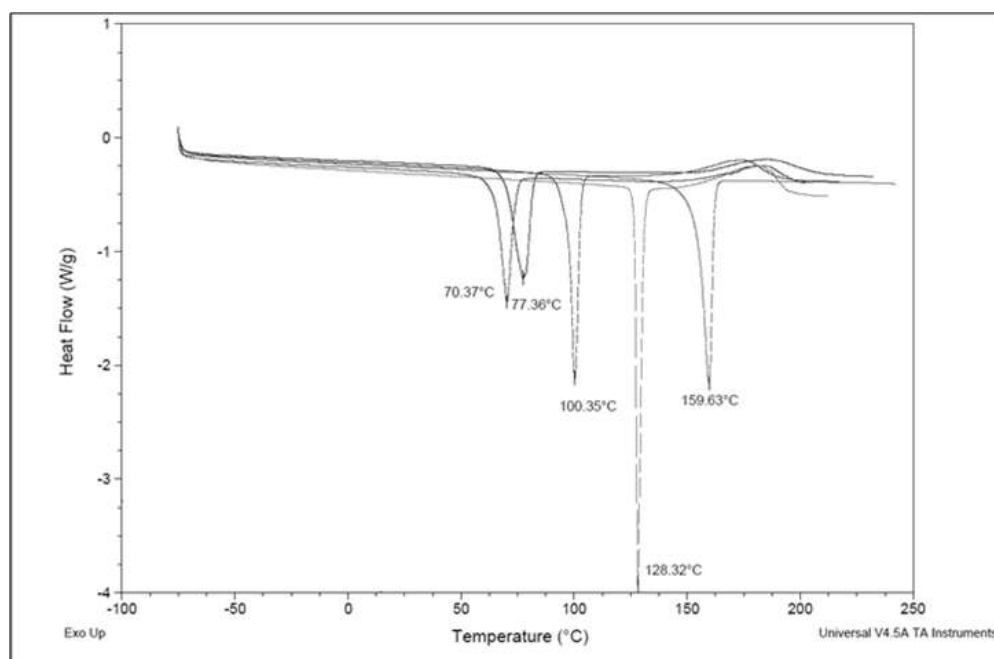
Figure 3.9: (Left to Right) Melting Points of KDCH18C6Tf$_2$N Complexes Formed From
Ismer D, E, A, C, and B

Table 3.5: Comparison of Uncomplexed and Complexed Stereoisomers of DCH18C6
Thermal Transitions

	Crown Ether Transition (°C)	Complex Transition (°C)
cis-syn-cis (A)	MP = 61.37	MP = 100.35
cis-anti-cis (B)	MP = 69.95	MP = 159.83
trans-syn-trans (C)	MP = 117.09	MP = 128.32
trans-anti-trans(D)	MP = 63.96	MP = 70.37
cis-trans (E)	GT = -38.6	MP = 77.36
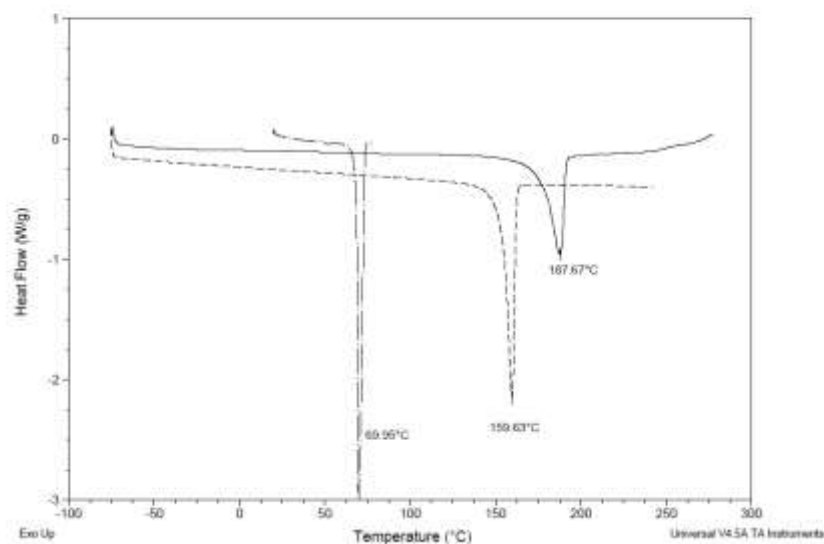
Figure 3.10: (Left to Right) Melting Point for the DCH18C6B, KDCH18C6BTf$_2$N, and KTf$_2$N

A change of melting point for the complex *vs.* the free crown ether is expected *(12)*. In fact, similar results have previously been obtained for nitro derivatives of benzo-15-crown-5 complexed with lithium, sodium, and potassium (*12*). In complex crown ethers, new interactions (especially inter-atomic interactions between the potassium ion in or just outside the crown ether cavity and the oxygens of the *bis*(trifluoromethylsulfonyl)imide anion) are occurring. (See the crystal structure of *cis-anti-cis*-dicyclohexano-18-crown-6 *bis*(trifluoromethylsulfonyl)imide shown in Figure 3.11.) These interactions appear to organize the complex more efficiently, thus allowing for higher melting points than for the uncomplexed crown ethers. It comes as no surprise then, that the one stereoisomer that yielded a crystalline solid not only exhibited the largest increase in melting point versus the uncomplexed form, but also the highest

melting point of all of the complexes. As was stated regarding the melting points of uncomplexed crown ethers in Chapter 2, additional packing studies (*13, 14*) would be necessary to fully decipher what occurs upon complexation for the other stereoisomers studied. In addition, computational studies similar to these carried out for traditional ILs in the prediction of melting points of traditional ionic liquids may be beneficial for these new crown-based ternary ionic liquids (*15-17*).
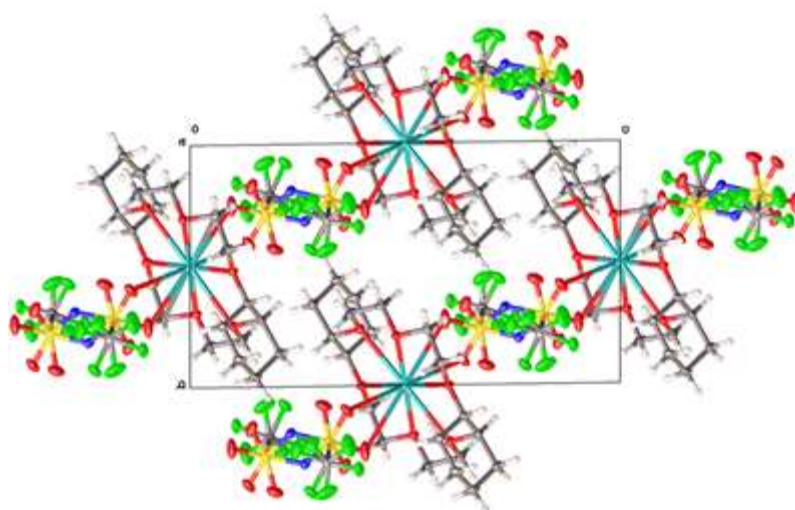
Figure 3.11: Crystal Structure of potassium *cis-anti-cis*-dicyclohexano-18-crown-6 *bis*(trifluoromethyl-sulfonyl)imide

3.3.3: Anion Effects on the Melting Points of the Other Crown Ether Complexes

Table 3.6 summarizes the results of melting point determinations on a series of complexes (*i.e.* prospective TILs) comprising various crown ethers and either potassium *bis*(trifluoromethylsulfonyl)imide or potassium bromide. In each case, the melting point of the complex is higher than that of the free crown ether, as anticipated. A comparison of

the change in melting point upon complexation of DCH18C6B by KTf$_2$N (Table 3.5) and KBr (Table 3.6), 90°C and 52°C, respectively, indicates that the anion plays an important role in determining the melting point of the complex/TIL. This is consistent with the behavior of conventional (*i.e.,* two component) ILs where the nature of the anion has long been known to influence the melting point of the ionic liquid. Interestingly, for conventional ILs, the Tf$_2$N$^-$ anion is well known for its ability to lower IL melting points. For example, among dialkylimidazolium ILs, the melting points observed with a given IL cation have been found to follow the order TFSI$^-$ (*a.k.a.* Tf$_2$N$^-$) < TfO$^-$ < BF$_4^-$ < PF$_6^-$ < Br$^-$ < Cl$^-$ (Figure 3.12) (*18)*. Here, in contrast, the complex formed by Tf$_2$N$^-$ melts at a higher temperature than does the analogous Br$^-$ complex. Given the limited data available, it is not yet possible to determine if this reversal is a general characteristic of ternary ILs or merely a peculiarity of these particular complexes. Nonetheless it suggests that the principles governing the design of "conventional" ILs may not be applicable to TILs.

Table 3.6: Comparison of Uncomplexed and Complexed Crown Ether Thermal Transitions

	Crown Ether Transition (°C)	Complex Transition (°C)
KBBr	MP = 69.95	MP = 121.78
KB18C6Tf$_2$N	MP = 44.8	MP = 60.45
K21C7Tf$_2$N	GT = -32.4	MP =96.3
K18C6Tf$_2$N	MP = 34.6	MP =164
K(15C5)$_2$Tf$_2$N	GT/MP = -36.4	MP = 79.9 / 94.2
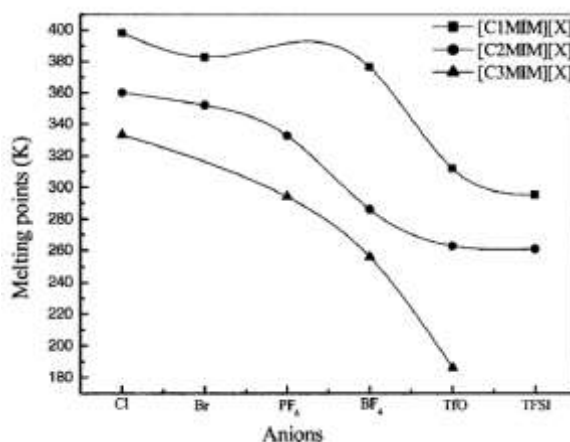
Figure 3.12: Melting Point Variation with Anions for Imidazolium-Based Ionic Liquids(*18)*

3.3.4: Attempts to Form Ternary Ionic Liquids for DCH18C6B and Traditional Crown Ethers and Sodium Based Ionic Liquid Anion Salts and Other Non-traditional Potassium Salts

A logical extension of the work described in prior sections of this chapter involves the preparation of prospective TILs *(i.e.,* metal-crown ether-anion complexes) that incorporate metal ions other than K^+. With this in mind, we sought to prepare ionic liquids incorporating sodium ion, paired either with dicyanamide or *bis*(trifluromethylsulfonyl)imide. Unfortunately, these efforts were largely unsuccessful. In many cases, (e.g., when 15-crown-5, 18-crown-6, or 21-crown-7 were employed as the crown ether) a complex could be isolated, but attempts to free it of excess reactant by washing inevitably led to the dissolution of the complexes, making the recovery impossible. This, along with the lower values of K_f for Na^+ complexes with the crown ethers considered (versus K^+), suggests that the cation-crown ether complex must be strong if the complex/TIL is to remain intact during purification. Otherwise the cation is

readily lost from the cavity, destroying the complex/TIL. In one instance, in which a sodium *bis*(trifluoromethylsulfonyl)imide complex with DCH18C6B was prepared and survived initial washings, the product was found to contain significant quantities of un-reacted starting materials (see Figures 3.13 and 3.14 for a comparison of the thermogram of a well behaved complex and the corresponding impure sodium complex.
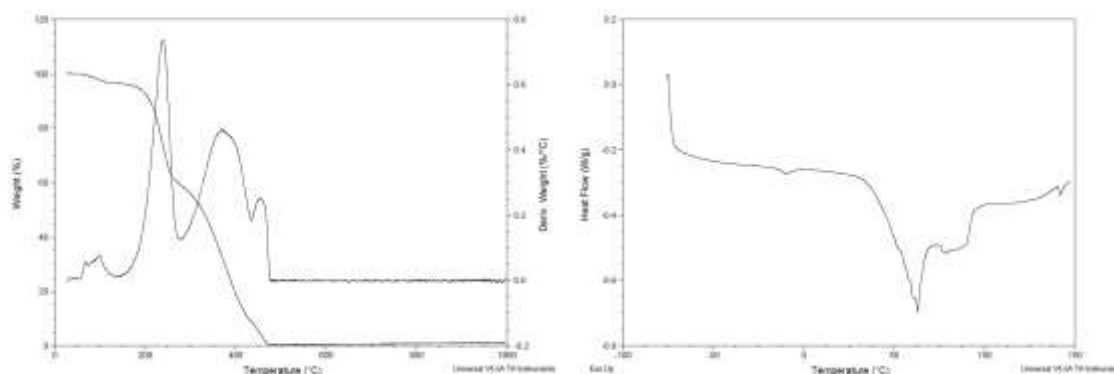
Figure 3.13: TGA and DSC Thermogram of sodium *cis-anti-cis*-dicyclohexano-18-crown-6 *bis*(trifluoromethylsulfonyl)imide
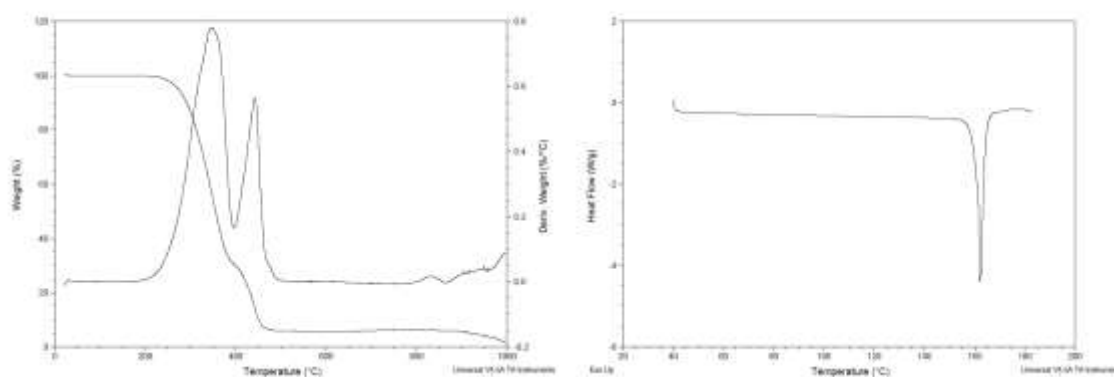
Figure 3.14: TGA and DSC Thermogram of potassium *cis-anti-cis*-dicyclohexano-18-crown-6 *bis*(trifluoromethylsulfonyl)imide

3.4: Conclusion

Preliminary studies of a new set of ternary complexes incorporating the stereoisomers of dicyclohexano-18-crown-6 or other "traditional" crown ethers (*e.g.* 21-crown-7) have led to the preparation of five new ionic liquids (eight, if the cutoff for melting points is taken to be 150°C). In the cases of TILs formed from KTf$_2$N, all of onset temperatures were higher than that of the uncomplexed crowns, indicating a strong influence of the complexation on the overall thermal properties of the TIL.

A further indication of the importance of the strength of complex formation to TIL synthesis and thermal stability is found in results obtained when sodium ion is substituted for potassium ion. Specifically, if the metal-crown ether formation constant is too low, it is very difficult to form a pure TIL. In addition, the magnitude of the formation constant also appears to influence the thermal stability of a formed TIL to a measureable extent. In contrast to traditional ionic liquids, the Tf$_2$N anion yielded ILs having a higher melting point than analogous bromide-containing TILs. Thus, while the anion plays a crucial role in determining the thermal stability of a TIL, it appears that trends derived from studies of conventional ILs may not apply to TILs.

3.5: References

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Chapter 4 : Study of the Complex Formation between the Dicyclohexano-18-Crown-6 Family of Isomers with Some Alkaline Earth Metal Ions in Methanol Using Isothermal Titration Calorimetry

4.1: Introduction

The complexation of metal ions by crown ethers has been an area of intense interest since the discovery of crown ethers nearly fifty years ago (*1*). Numerous studies performed during this time have shown these compounds to be excellent complexing agents for a wide variety of ions and molecules, most notably alkali and alkaline earth cations, ions not readily bound by most "classical ligands" (*2-5*). As a result of such studies, it is now recognized that a number of structural features of a crown ether can affect its complexation ability, among them the nature and number of donor atoms, ring size, and substituents. The stereochemistry of the crown ether has also been shown to play an important role in determining the strength and selectivity of metal ion binding (*2, 4, 6-8*). In contrast to the effects of other structural features, however, the influence of stereochemistry has received relatively little attention, a consequence of the difficulty in preparing or isolating individual crown ether isomers. To date, the few studies that have considered isomer effects on complexation have focused almost entirely on two of the five stereoisomers of dicyclohexano-18-crown-6 (DCH18C6) (Figure 4.1), in particular, the *cis-syn-cis* (A) and *cis-anti-cis* (B) forms. Recent developments in isomer specific synthesis, however, have made possible the gram-scale preparation of the *trans-syn-trans* (C), *trans-anti-trans* (D), and *cis-trans* (E) isomers, opening up the possibility of a systematic evaluation of the complexation properties of all five forms of the compound (*9, 10*).
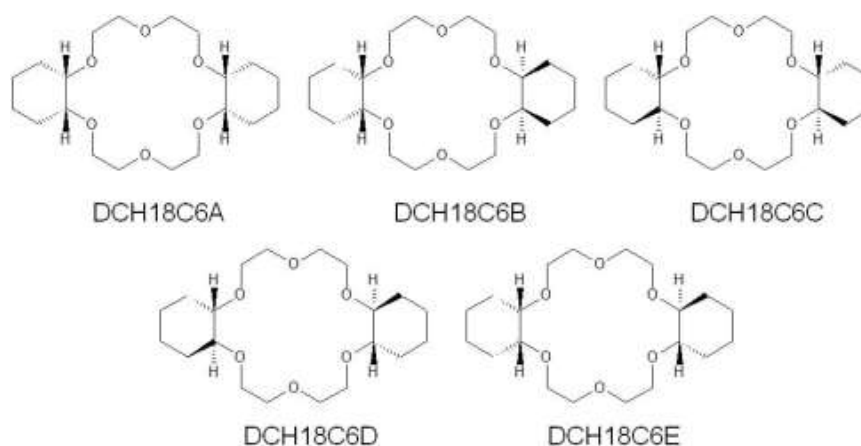
Figure: 4.1 Stereoisomers of Dicyclohexano-18-crown-6 (DCH18C6)

In this chapter, we describe the results of isothermal titration calorimetry (ITC) studies of these individual crown ether isomers. Specifically their interactions with divalent metal cations are examined in an effort to better understand the effect of stereochemistry on metal cation complexation. As will be shown, by combining the measured formation constants with thermodynamic and molecular mechanics calculations (*7*), we have extended previous reports of a relationship between ligand strain energy (*i.e.,* reorganization energy) and association constants (*8*) for crown ether complexes with monovalent cations (*i.e.,* K$^+$) to divalent cations (*i.e*., Sr^{2+}, Ba^{2+}). In so doing, we have laid the groundwork for the treatment of more complex, alkyl-substituted analogs of DCH18C6 such as di-*tert*-butylcyclohexano-18-crown-6 (DtBuCH18C6), the key component in the SREX process for the removal of radiostrontium from nuclear waste streams (*11*), and Sr resin, an extraction chromatographic material employed for the separation and preconcentration of Sr-89/90 from environmental and biological samples (*12*).

4.2: Experimental

4.2.1: Materials

The *cis-syn-cis* (A) and *cis-anti-cis* (B) isomers of DCH18C6 (99%) were purchased from Acros Organics (Geel, Belgium). The C, D, and E isomers were obtained as a generous gift from Professor Richard A. Bartsch (Texas Tech University, Lubbock, TX, USA). Potassium chloride (99%), strontium chloride hexahydrate (99%), calcium chloride dihydrate (99%), and barium chloride dihydrate (99%) were purchased from Aldrich (Milwaukee, WI USA). Methanol (DriSolv®) was purchased from EMD (Billerica, MA USA). All chemicals were used without further purification.

4.2.2: Instruments

ITC measurements were performed with a TA Instruments Nano ITC G2 (New Castle, DE USA). All measurements were performed at 25°C utilizing a 50 µl syringe and a low-volume gold cell (174 µL). The stir rate was 300 rpm and no degassing was performed. NanoAnalyze software was used to determine the formation constant (K_f), the change in enthaphy (ΔH), the change in entropy (ΔS), and the stoichiometry (n) of complexation. All measurements were carried out in at least duplicate (Appendix C).

4.2.3: Methods

In a typical experiment, a 40mM solution of the crown ether in methanol was titrated into a 5mM solution of the metal chloride in the same solvent. In cases where c (see 4.2.4) was not optimal, the concentrations of the crown ether and the metal salt were raised to 100mM and 10mM, respectively. All materials were stored in a dessicator for a

minimum of 48 hours priors to use. The anhydrous methanol was removed from its Drisolv® bottle under a dry nitrogen environment. All crown ether and metal chloride solutions were stored in a desiccator prior to use and between experiments, and were discarded 48 hours after preparation to avoid significant uptake of water.

4.2.4: Overview of Isothermal Titration Calorimetry

Isothermal Titration Calorimetry (ITC) is a method that monitors the thermodynamic events that occur when one solution interacts with another through titration in a temperature-controlled environment. In many cases, when the two components interact (whether it is a conformational change when a drug interacts with a protein or when a metal interacts with a crown ether), there is a measurable change in heat associated with this interaction. Measuring this change permits the determination of the thermodynamic (ΔH, ΔS, and ΔG) and complexation (n and K_f) variables of interest. For a given calorimetric instrument, there are three different methods of heat measurement: one that relies on a known temperature change, one that relies on heat conduction, and one that relies on power compensation (the ITC type used herein).

"In a temperature change instrument, the heat produced (or consumed) by the reaction occurring in the calorimeter results in a change in temperature of the calorimeter measuring cell. The raw calorimetric signal is simply the temperature of the calorimeter cell as a function of time… (*13*)"

"In a heat conduction instrument, the calorimeter measurement cell is passively maintained at a constant temperature by being coupled with heat flow sensors to a heat

sink that is actively controlled at a constant temperature. The raw signal in the heat conduction calorimeter is typically a small voltage that is proportional to the very small ΔT that is temporarily developed across the heat flow sensors as a result of the heat produced by the chemical reaction… (*13*)"

"In a power compensation instrument, the calorimeter measurement cell is controlled at a constant temperature. This is accomplished by means of applying constant cooling to the cell and then using a temperature controller and heater to keep the cell temperature constant. As a chemical reaction takes place, any heat input from the chemical reaction is sensed and the power applied to the control heater reduced so that again the temperature remains constant. The heating power from the two sources, reaction and controller heater, are obviously kept at a constant level so that a heat input from the reaction is compensated by a drop in the heat input from the controlled heater. The raw signal in the power compensation calorimeter is the power applied to the control heater that is required to keep the calorimeter cell from changing temperature as a function of time… (*13*)"

Although ITC can be used in a number of different applications, it is typically employed to determine the binding affinity of a ligand for a given molecule (*2-4, 14-18*). The instrument itself is composed of two identical cells (Figure 4.2) one a reference and the other where the experiment actually occurs. Typically these cells consist of a chemically inert metal or alloy like Hastalloy or gold. Temperature sensors are attached to each cell to measure any change that occurs during the typical experiment. Heaters

working in conjunction with the sensors are also attached to each cell to keep the cells at

the same temperature.
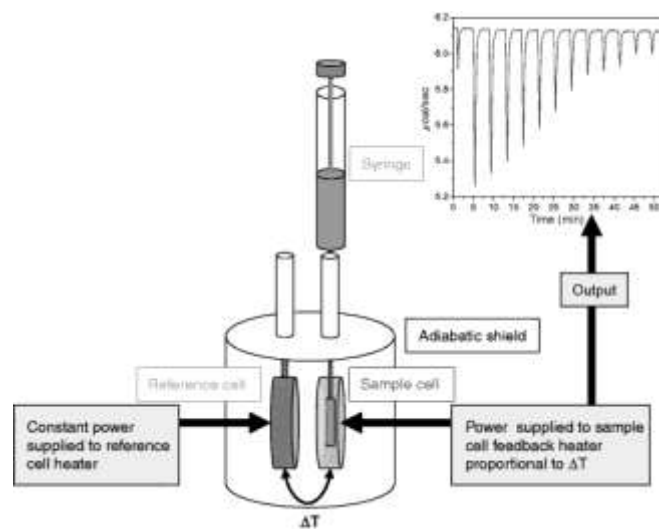
Figure 4.2: Schematic of Isothermal Titration Calorimetry (*14*)
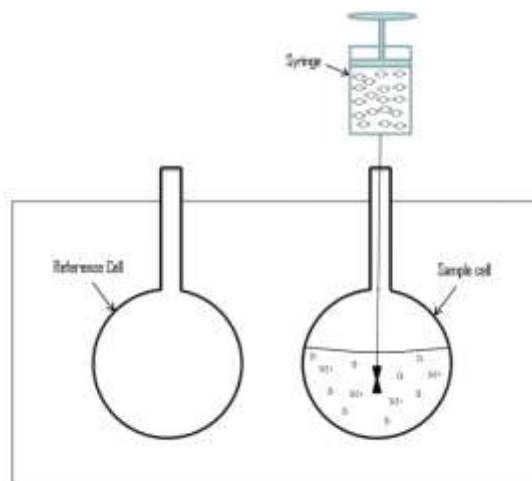
Figure 4.3: Syringe and Cell Makeup for Our Experiment

(image modified from Zhou *et al.(15)*)

In a typical experiment, a solution of the crown ether is loaded into the syringe and a solution of the metal chloride is placed in the sample cell (Figure 4.3). The precise concentrations chosen depend on c, a unitless value that provides an indication of the viability of a given set of experimental conditions:

$$c = n * K_a * [M_{Macrocycle}] \text{ (1)}$$

Values of c between 10 and 100 are ideal, but acceptable c values can range from ~1 to 1000, depending on the system (Figure 4.4).
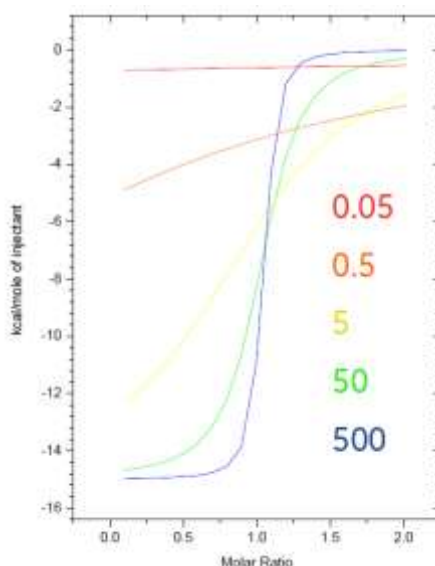
Figure 4.4: Graphical Representation of c Values (*16*)

The syringe, which has a paddle attached to its end to ensure proper solution mixing, is then placed into the cell. Multiple injections of a known volume of the crown ether solution are then performed automatically by the instrument, yielding an injection profile such as that shown in Figure 4.5. For an exothermic system, the temperature of the sample cell will increase with each injection; while in an endothermic system, the temperature of the sample cell will decrease with each injection. In either case, the

instrument manipulates the power applied to the heater to ensure that the sample and reference cell are maintained at the same temperature. From the data obtained, the formation constant of the complex, the reaction stoichiometry, and the enthalpy change for the reaction can then be determined. The entropy of reaction can then be determined from Equation 2 and 3.

$$\Delta G = -RT \ln K \text{ (2)}$$

$$\Delta G = \Delta H - T\Delta S \text{ (3)}$$
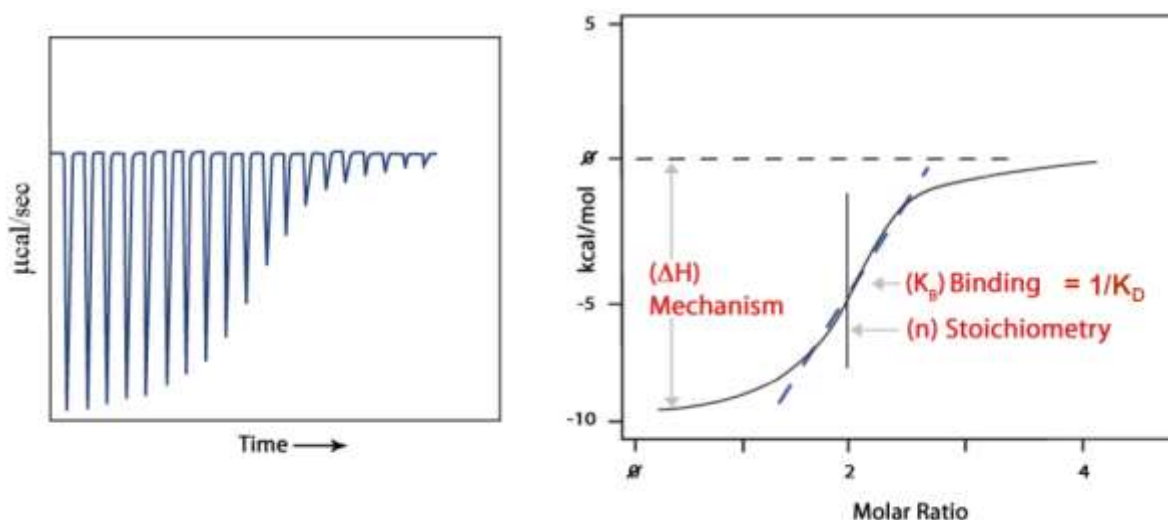
Figure 4.5: Typical Injection Profile and Methods to Determine Variables (*16*)

4.2.5: Instrument and Procedure Validation (*6*)

To ensure that the procedure followed to measure formation constants is experimentally sound, a validation procedure similar to that described by Vogel (*6*) was employed. In this procedure, the formation constants obtained for the complex of DCH18C6B with potassium ion (as the potassium chloride form) from three sources – the present work, unpublished studies carried out by Vogel using a Microcal MSC ITC (*6*)

and results published by Hay *et al. (8)* using a method employing an ion selective electrode – were compared. As shown in Table 4.1, the result obtained here agrees well with other published data.

Table 4.1: Formation Constants for DCH18C6B and KCl

for Instrument and Procedure Validation

log K_f	UWM - ITC[a]	TTU (15) - ITC	*Hay et al.* (9) - ISE
K^+	5.43	5.4	5.3

[a] average of three trials

4.2.6: Alternative Methods in the Determination of Association Constants

A number of approaches other than ITC can be used to determine the formation constants of various metal ion-crown ether complexes (*2-4, 18-20*). Some of the most commonly used methods are nuclear magnetic resonance (NMR) (*19, 21*), fluorescence spectroscopy (*22, 23*), UV-Vis spectroscopy (*24, 25*), potentiometric titrations (*26, 27*), and extraction experiments (*28, 29*). All of these methods have advantages and disadvantages. With NMR for example, formation constants below 10^5 can be determined, but deuterated solvents must be used, there is no direct measure of the thermodynamic properties of the system, and the exchange rate (slow or fast) of the complexation reaction must be taken into account (*30*). With fluorescence spectroscopy, K_f values exceeding 10^6 can be determined, but one of the two species involved in the complexation reaction must incorporate a fluorophore, which is a major disadvantage (*19*). (Even if a fluorophore is present, it is best if only one form of the complexing agent (*i.e.,* complexed or uncomplexed) is fluorescent.) With UV-vis spectrophotometry,

formation constants up to 10^9 can be measured, but a chromophore is required (*19*). Potentiometric titrations are selective and sensitive, but interfering ions can be an issue. Also, the redox potential has to be high enough for the complexation so that it is readily measureable (*30*). Lastly, liquid-liquid extraction can be used to measure formation constants spanning a wide range (10^4-10^{12}), but the method is limited in the solvents that can be used (*30*). That is, the metal ion is extracted from one solvent (typically water) into another (often chloroform or dichloromethane). Therefore immiscible solvents must be used. In addition, the complexing molecule must not be appreciably soluble in the aqueous layer. As already noted, ITC was chosen for use in this study. Its main advantage versus other methods is its ability to directly measure the enthalpy of complexation, which then permits the determination of the corresponding entropy and free energy (*31*). The principal disadvantage of the method is the requirement that an observable amount of heat be released or absorbed upon complex formation (if the heat transfer is too low or too high, then the system cannot measure the formation constants). The upper and lower limits for the determination of formation constants by ITC are 10^8 (*32*) and 10^3 (*33*), respectively.

4.3: Results

Complexation constants determined for the Ca^{2+}, Sr^{2+}, and Ba^{2+} complexes of four of the five isomers of DCH18C6 are shown in Table 4.2. It is clear from these values that the following trend in formation constants is seen regardless of metal cation: A>B>C>D.

Table 4.2: Average Formation Constants for Alkali Earth Metal Cations with the
Stereoisomers of DCH18C6

Compound	Cation	K	log K	N	ΔH (kJ/mol)	ΔS (kJ/mol•K)	ΔG (kJ/mol)	-TΔS (kJ/mol)
DCH18C6A	Ca^{2+}	1890	3.28	1	5.469	0.081	-18.666	-24.135
(cis-syn-cis)	Sr^{2+}	728000	5.86	1	-25.415	0.027	-33.449	-8.034
	Ba^{2+}	1620000	6.21	1	-29.615	0.020	-35.429	-5.814
DCH18C6B	Ca^{2+}	1540	3.19	1	8.521	0.090	-18.160	-26.681
(cis-anti-cis)	Sr^{2+}	155000	5.19	1	-10.720	0.063	-29.488	-18.768
	Ba^{2+}	684000	5.84	1	-22.825	0.035	-33.282	-10.457
DCH18C6C	Ca^{2+}	<1000	<3					
(trans-syn-trans)	Sr^{2+}	14800	4.17	1	-13.180	0.034	-23.309	-10.129
	Ba^{2+}	28000	4.45	1	-19.520	0.020	-25.380	-5.860
DCH18C6D	Ca^{2+}	<1000	<3					
(trans-anti-trans)	Sr^{2+}	10200	4.01	1	-12.735	0.034	-22.867	-10.132
	Ba^{2+}	5870	3.77	1	-12.395	0.031	-21.633	-9.238

4.3.1: Corey-Pauling-Koltun (CPK) Modeling as an Approach to Rationalizing Stereoisomer Effects on Metal Ion Complexation

Corey-Paulin-Koltun (CPK) models can provide a qualitative understanding of the complexation properties of the stereoisomers of dicyclohexano-18-crown-6 (*6*). As can be seen from Figure 4.6, for isomers A and B, the complexing cavity is round and symmetrical, and thus is comparable to that seen for 18-crown-6 (18C6), for which the ether oxygens are positioned in such a way as to maximize their interaction with the metal cation. In all three ligands, the unshared electron pairs on the ether oxygens are well positioned to participate in stabilizing the positive charge of the metal cation guest. In Isomers C and D, the overall size of the macro ring cavity is appropriate for complexing a metal ion, but it is not round; rather it is elongated in shape. As a result, the

unshared electron pairs of the ether oxygens are not well positioned for metal ion complexation. That is, instead of pointing toward the cavity, any possible conformation of the *trans* arrangement leads the unshared electron pairs to rotate out of the ring, where they cannot effectively participate in interaction with the metal cation. Isomer E is a combination of the two limiting conformations of the cyclohexano residues; one side of the molecule contains the *cis* conformer, while the other side contains a *trans* conformer. The resulting complexing cavity has some characteristics of each conformer, round on the *cis* side (the left side in the figure) and elongated on the *trans* side (the right side in the figure), resulting in a pear-shaped complexing cavity. This cavity is not as favorable for complexing metal cations as the all-*cis* (totally round) cavity, but better than an all-*trans* (completely elongated) cavity.
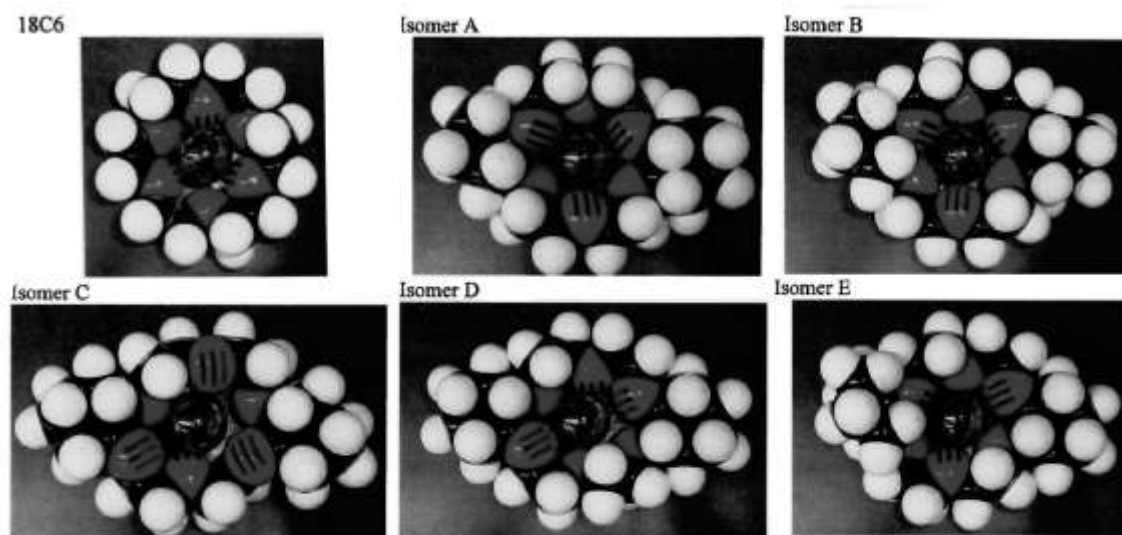
Figure 4.6: CPK Modeling of 18-crown-6 and the dicyclohexano-18-crown-6 Family (*6*)

4.3.2: Trends in Formation Constants for Stereoisomers of Dicyclohexano-18-crown-6 Explained through Molecular Mechanics Calculations of Ligand Reorganization Energy

Prior researchers have sought to explain the trends observed in the binding constants of various crown ether with a metal ion by use of molecular mechanics calculations (*8, 34*). This approach considers the free energy changes associated with the process of metal ion binding by the crown ether, in particular the change in free energy the crown undergoes as it converts from its minimal energy "free ligand" form to the "binding conformer" form and ultimately to its complexed form (Figure 4.7) (*8*). This process results in ligand (*i.e*., crown ether) "strain", the magnitude of which is inversely proportional to the binding constant. Stated another way, the greater the energy expended in ligand reorganization to enable binding (*i.e*., the greater strain induced in the ligand by binding), the less its propensity to complex a given metal ion (*7*). Table 4.3 summarizes the results of MM3 calculations for the five isomers of DCH18C6 for the complexation of Ca^{2+}, Sr^{2+}, and Ba^{2+} (*7*). From this table, trends in the reorganization (*i.e.,* strain) energy associated with metal ion binding can be seen. For example, the *cis-cis* isomers have lower strain energy than the *trans-tra*ns isomers, while a combination of *cis* and *trans* falls somewhere between. In addition, *syn* isomers exhibit lower strain energies than do the *anti* isomers. This leads to the complexing trend seen in the stereoisomers of DCH18C6, and to the conclusion that as is the case for K^+ complexation, smaller reorganization energies result in higher formation constants (*8*). It remains to be seen if this strong inverse linear relationship (Figure 4.8) holds true for more complex, substituted derivatives of dicyclohexano-18-crown-6.
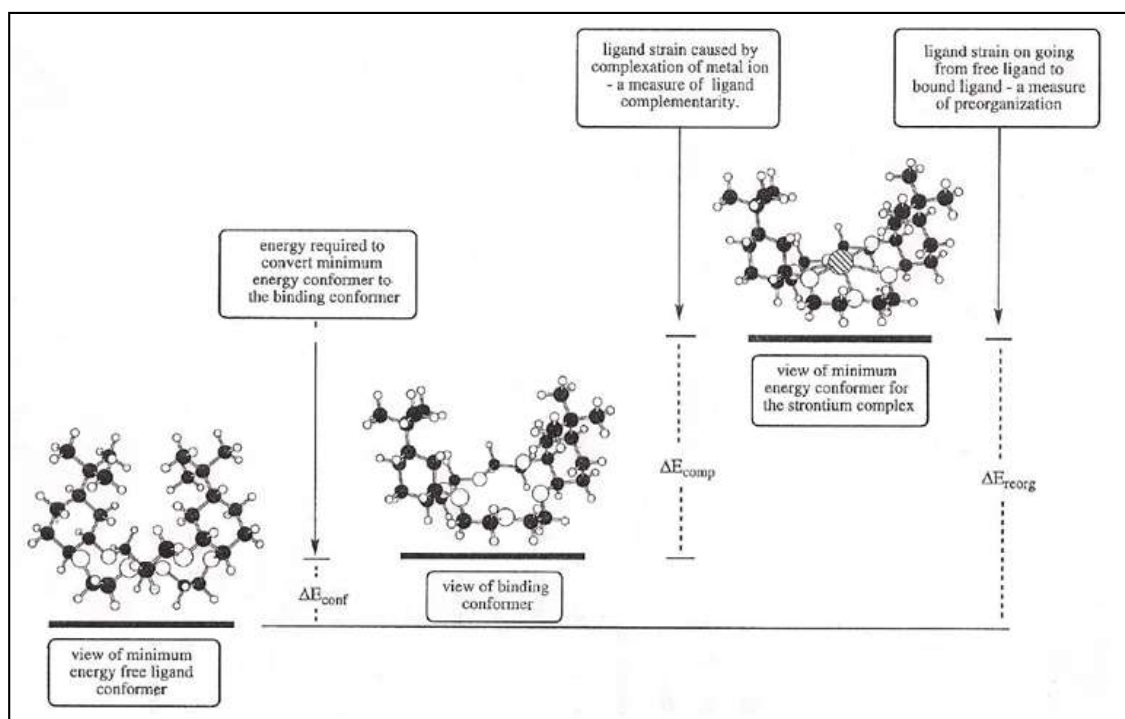
Figure 4.7: Reorganization Energy (ΔE_{reorg}) Determination

Table 4.3: Reorganization Energies for Metal Cation-Crown Ether Complexation (*7*)

$\Delta U_{reorganization}$ (kcal/mol)			
	Ca^{2+}	Sr^{2+}	Ba^{2+}
cis-syn-cis	12.87	11.23	10.67
cis-anti-cis	13.76	12.18	11.09
cis-trans	15.18	13.51	12.94
trans-syn-trans	16.92	14.92	14.25
trans-anti-trans	19.59	17.86	17.28
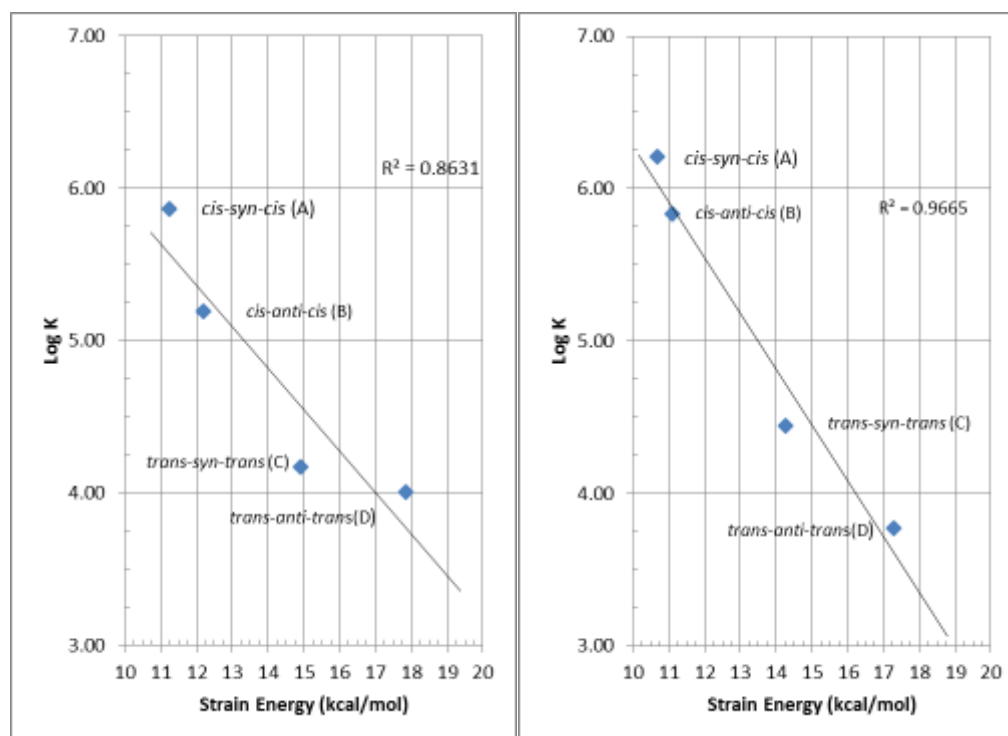
Figure 4.8: (left panel) Log K_f *vs*. Strain Energy for the Complexation of Strontium by the Stereoisomers of DCH18C6 and (right panel) Log K_f *vs.* Strain Energy for the Complexation of Barium by the Stereoisomers of DCH18C6

4.3.3: Thermodynamic Aspects of Alkaline Earth Cation Complexation by the Stereoisomers of Dicyclohexano-18-crown-6

As can be seen in Figure 4.9 and 4.10, the complexation of Ba^{2+} and Sr^{2+} by the stereoisomers of DCH18C6 is enthalpically favorable, as indicated by the negative values of the enthalpy of complexation. In contrast, calcium is too small to interact with the crown ether ring and therefore has a positive enthalpy of complexation, suggesting that it prefers to be solvated by the traces of water present rather than form a complex with the crown ether. All of the systems exhibit a positive T∆S, which indicates that complexation is entropically favorable. This is not unexpected given that complexation undoubtedly

results in loss of coordinated water molecules and their replacement with the crown ether. The use of methanol rather than water as the solvent also has a significant effect on the complexation of the metal ion by the crown ether (Table 4.4). The cations are more strongly solvated in water than methanol, directly influencing the complexing constants(*35*). Note that by using hydrated metal salts, the values of ΔH, ΔS, and TΔS have likely been altered when compared to the use of anhydrous metal salts, but the formation constants should be very similar regardless (formation constants obtained in dry methanol and 90:10 (%v/v) methanol:water for DCH18C6 showed minimal differences between the two (*36*)).
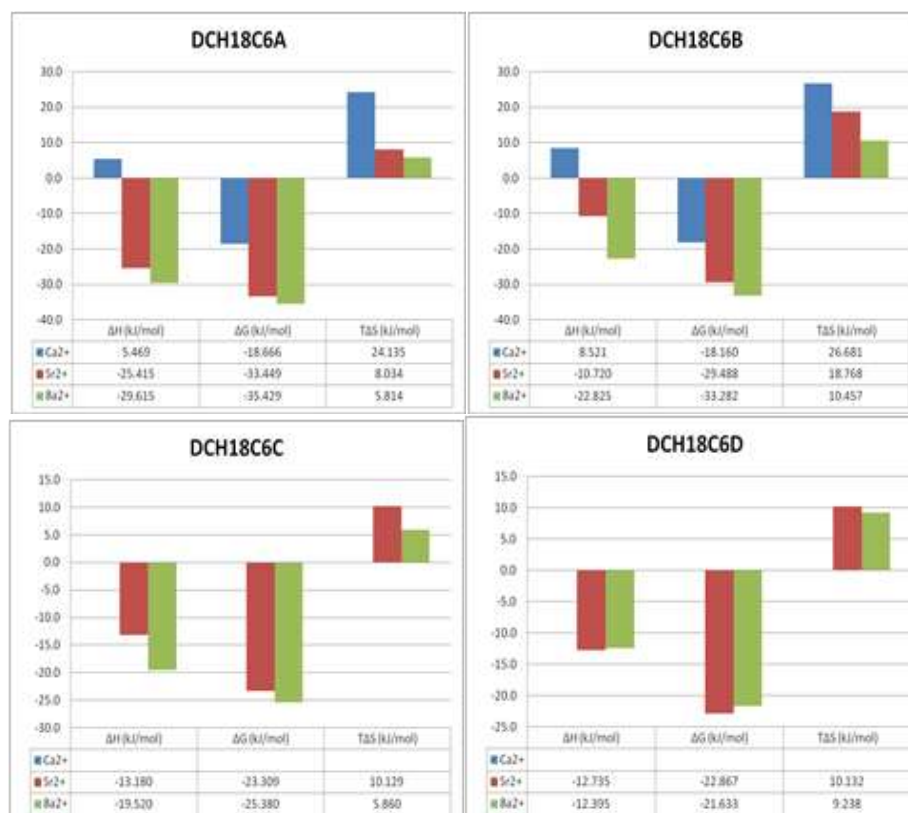
Figure 4.9: Thermodynamic Data for Each Isomer of DCH18C6 and Alkaline Earth Metal Cations
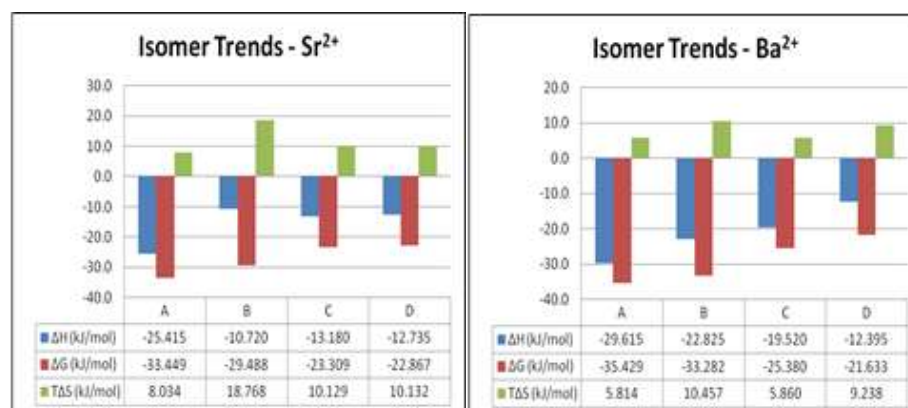
Figure 4.10: Trends inThermodynamic Data for Strontium (left panel) and Barium (right panel)

Table 4.4: Formation Constants and Thermodynamic Data for Alkaline Earth Cation Complexation by DCH18C6 (A and B Isomers) in Methanol[a] and Water[b]

Compound	Solvent	Cation	K	log K	N	ΔH (kJ/mol)	ΔS (kJ/mol•K)	ΔG (kJ/mol)	$T\Delta S$ (kJ/mol)
DCH18C6A	MeOH	Sr^{2+}	728000	5.86	1	-25.415	0.027	-33.461	8.046
(cis-syn-cis)	Water	Sr^{2+}	1738	3.24	1	-15.397	0.010	-18.514	3.117
	MeOH	Ba^{2+}	1620000	6.21	1	-29.615	0.020	-35.575	5.960
	Water	Ba^{2+}	3715	3.57	1	-20.585	-0.001	-20.336	-0.249
DCH18C6B	MeOH	Sr^{2+}	155000	5.19	1	-10.720	0.063	-29.494	18.774
(cis-anti-cis)	Water	Sr^{2+}	436.516	2.64	1	-13.221	0.006	-15.092	1.870
	MeOH	Ba^{2+}	684000	5.84	1	-22.825	0.035	-33.255	10.430
	Water	Ba^{2+}	1862.09	3.27	1	-25.941	-0.024	-18.709	-7.232

[a] This work [b] Ref. (*17*)

When considering the trends in complexation constants seen for the individual stereoisomers of DCH18C6, there also appears to be a relationship between the size of the cation and the observed formation constants. The cavity sizes of the dicyclohexano-18-crown-6 isomers are very similar to that of 18-crown-6, which ranges from 2.6-3.2 Å (*37*). Table 4.5 shows the ionic diameters of the three alkaline earth cations studied in this work. Figure 4.11 shows the formation constants and the size of the metal cation size. In

most cases, the following trend is observed: $Ba^{2+} > Sr^{2+} > Ca^{2+}$. Metals cations that are equal in size to the diameter of the cavity have been found to exhibit the largest formation constants, as illustrated by the work of *Izatt et al. (18)* with 18-crown-6 and various monovalent and divalent cations in water (Figure 4.12). Ions that are too large cannot interact fully with the oxygens present on the ring, leading to reduced formation constants. (Note that this metal cation size to crown ether cavity size relationship has been reported to break down for larger crown ethers, due to greater ring flexibility (*38*). This reinforces the notion that many factors influence the complexation of a metal cation to a crown ether (*2-4, 18*).

Table 4.5: Ionic Diameters (*39*)

Ionic diameter (Å)	
Ca^{2+}	2.00
Sr^{2+}	2.36
Ba^{2+}	2.70

Metal Ion Size Effects on Complexation

	Ca2+	Sr2+	Ba2+
DCH18C6A	3.28	5.86	6.21
DCH18C6B	3.19	5.19	5.84
DCH18C6C		4.17	4.45
DCH18C6D		4.01	3.77
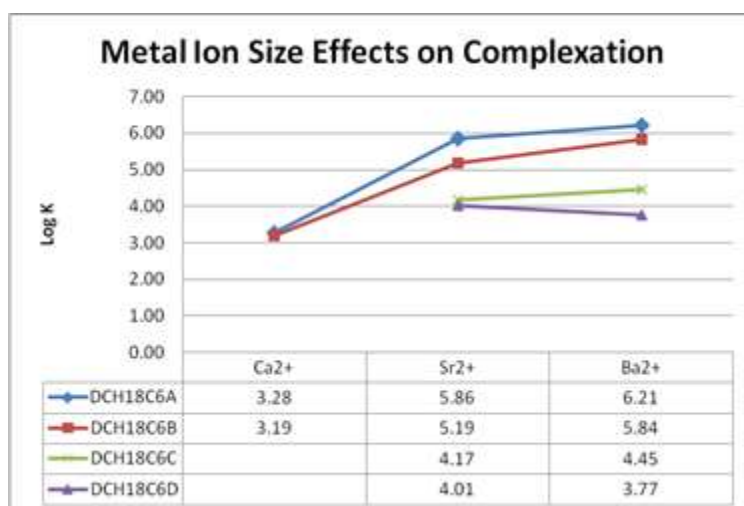
Figure 4.11: Metal Ion Size Influence on Complexation
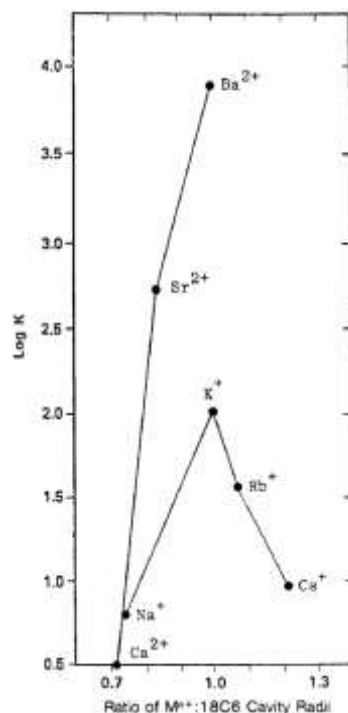
Figure 4.12: Selectivity of 18-Crown-6 (*18, 40*)

4.4: Conclusions

We have determined the complexation constants for four of the five stereoisomers of dicyclohexano-18-crown-6 with several divalent alkaline earth metal cations in methanol. Regardless of cation, the constants follow the trend: DCH18C6A > DCH18C6B > DCH18C6C > DCH18C6D. This trend can explained qualitatively by molecular models and quantitatively by molecular mechanics methods. Among the metal cations, barium forms the strongest complex and calcium the weakest with strontrium between. This trend can be explained by considering the match of the cation size to that of the crown ether cavity.

4.5: References

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Chapter 5 : Separation of the Stereoisomers of Di-*tert*-butylcyclohexano-18-crown-6

5.1: Introduction

Previous studies have shown that the two most prevalent stereoisomers of dicyclohexano-18-crown-6 (DCH18C6), the *cis-syn-cis* (A) and *cis-anti-cis* (B) forms, are excellent complexing agents for various metal ions, especially alkaline earth cations (*1*). In contrast to its aromatic precursor dibenzo-18-crown-6, the cyclohexano groups attached to the polyether ring donate electron density to the ring (*2*). This shifts the affinity of the macrocycle from "softer" alkali metal cations to "harder" alkaline earth cations, which makes DCH18C6 a prime candidate as an extractant for alkaline earths (*3*). Unfortunately, both the crown ether itself and the metal complexes it forms are often too water-soluble to provide the basis of a practical liquid-liquid extraction system, a result of the poor efficiency with which the complex is extracted and loss of the crown ether to the aqueous phase (*4, 5*). This high aqueous solubility also makes this crown ether a poor choice as the basis for an extraction chromatographic resin, as it would be readily leached from the support. In an attempt to address this issue, prior researchers have prepared alkyl-substituted analogs of DCH18C6 by adding, for example, a *tert*-butyl group to each of the cyclohexano- groups present in DCH18C6. Not only is the resultant crown ether, 4,4'(5')-di-*tert*-butylcyclohexano-18-crown-6 (DtBuCH18C6) much less water-soluble, but its ability to extract alkaline earth metal cations is greatly enhanced due to the increase in crown ether hydrophobicity resulting from the introduction of *tert*-butyl groups into the molecule (*5*). This improvement is accompanied by a new problem, however. That is, the number of possible stereoisomers is dramatically increased, and this

is reflected in the much greater complexity of the product produced by the hydrogenation of the aromatic precursor. Specifically while reduction of dibenzo-18-crown-6 can produce five isomers of dicyclohexano-18-crown-6 (two in appreciable quantities) (*3*), hydrogenation of di-*tert*-butylbenzo-18-crown-6 can result in the production of up to forty isomers, with more than a dozen forms (many of which differ significantly in their metal ion extraction behavior) being produced in measurable quantities. This is a result of the harsh reaction conditions required to reduce the more sterically hindered di-*tert*-butyl compound (*6*). Adding to the complexity of the product is the fact that it is mixed with a variety of contaminants, among them spent catalyst, unreacted and partially reacted starting material, and crown ether fragments. Taken together, these factors lead to significant lot-to-lot variability in the composition of the DtBuCH18C6 product, regardless of efforts taken to ensure uniformity. As a result, the extraction behavior of the commercially available DtBuCH18C6 is often found to vary substantially from one sample to the next. Because uniform and predictable behavior is required of any extractant employed in a "real world" extraction process, it is apparent that the separation of the DtBuCH18C6 stereoisomers, both from contaminants and from one another, is a very important task. This task is the focus of the work described in this chapter.

Prior work concerning the separation of individual crown ether stereoisomers is limited (*7, 8*). In fact, nearly all published studies have focused on the separation of the various forms of DCH18C6 (*9*). For example, *Izatt et al.* (*10*) exploited the differences in the abilities of the *cis-syn-cis* (A) and *cis-anti-cis* (B) forms of the crown to complex perchloric acid and lead perchlorate to selectively precipitate the individual isomers in

good yields. Similarly, Yakshin *et al.* (*11*) used perchloric acid precipitation to separate all five of the isomers of DCH18C6. The use of perchloric acid and its derivatives is hazardous, however, particularly on a large scale. Among these same lines, a method has been described involving formation of a complex of DCH18C6 with uranyl nitrate and its subsequent crystallization to isolate the *cis-anti-cis* isomer and distillation to isolate the *cis-syn-cis* isomer of DCH18C6 *(12)*.

Other means of crown ether separation utilizing chromatography have also been explored. For example, an alumina column was used to separate a mixture of *cis-syn-cis* and *cis-anti-cis* DCH18C6, but the incompleteness of the separation made crystallization necessary to ensure pure isomeric fractions (*1*). Metal-loaded cation-exchange resins relying on the principles of ion-dipole association chromatography have been used to separate crown ethers on an analytical scale from contaminants like open-chained analogs, as well as to separate crown ethers homologs that differ in the ring size (*13*). Both aminopropyl- and cyano-derivatized silica (on an analytical scale) have also been used to separate crown ethers. Specifically, it has been shown that aminopropyl silica can be used to partially separate isomers of DCH18C6 by HPLC based on the affinity of the crown ether for the amine group present (which interacts with the oxygens present in the ring) (*13-17*).

To date, only a single report describing an effort to separate the various forms of DtBuCH18C6, either from one another or from impurities, has appeared. In 1999, Dietz *et al.* (*18*) performed a preliminary evaluation of the utility of perchloric acid precipitation (similar to Izatt *et al. (10)* and Yakshin *et al. (11))* or classical column

chromatography for the removal of impurities from this crown ether. Both were found to provide a product that exhibited higher strontium extraction efficiency (a measure of the purity of the crown ether). In addition, under certain conditions, precipitation with perchloric acid yielded what subsequent HPLC showed to be a single isomer, reported to be the 4z, 4'z *cis-syn-cis* DtBuCH18C6 form (Figure 5.1).
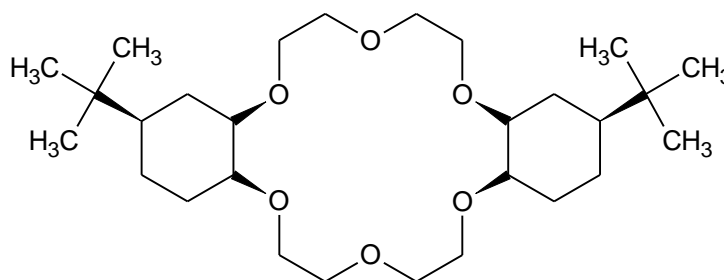
Figure 5.1: 4z, 4'z *cis-syn-cis*-di-*tert*-butylcyclohexano-18-crown-6

In this chapter, we describe our efforts to extend this work and to devise a method for the isolation of a number of DtBuCH18C6 stereoisomers, both from the variety of impurities present in the commercial material and from one another. In particular, we investigate the utility of a number of other complexing agents as a means of achieving selective precipitation of one or more DtBuCH18C6 isomers. In addition, we evaluate an automated version of classical column chromatography (*i.e.,* flash chromatography) employing a smaller particle size stationary phase as a means of purifying DtBuCH18C6. Lastly, we evaluate preparative-scale LC as a means of resolving individual DtBuCH18C6 isomers.

5.2: Experimental

5.2.1: Materials

A mixture of the *cis-syn-cis* and *cis-anti-cis* forms of dicyclohexano-18-crown-6 was obtained from Parish Chemical Company (Orem, UT USA). 4,4',(5')-di(*tert*-butylcyclohexano)-18-crown-6 (DtBuCH18C6) was obtained as a mixture of isomers from EiChroM, Inc. (Lisle, IL USA). Trace metal grade perchloric acid and HPLC grade methanol were obtained from Fisher Scientific (Waltham, MA USA). Hexane was obtained from EMD Millipore (Billerica, MA USA). BakerBond aminopropyl-functionalized silica (40 μm average pore diameter) was obtained from J.T. Baker (Phillipsburg, NJ USA). HPLC grade acetonitrile was obtained from Honeywell (Morris Township, NJ USA). RediSep® R_f Gold cartridges were provided by Teledyne Isco (Lincoln, NE USA). All aqueous solutions were prepared using deionized water with a specific resistance of 18MΩ·cm^{-1}. All chemicals were used without additional purification unless noted otherwise.

5.2.2: Instruments

Flash chromatographic analyses were performed on a Teledyne Isco Combi-Flash® Flash Chromatograph coupled to an evaporative light-scattering detector. Flash cartridges used on the Teledyne flash chromatograph had an average particle size of 20 to 40μm.

High performance liquid chromatography (HPLC) was performed on an Agilent 1200 Series Liquid Chromatograph equipped with analytical-scale quaternary pumps

utilizing an online degasser, a fixed 20 μL loop manual injection port, and a variable wavelength UV-Vis flow cell. In addition, when necessary, a Varian 380-LC Evaporative Light Scattering Detector (ELSD) was used. ChemStation software was used to run the instrument. For most analyses, a 3.0 x 75 mm Agilent Zorbax NH_2 LC-MS column with an average particle size of 5 microns was employed. For scale-up, a 4.6 x 250 mm Agilent Zorbax NH_2 Analytical column with an average particle size of 5 microns or 7 microns was used. In addition, an IDEX Micro-Splitter Valve (Oak Harbor, WA USA) was used when necessary to ensure that the ELSD was not overloaded with column effluent.

Preparative LC runs were performed on a Varian ProStar Solvent Delivery Module equipped with a custom 500μL loop injection port and a Varian 380-LC Evaporative Light Scattering Detector. In addition, an Analytical Scientific Instruments Semi-Preparative Adjustable Flow Splitter (Richmond, CA USA) was used to feed the effluent from the column to the ELSD and the fraction collector. All semi-preparative chromatographic runs used an Agilent Zorbax NH_2 Preparative column that has the dimensions of 21.2 x 250 mm and an average particle size of 7 μm.

Strontium distribution ratio determinations were performed on a Perkin Elmer 2480 Automatic Gamma Counter equipped with WIZARD2 software (Waltham, MA USA).

5.2.3: Methods

Classical column chromatography, perchloric acid precipitations, and strontium distribution ratios measurements were performed following methods similar to those described by *Dietz et al.(18).* For the perchloric acid treatment, a 0.5 M solution of the crown ether was prepared in hexane and the solution contacted with twice its volume of a 0.25 M to 6 M perchloric acid solution. The mixture was then vortexed and placed in refrigerator overnight, during which time a solid formed at the interface. The solid (a hydronium crown ether perchlorate) was removed, dissolved in methylene chloride, and washed with water to remove the acid. Once the water washing was complete (as indicated by a pH of approximately 5), the methylene chloride layer was removed and evaporated to yield a purified DtBuCH18C6 sample. Strontium-85 was used to determine the strontium distribution ratios of the crown ether isolated radiometrically. In each case, a 0.1M solution of the recovered DtBuCH18C6 was prepared in 1-octanol. This solution was then preconditioned with twice its volume of a 1M HNO_3 solution. After preconditioning, the sample was contacted with an equal volume of the same acid spiked with the radiotracer. Following mixing and centrifugation, aliquots of equal volume were removed from both the organic and aqueous layers for analysis by gamma spectroscopy.

For classical column chromatography, aminopropyl-silica was slurried in methanol and transferred under air pressure to a 1.55 cm x 30 cm glass (Ace Glass, Vineland, NJ USA) column modified with a glass frit and equipped with a Teflon stopcock. The slurry was added until a bed height of 16 cm had been reached, after which a plug of glass wool was placed atop the bed to ensure that it would not be disrupted

during sample introduction. In addition, samples were introduced to the column bed with a long Pasteur pipet to ensure bed integrity. After sample loading, the column was washed with 4 bed volumes of 10% (v/v) methanol-acetonitrile. Two different column studies were performed. First, the column was used solely to separate DtBuCH18C6 from non-extracting impurities. In this study, only two fractions were collected, the first corresponding to column loading and rinsing (to remove impurities) and a second corresponding to the stripping of sorbed DtBuCH18C6 from the column. In a typical run, a solution of crown ether (1 g in 10 mL of 10% (v/v) methanol-acetonitrile) was added in two 5 mL aliquots to the column. Next, 40 mL of 10% (v/v) methanol-acetonitrile was added and the effluent collected in the same container as the load fraction. This was followed by the introduction of 100 mL of pure methanol to strip the column of the crown ether. In a subsequent, more detailed study, the same experimental procedures were followed but the strip fraction was collected as a series of 2-mL aliquots in weighed scintillation vials.

For flash chromatographic analyses, a Reveleris® SRC aminopropyl 11 g or 28 g SNAP cartridge was used. A 0.5 g portion of the crown of interest (a mixture of dicyclohexano-18-crown-6 or 4,4'(5')-di(*tert*-butylcyclohexano)-18-crown-6) was dissolved in 10 mL of a solution comprising 90:10 (v/v) methanol: acetonitrile. Roughly half of this solution was loaded onto an aminopropyl cartridge and the crown ether eluted utilizing a solvent gradient that went from 100% acetonitrile to 100% methanol over a period of 30 minutes. The flow rate applied during the gradient was 32 mL/min.

For analytical HPLC analyses, samples of DtBuCH18C6 were dissolved in methanol to obtain a solution concentration of 1 mg/mL. For each run, 20 µL of this solution was loaded on a column using the manual injection port. For scale-up experiments, the concentrations of the crown ether dissolved in methanol varied from 1 mg/mL to 100 mg/mL. For all chromatographic runs, a 0-80% (v/v) methanol:acetonitrile gradient was applied for 90 minutes, and depending on the column carryover, the system was flushed with the final solvent mixture for 30 to 90 additional minutes. Between runs, the system was equilibrated at the initial conditions for 20 minutes. The flow rate used depended on the column length and particle size. For a 3.0 x 75 mm (5-micron average particle size) column, a flow rate of 0.235 mL/min was used. For a 4.6 x 250 mm (5-micron average particle size) column, a flow rate of 1.842 mL/min was used. Lastly, a flow rate of 1.316 mL/min was used for the 4.6 x 250 mm (7-micron average particle size) column. Regardless of the flow rate chosen, no more than 1.0 mL/min of the effluent was allowed to reach the ELSD; a splitter was used when necessary. The conditions of the ELSD for all experiments were as follows: nebulizer temperature: 50°C, evaporator temperature: 60°, and gas flow rate: 0.90 SLM (standard liter per minute).

For preparative LC analyses, samples of DtBuCH18C6 were dissolved in methanol to obtain solution ranging in concentrations from 20 mg/mL to 100 mg/mL. Aliquots of 300-500µL were loaded onto the column for each trial. For all chromatographic runs, a 0-80% (v/v) methanol:acetonitrile gradient was applied over 90 minutes. Between runs, the system was equilibrated at the starting conditions for 20 minutes. A flow rate of 28 mL/min was used on 21.2 x 250 mm column with an average

particle size of 7-micron. A semi-preparative adjustable flow splitter set at a split ratio of 100:1 was used to ensure that the ELSD was not overwhelmed and that the maximum amount of effluent was collected. The conditions of the ELSD for all experiments were as noted above.

5.3: Results

5.3.1: Perchloric Acid Precipitation

In a preliminary study of the effect of perchloric acid-induced precipitation on the extraction behavior of DtBuCH18C6, Dietz *et al*(*18*) demonstrated that the strontium distribution ratios obtainable can be improved by treatment of the crown ether with an acid solution of an appropriate concentration, an observation attributed to enrichment of the material in the isomer(s) most effective as strontium extractants. A systematic chromatographic study of the purified materials obtained was not performed however. To address this deficiency and to better understand the precipitation process, the methods of Dietz *et al.* (*18*) were again employed, but the resultant precipitates were analyzed by gradient elution HPLC. In a typical procedure, a solution of DtBuCH18C6 (0.5M) in hexane was contacted with twice its volume of a perchloric acid solution of known (0.25 − 6M) concentration. After mixing and refrigeration, the crown ether-perchloric acid complex formed at the interface was removed and washed to remove acid, yielding a purified crown ether sample. In agreement with the results of Dietz *et al.* (*18*), it was observed that solutions containing lower concentrations of perchloric acid yield less precipitate than those contacted with more acidic solutions. The strontium distribution ratios, however, were found to be highest for the samples treated with the most dilute

acid. This indicates that there is competition for the perchloric acid, and the most effective isomers for strontium extraction bind to the acid first. Studies of the crown ether samples recovered (following removal of perchloric acid) and of the residual hexane layer are consistent with this view. Figure 5.2 shows the chromatogram of an unpurified commercial lot of DtBuCH18C6, while Figure 5.3 shows the chromatograms of the same material following contact with 0.25 M perchloric acid and of the hexane layer (containing uncomplexed crown ether and contaminants) from this precipitation experiment. As expected, the solids formed upon acid treatment largely consist of a single material (*i.e.* one DtBuCH18C6 isomer), while in contrast, numerous peaks are observed in the chromatograms of the hexane layer. Similar results are obtained at higher perchloric acid concentrations, although the chromatograms for the hexane layer appear to be somewhat less complicated due to more material being precipitated (as a result of the abundance of perchloric acid available for complexation) (Figures 5.4 and 5.5).
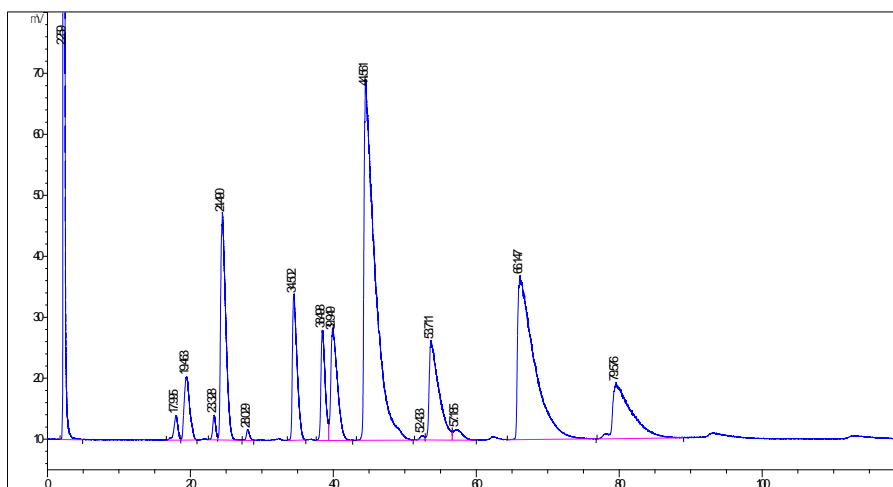
Figure 5.2: HPLC Chromatogram of an Untreated Commercial Sample of DtBuCH18C6 (Experimental Conditions: 20µL injection of a 1mg/mL crown ether sample in methanol, a 0-80% (v/v) methanol:acetonitrile gradient was applied for 90 minutes and then held at the final conditions for 30 minutes, Zorbax NH$_2$ 3.0 x 75 mm 5-micron particle size

column, flow rate: 0.235mL/min, Detection: Varian 380-LC ELSD: nebulizer
temperature: 50°C, evaporator temperature: 60°, and gas flow rate: 0.90 SLM
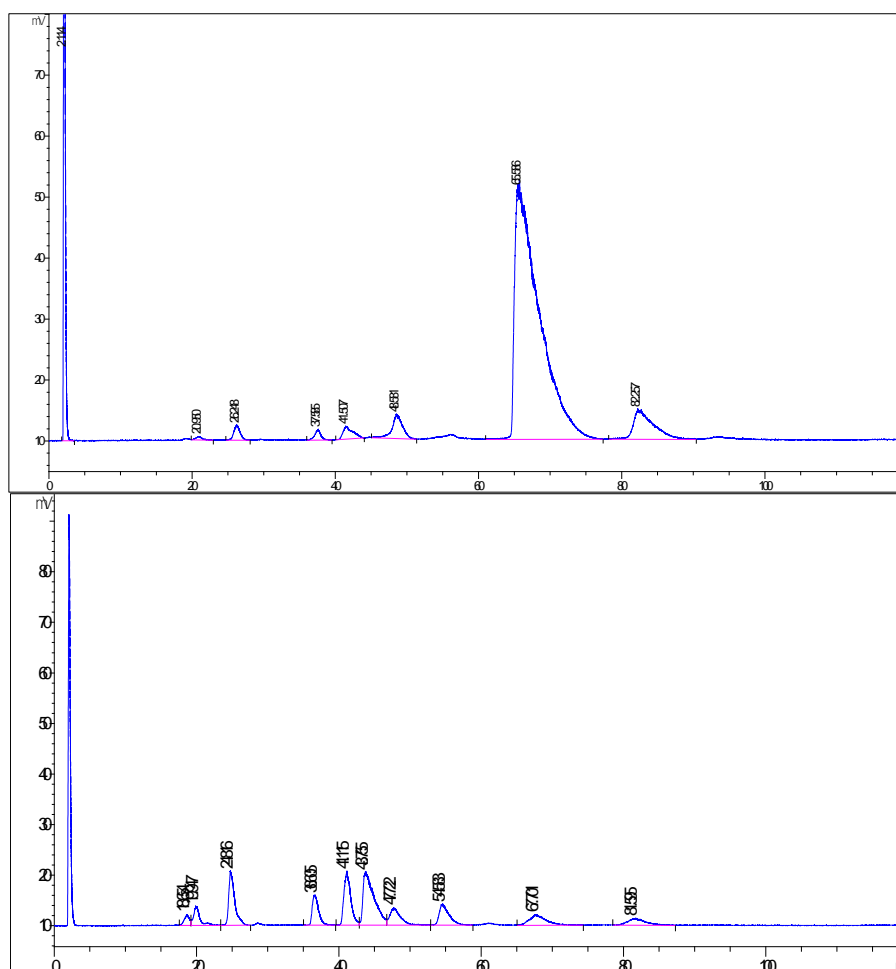
Figure 5.3: (top) 0.25M Perchloric Acid-Treated DtBuCH18C6 and (bottom) the 0.25M
Hexane Layer Containing Uncomplexed Crown Ether and Contaminants (Experimental
Conditions were the same as Figure 5.2)
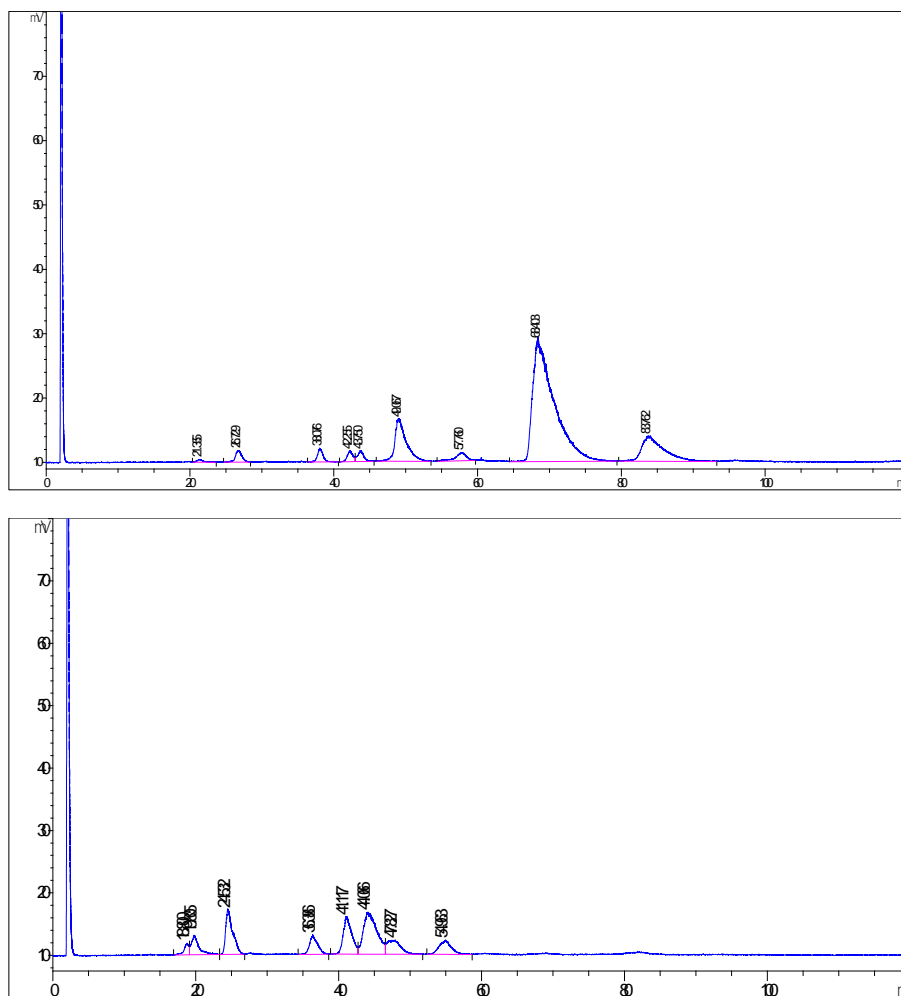
Figure 5.4: (top) 0.50M Perchloric Acid-Treated DtBuCH18C6, and (bottom) 0.50M Hexane Layer (Experimental Conditions were the same as Figure 5.2)
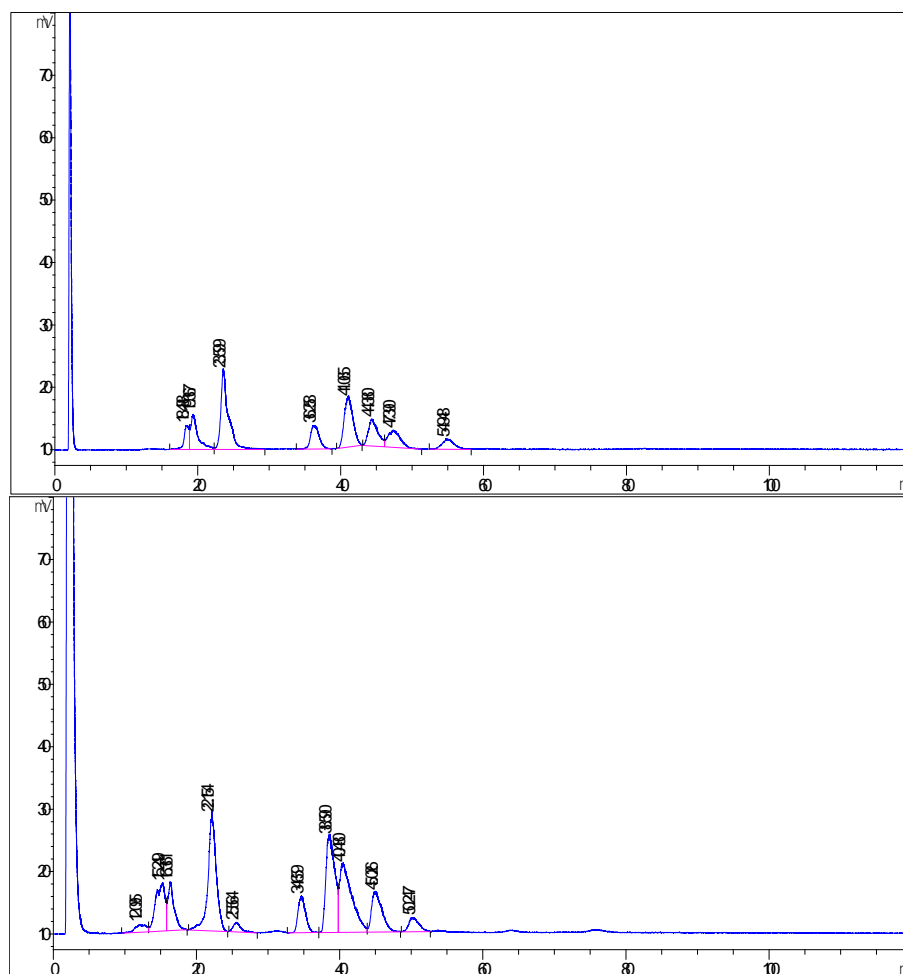
Figure 5.5: (top) 1.00M Hexane Layer and (bottom) 3.00M Hexane Layer Containing Uncomplexed Crown Ether and Contaminants (Experimental Conditions were the same as Figure 5.2)

5.3.2: Classical Column Chromatography of DtBuCH18C6

A preliminary investigation of classical column chromatography as a means of separating the individual isomers of DtBuCH18C6 was carried out by Dietz *et al.* (*18*) more than a decade ago. In this investigation, the strontium distribution experiments associated with a number of columns fractions were measured. Some of the fractions

were shown to yield higher distribution ratios than others, suggesting that they contain more of the most effective DtBuCH18C6 isomers. HPLC studies of the fractions were not performed however, leaving the composition undetermined. (Ideally of course, each fraction would contain only a single isomer of DtBuCH18C6.) To explore the composition of the individual fractions obtained in the treatment of a DtBuCH18C6 sample by column chromatography, an experiment analogous to those carried out by Dietz *et al.* (*18*) was performed. Figure 5.6 (top) shows the elution profile of one sample of DtBuCH18C6, expressed in terms of the mass of material found in each column fraction. Figure 5.6 (bottom) shows results for this same run, this time expressed as the cumulative percent recovery of material from the column. Because the large number of fractions make HPLC analysis of all of them impractical, fractions 14, 16, 18, and 20, which correspond to the peak in the elution profile, were selected (Figure 5.7). HPLC analyses of these fractions indicated that none of these samples contained only one isomer of DtBuCH18C6; rather all were complex mixtures. Given the particle size of the stationary phase used, this is not an entirely unexpected result.
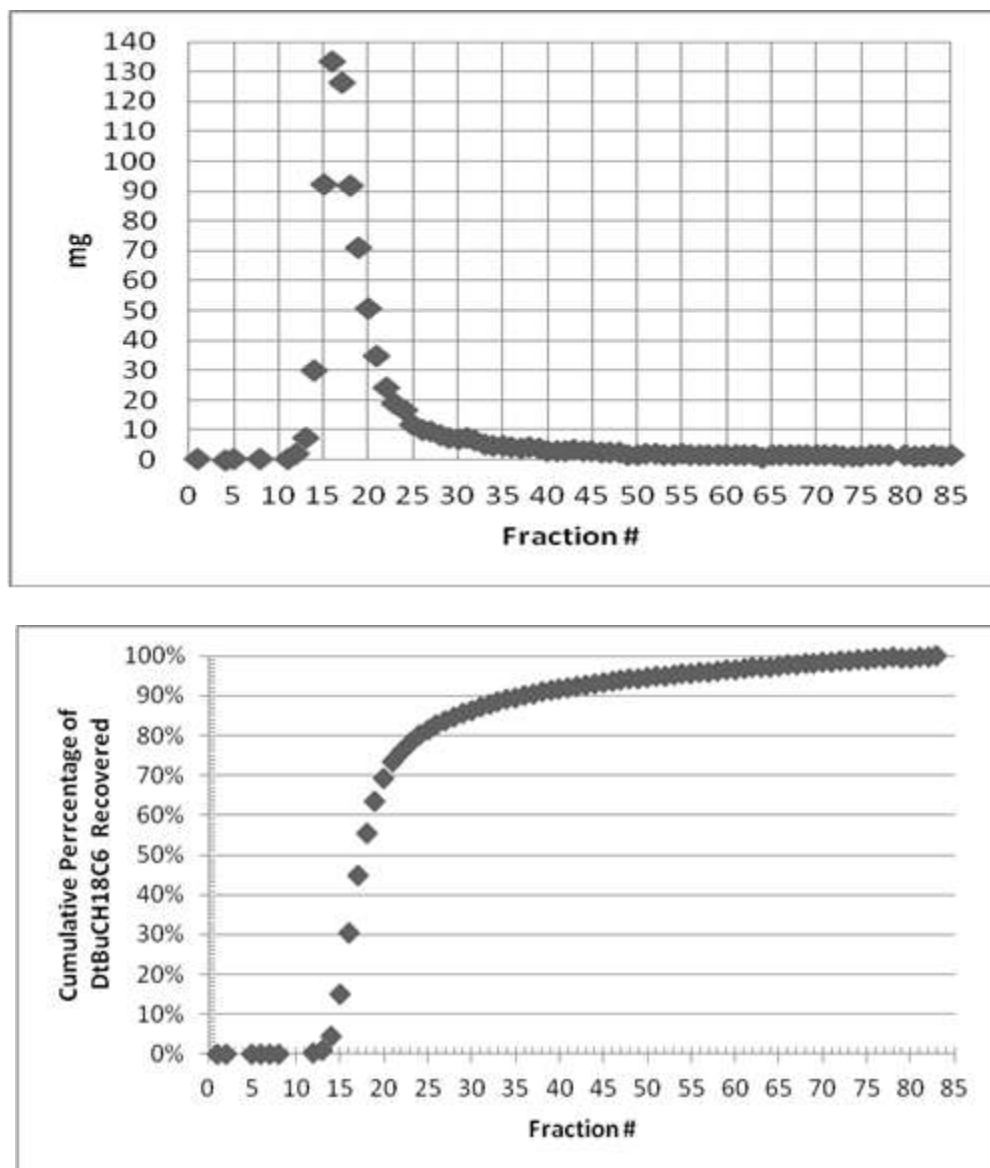
Figure 5.6: (top) Mass Recovered (mg) of Each Fraction Collected and (bottom) Cumulative % Recovery Chromatogram for Individual Fraction Collection
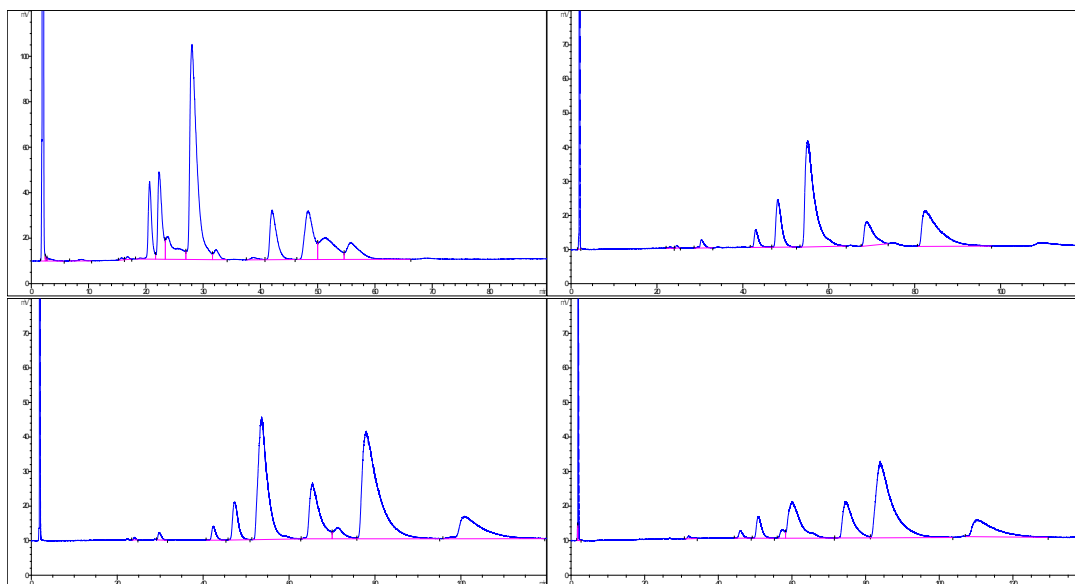
Figure 5.7: HPLC Chromatograms Associated with Mass Chromatogram (from left to right, top to bottom) fraction #14, 16, 18, 20 (Experimental Conditions were the same as Figure 5.2)

5.3.3: Flash Chromatography Analysis of DCH18C6 and DtBuCH18C6 Family of Stereoisomers

Flash chromatography is an automated form of classical column chromatography, that employs smaller particle size sorbents (an average particle size between 20 to 40 μm *vs.* an average particle size of 40μm for classical columns) and therefore requires pressurized gas to force the mobile phase solvent through the stationary phase (*19, 20*). Although typically employed for the separation of a molecule of interest from contaminants, the use of flash chromatography to separate isomers has been reported. Specifically, Marchi *et al.* (*21*) separated the isomers of phenol-oxazolines using mixtures of hexane/ethyl actetate as the mobile phase and 240-400 mesh silica gel as their stationary phase. When considered together with the initial results of *Dietz et al. (18)* showing that aminopropyl silica column treatment enables the removal of contaminants

from the crown ethers of interest, this suggests that flash chromatography may provide a fast and efficient means of obtaining individual isomers of DtBuCH18C6. As a first step in evaluating flash chromatography for this application, an attempt was made to resolve a commercial samples of dicyclohexano-18-crown-6 into its two component stereoisomers. (In a typical sample of DCH18C6, only isomers A and B are present in significant amounts, with isomers C, D, and E accounting for less than 1% of the overall mass of the mixture). The methodology used for this experiment was similar to that described by *Laskorin et al.* (*14*), with modifications as necessary to convert from an HPLC method to flash chromatography. Results from the initial experiment were unexpectedly disappointing, as no separation of the DCH18C6 isomers was observed. In HPLC, isomer A elutes first, followed by isomer B and a broad unresolved peak containing C, D, and E. No such results were seen with flash chromatography, however (*14*). Additional experiments performed with the assistance of the instrument manufacturer using a variety of stationary phases and solvent systems yielded the same result: no separation of the DCH18C6 isomers (Figure 5.8). Not unexpectedly, subsequent experiments using the DtBuCH18C6 family of isomers were equally disappointing, as no evidence of isomer separation was observed in any of the runs regardless of conditions (Figure 5.9). Apparently the particle size of the stationary phase of the flash chromatographic columns is simply too large to allow for efficient separation of the isomers. It therefore appears that preparative-scale liquid chromatography (Prep-LC) is required if macro quantities of individual DtBuCH18C6 isomers are to be obtained.
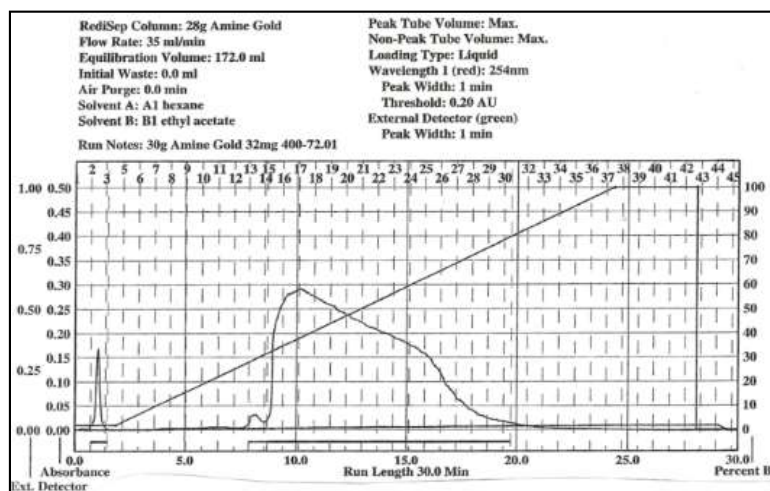
Figure 5.8: Flash Chromatogram of DCH18C6 from Teledyne-Isco
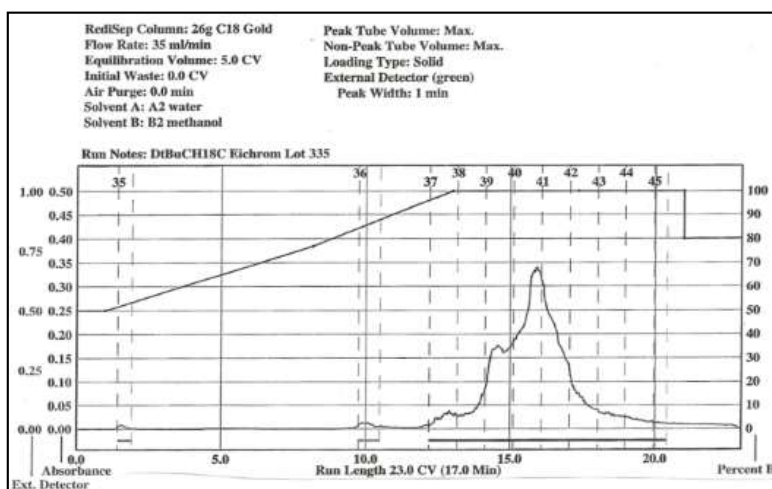
Figure 5.9: Flash Chromatogram of DtBuCH18C6 from Teledyne-Isco

5.3.4: Scale-up of Analytical-Scale HPLC to Preparative-Scale LC for the Separation of DtBuCH18C6 Isomers

It has been shown previously that HPLC can be used to separate many of the isomers present in a sample of DtBuCH18C6 (*18*). Collection of the column effluent from analytical-scale experiments would never yield a useful sample mass, however. Rather preparative-scale LC is required. Preparative-scale LC is essentially a large-scale

version of analytical HPLC, with pumps that can handle flow rates well in excess of those used in analytical HPLC. To transition from the analytical to the preparative scale, a variety of mass loading studies were performed on a number of different columns (all chromatograms are presented in Appendix D). Specifically, following analytical-scale runs on a Zorbax 3.0 x 75 mm, 5-micron column, the method was employed on a 4.6 x 250 mm, 5-micron column; a 4.6 x 250 mm, 7-micron column; and finally on a 21.2 x 250 mm, 7-micron column. Column loading studies were performed on samples purified through 0.5 and 1.0 M perchloric acid contacts, to reduce the possibility of column fouling with the direct use of a commercial sample of DtBuCH18C6. For scale up, the mobile phase flow rate was raised from 0.235 mL/min to 1.800 mL/min for the 4.6 x 250 mm, 5-micron column. Utilizing the 20 μL loop for the analytical scale HPLC, the typical mass on column at 1.0 mg/mL for an analytical-scale HPLC run is only 20 μg. At a concentration of 18 mg/mL (Figure 5.10) on the same 4.6 x 250 mm, 5-micron column, the resolution between peaks was still excellent (the critical pair [peaks at 22.050 and 23.584min] was still baseline resolved and had a resolution of 2.00 as calculated by Chemstation). When scaled up to preparative scale, however, this mass would still be very small relative to the large amount of solvent used. Samples with a concentration of 98 mg/mL (Figure 5.11) were too poorly resolved to guarantee the recovery of individual peaks without the contamination of neighboring peaks; therefore after additional studies, a mass of 54 mg/mL (Figure 5.12) was deemed to be the highest amount of material that could be used on this column while still achieving satisfying resolution for most peaks (critical pair was not fully resolved, having a resolution of 0.73). Unfortunately, in the

course of these studies, it became apparent that at the linear velocity of choice, backpressure could become an issue in the preparative runs. We therefore decided to switch to a 7-micron particle size packing. Initial experiments using the new 4.6 x 250 mm, 7-micron column were promising; not only was back-pressure no longer a problem, but at a solute concentration of 36 mg/mL (Figure 5.13), the critical pair of peaks was fully resolved (resolution of 1.55). Even at 71.4 mg/mL (Figure 5.14), the majority of the peaks (except for the critical pair with a resolution of 0.52) were sufficiently resolved to ensure contaminant-free fractions when scaled up. Following this success, the separation was attempted on a 21.2 x 250 mm, 7-micron column. With a 500-μL injection loop, a sample concentration of 20 mg/mL yielded the chromatogram with the best resolved peaks (Figure 5.15) but the small amount of material used makes these conditions impractical for preparative work. That is, the 10 mg of material on column is split among as many as sixteen peaks (*i.e.,* twelve *cis-cis* isomers of DtBuCH18C6 and four contaminants). Therefore, concentrations of 80 and 100 mg/mL (Figures 5.16 and 5.17) were used for all subsequent preparative-scale runs and fractions were collected for future analysis.
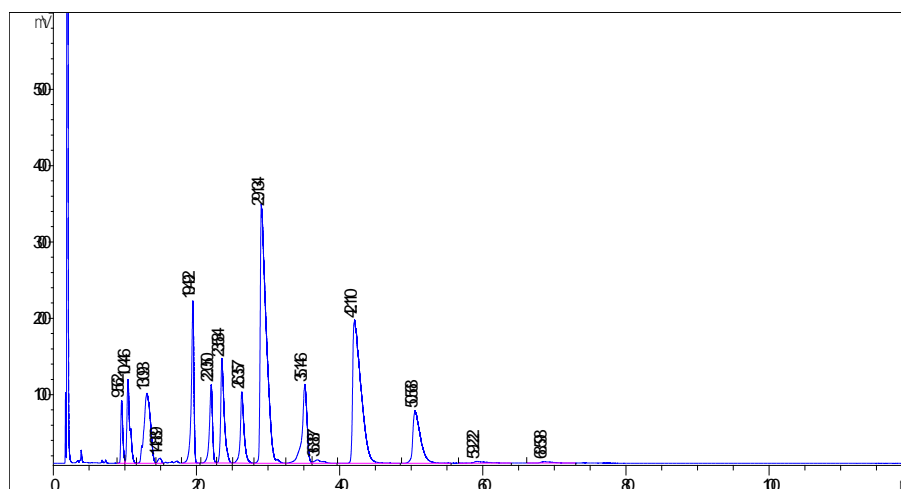
Figure 5.10: Perchloric Acid-Treated HPLC of 18 mg/mL DtBuCH18C6 (Experimental Conditions: 20µL injection of a 18mg/mL crown ether sample in methanol, a 0-80% (v/v) methanol:acetonitrile gradient was applied for 90 minutes, Zorbax NH_2 4.6 x 250 mm 5-micron particle size column, flow rate: 1.842mL/min (0.25mL/min was split to the detector), Detection: Varian 380-LC ELSD: nebulizer temperature: 50°C, evaporator temperature: 60°, and gas flow rate: 0.90 SLM
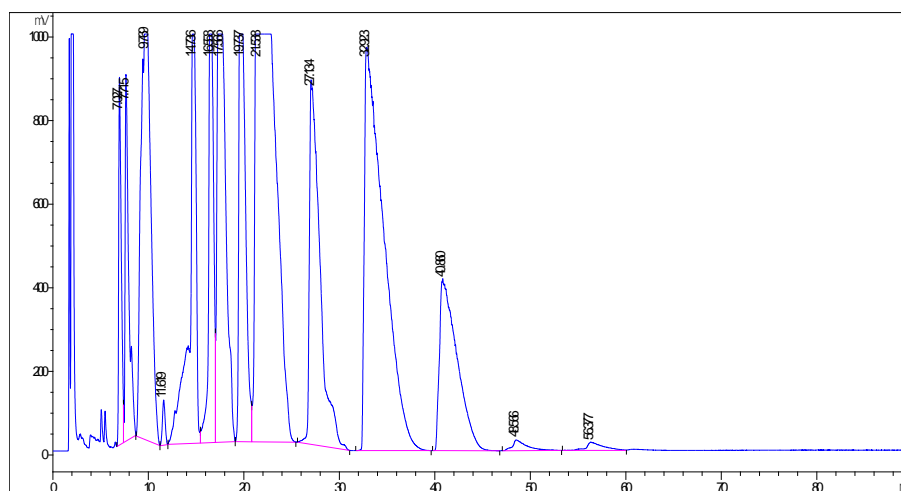
Figure 5.11: Perchloric Acid-Treated HPLC of 98 mg/mL DtBuCH18C6 (Experimental Conditions were Similar to Figure 5.9 but concentration of the sample is now 98 mg/mL)
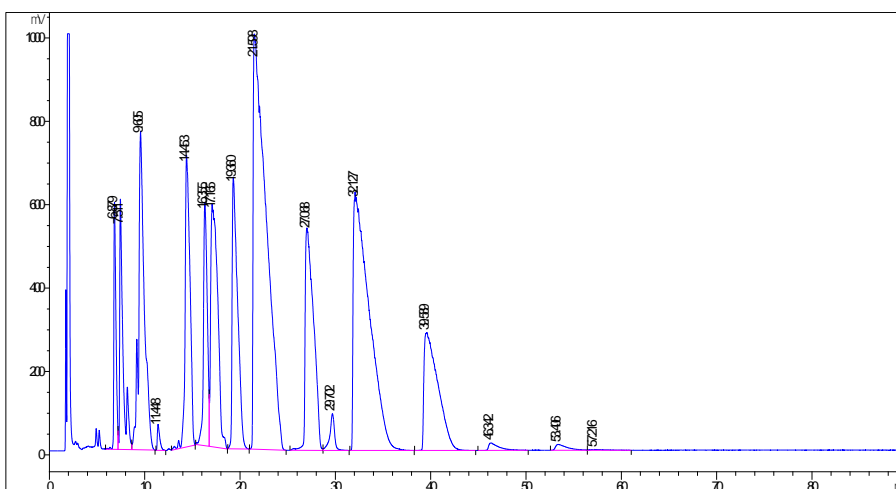
Figure 5.12: Perchloric Acid-Treated HPLC of 54.4 mg/mL DtBuCH18C6 (Experimental Conditions were Similar to Figure 5.9 but concentration of the sample is now 54.4 mg/mL)
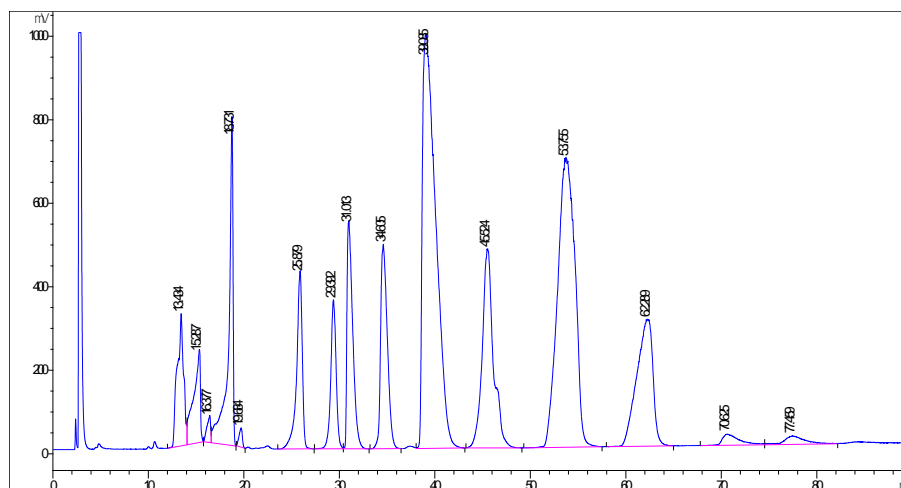
Figure 5.13: Perchloric Acid-Treated HPLC of 36.3 mg/mL DtBuCH18C6(Experimental Conditions: 20µL injection of a 36.3 mg/mL crown ether sample in methanol, a 0-80% (v/v) methanol:acetonitrile gradient was applied for 90 minutes, Zorbax NH$_2$ 4.6 x 250 mm 7-micron particle size column, flow rate: 1.316mL/min (0.25mL/min was split to the detector), Detection: Varian 380-LC ELSD: nebulizer temperature: 50°C, evaporator temperature: 60°, and gas flow rate: 0.90 SLM
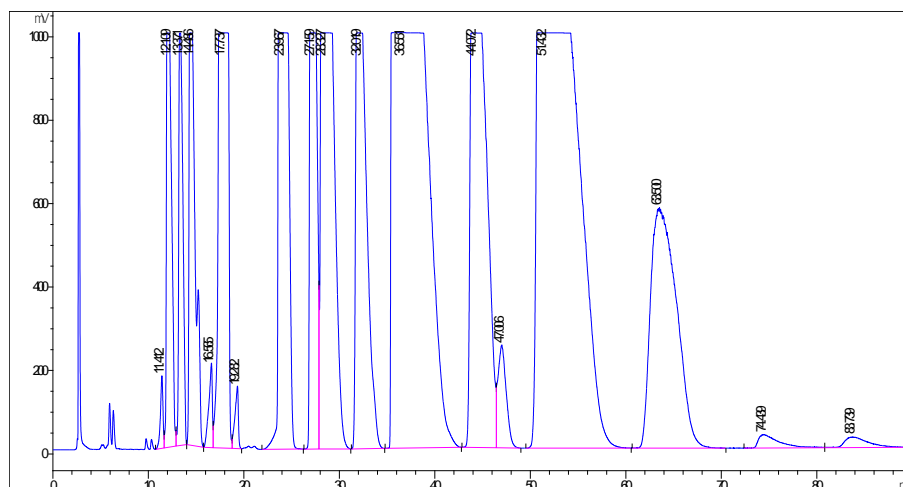
Figure 5.14: Perchloric Acid-Treated HPLC of 71.4 mg/mL DtBuCH18C6 (Experimental Conditions were Similar to Figure 5.9 but concentration of the sample is now 71.4 mg/mL)
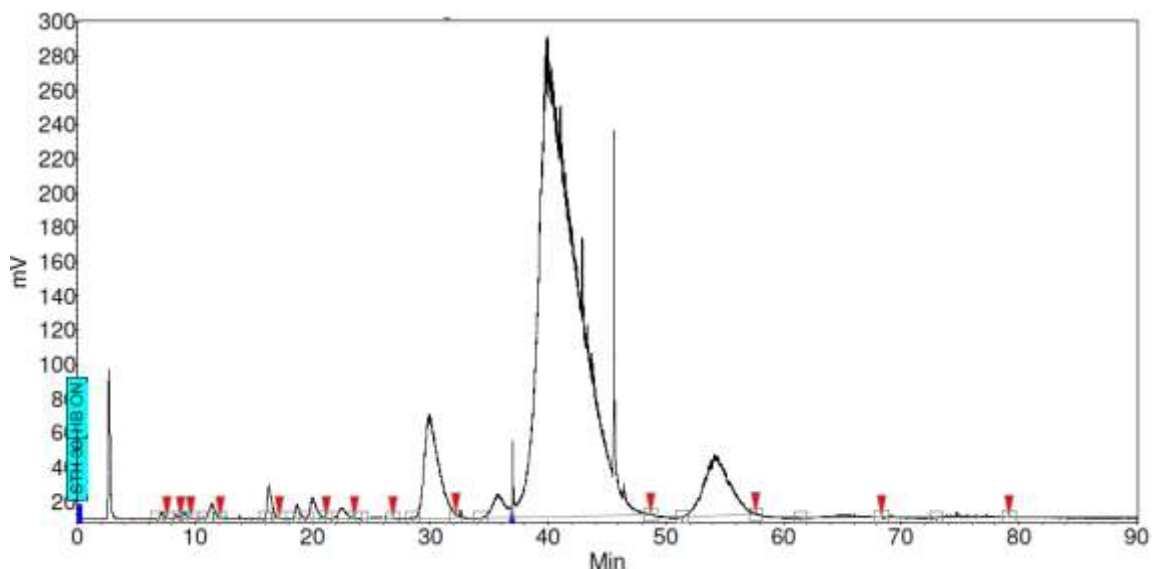
Figure 5.15: Perchloric Acid-Treated LC of 20 mg/mL DtBuCH18C6 (Experimental Conditions: 500μL injection of a 20 mg/mL crown ether sample in methanol, a 0-80% (v/v) methanol:acetonitrile gradient was applied for 90 minutes, Zorbax NH_2 21.2 x 250 mm 7-micron particle size column, flow rate: 28mL/min (0.28mL/min was split to the detector), Detection: Varian 380-LC ELSD: nebulizer temperature: 50°C, evaporator temperature: 60°, and gas flow rate: 0.90 SLM
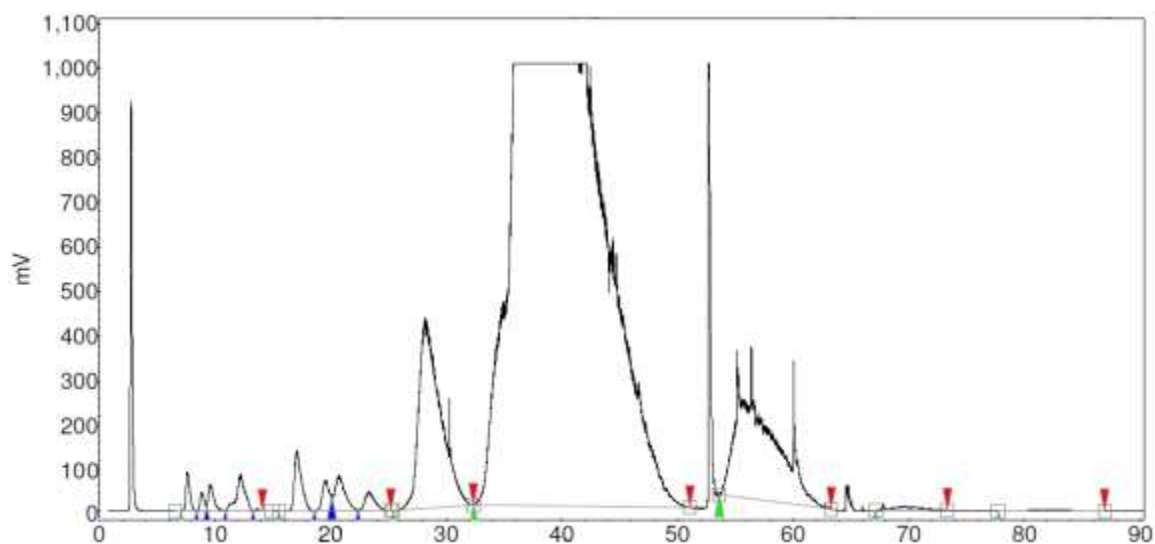
Figure 5.16: Perchloric Acid-Treated LC of 80 mg/mL DtBuCH18C6 (Experimental Conditions were Similar to Figure 5.12 but concentration of the sample is now 80 mg/mL)
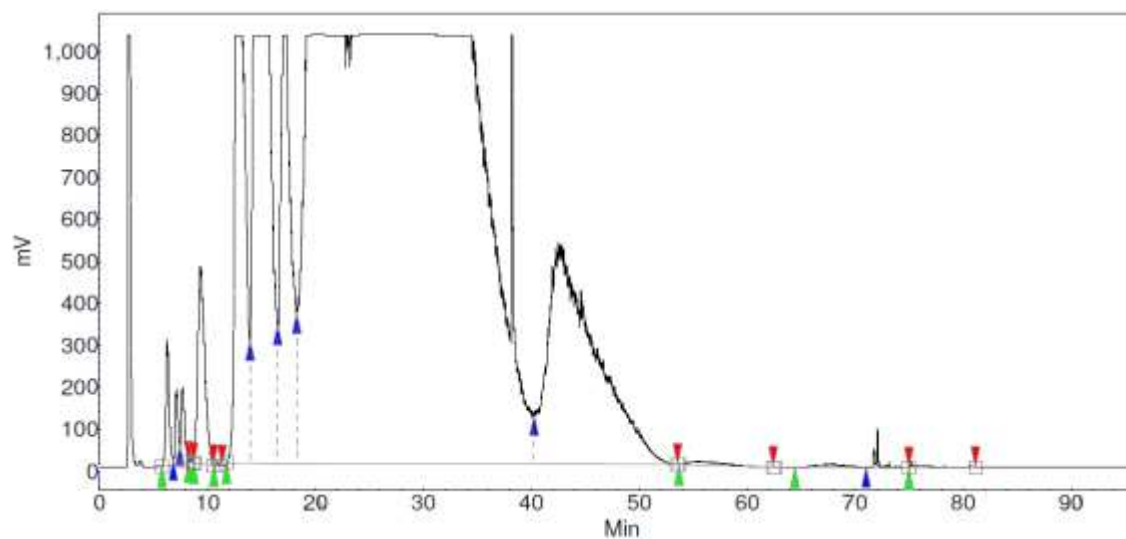
Figure 5.17: Perchloric Acid-Treated LC of 100 mg/mL DtBuCH18C6 (Experimental Conditions were Similar to Figure 5.12 but concentration of the sample is now 100 mg/mL)

5.3.5: HPLC Analyses of Individual Fractions Collected from Preparative LC

To determine if the peaks collected consisted of only a single isomer, all samples collected were examined by analytical-scale HPLC. Of the eleven peaks collected from the 100mg/mL sample run (Figure 5.17), six yielded a chromatogram consisting of a dominant single peak whose area corresponded to over 95% of the total peak area of the chromatogram. None of the samples examined yielded a single peak; rather all of them exhibited a least two peaks, with the majority having three. Samples of purity of 95% or greater were then further analyzed to determine if the identity of these peaks could be ascertained (Figure 5.18).
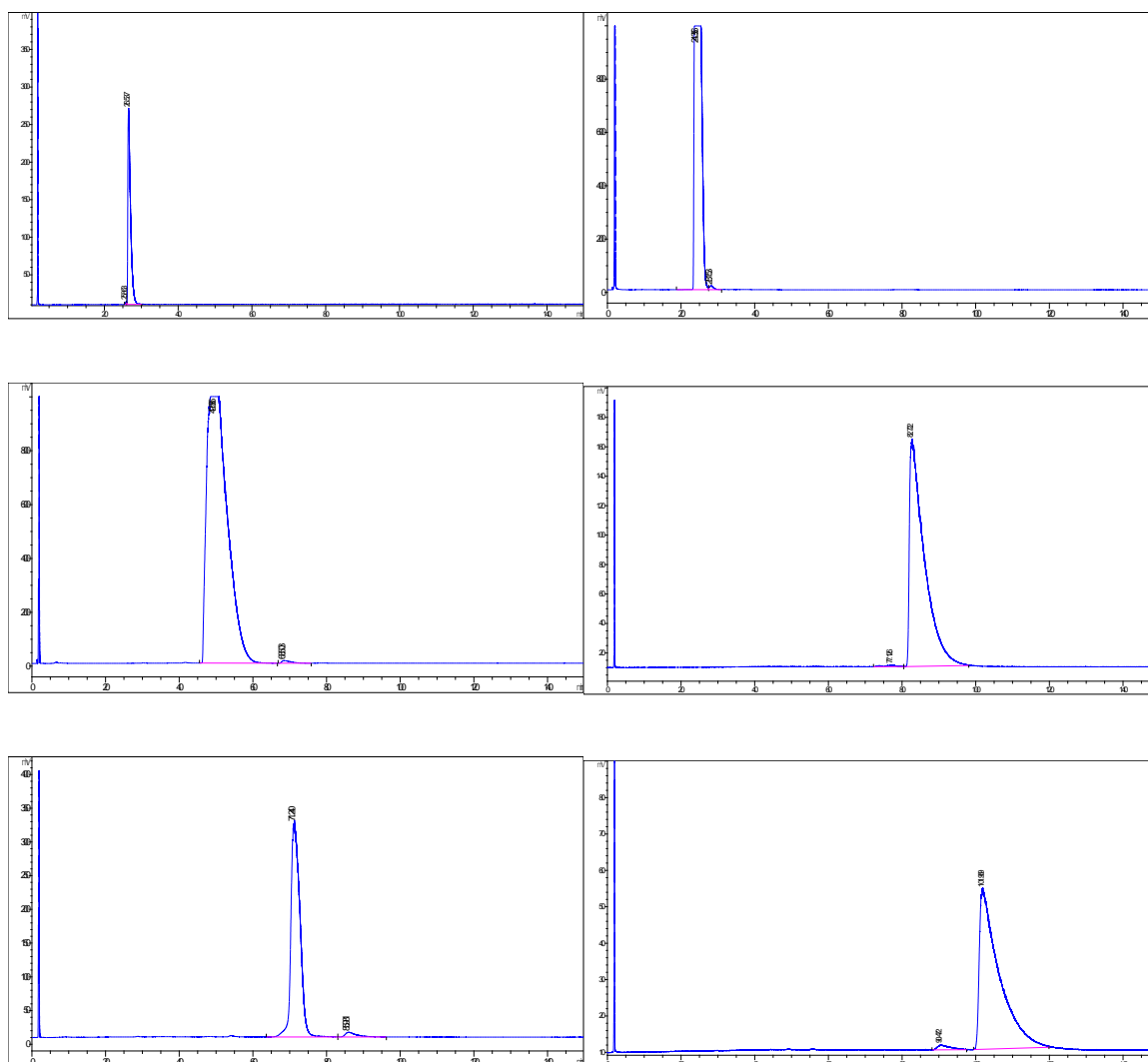
Figure 5.18: (top left) Prep Sample 6.8-7.4 minutes, (top right) Prep Sample 9-10 minutes (middle left) Prep Sample 16.5-17.5 minutes, (middle right) Prep Sample 29-31 minutes, (bottom left) Prep Sample 35-40 minutes and (bottom right) Prep Sample 42-47 minutes (Experimental Conditions: 20µL injection of a 1mg/mL crown ether sample in methanol, a 0-80% (v/v) methanol:acetonitrile gradient was applied for 90 minutes and then held at the final conditions for 30 minutes, Zorbax NH_2 3.0 x 75 mm 5-micron particle size column, flow rate: 0.235mL/min, Detection: Varian 380-LC ELSD: nebulizer temperature: 50°C, evaporator temperature: 60°, and gas flow rate: 0.90 SLM

5.4: Conclusions

In this work, several methods for separation of the various isomers of DtBuCH18C6 either from impurities or from one another have been investigated. Column chromatography (and its automated analog flash chromatography), although promising in principle, were not capable of separating the isomers of interest. Better results were achieved using perchloric acid precipitation in combination with analytical-scale HPLC. On the basis of the analytical-scale separation, preparative-scale LC experiments were undertaken, yielding not only baseline resolution of many of the peaks present in the chromatogram but measurable masses of individual DtBuCH18C6 stereoisomers. Finally, additional analytical-scale HPLC demonstrated that six of the peaks correspond to purities in excess of 95%.

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Chapter 6 : Identification of the Stereoisomers of Di-tert-butylcyclohexano-18-crown-6

6.1: Introduction

Isolating the individual stereoisomers of a crown ether is obviously of little value unless the isomers are also identified. This is not a simple task, however, as the compounds of interest differ only in the orientation of the hydrogen bound at the junctions of the crown ether and the cyclohexano ring and the location and orientation of the *tert*-butyl groups attached to the cyclohexano rings (Figures 6.1 and 6.2). As a result, many of the methods ordinarily applicable in organic qualitative analysis (*e.g*., UV-visible and IR spectroscopy, 1-D NMR, and mass spectroscopy) are of little or no use in this instance (*1*). For this reason, we have examined several alternatives. First, we have explored an approach that has been employed with considerable success with dicyclohexano-18-crown-6 (DCH18C6), a simpler analog of 4,4'(5')-di-*tert*-butylcyclohexano-18-crown-6 (DtBuCH18C6) lacking the *tert*-butyl groups and thus, existing in far fewer (*i.e.,* five) isomeric forms than DtBuCH18C6 (*i.e.,* forty) (Figure 6.3 and 6.4). That is, for DCH18C6, precipitation of individual isomers followed by single crystal X-ray studies has proven to be an effective means of definitively identifying both the *cis-syn-cis* (A) and *cis-anti-cis* (B) forms. For the A form, precipitation is readily accomplished with perchoric acid, while for the B form, addition of lead perchlorate to an aqueous solution of a mixture of isomers leads to its preferential precipitation (*2-4*). A variety of other reagents including (but not limited to) thionicotinamide (*5*), 4-aminobenzenesulfonamide (sulfanilamide) (*6*), 4-methylbenzenesulfonamide (*p*-toluenesulfonamide) (*7*), 4-aminobenzoic acid (*p*-aminobenzoic acid or PABA) (*8*),

sulfamic acid (*9*), 4-aminobenzenesulfamidine (sulfaguanidine) (*10*) and ammonium iodide (*11*) have been examined as alternate precipitating agents, in some cases with satisfactory results.
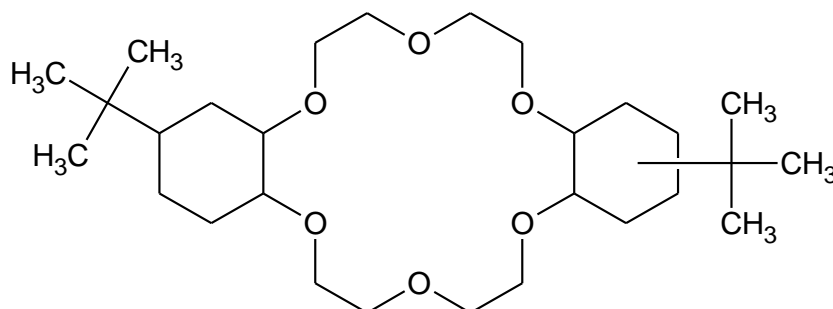
Figure 6.1: 4,4'(5')-di(*tert*-butylcyclohexano)-18-crown-6 (DtBuCH18C6)
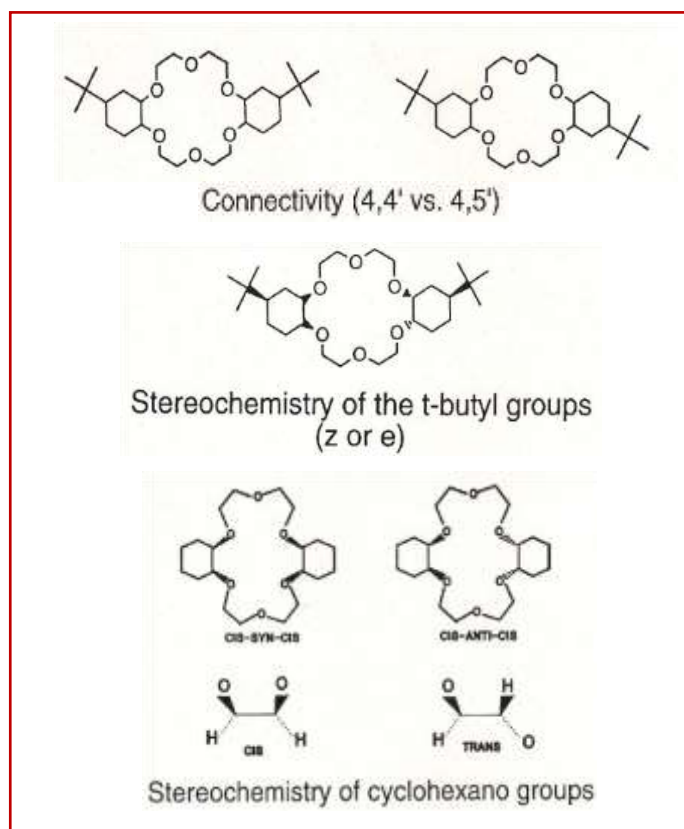
Figure 6.2: Stereochemistry of DtBuCH18C6
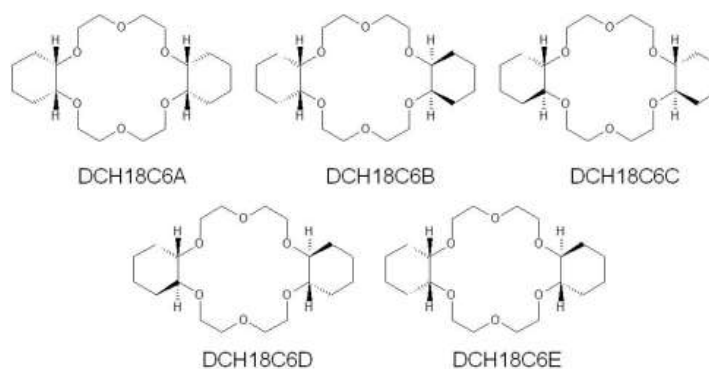
Figure 6.3: The Five Stereoisomers of DCH18C6
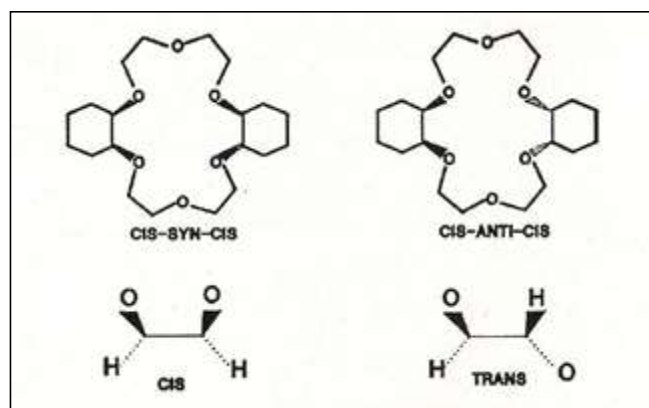
Figure 6.4: Stereochemistry of DCH18C6

As a first step in efforts to identify the individual stereoisomers of DtBuCH18C6, a number of these complexing agents have been applied to a purified (by 1M perchloric acid), commercial lot of DtBuCH18C6 to determine if the isolation of a single isomer of DtBuCH18C6 from a mixture of isomers is feasible and if the complex obtained is suitable for X-ray crystallography studies. Of course, growing X-ray quality crystals

remains more art than science, and as a result, a second approach to isomer identification, one involving a combination of strontium distribution ratio measurements and molecular mechanics calculations, has also been explored.

Molecular mechanics methods have previously been used to determine the strain associated with ligands in their free and bound (to metal ions) states (*e.g.,* complexes of nickel (*12, 13*) and cobalt (*14*) with amines, cobalt with thioethers (*15*), and lanthanides with water and nitrate (*16*)). It has been proposed that similar molecular mechanics calculations can be used for ligand design (*17*). For example, work by Hay *et al. (18, 19)* examined these methods to determine the amount of ligand strain energy associated with the process of binding metal ions by various crown ethers. Calculations performed to determine the energy change for complex formation between a potassium ion and four of the five stereoisomers of dicyclohexano-18-crown-6, for example, revealed a relationship between the reorganization energy and the formation constants for these isomers(*18*). Subsequent studies extended these calculations to the complexation of barium, calcium, and strontium ions by DCH18C6 (*20*) and to the *cis-cis* isomers of DtBuCH18C6 (*21*). In this instance, a relationship was noted between the ligand strain (reorganization) energy and the extent to which the metal ion was extracted into 1-octanol, with higher ligand strain energies yielding lower extraction efficiency. Interestingly, a plot of extraction efficiency *versus* ligand reorganization energy showed that a single line describes the results for strontium ion extraction by both DtBuCH18C6 (3 isomers) and DCH18C6 (5 isomers). Thus, if the strontium ion extraction efficiency associated with a given newly isolated DtBuCH18C6 stereoisomer can be determined, one can employ this plot to

estimate the ligand strain energy for the isomer. Because Hay *et al. (21)* have published a ranking of all of the *cis-cis* stereoisomers by strain energy, this estimate can be used to identify the unknown isomer.

Finally, as we have already noted, conventional (*i.e.* 1-D) NMR is not particularly useful in the identification of individual crown ether stereoisomers. More complex NMR techniques (*e.g.* NOESY) have, however, been successfully employed in structural elucidation studies of other complex molecules and may therefore be of value here (*22*). For this reason, in conjunction with collaborators, NMR (1-D and 2-D) has also been evaluated as a possible approach to stereoisomer identification. As will now be shown, best results were obtained using a combination of molecular mechanics and association constants (or metal ion distribution ratios) or crystallography.

6.2: Experimental

6.2.1: Materials

Strontium chloride hexahydrate, calcium chloride dihydrate, barium chloride dihydrate, potassium chloride, sodium chloride, acetone, isopropanol, and ammonium iodide were purchased from Aldrich (St. Louis, MO, USA). 4,4'(5')-di(*tert*-butylcyclohexano)-18-crown-6 was purchased from Eichrom (Lisle, IL, USA). 4-aminobenzenesulfamidine (sulfaguanidine), 4-aminobenzenesulfonamide (sulfanilamide) and thionicotinamide were purchased from Acros (Geel, Belgium). 4-methylbenzenesulfonamide (*p*-toluenesulfonamide), and 4-aminobenzoic acid (PABA) were purchased from Alfa Aesar (Ward Hill, MA, USA). Sulfamic acid was purchased

from EMD Chemical (Billerica, MA, USA). HPLC grade methanol was purchased from Fisher Scientific (Waltham, MA, USA). HPLC grade acetonitrile was purchased from Honeywell (Morristown, NJ, USA). All chemicals were used without additional purification unless noted.

6.2.2: Instruments.

Isothermal titration calorimetry (ITC) measurements were performed with a TA Instruments Nano ITC G2 (New Castle, DE, USA). All measurements were performed in least duplicate at 25°C utilizing a 50 µL syringe and a low-volume gold cell (174 µL). The stir rate was 300 rpm and no degassing was performed. NanoAnalyze software was used to determine the formation constant (K_f), change in enthalpy (ΔH), change in entropy (ΔS), and stoichiometry (n) for the reaction of interest. NMR experiments (Appendix G) were performed by Dr. Stephen McKenna (INEOS, Lisle, IL USA) utilizing a Varian Inova 500MHz NMR spectrometer (Santa Clara, CA, USA). Hydrogen-hydrogen distances were calculated by Dr. Dennis Bennett (UWM) with the use of Gaussian and Avogadro (Appendix H). HPLC-MS measurements were performed on a Shimadzu LCMS-2020 utilizing a DUIS-2020 dual ion source (both positive and negative electrospray ionization (ESI) and atmospheric-pressure chemical ionization (APCI)) with the help of Dr. Zhiqiang (Mark) Wang (UWM).

X-ray crystallographic experiments were performed in collaboration with Dr. Dennis Bennett (UWM), Dr. Nicholas Silvaggi (UWM), and Dr. Sergey Lindeman (Marquette University, Milwaukee, WI USA). Crystal structures were obtained by Dr. Sergey Lindeman using an Oxford SuperNova diffractometer using Mo (Kα) radiation at

100K (-173.15°C). Using Olex2, the structure was solved with the XS structure solution program using direct methods and refined with the XL refinement package using least square minimization (Appendix E and F).

6.2.3: Methods

The methodology employed for the ITC measurements was described in Chapter 4, section 2.3. Strontium distribution ratio measurements were conducted as outlined in Chapter 5, section 2.3. Analytical-scale HPLC experiments were performed as described in Chapter 5, section 2.3. The complex between thionictotinamide and DtBuCH18C6 was prepared as described by Fonari *et al*. (*5*) with minor modification. Briefly, a solution containing equimolar quantities of DtBuCH18C6 and thionicotinamide was prepared in 10mL of 1:1 (v/v) acetone:hexane. The solvent was then left to evaporate at room temperature, eventually yielding a solid complex. A complex between 4-aminobenzoic acid and DtBuCH18C6 was prepared in an essentially identical manner using isopropanol (*8*). The complex between 4-aminobenzenesulfonamide and DtBuCH18C6 was prepared by a modification of the procedure of Dvorkin *et al.* (*6*). Specifically, a solution of 4-aminobenzenesulfonamide in methanol was added to a solution containing an equimolar amount of DtBuCH18C6, also in methanol. Evaporation of the solvent at room temperature provided the complex. An essentially identical procedure was employed for the preparation of a complex between 4-methylbenzenesulfonamide and DtBuCH18C6 (*7*). Complex formation between DtBuCH18C6 and 4-aminobenzenesulfonidine (sulfaguanidine) was performed in acetone (*10*). For the formation of a complex between sulfamic acid and DtBuCH18C6, a modification of the procedure of Fonari *et al.* (*9*)

involving mixing solutions containing equimolar concentrations of DtBuCH18C6 and sulfamic acid in methanol and water, respectively, was employed. Evaporation of this solution yielded the complex. An analogous method was employed for the precipitation of a complex between DtBuCH18C6 and ammonium iodide. The oil that formed was removed and dissolved into a minimal amount of methanol to promote crystal growth.

6.3: Results

6.3.1: Complex Formation between DtBuCH18C6 and Various Organic Complexing Agents / Crystal Growth as an Approach to Stereoisomer Identification

Many crystallographic studies have been performed on the *cis-syn-cis* (A) and *cis-anti-cis* (B) stereoisomers of DCH18C6. As a result, a variety of reagents are now known to form complexes with one (*5, 6, 11*) or both (*7-10*) of these isomers, permitting their separation and in some cases identification. In contrast, such complexation studies of DtBuCH18C6 are rare. In fact, only one such study, described in a 1999 report by Dietz *et al. (3)* has employed this approach successfully in the identification of a DtBuCH18C6 isomer. Specifically, perchloric acid was employed in an attempt to complex various isomers of DtBuCH18C6, eventually leading to the isolation of the complex of the 4z,4'z-*cis-syn-cis*-di-*tert*-butylcyclohexano-18-crown-6 (4z,4'z csc DtBuCH18C6) with hydronium perchlorate. Although the identity of the complex was determined, no crystal structure was ever published (portions of the data having been lost). Therefore, our studies began with an attempt to replicate this work, eventually yielding single crystals of the complex (Figure 6.5) whose crystal structure is shown in Figure 6.6. In addition to yielding this complex, the perchloric acid treatment also yielded a second isomer, 4z,5'z-

cis-syn-cis-di-*tert*-butylcyclohexano-18-crown-6 (4z,5'z csc DtBuCH18C6), this time (unexpectedly) as the free ligand (Figure 6.7 and Figure 6.8). When it became apparent that perchloric acid treatment would yield no additional isomers, efforts were redirected toward an evaluation of complex formation between DtBuCH18C6 and the various reagents previously found to form stable (and sometimes isolable) complexes with one or more of the isomers of DCH18C6. It was anticipated that these reagents might also serve as complexing (and crystallizing) agents for various DtBuCH18C6 stereoisomers. With this in mind, samples of DtBuCH18C6, either as received from the manufacturer or following perchloric acid treatment and washing to remove contaminants, were treated with these same reagents. In all cases, complexation occurred, as indicated by oil or solid formation. Unfortunately, no crystals of X-ray quality were obtained with any of the reagents, despite multiple attempts to grow them under a number of different conditions, (*i.e.,* super-saturation, slow cooling, and growth in a NMR tube).
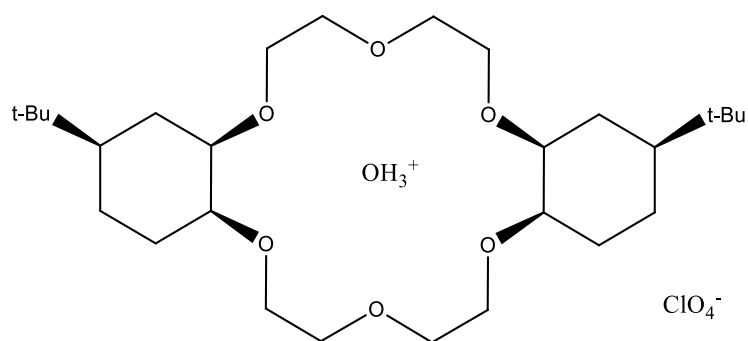
Figure 6.5: The Hydronium Perchlorate Complex of 4z,4'z-*cis-syn-cis*-di-*tert*-butylcyclohexano-18-crown-6
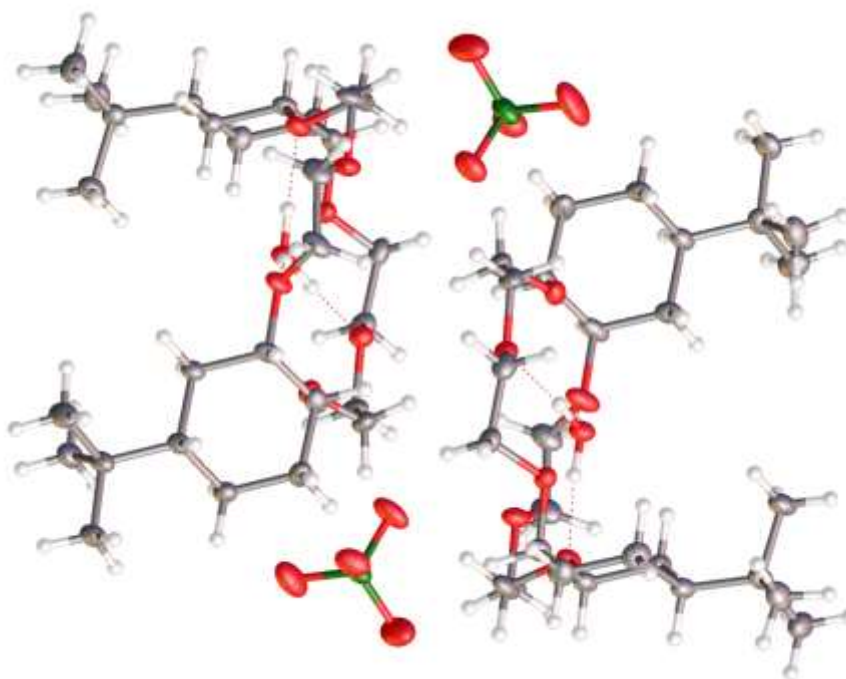
Figure 6.6: Packing Geometry of hydronium 4z,4'z cis-syn-cis di-tertbutylcyclohexano-18-crown-6
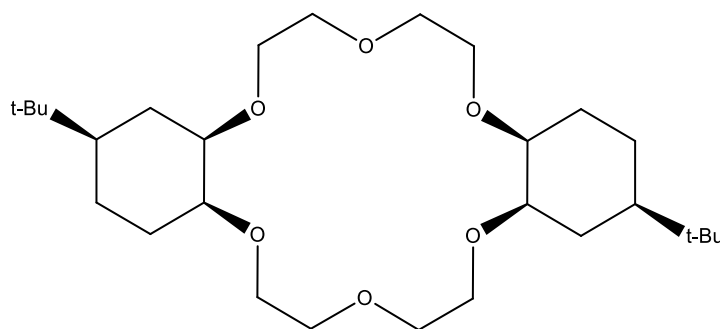
Figure 6.7: The 4z,5'z-*cis-syn-cis*-di-*tert*-butylcyclohexano-18-crown-6 Isomer
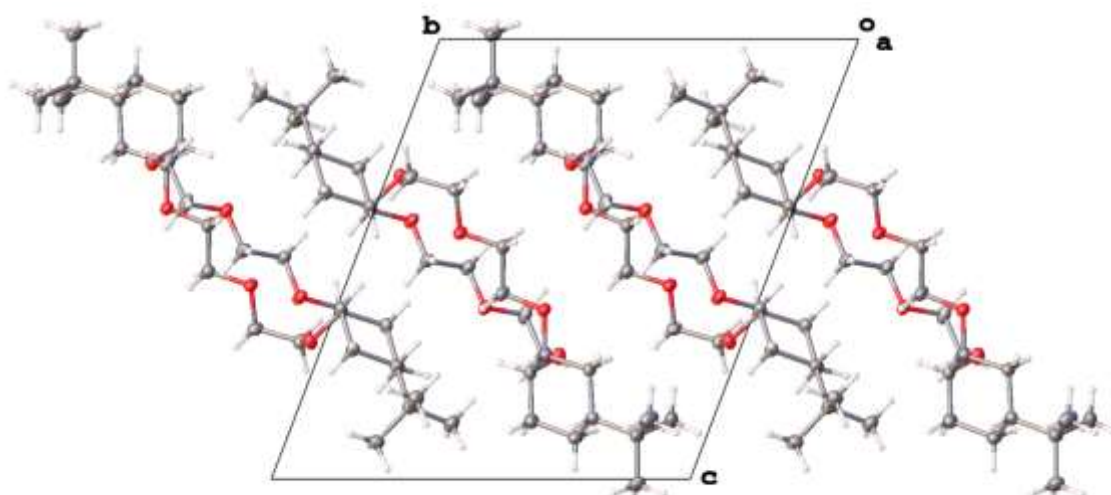
Figure 6.8: Packing Geometry of 4z,5'z *cis-syn-cis* di-*tert*-butylcyclohexano-18-crown-6

Because the work of Dietz *et al. (3)* suggests that complexing agents might also be employed to separate the various isomers, experiments were also performed to determine the effect of reagent addition on the extent of precipitation formation. It was observed that the addition of sulfamic acid results in precipitation similar that seen with perchloric acid. Sulfamic acid might therefore serve as a substitute for perchloric acid in the purification of DtBuCH18C6. Indeed, as shown in Figures 6.9, 6.10, and 6.11, aside

from retention time differences arising from column deterioration, similar results were obtained with perchloric acid, sulfamic acid, and sulfaguanidine (whose complex with the crown ether can be freed of sulfaguanidine by washing with 1M hydrochloric acid and then deionized water) (Figure 6.11). Here too then, this reagent may be able to serve as a substitute for perchloric acid in schemes to separate DtBuCH18C6 from various impurities. Additional work is required with both sulfamic acid and sulfaguanidine to determine if conditions can be identified under which a single DtBuCH18C6 isomer precipitates.
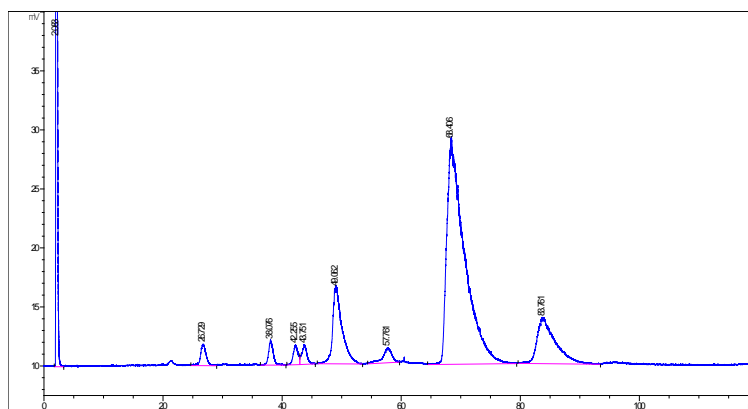
Figure 6.9: HPLC of 0.50M Perchloric Acid-Purified DtBuCH18C6 (Experimental Conditions: 20µL injection of a 1mg/mL crown ether sample in methanol; a 0-80% (v/v) methanol:acetonitrile gradient was applied for 90 minutes; Zorbax NH_2, 3.0 x 75 mm, 5-micron particle size column, flow rate: 0.235 mL/min, Detection: Varian 380-LC ELSD: nebulizer temperature: 50°C, evaporator temperature: 60°, and gas flow rate: 0.90 SLM (the largest peak is the second to last eluter)
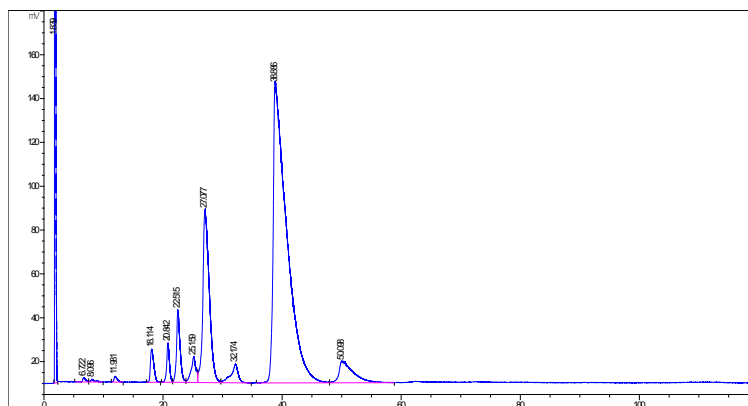
Figure 6.10: HPLC of Equimolar Sulfamic Acid-Purified DtBuCH18C6

(Experimental Conditions: 20µL injection of a 1mg/mL crown ether sample in methanol; a 0-80% (v/v) methanol:acetonitrile gradient was applied for 90 minutes; Zorbax NH_2, 3.0 x 75 mm, 5-micron particle size column, flow rate: 0.235 mL/min, Detection: Varian 380-LC ELSD: nebulizer temperature: 50°C, evaporator temperature: 60°, and gas flow rate: 0.90 SLM (the largest peak is the fourth to last eluter)
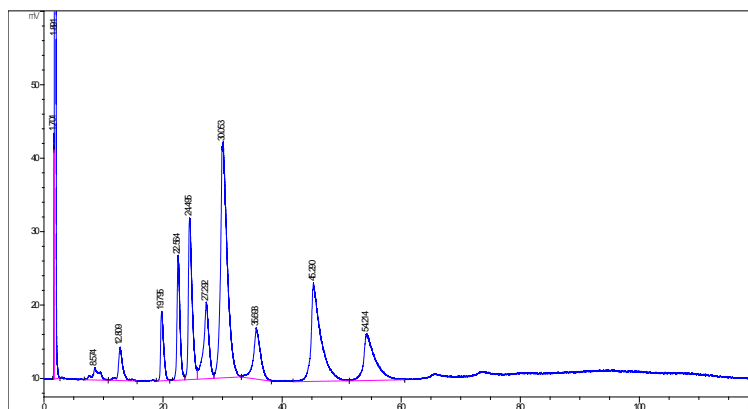
Figure 6.11: HPLC of Equimolar Sulfaguanidine-Purified DtBuCH18C6

(Experimental Conditions: 20µL injection of a 1mg/mL crown ether sample in methanol; a 0-80% (v/v) methanol:acetonitrile gradient was applied for 90 minutes; Zorbax NH_2, 3.0 x 75 mm, 5-micron particle size column, flow rate: 0.235 mL/min, Detection: Varian 380-LC ELSD: nebulizer temperature: 50°C, evaporator temperature: 60°, and gas flow rate: 0.90 SLM (the largest peak is the fourth to last eluter)

6.3.2: NMR Studies of 4z,5'z *cis-syn-cis*-di-*tert*-butylcyclohexano-18-crown-6

The use of nuclear magnetic resonance (NMR) spectroscopy to elucidate the structure of organic compounds, including their isomeric composition, is well established (*22*). For example, a combination of nuclear Overhauser effect (NOESY) in combination with other, more traditional NMR experiments and strain energy calculations were used to determine the stereochemistry of a metal complexed macrocycle (*23*), while in another case, NMR using Mosher's acid (a reagent that reacts with alcohols or amines to help determine stereochemistry through proton or fluorine NMR) helped elucidate the stereochemistry of another macrocyclic compound, this time a natural macrocyclic alkaloid (*24*). Many of the atoms present in a chemical compound have nuclei that are amenable for analysis by NMR. Due to the difficulties expected in establishing the stereoisomerism of the crown ethers of interest (a result of their size and high symmetry), our efforts to evaluate NMR began with a known isomer of DtBuCH18C6, 4z,5'z-*cis-syn-cis*-di-*tert*-butylcyclohexano-18-crown-6 (whose identity was previously verified by X-ray crystallography (see above)). For this crown, a -CH_3 is present at six locations, a -CH_2- present is at fourteen locations, a -CH- is present at six locations, and a C without hydrogens is present at two locations. Due to the rotational symmetry present in the molecule, the NMR analysis of the crown ether can be applied to half of the molecule (Figure 6.12). The three main methods explored were COSY, HSQC, and HMBC (Figure 6.13). In COSY (correlation spectroscopy), determination of three-bond coupling (proton to its carbon, the carbon-carbon bond, then to the adjacent carbon's proton) is possible; in HSQC (heteronuclear single quantum correlation), determination of carbon and its

adjacent hydrogen(s) can occur; and in HMBC (heteronuclear multiple bond correlation), determination of correlations between carbons and protons as far away as four bonds (but more typically, two to three bonds) can be found. In addition, NOESY (which looks at "through space" rather than "through bond" couplings like COSY) experiments in conjunction with molecular mechanics calculations were also explored to determine the stereochemical identity. For the crown ether of interest, the proton and carbon spectra (including DEPT (Distortionless Enhancement by Polarization Transfer, which can be used to distinguish carbons as either CH, CH_2, or CH_3) were both relatively resolved. Using a combination of the two, the carbon and hydrogen peaks for every bond location in the cyclohexano group can be identified (Figures 6.14 and 6.15). HSQC and COSY reiterate the identification of these atoms, but these techniques are not useful for the atoms present in the crown ether ring (because of overlap of signals). At first glance, HMBC does not appear promising for the analysis of the atoms present in the crown ether ring because of a resolution issue, but after additional exploration, it seems possible to determine the identity of all the atoms present (Figure 6.16). Looking at the specific region for the crown ether ring on the spectra, there seems to be an interaction between carbons #1 and r, as well as s with qa and qe, r with pe, and 2 with s, which should indicate s and q, and p and r are neighbors in the ring (a and e are used to arbitrarily designate the two protons present on carbons in the crown ether ring).
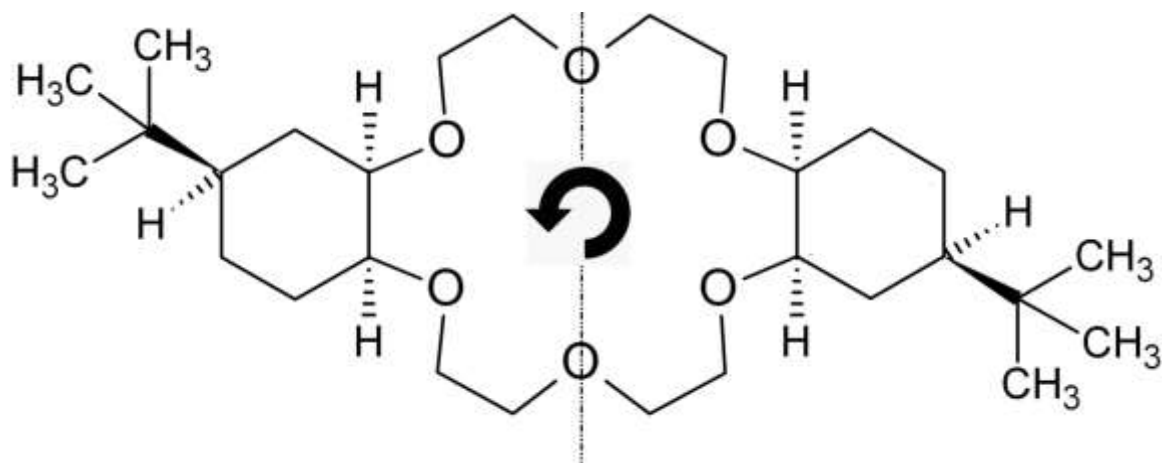
Figure 6.12: Rotation Symmetry of the Crown Ether Studied
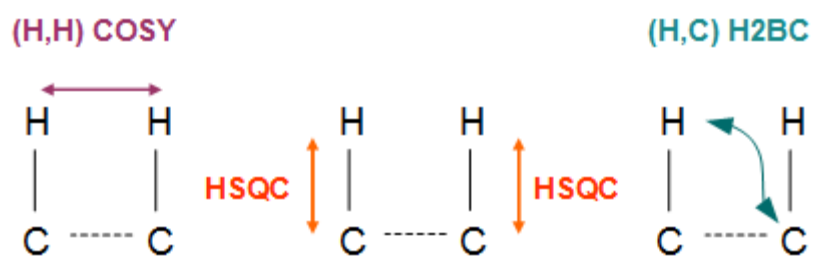
Figure 6.13: COSY, HSQC, and H2BC (also known as HMBC)
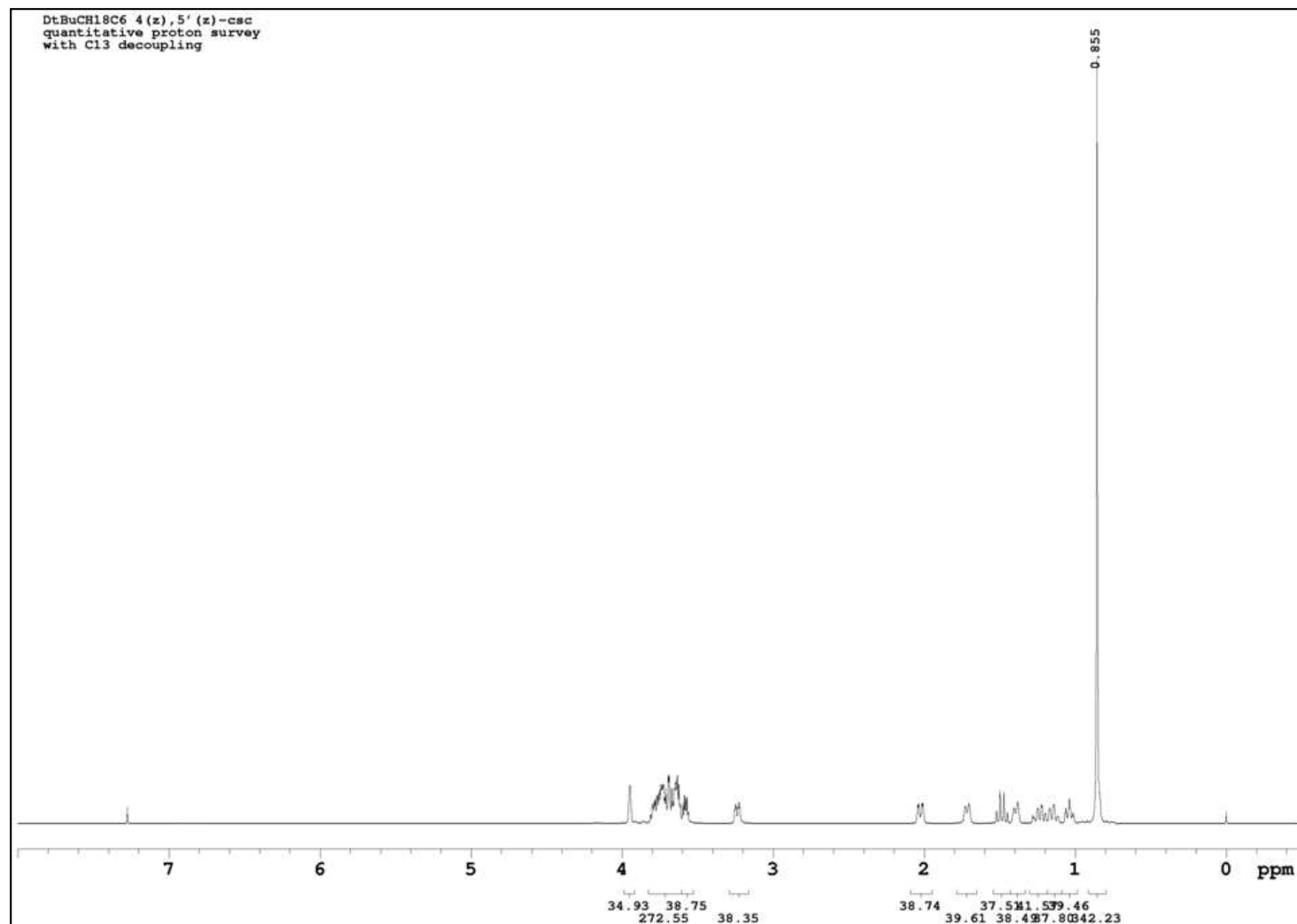
Figure 6.14: Proton NMR (in CDCl₃) of 4z,5'z csc DtBuCH18C6
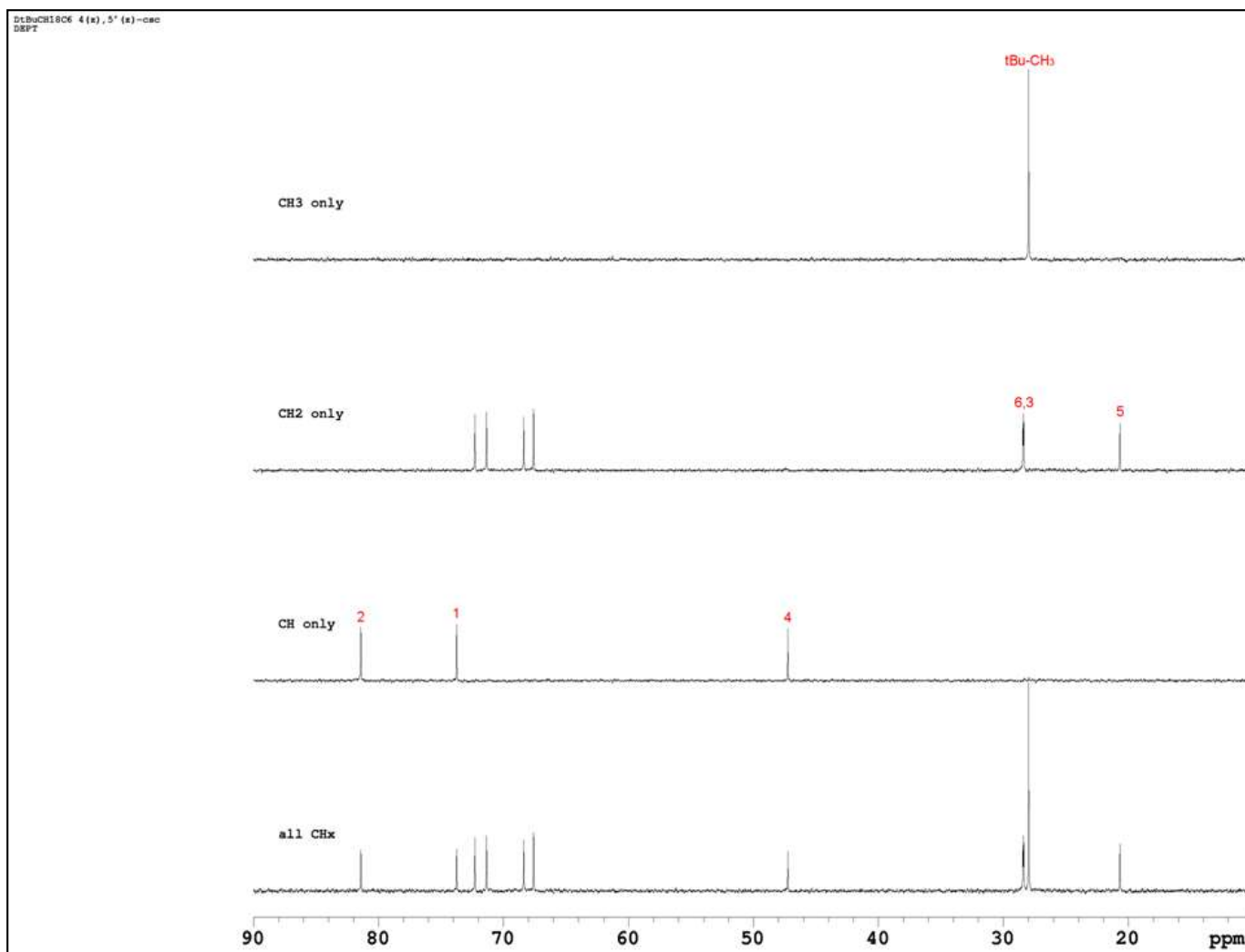
Figure 6.15: C-13 DEPT (in CDCl$_3$) of 4z,5'z csc DtBuCH18C6

Although we were able to identify all of the atoms present, the definitive determination of the ligand stereochemistry proved impossible. To establish the overall stereochemistry of an isomer, four factors must be determined: the stereochemistry of the hydrogens present at the junctions of the crown ether ring and the cyclohexano groups, the orientation of the hydrogens at these junctions, the location of the *tert*-butyl groups present on the cyclohexano groups, and the orientation of the *tert*-butyl groups (Figures 6.1 and 6.2). The identity of the atoms present in the cyclohexano rings should be fully definable for all isomers, leading to the determination of the stereochemistry of the junctions between the cyclohexano group and the crown ether ring (Figures 6.14 and 6.15) (Appendix G). Because the hydrogenation process used in the preparation of DtBuCH18C6 yields (overwhelmingly) *cis*-isomers, it is highly unlikely that any of the materials would be classified as *trans* (*25*). The determination of *e* versus *z* for the *tert*-butyl groups present should also be possible, but this may depend on the symmetry of the molecule. (The less symmetric the crown ether studied is, the more signals are present (in a small location on the NMR spectra) that can obscure the information necessary for analysis). The location of the *tert*-butyl groups present on the cyclohexano rings was expected to be one of the more difficult pieces of information to obtain, since it requires that all of the protons and carbons present in the crown ether ring and in the cyclohexano group be resolved (Figures 6.14 and 6.15). For this isomer, it was possible to distinguish between the 4,4' and. 4,5' substitution pattern using HMBC data (Figure 6.16). When looking across the crown ether ring, the two possible orientations present were q-s-2-1-r-p and p-r-1-2-s-q (indicating 4,5' classification) and q-s-2-1-r-p and q-s-2-1-r-p (indicating 4,4' classification). If p-q connections (p-qa, p-qa, q-pa, and q-pe) are seen in

the HMBC, it indicates the 4,5' classification while if p-p and q-q connections (p-pa, p-pe, q-qa, and q-qe) are seen, it indicated the 4,4' classification. Most of the connections are not visible due to overlapping peaks, but a strong q-pe peak and an absent q-qe peak seems to correctly indicate the 4,5' classification.

The most troublesome stereochemical determination for the crown ether was the *syn* or *anti* classification at the junctions of the crown ether and cyclohexano groups. In fact, none of the methods evaluated was able to provide this information. Because of this, it seems unlikely that NMR methods also can provide complete and definitive stereochemical information for the DtBuCH18C6 isomers (Figure 6.17). Better results may be achievable using a complexed (to lock in its orientation) crown ether or a higher field (900MHz) NMR spectrometer (*26, 27*).
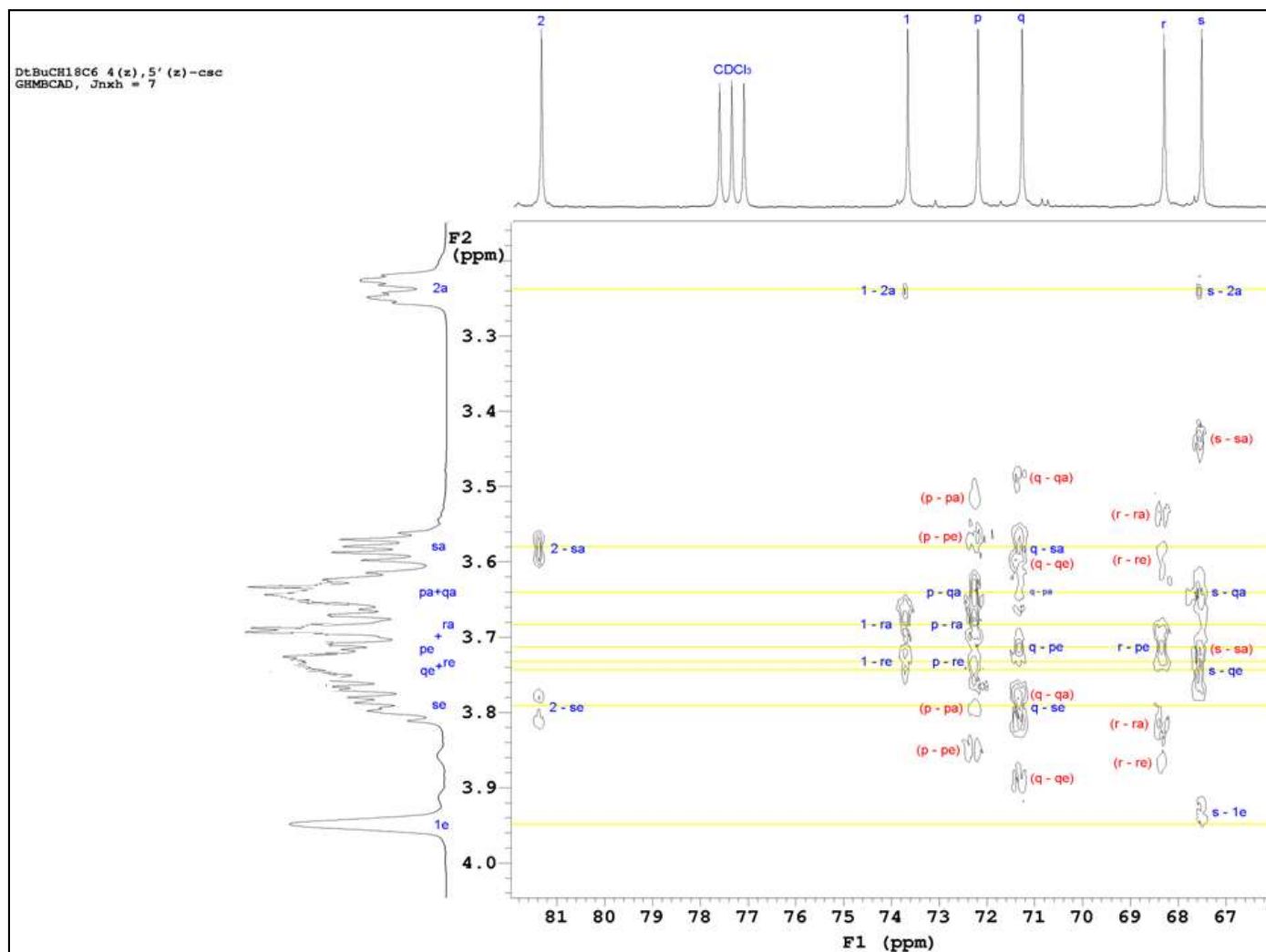
Figure 6.16: Partial HMBC NMR of of 4z,5'z csc DtBuCH18C6 with Cross Crown Ether Ring Assignments
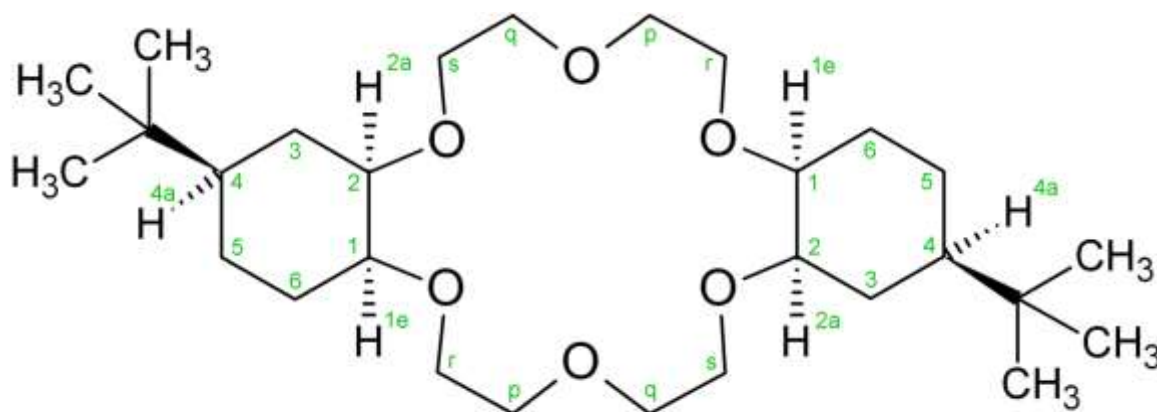
Figure 6.17: The Solved Structure of 4z,5'z *cis-syn-cis*-di-*tert*-butylcyclohexano-18-crown-6

6.3.3: Combining Ligand Strain Energy Calculations with Association Constants and Metal Ion Distribution Ratios to Determine the Identity of DtBuCH18C6 Isomers

As noted above, the formation constants for the binding of various alkali and alkaline earth metals to dicyclohexano-18-crown-6 stereoisomers are related to ligand strain energy (*18, 20*). This relationship can be exploited for identification of DtBuCH18C6 isomers. That is, each of the isomers of DtBuCH18C6 has a specific ligand strain energy associated with it that could be used to ascertain its identity (*21, 28*). For isomer identification, a plot is first prepared of the formation constant or the extent of extraction (reflected in, for example a strontium ion distribution ratio) *vs.* ligand strain energy for a series of known metal ion-DCH18C6 stereoisomer combinations. Then, using a measured formation constant (or metal ion distribution ratio) for interaction of the unknown isomer with the same metal ion, a ligand strain energy is estimated for the unknown isomer using published tables of ligand strain energies (*20, 21, 28*). From this, it may be possible to deduce the identity of the unknown isomer. To make this relationship stronger, we have added data for two DtBuCH18C6 isomers to the data for

DCH18C6 (Figure 6.18 and Table 6.1). One drawback for this method, is the need for a relatively large amount (~20mg) of purified sample. Although this may not seem like a large amount, for a typical preparative column run, the masses of the fractions collected ranged from 0.4mg to 15mg. (Moreover, even these small masses often represented more than one isomer).

When a strontium distribution ratio measurement was made on a perchloric acid-purified sample of DtBuCH18C6 (t_r = 57-59 minutes; see Figure 5.16), a value of 6.12 was observed. Such a value leads to a strain energy of 11.04 kcal/mol, which is consistent with only one isomer: 4*e*,4'*z-cis-syn-cis*-di-*tert*-butylcyclohexano-18-crown-6 (see Table 6.2). In addition, three more fractions were analyzed, two of which contained two major components, while the last one contained one major component. One of the two-component fractions, (which has a t_r = 5.8-6.6 minutes and is composed of two peaks: one corresponding to 47.9% of the total area and the other to 52.1%, see Figures 5.17 and 6.19) has a D_{Sr} of 0.038, which indicates that both components present are of low strontium complexing agents. The other two component fraction (which has a t_r = 14.5-16.25 minutes and is composed of two major peaks: one corresponding to 92.2% of the total area and the other to 7.8%, see Figures 5.17 and 6.19) has a D_{Sr} of 0.43, which indicates that the major component is a poor strontium complexing agent while the minor component is significantly better. Lastly, the one-component sample found at a t_r = 16.5-17.5 minutes (Figures 5.17 and 6.19) was shown to have a D_{Sr} of 3.27, which indicates that this fraction could be any of the following three isomers: 4*e*, 5'*e-cis-syn-cis*-di-*tert*-butylcyclohexano-18-crown-6, 4*z*,4'*e-cis-anti-cis*-di-*tert*-butylcyclohexano-18-crown-6, or 4e,5'e- *cis-anti-cis*-di-*tert*-butylcyclohexano-18-crown-6. HPLC spiking experiments

on an analytical scale were performed to indicate the identity of three peaks on a perchloric acid purified HPLC chromatogram (Figure 6.20).
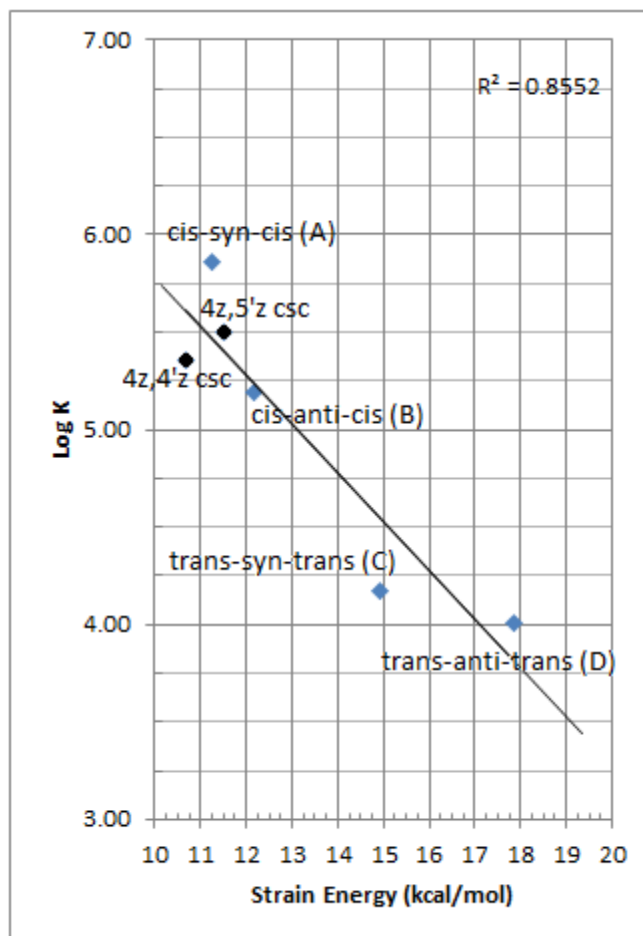
Figure 6.18: Log K vs. Strain Energy for Strontium for the Five Isomers of DCH18C6 (Chapter 4) and the Two Verified Isomers of DtBuCH18C6

Table 6.1: ITC Data for Strontium for the Two Verified Isomer of DtBuCH18C6

	Cation	log K	N

4z,4'z csc DtBuCH18C6	Sr^{2+}	5.36	1
4z,5'z csc DtBuCH18C6	Sr^{2+}	5.50	1

Table 6.2: Ligand Strain Energy and D$_{Sr}$ for DtBuCH18C6 Isomers(*28*)

Ligand	$\Delta E_{reorganization}$ Sr^{2+} (kcal/mol)	D$_{Sr}$ (Calc)	D$_{Sr}$ (Exp)
4(z),4'(z)-*cis-syn-cis*	10.67	9.5±1.6	7.5
4(z),4'(e)-*cis-syn-cis*	11.04	5.8±1.0	6.12
4(e),4'(e)-*cis-syn-cis*	11.16	4.9±0.8	
4(z),5'(e)-*cis-syn-cis*	11.22	4.6±0.8	
4(e),5'(e)-*cis-syn-cis*	11.38	3.7±0.6	
4(z),4'(e)-cis-anti-cis	11.48	3.2±0.5	
4(z),5'(z)-*cis-syn-cis*	11.53	3.0±0.5	3.57
4(e),5'(e)-*cis-anti-cis*	11.56	2.8±0.5	
4(z),5'(z)-*cis-anti-cis*	11.59	2.5±0.4	2.63
4(z),4'(z)-*cis-anti-cis*	14.4	0.052±0.009	
4(e),4'(e)-*cis-anti-cis*	14.55	0.06±0.01	
4(z),5'(e)-*cis-anti-cis*	15.21	0.022±0.004	
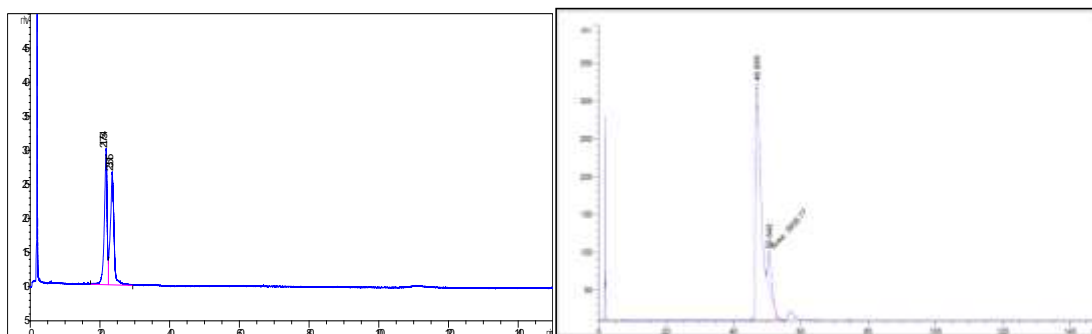
Figure 6.19: (left) Prep Sample 5.8-6.6 minutes and (right) Prep Sample 14.25-16.5 minutes(Experimental Conditions: 20µL injection of a 1mg/mL crown ether sample in methanol, a 0-80% (v/v) methanol:acetonitrile gradient was applied for 90 minutes and

then held at the final conditions for 30 minutes, Zorbax NH$_2$ 3.0 x 75 mm 5-micron particle size column, flow rate: 0.235mL/min, Detection: Varian 380-LC ELSD: nebulizer temperature: 50°C, evaporator temperature: 60°, and gas flow rate: 0.90 SLM
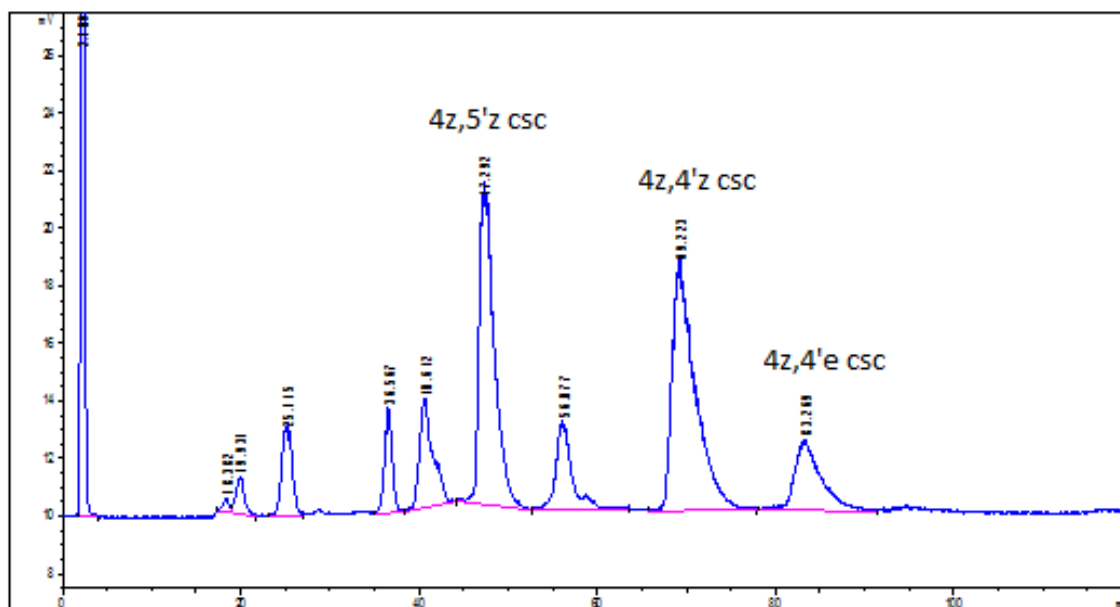
Figure 6.20: Representative Chromatogram Showing the Identity of Peaks Present in a Perchloric Acid Purified Sample of DtBuCH18C6 on a Zorbax NH$_2$ 3.0 x 75mm, 5-micron column (1mg/mL)

6.4: Conclusion

In this work, we have examined the utility of x-ray crystallography, NMR, and a combination of K_f or D_{Sr} determinations and MM3 calculations in identifying the various isomers of DtBuCH18C6. While some of these approaches provided little or no useful information, three isomers have been definitively identified using a combination of x-ray crystallography, ligand strain energy calculations, and strontium distribution ratios. The identity of an additional isomer has been narrowed down to one of three possibilities. The

identity of two additional isomers, both poor strontium complexing agents has been narrowed down to one of three possibilities. Improvements to the methods used here, along with other options to identify the other peaks observed in the chromatograms, will be explored in the last chapter.

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Chapter 7 : Recommendations for future work

7.1: Conclusions

In this work, the effect of stereochemistry on the thermal properties, ternary ionic liquid formation, and metal ion extraction behavior of crown ethers has been investigated. In the studies of the thermal properties, stereochemistry was found to have little or no effect on the onset temperatures of mass loss upon heating for a crown ether, but a much larger effect on the melting point and/or glass transition of the isomers. In addition, a relationship was observed between the enthalpy of vaporization and the onset temperature of mass loss for several crown ethers and between the molecular weight and onset temperatures for a series of aliphatic crown compounds. From these initial thermal studies, the characteristics of crown ethers best suited for use as the neutral complexing agent in a new series of ternary ionic liquids (TILs) have been identified. From examination of the onset temperature of these new ionic liquids, it is apparent that factors other than stereochemistry, specifically the choice of anion and the strength of complex formation between the crown ether and the metal ion, are more important in influencing the thermal properties of the TILs.

The stereochemistry of a crown ether has also been found to have important implications in metal ion extraction. Studies of the influence of stereochemistry on the complexation of alkaline earth metals in methanol by the isomers of dicyclohexano-18-crown-6 (DCH18C6) have revealed a relationship between metal-CE formation constants and the ligand strain energy, with lower strain leading to higher formation constants. Extraction efficiency, as reflected in D_{Sr}, strontium distribution ratio, was also been found

to be inversely related to ligand strain energy, and the extension of this relationship to the more complex 4,4'(5')-di(*tert*-butylcyclohexano)-18-crown-6 (DtBuCH18C6) family of stereoisomers has led to a possible means by which to identify individual stereoisomers of this crown ether.

An HPLC method similar to that used by *Dietz et al*. (*1*) has been implemented to separate the isomers of DtBuCH18C6 on the analytical scale. This method has been successfully scaled-up to yield a preparative-scale method that permits baseline resolution of many of the isomers.

In an effort to identify the various peak resolved, multiple NMR methods have been explored (since it has been used to determine the complete structure of many organic molecules in the past (*2*)), but the crown ethers of interest proved to be too complex to allow for more than a partial identification. In addition, the use of a variety of complexing agents to x-ray quality single crystals has been explored. Two isomers have been identified by this approach, one complexed to a hydronium perchlorate (hydronium 4*z*,4'z-*cis-syn-cis*-di-*tert*butylcyclohexano-18-crown-6 perchlorate) and the other (unexpectedly) uncomplexed (4*z*,5'*z-cis-syn-cis*-di-*tert*butylcyclohexano-18-crown-6). An additional isomer, 4z,4'e *cis-syn-cis*-di-*tert*butylcyclohexano-18-crown-6 observed in preparative column runs of perchloric acid-purified DtBuCH18C6 sample was identified via a combination of the metal ion distribution ratios and molecular mechanics methods. Lastly, the isomers present in three additional fractions were tentatively identified. Two of these fractions contained two prominent peaks each, while the other contained only one peak. For the fractions containing two peaks, the strontium distribution ratios indicate

that both components present are inefficient for the extraction of strontium, while the other fraction yielded a strontium distribution ratio consistent with that of any of three other isomers.

In summary, these results have laid the groundwork for an understanding of the effect of stereoisomerism of crown ethers on both ionic liquid design and metal ion extraction. While much progress has been made, a great deal of additional work is clearly necessary before a complete picture of these effects can be developed.

7.2: Recommendations

In the following sections, specific suggestions for future work are therefore provided.

7.2.1: Investigation of the Thermal Properties of Macrocyclic Polyethers

In the investigation of the thermal properties of crown ethers, TGA-GC-MS experiments should be pursued to determine if the crown ethers decompose following evaporation. Although evaporation or decomposition renders an ionic liquid incorporating a crown ether useless, the answer has important implications for the possible re-use or recycling of ternary ILs. Along these same lines, to further explore the relationship between the enthalpy of vaporization and the onset temperature of mass loss, further enthalpy of vaporization studies of crown ethers should be undertaken. If the trend holds true under further scrutiny, it will permit estimation of the onset temperature of mass loss for other crown ethers and provide further support for the notion that T_{onset} corresponds solely to an evaporation event.

7.2.2: Formation of a New Set of Ternary Ionic Liquids Utilizing the Dicyclohexano-18-crown-6 Family of Isomers

For the formation of ternary ionic liquids, additional combinations of crown ethers with various cations and anions (water soluble and insoluble) should be explored. Initial experiments mimicking Song *et al.(3)* using *cis-anti-cis*-dicyclohexano-18-crown-6 (instead of 18-crown-6) yielded ionic liquids, but these were subsequently determined to be impure. New experimental procedures are needed to synthesize these ionic liquids in pure form.

On this same subject, on the basis of results for a series of TILs incorporating K^+ there appears to be a relationship between the change (*vs.* the free ligand) in the temperature corresponding to the onset of mass loss for a complex/TIL and the formation constant for the metal cation-neutral ligand complex used in preparing the ternary ionic liquid. Here too, additional studies are needed to establish the generality of this observation for a range of cation-crown ether-anion combinations. In addition, once the factors governing the stability of TILs have been delineated, experiments to determine their practical utility should be undertaken.

7.2.3: Study of the Complex Formation Between the Dicyclohexano-18-crown-6 Family of Isomers with Some Alkaline Earth Metal Ions in Methanol Using Isothermal Titration Calorimetry

Isothermal titration calorimetry studies of *cis-trans*-dicyclohexano-18-crown-6 (Isomer E) with the various divalent metal chlorides studied here are needed, both to complete this work, and to obtain additional evidence supporting the trends observed thus far. Also, because previous work used anhydrous alkali metal chlorides, measurement of

the formation constants of metal-crown ether complex using anhydrous metal chlorides would permit the determination of the influence of trace amounts of H_2O an the measured constants (*4*).

7.2.4: Separation of the Stereoisomers of Di-*tert*-butylcyclohexano-18-crown-6

In the separation of the various isomers of DtBuCH18C6, additional experiments to fine tune the preparative scale LC runs would be of great value. The main limitation of the current method is the fact less than 5 mg is collected for many of the samples. Moreover, the collected material is not necessarily a single isomer. If conditions can be modified to minimize the cross-contamination of peaks and increase the purity of each collected fraction, then collection of such a small amount would be acceptable. Although aminopropyl-derivatized silica was used the separation of the DtBuCH18C6 stereoisomers, cyano-derivatized silica columns should also be explored for the separation of DtBuCH18C6. One issue with the use of aminopropyl derivatized-silica is the poor reproducibility of retention times arising (we suspect) from gradual column fouling. Along these same lines, due to the hazards associated with perchloric acid use, sulfamic acid should be systematically evaluated as a reagent for the precipitation and purification of DtBuCH18C6. Although, initial results were promising, much additional workup is necessary to determine if sulfamic acid is as effective as a precipitating agent for crown ethers as is perchloric acid.

7.2.5: Identification of the Stereoisomers of Di-*tert*-butylcyclohexano-18-crown-6

For the identification of DtBuCH186 stereoisomers, additional experiments using a higher field NMR spectrometer are recommended. The use of such an NMR

spectrometer would provide greater resolution, which is crucial for samples with minimal symmetry. Also, an NMR method employing a metal cation to "lock" the structure of the crown ether may be beneficial, since once locked the crown ether cannot change its orientation. Of course, additional molecular mechanics calculations would be necessary for these complexes.

It is lastly recommended that additional crystallographic studies be undertaken, as many of the experiments performed in this work failed to yield satisfactory results. Complexing agents used previously with dicyclohexano-18-crown-6 isomers would an obvious first choice, along with complexing agents for 18-crown-6. Among the more obvious choices are: 3,4-diaminofurazane(*5*), potassium 2-nitrophenoxide(*6*), lead(II) iodide(*7*), ferrioxamine B(*8*), and potassium chlorochromate(*9*).

7.2.6: Summary

The various studies described in this chapter represent what we consider to be the most promising avenues for further investigation. While the results of these studies obviously cannot be predicted, it seems likely that a successful outcome will significantly advance our understanding of isomer effects in crown ether and by analogy, other families of metal ion complexing agents.

7.3: References

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APPENDIX A

THERMOGRAMS (TGA and DSC) OF CROWN ETHERS AND CROWN ETHER-BASED TERNARY COMPLEXES (IONIC LIQUIDS)
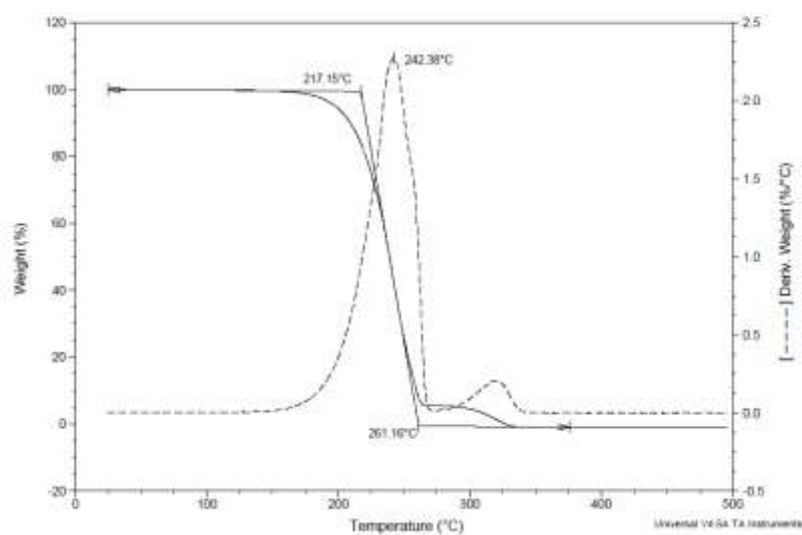
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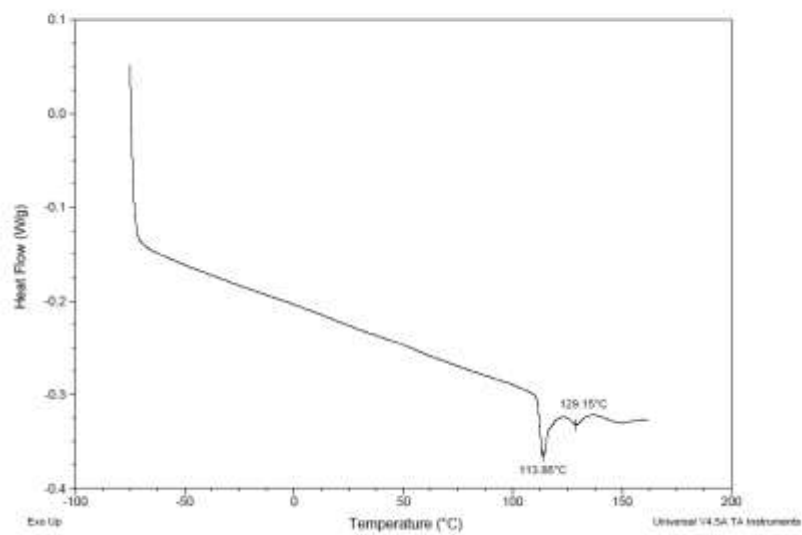
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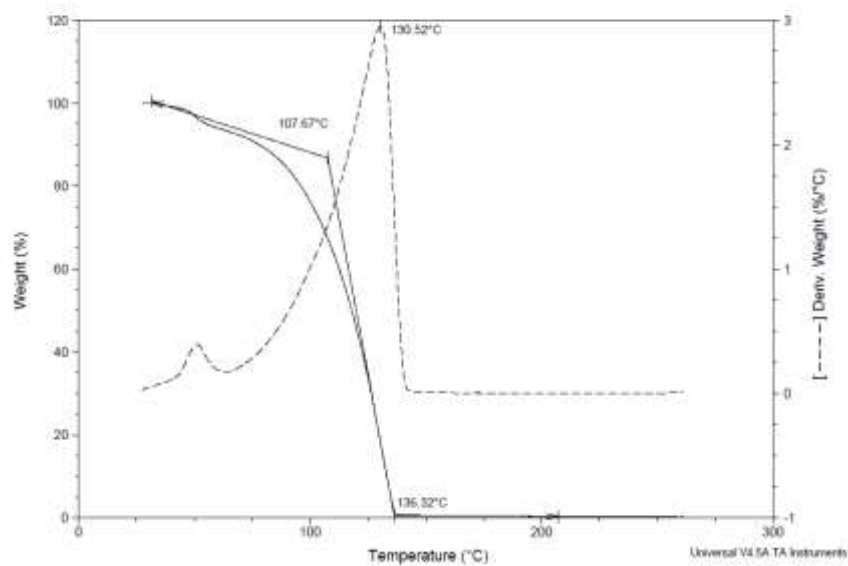
Figure A.3: TGA Thermogram of 1-aza-12-crown-4
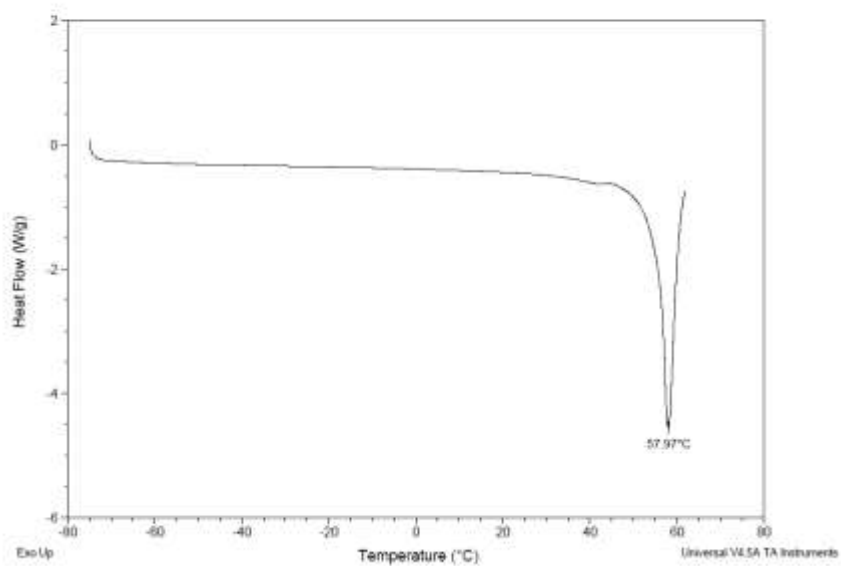
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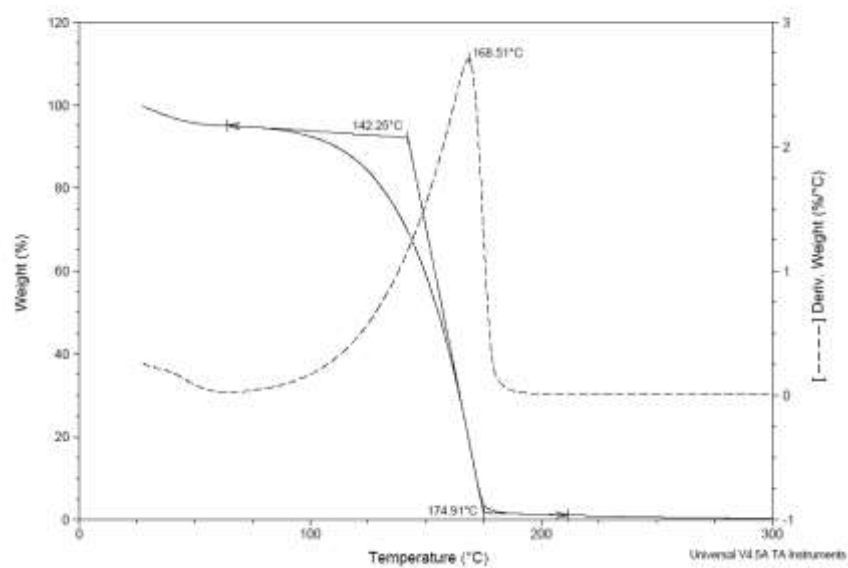
Figure A.5: TGA Thermogram of 1-aza-15-crown-5
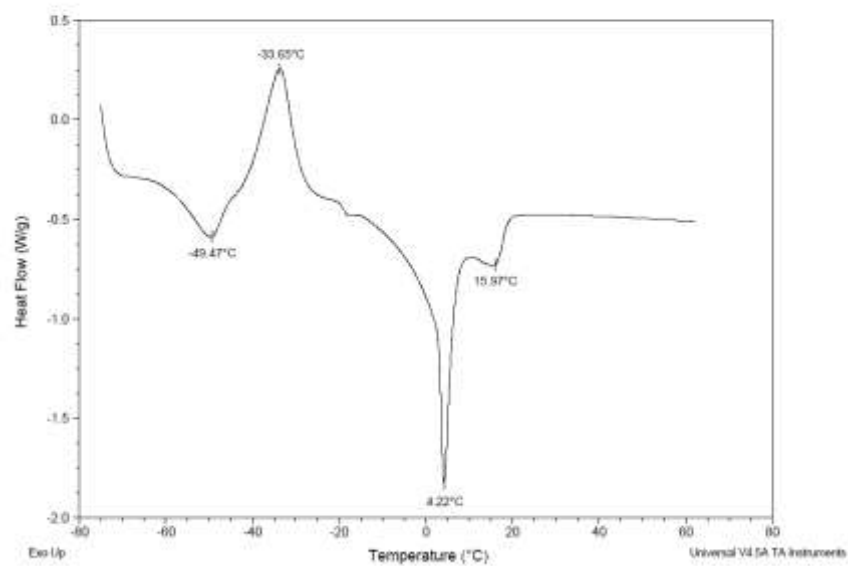
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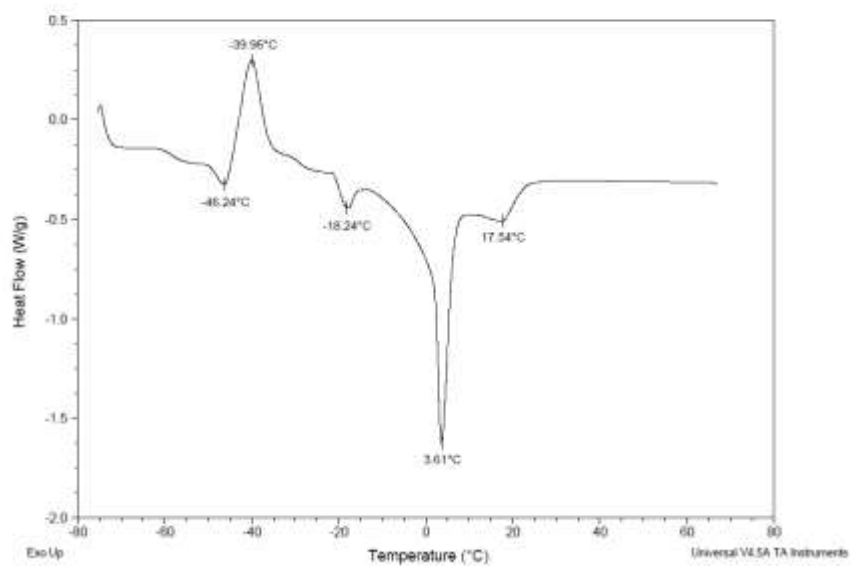
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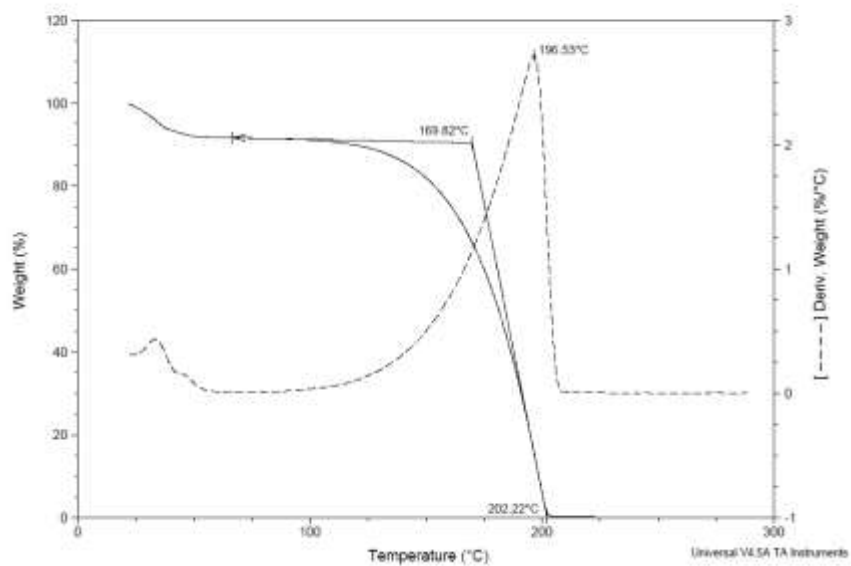
Figure A.8: TGA Thermogram of 1-aza-18-crown-6
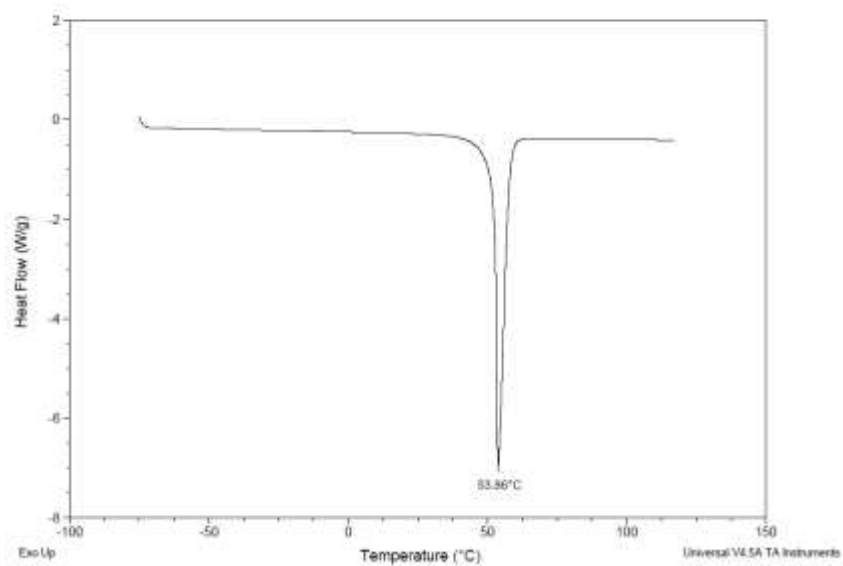
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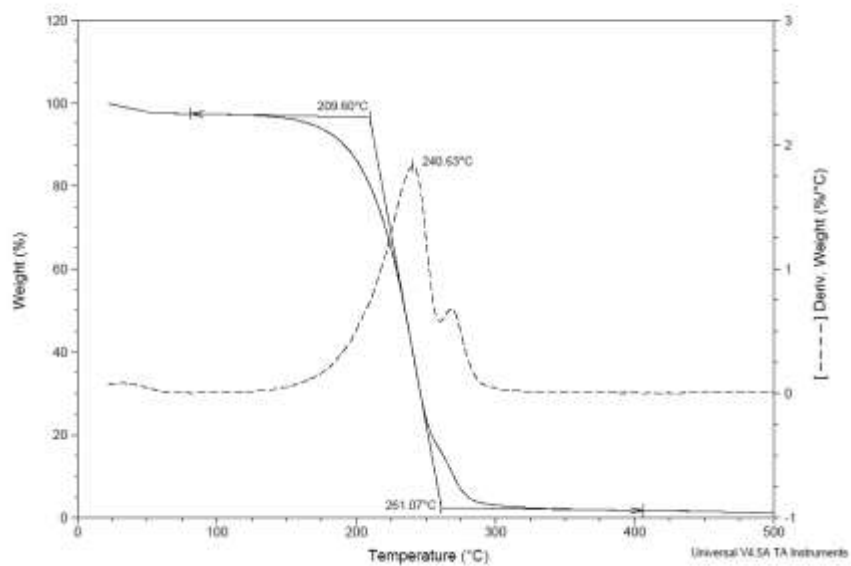
Figure A.10: TGA Thermogram of 4-*tert*-butylbenzo-18-crown-6
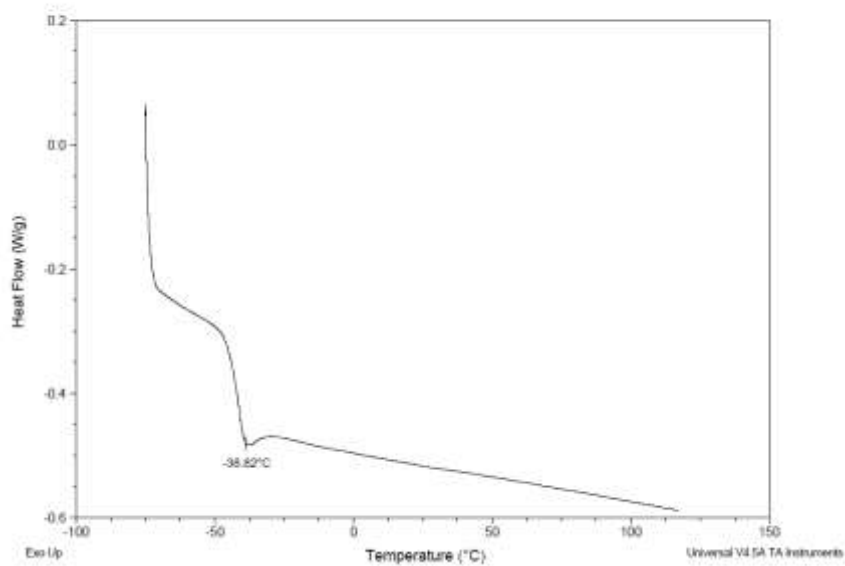
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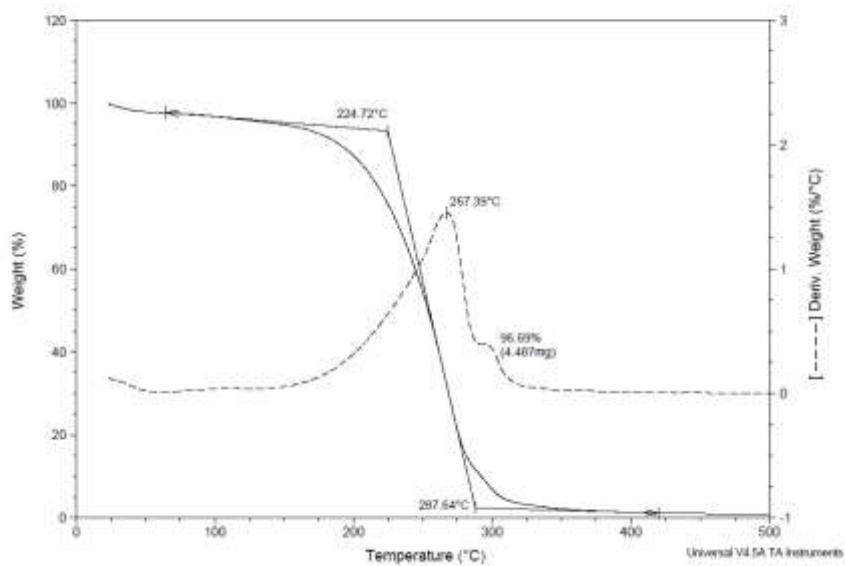
Figure A.12: TGA Thermogram of 4-*tert*-butylcyclohexano-18-crown-6
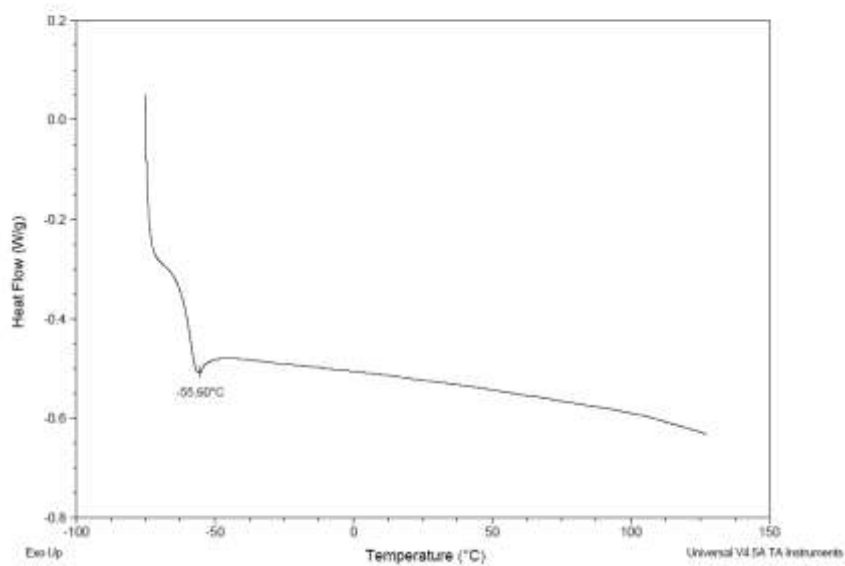
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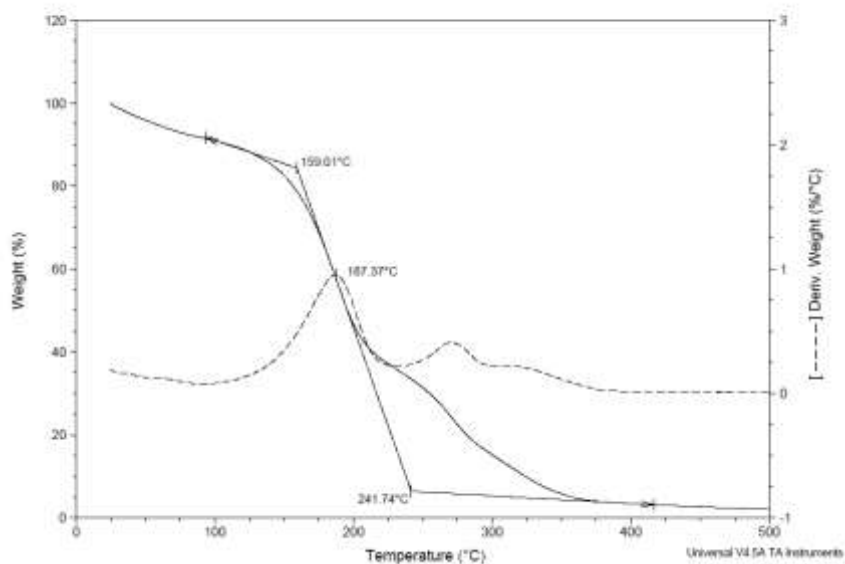
Figure A.14: TGA Thermogram of a mixture of cyclohexano-15-crown-5 isomers
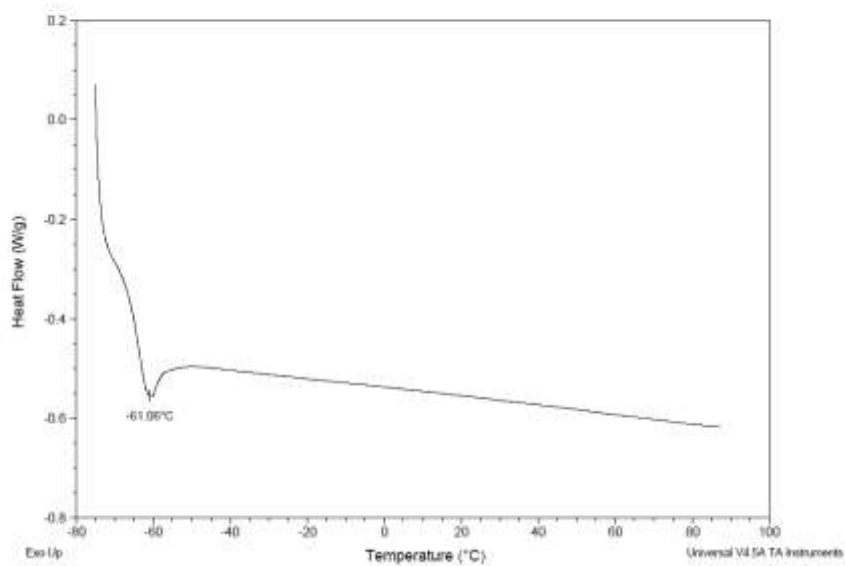
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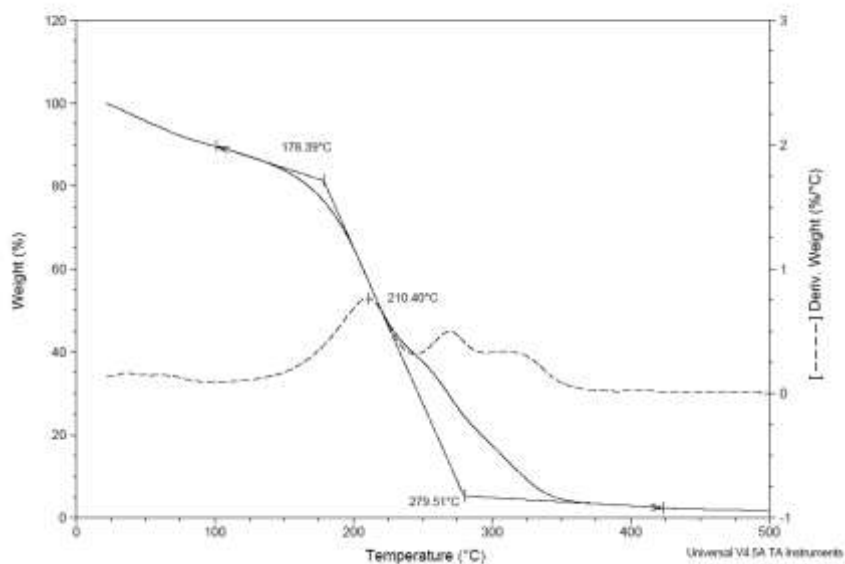
Figure A.16: TGA Thermogram of a mixture of cyclohexano-18-crown-6 isomers
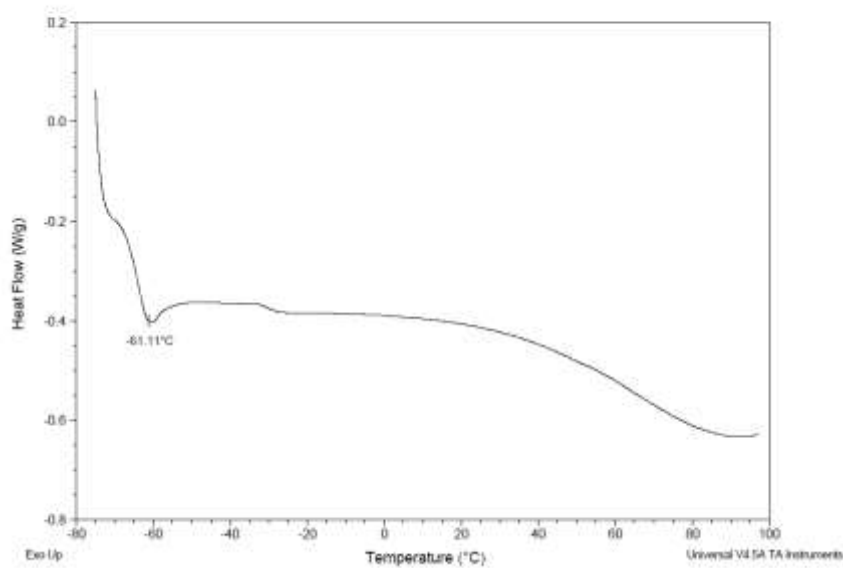
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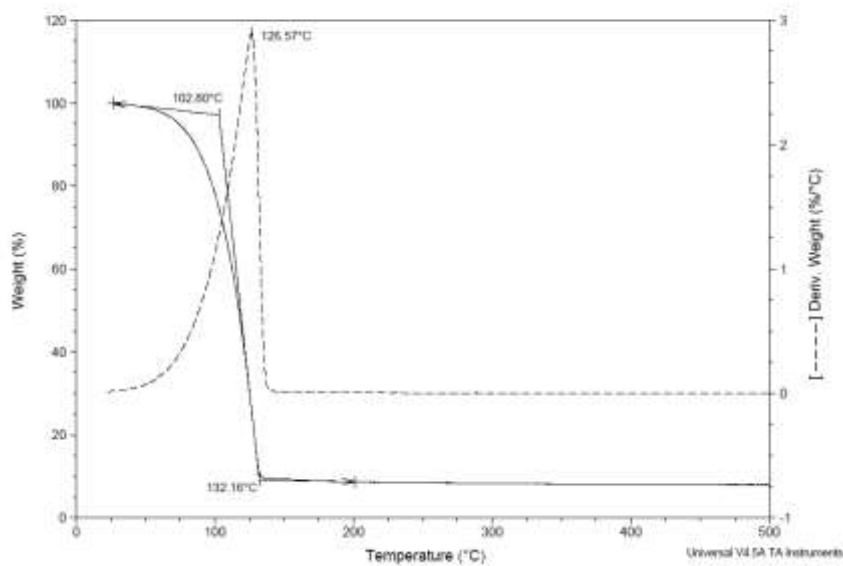
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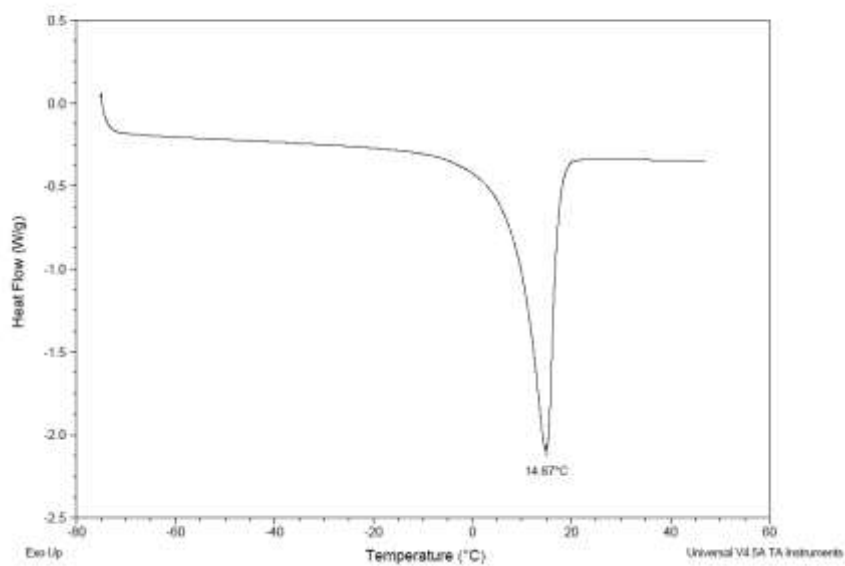
Figure A.19: DSC Thermogram of 12-crown-4
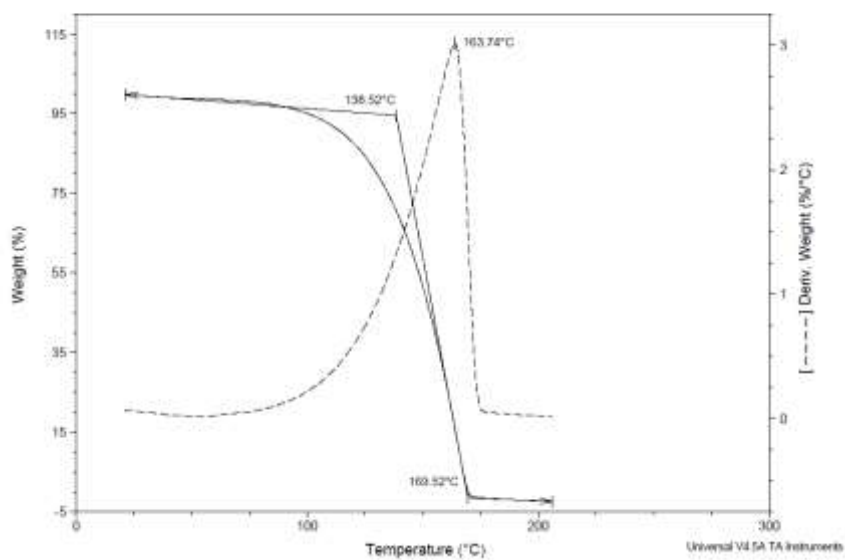
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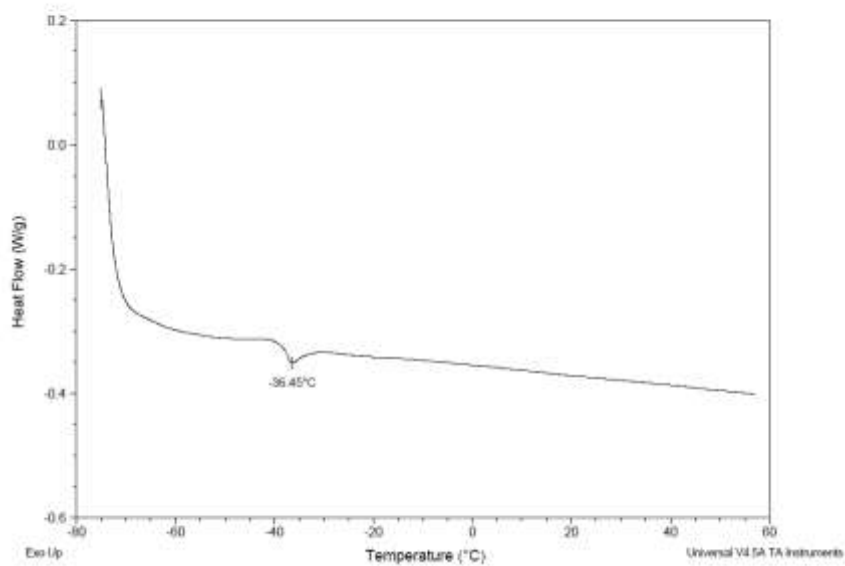
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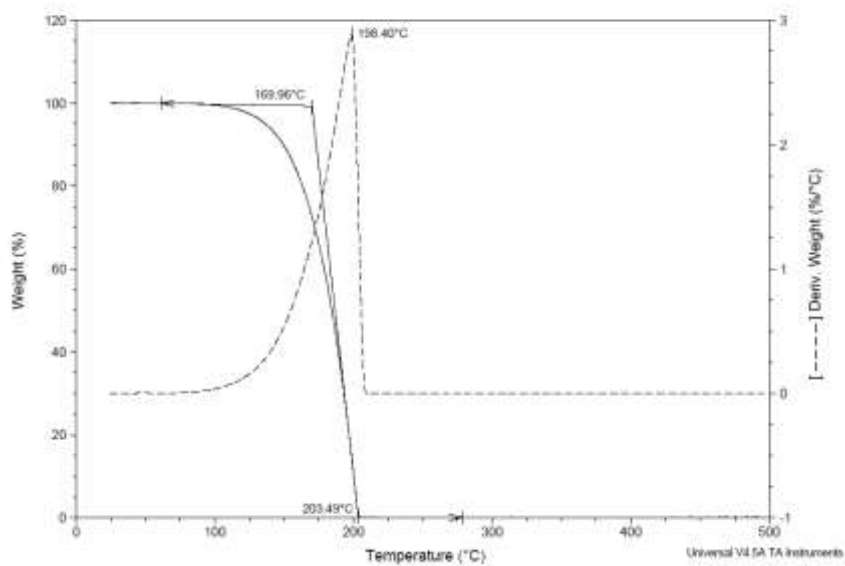
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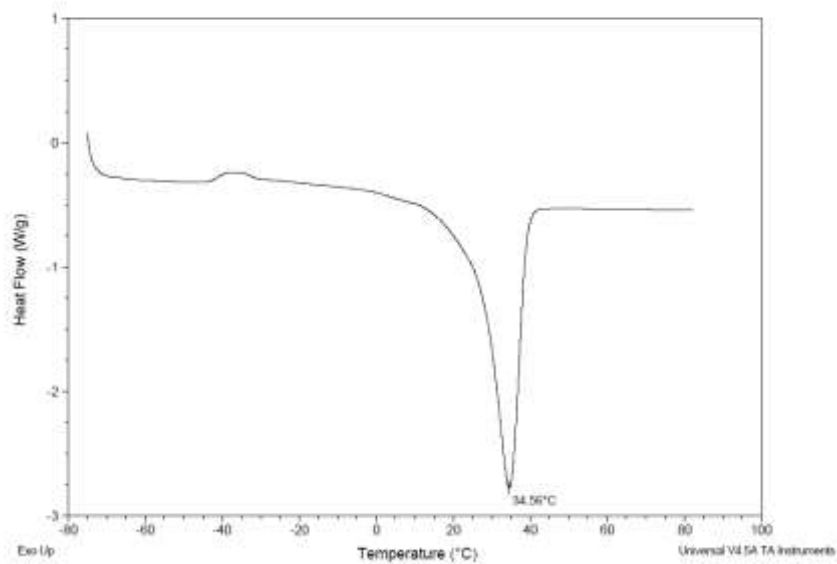
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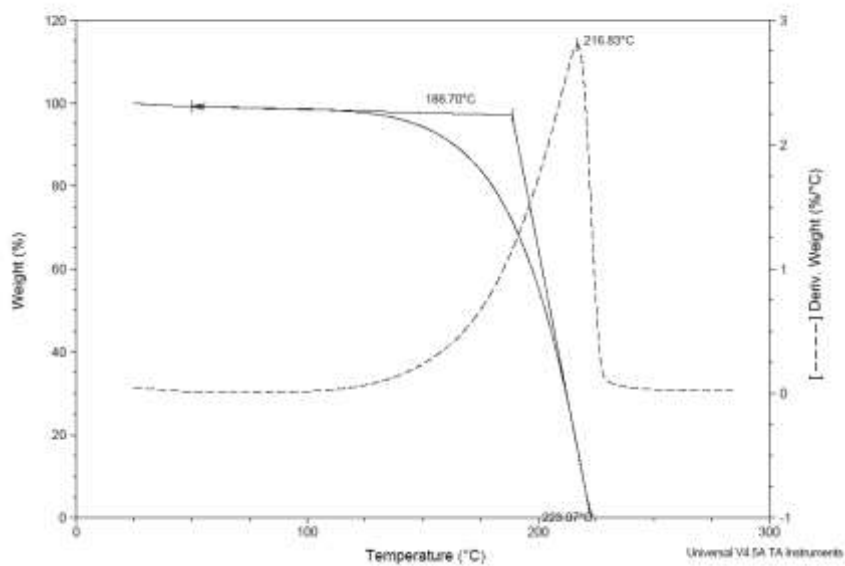
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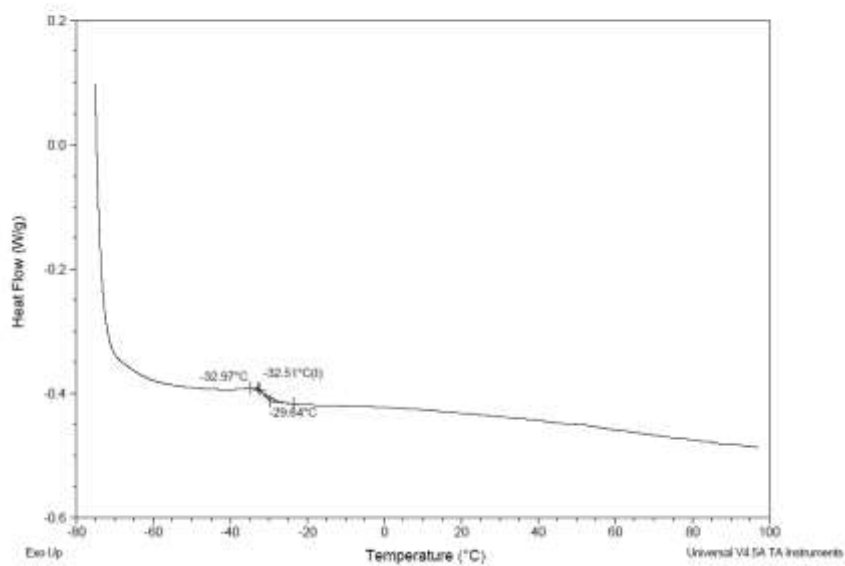
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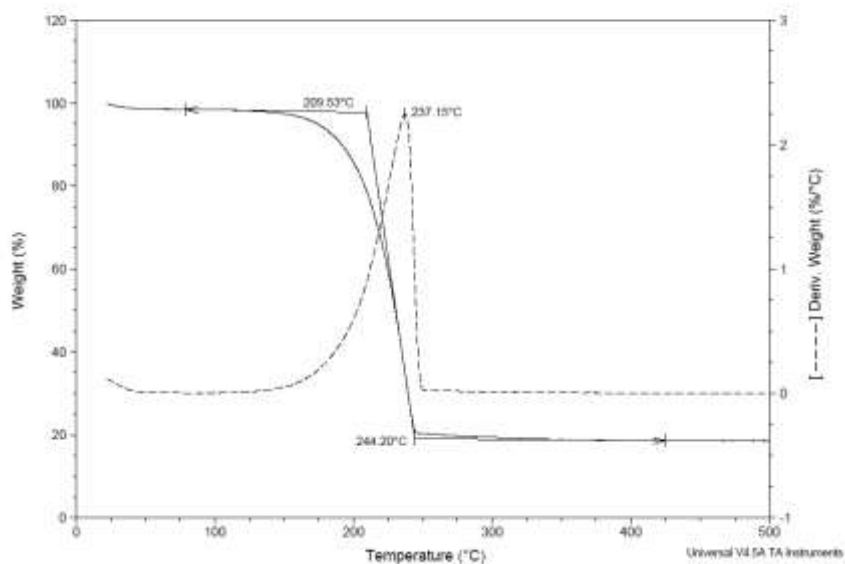
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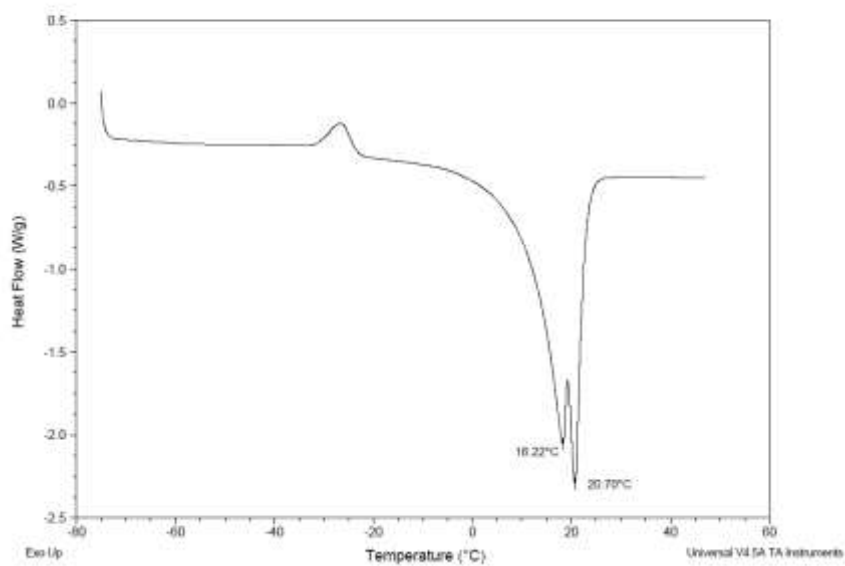
Figure A.27: DSC Thermogram of 24-crown-8
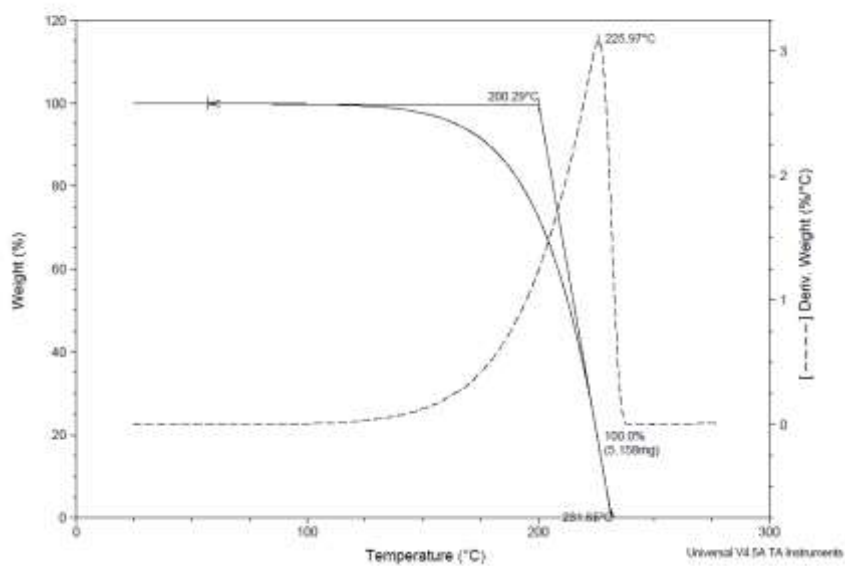
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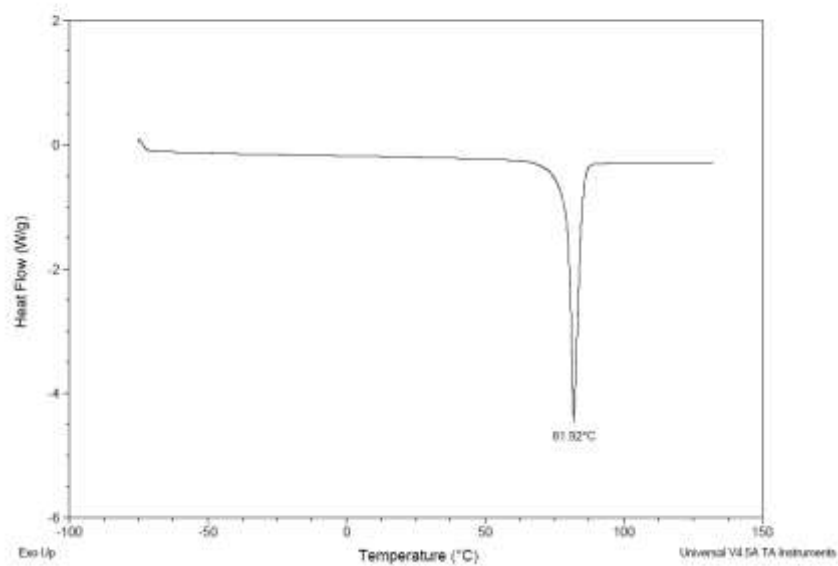
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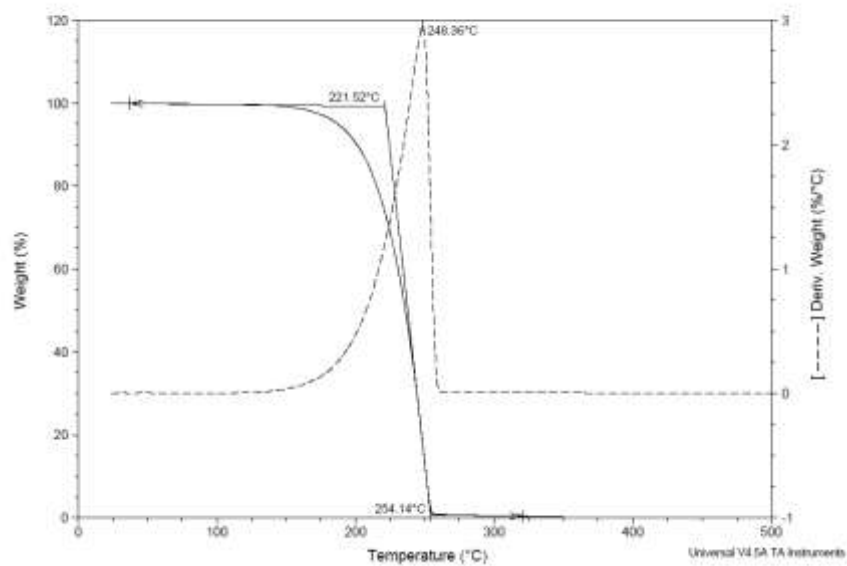
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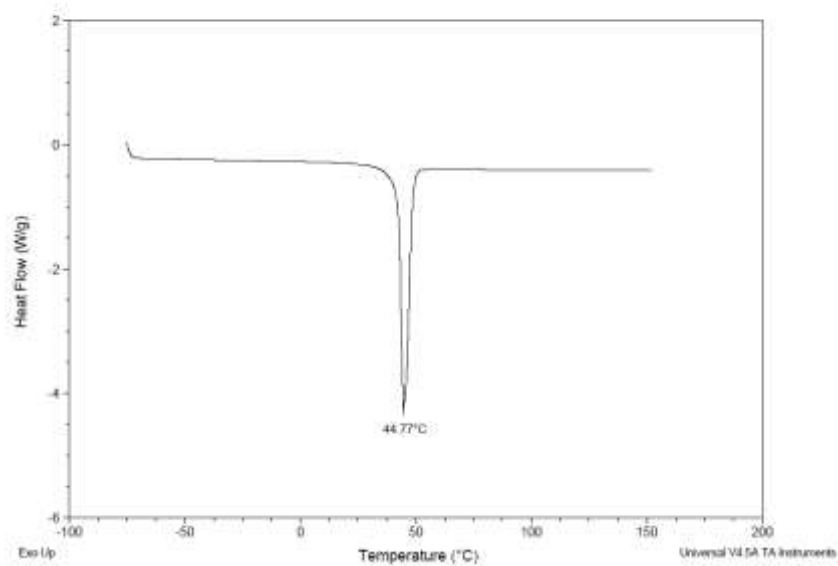
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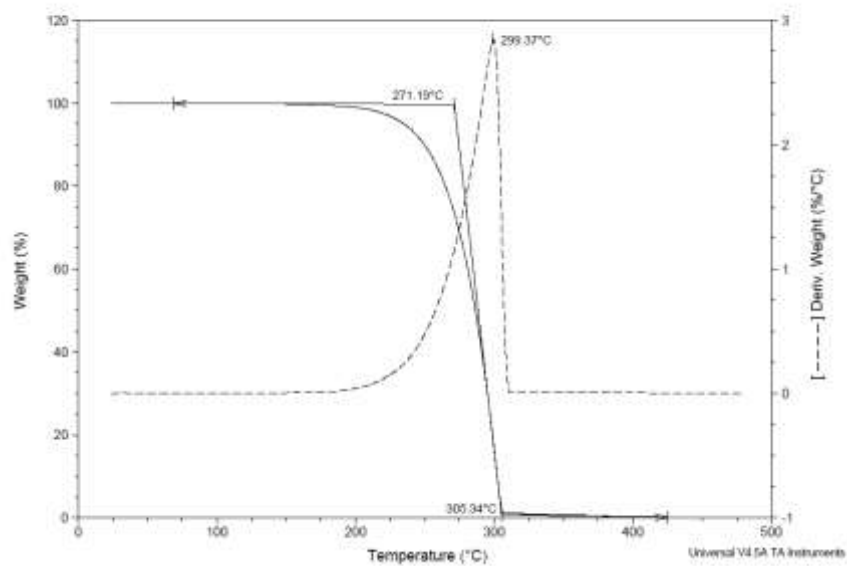
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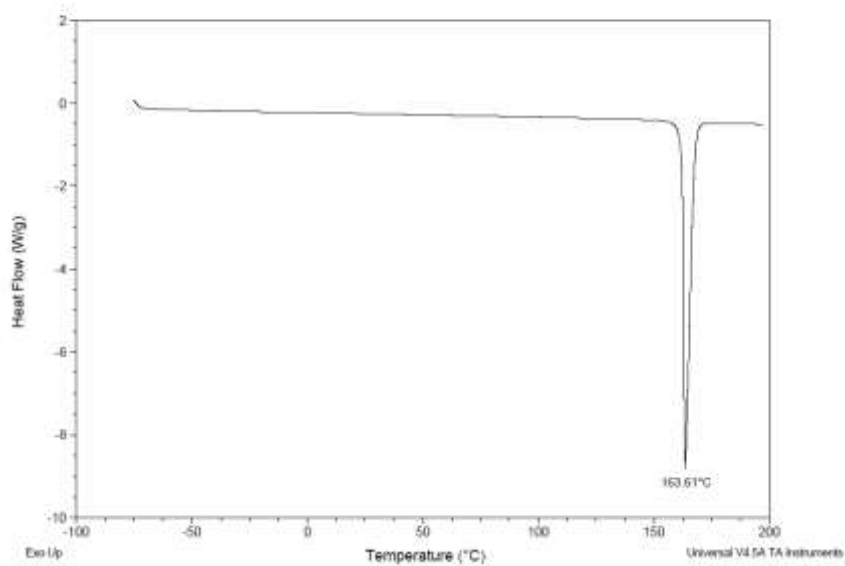
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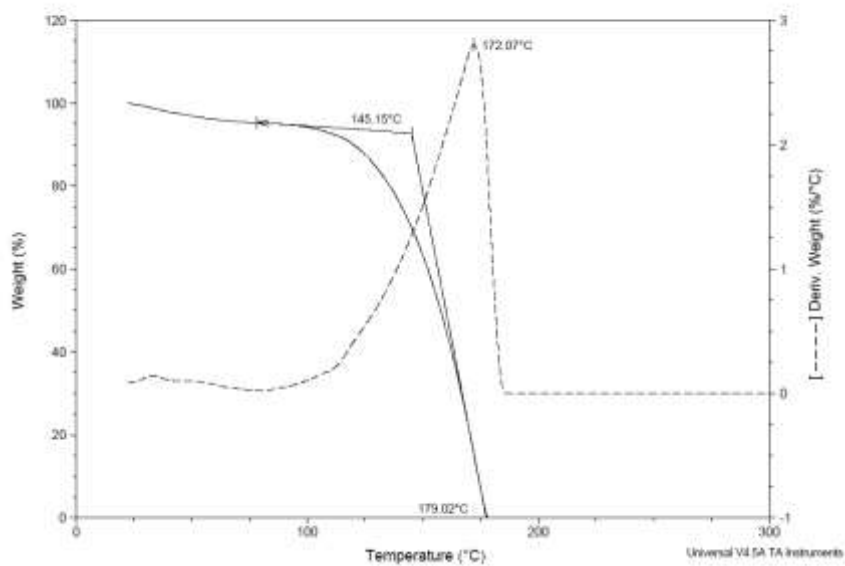
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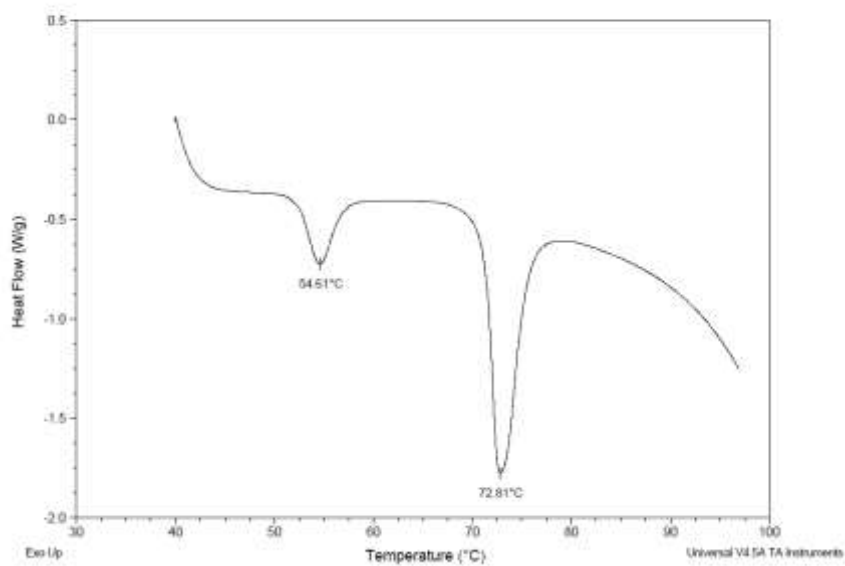
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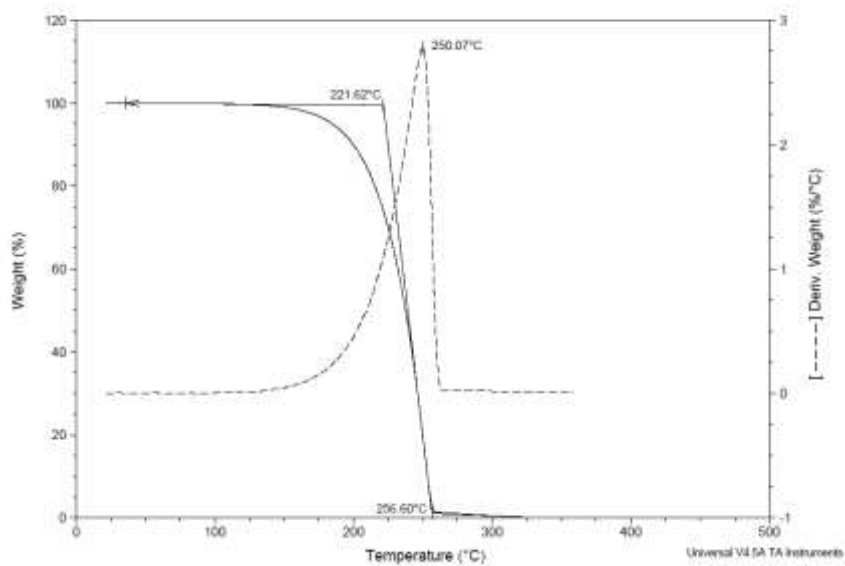
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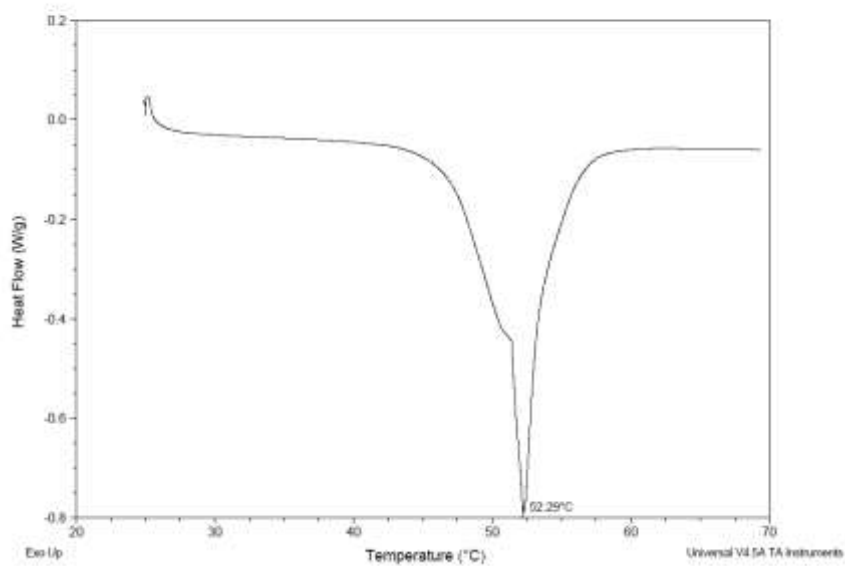
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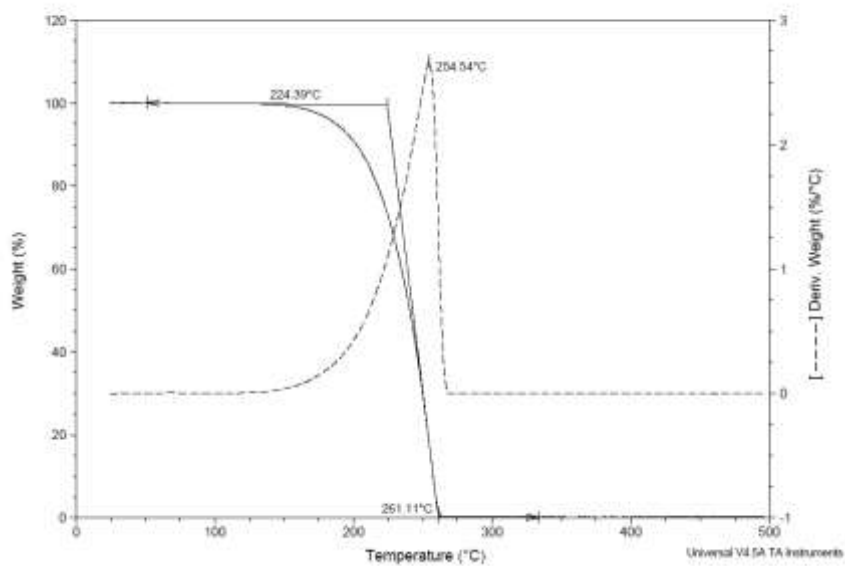
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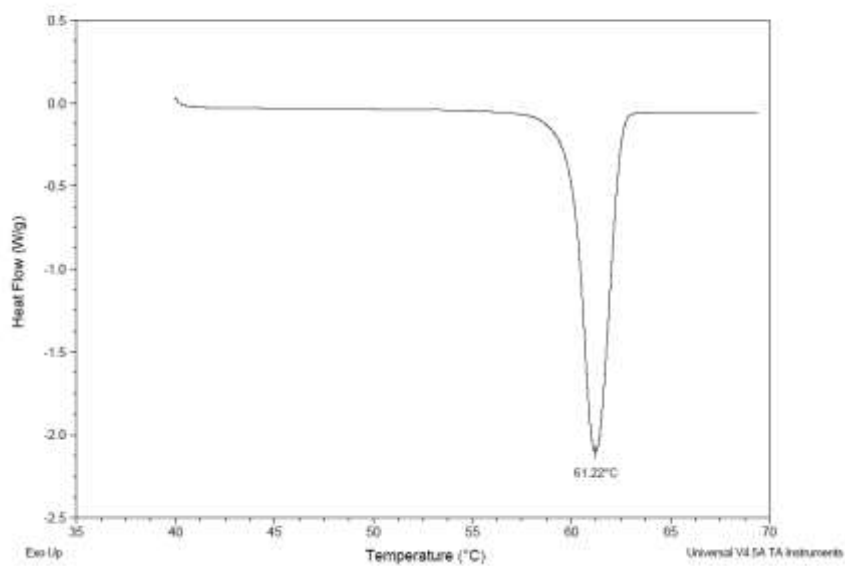
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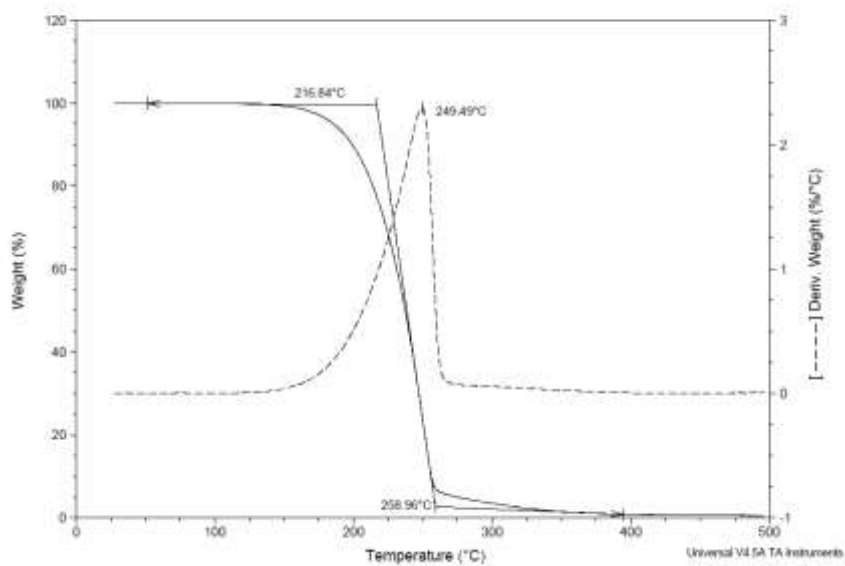
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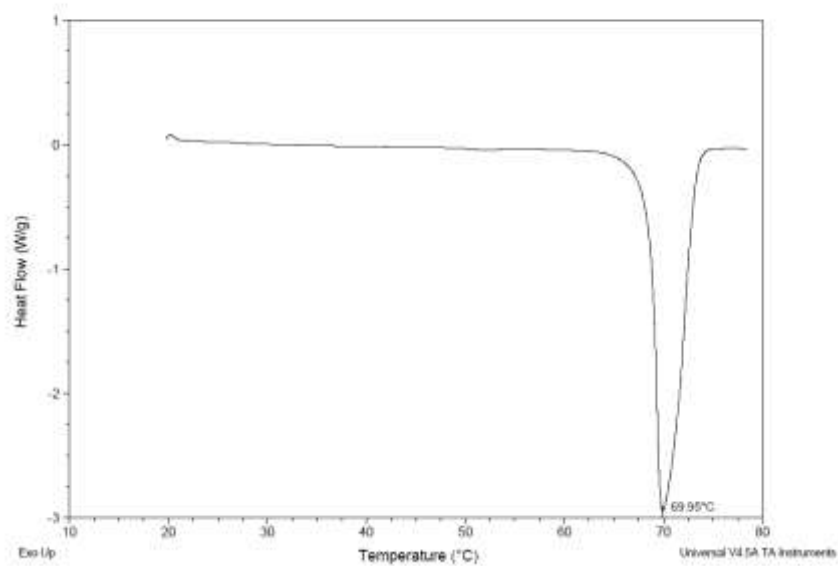
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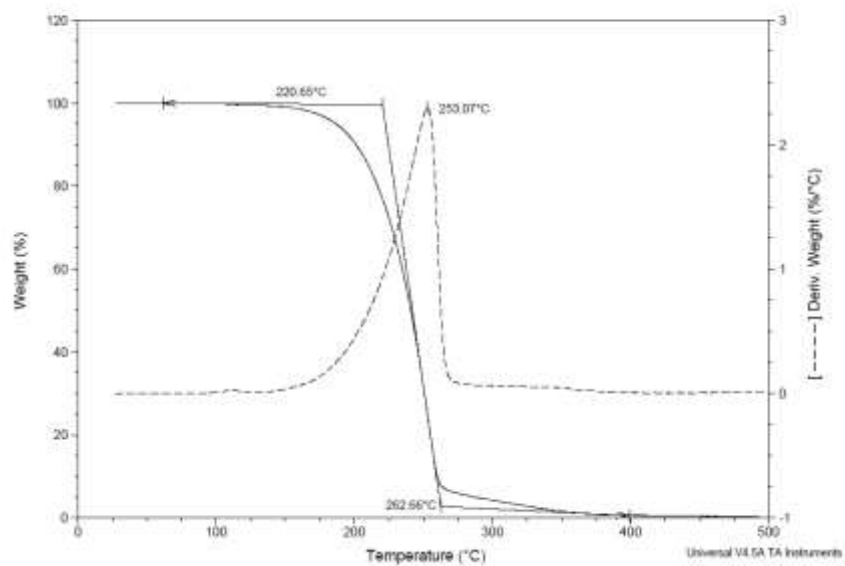
Figure A.42: TGA Thermogram of *trans-syn-trans*-dicyclohexano-18-crown-6
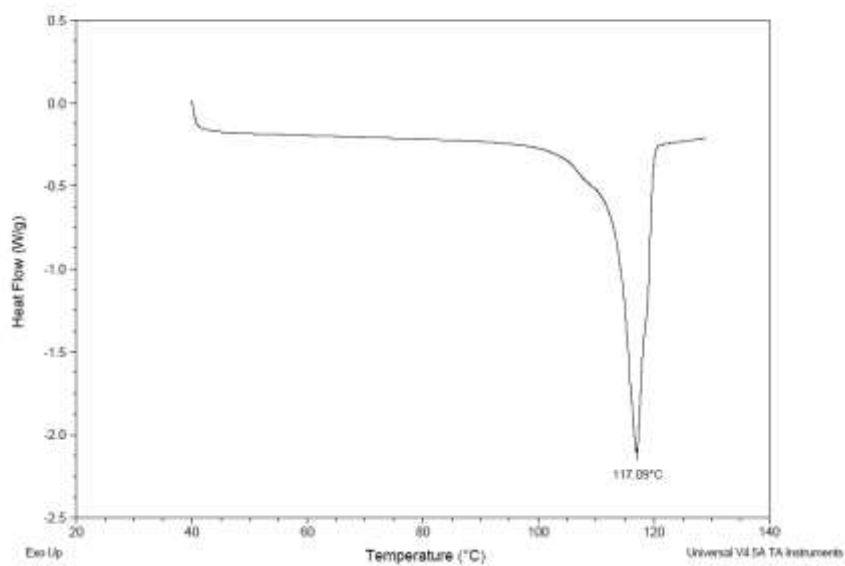
Figure A.43: DSC Thermogram of *trans-syn-trans*-dicyclohexanp-18-crown-6
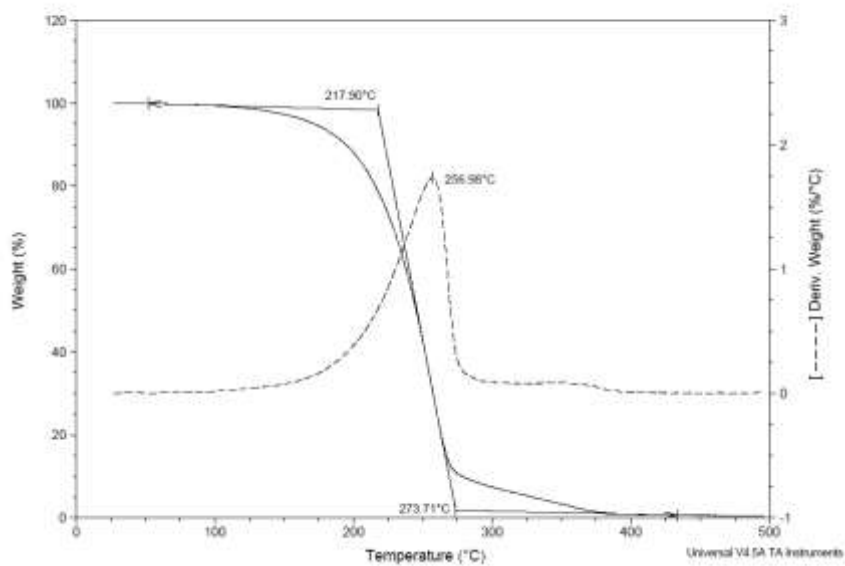
Figure A.44: TGA Thermogram of *trans-anti-trans*-dicyclohexano-18-crown-6
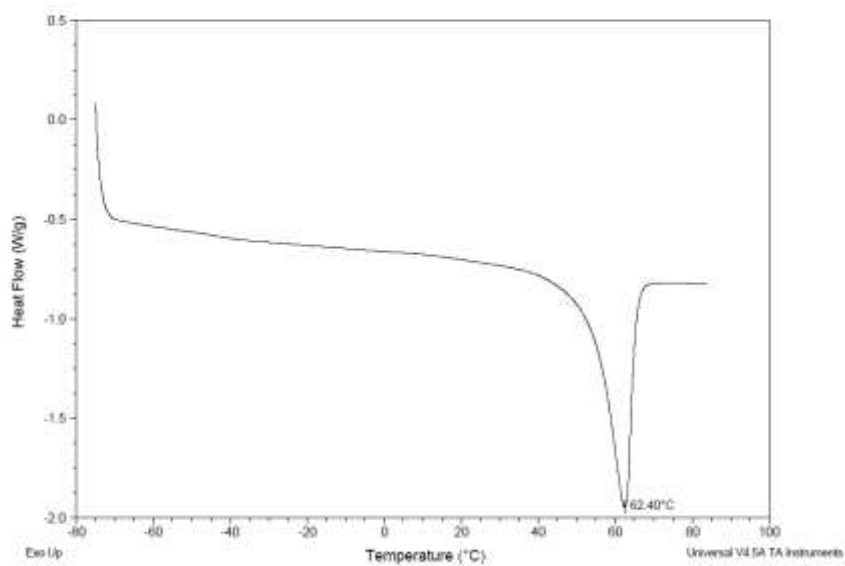
Figure A.45: DSC Thermogram of *trans-anti-trans*-dicyclohexano-18-crown-6
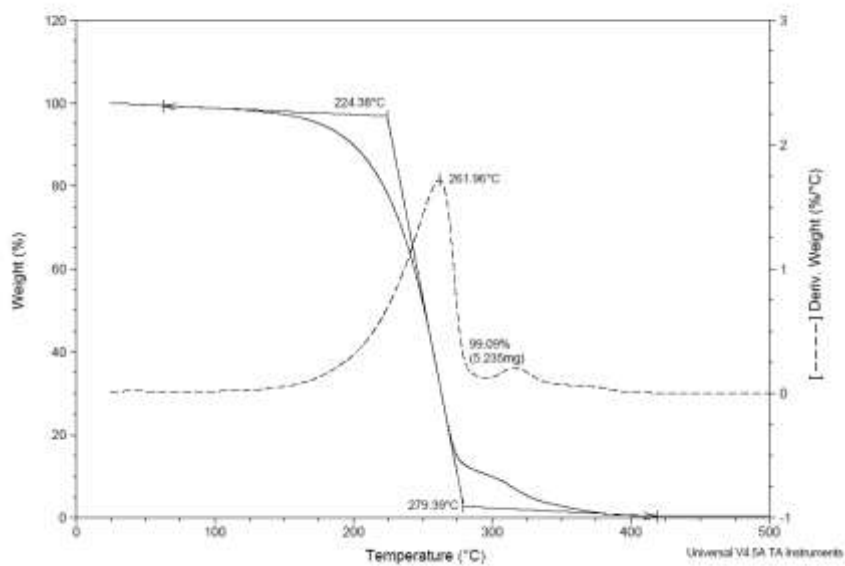
Figure A.46: TGA Thermogram of *cis-trans*-dicyclohexano-18-crown-6
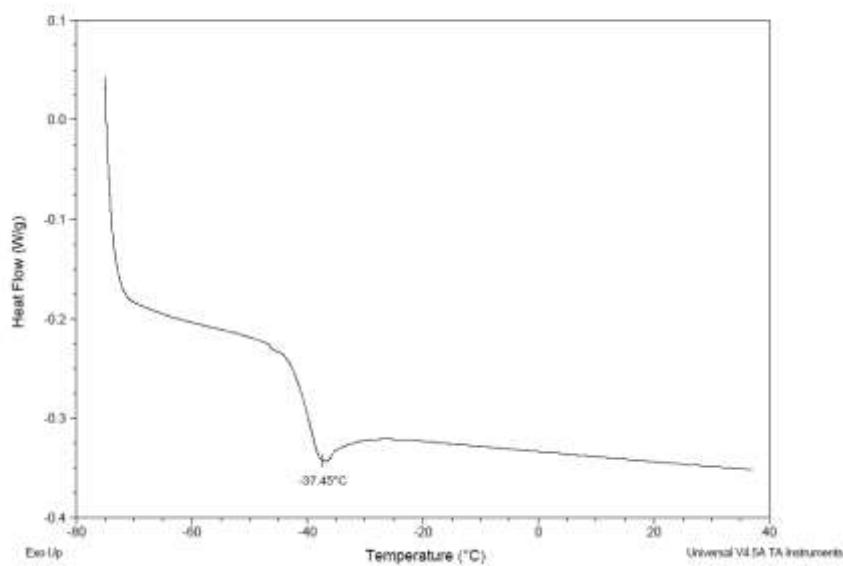
Figure A.47: DSC Thermogram of *cis-trans*-dicyclohexano-18-crown-6
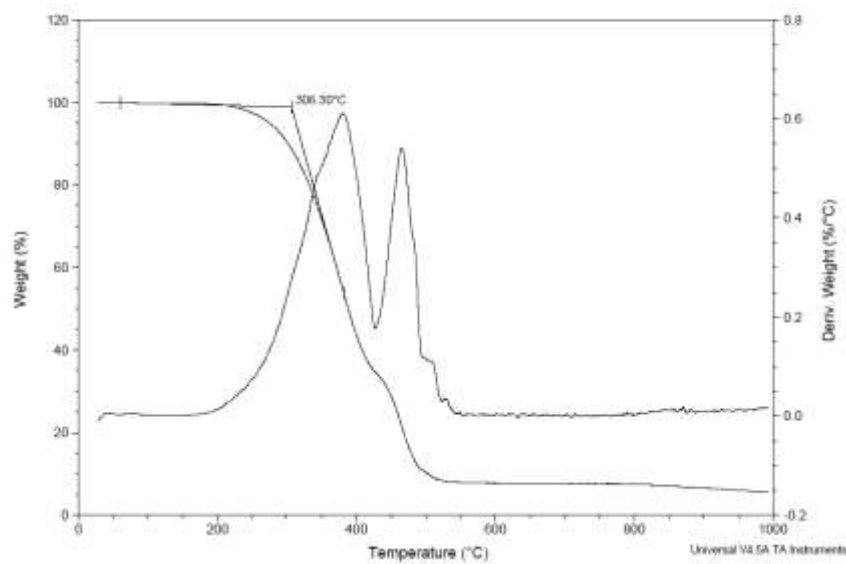
Figure A.48: TGA Thermogram of potassium *cis-syn-cis*-dicyclohexano-18-crown-6
bis(trifluroromethylsulfonyl)imide
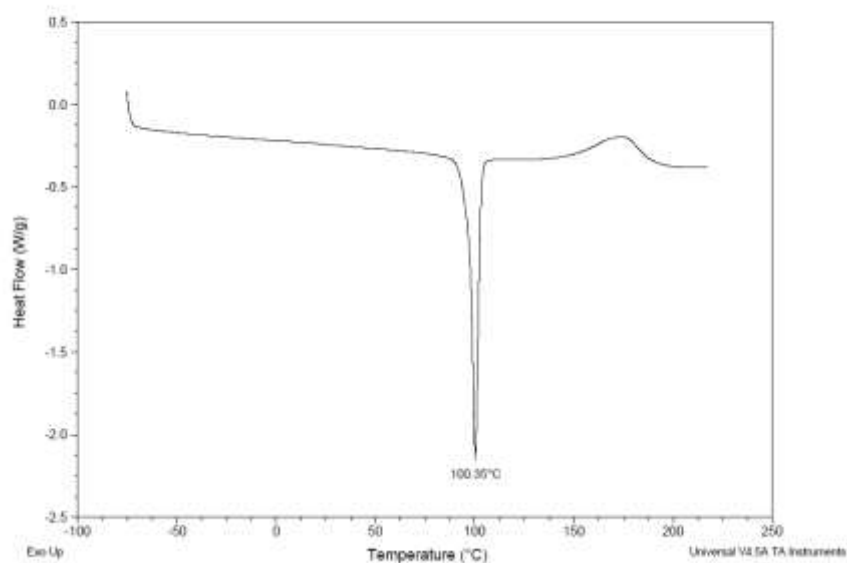
Figure A.49: DSC Thermogram of potassium *cis-syn-cis*-dicyclohexano-18-crown-6
bis(trifluroromethylsulfonyl)imide
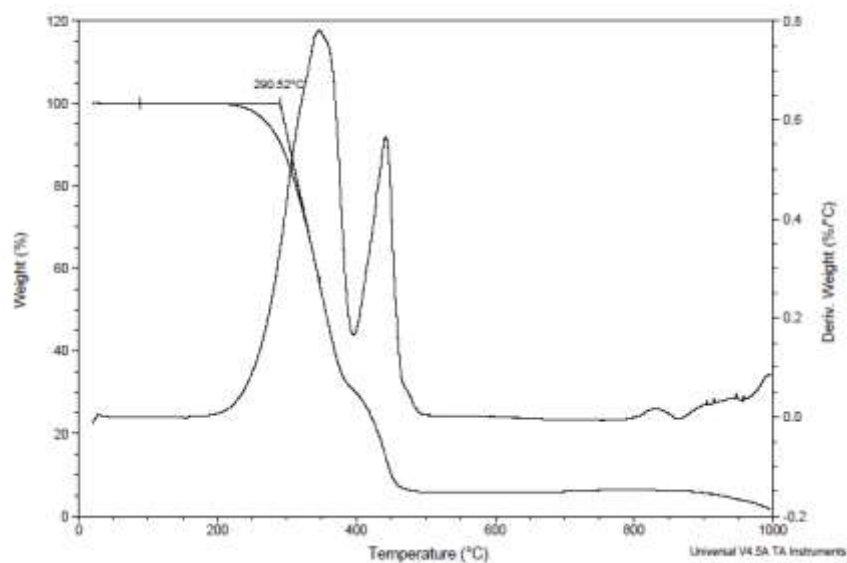
Figure A.50: TGA Thermogram of potassium *cis-anti-cis*-dicyclohexano-18-crown-6
bis(trifluroromethylsulfonyl)imide
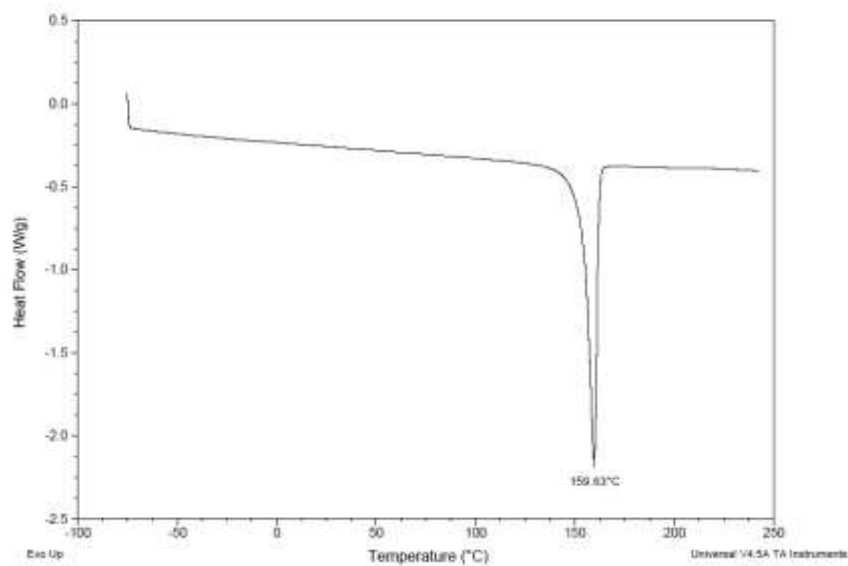
Figure A.51: DSC Thermogram of potassium *cis-anti-cis*-dicyclohexano-18-crown-6
bis(trifluroromethylsulfonyl)imide
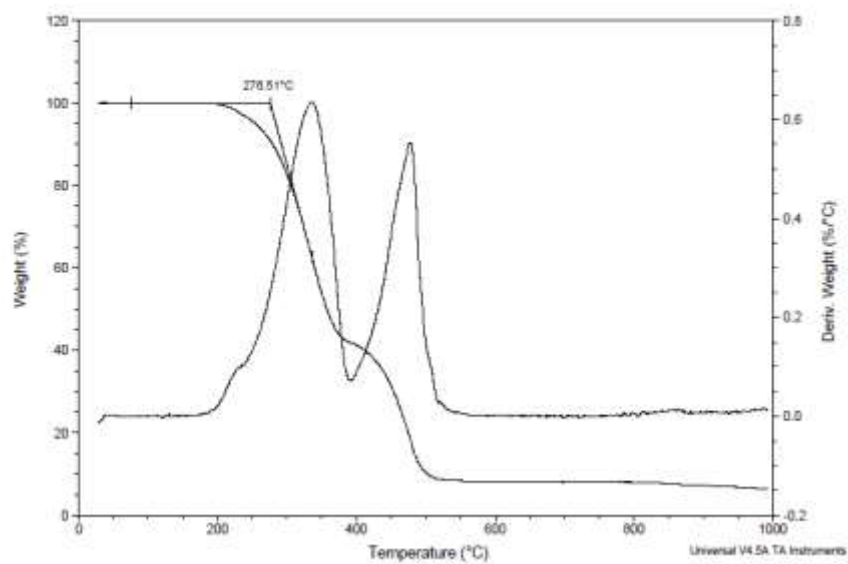
Figure A.52: TGA Thermogram of potassium *trans-syn-trans*-dicyclohexano-18-crown-6
bis(trifluroromethylsulfonyl)imide
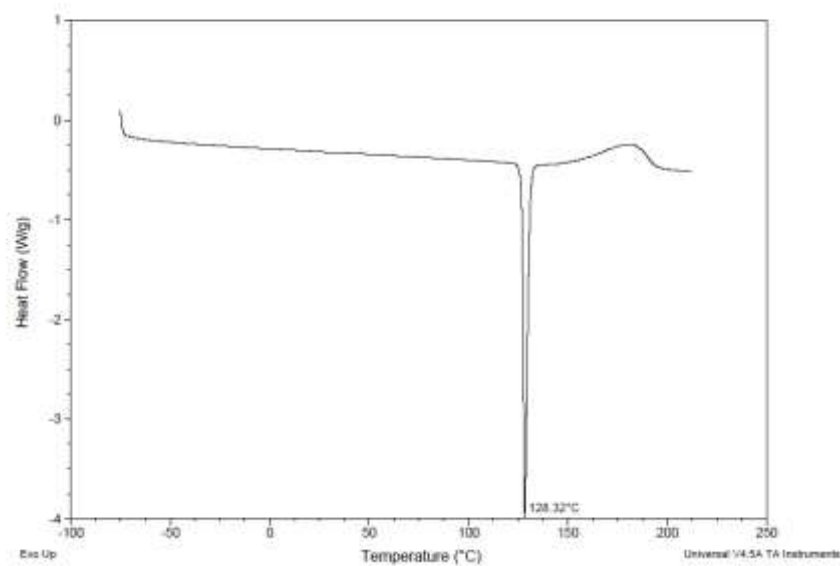
Figure A.53: DSC Thermogram of potassium *trans-syn-trans*-dicyclohexano-18-crown-6 *bis*(trifluroromethylsulfonyl)imide
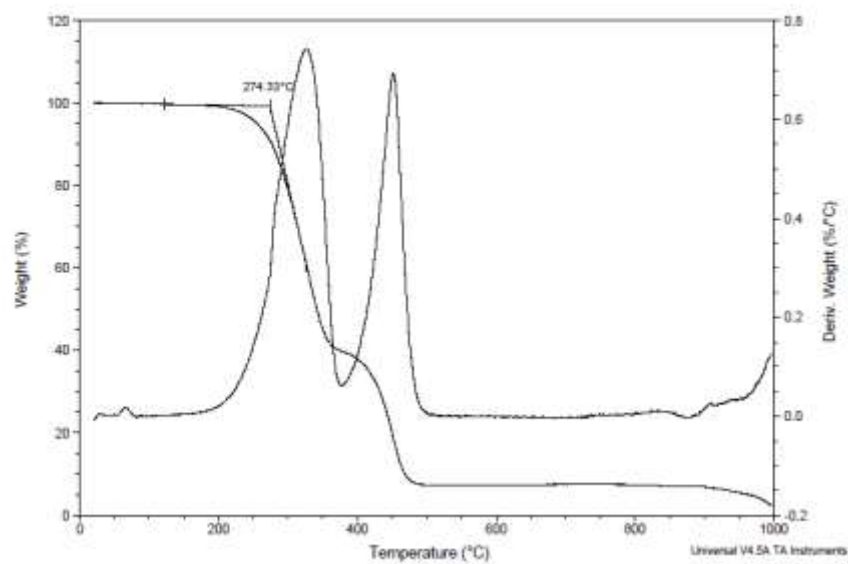
Figure A.54: TGA Thermogram of potassium *trans-anti-trans*-dicyclohexano-18-crown-6 *bis*(trifluroromethylsulfonyl)imide
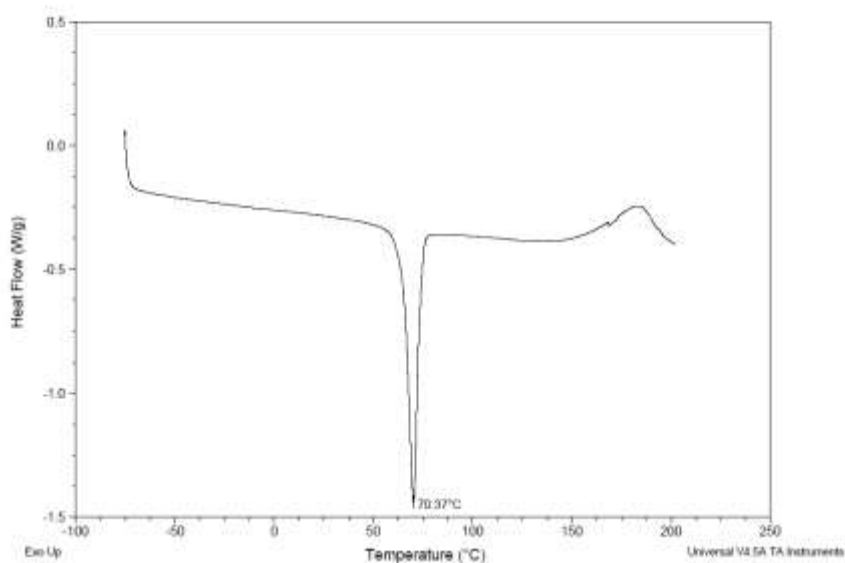
Figure A.55: DSC Thermogram of potassium trans-anti-trans-dicyclohexano-18-crown-6
bis(trifluoromethylsulfonyl)imide
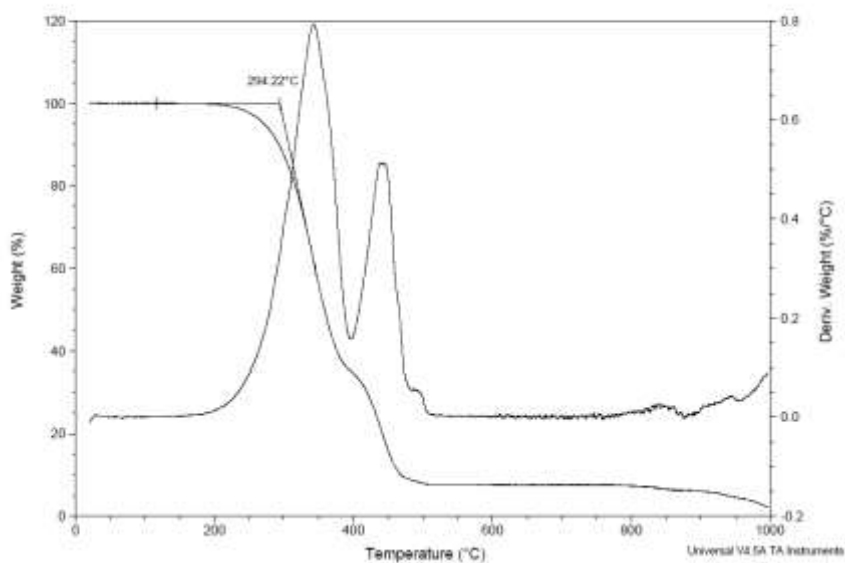
Figure A.56: TGA Thermogram of potassium *cis-trans*-dicyclohexano-18-crown-6
bis(trifluoromethylsulfonyl)imide
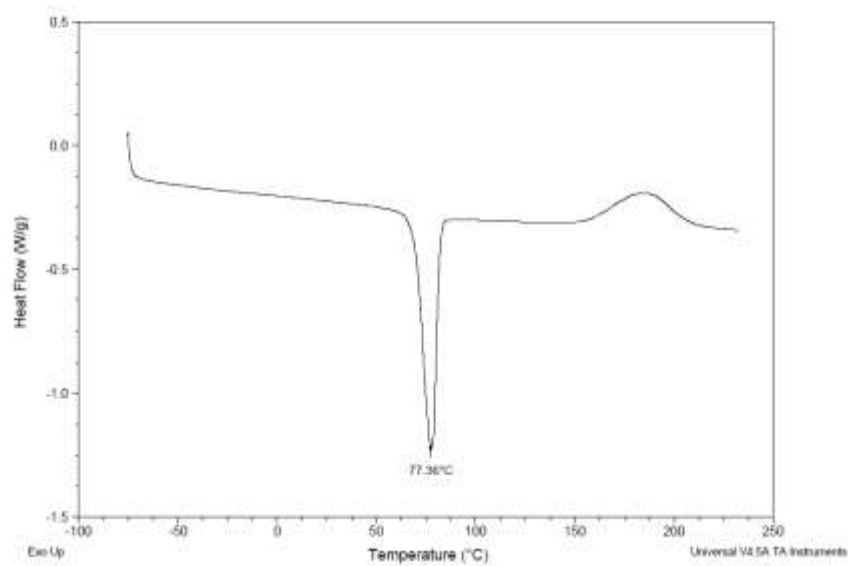
Figure A.57: DSC Thermogram of potassium *cis-trans*-dicyclohexano-18-crown-6
bis(trifluroromethylsulfonyl)imide
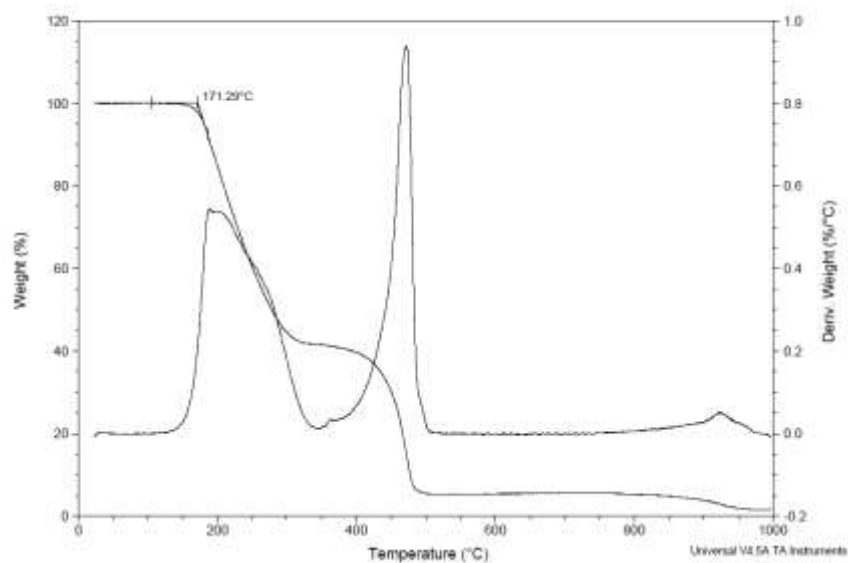
Figure A.58: TGA Thermogram of potassium 15-crown-5
bis(trifluroromethylsulfonyl)imide
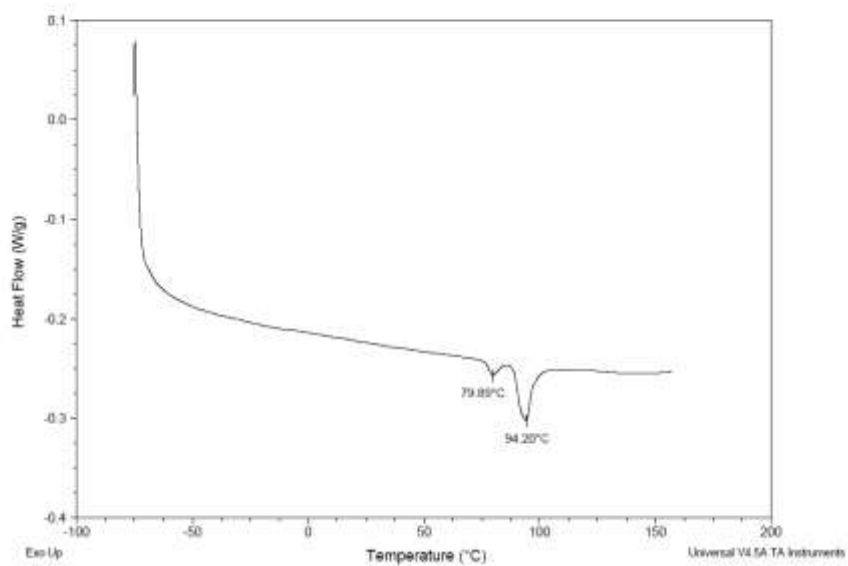
Figure A.59: DSC Thermogram of potassium 15-crown-5
bis(trifluromethylsulfonyl)imide
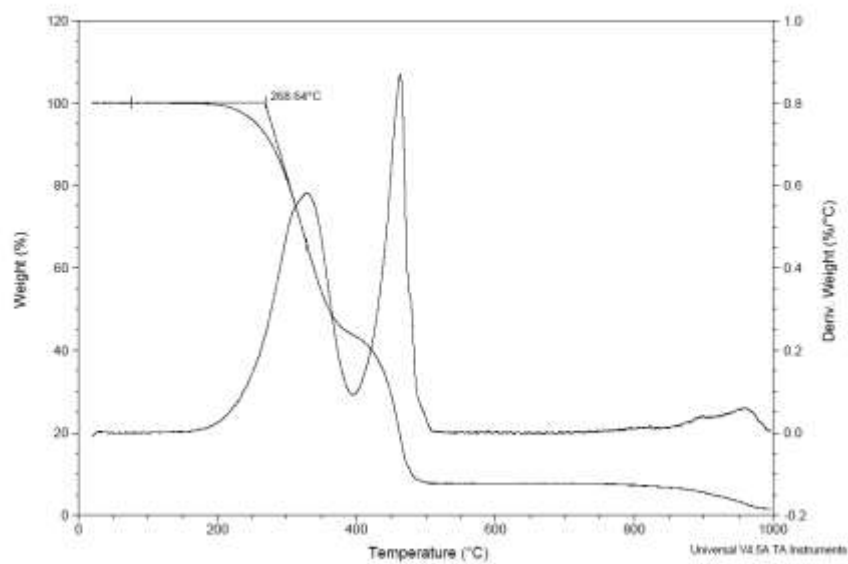
Figure A.60: TGA Thermogram of potassium 18-crown-6
bis(trifluromethylsulfonyl)imide
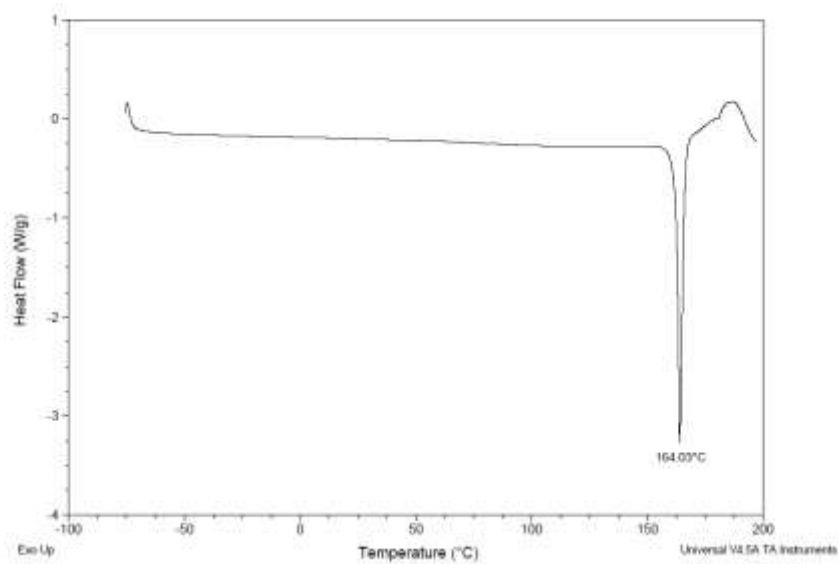
Figure A.61: DSC Thermogram of potassium 18-crown-6
bis(trifluroromethylsulfonyl)imide
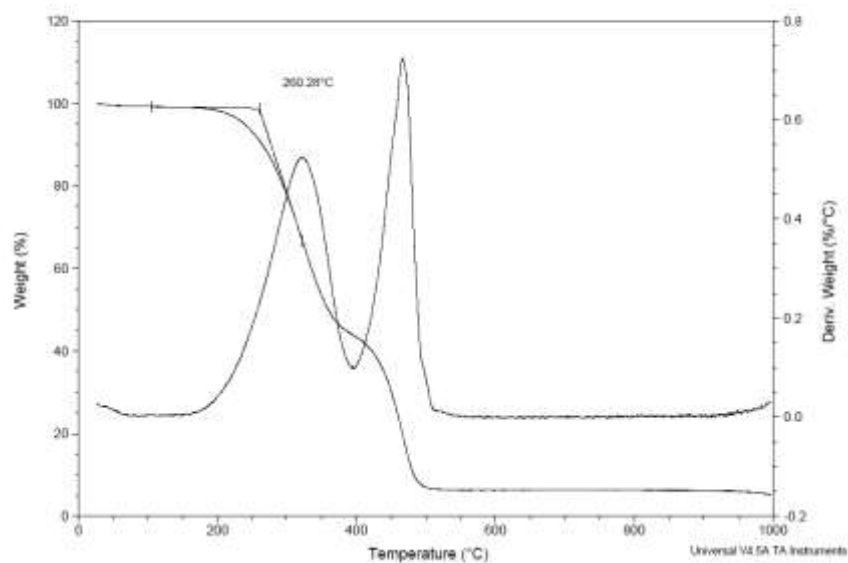
Figure A.62: TGA Thermogram of potassium 21-crown-7
bis(trifluroromethylsulfonyl)imide
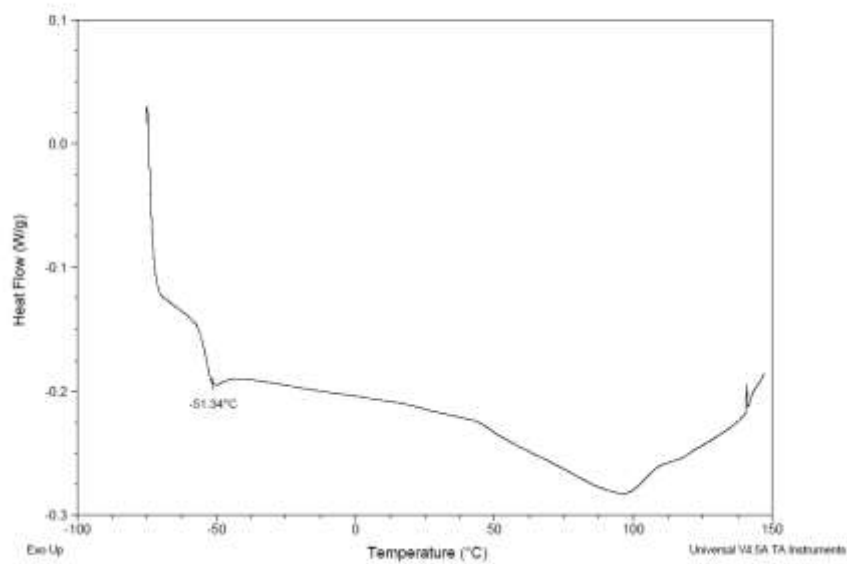
Figure A.63: DSC Thermogram of potassium 21-crown-7
bis(trifluroromethylsulfonyl)imide
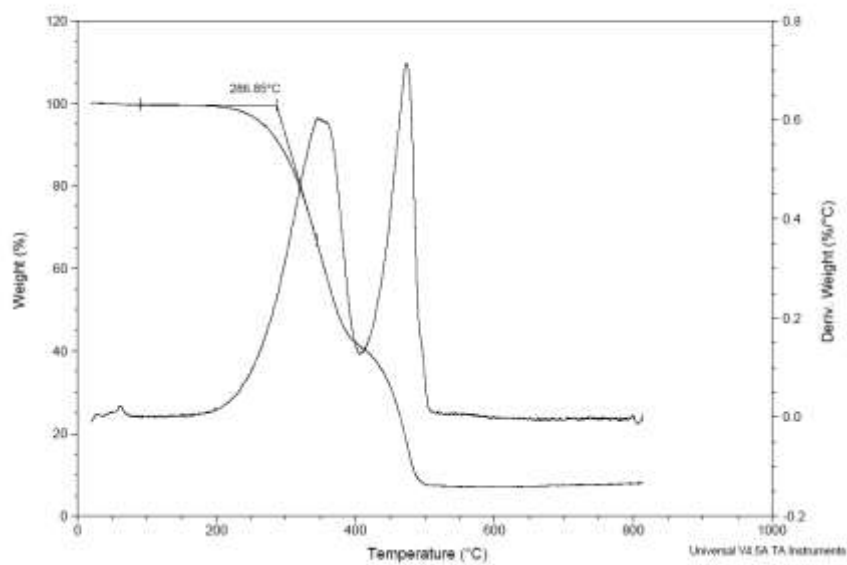
Figure A.64: TGA Thermogram of potassium benzo-18-crown-6
bis(trifluroromethylsulfonyl)imide
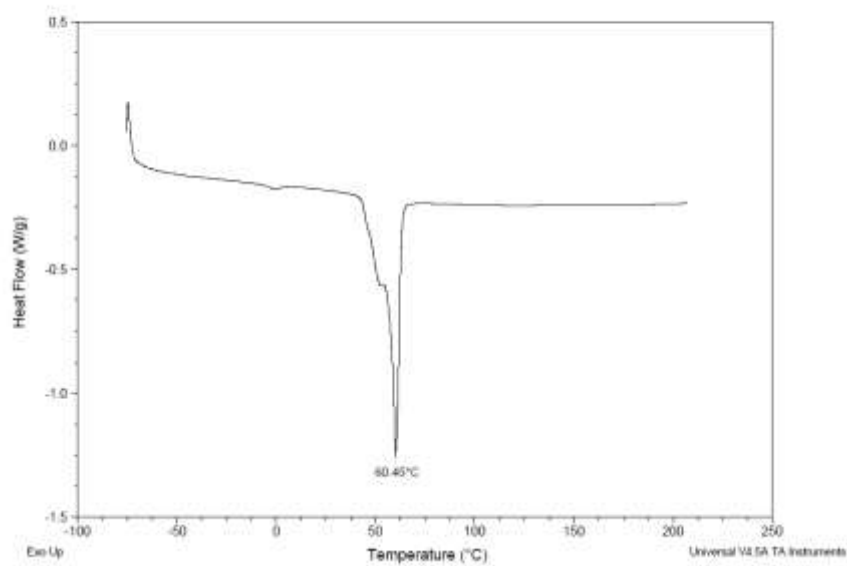
Figure A.65: DSC Thermogram of potassium benzo-18-crown-6
bis(trifluroromethylsulfonyl)imide
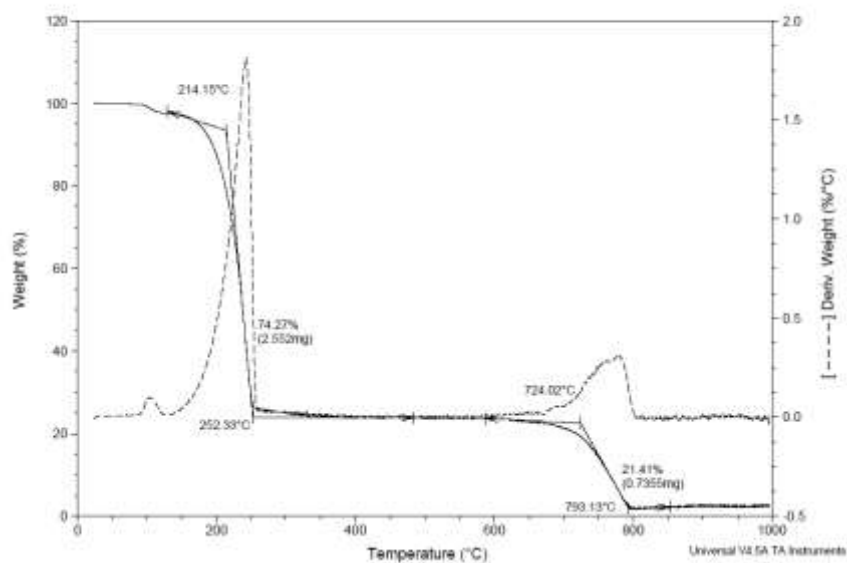
Figure A.66: TGA Thermogram of potassium *cis-anti-cis*-dicyclohexano-18-crown-6
bromide
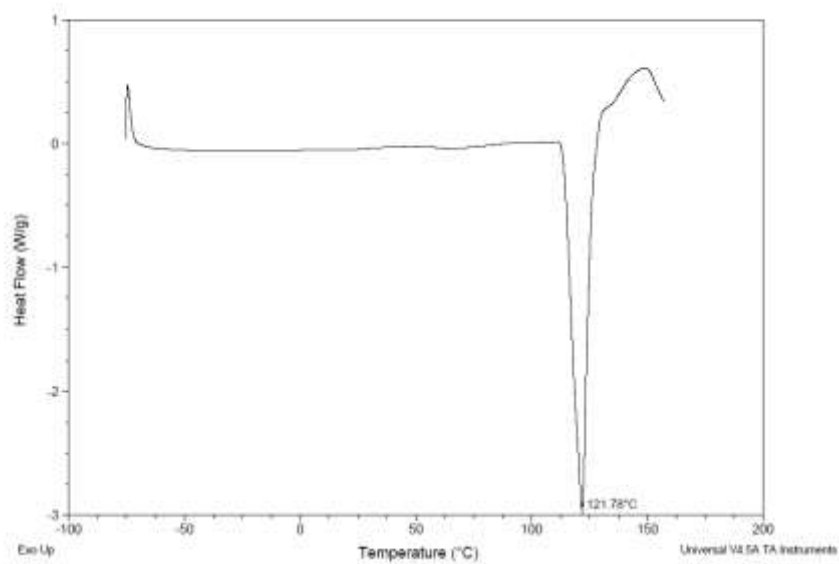
Figure A.67: DSC Thermogram of potassium *cis-anti-cis*-dicyclohexano-18-crown-6 bromide

APPENDIX B

CRYSTALLOGRAPHIC DATA FOR POTASSIUM *CIS-ANTI-CIS*-DICYCLOHEXANO-18-CROWN-6 *BIS*(TRIFLUOROMETHYLSULFONYL)IMIDE
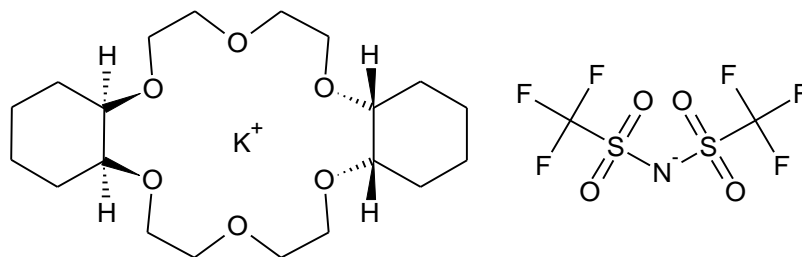
Colorless prisms. The experiment was done with Oxford SuperNova diffractometer using Cu(Kα) radiation at 100K.

Table B-1 Crystal Data

Empirical formula	$C_{22}H_{36}F_6KNO_{10}S_2$
Formula weight	691.74
Temperature/K	100.00(10)
Crystal system	triclinic
Space group	P-1
a/Å	9.2968(2)
b/Å	9.5458(2)
c/Å	17.0459(4)
α/°	90.323(2)
β/°	97.993(2)
γ/°	93.332(2)
Volume/Å^3	1495.38(6)
Z	2
ρ_{calc}mg/mm^3	1.536
m/mm^{-1}	0.407
F(000)	720.0
Crystal size/mm^3	$0.4451 \times 0.4061 \times 0.3394$
2Θ range for data collection	5.98 to 58.24°
Index ranges	$-12 \leq h \leq 12, -12 \leq k \leq 12, -23 \leq l \leq 22$
Reflections collected	35480

Independent reflections	7371[R(int) = 0.0320]
Data/restraints/parameters	7371/0/416
Goodness-of-fit on F^2	1.031
Final R indexes [I>=2σ (I)]	$R_1 = 0.0330$, $wR_2 = 0.0793$
Final R indexes [all data]	$R_1 = 0.0419$, $wR_2 = 0.0858$
Largest diff. peak/hole / e Å^{-3}	0.49/-0.49

Table B-2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for crystal. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	x	y	z	U(eq)
K1	5000	5000	0	18.37(10)
K2	5000	0	5000	15.84(9)
S1	4333.8(4)	2865.9(4)	1768.62(19)	19.56(9)
S2	5867.2(4)	2295.9(4)	3244.27(19)	18.58(8)
F1	2146.0(11)	2410.5(13)	2558.2(6)	35.7(3)
F2	2390.3(12)	778.4(13)	1734.3(9)	47.6(3)
F3	1557.3(11)	2729.2(16)	1321.4(7)	47.1(3)
F4	7575.6(12)	4369.8(12)	2821.9(6)	30.0(3)
F5	8524.2(11)	2377.5(12)	2840.3(7)	33.6(3)
F6	8352.3(10)	3439.4(12)	3934.6(5)	29.1(2)
O4	4515.0(13)	2521.8(16)	970.5(7)	35.8(3)
O5	4356.6(13)	4326.3(13)	1977.0(8)	32.9(3)
O6	6205.3(14)	1024.1(13)	3650.8(7)	32.3(3)
O7	5119.8(13)	3314.2(14)	3605.5(7)	29.5(3)
N1	5337.9(13)	1924.6(13)	2343.9(7)	17.6(3)
C11	2495.4(15)	2129.6(17)	1852.4(9)	24.6(3)
C12	7671.6(15)	3154.7(15)	3196.8(8)	20.6(3)
F1X	2418(11)	775(11)	2212(7)	30.0(3)
F2X	1453(10)	2722(11)	2138(6)	33.6(3)
F3X	1719(10)	1589(11)	1082(5)	29.1(2)
F4X	7859(12)	2640(12)	2461(6)	35.7(3)
F5X	7590(14)	4389(15)	3180(9)	47.6(3)
F6X	8454(10)	2460(16)	3697(7)	47.1(3)
O4X	3808(13)	4060(12)	1367(7)	32.3(3)
O5X	4924(12)	1725(13)	1428(7)	29.5(3)
O6X	5538(12)	2705(15)	4070(7)	35.8(3)

O7X	5660(13)	796(12)	3107(8)	32.9(3)
N1X	4655(12)	3186(12)	2681(7)	17.6(3)
O1	5810.5(10)	7468.4(10)	1002.8(5)	16.66(19)
O2	7551.8(9)	5214.7(9)	996.2(5)	15.56(19)
O3	2910.7(10)	6951.2(10)	148.4(5)	18.3(2)
C1	6896.0(15)	7240.2(14)	1667.9(7)	16.6(3)
C2	8121.9(14)	6535.7(13)	1342.1(8)	16.3(3)
C3	8811.5(16)	7476.2(15)	756.7(8)	21.3(3)
C4	9388.4(17)	8881.1(15)	1153.3(9)	27.2(3)
C5	8211.9(17)	9590.2(15)	1522.0(9)	26.5(3)
C6	7516.6(17)	8613.5(15)	2089.2(8)	22.8(3)
C7	8659.1(14)	4295.7(14)	878.9(9)	20.6(3)
C8	7953.4(14)	2892.5(14)	600.4(8)	17.7(3)
C9	3516.2(15)	8275.7(14)	464.4(9)	22.3(3)
C10	4538.0(16)	8057.3(16)	1211.9(9)	24.2(3)
O1A	5963(1)	2350(1)	6048.6(5)	16.79(19)
O2A	7577.3(9)	2.7(9)	6007.2(5)	14.95(19)
O3A	3046.7(10)	2049.4(9)	5197.7(5)	17.9(2)
C1A	7041.2(14)	2049.6(14)	6703.9(7)	16.3(3)
C2A	8218.6(14)	1293.2(13)	6365.7(8)	15.7(3)
C3A	8936.7(16)	2220.4(14)	5785.2(8)	20.9(3)
C4A	9573.2(17)	3607.6(15)	6182.9(10)	26.3(3)
C5A	8445.1(17)	4355.8(15)	6573.0(9)	26.0(3)
C6A	7737.8(16)	3387.3(15)	7136.6(8)	21.9(3)
C7A	8633.0(14)	-926.2(14)	5821.8(8)	18.9(3)
C8A	7867.1(14)	-2298.3(13)	5523.0(8)	16.7(3)
C9A	3727.2(16)	3321.6(14)	5545.1(9)	22.9(3)
C10A	4732.8(16)	2993.2(16)	6279.7(9)	23.9(3)

Table B-3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for crystal. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+...+2hka \times b \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
K1	19.2(2)	14.19(19)	20.6(2)	-2.88(15)	-2.66(15)	4.91(15)
K2	17.29(19)	13.78(19)	16.52(19)	-1.65(14)	1.28(14)	4.13(14)
S1	17.22(16)	26.53(19)	15.33(16)	4.05(13)	2.07(12)	4.77(13)
S2	19.93(16)	21.05(18)	13.93(16)	3.10(12)	1.02(12)	-2.88(13)

F1	25.8(5)	57.7(7)	25.0(5)	-7.0(5)	12.1(4)	-4.8(5)
F2	26.0(6)	37.8(7)	76.7(10)	-25.4(7)	4.8(6)	-10.7(5)
F3	16.6(5)	89.5(10)	35.3(6)	14.0(6)	-1.8(4)	15.1(6)
F4	26.5(5)	28.0(6)	32.8(6)	14.7(5)	-2.5(5)	-8.1(4)
F5	17.1(5)	45.4(7)	38.8(6)	-9.3(5)	4.6(4)	5.6(4)
F6	26.9(5)	38.8(6)	17.3(5)	2.1(4)	-6.2(4)	-11.6(4)
O4	22.7(6)	71.1(10)	14.9(6)	3.3(6)	4.4(5)	9.9(6)
O5	28.8(6)	22.2(6)	47.2(8)	10.6(5)	2.2(6)	4.1(5)
O6	34.8(7)	29.3(7)	28.9(7)	16.3(5)	-5.6(5)	-10.2(5)
O7	22.9(6)	42.8(8)	24.1(6)	-10.2(5)	10.0(5)	-2.8(5)
N1	15.6(6)	19.2(6)	17.4(6)	-2.3(5)	-0.7(5)	2.6(5)
C11	17.4(7)	36.7(9)	20.4(7)	-0.7(6)	3.1(5)	6.4(6)
C12	19.0(6)	25.1(7)	17.6(7)	3.4(5)	1.8(5)	1.0(5)
F1X	26.5(5)	28.0(6)	32.8(6)	14.7(5)	-2.5(5)	-8.1(4)
F2X	17.1(5)	45.4(7)	38.8(6)	-9.3(5)	4.6(4)	5.6(4)
F3X	26.9(5)	38.8(6)	17.3(5)	2.1(4)	-6.2(4)	-11.6(4)
F4X	25.8(5)	57.7(7)	25.0(5)	-7.0(5)	12.1(4)	-4.8(5)
F5X	26.0(6)	37.8(7)	76.7(10)	-25.4(7)	4.8(6)	-10.7(5)
F6X	16.6(5)	89.5(10)	35.3(6)	14.0(6)	-1.8(4)	15.1(6)
O4X	34.8(7)	29.3(7)	28.9(7)	16.3(5)	-5.6(5)	-10.2(5)
O5X	22.9(6)	42.8(8)	24.1(6)	-10.2(5)	10.0(5)	-2.8(5)
O6X	22.7(6)	71.1(10)	14.9(6)	3.3(6)	4.4(5)	9.9(6)
O7X	28.8(6)	22.2(6)	47.2(8)	10.6(5)	2.2(6)	4.1(5)
N1X	15.6(6)	19.2(6)	17.4(6)	-2.3(5)	-0.7(5)	2.6(5)
O1	19.9(5)	17.0(5)	13.3(4)	-1.0(3)	1.5(4)	5.2(4)
O2	14.8(4)	12.4(4)	19.3(5)	-1.8(3)	1.5(3)	1.6(3)
O3	22.1(5)	14.3(5)	18.7(5)	0.0(4)	2.3(4)	3.0(4)
C1	23.2(7)	14.1(6)	12.3(6)	0.4(5)	1.1(5)	1.5(5)
C2	20.1(6)	12.6(6)	15.2(6)	-0.1(5)	-0.3(5)	-1.6(5)
C3	24.2(7)	18.6(7)	21.4(7)	1.6(5)	5.7(5)	-3.1(5)
C4	31.7(8)	18.5(7)	29.4(8)	3.4(6)	0.6(6)	-8.1(6)
C5	38.2(9)	13.3(7)	25.2(7)	-1.0(5)	-2.8(6)	-4.0(6)
C6	33.0(8)	17.4(7)	16.5(7)	-3.3(5)	-1.5(6)	1.7(6)
C7	15.2(6)	17.7(7)	29.3(7)	-2.0(6)	3.9(5)	2.3(5)
C8	16.2(6)	15.5(6)	21.8(7)	0.2(5)	2.5(5)	4.5(5)
C9	23.3(7)	15.8(7)	27.6(7)	-6.2(5)	0.2(6)	7.0(5)
C10	25.0(7)	25.6(8)	22.9(7)	-8.6(6)	3.7(6)	8.2(6)

O1A	18.5(4)	17.4(5)	14.9(4)	-1.8(4)	2.7(4)	4.0(4)
O2A	14.0(4)	12.6(4)	18.6(5)	-1.6(3)	3.0(3)	1.5(3)
O3A	21.6(5)	12.9(4)	19.0(5)	-0.7(4)	1.5(4)	2.8(4)
C1A	20.4(6)	16.6(6)	12.1(6)	0.2(5)	3.0(5)	1.4(5)
C2A	18.2(6)	14.2(6)	14.3(6)	-1.3(5)	1.3(5)	-0.4(5)
C3A	24.1(7)	17.2(7)	22.5(7)	-0.3(5)	8.8(5)	-2.8(5)
C4A	27.4(8)	17.9(7)	33.4(8)	-0.7(6)	6.3(6)	-6.0(6)
C5A	30.1(8)	14.9(7)	31.8(8)	-4.6(6)	2.6(6)	-3.5(6)
C6A	27.0(7)	19.8(7)	18.2(7)	-5.2(5)	0.2(5)	2.4(6)
C7A	14.8(6)	16.6(7)	26.3(7)	-1.3(5)	5.5(5)	3.2(5)
C8A	16.1(6)	13.8(6)	21.2(7)	2.0(5)	4.2(5)	4.6(5)
C9A	23.2(7)	13.9(7)	31.3(8)	-6.5(6)	1.5(6)	5.3(5)
C10A	23.4(7)	24.4(7)	24.4(7)	-10.1(6)	3.6(6)	7.5(6)

Table B-4 Bond Lengths for crystal.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
K1	O4	2.9435(14)	F4	C12	1.3290(18)
K1	O4[1]	2.9436(14)	F5	C12	1.3210(17)
K1	O4X	2.845(12)	F6	C12	1.3458(16)
K1	O4X[1]	2.845(12)	C11	F1X	1.436(10)
K1	O1	2.9038(9)	C11	F2X	1.299(9)
K1	O1[1]	2.9038(9)	C11	F3X	1.482(8)
K1	O2	2.7153(9)	C12	F4X	1.381(10)
K1	O2[1]	2.7152(9)	C12	F5X	1.185(15)
K1	O3[1]	2.8033(9)	C12	F6X	1.259(11)
K1	O3	2.8032(9)	O1	C1	1.4358(15)
K1	C8	3.5380(13)	O1	C10	1.4265(16)
K1	C8[1]	3.5380(13)	O2	C2	1.4303(15)
K2	O6	2.8487(12)	O2	C7	1.4246(16)
K2	O6[2]	2.8487(12)	O3	C8[1]	1.4241(16)
K2	O6X[2]	3.090(14)	O3	C9	1.4251(16)
K2	O6X	3.090(14)	C1	C2	1.5232(18)
K2	O1A	2.8819(9)	C1	C6	1.5340(18)
K2	O1A[2]	2.8819(9)	C2	C3	1.5277(19)
K2	O2A[2]	2.7466(9)	C3	C4	1.5325(19)
K2	O2A	2.7466(9)	C4	C5	1.524(2)

Atom	Atom	Length/Å	Atom	Atom	Length/Å
K2	O3A²	2.7954(9)	C5	C6	1.528(2)
K2	O3A	2.7954(9)	C7	C8	1.5013(18)
S1	O4	1.4325(12)	C8	O3¹	1.4240(16)
S1	O5	1.4349(13)	C9	C10	1.503(2)
S1	N1	1.5790(13)	O1A	C1A	1.4353(15)
S1	C11	1.8343(15)	O1A	C10A	1.4298(16)
S1	O4X	1.409(11)	O2A	C2A	1.4322(15)
S1	O5X	1.405(11)	O2A	C7A	1.4261(15)
S1	N1X	1.568(11)	O3A	C8A²	1.4226(16)
S2	O6	1.4304(12)	O3A	C9A	1.4227(16)
S2	O7	1.4134(12)	C1A	C2A	1.5214(18)
S2	N1	1.5770(12)	C1A	C6A	1.5344(18)
S2	C12	1.8361(14)	C2A	C3A	1.5274(19)
S2	O6X	1.534(11)	C3A	C4A	1.5331(19)
S2	O7X	1.447(12)	C4A	C5A	1.526(2)
S2	N1X	1.653(11)	C5A	C6A	1.525(2)
F1	C11	1.3192(17)	C7A	C8A	1.5051(18)
F2	C11	1.3003(19)	C8A	O3A²	1.4226(16)
F3	C11	1.3235(18)	C9A	C10A	1.501(2)

¹1-X,1-Y,-Z; ²1-X,-Y,1-Z

Table B-5 Bond Angles for crystal.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O4	K1	O4¹	180.00(5)	O4X	S1	N1X	109.8(7)
O4¹	K1	C8¹	61.28(3)	O5X	S1	K1	88.8(5)
O4	K1	C8¹	118.72(3)	O5X	S1	O4	47.2(5)
O4¹	K1	C8	118.72(3)	O5X	S1	O5	151.6(5)
O4	K1	C8	61.28(3)	O5X	S1	N1	62.8(5)
O4X¹	K1	O4	143.6(3)	O5X	S1	C11	101.0(4)
O4X	K1	O4¹	143.6(3)	O5X	S1	O4X	126.1(7)
O4X	K1	O4	36.4(3)	O5X	S1	N1X	121.4(6)
O4X¹	K1	O4¹	36.4(3)	N1X	S1	K1	132.2(4)
O4X	K1	O4X¹	180.000(1)	N1X	S1	N1	58.5(4)
O4X¹	K1	O1¹	81.5(2)	N1X	S1	C11	91.8(4)
O4X	K1	O1¹	98.5(2)	O6	S2	N1	108.37(7)
O4X	K1	O1	81.5(2)	O6	S2	C12	102.82(7)
O4X¹	K1	O1	98.5(2)	O6	S2	O6X	80.8(5)

O4X	K1	C8[1]	92.6(2)	O6	S2	O7X	41.0(5)
O4X[1]	K1	C8	92.6(2)	O6	S2	N1X	148.0(4)
O4X	K1	C8	87.4(2)	O7	S2	O6	119.59(8)
O4X[1]	K1	C8[1]	87.4(2)	O7	S2	N1	117.54(7)
O1[1]	K1	O4[1]	110.45(3)	O7	S2	C12	104.14(7)
O1	K1	O4[1]	69.55(3)	O7	S2	O6X	40.7(5)
O1	K1	O4	110.45(3)	O7	S2	O7X	135.1(5)
O1[1]	K1	O4	69.55(3)	O7	S2	N1X	61.3(4)
O1	K1	O1[1]	180.0	N1	S2	C12	101.44(7)
O1	K1	C8	101.02(3)	N1	S2	N1X	56.8(4)
O1[1]	K1	C8[1]	101.02(3)	O6X	S2	N1	150.5(4)
O1	K1	C8[1]	78.98(3)	O6X	S2	C12	103.7(5)
O1[1]	K1	C8	78.98(3)	O6X	S2	N1X	100.4(6)
O2	K1	O4	81.60(3)	O7X	S2	N1	68.2(5)
O2[1]	K1	O4	98.40(3)	O7X	S2	C12	118.7(5)
O2[1]	K1	O4[1]	81.60(3)	O7X	S2	O6X	111.4(8)
O2	K1	O4[1]	98.40(3)	O7X	S2	N1X	112.9(6)
O2	K1	O4X	84.2(2)	N1X	S2	C12	107.8(4)
O2[1]	K1	O4X[1]	84.2(2)	S1	O4	K1	113.39(8)
O2	K1	O4X[1]	95.8(2)	S2	O6	K2	125.98(8)
O2[1]	K1	O4X	95.8(2)	S2	N1	S1	123.99(8)
O2[1]	K1	O1[1]	58.90(3)	F1	C11	S1	110.54(10)
O2	K1	O1[1]	121.10(3)	F1	C11	F3	107.51(12)
O2	K1	O1	58.90(3)	F1	C11	F1X	76.6(5)
O2[1]	K1	O1	121.10(3)	F1	C11	F3X	136.4(4)
O2[1]	K1	O2	180.0	F2	C11	S1	111.32(10)
O2[1]	K1	O3[1]	118.86(3)	F2	C11	F1	109.15(14)
O2[1]	K1	O3	61.14(3)	F2	C11	F3	109.54(14)
O2	K1	O3[1]	61.14(3)	F2	C11	F1X	34.0(5)
O2	K1	O3	118.86(3)	F2	C11	F3X	62.3(4)
O2	K1	C8[1]	137.80(3)	F3	C11	S1	108.70(11)
O2[1]	K1	C8	137.80(3)	F3	C11	F1X	130.7(4)
O2	K1	C8	42.20(3)	F3	C11	F3X	49.6(4)
O2[1]	K1	C8[1]	42.20(3)	F1X	C11	S1	115.6(4)
O3[1]	K1	O4[1]	110.44(3)	F1X	C11	F3X	92.7(6)
O3	K1	O4[1]	69.56(3)	F2X	C11	S1	128.4(5)
O3[1]	K1	O4	69.56(3)	F2X	C11	F1	42.8(5)

O3	K1	O4	110.44(3)	F2X	C11	F2	119.0(5)
O3	K1	O4X[1]	102.6(3)	F2X	C11	F3	65.0(5)
O3[1]	K1	O4X	102.6(3)	F2X	C11	F1X	100.6(7)
O3	K1	O4X	77.4(3)	F2X	C11	F3X	100.8(6)
O3[1]	K1	O4X[1]	77.4(3)	F3X	C11	S1	112.2(4)
O3[1]	K1	O1[1]	60.92(3)	F4	C12	S2	111.53(10)
O3	K1	O1[1]	119.08(3)	F4	C12	F6	106.96(12)
O3[1]	K1	O1	119.08(3)	F4	C12	F4X	83.5(5)
O3	K1	O1	60.92(3)	F5	C12	S2	113.27(10)
O3	K1	O3[1]	180.0	F5	C12	F4	107.78(12)
O3[1]	K1	C8[1]	157.67(3)	F5	C12	F6	107.29(12)
O3	K1	C8[1]	22.33(3)	F5	C12	F4X	37.9(5)
O3[1]	K1	C8	22.33(3)	F6	C12	S2	109.73(9)
O3	K1	C8	157.67(3)	F6	C12	F4X	143.8(5)
C8	K1	C8[1]	180.00(3)	F4X	C12	S2	97.5(4)
O6[2]	K2	O6	180.00(3)	F5X	C12	S2	109.8(7)
O6	K2	O6X	37.5(2)	F5X	C12	F4	27.3(7)
O6[2]	K2	O6X	142.5(2)	F5X	C12	F5	128.5(7)
O6[2]	K2	O6X[2]	37.5(2)	F5X	C12	F6	82.7(7)
O6	K2	O6X[2]	142.5(2)	F5X	C12	F4X	110.6(9)
O6[2]	K2	O1A	82.41(3)	F5X	C12	F6X	127.4(10)
O6	K2	O1A	97.59(3)	F6X	C12	S2	101.0(6)
O6	K2	O1A[2]	82.41(3)	F6X	C12	F4	144.6(6)
O6[2]	K2	O1A[2]	97.59(3)	F6X	C12	F5	69.5(6)
O6X[2]	K2	O6X	179.999(1)	F6X	C12	F6	46.5(7)
O1A[2]	K2	O6X[2]	68.4(2)	F6X	C12	F4X	106.2(8)
O1A	K2	O6X[2]	111.6(2)	S1	O4X	K1	119.8(7)
O1A[2]	K2	O6X	111.6(2)	S2	O6X	K2	108.8(7)
O1A	K2	O6X	68.4(2)	S1	N1X	S2	119.8(7)
O1A[2]	K2	O1A	180.0	C1	O1	K1	113.83(7)
O2A[2]	K2	O6	83.33(3)	C10	O1	K1	109.96(7)
O2A	K2	O6	96.67(3)	C10	O1	C1	113.81(10)
O2A[2]	K2	O6[2]	96.67(3)	C2	O2	K1	121.07(7)
O2A	K2	O6[2]	83.33(3)	C7	O2	K1	118.79(7)
O2A	K2	O6X	100.1(2)	C7	O2	C2	112.88(10)
O2A[2]	K2	O6X[2]	100.1(2)	C8[1]	O3	K1	109.24(7)
O2A	K2	O6X[2]	79.9(2)	C8[1]	O3	C9	111.04(10)

O2A²	K2	O6X	79.9(2)	C9	O3	K1	113.57(7)
O2A²	K2	O1A²	59.00(3)	O1	C1	C2	106.55(10)
O2A	K2	O1A²	121.00(3)	O1	C1	C6	112.47(11)
O2A	K2	O1A	59.00(3)	C2	C1	C6	108.71(11)
O2A²	K2	O1A	121.00(3)	O2	C2	C1	108.20(10)
O2A	K2	O2A²	180.0	O2	C2	C3	112.43(11)
O2A²	K2	O3A	60.87(3)	C1	C2	C3	111.51(11)
O2A	K2	O3A²	60.87(3)	C2	C3	C4	110.33(12)
O2A	K2	O3A	119.13(3)	C5	C4	C3	111.58(12)
O2A²	K2	O3A²	119.13(3)	C4	C5	C6	111.48(12)
O3A²	K2	O6	78.91(3)	C5	C6	C1	110.91(11)
O3A	K2	O6	101.09(3)	O2	C7	C8	108.74(10)
O3A²	K2	O6²	101.09(3)	O3¹	C8	K1	48.42(6)
O3A	K2	O6²	78.91(3)	O3¹	C8	C7	109.04(11)
O3A²	K2	O6X²	66.7(2)	C7	C8	K1	81.10(7)
O3A²	K2	O6X	113.3(2)	O3	C9	C10	109.51(11)
O3A	K2	O6X	66.7(2)	O1	C10	C9	108.30(11)
O3A	K2	O6X²	113.3(2)	C1A	O1A	K2	114.81(7)
O3A	K2	O1A	61.16(3)	C10A	O1A	K2	109.84(7)
O3A²	K2	O1A²	61.16(3)	C10A	O1A	C1A	113.49(10)
O3A²	K2	O1A	118.84(3)	C2A	O2A	K2	119.74(7)
O3A	K2	O1A²	118.84(3)	C7A	O2A	K2	117.52(7)
O3A²	K2	O3A	180.00(3)	C7A	O2A	C2A	112.81(9)
O4	S1	K1	46.09(6)	C8A²	O3A	K2	111.51(7)
O4	S1	O5	117.33(9)	C8A²	O3A	C9A	111.44(10)
O4	S1	N1	108.20(7)	C9A	O3A	K2	113.62(7)
O4	S1	C11	103.39(7)	O1A	C1A	C2A	106.90(10)
O4	S1	N1X	162.2(4)	O1A	C1A	C6A	112.22(11)
O5	S1	K1	71.27(6)	C2A	C1A	C6A	108.63(11)
O5	S1	N1	116.59(7)	O2A	C2A	C1A	108.22(10)
O5	S1	C11	106.37(7)	O2A	C2A	C3A	112.43(10)
O5	S1	N1X	65.6(4)	C1A	C2A	C3A	111.11(11)
N1	S1	K1	132.58(5)	C2A	C3A	C4A	110.94(11)
N1	S1	C11	103.09(7)	C5A	C4A	C3A	111.80(12)
C11	S1	K1	119.96(5)	C6A	C5A	C4A	111.15(12)
O4X	S1	K1	41.2(5)	C5A	C6A	C1A	110.94(11)
O4X	S1	O4	79.0(5)	O2A	C7A	C8A	108.89(10)

O4X	S1	O5	46.1(5)		O3A[2]	C8A	C7A	108.36(11)
O4X	S1	N1	160.1(5)		O3A	C9A	C10A	109.23(12)
O4X	S1	C11	92.8(5)		O1A	C10A	C9A	108.43(11)

[1]1-X,1-Y,-Z; [2]1-X,-Y,1-Z

Table B-6 Torsion Angles for crystal.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
K1	S1	N1	S2	112.33(8)	N1X	S1	C11	F1X	-73.1(7)
K1	S1	C11	F1	-131.05(10)	N1X	S1	C11	F2X	56.8(8)
K1	S1	C11	F2	107.47(11)	N1X	S1	C11	F3X	-177.7(6)
K1	S1	C11	F3	-13.28(13)	N1X	S1	O4X	K1	132.3(6)
K1	S1	C11	F1X	144.4(5)	N1X	S2	O6	K2	-68.0(8)
K1	S1	C11	F2X	-85.7(7)	N1X	S2	N1	S1	7.9(5)
K1	S1	C11	F3X	39.8(5)	N1X	S2	C12	F4	8.5(4)
K1	S1	N1X	S2	-113.6(7)	N1X	S2	C12	F5	-113.3(4)
K1	O1	C1	C2	49.68(11)	N1X	S2	C12	F6	126.9(4)
K1	O1	C1	C6	168.69(8)	N1X	S2	C12	F4X	-77.4(7)
K1	O1	C10	C9	-52.42(13)	N1X	S2	C12	F5X	37.7(9)
K1	O2	C2	C1	47.12(12)	N1X	S2	C12	F6X	174.4(8)
K1	O2	C2	C3	-76.48(12)	N1X	S2	O6X	K2	126.6(5)
K1	O2	C7	C8	-35.62(13)	O1[1]	K1	S1	O4	15.20(7)
K1	O3	C9	C10	-50.76(13)	O1	K1	S1	O4	-164.80(7)
K2	O1A	C1A	C2A	49.05(11)	O1[1]	K1	S1	O5	-162.73(6)
K2	O1A	C1A	C6A	168.04(8)	O1	K1	S1	O5	17.27(6)
K2	O1A	C10A	C9A	-52.88(13)	O1	K1	S1	N1	-92.01(7)
K2	O2A	C2A	C1A	47.75(12)	O1[1]	K1	S1	N1	87.99(7)
K2	O2A	C2A	C3A	-75.33(12)	O1[1]	K1	S1	C11	-64.21(6)
K2	O2A	C7A	C8A	-39.74(13)	O1	K1	S1	C11	115.79(6)
K2	O3A	C9A	C10A	-50.21(13)	O1	K1	S1	O4X	60.8(7)
O4[1]	K1	S1	O4	180.0	O1[1]	K1	S1	O4X	-119.2(7)
O4	K1	S1	O5	-177.92(9)	O1	K1	S1	O5X	-142.2(4)
O4[1]	K1	S1	O5	2.08(9)	O1[1]	K1	S1	O5X	37.8(4)
O4	K1	S1	N1	72.79(9)	O1[1]	K1	S1	N1X	170.9(6)
O4[1]	K1	S1	N1	-107.21(9)	O1	K1	S1	N1X	-9.1(6)
O4	K1	S1	C11	-79.41(9)	O1	K1	O4	S1	16.24(7)

O4¹	K1	S1	C11	100.59(9)	O1¹	K1	O4	S1	-163.76(7)
O4¹	K1	S1	O4X	45.6(7)	O1¹	K1	O4X	S1	61.9(7)
O4	K1	S1	O4X	-134.4(7)	O1	K1	O4X	S1	-118.1(7)
O4	K1	S1	O5X	22.6(4)	O1¹	K1	O1	C1	-62(10)
O4¹	K1	S1	O5X	-157.4(4)	O1¹	K1	O1	C10	169(10)
O4	K1	S1	N1X	155.7(6)	O1	K1	O2	C2	-15.46(8)
O4¹	K1	S1	N1X	-24.3(6)	O1¹	K1	O2	C2	164.54(8)
O4¹	K1	O4	S1	-158(27)	O1¹	K1	O2	C7	16.42(10)
O4¹	K1	O4X	S1	-155.0(4)	O1	K1	O2	C7	-163.58(10)
O4	K1	O4X	S1	25.0(4)	O1	K1	O3	C8¹	141.08(8)
O4	K1	O1	C1	45.88(8)	O1¹	K1	O3	C8¹	-38.92(8)
O4¹	K1	O1	C1	-134.12(8)	O1	K1	O3	C9	16.53(8)
O4¹	K1	O1	C10	96.84(9)	O1¹	K1	O3	C9	-163.47(8)
O4	K1	O1	C10	-83.16(9)	O1¹	K1	C8	O3¹	34.01(7)
O4	K1	O2	C2	-135.56(9)	O1	K1	C8	O3¹	-145.99(7)
O4¹	K1	O2	C2	44.44(9)	O1	K1	C8	C7	-20.51(8)
O4¹	K1	O2	C7	-103.68(9)	O1¹	K1	C8	C7	159.49(8)
O4	K1	O2	C7	76.32(9)	O1	C1	C2	O2	-62.26(12)
O4	K1	O3	C8¹	-116.25(8)	O1	C1	C2	C3	61.89(13)
O4¹	K1	O3	C8¹	63.75(8)	O1	C1	C6	C5	-59.33(15)
O4	K1	O3	C9	119.20(9)	O2¹	K1	S1	O4	72.59(7)
O4¹	K1	O3	C9	-60.80(9)	O2	K1	S1	O4	-107.41(7)
O4	K1	C8	O3¹	106.61(8)	O2	K1	S1	O5	74.67(6)
O4¹	K1	C8	O3¹	-73.39(8)	O2¹	K1	S1	O5	-105.33(6)
O4	K1	C8	C7	-127.92(9)	O2	K1	S1	N1	-34.62(7)
O4¹	K1	C8	C7	52.08(9)	O2¹	K1	S1	N1	145.38(7)
O4	S1	N1	S2	158.75(9)	O2¹	K1	S1	C11	-6.82(6)
O4	S1	C11	F1	-177.76(12)	O2	K1	S1	C11	173.18(6)
O4	S1	C11	F2	60.76(14)	O2¹	K1	S1	O4X	-61.8(7)
O4	S1	C11	F3	-59.99(13)	O2	K1	S1	O4X	118.2(7)
O4	S1	C11	F1X	97.7(5)	O2¹	K1	S1	O5X	95.2(4)
O4	S1	C11	F2X	-132.4(7)	O2	K1	S1	O5X	-84.8(4)
O4	S1	C11	F3X	-6.9(5)	O2¹	K1	S1	N1X	-131.7(6)
O4	S1	O4X	K1	-31.6(5)	O2	K1	S1	N1X	48.3(6)
O4	S1	N1X	S2	-37(2)	O2¹	K1	O4	S1	-111.51(6)
O5	S1	O4	K1	2.21(9)	O2	K1	O4	S1	68.48(6)
O5	S1	N1	S2	23.92(13)	O2	K1	O4X	S1	-58.7(7)

O5	S1	C11	F1	-53.58(13)	O2[1]	K1	O4X	S1	121.3(7)
O5	S1	C11	F2	-175.06(12)	O2[1]	K1	O1	C1	159.90(7)
O5	S1	C11	F3	64.20(12)	O2	K1	O1	C1	-20.10(7)
O5	S1	C11	F1X	-138.2(5)	O2[1]	K1	O1	C10	30.86(9)
O5	S1	C11	F2X	-8.3(7)	O2	K1	O1	C10	-149.14(9)
O5	S1	C11	F3X	117.2(5)	O2[1]	K1	O2	C2	-71(10)
O5	S1	O4X	K1	115.1(8)	O2[1]	K1	O2	C7	141(10)
O5	S1	N1X	S2	-141.1(9)	O2[1]	K1	O3	C8[1]	-27.82(7)
O6[2]	K2	O6	S2	67(10)	O2	K1	O3	C8[1]	152.18(7)
O6[2]	K2	O6X	S2	-163.1(3)	O2	K1	O3	C9	27.63(9)
O6	K2	O6X	S2	16.9(3)	O2[1]	K1	O3	C9	-152.37(9)
O6[2]	K2	O1A	C1A	67.62(8)	O2[1]	K1	C8	O3[1]	37.47(10)
O6	K2	O1A	C1A	-112.38(8)	O2	K1	C8	O3[1]	-142.53(10)
O6[2]	K2	O1A	C10A	-61.69(9)	O2[1]	K1	C8	C7	162.95(7)
O6	K2	O1A	C10A	118.30(9)	O2	K1	C8	C7	-17.05(7)
O6	K2	O2A	C2A	78.59(8)	O2	C2	C3	C4	179.36(11)
O6[2]	K2	O2A	C2A	-101.41(8)	O2	C7	C8	K1	23.36(9)
O6[2]	K2	O2A	C7A	115.37(9)	O2	C7	C8	O3[1]	63.48(14)
O6	K2	O2A	C7A	-64.63(9)	O3[1]	K1	S1	O4	-45.61(7)
O6	K2	O3A	C8A[2]	50.50(8)	O3	K1	S1	O4	134.39(7)
O6[2]	K2	O3A	C8A[2]	-129.50(8)	O3[1]	K1	S1	O5	136.47(6)
O6	K2	O3A	C9A	-76.45(9)	O3	K1	S1	O5	-43.53(6)
O6[2]	K2	O3A	C9A	103.55(9)	O3	K1	S1	N1	-152.82(7)
O6	S2	N1	S1	156.15(9)	O3[1]	K1	S1	N1	27.18(7)
O6	S2	C12	F4	179.17(11)	O3[1]	K1	S1	C11	-125.02(6)
O6	S2	C12	F5	57.37(12)	O3	K1	S1	C11	54.98(6)
O6	S2	C12	F6	-62.49(12)	O3	K1	S1	O4X	0.0(7)
O6	S2	C12	F4X	93.2(5)	O3[1]	K1	S1	O4X	180.0(7)
O6	S2	C12	F5X	-151.7(8)	O3	K1	S1	O5X	157.0(4)
O6	S2	C12	F6X	-15.0(7)	O3[1]	K1	S1	O5X	-23.0(4)
O6	S2	O6X	K2	-20.9(3)	O3[1]	K1	S1	N1X	110.1(6)
O6	S2	N1X	S1	-78.0(11)	O3	K1	S1	N1X	-69.9(6)
O7	S2	O6	K2	14.32(11)	O3[1]	K1	O4	S1	130.74(7)
O7	S2	N1	S1	16.70(13)	O3	K1	O4	S1	-49.26(7)
O7	S2	C12	F4	-55.41(12)	O3[1]	K1	O4X	S1	0.0(7)
O7	S2	C12	F5	-177.22(11)	O3	K1	O4X	S1	180.0(7)
O7	S2	C12	F6	62.92(12)	O3[1]	K1	O1	C1	-31.47(9)

O7	S2	C12	F4X	-141.3(5)	O3	K1	O1	C1	148.53(9)
O7	S2	C12	F5X	-26.3(8)	O3[1]	K1	O1	C10	-160.51(8)
O7	S2	C12	F6X	110.5(7)	O3	K1	O1	C10	19.49(8)
O7	S2	O6X	K2	142.2(9)	O3[1]	K1	O2	C2	153.20(9)
O7	S2	N1X	S1	-178.7(10)	O3	K1	O2	C2	-26.80(9)
N1	S1	O4	K1	-132.23(6)	O3	K1	O2	C7	-174.92(8)
N1	S1	C11	F1	69.60(12)	O3[1]	K1	O2	C7	5.08(8)
N1	S1	C11	F2	-51.88(13)	O3[1]	K1	O3	C8[1]	-141(29)
N1	S1	C11	F3	-172.63(11)	O3[1]	K1	O3	C9	94(29)
N1	S1	C11	F1X	-15.0(5)	O3	K1	C8	O3[1]	180.0
N1	S1	C11	F2X	114.9(7)	O3[1]	K1	C8	C7	125.48(12)
N1	S1	C11	F3X	-119.6(5)	O3	K1	C8	C7	-54.52(12)
N1	S1	O4X	K1	81.9(17)	O3	C9	C10	O1	71.58(15)
N1	S1	N1X	S2	7.4(5)	C1	O1	C10	C9	178.52(11)
N1	S2	O6	K2	-124.15(8)	C1	C2	C3	C4	57.63(15)
N1	S2	C12	F4	67.10(12)	C2	O2	C7	C8	173.79(11)
N1	S2	C12	F5	-54.71(12)	C2	C1	C6	C5	58.41(15)
N1	S2	C12	F6	-174.57(10)	C2	C3	C4	C5	-53.98(16)
N1	S2	C12	F4X	-18.8(5)	C3	C4	C5	C6	53.88(16)
N1	S2	C12	F5X	96.2(8)	C4	C5	C6	C1	-56.37(16)
N1	S2	C12	F6X	-127.0(7)	C6	C1	C2	O2	176.30(10)
N1	S2	O6X	K2	90.2(10)	C6	C1	C2	C3	-59.55(14)
N1	S2	N1X	S1	-7.6(5)	C7	O2	C2	C1	-163.04(11)
C11	S1	O4	K1	118.90(7)	C7	O2	C2	C3	73.36(14)
C11	S1	N1	S2	-92.18(10)	C8	K1	S1	O4	-63.26(7)
C11	S1	O4X	K1	-134.7(5)	C8[1]	K1	S1	O4	116.74(7)
C11	S1	N1X	S2	111.7(7)	C8	K1	S1	O5	-61.19(6)
C12	S2	O6	K2	128.99(7)	C8	K1	S1	O5	118.81(6)
C12	S2	N1	S1	-96.05(10)	C8[1]	K1	S1	N1	-170.47(7)
C12	S2	O6X	K2	-121.9(3)	C8	K1	S1	N1	9.53(7)
C12	S2	N1X	S1	84.6(7)	C8	K1	S1	C11	-142.67(6)
O4X	K1	S1	O4	134.4(7)	C8[1]	K1	S1	C11	37.33(6)
O4X[1]	K1	S1	O4	-45.6(7)	C8[1]	K1	S1	O4X	-17.7(7)
O4X[1]	K1	S1	O5	136.5(7)	C8	K1	S1	O4X	162.3(7)
O4X	K1	S1	O5	-43.5(7)	C8	K1	S1	O5X	-40.7(4)
O4X	K1	S1	N1	-152.8(7)	C8[1]	K1	S1	O5X	139.3(4)
O4X[1]	K1	S1	N1	27.2(7)	C8[1]	K1	S1	N1X	-87.6(6)

O4X[1]	K1	S1	C11	-125.0(7)	C8	K1	S1	N1X	92.4(6)
O4X	K1	S1	C11	55.0(7)	C8[1]	K1	O4	S1	-72.13(7)
O4X[1]	K1	S1	O4X	180.001(1)	C8	K1	O4	S1	107.87(7)
O4X[1]	K1	S1	O5X	-23.0(8)	C8	K1	O4X	S1	-16.5(7)
O4X	K1	S1	O5X	157.0(8)	C8[1]	K1	O4X	S1	163.5(7)
O4X[1]	K1	S1	N1X	110.1(9)	C8[1]	K1	O1	C1	162.61(8)
O4X	K1	S1	N1X	-69.9(9)	C8	K1	O1	C1	-17.39(8)
O4X[1]	K1	O4	S1	156.9(4)	C8	K1	O1	C10	-146.43(8)
O4X	K1	O4	S1	-23.1(4)	C8[1]	K1	O1	C10	33.57(8)
O4X[1]	K1	O4X	S1	109(23)	C8	K1	O2	C2	168.51(10)
O4X[1]	K1	O1	C1	-111.8(3)	C8[1]	K1	O2	C2	-11.49(10)
O4X	K1	O1	C1	68.2(3)	C8[1]	K1	O2	C7	-159.61(8)
O4X[1]	K1	O1	C10	119.2(3)	C8	K1	O2	C7	20.39(8)
O4X	K1	O1	C10	-60.8(3)	C8	K1	O3	C8[1]	180.0
O4X[1]	K1	O2	C2	81.0(3)	C8	K1	O3	C9	55.45(12)
O4X	K1	O2	C2	-99.0(3)	C8[1]	K1	O3	C9	-124.55(12)
O4X[1]	K1	O2	C7	112.9(3)	C8[1]	K1	C8	O3[1]	12(8)
O4X	K1	O2	C7	-67.1(3)	C8[1]	K1	C8	C7	137(8)
O4X[1]	K1	O3	C8[1]	-131.8(2)	C8[1]	O3	C9	C10	-174.34(11)
O4X	K1	O3	C8[1]	48.2(2)	C10	O1	C1	C2	176.75(11)
O4X	K1	O3	C9	103.7(3)	C10	O1	C1	C6	-64.24(15)
O4X[1]	K1	O3	C9	-76.3(3)	O1A[2]	K2	O6	S2	120.18(8)
O4X[1]	K1	C8	O3[1]	-46.8(2)	O1A	K2	O6	S2	-59.82(8)
O4X	K1	C8	O3[1]	133.2(2)	O1A	K2	O6X	S2	155.4(6)
O4X[1]	K1	C8	C7	78.7(2)	O1A[2]	K2	O6X	S2	-24.6(6)
O4X	K1	C8	C7	-101.3(2)	O1A[2]	K2	O1A	C1A	16(16)
O4X	S1	O4	K1	28.6(5)	O1A[2]	K2	O1A	C10A	-113(16)
O4X	S1	N1	S2	50.1(16)	O1A	K2	O2A	C2A	-16.28(8)
O4X	S1	C11	F1	-98.4(5)	O1A[2]	K2	O2A	C2A	163.72(8)
O4X	S1	C11	F2	140.1(5)	O1A[2]	K2	O2A	C7A	20.49(9)
O4X	S1	C11	F3	19.4(5)	O1A	K2	O2A	C7A	-159.51(9)
O4X	S1	C11	F1X	177.0(7)	O1A	K2	O3A	C8A[2]	143.12(8)
O4X	S1	C11	F2X	-53.1(8)	O1A[2]	K2	O3A	C8A[2]	-36.88(8)
O4X	S1	C11	F3X	72.4(7)	O1A[2]	K2	O3A	C9A	-163.82(8)
O4X	S1	N1X	S2	-154.7(8)	O1A	K2	O3A	C9A	16.18(8)
O5X	S1	O4	K1	-148.4(6)	O1A	C1A	C2A	O2A	-62.34(13)
O5X	S1	N1	S2	172.0(5)	O1A	C1A	C2A	C3A	61.54(13)

O5X	S1	C11	F1	134.0(5)	O1A	C1A	C6A	C5A	-58.33(15)
O5X	S1	C11	F2	12.5(5)	O2A[2]	K2	O6	S2	60.68(8)
O5X	S1	C11	F3	-108.2(5)	O2A	K2	O6	S2	-119.32(8)
O5X	S1	C11	F1X	49.4(7)	O2A	K2	O6X	S2	104.6(5)
O5X	S1	C11	F2X	179.3(8)	O2A[2]	K2	O6X	S2	-75.4(5)
O5X	S1	C11	F3X	-55.2(7)	O2A	K2	O1A	C1A	-19.14(7)
O5X	S1	O4X	K1	-28.9(10)	O2A[2]	K2	O1A	C1A	160.86(7)
O5X	S1	N1X	S2	7.6(11)	O2A[2]	K2	O1A	C10A	31.55(9)
O6X[2]	K2	O6	S2	158.6(4)	O2A	K2	O1A	C10A	-148.45(9)
O6X	K2	O6	S2	-21.4(4)	O2A[2]	K2	O2A	C2A	73(5)
O6X[2]	K2	O6X	S2	12(17)	O2A[2]	K2	O2A	C7A	-70(5)
O6X[2]	K2	O1A	C1A	43.6(2)	O2A[2]	K2	O3A	C8A[2]	-25.34(7)
O6X	K2	O1A	C1A	-136.4(2)	O2A	K2	O3A	C8A[2]	154.66(7)
O6X[2]	K2	O1A	C10A	-85.7(2)	O2A[2]	K2	O3A	C9A	-152.29(9)
O6X	K2	O1A	C10A	94.3(2)	O2A	K2	O3A	C9A	27.71(9)
O6X	K2	O2A	C2A	40.8(2)	O2A	C2A	C3A	C4A	178.43(11)
O6X[2]	K2	O2A	C2A	-139.2(2)	O2A	C7A	C8A	O3A[2]	64.10(13)
O6X	K2	O2A	C7A	-102.4(2)	O3A[2]	K2	O6	S2	-177.84(9)
O6X[2]	K2	O2A	C7A	77.6(2)	O3A	K2	O6	S2	2.16(9)
O6X	K2	O3A	C8A[2]	65.8(3)	O3A	K2	O6X	S2	-137.9(6)
O6X[2]	K2	O3A	C8A[2]	-114.2(3)	O3A[2]	K2	O6X	S2	42.1(6)
O6X	K2	O3A	C9A	-61.1(3)	O3A[2]	K2	O1A	C1A	-30.90(9)
O6X[2]	K2	O3A	C9A	118.9(3)	O3A	K2	O1A	C1A	149.10(9)
O6X	S2	O6	K2	26.9(5)	O3A	K2	O1A	C10A	19.79(8)
O6X	S2	N1	S1	52.1(11)	O3A[2]	K2	O1A	C10A	-160.21(8)
O6X	S2	C12	F4	-97.4(5)	O3A[2]	K2	O2A	C2A	151.93(9)
O6X	S2	C12	F5	140.8(5)	O3A	K2	O2A	C2A	-28.07(9)
O6X	S2	C12	F6	21.0(5)	O3A	K2	O2A	C7A	-171.30(8)
O6X	S2	C12	F4X	176.7(7)	O3A[2]	K2	O2A	C7A	8.70(8)
O6X	S2	C12	F5X	-68.2(10)	O3A[2]	K2	O3A	C8A[2]	-132(9)
O6X	S2	C12	F6X	68.5(8)	O3A[2]	K2	O3A	C9A	101(9)
O6X	S2	N1X	S1	-167.1(8)	O3A	C9A	C10A	O1A	71.44(15)
O7X	S2	O6	K2	-111.7(7)	C1A	O1A	C10A	C9A	177.10(11)
O7X	S2	N1	S1	147.4(5)	C1A	C2A	C3A	C4A	56.98(15)
O7X	S2	C12	F4	138.4(6)	C2A	O2A	C7A	C8A	174.59(10)
O7X	S2	C12	F5	16.6(6)	C2A	C1A	C6A	C5A	59.64(15)
O7X	S2	C12	F6	-103.3(6)	C2A	C3A	C4A	C5A	-53.07(17)

O7X	S2	C12	F4X	52.5(8)		C3A	C4A	C5A	C6A	53.17(17)
O7X	S2	C12	F5X	167.6(10)		C4A	C5A	C6A	C1A	-56.81(16)
O7X	S2	C12	F6X	-55.7(9)		C6A	C1A	C2A	O2A	176.36(10)
O7X	S2	O6X	K2	6.9(7)		C6A	C1A	C2A	C3A	-59.76(14)
O7X	S2	N1X	S1	-48.4(10)		C7A	O2A	C2A	C1A	-167.42(10)
N1X	S1	O4	K1	-93.0(14)		C7A	O2A	C2A	C3A	69.49(14)
N1X	S1	N1	S2	-8.2(5)		C8A[2]	O3A	C9A	C10A	-177.20(11)
N1X	S1	C11	F1	11.5(4)		C10A	O1A	C1A	C2A	176.54(11)
N1X	S1	C11	F2	-110.0(4)		C10A	O1A	C1A	C6A	-64.47(14)
N1X	S1	C11	F3	129.3(4)						

[1]1-X,1-Y,-Z; [2]1-X,-Y,1-Z

Table B-7 Hydrogen Atom Coordinates ($\mathring{A}\times10^4$) and Isotropic Displacement Parameters ($\mathring{A}^2\times10^3$) for crystal.

Atom	x	y	z	U(eq)
H1	6473	6605	2052	20
H2	8889	6353	1796	20
H3A	8079	7644	293	26
H3B	9621	7002	568	26
H4A	10215	8721	1570	33
H4B	9752	9509	754	33
H5A	7452	9875	1097	32
H5B	8644	10448	1814	32
H6A	6727	9087	2298	27
H6B	8255	8402	2543	27
H7A	9317	4192	1381	25
H7B	9242	4687	479	25
H8A	8709	2220	552	21
H8B	7335	2522	989	21
H9A	2728	8866	580	27
H9B	4048	8766	72	27
H10A	4802	8964	1495	29
H10B	4064	7415	1566	29
H1A	6592	1426	7084	20
H2A	8980	1066	6813	19

H3AA	8208	2417	5324	25
H3AB	9722	1718	5590	25
H4AA	10407	3419	6588	32
H4AB	9939	4227	5781	32
H5AA	8920	5192	6870	31
H5AB	7687	4678	6159	31
H6AA	6984	3886	7364	26
H6AB	8482	3132	7578	26
H7AA	9336	-1084	6300	23
H7AB	9175	-509	5411	23
H8AA	8589	-2982	5431	20
H8AB	7277	-2690	5920	20
H9AA	2979	3943	5681	27
H9AB	4283	3815	5164	27
H10C	5054	3866	6587	29
H10D	4223	2349	6617	29

Experimental

Single crystals of $C_{22}H_{36}F_6KNO_{10}S_2$. A suitable crystal was selected and run on a SuperNova, Dual, Cu at zero, Eos diffractometer. The crystal was kept at 100.00(10) K during data collection. Using Olex2 [1], the structure was solved with the XS [2] structure solution program using Direct Methods and refined with the XL [3] refinement package using Least Squares minimization.

1. O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, OLEX2: a complete structure solution, refinement and analysis program. J. Appl. Cryst. (2009). 42, 339-341.
2. XS, G.M. Sheldrick, Acta Cryst. (2008). A64, 112-122
3. XL, G.M. Sheldrick, Acta Cryst. (2008). A64, 112-122

Crystal Data for $C_{22}H_{36}F_6KNO_{10}S_2$ (M =691.74): triclinic, space group P-1 (no. 2), a = 9.2968(2) Å, b = 9.5458(2) Å, c = 17.0459(4) Å, α = 90.323(2)°, β = 97.993(2)°, γ = 93.332(2)°, V = 1495.38(6) Å^3, Z = 2, T = 100.00(10) K, μ(Mo Kα) = 0.407 mm^{-1}, $Dcalc$ = 1.536 g/mm^3, 35480 reflections measured (5.98 ≤ 2Θ ≤ 58.24), 7371 unique (R_{int} = 0.0320) which were used in all calculations. The final R_1 was 0.0330 (>2sigma(I)) and wR_2 was 0.0858 (all data).

Initial workup was performed by Dr. Nicholas Silvaggi; University of Wisconsin-Milwaukee; Milwaukee, WI

Follow-up work was done by Dr. Sergey Lindeman; Marquette University; Milwaukee, WI
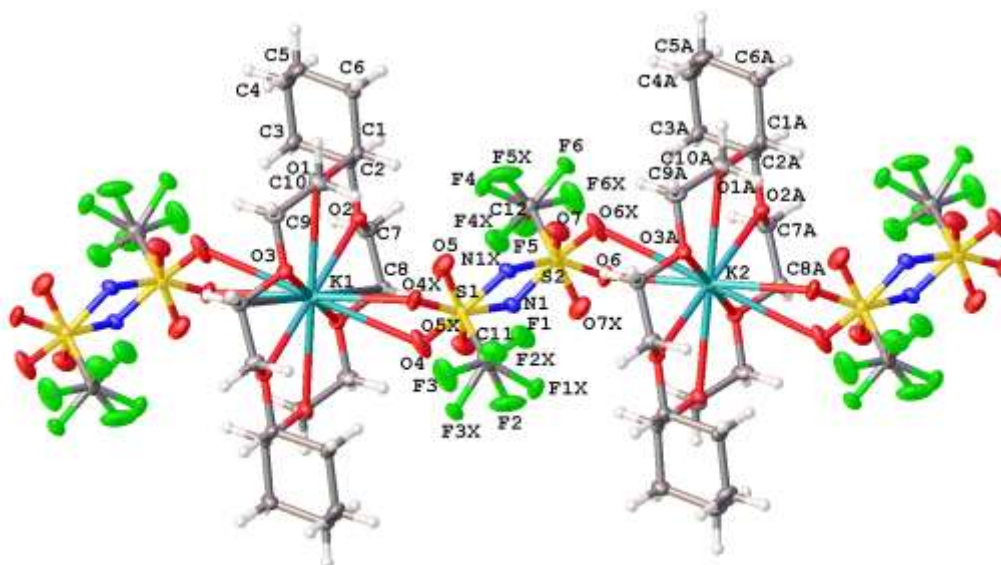
Molecular geometry:

The potassium-crown complex (both symmetrically independent units) occupies crystallographic inversion center. The sulfamide counter ion is positioned between two complex units being 10% disordered by pseudo (non-crystallographic) inversion center.

The cyclohexane units have a chair conformation.
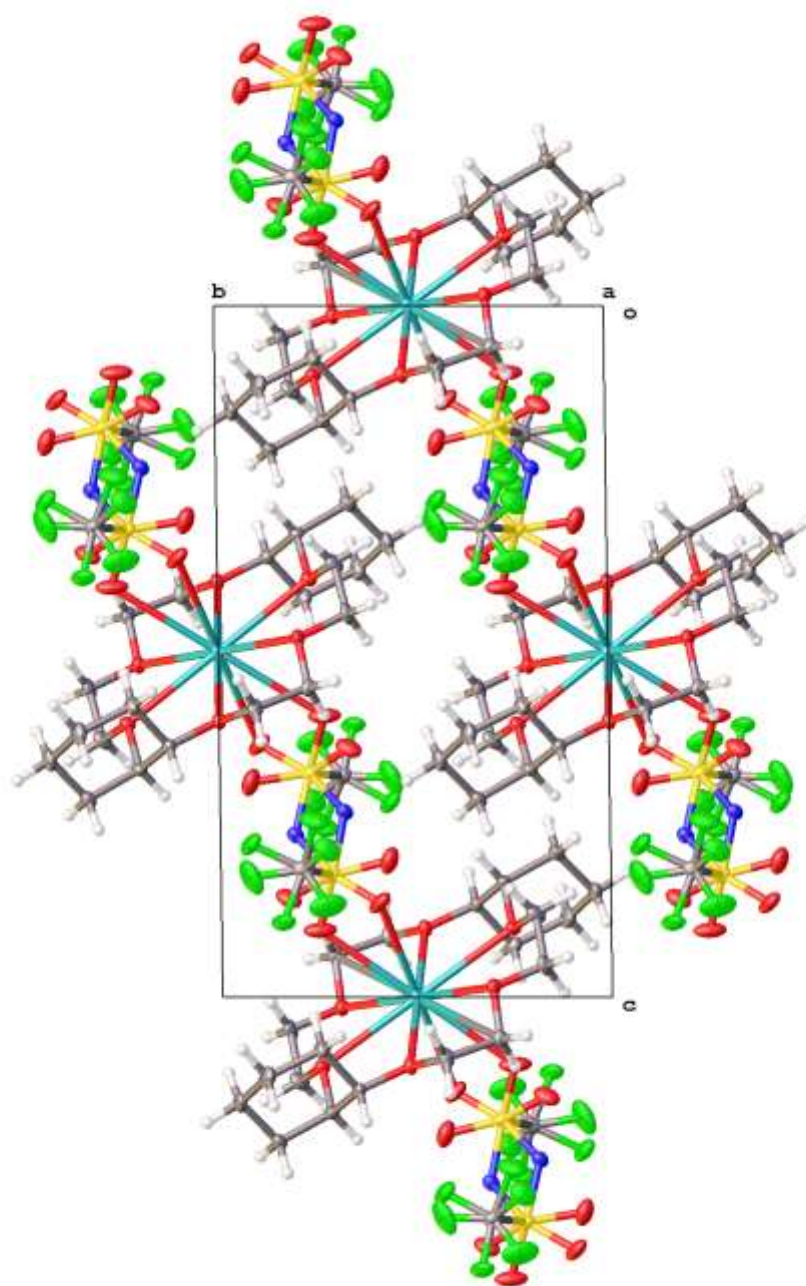
Molecular packing:

In the crystal structure, the ions form chains along [01-1].

APPENDIX C

ITC THERMOGRAMS
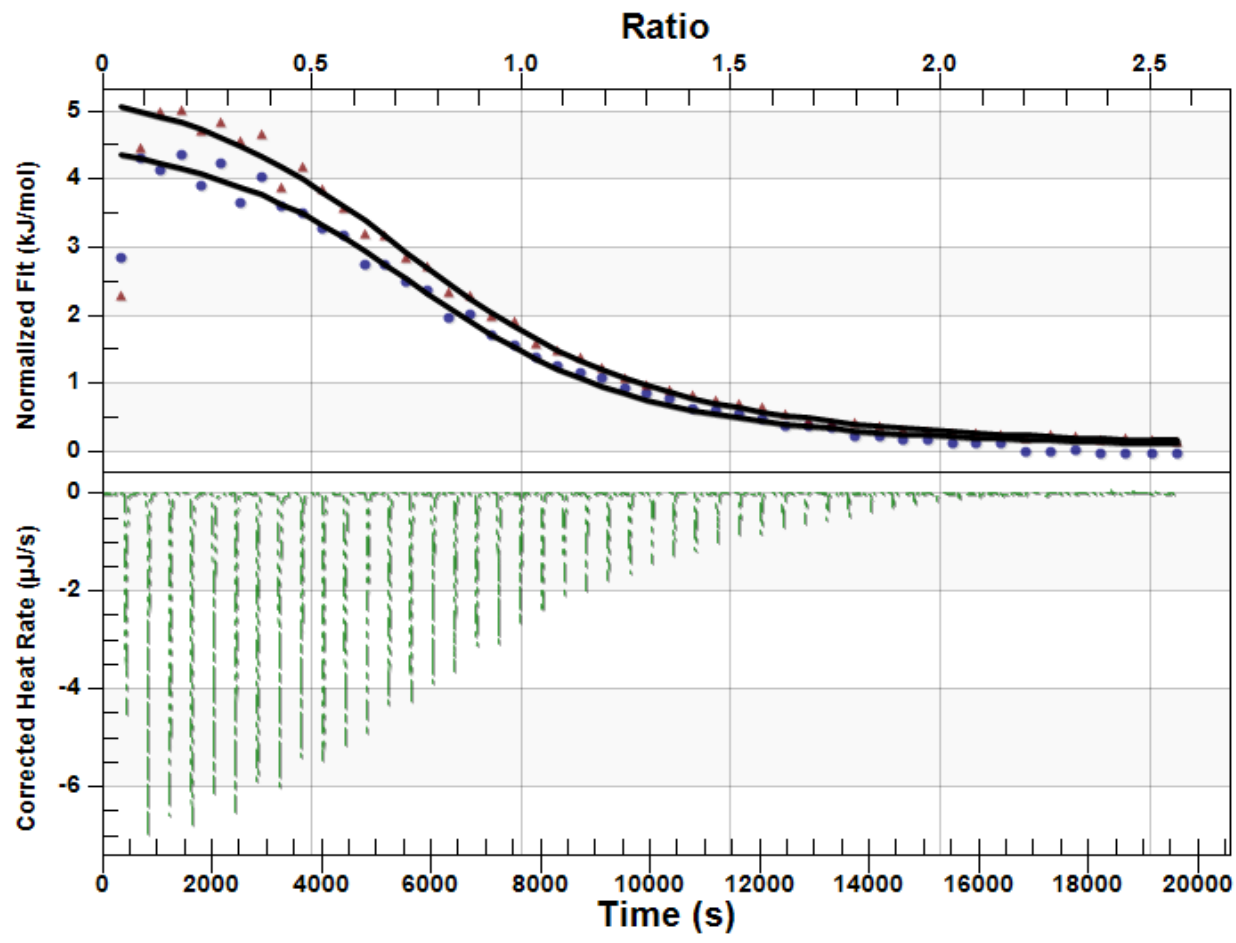
Figure C-1: ITC Thermogram of DCH18C6A Isomer Complexed with $CaCl_2 \cdot 2H_2O$ in Anhydrous Methanol
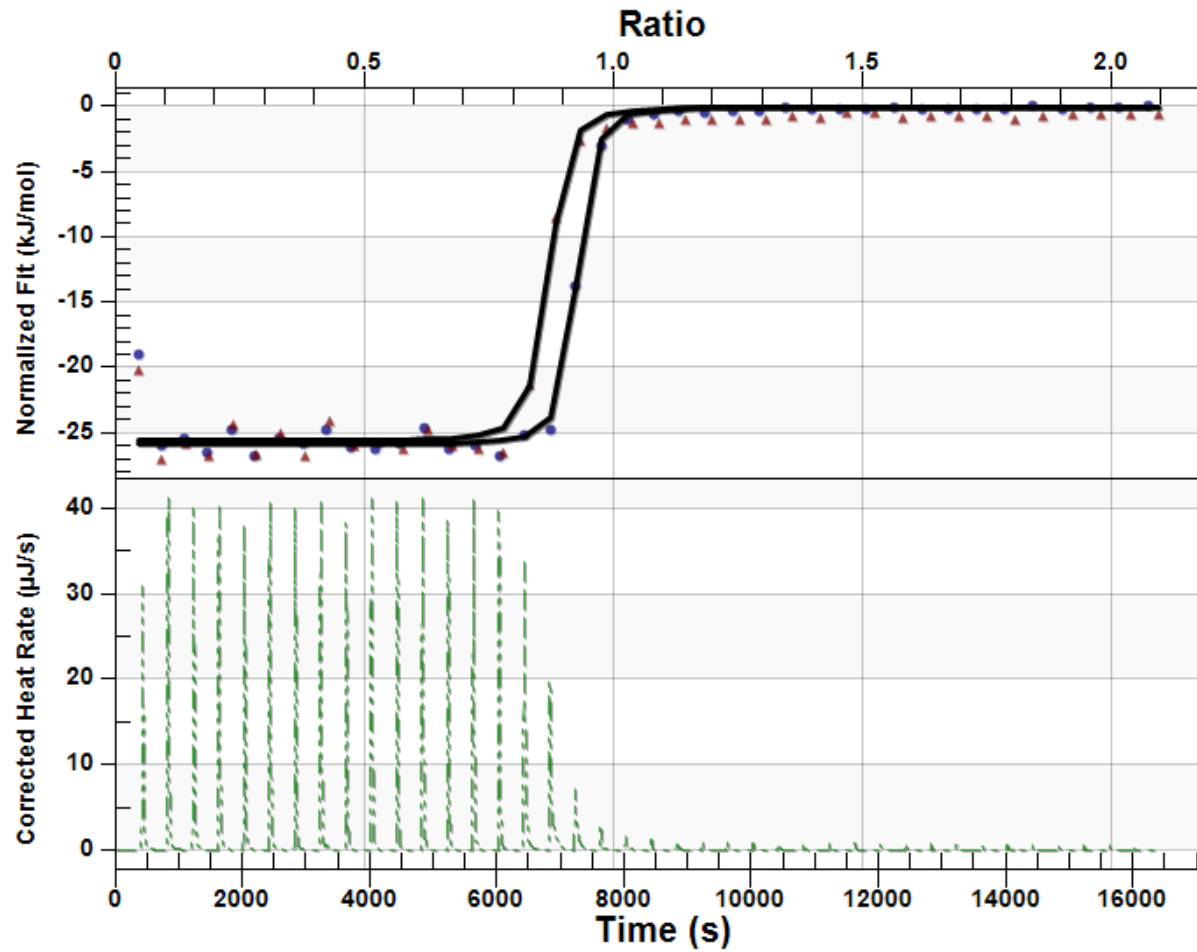
Figure C-2: ITC Thermogram of DCH18C6A Isomer Complexed with $SrCl_2 \cdot 6H_2O$ in Anhydrous Methanol
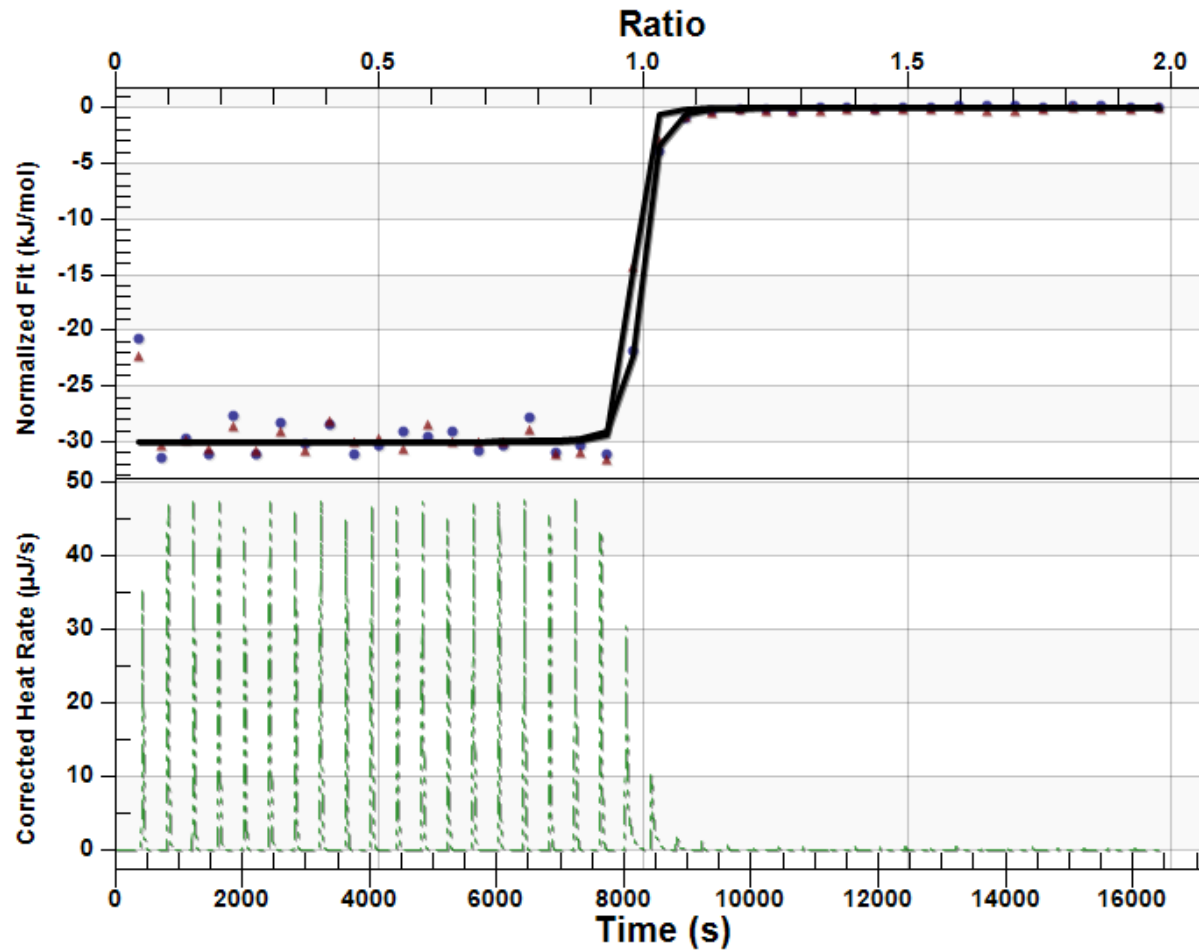
Figure C-3: ITC Thermogram of DCH18C6A Isomer Complexed with $BaCl_2 \cdot 6H_2O$ in Anhydrous Methanol
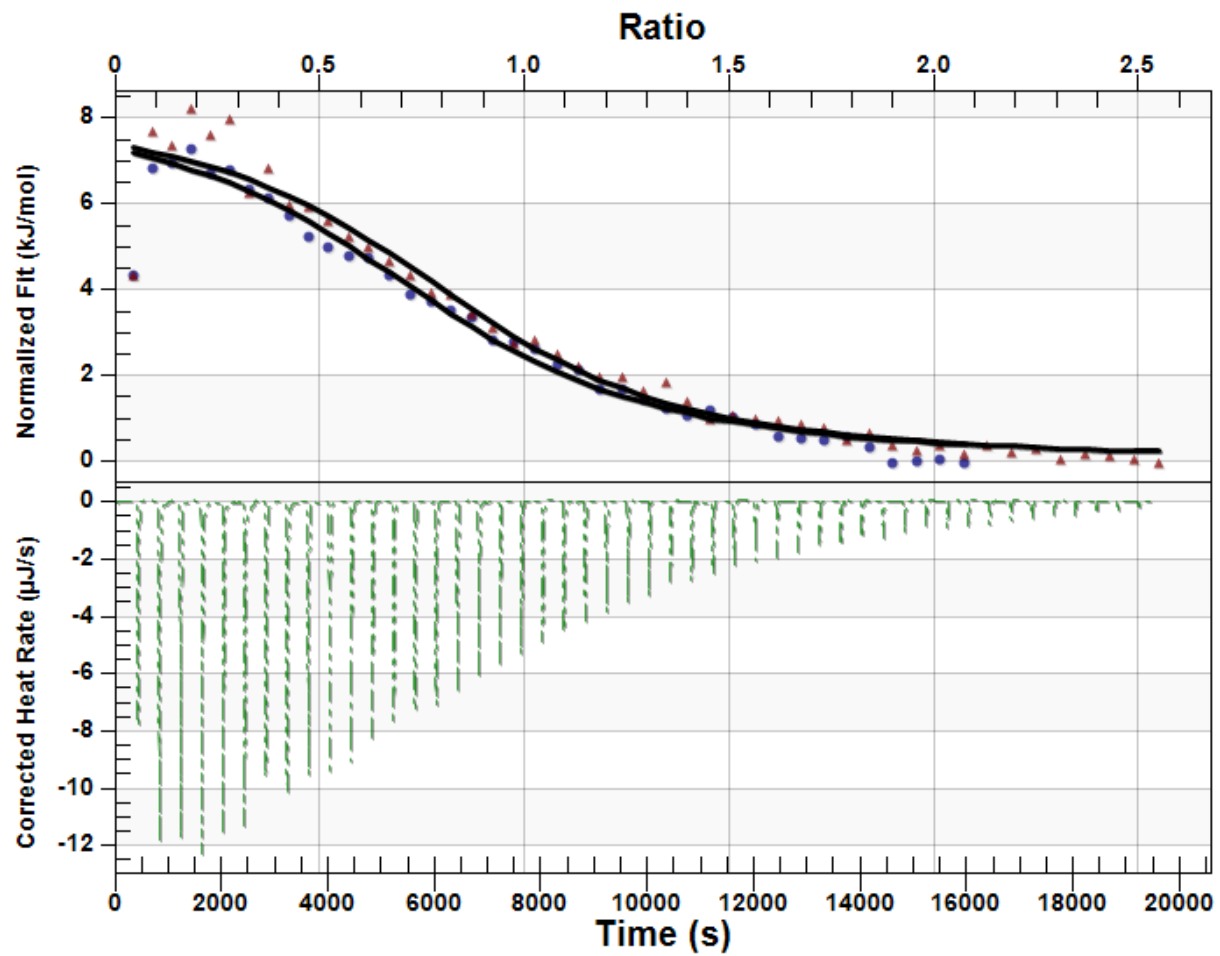
Figure C-4: ITC Thermogram of DCH18C6B Isomer Complexed with $CaCl_2 \cdot 2H_2O$ in Anhydrous Methanol
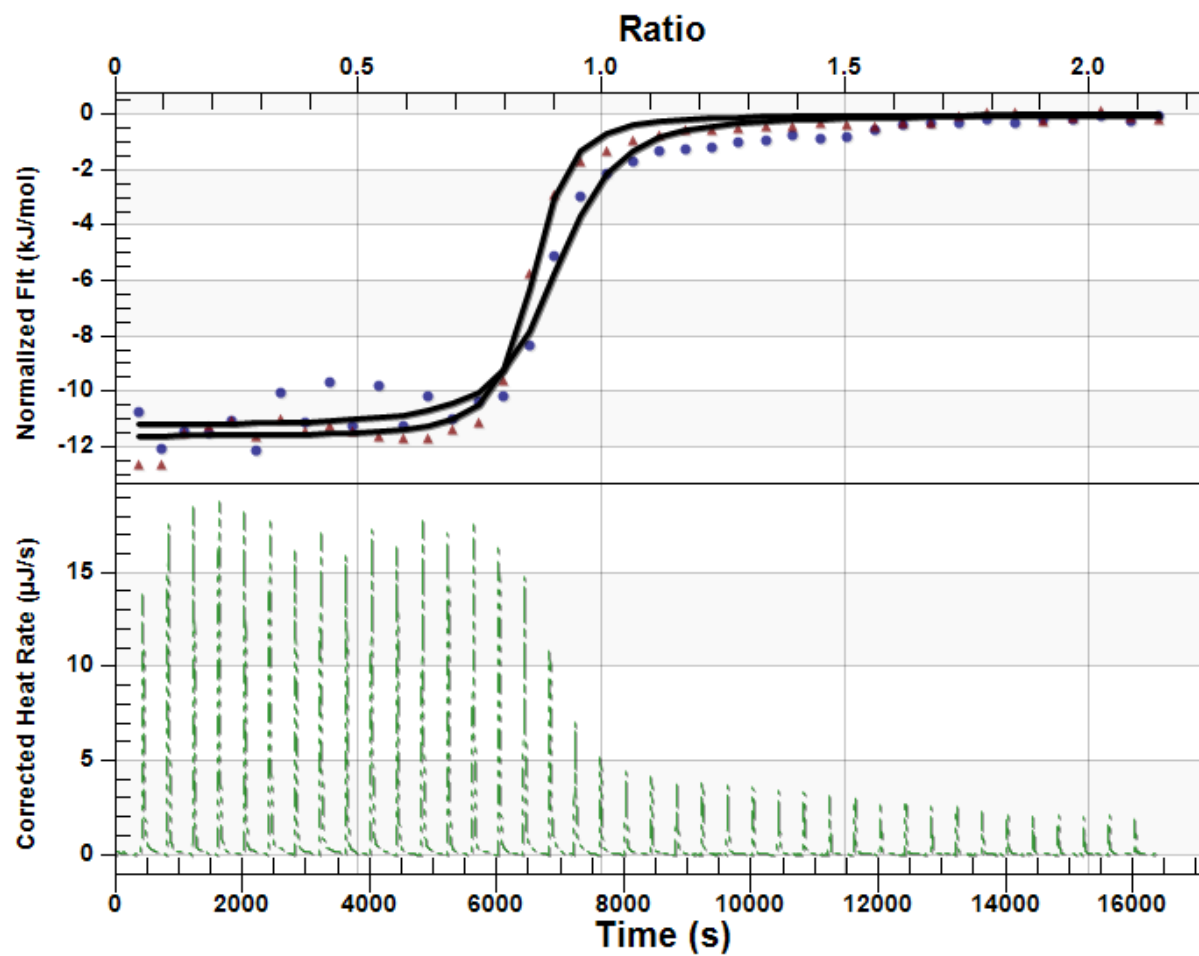
Figure C-5: ITC Thermogram of DCH18C6B Isomer Complexed with $SrCl_2 \cdot 6H_2O$ in Anhydrous Methanol
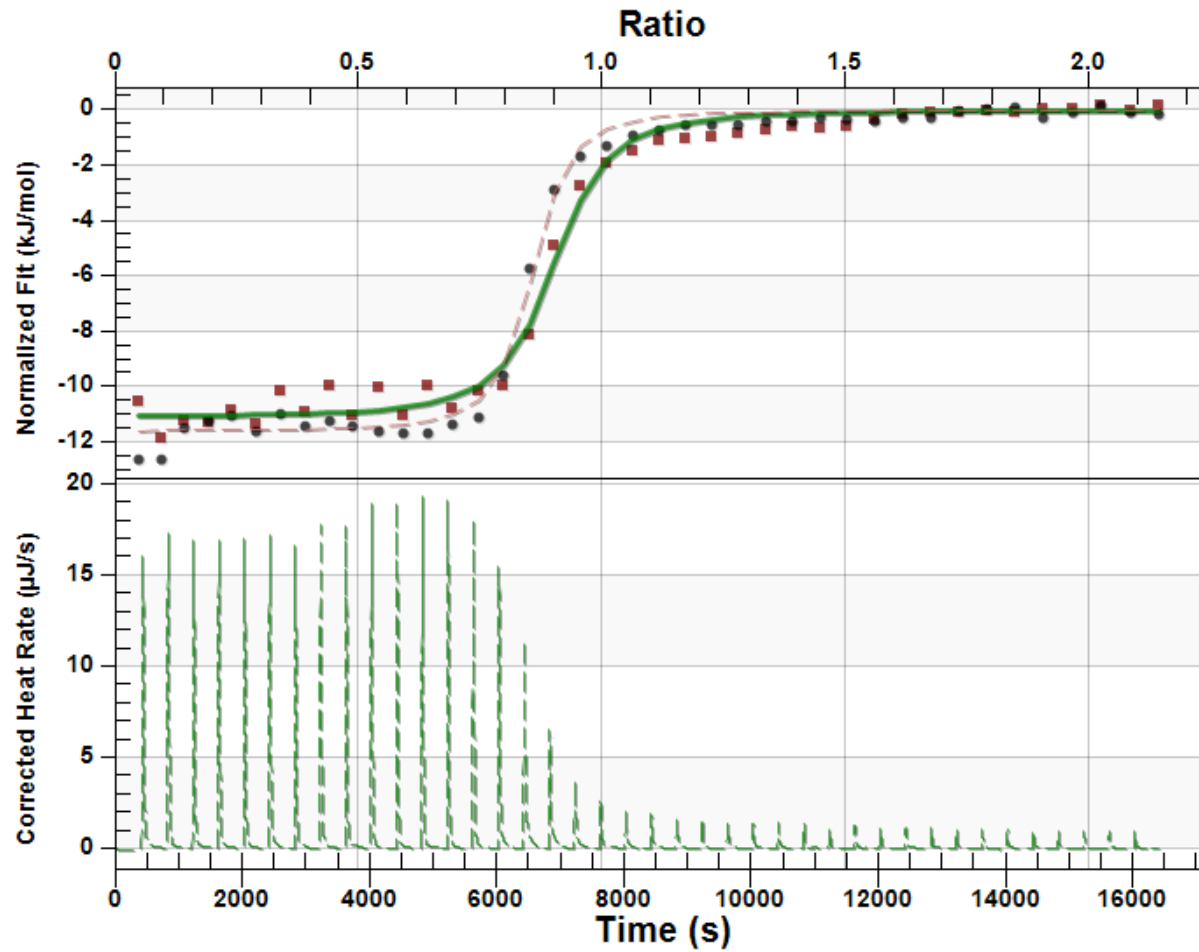
Figure C-6: ITC Thermogram of DCH18C6B Isomer Complexed with $BaCl_2 \cdot 2H_2O$ in Anhydrous Methanol
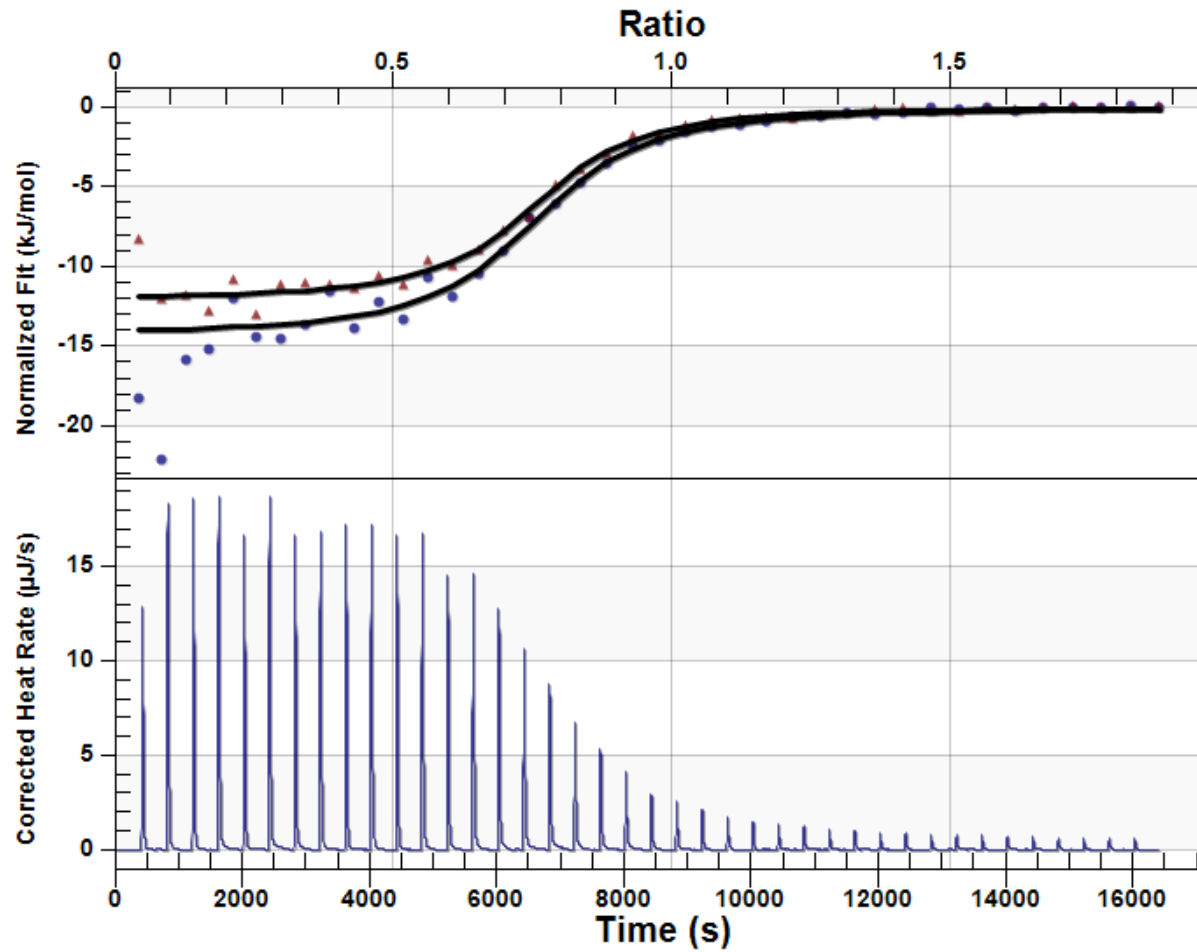
Figure C-7: ITC Thermogram of DCH18C6C Isomer Complexed with $SrCl_2 \cdot 6H_2O$ in Anhydrous Methanol
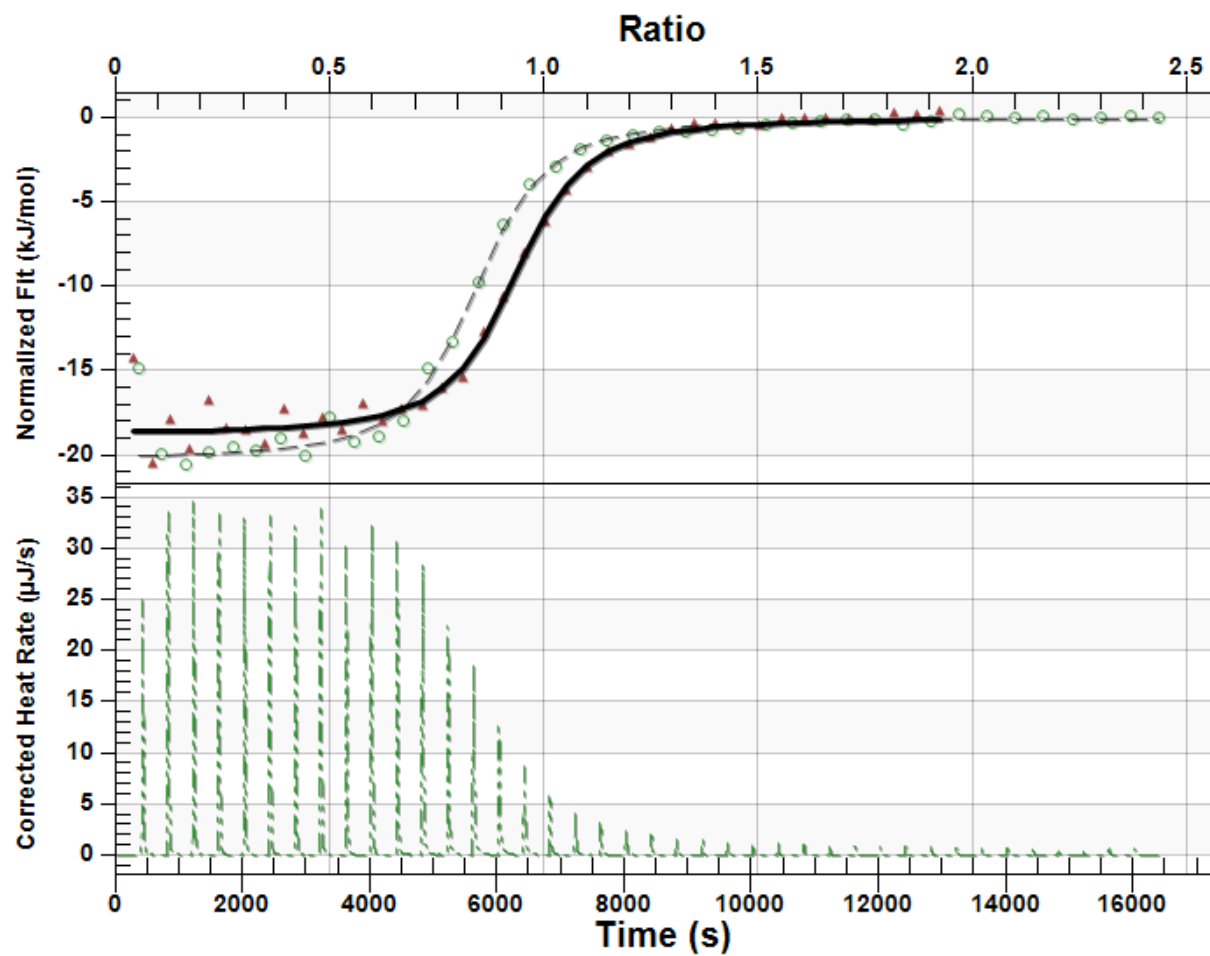
Figure C-8: ITC Thermogram of DCH18C6C Isomer Complexed with BaCl$_2$·2H$_2$O in Anhydrous Methanol
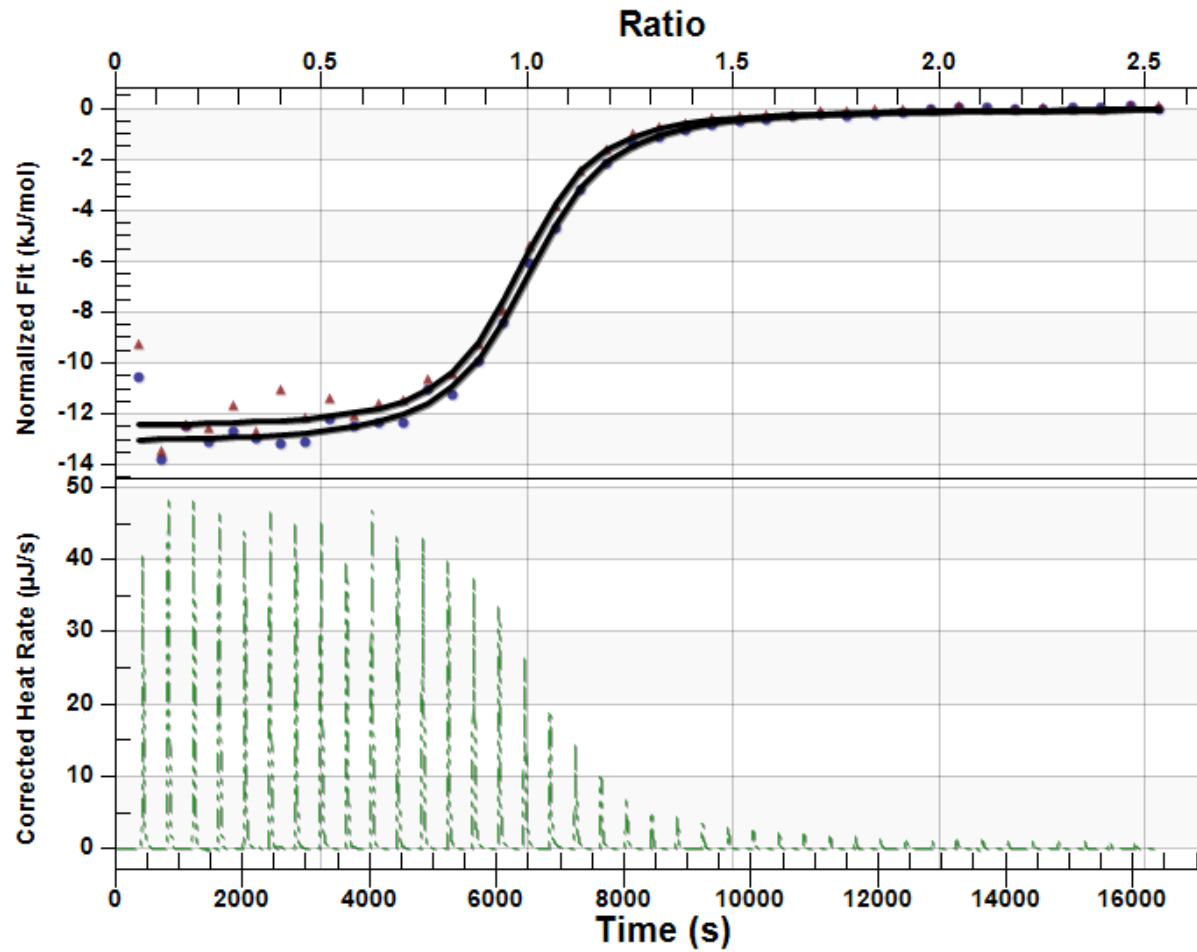
Figure C-9: ITC Thermogram of DCH18C6D Isomer Complexed with $SrCl_2 \cdot 6H_2O$ in Anhydrous Methanol
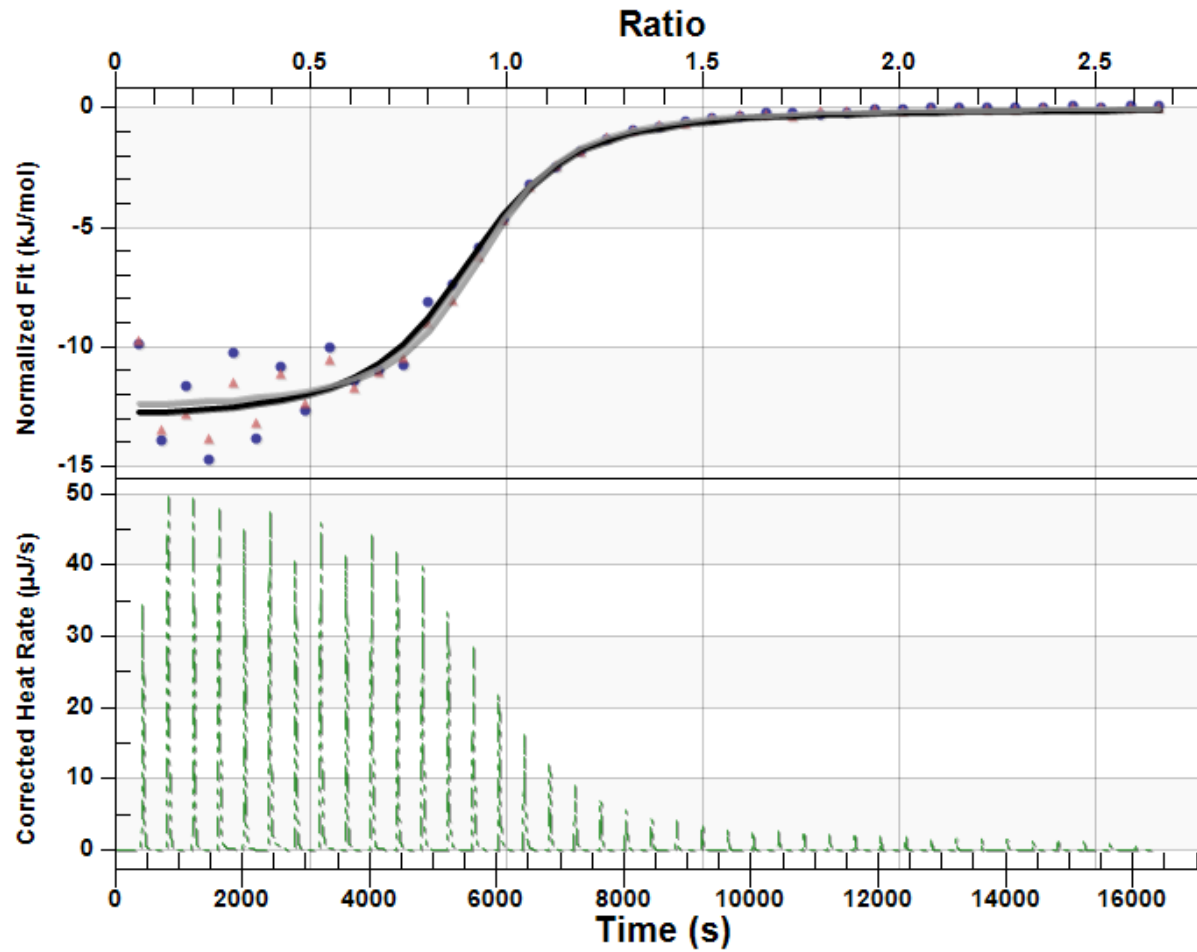
Figure C-10: ITC Thermogram of DCH18C6D Isomer Complexed with $BaCl_2 \cdot 2H_2O$ in Anhydrous Methanol
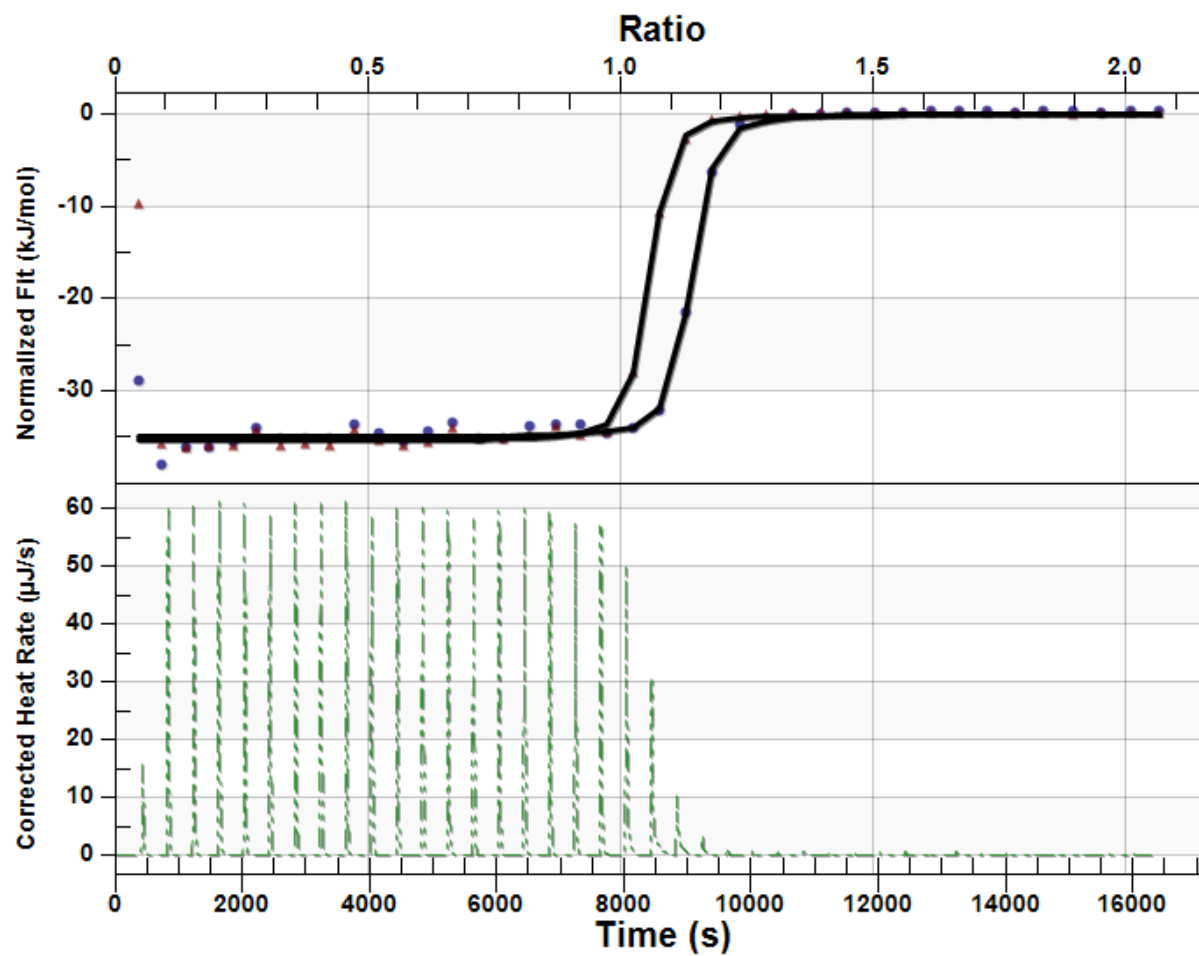
Figure C-11: ITC Thermogram of 4z,4'z *cis-syn-cis*-di-*tert*-butylcyclohexano-18-crown-6 Complexed with KCl in Anhydrous Methanol
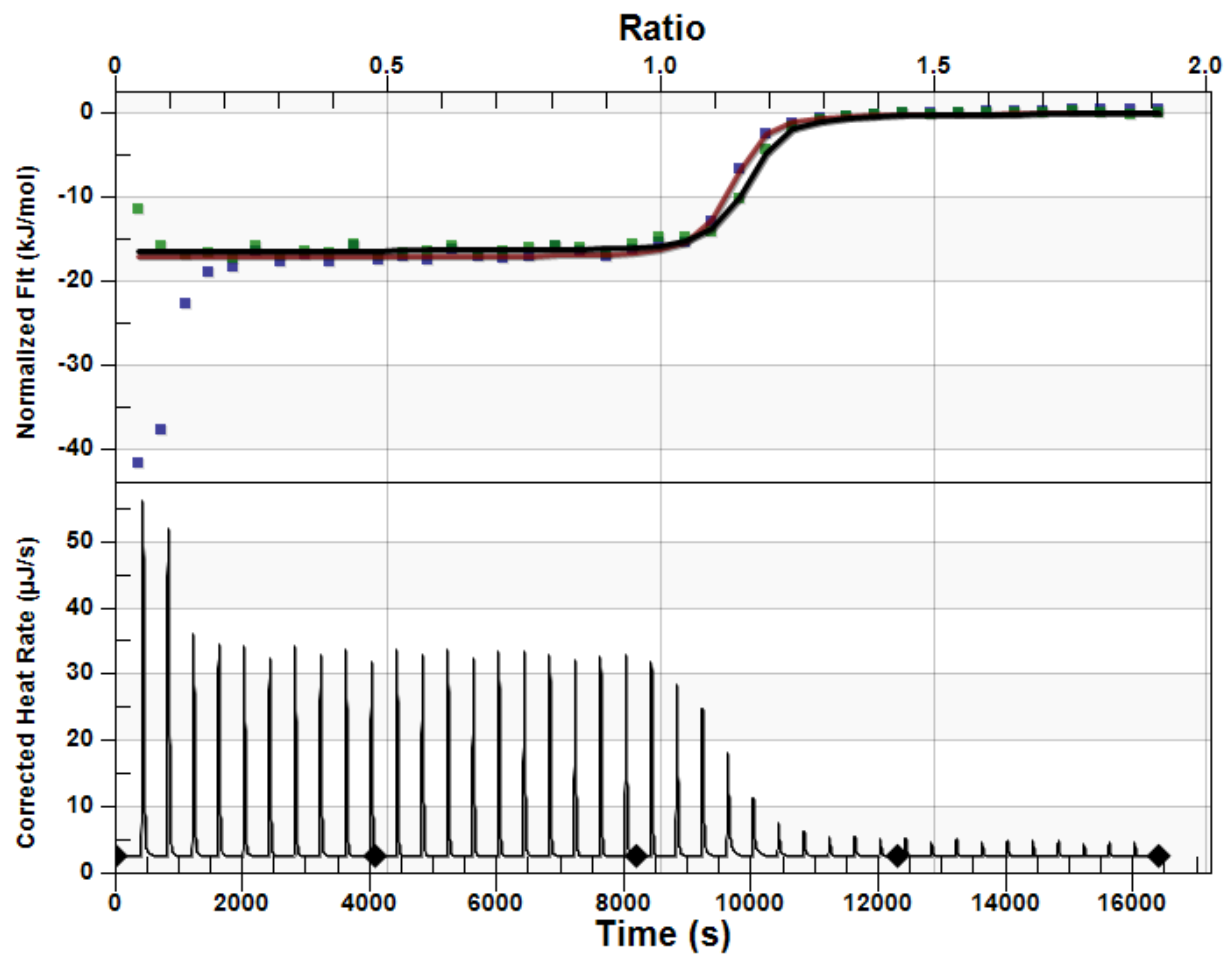
Figure C-12: ITC Thermogram of 4z,4'z *cis-syn-cis*-di-*tert*-butylcyclohexano-18-crown-6 Complexed with $SrCl_2 \cdot 6H_2O$ in Anhydrous Methanol
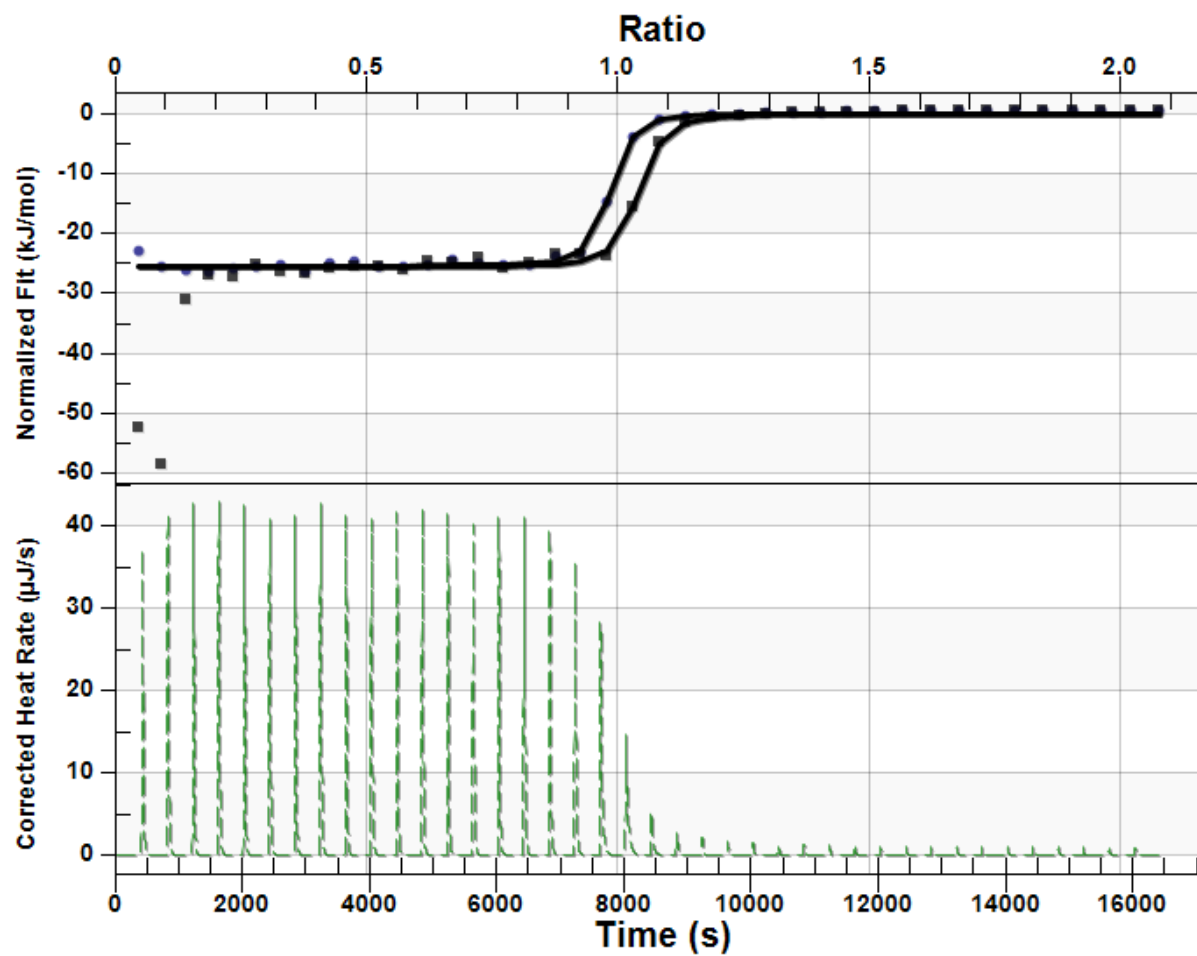
Figure C-13: ITC Thermogram of 4z,4'z *cis-syn-cis*-di-*tert*-butylcyclohexano-18-crown-6 Complexed with $BaCl_2 \cdot 2H_2O$ in Anhydrous Methanol
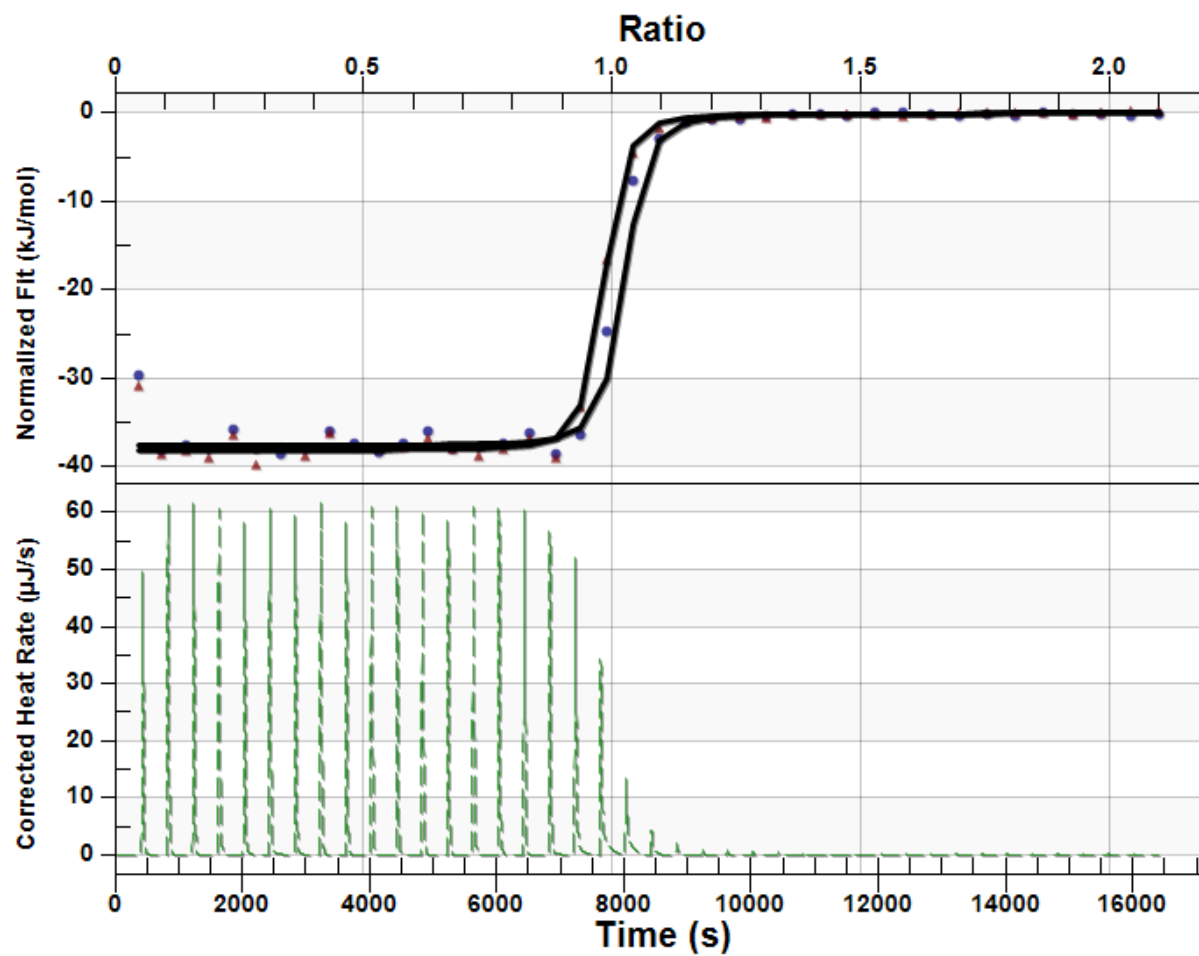
Figure C-14: ITC Thermogram of 4z,5'z *cis-syn-cis*-di-*tert*-butylcyclohexano-18-crown-6 Complexed with KCl in Anhydrous Methanol
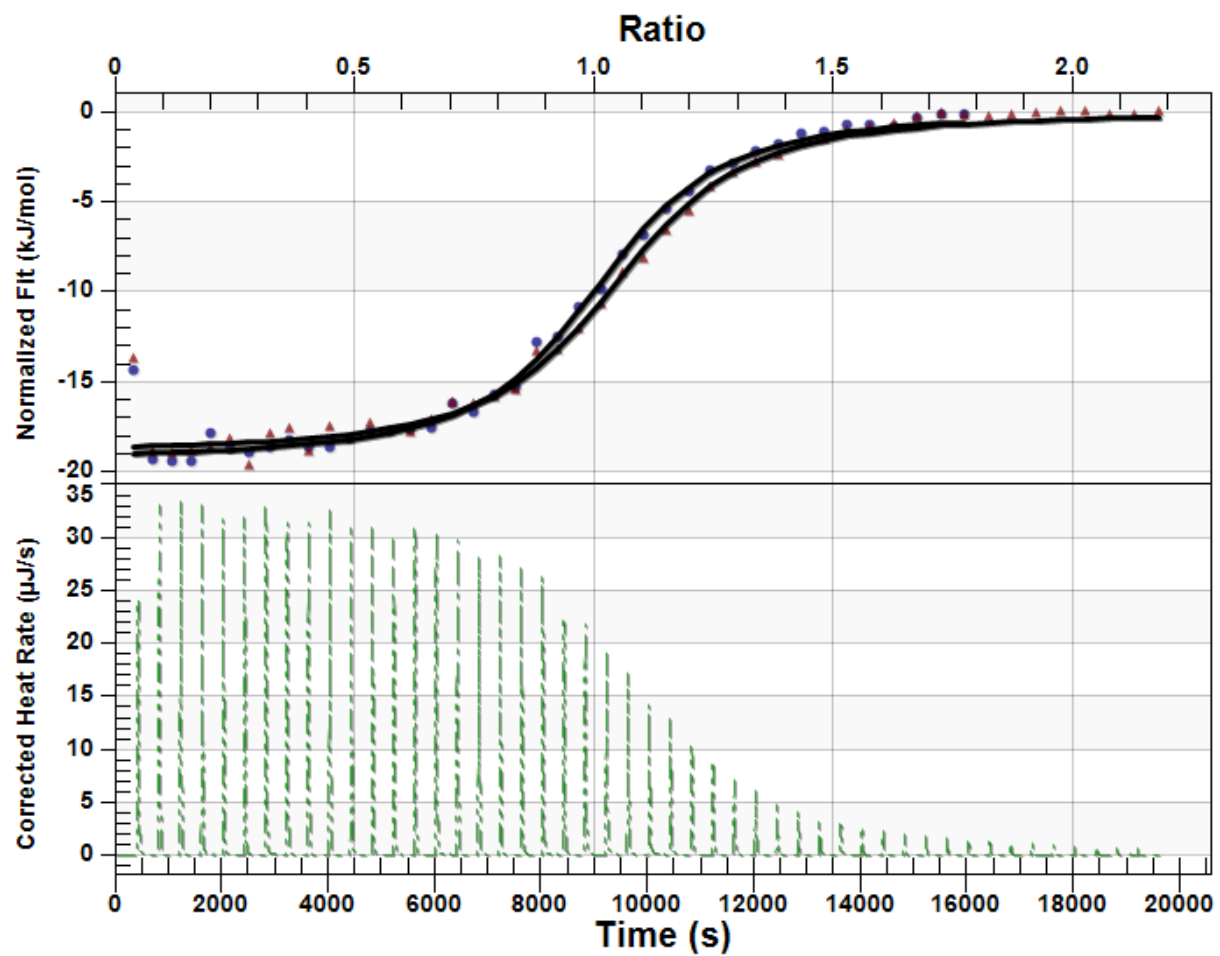
Figure C-15: ITC Thermogram of 4z,5'z *cis-syn-cis*-di-*tert*-butylcyclohexano-18-crown-6 Complexed with NaCl in Anhydrous Methanol
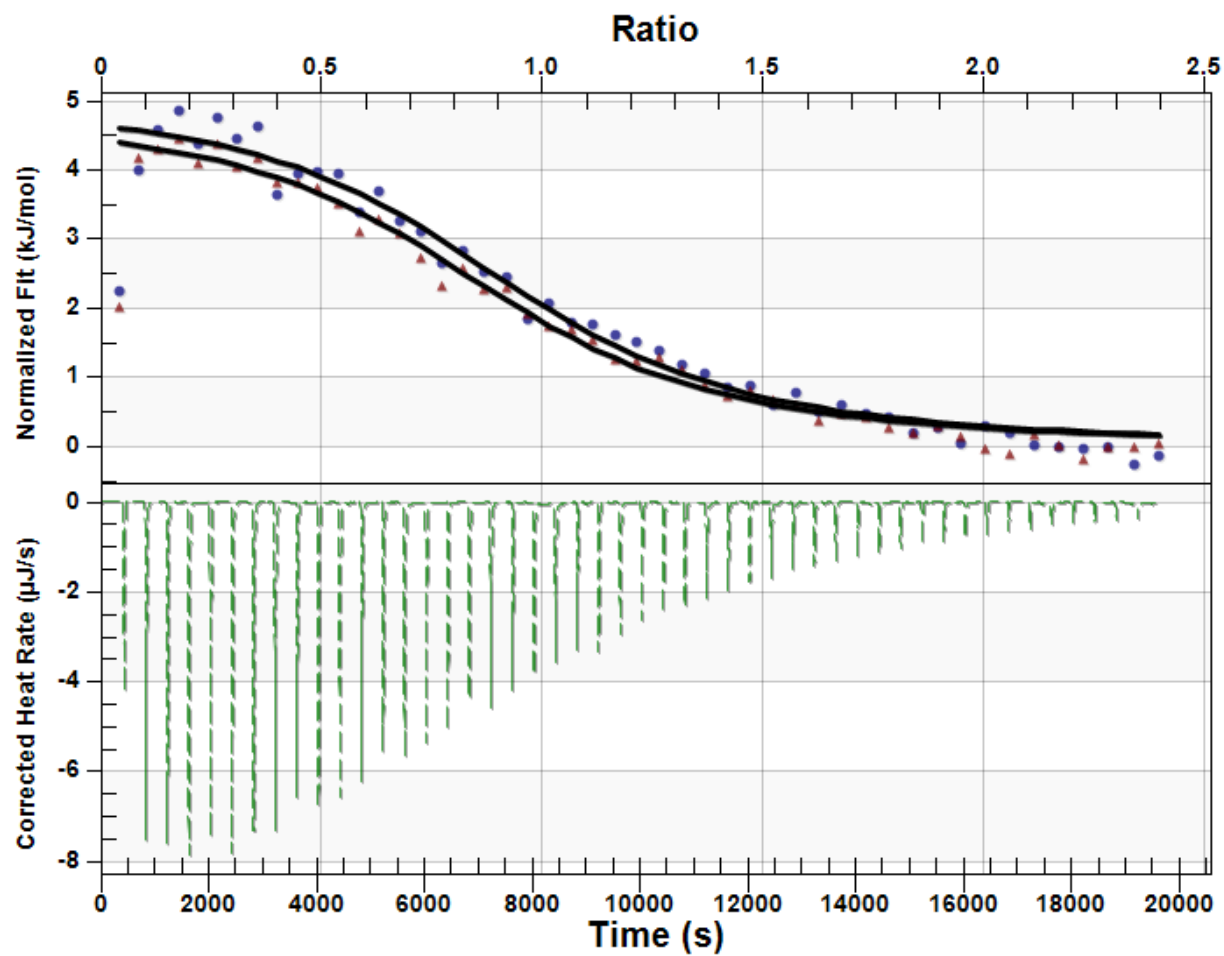
Figure C-16: ITC Thermogram of 4z,5'z *cis-syn-cis*-di-*tert*-butylcyclohexano-18-crown-6 Complexed with $CaCl_2 \cdot 2H_2O$ in Anhydrous Methanol
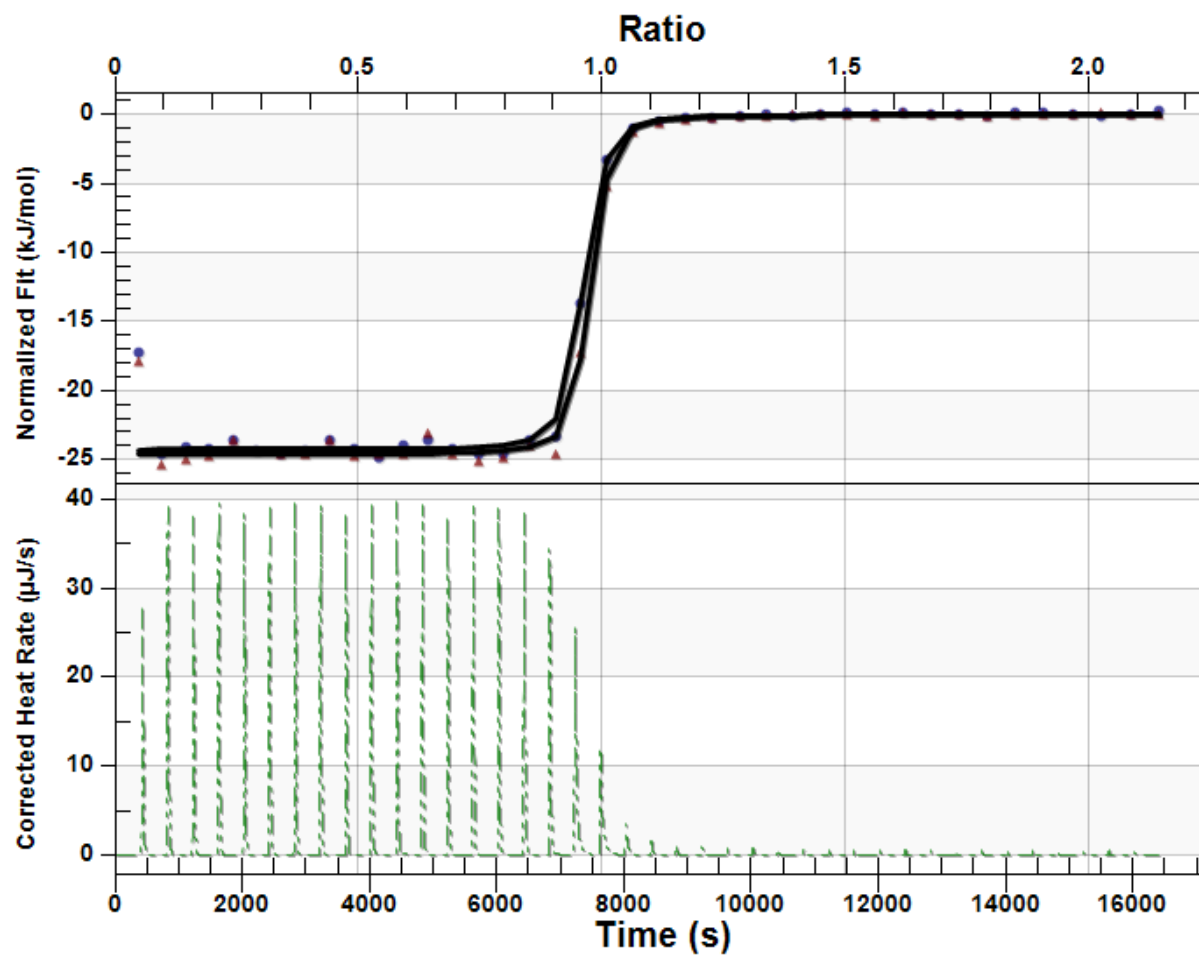
Figure C-17: ITC Thermogram of 4z,5'z *cis-syn-cis*-di-*tert*-butylcyclohexano-18-crown-6 Complexed with BaCl$_2$·2H$_2$O in Anhydrous Methanol
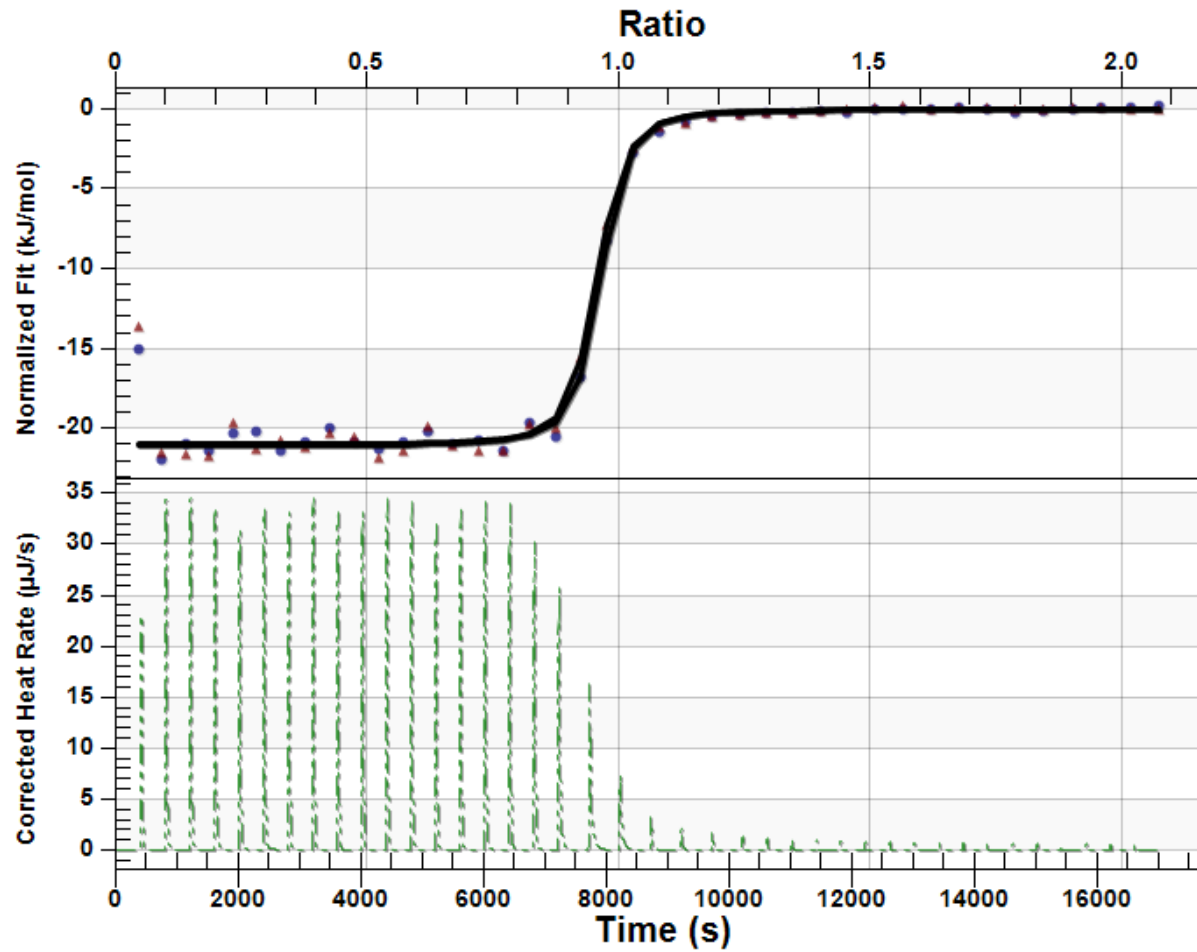
Figure C-18: ITC Thermogram of 4z,5'z *cis-syn-cis*-di-*tert*-butylcyclohexano-18-crown-6 Complexed with $SrCl_2 \cdot 6H_2O$ in Anhydrous Methanol

Table C-1: ITC Data for 4z,4'z *cis-syn-cis*-di-*tert*-butylcyclohexano-18-crown-6 with Various Metal Cations in Anhydrous Methanol

4z,4'zcscDtBuCh18C6		SrCl2		
		Run 1	Run 2	Average
	Ka	2.48E+05	2.09E+05	2.28E+05
	Log Ka	5.394	5.320	5.36
	n	1.106	1.136	1.12
J/mol*K	dS	45.890	46.900	46.40
kJ/mol*K	dS	0.046	0.047	0.05
kJ/mol	dH	-17.110	-16.380	-16.75
K	Temp	298.000	298.000	298.00
kJ/mol	dG	-30.785	-30.356	-30.57
kJ/mol	-TdS	-13.67522	-13.9762	-13.83
4z,4'zcscDtBuCh18C6		BaCl2		
		Run 1	Run 2	Average
	Ka	4.14E+05	4.92E+05	4.53E+05
	Log Ka	5.617	5.692	5.654
	n	1.017	0.960	0.989
J/mol*K	dS	21.560	23.650	22.605
kJ/mol*K	dS	0.022	0.024	0.023
kJ/mol	dH	-25.630	-25.440	-25.535
K	Temp	298.000	298.000	298.000
kJ/mol	dG	-32.055	-32.488	-32.271
kJ/mol	-TdS	-6.42488	-7.0477	-6.736
4z,4'zcscDtBuCh18C6		KCl		
		Run 1	Run 2	Average
	Ka	5.53E+05	5.81E+05	5.67E+05
	Log Ka	5.743	5.764	5.754
	n	1.116	1.032	1.074
J/mol*K	dS	-7.332	-8.253	-7.793
kJ/mol*K	dS	-0.007	-0.008	-0.008
kJ/mol	dH	-34.960	-35.360	-35.160
K	Temp	298.000	298.000	298.000
kJ/mol	dG	-32.775	-32.901	-32.838
kJ/mol	-TdS	2.184936	2.459394	2.322

Table C-2: ITC Data for 4z,5'z *cis-syn-cis*-di-*tert*-butylcyclohexano-18-crown-6 with Various Metal Cations in Anhydrous Methanol

4z,5'z csc		CaCl2		
		Run 1	Run 2	Average
	Ka	2.10E+03	2.03E+03	2.06E+03
	Log Ka	3.323	3.307	3.315
	n	0.972	0.933	0.953
J/mol*K	dS	80.530	79.550	80.040
kJ/mol*K	dS	0.081	0.080	0.080
kJ/mol	dH	5.046	4.844	4.945
K	Temp	298.000	298.000	298.000
kJ/mol	dG	-18.952	-18.862	-18.907
kJ/mol	-TdS	-23.99794	-23.7059	-23.852
4z,5'z csc		SrCl2		
		Run 1	Run 3	Average
	Ka	3.37E+05	2.98E+05	3.18E+05
	Log Ka	5.528	5.475	5.501
	n	0.942	0.934	0.938
J/mol*K	dS	35.650	34.120	34.885
kJ/mol*K	dS	0.036	0.034	0.035
kJ/mol	dH	-20.920	-21.070	-20.995
K	Temp	298.000	298.000	298.000
kJ/mol	dG	-31.544	-31.238	-31.391
kJ/mol	-TdS	-10.6237	-10.16776	-10.396
4z,5'z csc		BaCl2		
		Run 1	Run 2	Average
	Ka	7.21E+05	6.76E+05	6.98E+05
	Log Ka	5.858	5.830	5.844
	n	0.938	0.952	0.945
J/mol*K	dS	30.620	29.280	29.950
kJ/mol*K	dS	0.031	0.029	0.030
kJ/mol	dH	-24.310	-24.540	-24.425
K	Temp	298.000	298.000	298.000
kJ/mol	dG	-33.435	-33.265	-33.350
kJ/mol	-TdS	-9.12476	-8.72544	-8.925

APPENDIX D

HPLC CHROMATOGRAMS

Figures D-1 to D-10 - Perchloric Acid Contacts / Remaining Hexane Layers – (Experimental Parameters Were the Same as Figure 5.2)

Figures D-11 to D-14 - Chromatograms Associated with Mass Chromatograms (#14, 16, 18, 20) – (Experimental Parameters Were the Same as Figure 5.2)

Figures D-15 to D-19 - Column Loading Studies (Experimental Parameters for D-15-D17 Were the Same as Figure 5.9 With Different Masses and Experimental Parameters for D-18 and D-19 Were the Same as Figure 5.13 With Different Masses)

Figure D-20 – Sulfamic Acid Treated DtBuCH18C6 (Experimental Parameters Were the Same as Figure 6.10)

Figure D-21 – Sulfaguanidine Treated DtBuCH18C6 (Experimental Parmeters Were the Same as Figure 6.11)

Figures D-22 to D-31 – Chromatograms Assoicated with Prep Sample Fractions (Experimental Parameters Were the Same as Figure 5.2)

Figures D-32 to D-35 – Spiking Experiments (Experimental Parameters Were the Same as Figure 5.2)

Figure D-36 - HPLC-ELSD Chromatograms for Spiked (with the 4z, 5'z *cis-syn-cis* isomer) and Unspiked DtBuCH18C6 Samples

Figure D-37 - Representative Chromatogram Showing the Identity of Peaks Present in a Perchloric Acid Purified Sample of DtBuCH18C6

ELS1 A, Voltage (EICHROM B1 2010-04-08 11-24-56/EICHROM NC-1.D)

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Area Percent Report

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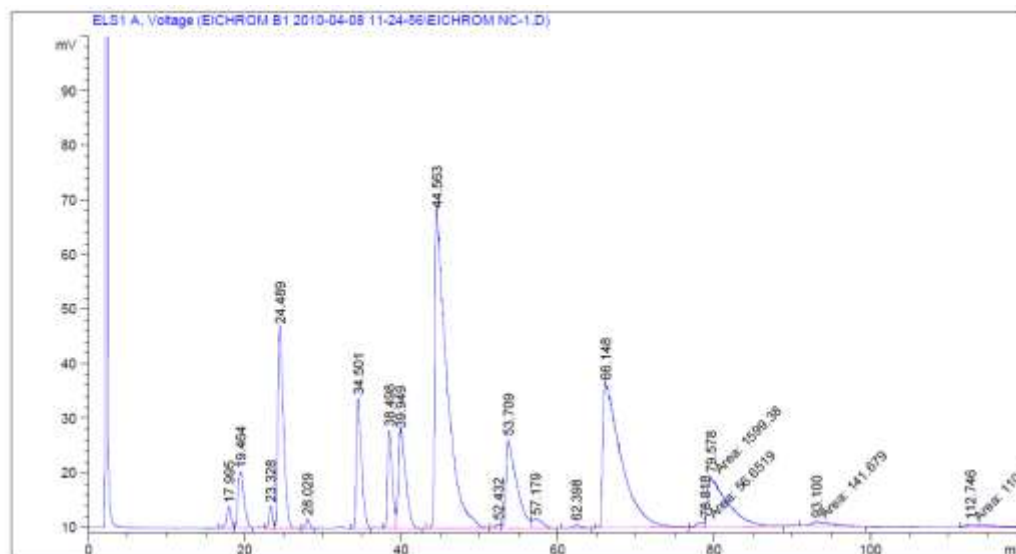
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Multiplier: :   1.0000
Dilution: :   1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: ELS1 A, Voltage

| Peak | RetTime | Type | Width | Area | Height | Area |
#	[min]		[min]	[mV*s]	[mV]	%
1	17.995	BV	0.6019	154.20039	3.92913	0.7770
2	19.464	VB	0.8575	554.44598	10.21050	2.7939
3	23.328	BV	0.4682	117.08266	4.01466	0.5900
4	24.489	VB	0.7738	1833.40076	36.76768	9.2386
5	28.029	BB	0.5154	53.92912	1.69394	0.2718
6	34.501	BB	0.6728	1077.18396	23.76514	5.4280
7	38.498	BV	0.6408	740.27356	17.96422	3.7303

| Peak | RetTime | Type | Width | Area | Height | Area |
#	[min]		[min]	[mV*s]	[mV]	%
8	39.949	VB	0.9758	1165.52771	17.70972	5.8731
9	44.563	BB	1.4886	6209.68799	58.02436	31.2908
10	52.432	BV	0.6733	30.45936	7.14635e-1	0.1535
11	53.709	VV	1.3160	1521.20801	16.25181	7.6654
12	57.179	VB	1.1533	154.01924	1.67413	0.7761
13	62.358	BB	1.0161	39.52498	5.38619e-1	0.1992
14	66.148	BB	2.1222	4285.80908	26.34118	21.5963
15	78.818	MF	0.9755	56.65186	9.67888e-1	0.2855
16	79.578	FM	2.8901	1599.38049	9.22339	8.0593
17	93.100	MM	2.8204	141.67867	8.37216e-1	0.7139
18	112.746	MM	3.3374	110.63864	5.52515e-1	0.5575

Totals :   1.98451e4   231.18074

Figure D-1: Untreated Commerical Material
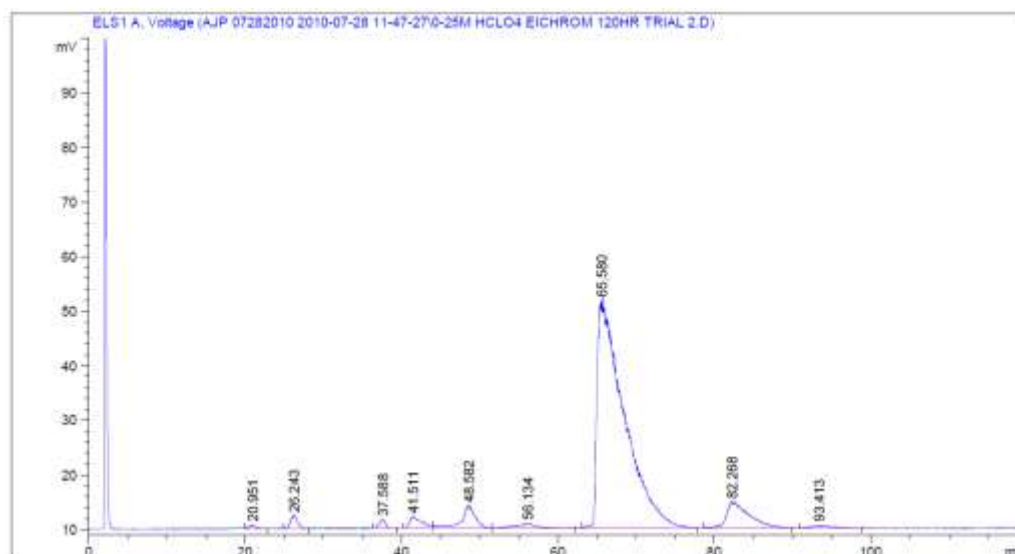
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=================================================================
                    Area Percent Report
=================================================================

Sorted By           :       Signal
Multiplier:                 :      1.0000
Dilution:                   :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: ELS1 A, Voltage

Peak RetTime Type  Width      Area        Height     Area
  #   [min]        [min]    [mV*s]        [mV]        %
----|-------|----|-------|----------|----------|--------|
  1  20.951 VB    0.9285   39.39772 5.85933e-1   0.3207
  2  26.243 BB    0.9824  146.37407   2.30036    1.1914
  3  37.588 BB    0.8425   92.85360   1.58733    0.7558
  4  41.511 BV    1.4835  233.34235   2.13425    1.8993
  5  48.582 VV    1.6308  511.93103   4.10551    4.1668
  6  56.134 VB    2.9410  195.23633 9.53406e-1   1.5891
  7  65.580 BB    3.0076 9991.48535  41.63720   81.3243
  8  82.268 BB    2.5805  978.33087   4.81086    7.9630


Peak RetTime Type  Width      Area        Height     Area
  #   [min]        [min]    [mV*s]        [mV]        %
----|-------|----|-------|----------|----------|--------|
  9  93.413 BB    2.8024   97.02283 4.18242e-1   0.7897

Totals :                   1.22860e4   58.43310
```

Figure D-2: 0.25M Perchloric Acid Treated DtBuCH18C6

Figure D-3: 0.50M Perchloric Acid Treated DtBuCH18C6

Figure D-4: 1.00M Perchloric Acid Treated DtBuCH18C6

Figure D-5: 3.00M Perchloric Acid Treated DtBuCH18C6

Figure D-6: 6.00M Perchloric Acid Treated DtBuCH18C6

ELS1 A, Voltage (HEXANE LAYER HCLO4 TREATMENT 2010-09-14 14-55-23\HEXANE LAYER 0-25M.D)

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==================================================================
                    Area Percent Report
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Sorted By            :        Signal
Multiplier:          :        1.0000
Dilution:            :        1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: ELS1 A, Voltage

Peak RetTime Type  Width      Area       Height      Area
  #   [min]        [min]     [mV*s]       [mV]         %
----|-------|----|-------|----------|----------|--------|
  1  18.654 BV    0.7902   104.39639    2.03600    2.3243
  2  19.947 VV    0.9189   234.00165    3.67473    5.2099
  3  24.816 VB    0.8970   620.24158   10.50264   13.8093
  4  36.605 BB    0.9875   368.05780    5.74451    8.1946
  5  41.115 BV    1.0879   705.08795   10.49360   15.6984
  6  43.755 VV    1.4415  1135.45300   10.33729   25.2802


Peak RetTime Type  Width      Area       Height      Area
  #   [min]        [min]     [mV*s]       [mV]         %
----|-------|----|-------|----------|----------|--------|
  7  47.722 VB    1.4881   350.92645    3.36667    7.8132
  8  54.583 BB    1.3867   396.08112    4.08681    8.8185
  9  67.701 BB    2.1008   340.39810    2.02945    7.5788
 10  81.595 BB    2.3720   236.83116    1.27680    5.2729

Totals :                  4491.47520   53.54850
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Figure D-7: 0.25M Hexane Layer Containing Uncomplexed Crown Ether and Contaminants
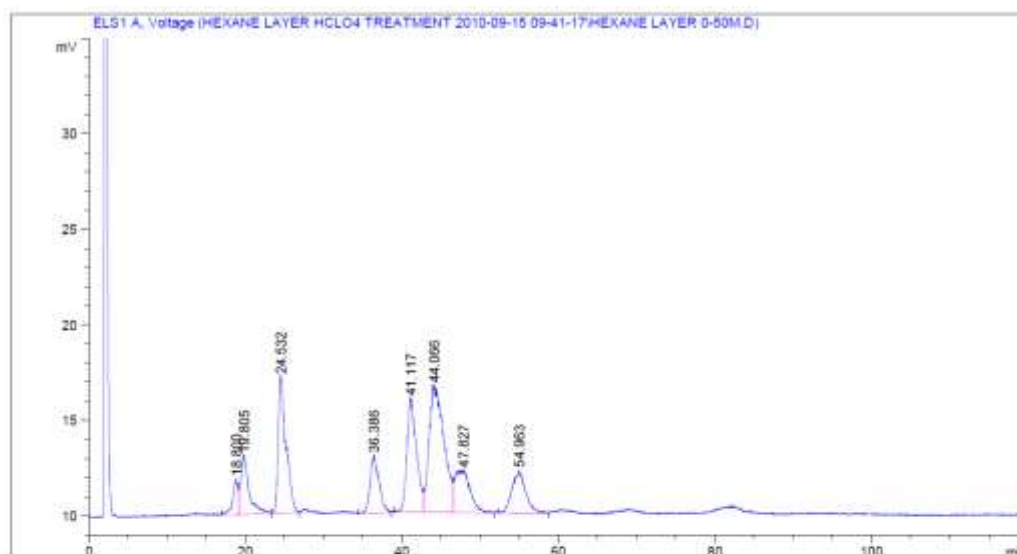
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                        Area Percent Report
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Sorted By   :   Signal
Multiplier: :   1.0000
Dilution: :   1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: ELS1 A, Voltage

Peak #	RetTime [min]	Type	Width [min]	Area [mV*s]	Height [mV]	Area %
1	18.800	BV	0.7185	86.76897	1.81258	2.9029
2	19.805	VV	1.0182	227.21574	3.03231	7.6016
3	24.532	VB	1.0218	493.17615	7.07027	16.4995
4	36.386	BB	1.1308	238.36314	2.96231	7.9746
5	41.117	BV	1.1436	499.10922	5.91983	16.6980
6	44.066	VV	1.6701	879.87830	6.58851	29.4369

Peak #	RetTime [min]	Type	Width [min]	Area [mV*s]	Height [mV]	Area %
7	47.827	VB	1.7663	297.13638	2.17986	9.9409
8	54.963	BB	1.4909	267.38458	2.21092	8.9455

Totals :   2989.03249   31.77658

Figure D-8: 0.50M Hexane Layer Containing Uncomplexed Crown Ether and
Contaminants

Figure D-9: 1.00M Hexane Layer Containing Uncomplexed Crown Ether and Contaminants

Figure D-10: 3.00M Hexane Layer Containing Uncomplexed Crown Ether and
Contaminants

Figure D-11: Fraction #14 Associated with Mass Chromatogram (Bench-Top Chromatography)
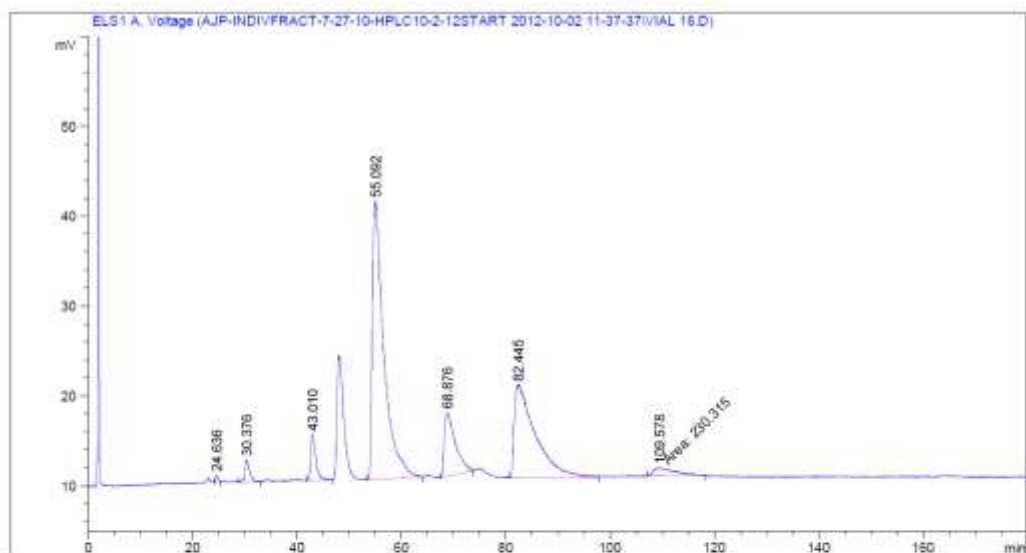
ELS1 A, Voltage (AJP-INDIVFRACT-7-27-10-HPLC10-2-12START 2012-10-02 11-37-37/VIAL 16.D)

```
=================================================================
                     Area Percent Report
=================================================================

Sorted By            :        Signal
Multiplier:          :        1.0000
Dilution:            :        1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: ELS1 A, Voltage

Peak RetTime Type  Width     Area        Height      Area
  #   [min]        [min]    [mV*s]       [mV]         %
----|-------|----|-------|----------|----------|--------|
  1  24.636 BB    0.5632   29.00881 8.07390e-1  0.3057
  2  30.376 BB    0.9316  161.36515   2.43982   1.7004
  3  43.010 BV    1.0063  355.40250   5.09174   3.7450
  4  55.092 BB    2.1155 4760.58008  30.93371  50.1643
  5  68.876 BB    2.0731 1050.45654   7.05487  11.0691
  6  82.445 BB    3.5766 2902.84839  10.24817  30.5886

Peak RetTime Type  Width     Area        Height      Area
  #   [min]        [min]    [mV*s]       [mV]         %
----|-------|----|-------|----------|----------|--------|
  7 109.578 MM    4.3590  230.31539 9.80609e-1  2.4269

Totals :                  9489.97689  57.45631
```

Figure D-12: Fraction #16 Associated with Mass Chromatogram (Bench-Top Chromatography)
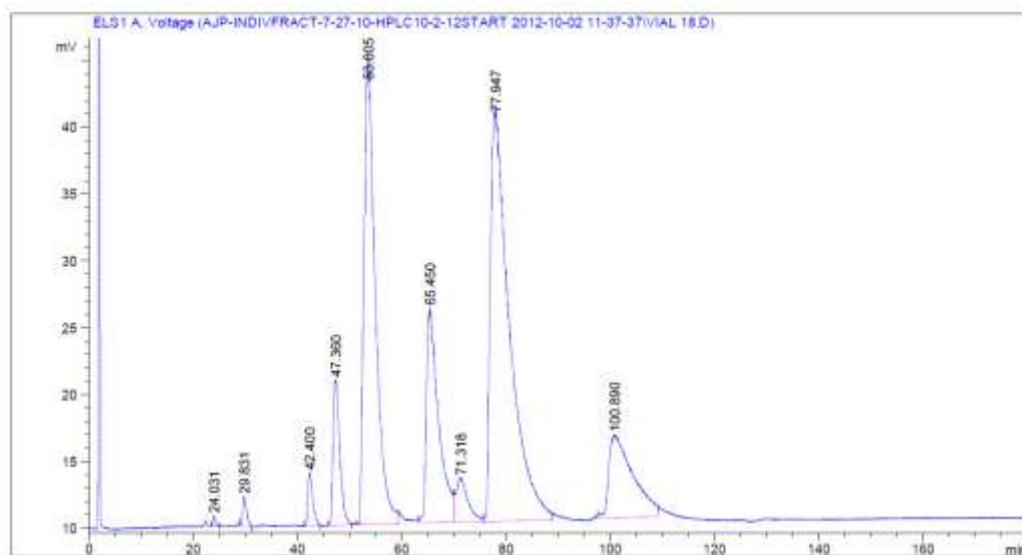
ELS1 A, Voltage (AJP-INDIVFRACT-7-27-10-HPLC10-2-12START 2012-10-02 11-37-37(VIAL 18.D)

```
========================================================================
                         Area Percent Report
========================================================================

Sorted By            :       Signal
Multiplier:                  :        1.0000
Dilution:                    :        1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: ELS1 A, Voltage

Peak RetTime Type  Width     Area       Height    Area
 #   [min]        [min]   [mV*s]     [mV]      %
----|-------|----|-------|----------|----------|--------|
  1   24.031 BB    0.6418    31.06918 7.52281e-1  0.1584
  2   29.831 BB    0.8988   123.23663   2.13059   0.6282
  3   42.400 BB    1.0224   255.43542   3.88844   1.3021
  4   47.360 BB    1.3886   961.06354  10.81667   4.8992
  5   53.605 BB    2.2445  5279.05127  34.90538  26.9109
  6   65.450 BV    2.4166  2608.40747  15.97781  13.2968
Peak RetTime Type  Width     Area       Height    Area
 #   [min]        [min]   [mV*s]     [mV]      %
----|-------|----|-------|----------|----------|--------|
  7   71.318 VB    2.3070   528.37347   3.20562   2.6935
  8   77.947 BB    3.5270  7837.27734  30.32670  39.9520
  9  100.890 BB    4.4286  1992.83057   6.13682  10.1588

Totals :                  1.96167e4  109.14030
```

Figure D-13: Fraction #18 Associated with Mass Chromatogram (Bench-Top Chromatography)

Figure D-14: Fraction #20 Associated with Mass Chromatogram (Bench-Top Chromatography)

Figure D-15 : Perchloric Acid Treated 18.13mg/mL Sample of DtBuCH18C6
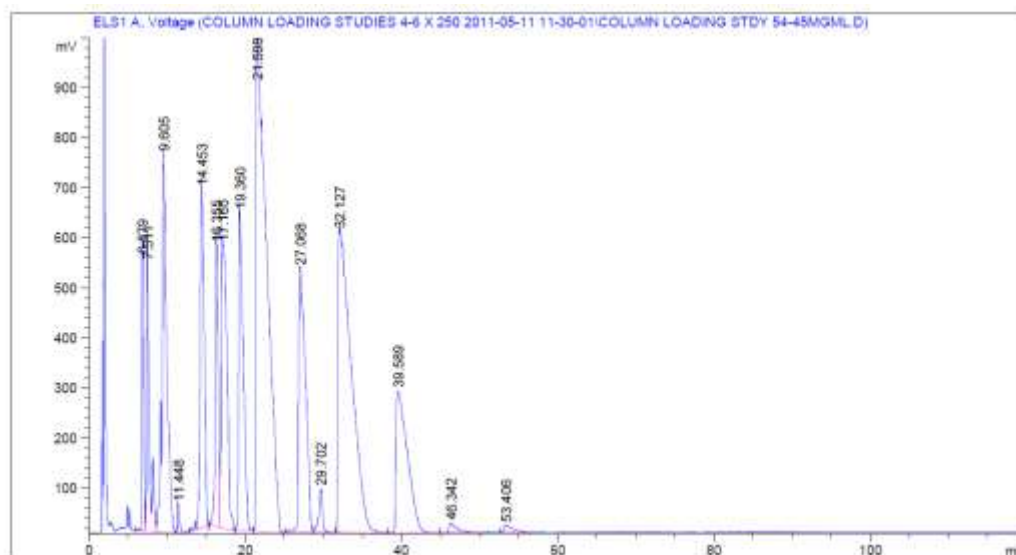
```
============================================================
              Area Percent Report with Performance
============================================================

Multiplier:                    :      1.0000
Dilution:                      :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: ELS1 A, Voltage
```

RetTime [min]	k'	Area [mV*s]	Height [mV]	Symm.	Width [min]	Plates	Resolution	Selectivity
6.879	-	9003.39648	547.18640	0.81	0.2483	4250	-	-
7.511	-	1.42897e4	535.07275	0.43	0.3267	2929	1.29	1.09
9.605	-	3.19203e4	753.67499	0.63	0.5150	1927	2.92	1.28
11.448	-	1083.38293	54.89536	0.65	0.2817	9152	2.72	1.19
14.453	-	2.47146e4	677.45197	0.66	0.5717	3541	4.14	1.26
16.355	-	1.60470e4	561.98151	0.84	0.4417	7597	2.21	1.13

RetTime [min]	k'	Area [mV*s]	Height [mV]	Symm.	Width [min]	Plates	Resolution	Selectivity
17.165	-	2.98570e4	565.25623	0.44	0.8683	2165	0.73	1.05
19.360	-	2.58156e4	634.76624	0.40	0.6400	5069	1.71	1.13
21.598	-	9.41524e4	980.21313	0.16	1.5667	1053	1.19	1.12
27.068	-	3.24569e4	525.94324	0.32	1.0450	3717	2.46	1.25
29.702	-	2959.69653	87.56612	1.26	0.4367	25631	2.09	1.10
32.127	-	7.20581e4	600.52783	0.15	1.8717	1632	1.23	1.08
39.589	-	2.89114e4	282.33960	0.22	1.6650	3132	2.48	1.23
46.342	-	1337.71936	17.91103	0.27	1.0350	11107	2.94	1.17
53.406	-	1211.76306	13.89697	0.29	1.2567	10006	3.62	1.15

Figure D-16 : Perchloric Acid Treated 54.45mg/mL Sample of DtBuCH18C6
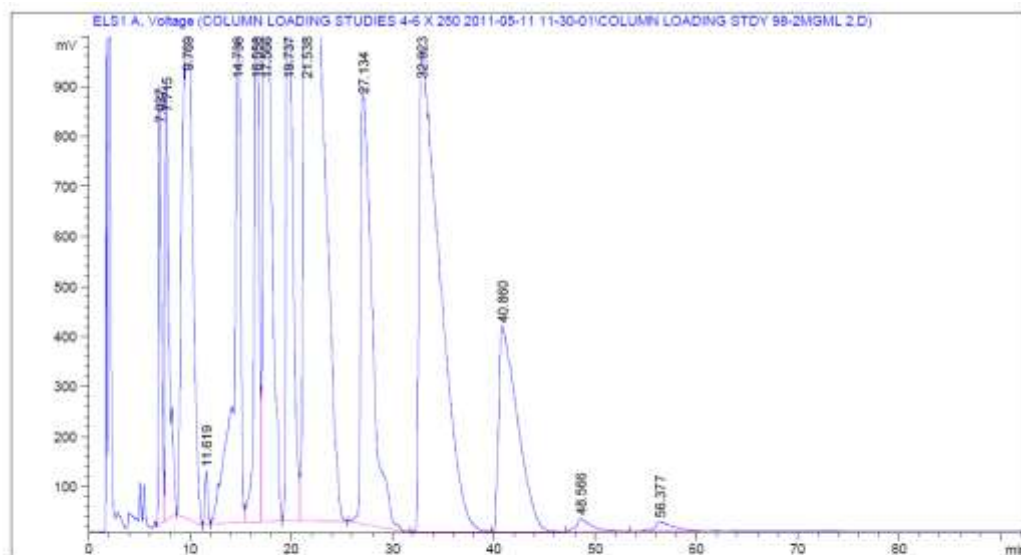
ELS1 A, Voltage (COLUMN LOADING STUDIES 4-6 X 250 2011-05-11 11-30-01\COLUMN LOADING STDY 98-2MGML 2.D)

```
=================================================================
                  Area Percent Report with Performance
=================================================================

Multiplier:                        :      1.0000
Dilution:                          :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: ELS1 A, Voltage
```

RetTime [min]	k'	Area [mV*s]	Height [mV]	Symm.	Width [min]	Plates	Resolution	Selectivity
7.027	-	1.64027e4	795.02533	0.72	0.3167	2728	-	-
7.715	-	2.34353e4	807.89081	0.47	0.3750	2345	1.17	1.10
9.769	-	7.35409e4	971.21692	1.01	1.2633	331	1.47	1.27
11.619	-	2127.65112	106.47315	0.96	0.3133	7618	1.38	1.19
14.736	-	5.01195e4	982.92609	1.74	0.5450	4050	4.27	1.27
16.558	-	3.61801e4	979.36255	0.88	0.5550	4931	1.95	1.12

RetTime [min]	k'	Area [mV*s]	Height [mV]	Symm.	Width [min]	Plates	Resolution	Selectivity
17.566	-	6.62932e4	976.28387	0.58	1.0267	1622	0.75	1.06
19.737	-	4.98207e4	975.04034	0.52	0.7867	3487	1.41	1.12
21.538	-	1.57247e5	975.45691	0.18	2.6400	369	0.62	1.09
27.134	-	6.72079e4	852.04755	0.27	1.1600	3031	1.73	1.26
32.923	-	1.36110e5	963.26263	0.16	2.2683	1167	1.98	1.21
40.860	-	5.26717e4	409.16028	0.24	2.0267	2252	2.17	1.24
48.566	-	2613.32861	25.37505	0.40	1.2733	8059	2.74	1.19
56.377	-	2435.44775	19.30818	0.41	1.6117	6779	3.18	1.16

Figure D-17 : Perchloric Acid Treated 98.2mg/mL Sample of DtBuCH18C6

Figure D-18 : Perchloric Acid Treated 36.3mg/mL Sample of DtBuCH18C6

Figure D-19 : Perchloric Acid Treated 71.4mg/mL Sample of DtBuCH18C6
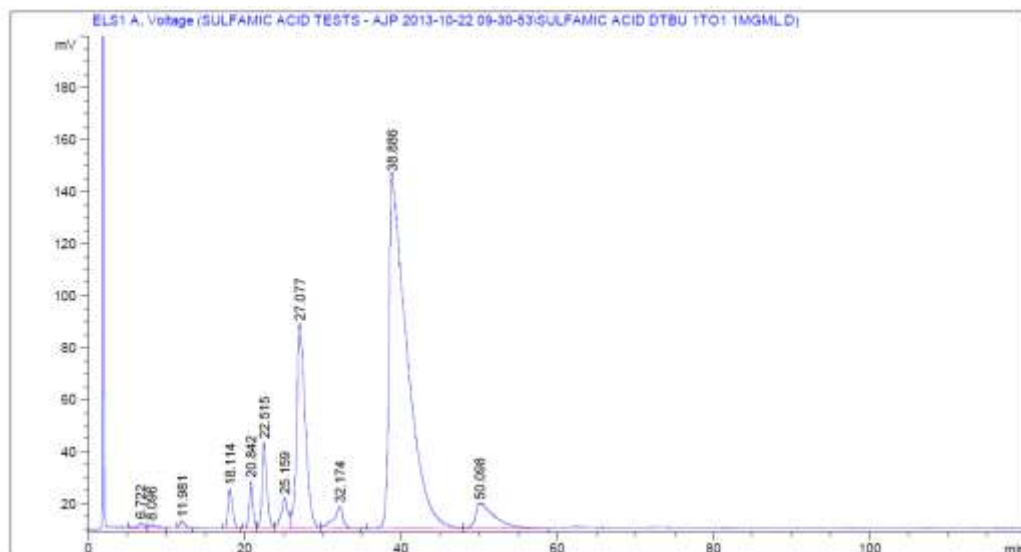
```
================================================================
                     Area Percent Report
================================================================

Sorted By            :        Signal
Multiplier:          :        1.0000
Dilution:            :        1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: ELS1 A, Voltage

Peak RetTime Type  Width    Area        Height      Area
 #   [min]         [min]    [mV*s]      [mV]         %
----|-------|----|-------|----------|----------|--------|
  1   6.722 BV    0.5491   69.75668    1.86202   0.2087
  2   8.096 VB    0.7044   60.61063    1.16227   0.1814
  3  11.981 BB    0.5728   97.36393    2.55390   0.2914
  4  18.114 BB    0.6254  597.04810   14.96827   1.7867
  5  20.842 BV    0.4857  567.84442   17.72591   1.6993
  6  22.515 VV    0.6084 1355.11072   32.90879   4.0552

Peak RetTime Type  Width    Area        Height      Area
 #   [min]         [min]    [mV*s]      [mV]         %
----|-------|----|-------|----------|----------|--------|
  7  25.159 VV    0.7825  654.37720   11.66410   1.9582
  8  27.077 VV    1.0929 5964.15430   78.63379  17.8478
  9  32.174 VB    1.1756  717.36340    8.50900   2.1467
 10  38.886 BV    2.0521 2.16912e4   136.05058  64.9112
 11  50.098 VB    2.2142 1641.89673    9.47262   4.9134

Totals :                 3.34168e4   315.51125
```

Figure D-20: Sulfamic Acid Treated DtBuCH18C6

Figure D-21: Sulfaguanidine Treated DtBuCH18C6

```
                              Area Percent Report
```

```
Sorted By              :       Signal
Multiplier:            :       1.0000
Dilution:              :       1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: ELS1 A, Voltage

Peak RetTime Type  Width     Area        Height    Area
 #   [min]        [min]    [mV*s]       [mV]        %
----|-------|----|-------|----------|----------|--------|
 1  21.755 BV  0.8185 1076.71558   19.55058  47.8613
 2  23.514 VB  1.0764 1172.94226   16.36160  52.1387

Totals :                2249.65784  35.91218
```

Figure D-22: Chromatogram of Prep Sample Fraction 5.8-6.6 Minutes
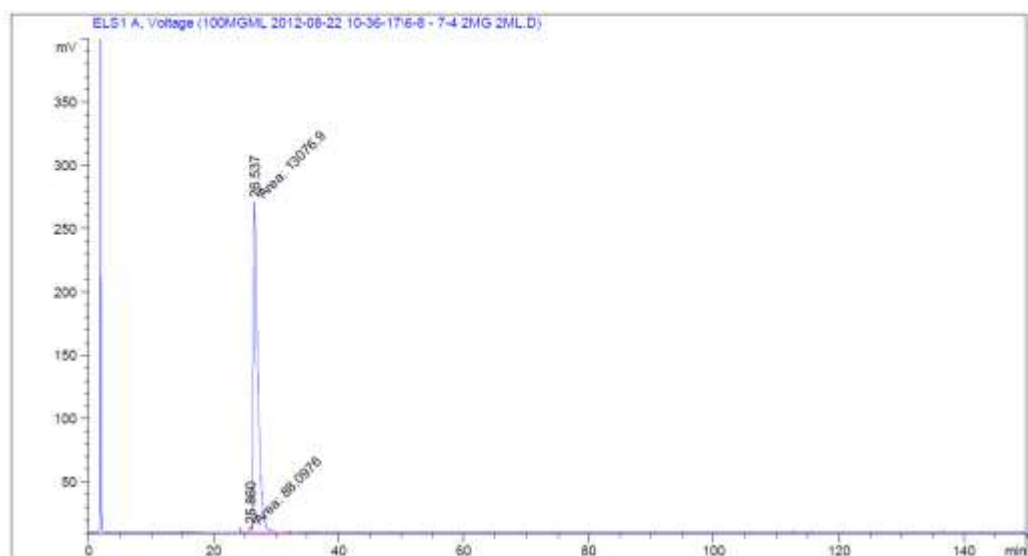
Figure D-23: Chromatogram of Prep Sample Fraction 6.8-7.4 Minutes
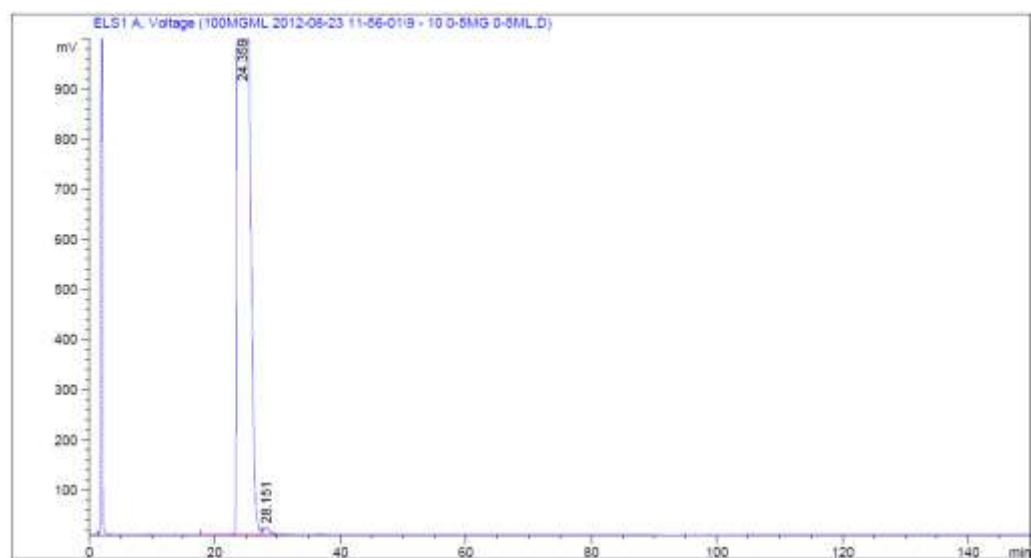
```
========================================================================
                         Area Percent Report
========================================================================

Sorted By            :      Signal
Multiplier:                 :       1.0000
Dilution:                   :       1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: ELS1 A, Voltage

Peak RetTime Type  Width     Area       Height      Area
  #   [min]        [min]    [mV*s]       [mV]         %
----|-------|----|-------|----------|-----------|--------|
  1  24.359 BV   1.8966 1.47311e5   989.66949   99.1990
  2  28.151 VV   1.1623 1189.44666   15.04630    0.8010

Totals :                 1.48500e5  1004.71579
```

Figure D-24: Chromatogram of Prep Sample Fraction 9-10 Minutes
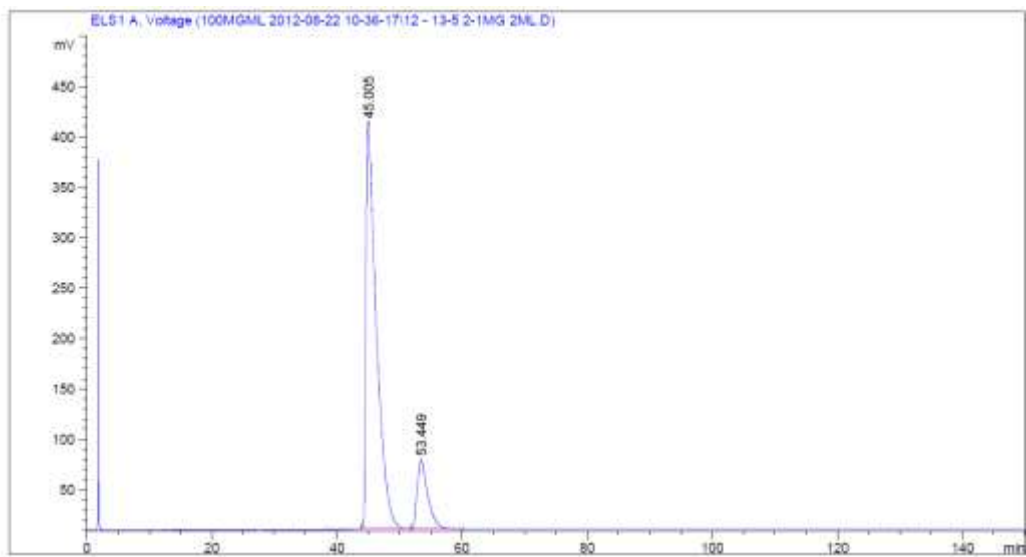
```
==================================================================
                        Area Percent Report
==================================================================

Sorted By           :        Signal
Multiplier:                  :      1.0000
Dilution:                    :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: ELS1 A, Voltage

Peak RetTime Type  Width     Area       Height      Area
 #    [min]        [min]     [mV*s]     [mV]          %
----|-------|----|-------|----------|----------|--------|
 1   45.005 BV    1.5823 4.64974e4   404.11984   85.1038
 2   53.449 VB    1.6480 8138.71338   69.00362   14.8962

Totals :                    5.46361e4   473.12347
```

Figure D-25: Chromatogram of Prep Sample Fraction 12-13.5 Minutes
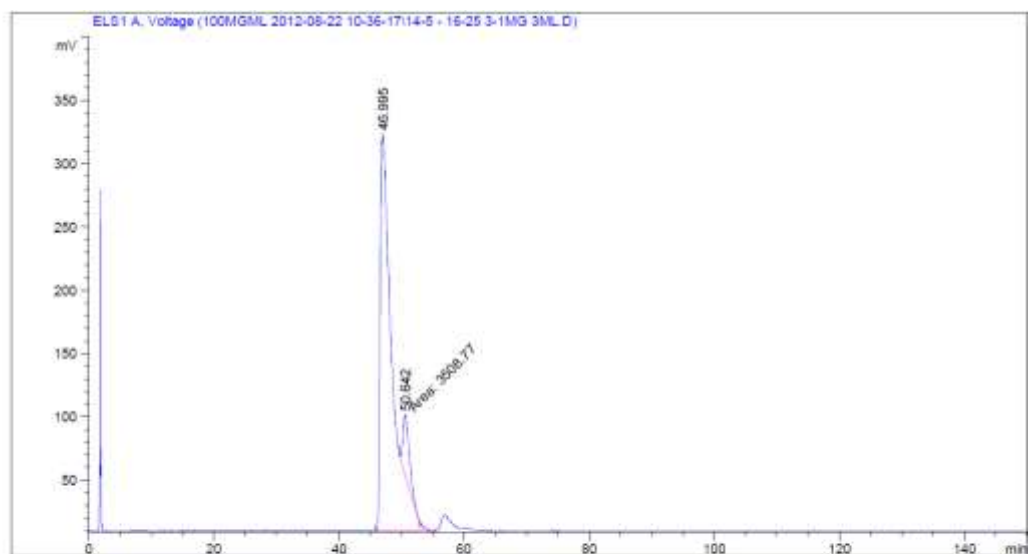
Figure D-26: Chromatogram of Prep Sample Fraction 14.5-16.25 Minutes
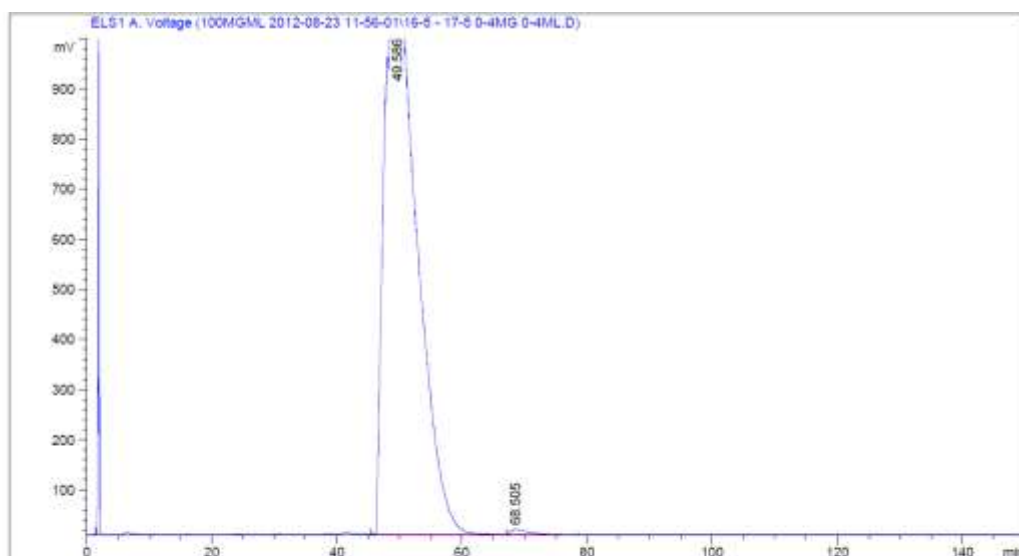
```
                           Area Percent Report
=========================================================================

Sorted By            :         Signal
Multiplier:                 :     1.0000
Dilution:                   :     1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: ELS1 A, Voltage

Peak RetTime Type  Width    Area        Height     Area
  #   [min]        [min]    [mV*s]      [mV]        %
----|-------|----|-------|----------|----------|--------|
  1   49.586 VB   4.7105 3.94375e5   990.22028  99.5767
  2   68.505 BB   2.2365 1676.58826    9.87636   0.4233

Totals :                   3.96052e5  1000.09664
```

Figure D-27: Chromatogram of Prep Sample Fraction 16.5-17.5 Minutes
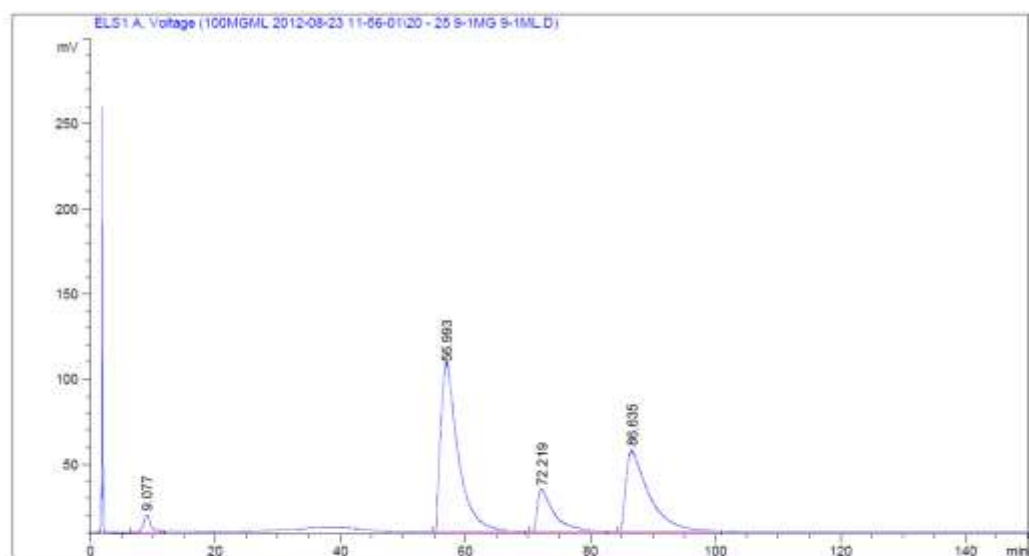
```
ELS1 A, Voltage (100MGML 2012-08-23 11-56-01(20 - 25 9-1MG 9-1ML.D)
```

```
==================================================================
                     Area Percent Report
==================================================================

Sorted By           :       Signal
Multiplier:                 :      1.0000
Dilution:                   :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: ELS1 A, Voltage

Peak RetTime Type  Width     Area       Height     Area
 #   [min]         [min]     [mV*s]     [mV]        %
----|-------|----|-------|----------|----------|--------|
  1   9.077 BV   1.1572  829.54224   10.37051   2.2783
  2  56.993 BB   2.6481 1.90444e4    97.44607  52.3056
  3  72.219 BB   2.4594 4547.36523   24.79755  12.4894
  4  86.635 BB   3.0867 1.19886e4    47.78934  32.9267

Totals :                 3.64099e4  180.40347
```

Figure D-28: Chromatogram of Prep Sample Fraction 20-25 Minutes
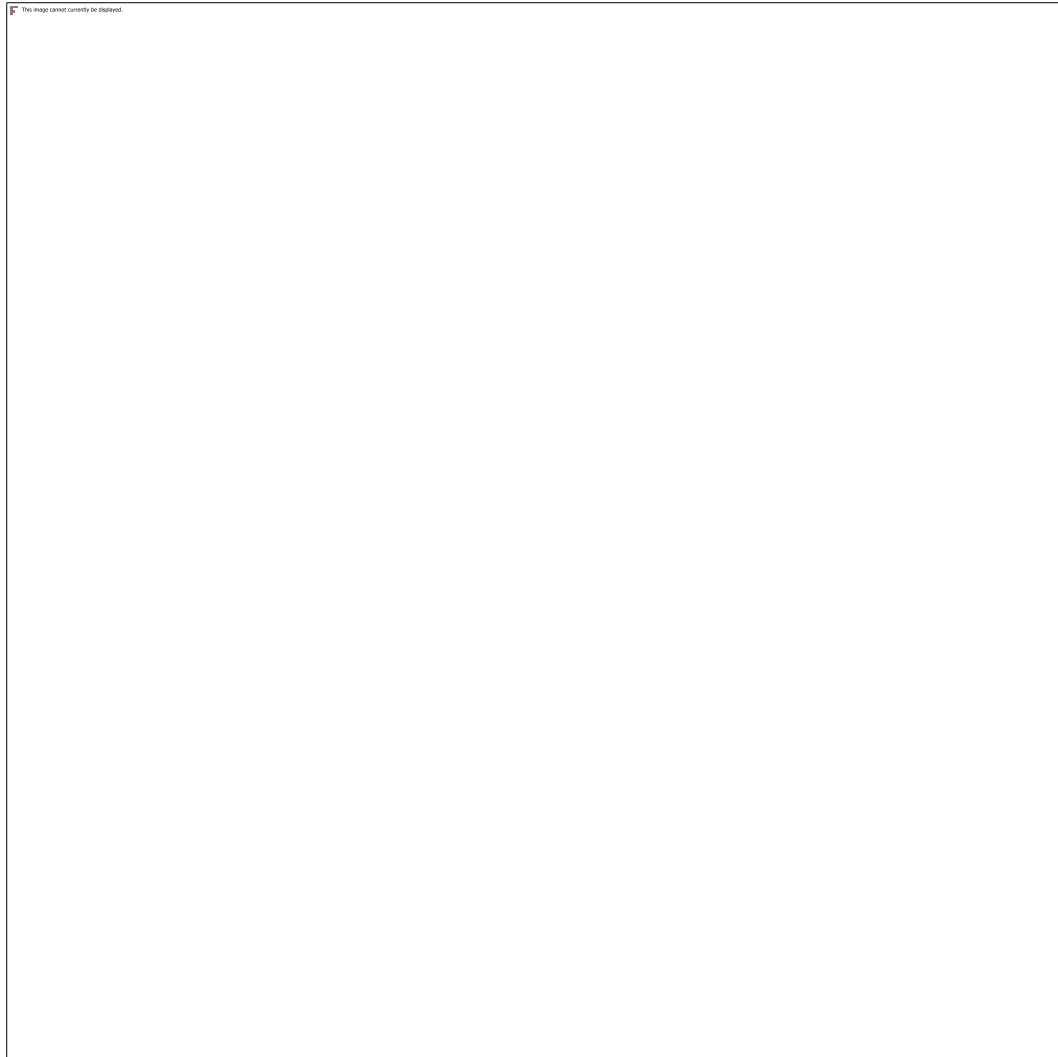
Figure D-29: Chromatogram of Prep Sample Fraction 29-31 Minutes

This image cannot currently be displayed.
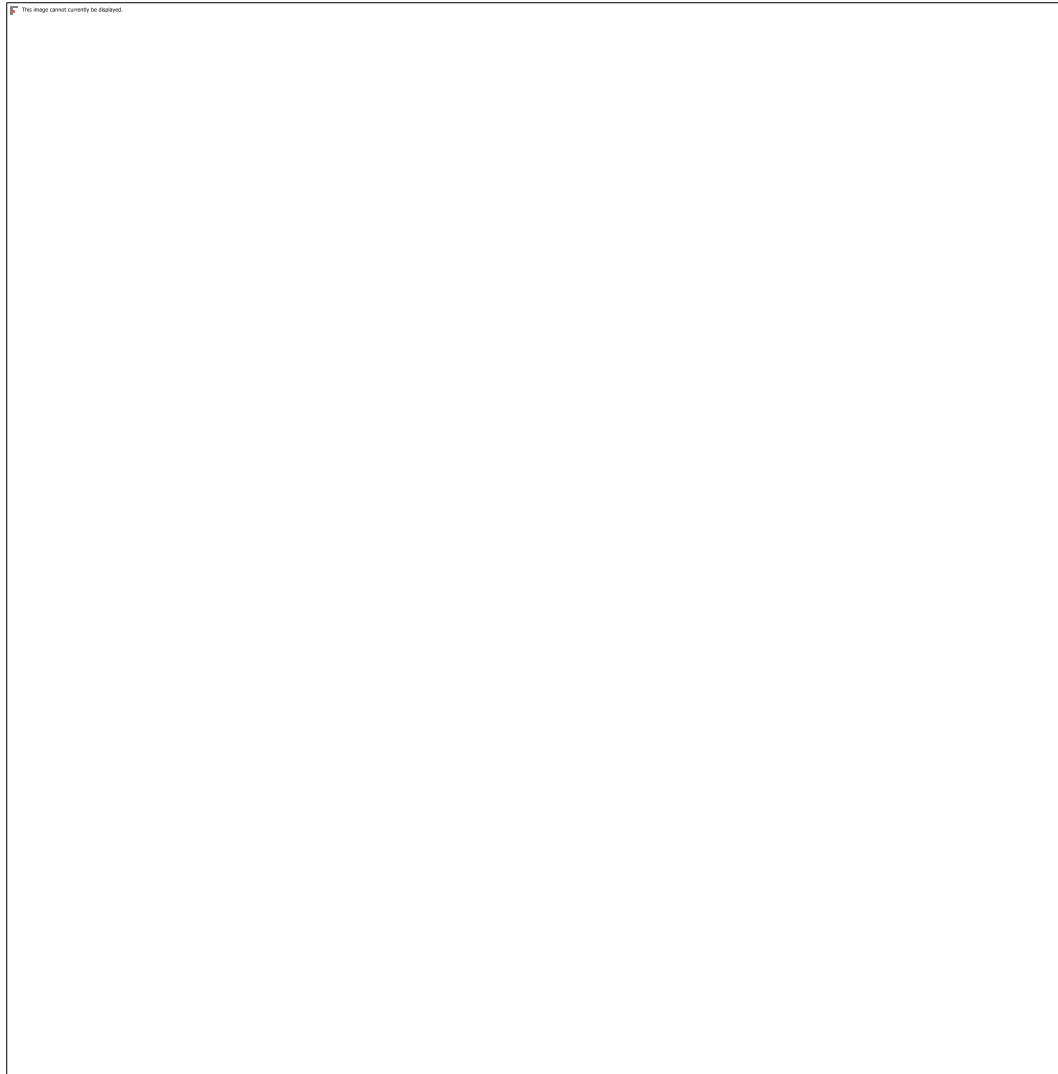
Figure D-30: Chromatogram of Prep Sample Fraction 35-40 Minutes
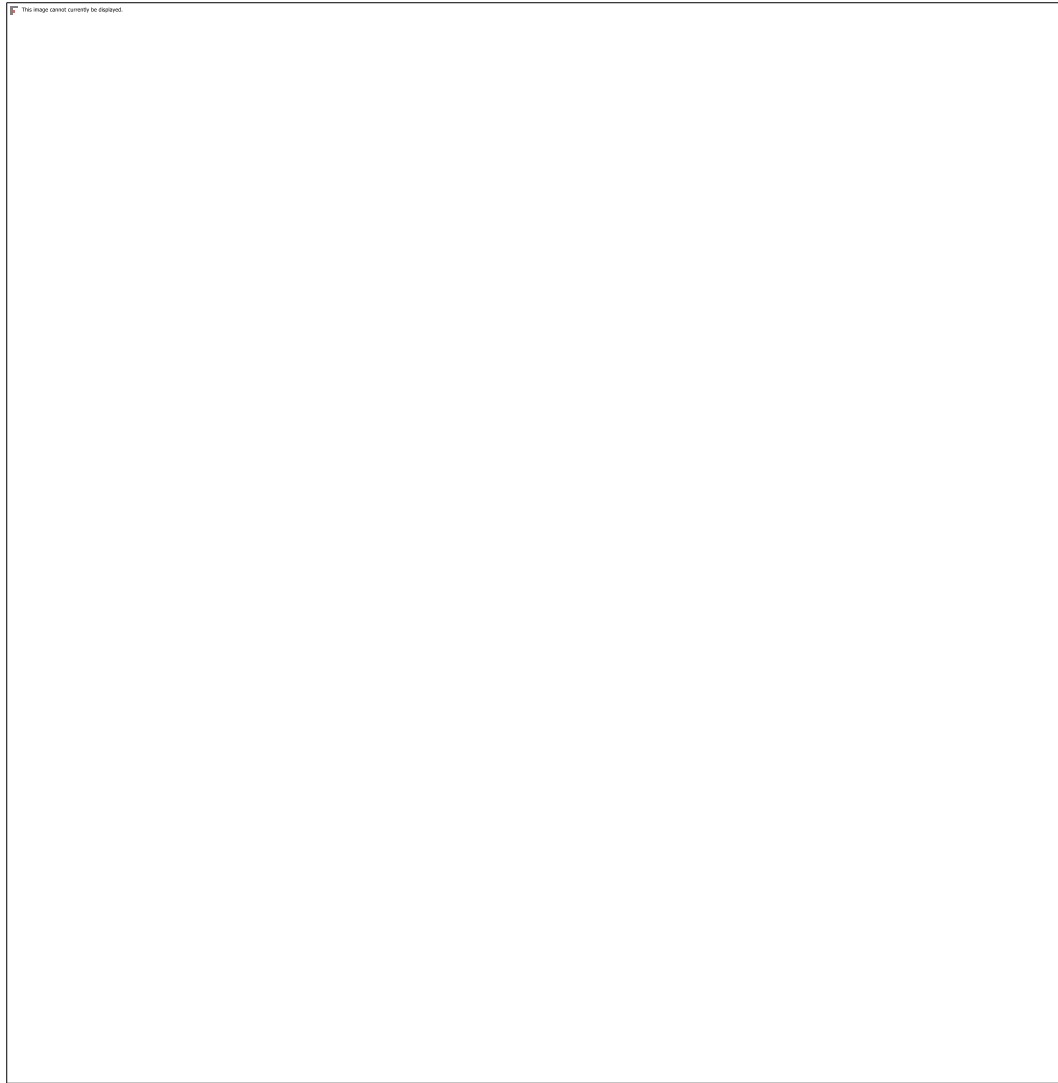
Figure D-31: Chromatogram of Prep Sample Fraction 41-47 Minutes

```
Peak RetTime Type   Width    Area     Height    Area
 #    [min]        [min]    [mV*s]    [mV]       %
----|-------|----|-------|----------|----------|--------|
 7  53.985 BB    2.3953  659.53467  3.57012  21.3388
 8  64.404 BB    2.4972  308.96335  1.54224   9.9963
```

Figre D-32: 3.0M Perchloric Acid Treated for Spiking Experiments

This image cannot currently be displayed.

```
Peak RetTime Type  Width     Area     Height    Area
  #    [min]       [min]    [mV*s]     [mV]       %
----|-------|----|-------|----------|----------|--------|
  7   60.734 MM   3.7498   537.26263   2.38796   9.9203
```
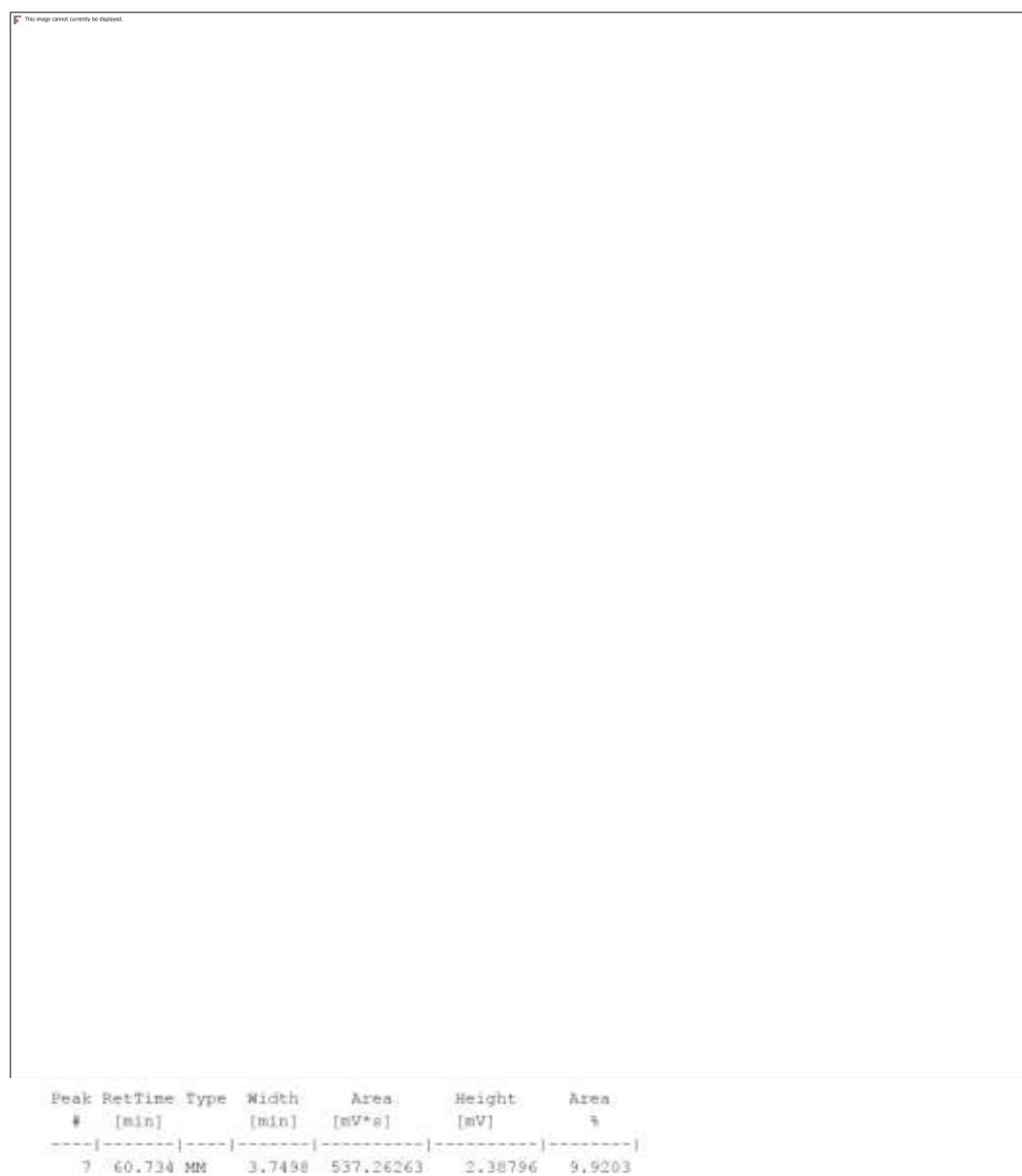
Figre D-33: 3.0M Perchloric Acid Treated Spiked with 4*z*,4'*z cis-syn-cis*-di-*tert*-butylcyclohexano-18-crown-6
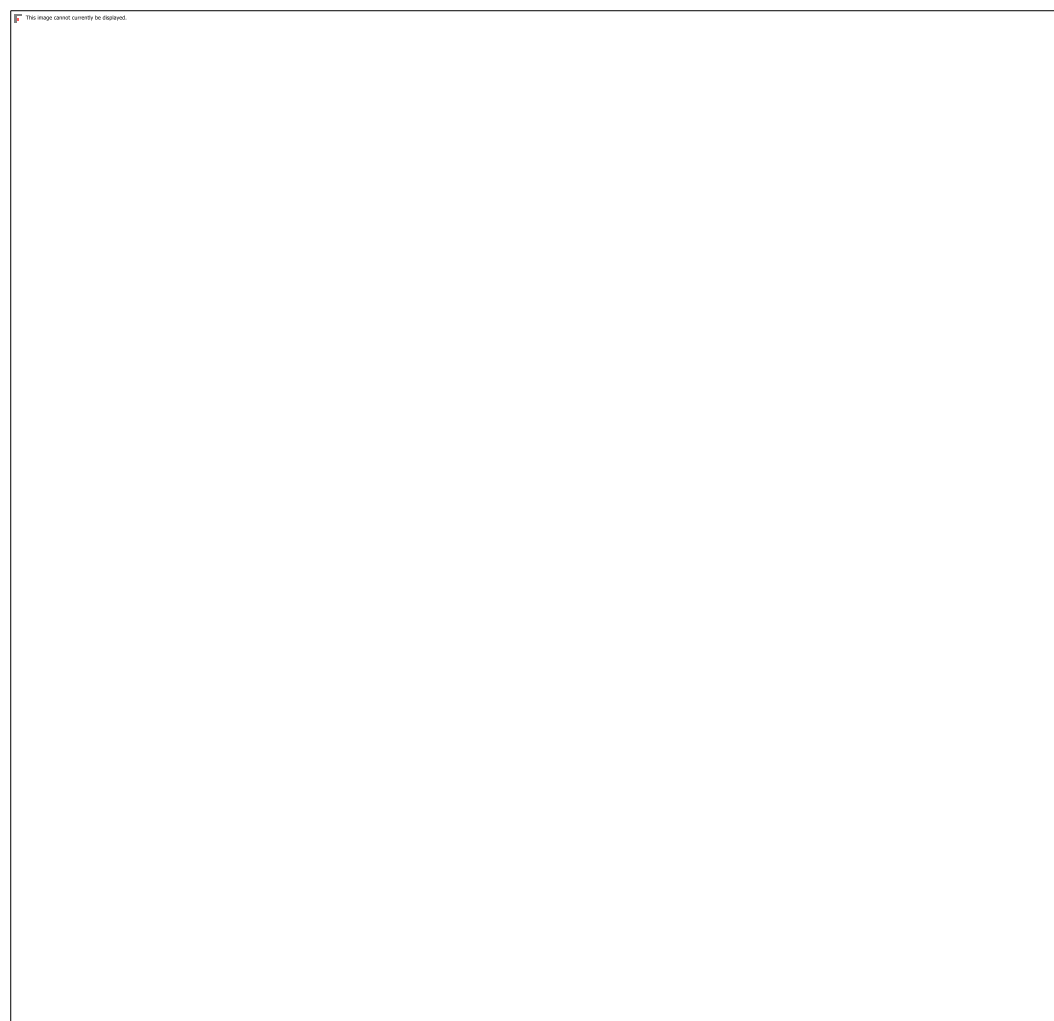
Peak #	RetTime [min]	Type	Width [min]	Area [mV*s]	Height [mV]	Area %
4	32.313	BV	1.3311	1756.21094	17.49574	29.8909
5	34.439	VB	1.4604	1080.52600	9.13212	18.3907
6	41.621	BB	1.8235	429.37759	3.04052	7.3080
7	50.452	BV	2.3105	892.77496	4.95305	15.1951
8	60.301	VB	2.6802	422.33377	1.93055	7.1892

Totals : 5875.40684 57.94210

Figre D-34: 3.0M Perchloric Acid Treated Spiked with 4*z*,5'*z cis-syn-cis*-di-*tert*-butylcyclohexano-18-crown-6

```
Peak RetTime Type  Width    Area      Height     Area
 #    [min]        [min]    [mV*s]     [mV]        %
----|-------|----|-------|----------|----------|--------|
  7  58.917 VB   2.9606 1259.20178   5.18623  31.4319

Totals :                  4006.12311  29.11746
```

Figre D-35: 3.0M Perchloric Acid Treated Spiked with 4z,4'e *cis-syn-cis*-di-*tert*-butylcyclohexano-18-crown-6
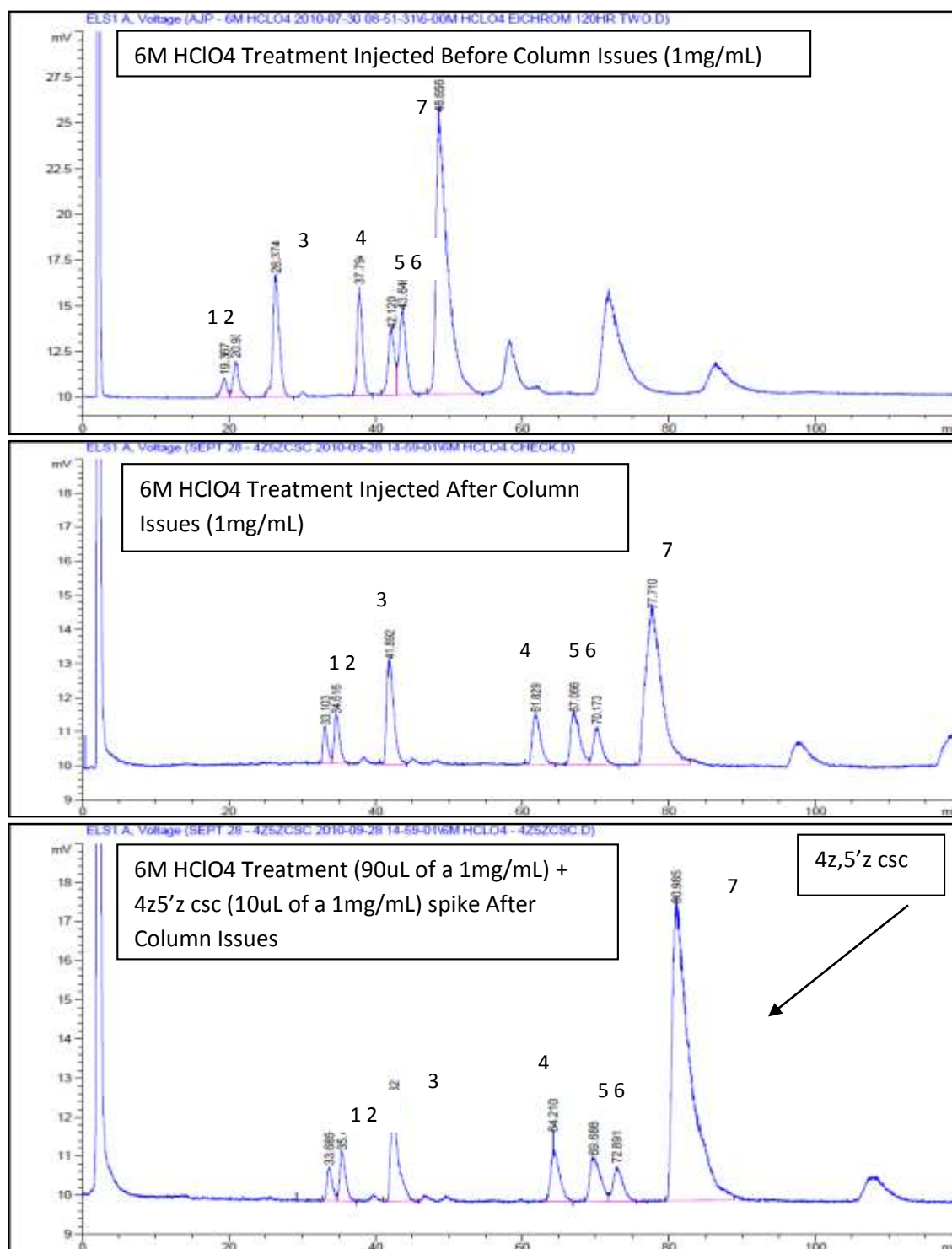
Figure D-36. HPLC-ELSD Chromatograms for Spiked (with the 4z, 5'z *cis-syn-cis* isomer) and Unspiked DtBuCH18C6 samples.
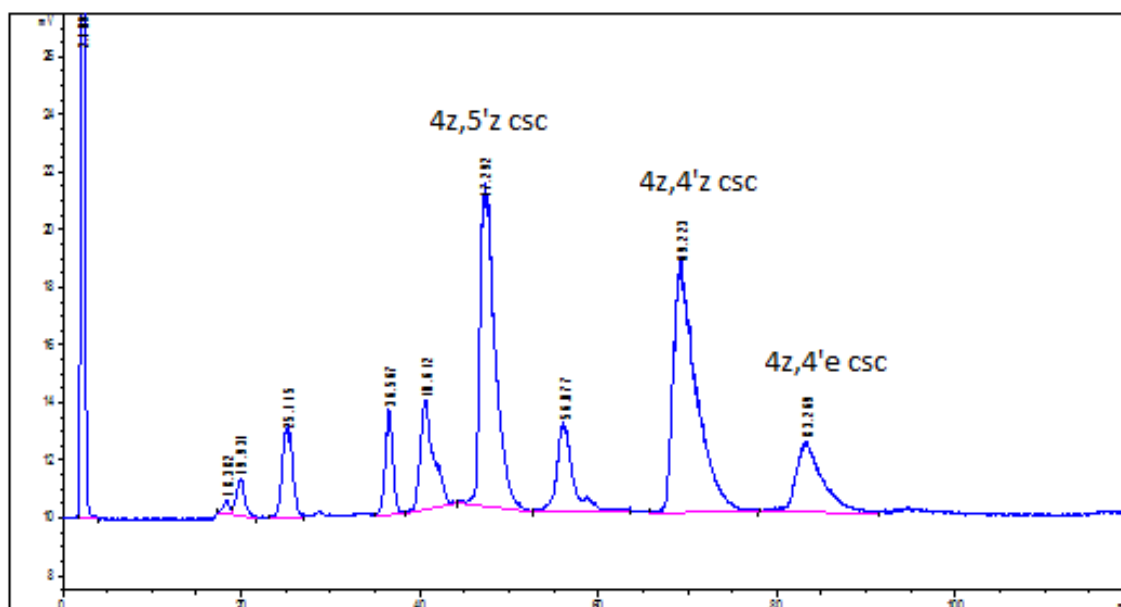
Figure D-37: Representative Chromatogram Showing the Identity of Peaks Present in a Perchloric Acid Purified Sample of DtBuCH18C6

APPENDIX E

CRYSTALLOGRAPHIC DATA FOR HYDRONIUM 4Z,4'Z-*CIS-SYN-CIS*-DI-*TERT*-BUTYLCYCLOHEXANO-18-CROWN-6 PERCHLORATE
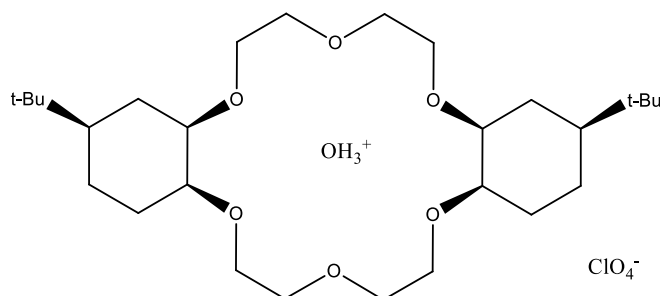
Colorless prisms. The experiment was done with Oxford SuperNova diffractometer using Cu(Kα) radiation at 100K.

Table E-1 Crystal Data

Empirical formula	$C_{28}H_{55}ClO_{11}$
Formula weight	603.17
Temperature/K	100.00(10)
Crystal system	orthorhombic
Space group	$Pna2_1$
a/Å	22.6891(4)
b/Å	10.5108(2)
c/Å	26.9322(4)
α/°	90.00
β/°	90.00
γ/°	90.00
Volume/Å^3	6422.8(2)
Z	8
ρ_{calc}mg/mm^3	1.248
m/mm^{-1}	1.512
F(000)	2624.0
Crystal size/mm^3	$0.4366 \times 0.3472 \times 0.1021$
2Θ range for data collection	6.56 to 147.82°
Index ranges	$-27 \leq h \leq 27, -12 \leq k \leq 8, -32 \leq l \leq 33$
Reflections collected	31583
Independent reflections	11677[R(int) = 0.0285]
Data/restraints/parameters	11677/7/758

Goodness-of-fit on F^2	1.034
Final R indexes [I>=2σ (I)]	$R_1 = 0.0481$, $wR_2 = 0.1276$
Final R indexes [all data]	$R_1 = 0.0509$, $wR_2 = 0.1318$
Largest diff. peak/hole / e Å^{-3}	1.06/-0.66
Flack parameter	0.00(2)

Table E-2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{Å}^2 \times 10^3$) for crystal. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	x	y	z	U(eq)
Cl1	2276.1(3)	413.0(6)	6988.5(2)	26.42(14)
O1	2154.9(8)	1738.1(19)	6983.2(9)	35.8(5)
O2	1874.1(11)	-204(3)	6650(1)	55.4(7)
O3	2190.6(10)	-61(3)	7480.9(9)	45.3(6)
O4	2875.4(9)	178(2)	6830.6(9)	39.7(5)
Cl1A	5257.5(3)	9512.6(6)	6120.4(2)	30.29(15)
O1A	4668.9(9)	9802(2)	6294.4(8)	38.7(5)
O2A	5334.9(12)	9975(3)	5625(1)	57.2(8)
O3A	5690.7(11)	10091(3)	6445.3(12)	62.4(8)
O4A	5354.4(9)	8182(2)	6129.9(9)	38.6(5)
O5	3746.3(8)	7346.0(17)	7636.0(7)	23.3(4)
O6	4883.7(8)	7302.7(18)	7288.1(7)	24.0(4)
O7	5470.5(7)	5345.4(17)	7769.9(6)	22.4(4)
O8	5090.4(7)	2934.9(18)	7564.6(6)	21.8(4)
O9	3971.3(7)	3244.7(17)	7138.9(6)	22.3(4)
O10	3126.0(7)	5183.3(17)	7365.8(6)	22.3(3)
C1	2871.9(11)	6401(3)	7255.9(9)	25.2(5)
C2	3106.9(11)	7342(3)	7629.7(10)	22.6(5)
C3	2889.5(10)	7090(2)	8156.0(9)	20.8(5)
C4	2207(1)	7151(3)	8166.2(9)	20.6(5)
C5	1976.5(10)	6131(3)	7811.5(9)	22.9(5)
C6	2196.5(11)	6381(3)	7281.1(9)	28.2(6)
C7	1947.5(11)	7118(3)	8698.5(10)	23.5(5)
C8	2140.4(12)	5943(3)	8987.5(10)	30.3(6)

C9	2143.9(13)	8308(3)	8988.2(11)	33.8(6)
C10	1267.5(11)	7167(3)	8671.6(10)	29.1(6)
C11	3984.7(11)	8387(3)	7366.9(10)	28.5(6)
C12	4632.8(12)	8458(3)	7450.1(11)	31.2(6)
C13	5511.9(12)	7304(3)	7333.2(12)	32.8(7)
C14	5713.9(11)	5946(3)	7332.0(11)	33.0(6)
C15	5800.7(10)	4242(3)	7936.3(9)	21.5(5)
C16	5718.0(11)	3124(3)	7591.0(8)	23.4(5)
C17	6032.8(12)	1954(3)	7797.9(9)	27.7(6)
C18	5827.8(11)	1648(3)	8327.3(9)	25.3(5)
C19	5915.8(10)	2769(3)	8675.7(9)	21.4(5)
C20	5594.7(10)	3949(2)	8460.2(8)	20.0(5)
C21	5758.1(11)	2525(3)	9232.1(9)	22.7(5)
C22	5091.4(12)	2332(3)	9307.8(11)	31.3(6)
C23	6075.7(12)	1340(3)	9423.7(10)	30.1(6)
C24	5967.2(13)	3661(3)	9538.5(10)	32.8(6)
C25	4910.7(12)	2180(3)	7158.8(9)	24.8(5)
C26	4256.4(12)	2018(3)	7188.9(9)	24.9(5)
C27	3341.9(11)	3077(3)	7102.1(9)	25.7(5)
C28	3051.2(11)	4300(3)	6968.5(9)	26.3(5)
O5A	2049.1(7)	4469.9(17)	5313.4(6)	21.3(4)
O6A	2640.6(8)	2570.2(17)	5823.6(7)	24.3(4)
O7A	3777.4(8)	2583(2)	5487.1(8)	32.2(5)
O8A	4377.5(8)	4815.5(19)	5728.5(6)	24.8(4)
O9A	3505.7(8)	6713.5(18)	5933.4(6)	24.0(4)
O10A	2386.9(7)	6931.6(17)	5484.3(6)	21.2(3)
C1A	1766.9(10)	6688(3)	5449.2(9)	22.9(5)
C2A	1709.1(10)	5520(2)	5122.4(9)	21.6(5)
C3A	1920.2(10)	5776(2)	4595.2(8)	20.5(5)
C4A	1577.1(10)	6875(2)	4355.1(9)	20.8(5)
C5A	1635.2(12)	8058(3)	4683(1)	28.5(6)
C6A	1432.4(12)	7795(3)	5219(1)	29.2(6)
C7A	1734.7(11)	7084(3)	3799.0(9)	22.8(5)
C8A	2399.4(11)	7251(3)	3725.1(11)	29.0(6)
C9A	1531.8(12)	5927(3)	3495.4(10)	31.9(6)
C10A	1419.9(13)	8263(3)	3593.9(10)	32.2(6)
C11A	1806.8(11)	3901(3)	5756.8(10)	31.0(6)

C12A	2014.5(12)	2551(3)	5779.8(12)	30.1(6)
C13A	2905.0(13)	1440(3)	5656.5(11)	32.4(6)
C14A	3552.6(12)	1527(3)	5743.0(11)	31.3(6)
C15A	4420.7(12)	2620(3)	5488.4(11)	28.1(6)
C16A	4643.1(11)	3622(3)	5852.4(9)	28.9(6)
C17A	5318.7(11)	3678(4)	5823.5(10)	35.8(7)
C18A	5529.8(11)	3887(3)	5287.8(10)	26.6(5)
C19A	5317.3(11)	2800(3)	4955.3(9)	22.3(5)
C20A	4641.1(11)	2795(3)	4965.7(10)	24.3(5)
C21A	5580.8(12)	2761(3)	4423.4(10)	25.2(5)
C22A	5356.1(14)	3853(3)	4104.9(10)	34.7(7)
C23A	6255.5(12)	2851(3)	4451.2(10)	30.7(6)
C24A	5427.5(13)	1491(3)	4174.6(12)	38.4(7)
C25A	4431.8(11)	5717(3)	6121.6(10)	30.8(6)
C26A	4132.6(11)	6926(3)	5977.6(10)	28.7(6)
C27A	3198.4(12)	7904(3)	5880.1(10)	27.8(5)
C28A	2543.8(12)	7674(3)	5902.1(10)	25.6(5)
O11	4330.6(7)	5113.7(17)	7725.6(6)	20.3(3)
O11A	3175.8(7)	4764.8(18)	5366.3(7)	22.3(4)

Table E-3 Anisotropic Displacement Parameters ($\text{Å}^2 \times 10^3$) for paw1a. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+...+2hka\times b\times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cl1	23.7(3)	21.9(3)	33.6(3)	1.2(2)	9.1(2)	-0.3(2)
O1	25.6(9)	27.1(10)	54.7(12)	7.6(10)	4.1(9)	6.8(8)
O2	43.1(12)	65.9(17)	57.1(15)	-30.2(14)	8.6(11)	-16.1(12)
O3	39.8(11)	50.8(14)	45.4(12)	21.0(11)	14(1)	10.0(11)
O4	27.1(10)	35.2(12)	56.7(13)	8.7(10)	20.2(9)	9.0(9)
Cl1A	29.5(3)	24.6(3)	36.8(3)	1.9(3)	12.7(2)	-0.3(2)
O1A	30.5(10)	38.3(12)	47.4(12)	2.3(10)	14.4(9)	8.0(9)
O2A	58.6(15)	60.4(18)	52.7(14)	30.6(13)	28.2(12)	21.4(13)
O3A	37.9(12)	73.2(19)	76.0(18)	-34.3(16)	7.9(12)	-14.4(13)
O4A	29.9(10)	32.5(11)	53.5(12)	7.5(10)	6.0(9)	5.7(9)
O5	17.9(9)	22.2(9)	29.8(9)	10.0(7)	4.5(7)	-0.2(7)
O6	15.1(9)	25.7(10)	31.1(9)	3.0(8)	-0.9(7)	-1.3(7)
O7	14.9(7)	25.1(9)	27.1(8)	5.7(7)	2.3(6)	1.3(7)

O8	17.9(8)	27.8(10)	19.7(8)	-4.8(7)	-1.0(6)	2.4(7)
O9	19.4(8)	22.0(9)	25.7(8)	-1.8(7)	-1.5(6)	0.9(7)
O10	21.3(8)	25.3(9)	20.3(8)	0.0(7)	-3.2(6)	2.9(7)
C1	21.1(11)	32.0(15)	22.4(11)	5.1(11)	-1.0(9)	8.6(11)
C2	14.4(11)	21.2(13)	32.1(13)	4.9(10)	1.7(9)	3.4(9)
C3	16.7(11)	20.2(12)	25.5(11)	1.6(10)	1.3(9)	-0.8(10)
C4	17.9(12)	19.4(12)	24.5(11)	0(1)	1.4(9)	0.2(10)
C5	17.2(10)	26.0(13)	25.4(11)	-2(1)	-0.8(8)	1.3(10)
C6	20.8(12)	41.2(17)	22.7(11)	-1.6(11)	-2.6(9)	8.0(11)
C7	19.8(12)	23.9(13)	26.9(11)	-4.9(11)	4.2(9)	-2.4(10)
C8	26.8(12)	34.9(16)	29.3(12)	7.3(12)	2.3(10)	-3.3(12)
C9	28.7(13)	32.5(16)	40.2(14)	-13.2(13)	6.5(11)	-4.6(12)
C10	20.4(13)	34.9(15)	32.0(13)	-3.7(12)	5.2(10)	-2.5(11)
C11	25.2(12)	21.9(13)	38.3(13)	8.6(11)	9.4(10)	0.5(10)
C12	31.5(14)	20.1(13)	41.9(14)	0.9(12)	8.1(11)	-5.1(11)
C13	15.5(13)	36.8(16)	46.2(16)	16.9(13)	-0.4(11)	-6.5(11)
C14	20.6(11)	44.2(18)	34.3(13)	14.7(12)	7.6(10)	5.0(12)
C15	13.3(10)	23.6(13)	27.5(11)	4.4(10)	0.0(8)	2.6(9)
C16	18.2(11)	29.3(14)	22.6(11)	0.8(10)	2.3(8)	4.9(10)
C17	27.1(13)	29.8(14)	26.2(11)	-4.2(11)	-0.9(9)	10.6(11)
C18	27.4(12)	22.9(13)	25.5(11)	-0.1(10)	-4.1(9)	7.1(10)
C19	15.5(10)	26.0(13)	22.7(11)	-0.9(10)	-1.6(8)	5.1(9)
C20	17.2(10)	19.5(12)	23.2(10)	-0.2(9)	-2.1(8)	2.5(9)
C21	18.5(11)	25.2(13)	24.4(11)	-1.1(10)	-0.5(9)	4.7(10)
C22	21.2(13)	39.8(17)	32.8(14)	6.2(12)	3.8(10)	4.5(12)
C23	30.5(13)	32.2(15)	27.7(11)	3.8(11)	-3.5(10)	10.0(12)
C24	40.6(15)	31.2(15)	26.7(12)	-1.8(11)	-4.3(10)	0.7(12)
C25	32.2(14)	23.2(13)	19.1(11)	-2.4(10)	-3.1(9)	4.6(11)
C26	29.6(13)	18.4(13)	26.7(11)	-0.8(10)	-3.9(10)	2.8(10)
C27	18.2(11)	29.9(14)	28.9(12)	-4.1(11)	-3.7(9)	-4(1)
C28	18.4(11)	35.9(15)	24.6(11)	-6.3(11)	-4.4(9)	-0.2(10)
O5A	16.4(7)	22.4(9)	25.2(8)	8.3(7)	1.6(6)	1.0(7)
O6A	15.8(9)	22.9(9)	34.2(10)	7.1(8)	-1.6(7)	-1.1(7)
O7A	17.3(9)	30.9(11)	48.6(12)	19.6(9)	4.7(8)	4.5(8)
O8A	21.8(8)	33.9(11)	18.6(7)	1.2(7)	-1.0(6)	4.9(8)
O9A	21.3(8)	27.0(9)	23.8(8)	-1.7(7)	-1.3(6)	-2.6(7)
O10A	19.0(8)	23.7(9)	21.0(8)	-2.4(7)	-1.5(6)	3.0(7)

C1A	16.8(11)	27.2(13)	24.8(11)	3.8(10)	-0.8(8)	6(1)
C2A	15(1)	24.6(13)	25.3(11)	6.3(10)	-1.9(8)	2.3(9)
C3A	19.6(10)	20.5(12)	21.3(10)	4.6(10)	-1.8(8)	1.3(9)
C4A	17(1)	21.0(12)	24.4(11)	5.2(10)	-1.5(8)	1.1(9)
C5A	29.8(13)	20.9(13)	34.8(13)	4.4(11)	-5.2(10)	7.5(10)
C6A	26.0(12)	31.4(15)	30.3(12)	-1.2(11)	0.8(10)	11.0(12)
C7A	17.8(11)	24.7(13)	25.8(11)	9(1)	-0.2(9)	3.1(10)
C8A	18.2(12)	34.9(15)	34.0(13)	7.9(12)	1.7(10)	-0.4(11)
C9A	33.5(14)	36.0(16)	26.0(12)	7.5(12)	-5.2(10)	-5.3(12)
C10A	31.6(13)	35.0(16)	30.1(12)	10.9(12)	2.2(10)	8.5(12)
C11A	19.0(11)	42.7(17)	31.2(12)	17.0(12)	5.6(9)	1.1(11)
C12A	13.9(12)	36.9(16)	39.5(15)	22.1(12)	-4.8(10)	-4.4(10)
C13A	30.1(14)	24.1(14)	43.0(15)	-0.7(12)	6.4(11)	-4.1(11)
C14A	27.4(13)	23.3(14)	43.2(14)	7.6(12)	7.8(11)	2.5(11)
C15A	15.6(12)	32.0(15)	36.6(14)	16.5(12)	5.6(10)	6.7(10)
C16A	19.9(12)	44.2(17)	22.5(11)	13.1(12)	4.1(9)	9.9(11)
C17A	19.1(12)	61(2)	27.0(13)	0.1(13)	-3.5(9)	11.4(13)
C18A	15.6(10)	33.9(15)	30.1(12)	-1.8(11)	0.3(9)	0.3(10)
C19A	17.1(12)	25.6(13)	24.2(11)	7.8(10)	1.3(9)	3.7(10)
C20A	19.2(12)	21.6(13)	32.2(12)	2.3(11)	-1.3(9)	1(1)
C21A	22.1(12)	28.5(14)	25.0(11)	4.2(11)	0.8(9)	8.0(11)
C22A	36.4(15)	39.0(17)	28.8(13)	8.6(12)	4.5(10)	15.5(13)
C23A	22.4(13)	37.7(16)	31.8(13)	0.6(12)	5.1(10)	9.5(12)
C24A	29.5(14)	42.5(18)	43.2(15)	-10.4(14)	-2.9(12)	7.6(13)
C25A	22.5(11)	48.4(18)	21.5(11)	-3.0(12)	-2.0(9)	-0.3(12)
C26A	23.1(12)	35.3(16)	27.6(12)	-5.3(11)	-0.8(9)	-7.5(11)
C27A	35.8(14)	22.1(13)	25.5(11)	-0.5(11)	-1.8(10)	-2.7(11)
C28A	27.0(13)	28.2(14)	21.5(11)	-5.9(10)	-2.1(9)	4.3(11)
O11	16.2(7)	17.6(9)	27.1(8)	1.1(7)	-0.2(6)	0.3(7)
O11A	18.0(8)	19.9(9)	29.0(8)	4.1(7)	-0.2(6)	-1.2(7)

Table E-4 Bond Lengths for crystal.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cl1	O1	1.420(2)	C21	C23	1.528(4)
Cl1	O2	1.443(2)	C21	C24	1.527(4)
Cl1	O3	1.430(2)	C25	C26	1.496(4)

Cl1	O4	1.446(2)	C27	C28	1.489(4)
Cl1A	O1A	1.448(2)	O5A	C2A	1.442(3)
Cl1A	O2A	1.431(2)	O5A	C11A	1.444(3)
Cl1A	O3A	1.449(3)	O6A	C12A	1.426(3)
Cl1A	O4A	1.416(2)	O6A	C13A	1.405(3)
O5	C2	1.451(3)	O7A	C14A	1.402(3)
O5	C11	1.419(3)	O7A	C15A	1.460(3)
O6	C12	1.410(3)	O8A	C16A	1.431(3)
O6	C13	1.430(3)	O8A	C25A	1.426(3)
O7	C14	1.447(3)	O9A	C26A	1.445(3)
O7	C15	1.452(3)	O9A	C27A	1.439(3)
O8	C16	1.440(3)	O10A	C1A	1.433(3)
O8	C25	1.411(3)	O10A	C28A	1.415(3)
O9	C26	1.449(3)	C1A	C2A	1.516(4)
O9	C27	1.442(3)	C1A	C6A	1.521(4)
O10	C1	1.434(3)	C2A	C3A	1.523(3)
O10	C28	1.426(3)	C3A	C4A	1.535(3)
C1	C2	1.509(4)	C4A	C5A	1.531(4)
C1	C6	1.534(3)	C4A	C7A	1.555(3)
C2	C3	1.524(3)	C5A	C6A	1.540(4)
C3	C4	1.550(3)	C7A	C8A	1.531(3)
C4	C5	1.529(4)	C7A	C9A	1.536(4)
C4	C7	1.550(3)	C7A	C10A	1.533(4)
C5	C6	1.536(3)	C11A	C12A	1.497(4)
C7	C8	1.524(4)	C13A	C14A	1.491(4)
C7	C9	1.540(4)	C15A	C16A	1.525(4)
C7	C10	1.545(3)	C15A	C20A	1.505(4)
C11	C12	1.489(4)	C16A	C17A	1.536(3)
C13	C14	1.499(4)	C17A	C18A	1.536(4)
C15	C16	1.510(4)	C18A	C19A	1.530(4)
C15	C20	1.518(3)	C19A	C20A	1.535(3)
C16	C17	1.527(4)	C19A	C21A	1.553(3)
C17	C18	1.534(3)	C21A	C22A	1.521(4)
C18	C19	1.519(4)	C21A	C23A	1.536(4)
C19	C20	1.551(3)	C21A	C24A	1.534(4)
C19	C21	1.562(3)	C25A	C26A	1.491(4)
C21	C22	1.540(4)	C27A	C28A	1.506(4)

Table E-5 Bond Angles for crystal.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	Cl1	O2	108.17(16)	C24	C21	C22	109.7(2)
O1	Cl1	O3	108.95(15)	C24	C21	C23	107.9(2)
O1	Cl1	O4	110.30(13)	O8	C25	C26	108.0(2)
O2	Cl1	O4	109.37(15)	O9	C26	C25	109.7(2)
O3	Cl1	O2	110.10(17)	O9	C27	C28	110.5(2)
O3	Cl1	O4	109.92(14)	O10	C28	C27	109.1(2)
O1A	Cl1A	O3A	110.01(15)	C2A	O5A	C11A	114.10(18)
O2A	Cl1A	O1A	110.10(14)	C13A	O6A	C12A	112.8(2)
O2A	Cl1A	O3A	109.7(2)	C14A	O7A	C15A	112.5(2)
O4A	Cl1A	O1A	110.18(13)	C25A	O8A	C16A	111.91(19)
O4A	Cl1A	O2A	109.46(16)	C27A	O9A	C26A	110.5(2)
O4A	Cl1A	O3A	107.32(17)	C28A	O10A	C1A	113.45(19)
C11	O5	C2	112.16(19)	O10A	C1A	C2A	105.54(18)
C12	O6	C13	112.0(2)	O10A	C1A	C6A	112.3(2)
C14	O7	C15	113.79(19)	C2A	C1A	C6A	109.8(2)
C25	O8	C16	113.69(18)	O5A	C2A	C1A	111.50(19)
C27	O9	C26	109.9(2)	O5A	C2A	C3A	107.44(19)
C28	O10	C1	112.20(18)	C1A	C2A	C3A	111.8(2)
O10	C1	C2	107.78(19)	C2A	C3A	C4A	111.47(19)
O10	C1	C6	112.3(2)	C3A	C4A	C7A	113.3(2)
C2	C1	C6	109.4(2)	C5A	C4A	C3A	108.94(19)
O5	C2	C1	111.3(2)	C5A	C4A	C7A	114.9(2)
O5	C2	C3	108.3(2)	C4A	C5A	C6A	111.6(2)
C1	C2	C3	113.1(2)	C1A	C6A	C5A	111.7(2)
C2	C3	C4	109.4(2)	C8A	C7A	C4A	111.6(2)
C3	C4	C7	113.3(2)	C8A	C7A	C9A	108.5(2)
C5	C4	C3	107.6(2)	C8A	C7A	C10A	108.6(2)
C5	C4	C7	115.6(2)	C9A	C7A	C4A	109.4(2)
C4	C5	C6	110.5(2)	C10A	C7A	C4A	110.7(2)
C1	C6	C5	111.6(2)	C10A	C7A	C9A	107.9(2)
C8	C7	C4	112.4(2)	O5A	C11A	C12A	107.9(2)
C8	C7	C9	108.5(2)	O6A	C12A	C11A	107.7(2)
C8	C7	C10	109.7(2)	O6A	C13A	C14A	108.6(2)

C9	C7	C4	109.9(2)	O7A	C14A	C13A	109.3(2)
C9	C7	C10	106.6(2)	O7A	C15A	C16A	110.5(2)
C10	C7	C4	109.6(2)	O7A	C15A	C20A	109.4(2)
O5	C11	C12	109.8(2)	C20A	C15A	C16A	114.0(2)
O6	C12	C11	108.0(2)	O8A	C16A	C15A	108.44(19)
O6	C13	C14	107.7(2)	O8A	C16A	C17A	112.0(2)
O7	C14	C13	107.3(2)	C15A	C16A	C17A	108.9(2)
O7	C15	C16	111.55(19)	C16A	C17A	C18A	111.4(2)
O7	C15	C20	106.86(19)	C19A	C18A	C17A	110.2(2)
C16	C15	C20	112.1(2)	C18A	C19A	C20A	107.9(2)
O8	C16	C15	105.12(18)	C18A	C19A	C21A	116.0(2)
O8	C16	C17	111.7(2)	C20A	C19A	C21A	113.7(2)
C15	C16	C17	110.1(2)	C15A	C20A	C19A	110.5(2)
C16	C17	C18	111.5(2)	C22A	C21A	C19A	111.8(2)
C19	C18	C17	111.8(2)	C22A	C21A	C23A	108.4(2)
C18	C19	C20	109.09(19)	C22A	C21A	C24A	109.5(2)
C18	C19	C21	115.8(2)	C23A	C21A	C19A	109.7(2)
C20	C19	C21	112.51(19)	C24A	C21A	C19A	109.8(2)
C15	C20	C19	111.42(19)	C24A	C21A	C23A	107.5(2)
C22	C21	C19	111.9(2)	O8A	C25A	C26A	109.5(2)
C23	C21	C19	110.5(2)	O9A	C26A	C25A	109.8(2)
C23	C21	C22	108.2(2)	O9A	C27A	C28A	109.5(2)
C24	C21	C19	108.6(2)	O10A	C28A	C27A	107.8(2)

Table E-6 Hydrogen Bonds for crystal.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
O11	H11H	O9	0.911(19)	1.75(2)	2.650(2)	167(5)
O11	H11I	O7	0.907(19)	1.70(2)	2.601(2)	170(4)
O11	H11J	O5	0.890(19)	1.82(2)	2.706(3)	172(4)
O11A	H11E	O9A	0.906(18)	1.762(19)	2.662(3)	172(3)
O11A	H11F	O5A	0.916(19)	1.67(2)	2.579(2)	170(4)
O11A	H11G	O7A	0.92(2)	1.79(2)	2.689(3)	164(6)

Table E-7 Torsion Angles for crystal.

A	B	C	D	Angle/°
O5	C2	C3	C4	177.0(2)
O5	C11	C12	O6	59.4(3)
O6	C13	C14	O7	-63.8(3)
O7	C15	C16	O8	-55.3(2)
O7	C15	C16	C17	-175.72(19)
O7	C15	C20	C19	179.42(19)
O8	C16	C17	C18	-61.1(3)
O8	C25	C26	O9	63.2(3)
O9	C27	C28	O10	-65.8(3)
O10	C1	C2	O5	54.7(3)
O10	C1	C2	C3	-67.4(3)
O10	C1	C6	C5	65.7(3)
C1	O10	C28	C27	178.2(2)
C1	C2	C3	C4	-59.2(3)
C2	O5	C11	C12	171.3(2)
C2	C1	C6	C5	-54.0(3)
C2	C3	C4	C5	60.1(3)
C2	C3	C4	C7	-170.9(2)
C3	C4	C5	C6	-60.5(3)
C3	C4	C7	C8	-57.0(3)
C3	C4	C7	C9	63.9(3)
C3	C4	C7	C10	-179.3(2)
C4	C5	C6	C1	58.7(3)
C5	C4	C7	C8	67.7(3)
C5	C4	C7	C9	-171.4(2)
C5	C4	C7	C10	-54.6(3)
C6	C1	C2	O5	177.1(2)
C6	C1	C2	C3	55.0(3)
C7	C4	C5	C6	171.8(2)
C11	O5	C2	C1	100.8(2)
C11	O5	C2	C3	-134.3(2)
C12	O6	C13	C14	160.0(2)
C13	O6	C12	C11	177.4(2)
C14	O7	C15	C16	-72.0(3)
C14	O7	C15	C20	165.1(2)
C15	O7	C14	C13	-156.0(2)

C15	C16	C17	C18	55.3(3)
C16	O8	C25	C26	177.7(2)
C16	C15	C20	C19	56.9(3)
C16	C17	C18	C19	-56.8(3)
C17	C18	C19	C20	55.7(3)
C17	C18	C19	C21	-176.2(2)
C18	C19	C20	C15	-55.7(3)
C18	C19	C21	C22	-68.1(3)
C18	C19	C21	C23	52.5(3)
C18	C19	C21	C24	170.7(2)
C20	C15	C16	O8	64.5(2)
C20	C15	C16	C17	-55.9(3)
C20	C19	C21	C22	58.3(3)
C20	C19	C21	C23	178.9(2)
C20	C19	C21	C24	-62.9(3)
C21	C19	C20	C15	174.4(2)
C25	O8	C16	C15	163.1(2)
C25	O8	C16	C17	-77.5(2)
C26	O9	C27	C28	-170.80(19)
C27	O9	C26	C25	172.49(19)
C28	O10	C1	C2	-165.5(2)
C28	O10	C1	C6	73.8(2)
O5A	C2A	C3A	C4A	179.25(19)
O5A	C11A	C12A	O6A	63.1(3)
O6A	C13A	C14A	O7A	-58.9(3)
O7A	C15A	C16A	O8A	-55.0(3)
O7A	C15A	C16A	C17A	-177.2(2)
O7A	C15A	C20A	C19A	-178.4(2)
O8A	C16A	C17A	C18A	-66.1(3)
O8A	C25A	C26A	O9A	65.9(3)
O9A	C27A	C28A	O10A	-64.9(3)
O10A	C1A	C2A	O5A	55.3(2)
O10A	C1A	C2A	C3A	-65.0(2)
O10A	C1A	C6A	C5A	61.9(3)
C1A	O10A	C28A	C27A	-177.5(2)
C1A	C2A	C3A	C4A	-58.1(3)
C2A	O5A	C11A	C12A	154.5(2)

C2A C1A C6A C5A -55.2(3)
C2A C3A C4A C5A 56.5(3)
C2A C3A C4A C7A -174.3(2)
C3A C4A C5A C6A -55.5(3)
C3A C4A C7A C8A -53.9(3)
C3A C4A C7A C9A 66.2(3)
C3A C4A C7A C10A -175.0(2)
C4A C5A C6A C1A 56.2(3)
C5A C4A C7A C8A 72.2(3)
C5A C4A C7A C9A -167.8(2)
C5A C4A C7A C10A -48.9(3)
C6A C1A C2A O5A 176.61(19)
C6A C1A C2A C3A 56.3(3)
C7A C4A C5A C6A 176.2(2)
C11A O5A C2A C1A 72.1(3)
C11A O5A C2A C3A -165.1(2)
C12A O6A C13A C14A -177.0(2)
C13A O6A C12A C11A -156.5(2)
C14A O7A C15A C16A -104.5(3)
C14A O7A C15A C20A 129.2(3)
C15A O7A C14A C13A -170.9(2)
C15A C16A C17A C18A 53.9(3)
C16A O8A C25A C26A -178.4(2)
C16A C15A C20A C19A 57.2(3)
C16A C17A C18A C19A -59.9(3)
C17A C18A C19A C20A 60.9(3)
C17A C18A C19A C21A -170.3(2)
C18A C19A C20A C15A -59.1(3)
C18A C19A C21A C22A -69.6(3)
C18A C19A C21A C23A 50.6(3)
C18A C19A C21A C24A 168.6(2)
C20A C15A C16A O8A 68.7(3)
C20A C15A C16A C17A -53.4(3)
C20A C19A C21A C22A 56.3(3)
C20A C19A C21A C23A 176.6(2)
C20A C19A C21A C24A -65.5(3)
C21A C19A C20A C15A 170.8(2)

C25A O8A C16A C15A 164.2(2)
C25A O8A C16A C17A -75.6(3)
C26A O9A C27A C28A -172.63(19)
C27A O9A C26A C25A 170.0(2)
C28A O10A C1A C2A -158.7(2)
C28A O10A C1A C6A   81.7(3)

Table E-8 Hydrogen Atom Coordinates ($\mathring{A}\times10^4$) and Isotropic Displacement Parameters ($\mathring{A}^2\times10^3$) for crystal.

Atom	x	y	z	U(eq)
H1	2997	6669	6915	30
H2	2971	8210	7530	27
H3A	3055	7734	8385	25
H3B	3023	6240	8267	25
H4	2094	7991	8020	25
H5A	1540	6132	7815	27
H5B	2113	5283	7923	27
H6A	2045	5709	7058	34
H6B	2041	7208	7164	34
H8A	2019	5176	8807	46
H8B	1956	5949	9316	46
H8C	2570	5947	9024	46
H9A	2573	8301	9026	51
H9B	1958	8309	9317	51
H9C	2025	9074	8806	51
H10D	1145	7922	8484	44
H10E	1105	7209	9008	44
H10F	1121	6401	8505	44
H11C	3797	9188	7478	34
H11D	3903	8277	7008	34
H12C	4802	9179	7261	37
H12D	4717	8591	7807	37
H13C	5631	7726	7646	39
H13D	5691	7771	7052	39
H14C	5573	5508	7029	40
H14D	6150	5906	7339	40

H15	6229	4466	7947	26
H16	5876	3335	7254	28
H17C	6463	2108	7799	33
H17D	5954	1215	7580	33
H18C	5405	1415	8321	30
H18D	6051	908	8454	30
H19	6346	2972	8668	26
H20C	5165	3791	8458	24
H20D	5671	4694	8676	24
H22D	4883	3125	9230	47
H22E	5015	2095	9654	47
H22F	4952	1654	9088	47
H23D	6003	1246	9780	45
H23E	6500	1427	9365	45
H23F	5928	588	9248	45
H24D	5752	4425	9435	49
H24E	6390	3789	9486	49
H24F	5893	3498	9891	49
H25C	5107	1339	7172	30
H25D	5019	2599	6843	30
H26C	4121	1443	6921	30
H26D	4149	1632	7512	30
H27C	3186	2769	7424	31
H27D	3252	2429	6846	31
H28C	3229	4647	6661	32
H28D	2626	4156	6908	32
H1A	1604	6501	5787	28
H2A	1285	5264	5110	26
H3AA	1869	4998	4393	25
H3AB	2345	5989	4601	25
H4A	1152	6626	4364	25
H5AA	1395	8755	4541	34
H5AB	2051	8340	4686	34
H6AA	1495	8567	5423	35
H6AB	1005	7601	5219	35
H8AA	2541	7947	3936	44
H8AB	2480	7453	3376	44

H8AC	2602	6462	3815	44
H9AA	1710	5153	3632	48
H9AB	1655	6031	3149	48
H9AC	1101	5859	3511	48
H10A	995	8188	3655	48
H10B	1492	8328	3236	48
H10C	1571	9025	3760	48
H11A	1371	3929	5746	37
H11B	1941	4373	6054	37
H12A	1838	2114	6069	36
H12B	1897	2090	5475	36
H13A	2825	1319	5298	39
H13B	2741	703	5839	39
H14A	3632	1617	6103	38
H14B	3748	741	5624	38
H15A	4564	1773	5607	34
H16A	4523	3377	6197	35
H17A	5486	2872	5952	43
H17B	5464	4380	6036	43
H18A	5374	4706	5162	32
H18B	5966	3928	5281	32
H19A	5445	1995	5121	27
H20A	4491	3610	4831	29
H20B	4491	2097	4754	29
H22A	4934	3737	4040	52
H22B	5571	3867	3789	52
H22C	5418	4660	4280	52
H23A	6369	3695	4573	46
H23B	6423	2718	4120	46
H23C	6406	2199	4678	46
H24A	5534	789	4396	58
H24B	5647	1412	3863	58
H24C	5004	1460	4106	58
H25A	4854	5883	6190	37
H25B	4250	5373	6427	37
H26A	4209	7586	6232	34
H26B	4292	7232	5657	34

H27A	3303	8302	5559	33
H27B	3316	8491	6150	33
H28A	2440	7218	6212	31
H28B	2329	8494	5897	31
H11H	4160(20)	4550(40)	7511(15)	76(15)
H11I	4721(9)	5290(40)	7748(17)	66(14)
H11J	4169(16)	5880(20)	7683(15)	48(11)
H11E	3283(14)	5480(20)	5534(11)	30(8)
H11F	2772(8)	4740(40)	5371(16)	54(12)
H11G	3350(20)	4020(30)	5460(20)	98(19)

Experimental

Single crystals of $C_{28}H_{55}ClO_{11}$. A suitable crystal was selected and run on an Oxford SuperNova diffractometer. The crystal was kept at 100.00(10) K during data collection. Using Olex2 [1], the structure was solved with the XS [2] structure solution program using Direct Methods and refined with the XL [3] refinement package using Least Squares minimization.

1. O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, OLEX2: a complete structure solution, refinement and analysis program. J. Appl. Cryst. (2009). 42, 339-341.
2. SHELXS-97 (Sheldrick, 2008)
3. XL, G.M. Sheldrick, Acta Cryst. (2008). A64, 112-122

Crystal Data. $C_{28}H_{55}ClO_{11}$, M =603.17, orthorhombic, a = 22.6891(4) Å, b = 10.5108(2) Å, c = 26.9322(4) Å, V = 6422.8(2) Å^3, T = 100.00(10), space group Pna2$_1$ (no. 33), Z = 8, μ(Cu Kα) = 1.512, 31583 reflections measured, 11677 unique (R_{int} = 0.0285) which were used in all calculations. The final wR_2 was 0.1318 (all data) and R_1 was 0.0481 (>2sigma(I)).

All work was done by Dr. Sergey Lindeman; Marquette University; Milwaukee, WI
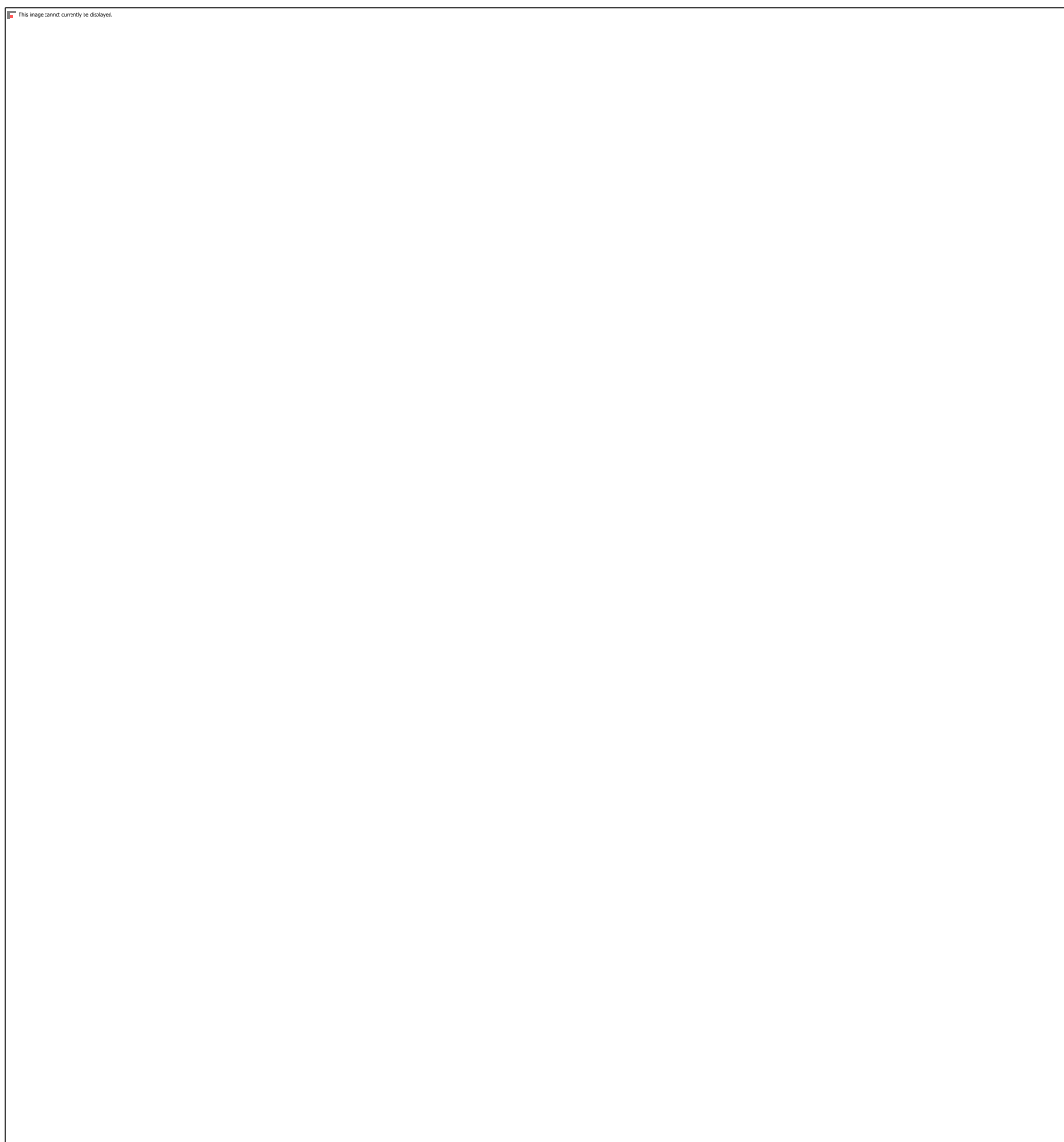
Molecular geometry:

The crystal contains two symmetrically independent formula units having almost identical structure. The crown-ether molecule has an approximate (non-crystallographic) mirror symmetry (with m-plane through O6 and O9 perpendicular to the mean plane f the macrocycle). The ethylene bridges are in alternated g^+g^- conformations. The cis-fused cyclohexane rings are both in a chair conformation with t-Bu groups positioned equatorially. The oxonium ion is positioned over the center of the crown-ether making H-bonds O-H…O with 3 (out of 6) of its oxygens.

Two symmetrically independent units form almost ideal (non-crystallographic) centrosymmetric dimer albeit the crystal itself is non-centrosymmetric (polar).
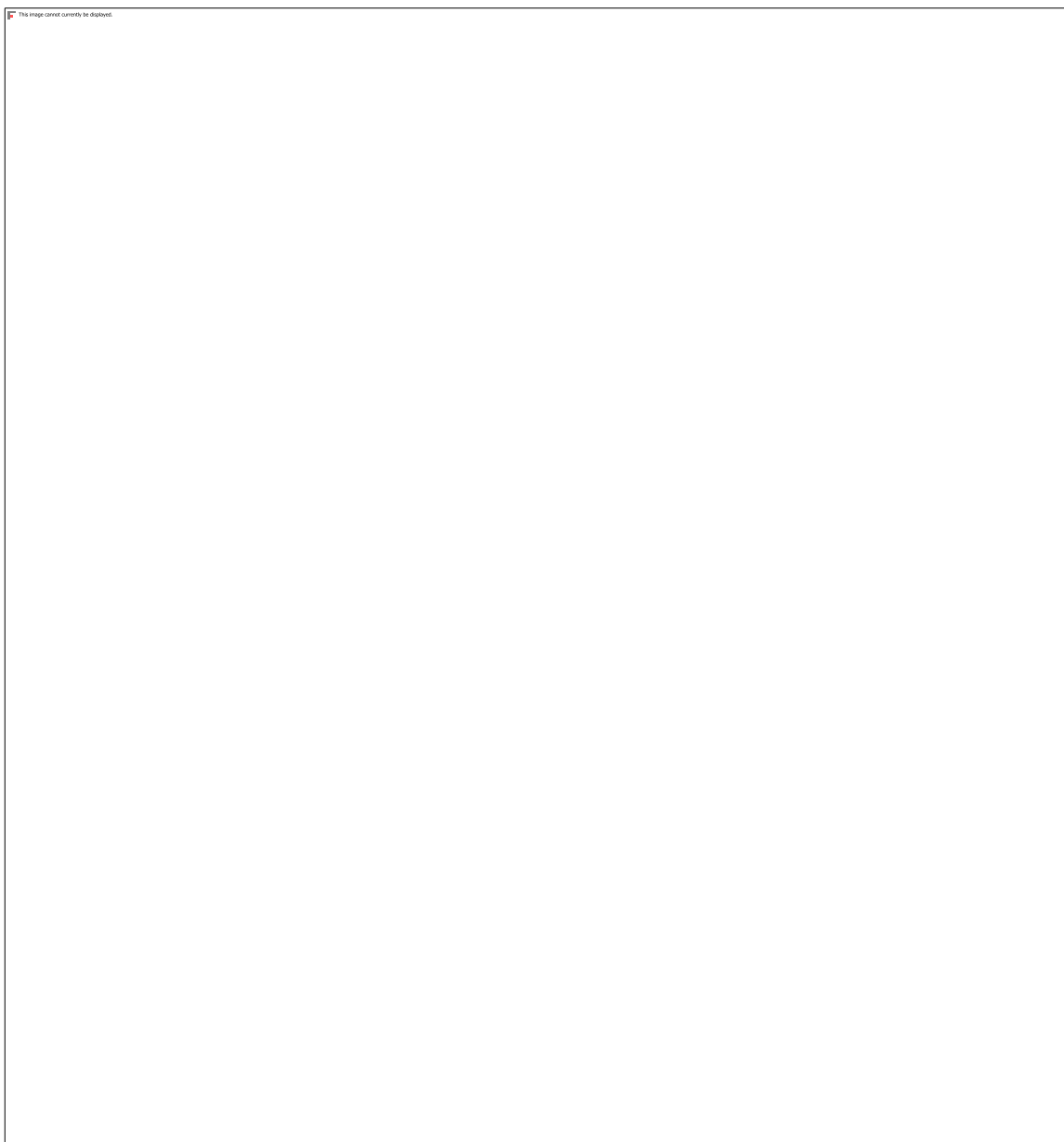
Molecular packing:

In the crystal structure, hydrophilic and hydrophobic parts of the molecules form alternated layers along c axis. There are multiple C-H…O interactions. The crystals represent a partial (3:1) racemic twin.

APPENDIX F

CRYSTALLOGRAPHIC DATA FOR 4Z,5'Z-*CIS-SYN-CIS*-DI-*TERT*-
BUTYLCYCLOHEXANO-18-CROWN-6
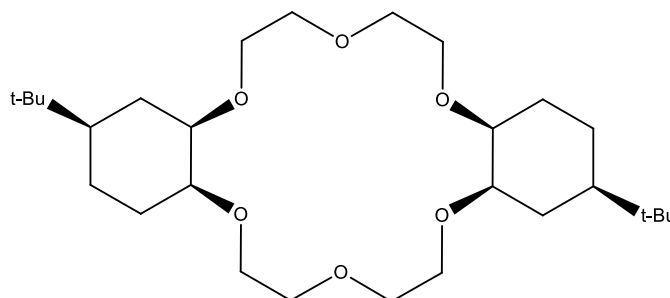
Colorless prisms. The experiment was done with Oxford SuperNova diffractometer using
Cu(Kα) radiation at 100K.

Table F-1 Crystal Data

Empirical formula	$C_{28}H_{52}O_6$
Formula weight	484.70
Temperature/K	100.00(10)
Crystal system	triclinic
Space group	P-1
a/Å	7.7239(3)
b/Å	13.3138(6)
c/Å	14.9144(7)
α/°	68.539(5)
β/°	83.898(4)
γ/°	84.192(4)
Volume/Å^3	1416.07(11)
Z	2
ρ_{calc}mg/mm^3	1.137
m/mm^{-1}	0.618
F(000)	536.0
Crystal size/mm^3	$0.15 \times 0.12 \times 0.1$
2Θ range for data collection	7.16 to 147.78°
Index ranges	$-9 \le h \le 9$, $-16 \le k \le 16$, $-18 \le l \le 17$

Reflections collected	21303	
Independent reflections	5635[R(int) = 0.0259]	
Data/restraints/parameters	5635/0/313	
Goodness-of-fit on F^2	1.023	
Final R indexes [I>=2σ (I)]	$R_1 = 0.0358$, $wR_2 = 0.0900$	
Final R indexes [all data]	$R_1 = 0.0423$, $wR_2 = 0.0960$	
Largest diff. peak/hole / e Å^{-3}	0.21/-0.23	

Table F-2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{Å}^2 \times 10^3$) for crystal. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	x	y	z	U(eq)
O1	3552.8(9)	4964.3(6)	3845.0(5)	21.19(17)
O2	3532.8(10)	2261.1(6)	5594.7(5)	22.63(17)
O5	8428.6(10)	3528.3(6)	3895.1(6)	21.87(17)
O6	6745.2(9)	5734.4(6)	2793.4(6)	23.61(18)
O3	5262.1(9)	328.6(6)	6875.6(6)	22.59(17)
C3	3221.1(13)	6596.7(8)	2485.3(8)	19.5(2)
C17	8763.9(13)	-758.3(8)	7062.6(8)	20.8(2)
C19	6356.4(14)	-2014.0(9)	7477.6(8)	21.7(2)
C14	3418.0(14)	556.4(9)	6867.8(9)	24.6(2)
C2	3781.5(13)	5396.9(8)	2816.5(8)	19.8(2)
C11	3870.8(14)	3819.0(9)	4221.2(8)	23.5(2)
C12	3294.1(14)	3407.5(9)	5281.4(8)	22.2(2)
C18	8345.3(13)	-1951.5(8)	7421.7(8)	19.4(2)
C1	5638.3(14)	5205.6(9)	2419.6(8)	21.4(2)
C15	6005.2(13)	-146.5(8)	6194.8(8)	19.8(2)
C16	7982.6(13)	-84.5(8)	6116.5(8)	20.4(2)
C21	9209.8(14)	-2644.2(9)	8372.6(8)	21.6(2)
C13	2958.7(14)	1751.3(9)	6582.3(8)	23.6(2)
C4	3282.9(13)	7111.1(9)	1375.3(8)	20.4(2)
C9	2794.8(16)	8772.9(10)	-115.8(9)	29.1(3)
C7	2662.2(14)	8332.2(9)	992.5(8)	23.2(2)
C20	5607.5(14)	-1334.5(9)	6515.2(8)	22.0(2)
C5	5105.0(14)	6879.7(9)	943.8(8)	24.4(2)
C27	9050.4(14)	4553.5(9)	3739.1(9)	27.5(3)
C23	8757.0(15)	-2161(1)	9164.0(8)	26.8(2)
C22	8591.4(16)	-3795.3(9)	8746.1(9)	29.1(3)

C6	5706.0(15)	5679.1(9)	1319.3(8)	26.2(2)
C24	11203.7(14)	-2716.3(10)	8169.9(9)	26.6(2)
C8	747.3(16)	8473.9(11)	1344.5(10)	36.1(3)
C10	3747.9(17)	9007.7(10)	1331.7(10)	32.3(3)
O4	8525.9(10)	982.5(6)	5871.7(6)	23.60(18)
C25	8023.0(14)	1725.6(8)	4964.7(8)	21.5(2)
C26	8859.7(14)	2759.2(9)	4806.1(8)	24.0(2)
C28	8539.1(14)	5368.7(9)	2783.0(9)	28.8(3)

Table F-3 Anisotropic Displacement Parameters ($\text{Å}^2 \times 10^3$) for crystal. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a*^2U_{11}+...+2hka\times b\times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	23.0(4)	17.7(4)	20.3(4)	-3.9(3)	-0.8(3)	-1.7(3)
O2	25.2(4)	18.7(4)	19.9(4)	-3.4(3)	2.6(3)	-0.2(3)
O5	22.2(4)	16.3(4)	24.3(4)	-3.4(3)	-2.6(3)	-2.5(3)
O6	16.0(4)	22.0(4)	32.3(4)	-9.2(3)	-3.5(3)	0.8(3)
O3	19.4(4)	24.2(4)	27.1(4)	-12.5(3)	-5.0(3)	1.1(3)
C3	16.9(5)	19.1(5)	21.4(5)	-6.3(4)	-1.6(4)	-0.1(4)
C17	17.9(5)	20.8(5)	22.5(6)	-5.4(4)	-4.0(4)	-3.0(4)
C19	21.4(5)	18.8(5)	23.8(6)	-5.8(4)	-2.3(4)	-3.9(4)
C14	19.6(5)	23.4(6)	26.5(6)	-4.0(5)	-0.6(4)	-2.6(4)
C2	19.5(5)	19.9(5)	19.4(5)	-5.7(4)	-1.9(4)	-3.0(4)
C11	21.7(5)	18.5(5)	25.4(6)	-3.5(4)	0.3(4)	1.7(4)
C12	22.1(5)	19.4(5)	23.8(6)	-6.3(4)	-2.8(4)	-0.9(4)
C18	19.3(5)	19.8(5)	18.8(5)	-6.6(4)	-1.6(4)	-1.3(4)
C1	20.9(5)	18.0(5)	24.7(6)	-7.6(4)	-0.8(4)	-1.0(4)
C15	20.9(5)	19.7(5)	19.8(5)	-7.2(4)	-4.6(4)	-2.1(4)
C16	20.7(5)	18.1(5)	21.7(5)	-5.6(4)	-1.9(4)	-3.8(4)
C21	21.9(5)	21.0(5)	20.8(5)	-5.9(4)	-2.9(4)	-1.5(4)
C13	22.0(5)	25.2(6)	19.7(6)	-4.8(4)	2.6(4)	-0.2(4)
C4	19.4(5)	20.9(5)	21.1(5)	-7.2(4)	-2.9(4)	-1.8(4)
C9	29.8(6)	27.5(6)	25.1(6)	-2.9(5)	-6.9(5)	-0.2(5)
C7	22.5(5)	22.3(5)	22.5(6)	-5.1(4)	-4.3(4)	0.9(4)
C20	21.5(5)	20.6(5)	25.2(6)	-8.1(4)	-5.1(4)	-3.9(4)
C5	24.9(5)	23.7(6)	20.7(6)	-4.6(4)	1.4(4)	-0.3(4)
C27	18.3(5)	18.9(5)	41.9(7)	-5.1(5)	-6.6(5)	-3.2(4)

C23	27.6(6)	30.6(6)	21.9(6)	-8.2(5)	-3.5(4)	-3.2(5)
C22	32.0(6)	22.4(6)	29.1(6)	-3.0(5)	-8.0(5)	-2.4(5)
C6	27.9(6)	24.5(6)	24.9(6)	-9.1(5)	2.7(5)	0.5(4)
C24	22.9(5)	28.0(6)	27.8(6)	-8.6(5)	-5.5(5)	2.2(4)
C8	28.6(6)	33.3(7)	35.6(7)	-3.1(6)	-0.2(5)	8.7(5)
C10	43.1(7)	21.2(6)	34.0(7)	-9.7(5)	-12.5(5)	1.5(5)
O4	25.7(4)	18.7(4)	23.3(4)	-1.3(3)	-6.7(3)	-6.7(3)
C25	20.4(5)	19.8(5)	21.6(6)	-3.2(4)	-3.7(4)	-2.8(4)
C26	23.6(5)	20.5(5)	25.2(6)	-3.7(4)	-5.2(4)	-3.6(4)
C28	15.9(5)	22.0(5)	39.7(7)	-1.4(5)	1.2(5)	-2.1(4)

Table F-4 Bond Lengths for crystal.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C2	1.4256(13)	C11	C12	1.5049(15)
O1	C11	1.4239(13)	C18	C21	1.5580(15)
O2	C12	1.4218(13)	C1	C6	1.5246(16)
O2	C13	1.4203(13)	C15	C16	1.5276(14)
O5	C27	1.4229(13)	C15	C20	1.5292(14)
O5	C26	1.4194(13)	C16	O4	1.4269(12)
O6	C1	1.4310(13)	C21	C23	1.5336(15)
O6	C28	1.4218(13)	C21	C22	1.5343(15)
O3	C14	1.4263(12)	C21	C24	1.5377(15)
O3	C15	1.4259(13)	C4	C7	1.5556(15)
C3	C2	1.5203(14)	C4	C5	1.5345(14)
C3	C4	1.5402(15)	C9	C7	1.5341(16)
C17	C18	1.5361(14)	C7	C8	1.5329(16)
C17	C16	1.5184(15)	C7	C10	1.5309(16)
C19	C18	1.5387(14)	C5	C6	1.5279(15)
C19	C20	1.5277(15)	C27	C28	1.5059(17)
C14	C13	1.5033(15)	O4	C25	1.4193(13)
C2	C1	1.5258(14)	C25	C26	1.5088(14)

Table F-5 Bond Angles for crystal.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°

A	B	C	Angle	A	B	C	Angle
C11	O1	C2	112.10(8)	O4	C16	C15	114.03(8)
C13	O2	C12	112.31(8)	C23	C21	C18	111.87(9)
C26	O5	C27	111.21(8)	C23	C21	C22	108.57(9)
C28	O6	C1	115.23(8)	C23	C21	C24	108.84(9)
C15	O3	C14	114.58(8)	C22	C21	C18	109.80(9)
C2	C3	C4	111.32(9)	C22	C21	C24	108.15(9)
C16	C17	C18	112.91(8)	C24	C21	C18	109.53(9)
C20	C19	C18	111.42(9)	O2	C13	C14	108.27(9)
O3	C14	C13	110.86(9)	C3	C4	C7	113.73(9)
O1	C2	C3	107.88(8)	C5	C4	C3	109.58(9)
O1	C2	C1	113.49(9)	C5	C4	C7	113.00(9)
C3	C2	C1	111.23(9)	C9	C7	C4	109.81(9)
O1	C11	C12	108.73(9)	C8	C7	C4	109.59(9)
O2	C12	C11	105.83(8)	C8	C7	C9	108.09(9)
C17	C18	C19	108.96(8)	C10	C7	C4	112.25(9)
C17	C18	C21	112.50(8)	C10	C7	C9	108.38(10)
C19	C18	C21	114.39(9)	C10	C7	C8	108.61(10)
O6	C1	C2	106.60(8)	C19	C20	C15	111.82(8)
O6	C1	C6	111.74(9)	C6	C5	C4	112.80(9)
C6	C1	C2	108.52(9)	O5	C27	C28	110.61(9)
O3	C15	C16	108.04(8)	C1	C6	C5	111.94(9)
O3	C15	C20	111.70(9)	C25	O4	C16	114.57(8)
C16	C15	C20	108.44(8)	O4	C25	C26	106.03(8)
C17	C16	C15	111.54(9)	O5	C26	C25	108.46(9)
O4	C16	C17	105.94(8)	O6	C28	C27	113.19(10)

Table F-6 Torsion Angles for crystal.

A	B	C	D	Angle/°
O1	C2	C1	O6	-60.78(11)
O1	C2	C1	C6	178.71(8)
O1	C11	C12	O2	176.07(8)
O5	C27	C28	O6	74.97(12)
O6	C1	C6	C5	-60.51(12)
O3	C14	C13	O2	68.37(11)
O3	C15	C16	C17	64.37(11)
O3	C15	C16	O4	-55.58(11)

O3	C15	C20	C19	-60.92(11)
C3	C2	C1	O6	61.09(11)
C3	C2	C1	C6	-59.42(11)
C3	C4	C7	C9	179.23(9)
C3	C4	C7	C8	-62.18(12)
C3	C4	C7	C10	58.59(12)
C3	C4	C5	C6	52.25(12)
C17	C18	C21	C23	53.63(12)
C17	C18	C21	C22	174.24(9)
C17	C18	C21	C24	-67.14(11)
C17	C16	O4	C25	175.80(8)
C19	C18	C21	C23	-71.40(11)
C19	C18	C21	C22	49.21(12)
C19	C18	C21	C24	167.83(9)
C14	O3	C15	C16	166.35(8)
C14	O3	C15	C20	-74.46(11)
C2	O1	C11	C12	-169.90(8)
C2	C3	C4	C7	178.04(8)
C2	C3	C4	C5	-54.42(11)
C2	C1	C6	C5	56.75(12)
C11	O1	C2	C3	173.86(8)
C11	O1	C2	C1	-62.42(11)
C12	O2	C13	C14	-174.74(8)
C18	C17	C16	C15	56.96(12)
C18	C17	C16	O4	-178.42(8)
C18	C19	C20	C15	-58.33(12)
C1	O6	C28	C27	-97.70(12)
C15	O3	C14	C13	-116.93(10)
C15	C16	O4	C25	-61.15(12)
C16	C17	C18	C19	-54.17(12)
C16	C17	C18	C21	177.88(8)
C16	C15	C20	C19	58.02(11)
C16	O4	C25	C26	-174.82(8)
C13	O2	C12	C11	-177.15(8)
C4	C3	C2	O1	-175.31(8)
C4	C3	C2	C1	59.61(11)
C4	C5	C6	C1	-54.92(13)

C7	C4	C5	C6	-179.80(9)
C20	C19	C18	C17	54.29(11)
C20	C19	C18	C21	-178.84(8)
C20	C15	C16	C17	-56.86(11)
C20	C15	C16	O4	-176.81(8)
C5	C4	C7	C9	53.48(12)
C5	C4	C7	C8	172.07(10)
C5	C4	C7	C10	-67.16(12)
C27	O5	C26	C25	174.81(9)
O4	C25	C26	O5	178.78(8)
C26	O5	C27	C28	-178.38(9)
C28	O6	C1	C2	159.99(9)
C28	O6	C1	C6	-81.59(11)

Table F-7 Hydrogen Atom Coordinates ($\mathring{A}\times10^4$) and Isotropic Displacement Parameters ($\mathring{A}^2\times10^3$) for crystal.

Atom	x	y	z	U(eq)
H3A	4002	6968	2730	23
H3B	2019	6695	2759	23
H17A	8312	-450	7561	25
H17B	10046	-715	6976	25
H19A	6085	-2777	7655	26
H19B	5799	-1753	7988	26
H14A	2861	173	7518	30
H14B	2963	289	6406	30
H2	2981	5039	2559	24
H11A	5130	3623	4127	28
H11B	3215	3487	3878	28
H12A	4008	3689	5640	27
H12B	2053	3636	5386	27
H18	8860	-2244	6915	23
H1	5979	4413	2643	26
H15	5542	265	5550	24
H16	8504	-373	5609	24
H13A	1681	1890	6676	28
H13B	3535	2044	6988	28

H4	2453	6729	1161	25
H9A	4026	8804	-358	44
H9B	2214	9501	-352	44
H9C	2229	8296	-346	44
H20A	4328	-1387	6579	26
H20B	6108	-1627	6014	26
H5A	5094	7139	232	29
H5B	5953	7290	1100	29
H27A	10337	4483	3749	33
H27B	8557	4807	4266	33
H23A	9318	-1479	8982	40
H23B	9174	-2670	9775	40
H23C	7489	-2025	9240	40
H22A	7363	-3782	8989	44
H22B	9298	-4262	9269	44
H22C	8719	-4076	8218	44
H6A	4952	5279	1089	31
H6B	6916	5585	1054	31
H24A	11505	-3005	7652	40
H24B	11741	-3196	8756	40
H24C	11636	-1994	7973	40
H8A	42	8028	1149	54
H8B	330	9236	1059	54
H8C	646	8248	2050	54
H10A	3582	8786	2036	48
H10B	3372	9775	1035	48
H10C	4984	8895	1141	48
H25A	6737	1852	4973	26
H25B	8437	1445	4444	26
H26A	8428	3039	5325	29
H26B	10142	2621	4819	29
H28A	9257	5998	2603	35
H28B	8799	5040	2282	35

Experimental

Single crystals of $C_{28}H_{52}O_6$. A suitable crystal was selected and run on a Oxford SuperNova diffractometer. The crystal was kept at 100.00(10) K during data collection. Using Olex2 [1], the structure was solved with the XS [2] structure solution program using Direct Methods and refined with the XL [3] refinement package using Least Squares minimization.

1. O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, OLEX2: a complete structure solution, refinement and analysis program. J. Appl. Cryst. (2009). 42, 339-341.
2. SHELXS-97 (Sheldrick, 2008)
3. XL, G.M. Sheldrick, Acta Cryst. (2008). A64, 112-122

Crystal Data. $C_{28}H_{52}O_6$, M =484.70, triclinic, a = 7.7239(3) Å, b = 13.3138(6) Å, c = 14.9144(7) Å, α = 68.539(5)°, β = 83.898(4)°, γ = 84.192(4)°, V = 1416.07(11) Å^3, T = 100.00(10), space group P-1 (no. 2), Z = 2, μ(Cu Kα) = 0.618, 21303 reflections measured, 5635 unique (R_{int} = 0.0259) which were used in all calculations. The final wR_2 was 0.0960 (all data) and R_1 was 0.0358 (>2sigma(I)).

Initial workup was performed by Dr. Dennis W. Bennett; University of Wisconsin-Milwaukee; Milwaukee, WI

Follow-up work was done by Dr. Sergey Lindeman; Marquette University; Milwaukee, WI
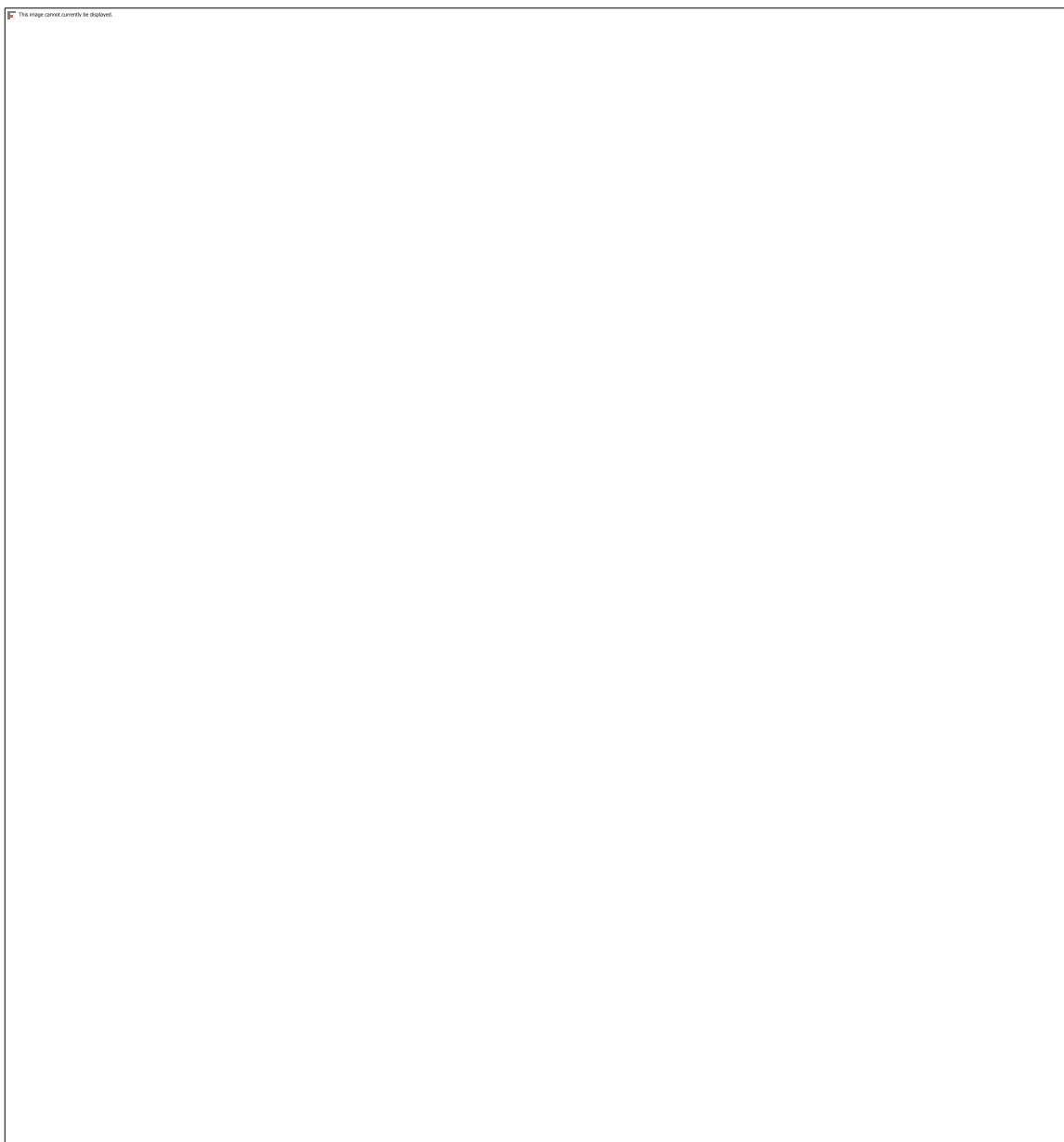
Molecular geometry:

The crown-ether molecule has an approximate (non-crystallographic) two-fold symmetry (with the axis perpendicular to the mean plane of the macrocycle). The ethylene bridges are in extended g^+t conformations. Apparently, there are some intra-molecular C-H…O hydrogen bonds. The cis-fused cyclohexane rings are both in a chair conformation with t-Bu groups oriented equatorially.

This image cannot currently be displayed.
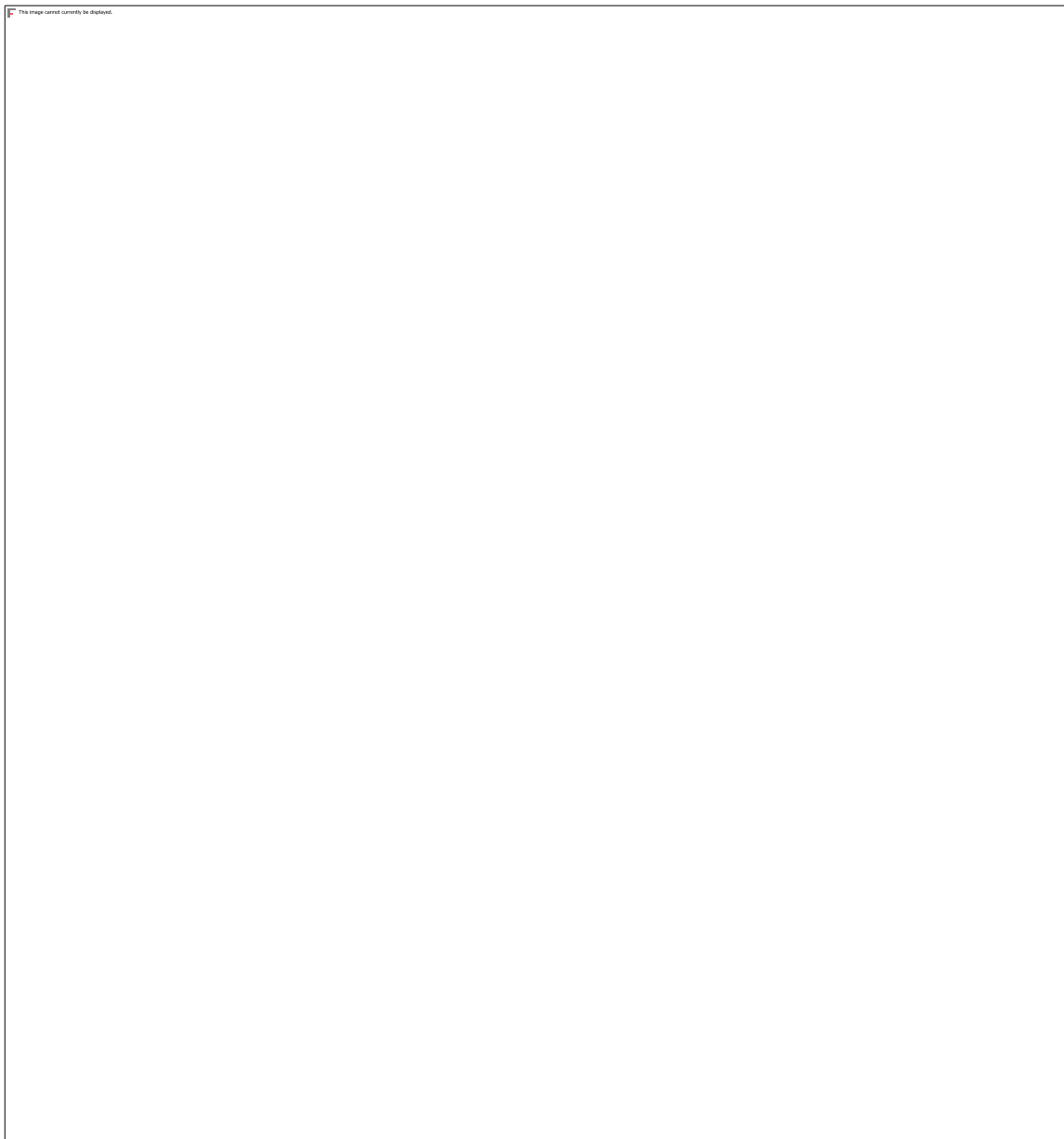
Molecular packing:

In the crystal, the molecules form stacks along b axis, probably – as a result of multiple inter-molecular C-H…O interactions within the stacks. The crystal represents a racemate

APPENDIX G

NMR OF 4Z,5'Z *CIS-SYN-CIS*-DI-*TERT*-BUTYLCYCLOHEXANO-18-CROWN-6

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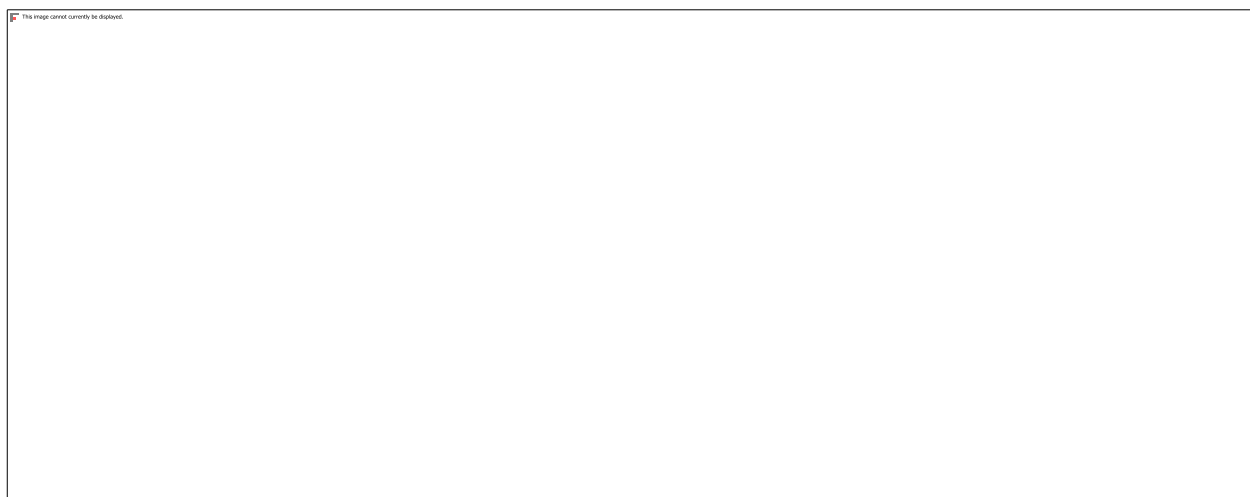
Figure G-1: Structure of 4z,5'z *cis-syn-cis*-di-*tert*-butylcyclohexano-18-crown-6
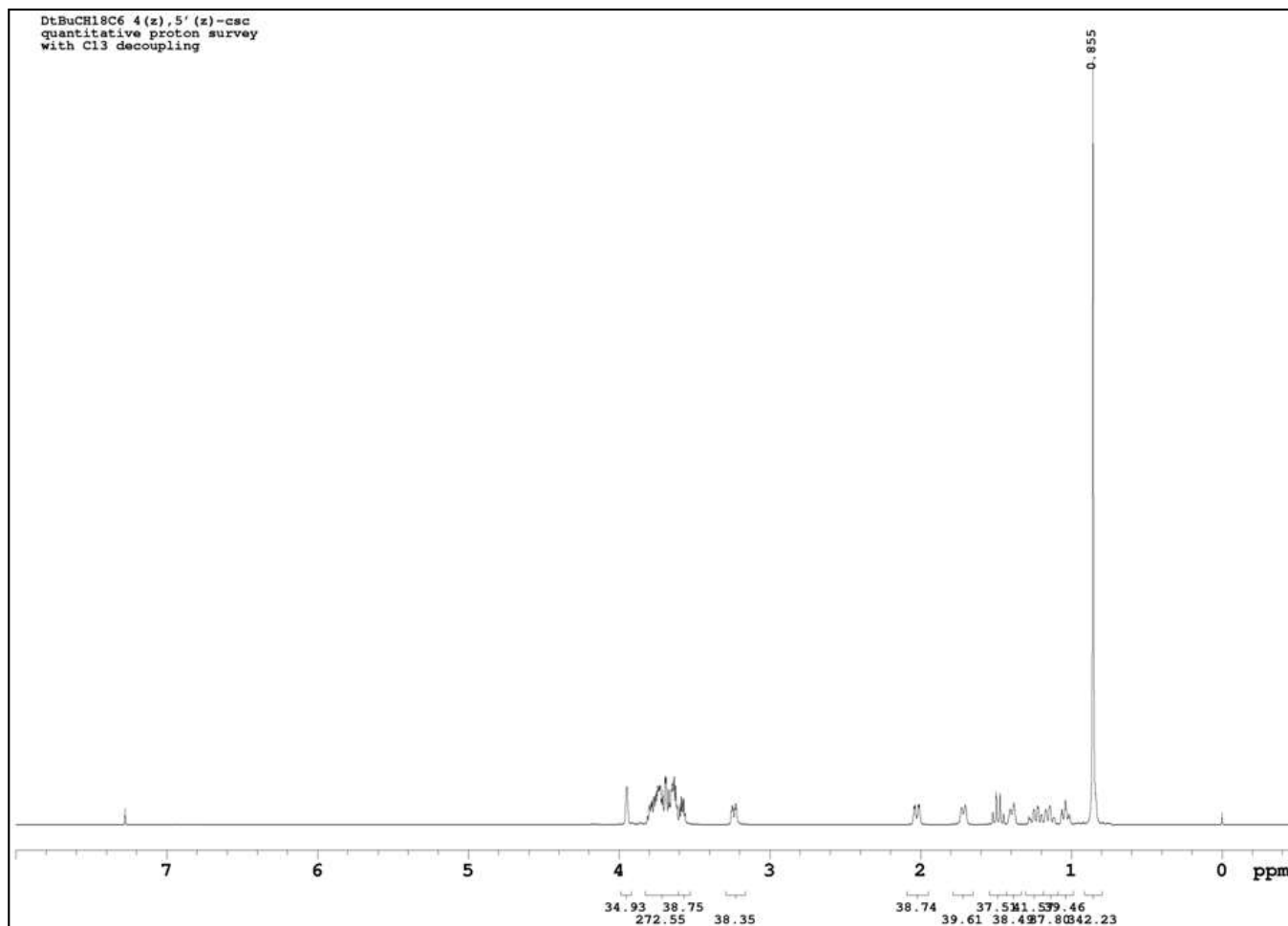
Figure G-2: ^{1}H NMR of 4z,5'z *csc* DtBuCH18C6
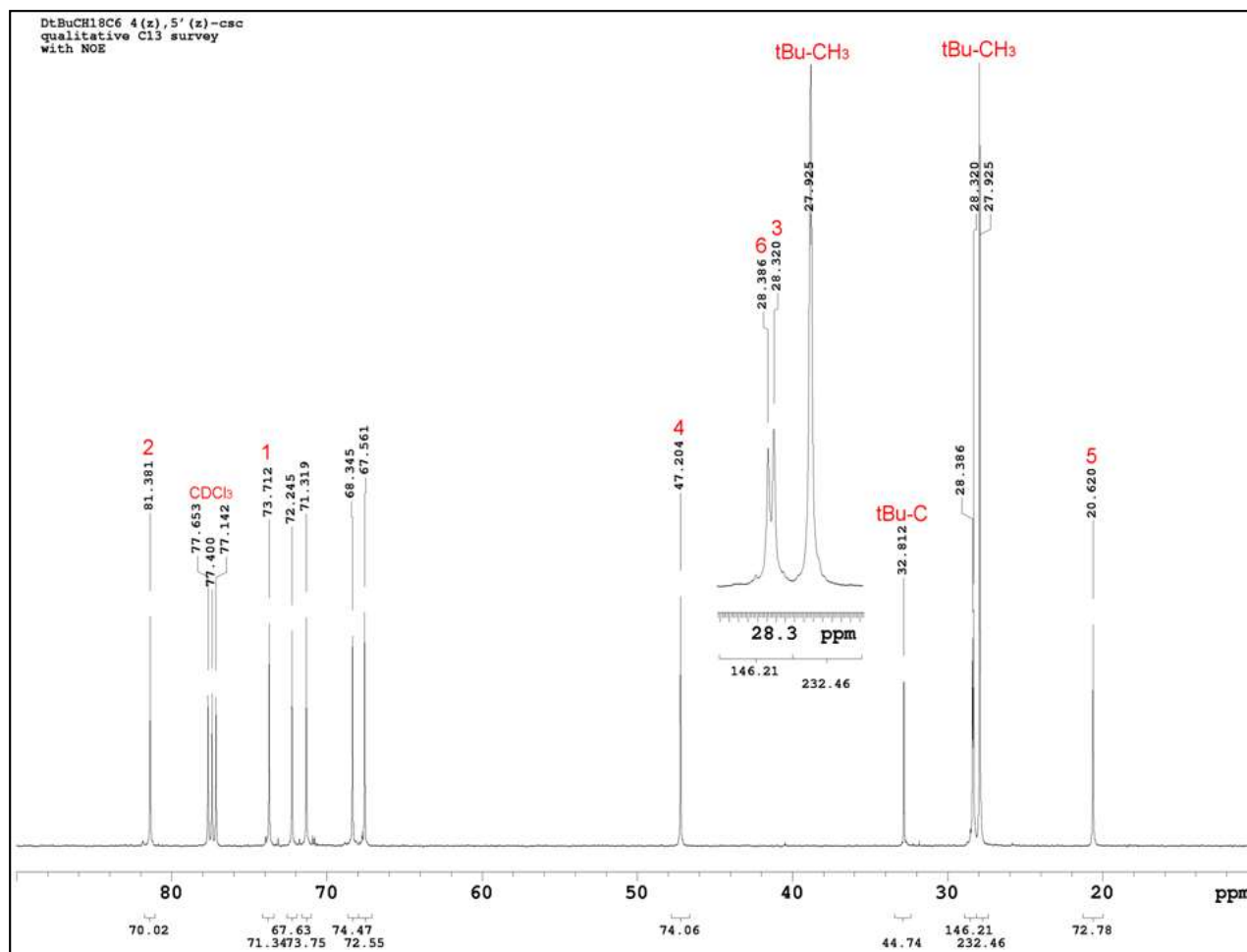
Figure G-3: ^{13}C NMR of 4z,5'z *csc* DtBuCH18C6
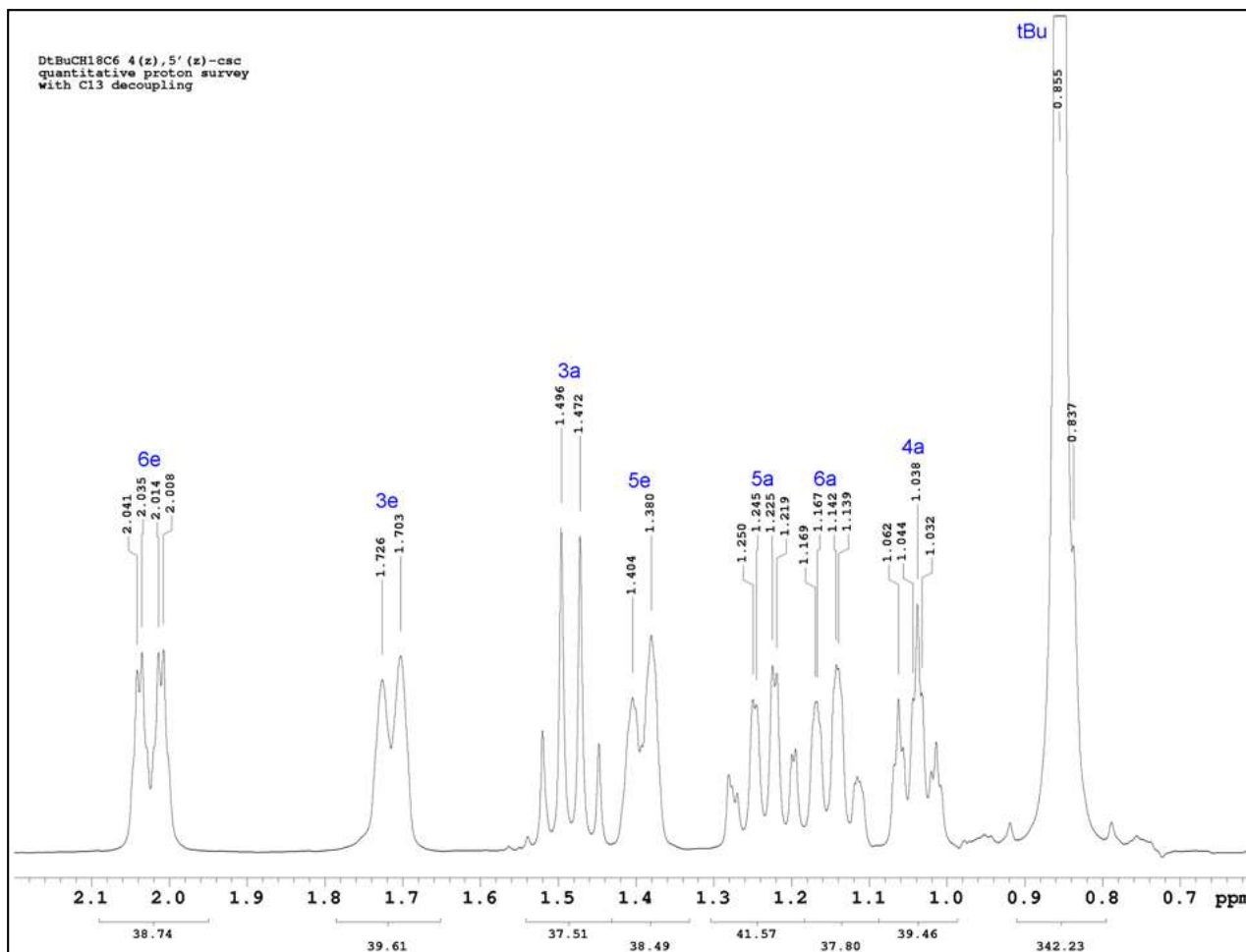
Figure G-4: Partial ¹H NMR of 4z,5'z *csc* DtBuCH18C6 with Peak Assignments
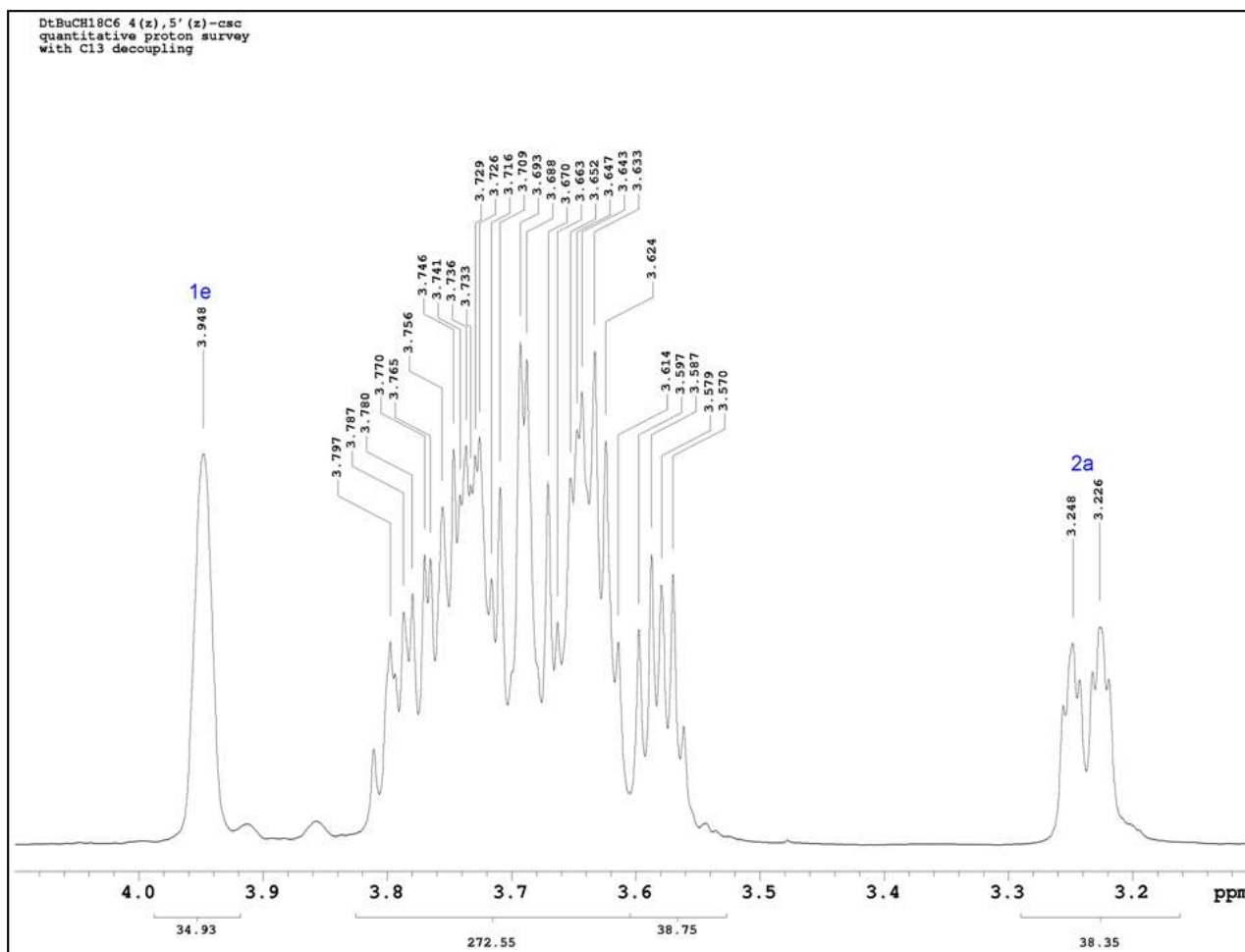
Figure G-5: Partial ^{1}H NMR of 4z,5'z *csc* DtBuCH18C6 with Peak Assignments
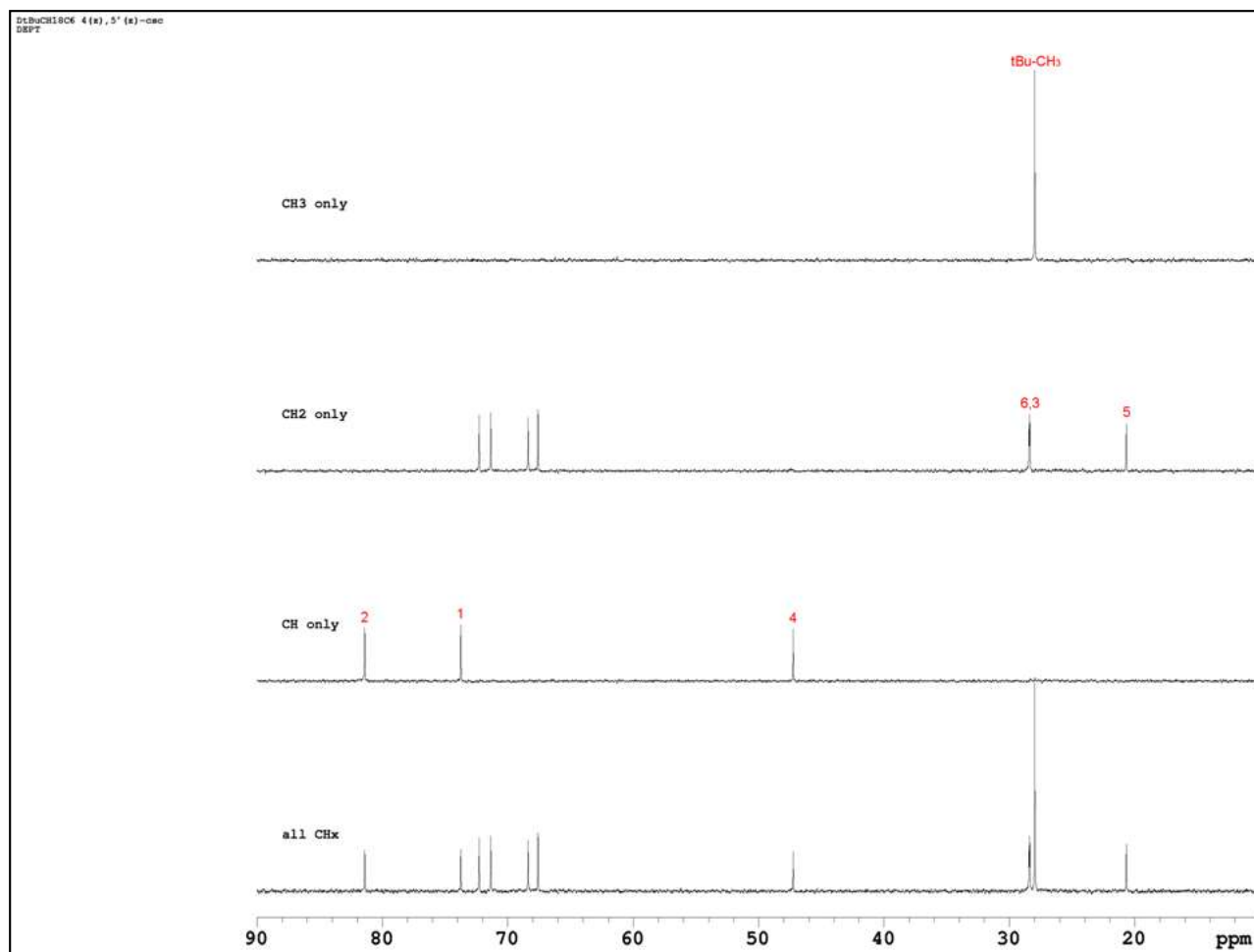
Figure G-6: Carbon DEPT NMR of 4z,5'z *csc* DtBuCH18C6 with Peak Assignments
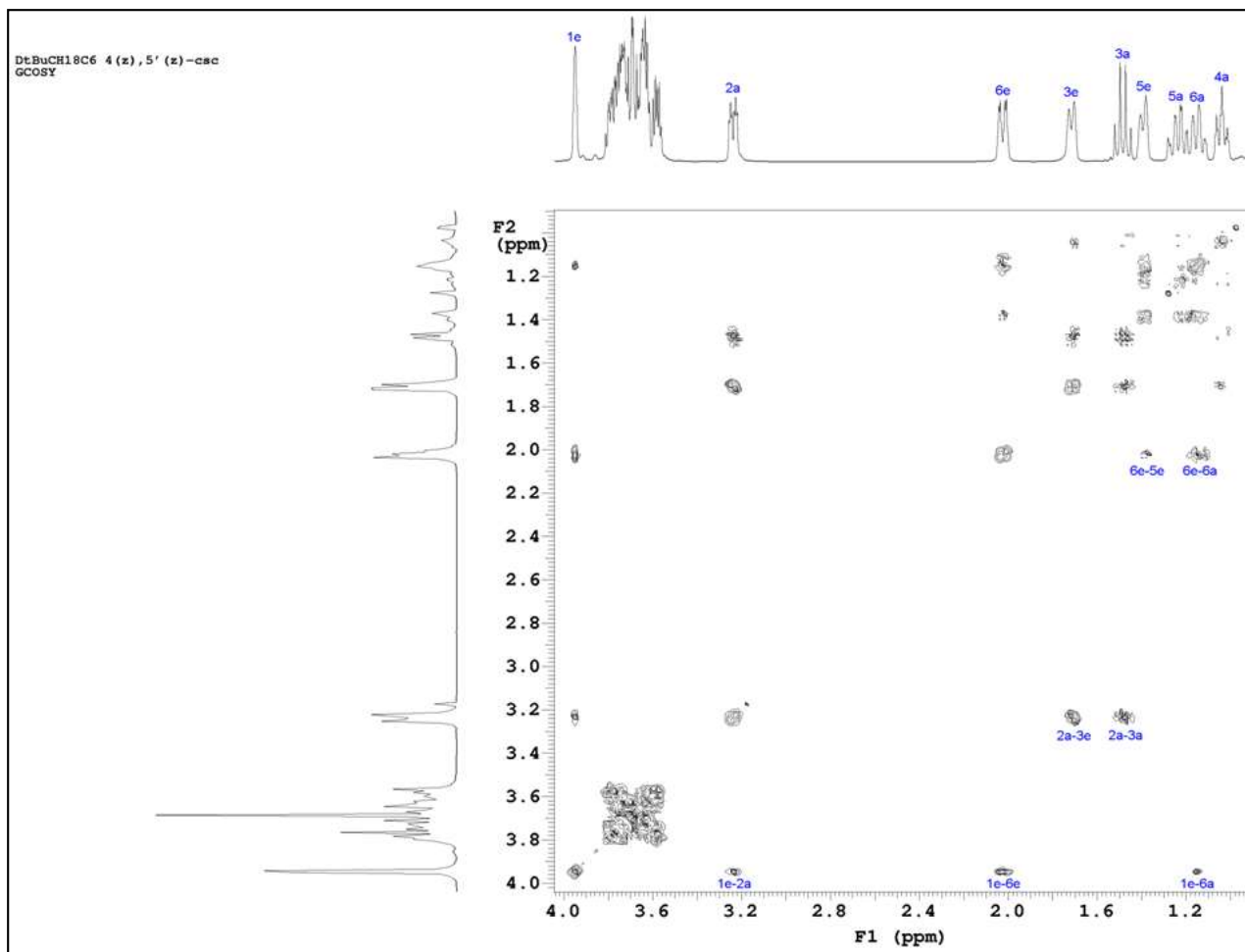
Figure G-7: Partial COSY NMR of 4z,5'z *csc* DtBuCH18C6 with Peak Assignments
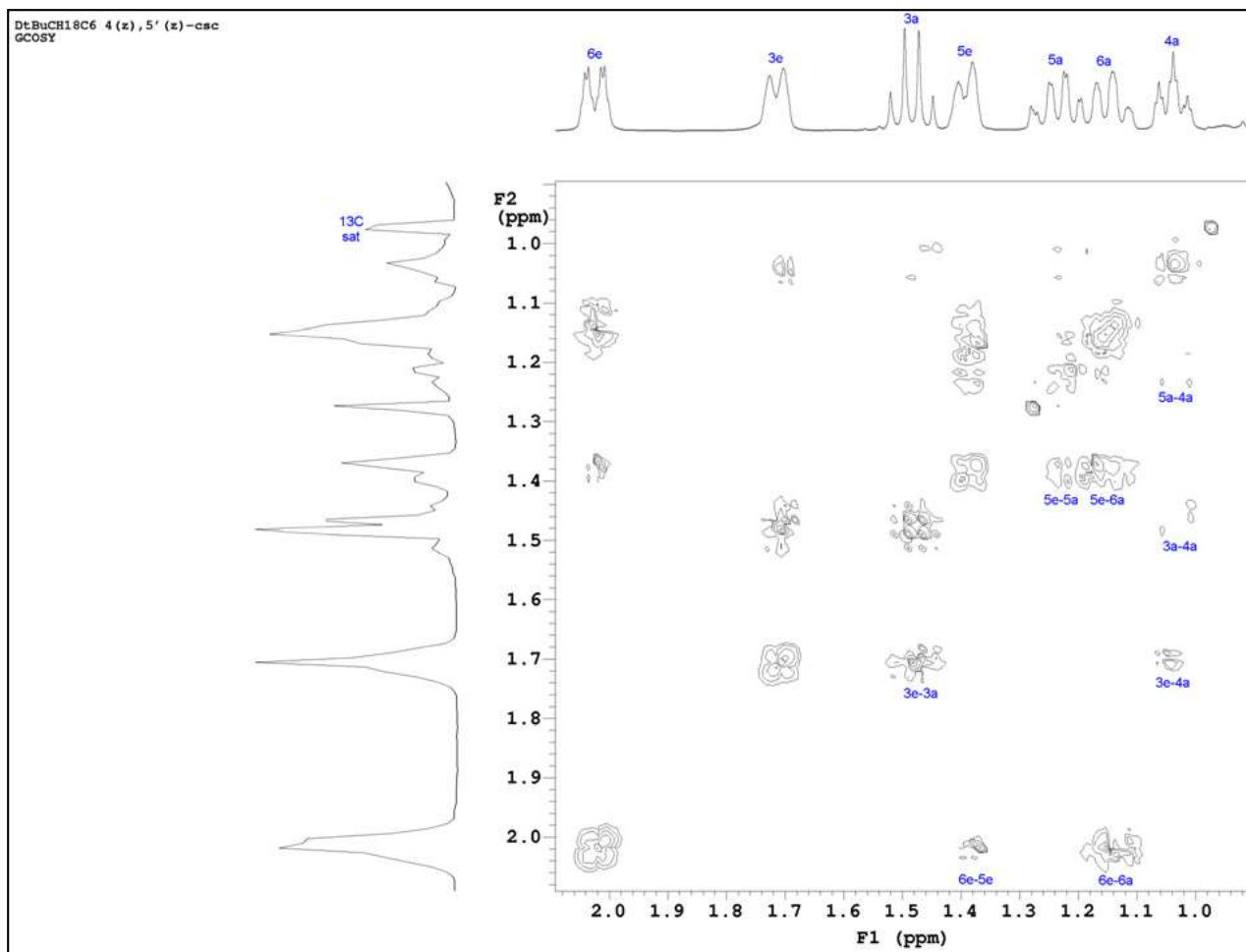
Figure G-8: Partial COSY NMR of 4z,5'z *csc* DtBuCH18C6 with Peak Assignments
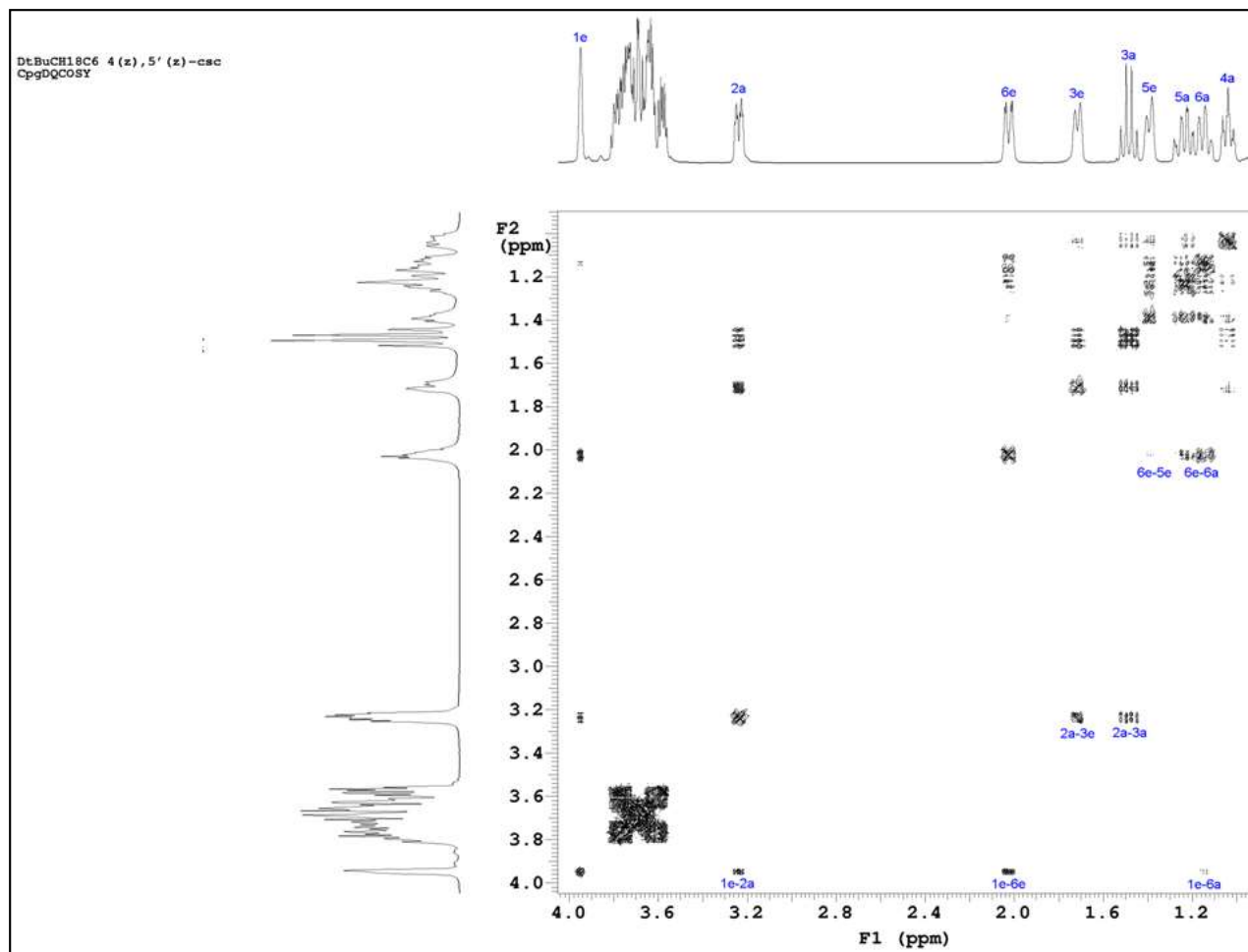
Figure G-9: Partial COSY NMR of of 4z,5'z *csc* DtBuCH18C6 with Peak Assignments
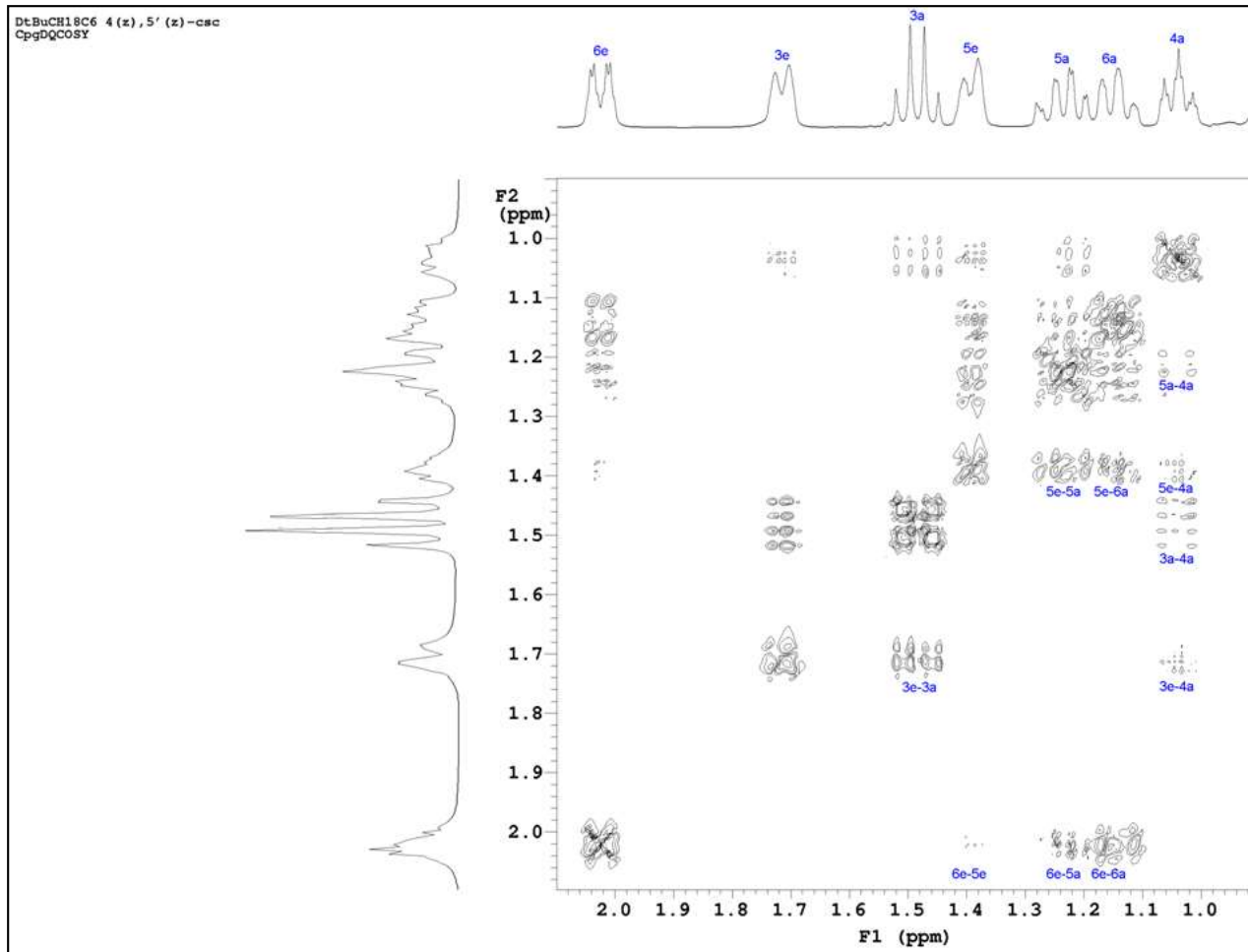
Figure G-10: Partial COSY NMR of 4z,5'z *csc* DtBuCH18C6 with Peak Assignments
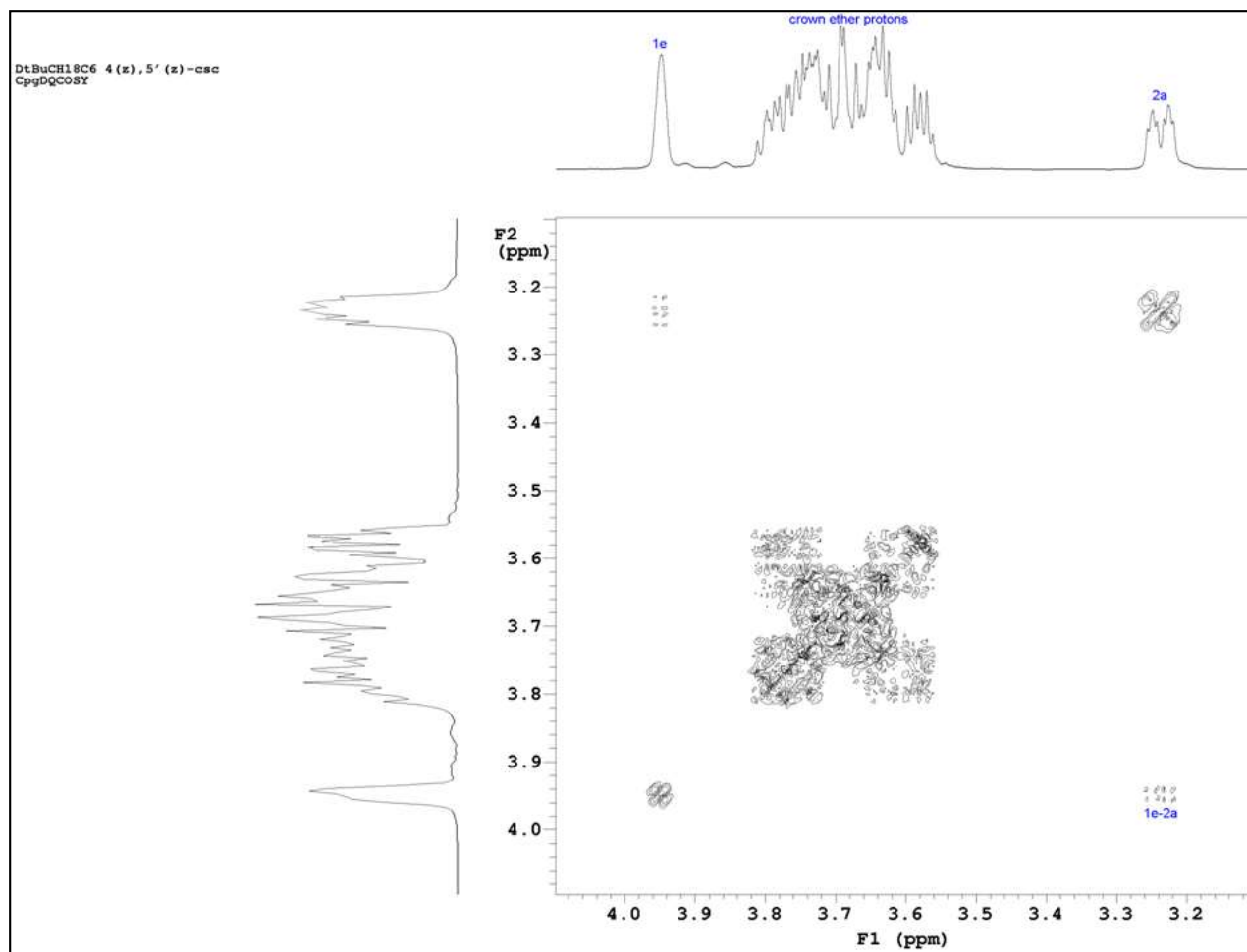
Figure G-11: Partial COSY NMR of 4z,5'z *csc* DtBuCH18C6 with Peak Assignments
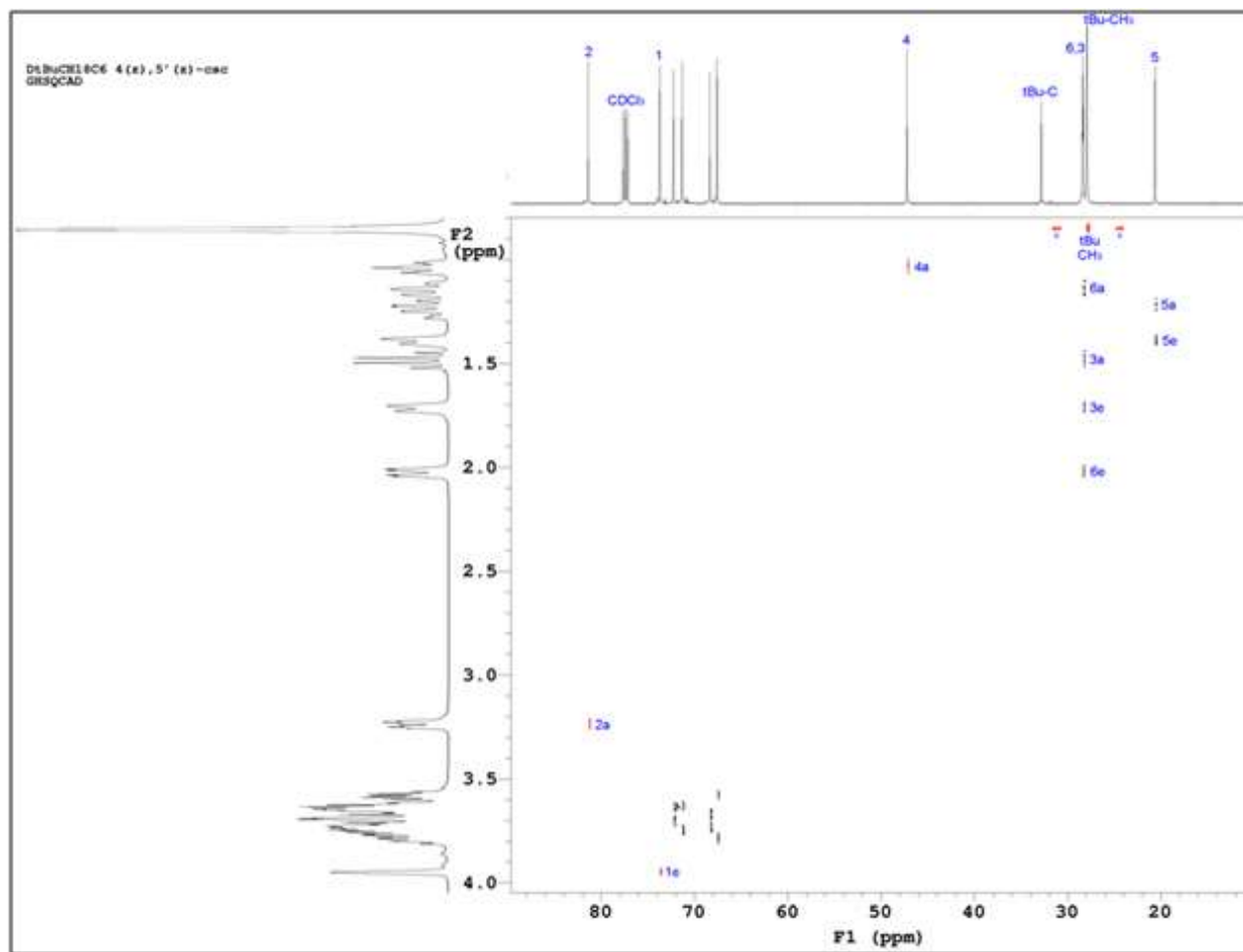
Figure G-12: Partial HSQC NMR of 4z,5'z *csc* DtBuCH18C6 with Peak Assignments
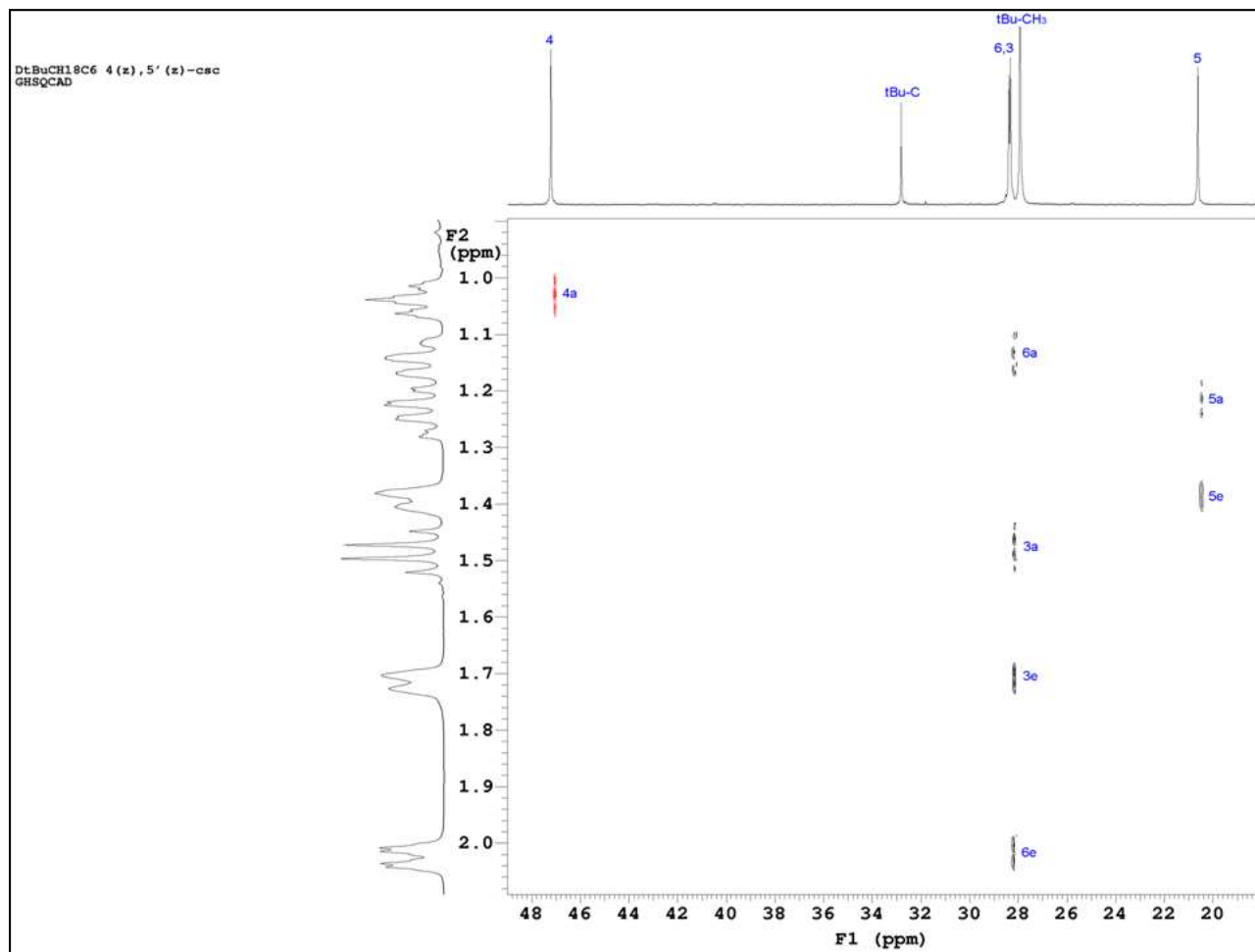
Figure G-13: Partial HSQC NMR of 4z,5'z *csc* DtBuCH18C6 with Peak Assignments
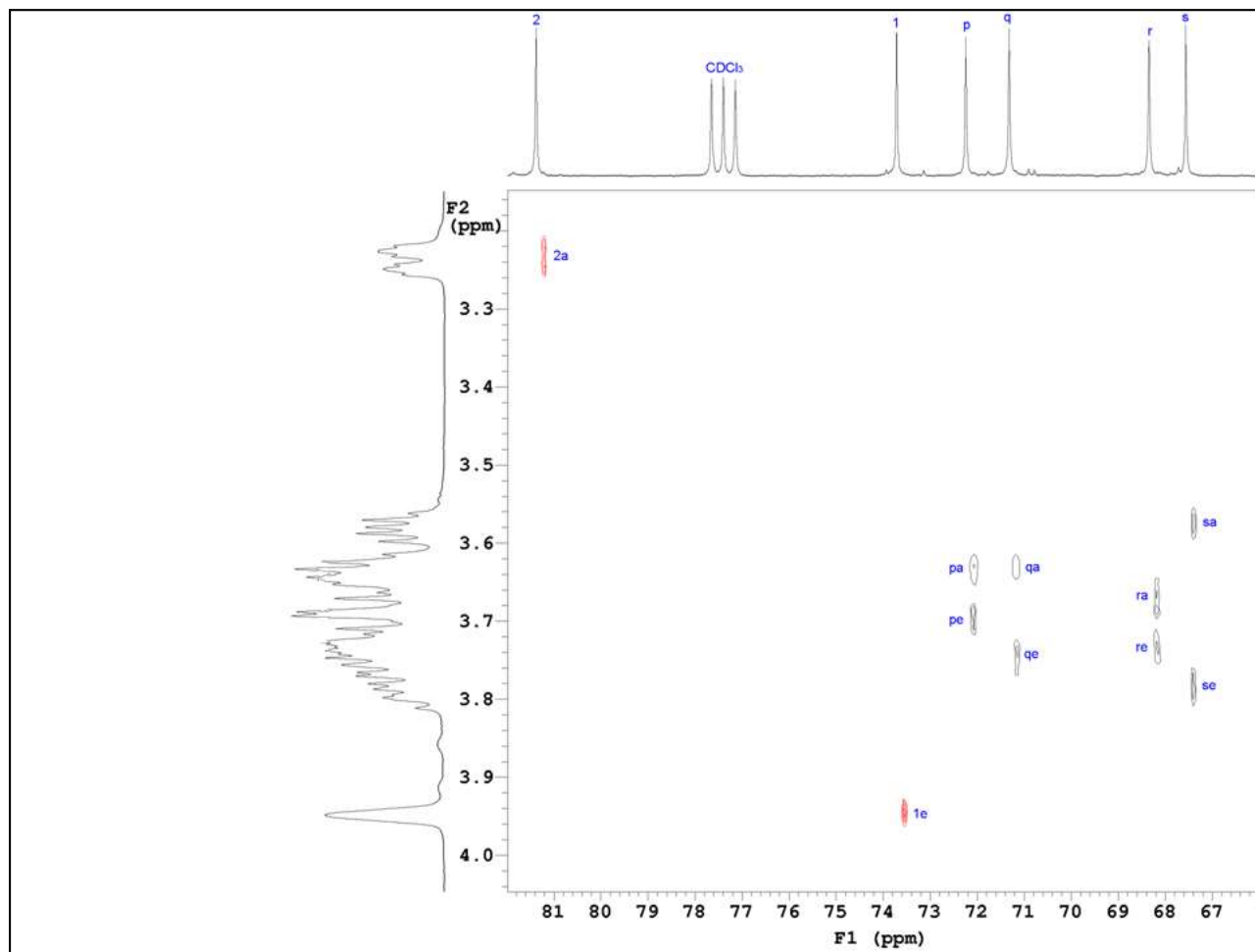
Figure G-14: Partial HSQC NMR of 4z,5'z *csc* DtBuCH18C6 with Peak Assignments
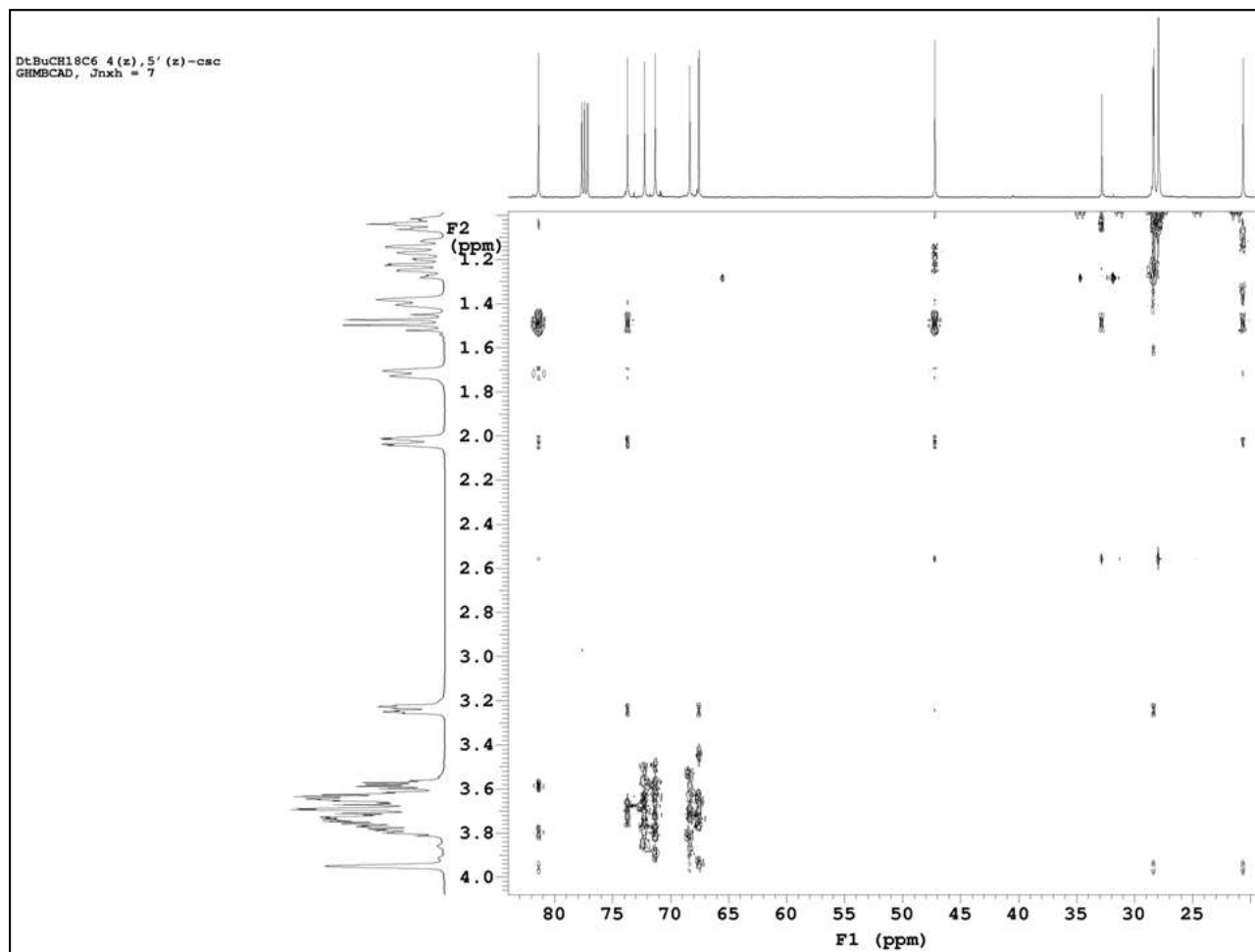
Figure G-15: Partial HMBC NMR of 4z,5'z *csc* DtBuCH18C6

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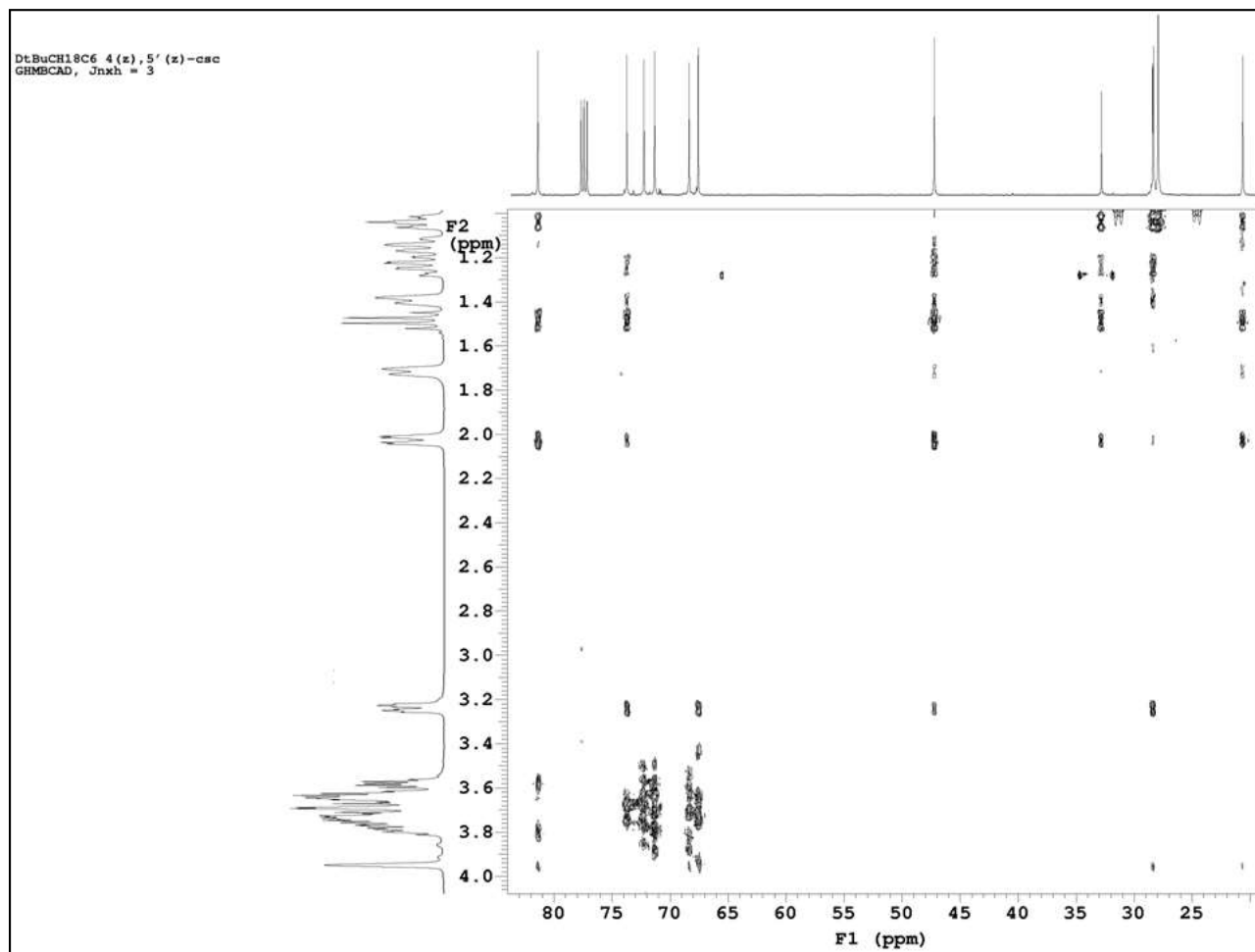
Figure G-16: Partial HMBC NMR of 4z,5'z *csc* DtBuCH18C6
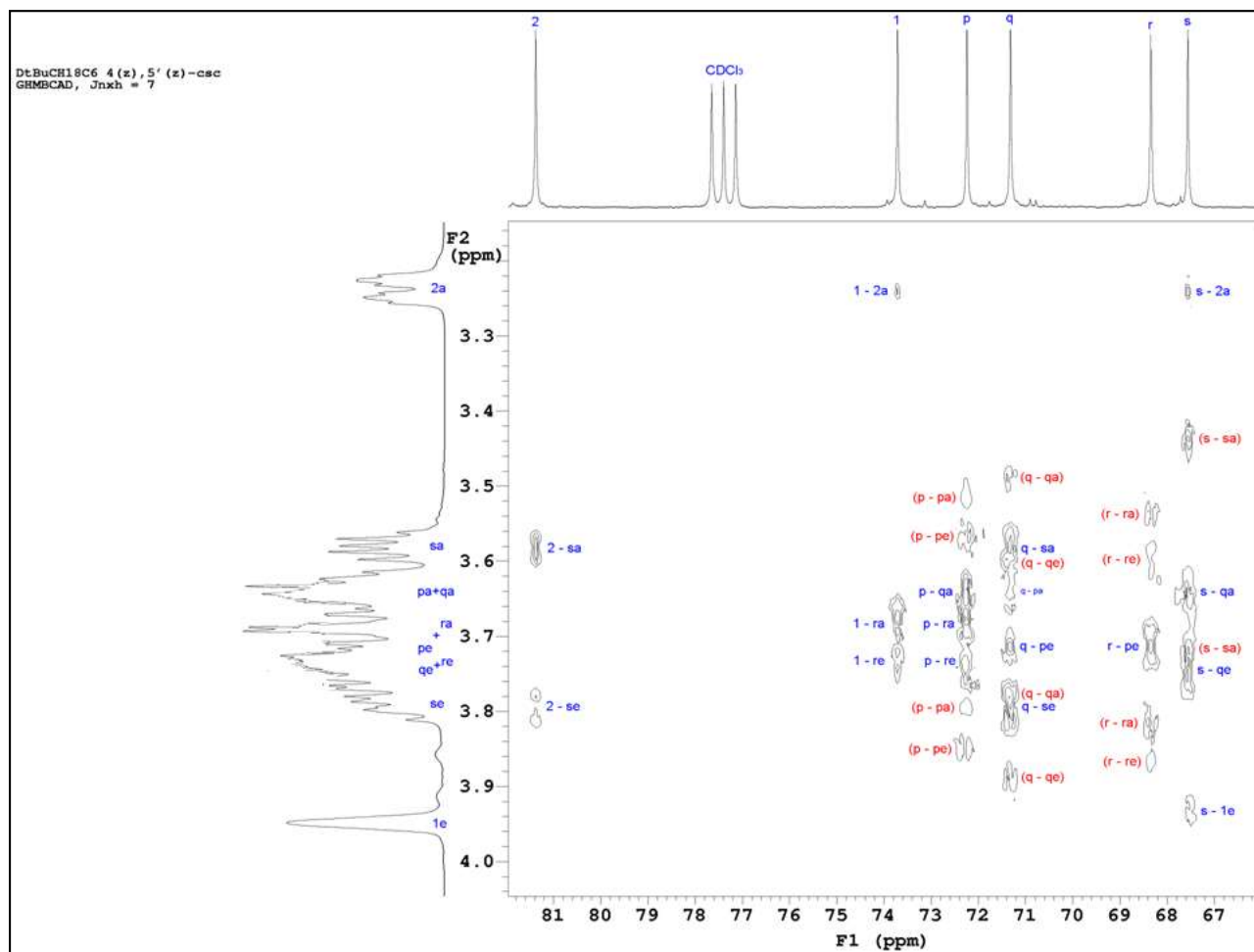
Figure G-17: Partial HMBC NMR of 4z,5'z *csc* DtBuCH18C6 with Peak Assignments
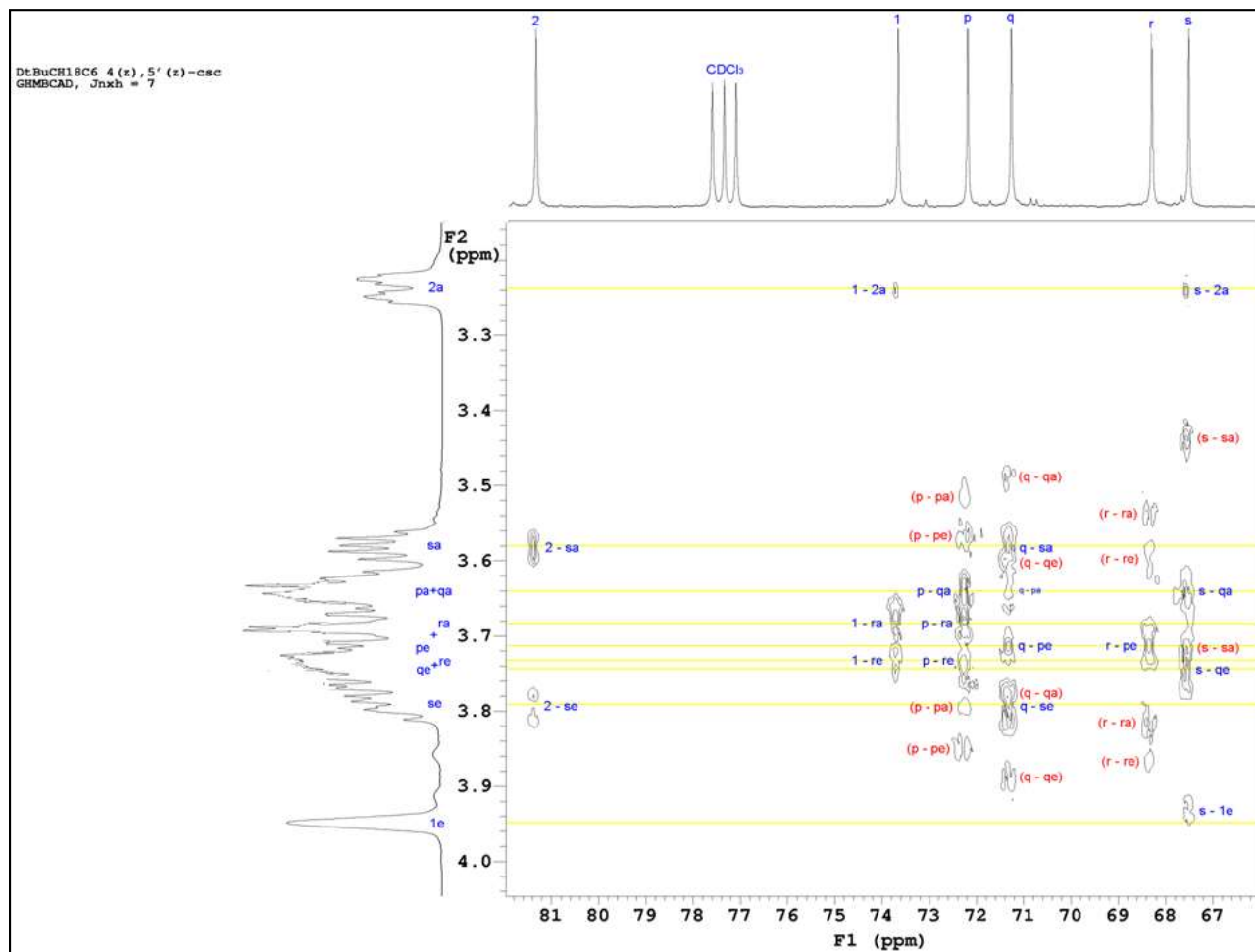
Figure G-18: Partial HMBC NMR of 4z,5'z *csc* DtBuCH18C6 with Cross Crown Ether Ring Assignments

MOLECULAR MECHANICS CALCULATIONS FOR THE *CIS-CIS* ISOMERS OF DTBUCH18C6
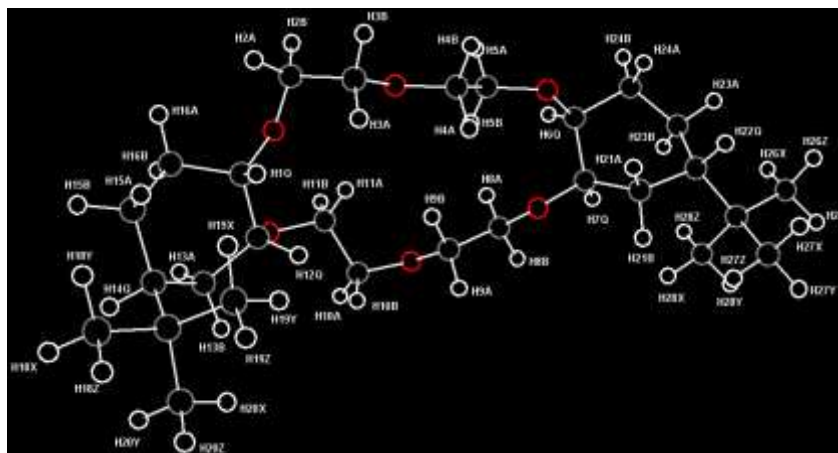
Figure H.1: Optimized Structure of 4e,4'e *cis-anti-cis* DtBuCH18C6 with Hydrogen Labels

Figure H.2: Optimized Structure of 4e,4'e *cis-anti-cis* DtBuCH18C6 with Carbon and Oxygen Labels

Table H.1: Hydrogen Distances for the Optimized Structure of 4e,4'e *cis-anti-cis* DtBuCH18C6

	H28X	H28Y	H28Z	H26X	H26Y	H26Z	H27X	H27Y	H27Z	H20X	H20Y	H20Z	H18X	H18Y	H18Z	H19X	H19Y	H19Z	H15A	H15B	H16A	H16B	H13A	H13B	H2A	H2B
H28X	0	1.7656	1.7731	3.7808	3.7689	4.3525	3.7967	3.0941	2.6065	11.0141	12.7687	12.1874	14.2786	13.7873	13.6107	11.3074	10.0218	11.2032	12.7368	13.832	12.6647	12.4451	11.7199	10.7971	11.284	10.6816
H28Y	1.7656	0	1.7651	3.0317	2.5355	3.7536	3.748	2.5162	3.1272	12.6827	14.4415	13.8225	15.9942	15.5099	15.2847	13.0231	11.7404	12.865	14.4898	15.5968	14.4121	14.1979	13.4584	12.518	12.9786	12.3297
H28Z	1.7731	1.7651	0	2.5707	3.1717	3.7868	4.3513	3.7552	3.814	12.3908	14.1175	13.6506	15.5748	15.0343	15.0007	12.5393	11.3263	12.6087	13.8039	14.8417	13.4595	13.2455	12.6938	11.95	11.9631	11.1319
H26X	3.7808	3.0317	2.5707	0	1.766	1.7728	3.777	3.7147	4.3559	14.3374	16.0708	15.4693	17.2922	16.5521	16.5908	13.9715	12.9662	14.1278	15.2835	16.4592	14.8834	14.915	14.6395	13.9541	13.1034	12.2622
H26Y	3.7689	2.5355	3.1717	1.766	0	1.7702	3.0077	2.4473	3.7066	14.4961	16.2599	15.5188	17.5651	16.8752	16.7371	14.299	13.2275	14.2473	15.802	17.0442	15.6562	15.6802	15.2239	14.3576	13.943	13.2776
H26Z	4.3525	3.7536	3.7868	1.7728	1.7702	0	2.5728	3.1313	3.7956	14.3858	16.1237	15.3509	17.1918	16.3433	16.3346	13.7336	12.8467	13.8343	15.1896	16.5022	14.9612	15.1638	14.9591	14.1967	13.0797	12.4213
H27X	3.7967	3.748	4.3513	3.777	3.0077	2.5728	0	1.7713	1.7705	12.6729	14.4163	13.461	15.4906	14.6793	14.477	12.1007	11.1811	11.9669	13.7905	15.1965	13.9397	14.1673	13.7776	12.8046	12.1945	11.8562
H27Y	3.0941	2.5162	3.7552	3.7147	2.4473	3.1313	1.7713	0	1.7662	12.817	14.5852	13.6879	15.9228	15.2898	14.9654	12.7599	11.6368	12.4817	14.4629	15.7733	14.6578	14.686	14.0404	12.9743	13.0899	12.7042
H27Z	2.6065	3.1272	3.814	4.3559	3.7066	3.7956	1.7705	1.7662	0	11.1906	12.9525	12.0462	14.207	13.5386	13.2504	10.9998	9.9071	10.7572	12.7097	14.0427	12.9532	13.0211	12.4153	11.3537	11.4122	11.1201
H20X	11.0141	12.6827	12.3908	14.3374	14.4961	14.3858	12.6729	12.817	11.1906	0	1.7719	1.7639	3.7874	4.3567	3.6995	3.7747	2.5491	3.0281	4.6216	5.0356	6.1684	5.4851	3.6917	2.1193	7.0894	7.982
H20Y	12.7687	14.4415	14.1175	16.0708	16.2599	16.1237	14.4163	14.5852	12.9525	1.7719	0	1.7706	2.588	3.8035	3.6933	4.3543	3.7693	3.7516	4.5654	4.4922	6.2758	5.5296	3.8201	2.835	6.7893	8.7255
H20Z	12.1874	13.8225	13.6506	15.4693	15.5188	15.3509	13.461	13.6879	12.0462	1.7639	1.7706	0	3.0126	3.6933	2.4228	3.7686	3.155	2.5329	4.7673	5.2794	6.803	6.4258	4.9732	3.6852	7.7939	8.9666
H18X	14.2786	15.9942	15.5748	17.2922	17.5651	17.1918	15.4906	15.9228	14.207	3.7874	2.588	3.0126	0	1.7707	1.7709	3.8061	4.3491	3.7443	3.3504	3.2054	5.4408	5.2753	4.6437	4.4055	7.076	8.4661
H18Y	13.7873	15.5099	15.0343	16.5521	16.8752	16.3433	14.6793	15.2898	13.5386	4.3567	3.8035	3.6933	1.7707	0	1.7661	2.6146	3.8129	3.1032	2.1779	2.8111	4.524	4.9161	4.9364	4.8069	5.8329	7.4033
H18Z	13.6107	15.2847	15.0007	16.5908	16.7371	16.3346	14.477	14.9654	13.2504	3.6995	3.6933	2.4228	1.7709	1.7661	0	3.1196	3.7522	2.5116	3.6654	4.293	5.566	4.9048	4.68	4.9048	7.1605	8.6586
H19X	11.3074	13.0231	12.5393	13.9715	14.299	13.7336	12.1007	12.7599	10.9998	3.7747	4.3543	3.7686	3.8061	2.6146	3.1196	0	1.7741	1.7632	2.2051	3.7897	4.0992	4.6238	4.6046	4.0966	4.4069	5.8548
H19Y	10.0218	11.7404	11.3263	12.9662	13.2275	12.8467	11.1811	11.6368	9.9071	2.5491	3.7693	3.155	4.3491	3.8129	3.7522	1.7741	0	1.7654	3.4005	4.6073	4.8774	4.8483	4.068	3.008	5.1034	6.1541
H19Z	11.2032	12.865	12.6087	14.1278	14.2473	13.8343	11.9669	12.4817	10.7572	3.0281	3.7516	2.5329	3.7443	3.1032	2.5116	1.7632	1.7654	0	3.6741	4.9607	5.7374	5.9587	5.2897	4.2458	6.0973	7.4298
H15A	12.7368	14.4898	13.8039	15.2835	15.802	15.1896	13.7905	14.4629	12.7097	4.6216	4.5654	4.7673	3.3504	2.1779	3.6654	2.2051	3.4005	3.6741	0	1.7466	2.4065	3.0665	3.8175	4.1717	3.7604	5.2682
H15B	13.832	15.5968	14.8417	16.4592	17.0442	16.5022	15.1965	15.7733	14.0427	5.0356	4.4922	5.2794	3.2054	2.8111	4.293	3.7897	4.6073	4.9607	1.7466	0	2.5203	2.5063	3.331	4.2205	4.6644	5.8999
H16A	12.6647	14.4121	13.4595	14.915	15.6562	14.9612	14.1673	14.6578	12.9532	6.1684	6.2758	6.803	5.4408	4.524	5.566	4.0992	4.8774	5.7374	2.4065	2.5203	0	1.7599	2.3755	4.9105	2.3644	3.4606
H16B	12.4451	14.1979	13.2455	14.915	15.6802	15.1638	14.1673	14.686	13.0211	5.4851	5.5296	6.4258	5.2753	4.9161	4.9048	4.6238	4.8483	5.9587	3.0665	2.5063	1.7599	0	3.6395	3.8183	3.6395	4.1763
H13A	11.7199	13.4584	12.6938	14.6395	15.2239	14.9591	13.7776	14.0404	12.4153	3.6917	3.8201	4.9732	4.6437	4.9364	4.68	4.6046	4.068	5.2897	3.8175	3.331	2.3755	3.6395	0	1.74	5.3504	5.8174
H13B	10.7971	12.518	11.95	13.9541	14.3576	14.1967	12.8046	12.9743	11.3537	2.1193	2.835	3.6852	4.4055	4.8069	4.9048	4.0966	3.008	4.2458	4.1717	4.2205	4.9105	3.8183	1.74	0	5.9929	6.5778
H2A	11.284	12.9786	11.9631	13.1034	13.943	13.0797	12.1945	13.0899	11.4122	7.0894	6.7893	7.7939	7.076	5.8329	7.1605	4.4069	5.1034	6.0973	3.7604	4.6644	2.3644	3.6395	5.3504	5.9929	0	1.7757
H2B	10.6816	12.3297	11.1319	12.2622	13.2776	12.4213	11.8562	12.7042	11.1201	7.982	8.7255	8.9666	8.4661	7.4033	8.6586	5.8548	6.1541	7.4298	5.2682	5.8999	3.4606	4.1763	5.8174	6.5778	1.7757	0
H3A	8.9858	10.6769	9.8223	10.9617	11.6371	10.8298	9.7397	10.6194	8.913	6.3904	7.5111	7.1862	7.4832	6.2973	7.0874	3.9766	4.0622	5.2217	4.6379	5.9803	4.3093	5.0482	5.7785	5.701	2.567	3.0634
H3B	9.7594	11.3609	10.3542	11.1745	12.0197	10.0012	9.6446	11.2723	9.0452	8.0696	9.045	8.7172	7.369	8.3911	5.316	5.7348	6.731	5.5677	6.0084	4.7104	5.7771	7.0288	7.2452		2.3952	2.5287
H11A	8.1664	9.8956	8.8725	10.6195	11.4154	10.0129	10.2104	10.6	9.0383	5.8283	7.0326	7.2933	7.9028	7.4018	8.0234	5.4772	4.637	6.3707	5.6795	6.2756	4.8781	4.3866	4.2901	4.3533	4.2696	3.7218
H11B	8.4477	10.5061	9.3902	11.3164	12.1986	11.9457	11.3495	11.5555	10.1155	6.4271	7.4363	8.0481	8.517	8.2971	8.9405	6.7493	5.8448	7.5906	6.5809	6.7397	5.5061	4.5337	4.2116	4.6062	5.3924	4.586
H10A	8.1668	9.7943	8.9956	11.2359	11.8278	11.8858	11.0013	10.8946	9.5126	5.3827	6.587	7.1333	8.3285	8.4642	8.6319	6.9474	5.5454	7.2212	7.2485	7.4068	6.9214	5.7552	4.3529	3.9428	7.0664	6.655
H10B	7.6437	9.3578	8.7117	10.8078	11.2628	11.2063	10.0296	10.0708	8.5434	4.289	5.7716	5.9383	7.4031	7.3475	7.3997	5.5357	4.0196	5.6911	6.2595	6.3403	5.5014	4.163	3.2868		6.2695	6.185
H4A	6.6669	8.2937	7.3934	8.4178	9.1307	8.3144	7.3899	8.2812	6.6468	7.6664	9.1148	8.6493	9.5837	8.5513	9.0397	6.032	5.5576	6.8098	7.0505	8.339	6.6759	7.1029	7.4183	7.061	4.8442	4.5496
H4B	7.7953	9.2815	8.2354	8.8378	9.7343	8.6511	8.0585	9.1855	7.6659	9.0353	10.3336	9.9166	10.4485	9.2216	9.9516	6.8429	6.7679	7.8896	7.5607	8.8402	6.8415	7.5743	8.3822	8.3063	4.6409	4.1638
H5A	7.2671	8.6642	7.2644	8.0141	9.2433	8.3051	8.3299	9.1999	7.9069	9.9783	11.3011	11.1762	11.7383	10.7372	11.513	8.4613	8.089	9.5152	8.8737	9.9272	7.6811	8.7351	8.85		5.5729	4.4962
H5B	6.1292	7.6891	6.387	7.6492	8.7061	8.0556	7.7805	8.3919	7.0129	8.7094	10.1405	10.0231	10.9091	10.102	10.6801	7.7653	7.06	8.5995	9.295	7.4441	7.4743	7.7344	7.6286		5.8117	4.7648
H9A	5.2885	7.0297	6.4684	8.4931	8.8577	8.8178	7.6077	7.6404	6.1173	5.9903	7.6813	7.3785	9.1895	8.8559	8.7959	6.5868	5.1269	6.614	7.7846	8.7006	7.8717	7.4247	6.4703	5.5239	7.0925	6.8428
H9B	6.0787	7.8313	6.9475	8.8745	9.3517	9.0147	8.0721	8.4159	6.8454	6.3056	7.8513	7.6849	8.9586	8.3951	8.6841	6.071	4.9521	6.5575	6.9691	7.9014	6.6436	6.3781	5.9655	5.4395	5.5945	5.1525
H8A	4.8826	6.4607	5.202	7.075	8.0037	7.8036	7.5167	6.6559	6.4287	8.5559	10.0894	10.0441	11.3475	10.8439	11.1671	8.564	7.4459	9.0687	9.2972	10.0755	8.5895	8.2085	7.8632	7.5154	7.3904	6.4266
H8B	3.704	5.3306	4.4209	6.6629	7.2598	7.394	6.8139	6.616	5.453	8.3672	10.0109	9.8291	11.5595	11.2071	11.2524	8.9133	7.5533	9.0744	9.9325	10.7552	9.5989	9.111	8.3431	7.6527	8.5665	7.8481
H24A	5.2668	6.124	4.9738	4.6664	5.8315	4.5584	5.0295	6.1584	5.2886	12.0198	13.6012	13.0651	14.2627	13.2279	13.6345	10.677	10.1085	11.2811	11.7198	12.9602	11.069	11.4572	11.7772	11.4143	9.008	8.1749
H24B	5.5256	6.2585	4.7618	4.5944	6.1175	5.0863	6.1207	6.9181	6.2684	12.6594	14.2119	13.869	14.9844	14.0434	14.5342	11.5612	10.9135	12.2365	12.385	13.1051	11.4648	11.6886	12.0217	11.8073	9.4988	8.3795
H23A	4.435	4.5845	3.4823	2.3189	3.7936	2.6899	4.2718	4.9734	4.8306	13.5518	15.2206	14.6768	16.1734	15.2814	15.5296	12.7036	11.9066	13.1089	13.8499	15.0389	13.2545	13.3481	13.4941	13.0023	11.3188	10.4082
H23B	3.3474	3.7997	2.2468	2.6015	4.0392	3.6355	4.717	4.9484	4.6371	12.5574	14.2289	13.8129	15.3806	14.6433	14.8548	12.113	11.1431	12.4756	13.1971	14.2637	12.5784	12.5596	12.4118	11.9086	10.8426	9.8625
H21A	3.8197	5.1022	4.5192	5.0665	5.5139	4.704	3.7133	4.7059	3.2451	10.0258	11.7042	10.971	12.5772	11.7747	11.9964	9.0635	8.2589	9.3061	10.0485	11.8323	10.0362	10.0688	10.5199	9.7973	8.572	8.1469
H21B	2.2772	3.7379	2.4743	4.6638	4.7964	4.5714	3.3152	3.6409	2.1225	9.8302	11.5766	10.8561	12.7819	12.093	11.9964	9.5299	8.4396	9.522	11.0457	12.3008	10.1686	10.0952	11.0952	10.6068	9.7035	9.1136
H14Q	13.0831	14.8265	14.2272	16.0811	16.5184	16.2007	14.7541	15.0985	13.4115	3.1656	2.4127	3.6387	2.4202	3.0889	3.6494	3.8452	3.839	4.2861	2.9196	2.2649	4.1458	3.3236	2.2705	2.536	5.9677	6.9874
H1Q	10.4823	12.2353	11.4514	12.9052	13.5082	12.8841	11.6462	12.3235	10.5916	4.7015	5.4606	5.4741	5.2818	4.2795	5.2461	2.4453	2.748	3.954	2.4528	3.6564	2.5434	3.0475	3.7064	3.8405	2.4124	3.5372
H12Q	9.1278	10.8896	10.2024	11.9934	12.4949	12.1521	11.0806	11.2314	9.5554	4.3776	4.7253	5.6629	5.2712	5.6445	3.4112	2.2925	4.0445	3.9909	4.764	4.2721	3.7806	2.9981	2.4023	4.3633	4.8013	
H7Q	2.6231	4.0435	2.7304	4.4792	5.3544	5.2112	5.1457	5.2252	4.2687	10.26	11.9342	11.574	13.213	12.6023	12.7443	10.125	9.0069	10.4095	11.2284	12.2391	10.7589	10.588	10.2147	9.6194	9.2635	8.4165
H6Q	4.9467	6.19	4.6474	5.6527	6.9446	6.318	6.6582	7.1738	6.1607	10.6277	12.1584	11.9626	13.093	12.3119	12.7803	9.899	9.0871	10.5763	10.6415	11.5848	9.7305	9.7241	9.8601	9.6487	8.0247	6.883
H22Q	3.8044	4.3005	3.8569	3.2538	3.7175	2.5229	2.4133	3.6519	3.0064	12.2418	13.9417	13.1774	14.8467	13.9235	14.0051	11.3097	10.5248	11.5212	12.7311	14.0772	12.5163	12.8097	12.7275	12.0195	10.6087	10.0466

(cont.) Table H.1: Hydrogen Distances for the Optimized Structure of 4e,4'e *cis-anti-cis* DtBuCH18C6

	H3A	H3B	H11A	H11B	H10A	H10B	H4A	H4B	H5A	H5B	H9A	H9B	H8A	H8B	H24A	H24B	H23A	H23B	H21A	H21B	H14Q	H1Q	H12Q	H7Q	H6Q	H22Q	
	8.9858	9.7594	8.1664	8.8477	8.1668	7.6437	6.6669	7.7953	7.2671	6.1292	5.2885	6.0787	4.8826	3.704	5.2668	5.5256	4.435	3.3474	3.8197	2.2772	13.0831	10.4823	9.1278	2.6231	4.9467	3.8044	H28X
	10.6769	11.3609	9.8956	10.5061	9.7943	9.3578	8.2937	9.2815	8.6642	7.6891	7.0297	7.8313	6.4607	5.3306	6.124	6.2585	4.5845	3.7997	5.1022	3.7379	14.8265	12.2353	10.8896	4.0435	6.19	4.3005	H28Y
	9.8223	10.3542	8.8725	9.3902	8.9956	8.7117	7.3934	8.2354	7.2644	6.387	6.4684	6.9475	5.202	4.4209	4.9738	4.7618	3.4823	2.2468	4.5192	3.4743	14.2272	11.4514	10.2024	2.7304	4.6474	3.8569	H28Z
	10.9617	11.1745	10.6195	11.3164	11.2359	10.8078	8.4178	8.8378	8.0141	7.6492	8.4931	8.7045	7.075	6.6629	4.6664	4.5944	2.3189	2.6015	5.0665	4.6638	16.0811	12.9052	11.9934	4.4792	6.6527	3.2538	H26X
	11.6371	12.0197	11.4154	12.1986	11.8278	11.2628	9.1307	9.7343	9.2433	8.7061	8.8577	9.3517	8.0037	7.2598	5.8315	6.1175	3.7936	4.0392	5.5139	4.7964	16.5184	13.5082	12.4949	5.3544	6.9446	3.7175	H26Y
	10.8298	11.0012	11.0129	11.9457	11.8858	11.2063	8.6511	8.6511	8.3051	8.0556	8.8178	9.0147	7.394		4.5584	5.0863	2.6899	3.6355	4.704	4.5714	16.2007	12.8841	12.1521	5.2112	6.318	2.5229	H26Z
	9.7397	10.2031	10.2104	11.3495	11.0013	10.0296	7.3899	8.0585	8.3299	7.7805	7.6077	8.0721	7.5167	6.8139	5.0295	6.1207	4.2718	4.717	3.7133	3.3152	14.7541	11.6462	10.8606	5.1457	6.6582	2.4133	H27X
	10.6194	11.2723	10.6	11.5555	10.8946	10.0708	8.2812	9.1855	9.1999	8.3919	7.6404	8.4159	7.6559	6.616	6.1584	6.9181	4.9734	4.9484	4.7059	3.6409	15.0985	12.3235	11.2314	5.2252	7.1738	3.6519	H27Y
	8.913	9.6446	9.0383	10.1155	9.5126	8.5434	6.6468	7.6659	7.9069	7.0129	6.1173	6.8454	6.4287	5.453	5.2886	6.2684	4.8306	4.6371	3.2451	2.1225	13.4115	10.5916	9.5554	4.2687	6.1607	3.0064	H27Z
	6.3904	8.0696	5.8283	6.4271	5.3827	4.289	7.6664	9.0353	9.9783	8.7094	5.9903	6.3056	8.5559	8.3672	12.0198	12.6594	13.5518	12.5574	10.0258	9.8302	3.1656	4.7015	3.4776	10.26	10.6277	12.2418	H20X
	7.5111	9.0545	7.0326	7.4363	6.587	5.7716	9.1148	10.3336	11.3011	10.1405	7.6813	7.8513	10.0894	10.0109	13.6012	14.2119	15.2206	14.2289	11.7042	11.5766	4.2127	5.4606	4.7255	11.9342	12.1584	13.9417	H20Y
	7.1862	8.7922	7.2933	8.0481	7.1333	5.9383	8.6493	9.9166	11.1762	10.0231	7.3785	7.6849	10.0441	9.8291	13.0651	13.869	14.6768	13.8129	10.971	10.8561	3.6387	5.4741	4.8382	11.574	11.9626	13.1774	H20Z
	7.4832	8.7172	7.9028	8.517	8.3285	7.4031	9.5837	10.4485	11.7383	10.9091	9.1895	8.9586	11.3475	11.5595	14.2627	14.9844	16.1734	15.3806	12.5772	12.7819	4.2202	5.2818	5.6529	13.213	13.093	14.8467	H18X
	6.2973	7.369	7.4018	8.2971	8.4642	7.3475	8.5513	9.2216	10.7372	10.102	8.8559	8.3951	10.8439	11.2071	13.2279	14.0434	15.2814	14.6433	11.7747	12.093	3.0889	4.2795	5.2712	12.6023	12.3119	13.9235	H18Y
	7.0874	8.3911	8.0234	8.9405	8.6319	7.3997	9.0397	9.9516	11.513	10.6801	8.7959	8.6841	11.1671	11.2524	13.6345	14.5342	15.5296	14.8548	11.7747	11.9964	3.6494	5.2461	5.6445	12.7443	12.7803	14.0051	H18Z
	3.9766	5.316	5.4772	6.7493	6.9474	5.5357	6.032	6.8429	8.4613	7.7653	6.5868	6.071	8.564	8.9133	10.677	11.5612	12.7036	12.113	9.0635	9.5299	3.8452	2.4453	3.4112	10.125	9.899	11.3097	H19X
	4.0622	5.7348	4.637	5.8448	5.5454	4.0196	5.5576	6.7679	8.089	7.06	5.1269	4.9521	7.4459	7.5533	10.1085	10.9135	11.9066	11.1431	8.2589	8.4396	3.839	2.748	2.2925	9.0069	9.0871	10.5248	H19Y
	5.2217	6.731	6.3707	7.5906	7.2212	5.6911	6.8098	7.8896	9.5152	8.5995	6.614	6.5675	9.0687	9.0744	11.2811	12.2541	13.1089	12.4756	9.3061	9.522	4.2861	3.954	4.0445	10.4095	10.5763	11.5212	H19Z
	4.6379	5.5677	5.6795	6.5809	7.2485	6.2595	7.0505	7.5607	8.8737	8.3683	7.7846	6.9691	9.2972	9.9325	11.7198	12.3865	13.8499	13.1971	10.4885	11.0457	2.9196	2.4528	3.9909	11.2284	10.6415	12.7311	H15A
	5.9803	6.8084	6.2756	6.7397	7.438	6.8113	8.339	8.8402	9.8272	9.295	8.7006	7.9014	10.0755	10.7552	12.9602	13.4552	15.0389	14.2637	11.8323	12.3008	2.2649	3.6564	4.764	12.2391	11.5848	14.0772	H15B
	4.3093	4.7104	4.8781	5.5061	6.9214	6.3403	6.6759	6.8415	7.6811	7.4441	7.8717	6.6436	5.8895	5.5989	11.069	11.4648	13.2545	12.5784	10.3662	10.6686	4.1458	2.5434	4.2721	10.7589	9.7305	12.5163	H16B
	5.0482	5.7771	4.3866	4.5337	5.7552	5.5014	7.1029	7.5743	8.0112	7.4743	7.4247	6.3781	8.2085	9.111	11.4572	11.6886	13.4481	12.5596	10.6388	11.0952	3.3236	3.0475	3.7806	10.588	9.7241	12.8097	H13A
	5.7785	7.0288	4.2901	4.2116	4.3529	4.163	7.4183	8.3822	8.7351	7.7344	6.4703	5.9655	7.8632	8.3431	11.7772	12.0217	13.4941	12.4118	10.5199	10.6068	2.2705	3.7064	2.9981	10.2147	9.8601	12.7275	H13B
	5.701	7.2452	4.3533	4.6062	3.9428	3.2868	7.061	8.85	8.7286	7.6286	5.5239	5.4395	7.5154	7.6527	11.4143	11.8073	13.0023	11.9086	9.7973	9.7035	2.536	3.8405	2.4023	9.6194	9.6487	12.0195	H2A
	3.0634	2.5287	3.7218	4.586	6.655	6.185	4.5496	4.1638	4.4962	4.7648	6.8428	5.1525	6.4266	7.8481	8.1749	8.3795	10.4082	9.8625	8.1469	9.1136	6.9874	3.5372	4.8013	8.4165	6.883	10.0466	H2B
	0	1.7781	3.4005	5.0748	6.1874	4.9706	2.5466	2.9737	4.5693	4.2478	5.0675	3.6965	5.7341	6.6438	7.1115	7.8661	9.3397	8.8777	6.1932	7.1061	6.505	2.4043	3.446	7.2128	6.3855	8.3364	H3A
	1.7781	0	4.4955	5.9748	7.5213	6.5209	3.115	2.4017	4.1016	4.5002	6.4695	4.9066	6.4298	6.8756	7.5741	7.6143	9.2897	9.055	6.619	7.842	7.7728	3.6604	5.0694	7.76	6.4572	8.5186	H3B
	3.4005	4.4955	0	1.7615	3.0819	2.6246	3.7762	4.8115	4.6265	3.4575	3.5598	2.2008	3.8398	4.8062	6.6143	7.7396	9.3091	8.2671	6.732	7.0046	6.0561	4.4725	2.4694	6.2263	5.5837	8.8051	H11A
	5.0748	5.9748	1.7615	0	2.4358	3.0733	5.3828	6.295	5.5448	4.4019	4.4526	3.4644	4.2484	5.2092	8.6682	8.4716	10.1204	8.8883	8	8.0755	6.3556	4.7378	3.5525	6.8762	6.2111	9.9202	H11B
	6.1874	7.5213	3.0819	2.4358	0	1.7708	6.2073	7.5866	5.5268	5.391	3.591	2.674	4.597	4.373	9.3979	9.3292	10.4898	9.0874	7.1019	7.026	6.2999	5.6358	5.3913	6.822	7.0011	10.038	H10A
	4.9706	6.5209	2.6246	3.0733	1.7708	0	5.0676	6.6095	6.6522	5.0814	2.4439	2.674	4.234	4.373	8.7188	8.9762	10.0017	8.774	7.1019	6.7855	5.701	4.5288	2.3176	6.4427	6.7541	9.1898	H10B
	2.5466	3.115	3.7762	5.3828	6.2073	5.0676	0	1.7817	3.0661	2.494	3.978	2.685	4.0058	4.8555	4.7009	5.546	6.825	6.3865	3.7319	4.7596	8.4911	4.6915	4.6696	4.8566	4.1777	5.8446	H4A
	2.9737	2.4017	4.8115	6.295	7.5866	6.6095	1.7817	0	2.4967	3.0588	5.708	4.2485	5.0945	6.2467	5.3061	6.909	6.7992	4.4798	5.8856	5.94	9.4071	5.3327	5.9175	5.789	4.4775	6.2018	H4B
	4.5693	4.1016	4.6265	5.5448	5.5268	6.6522	3.0661	2.4967	0	1.772	5.7306	4.2017	3.8203	5.3898	3.8878	6.0346	5.6058	4.8292	4.8292	5.94	10.2525	5.9225	6.5929	4.7845	2.7372	6.1689	H5A
	4.2478	4.5002	3.4575	4.4019	5.391	5.0814	2.494	3.0588	1.772	0	4.0255	2.5867	2.1952	3.7331	4.2946	4.2941	6.0371	5.1952	4.2335	4.9143	9.3439	5.9225	5.4379	3.692	2.2992	5.9085	H5B
	5.0675	6.4695	3.5598	4.4526	3.591	2.4439	3.978	5.708	5.7306	4.0255	0	1.7751	3.0639	2.4882	6.7759	7.1816	7.8291	6.649	4.879	4.3614	7.8156	5.6935	3.9374	4.3065	5.1515	6.8741	H9A
	3.6965	4.9066	2.2008	3.4644	2.674	2.674	2.685	4.2485	4.2017	2.5867	1.7751	0	2.514	3.063	6.0895	6.4291	7.5834	6.5388	4.7437	4.8348	7.4504	4.637	3.3701	4.3647	4.3229	6.8425	H9B
	5.7341	6.4298	3.8398	4.2484	4.597	4.234	4.0058	5.0945	3.8203	2.1952	3.0639	2.514	0	1.7762	5.1376	4.8653	6.0572	4.6957	4.5366	4.3877	6.6444	6.9259	5.6988	2.6543	5.2672	6.0331	H8A
	6.6438	6.8756	4.8062	5.2092	4.373	4.373	4.8555	6.2467	5.3898	3.7331	2.4882	3.063	1.7762	0	5.768	5.6986	6.2021	4.7125	4.4737	3.6544	9.9904	7.6715	6.0843	2.4062	3.712	5.8683	H8B
	7.1115	6.8756	7.6143	8.6682	9.3979	8.7188	4.7009	5.3061	3.8878	4.2946	6.7759	6.4291	5.1376	5.768	0	1.7571	2.5114	2.5452	2.7829	4.0639	13.1007	9.349	9.1146	2.4062	2.9686	2.2265	H24A
	7.8661	7.5741	7.7396	8.4716	9.3292	8.9762	5.546	5.3061	4.2946	4.2941	7.1816	6.4291	4.8653	5.6986	1.7571	0	2.4511	2.5452	4.0845	4.936	13.5807	9.9594	9.5943	3.6179	3.2404	3.7876	H24B
	9.3397	9.2897	9.3091	10.1204	10.4898	10.0017	6.825	6.909	5.6058	6.0371	7.8291	7.5834	6.0572	6.2021	2.5114	2.4511	0	1.7512	3.9337	4.3186	14.937	9.8979	10.853	3.7961	4.041	2.3619	H23A
	8.8777	9.055	8.2671	8.8883	9.0874	8.774	6.3865	6.7992	5.6058	5.1952	6.649	6.5388	4.6957	4.7125	2.5452	2.5452	1.7512	0	3.6977	3.6977	13.9878	8.2078	9.8979	2.3679	3.0879	3.0443	H23B
	6.1932	6.619	6.732	8	7.1019	6.7855	3.7319	5.8856	4.8292	4.2335	4.879	4.7437	4.5366	4.4737	2.7829	4.0845	3.9337	3.6977	0	1.751	11.6219	8.8033	7.6232	3.0442	3.7659	2.2779	H21A
	7.1061	7.842	7.0046	8.0755	7.026	6.7855	4.7596	5.94	5.94	4.9143	4.3614	4.8348	4.3877	3.6544	4.0639	4.936	4.3186	3.6977	1.751	0	11.7697	8.8033	7.7746	2.5244	4.2842	2.7993	H21B
	6.505	7.7728	6.0561	6.3556	6.2999	5.701	8.4911	9.4071	10.2525	9.3439	7.8156	7.4504	9.6444	9.9904	13.1007	13.5807	14.937	13.9878	11.6219	11.7697	0	4.1464	4.0992	11.7834	11.5344	13.891	H14Q
	2.4043	3.6604	4.4725	5.6358	5.4288	4.6915	5.3327	6.5096	5.9225	5.6935	4.637	6.9259	7.6715	9.349	11.4442	10.7659	9.8979	8.2078	8.8033	8.8033	4.1464	0	2.2879	8.8328	8.1899	10.4385	H1Q
	3.446	5.0694	2.4694	3.5525	5.3913	2.3176	4.6696	5.9175	6.5929	5.4379	3.9374	3.3701	5.6988	6.0843	9.1146	9.5943	10.853	9.8979	7.6232	7.7746	4.0992	2.2879	0	7.7107	7.5449	9.8688	H12Q
	7.2128	7.76	6.2263	6.8762	6.822	6.4427	4.8566	5.789	4.7845	3.692	4.3065	4.3647	2.6543	2.4062	3.7114	3.6179	3.7961	2.3679	3.0442	2.5244	11.7834	8.8328	7.7107	0	2.3773	3.7694	H7Q
	6.3855	6.4572	5.5837	6.2111	7.0011	6.7541	4.1777	4.4775	2.7372	2.2992	5.1515	4.3229	2.5672	3.712	2.9686	3.2404	4.041	3.0879	3.7659	4.2842	11.5344	8.1899	7.5449	2.3773	0	4.5987	H6Q
	8.3364	8.5186	8.8051	9.9202	10.038	9.1898	5.8446	6.2018	6.1689	5.9085	6.8741	6.8425	6.0331	5.8683	2.6265	3.7876	2.3619	3.0443	2.2779	2.7993	13.891	10.4385	9.8688	3.7694	4.5987	0	H22Q

Figure H.3: Optimized Structure of 4z,4'e *cis-anti-cis* DtBuCH18C6 with Hydrogen Labels

Figure H.4: Optimized Structure of 4z,4'e *cis-anti-cis* DtBuCH18C6 with Carbon and Oxygen Labels

Table H.2: Hydrogen Distances for the Optimized Structure of 4z,4'e *cis-anti-cis* DtBuCH18C6

	H28X	H28Y	H28Z	H27X	H27Y	H27Z	H26X	H26Y	H26Z	H18X	H18Y	H18Z	H20X	H20Y	H20Z	H19X	H19Y	H19Z	H15A	H15B	H13A	H13B	H16A	H16B	H11A	H11B
H28X	0	1.7722	1.7644	3.7961	4.3558	3.7051	2.5656	3.111	3.7902	15.1224	15.1546	14.513	13.243	12.4685	11.5613	14.1458	12.6123	14.0475	14.063	13.8419	10.6602	10.2231	12.0653	13.4213	8.5573	8.6728
H28Y	1.7722	0	1.7702	2.5805	3.7879	3.0441	3.775	3.7632	4.3536	15.5476	15.5918	14.7857	12.7613	12.0752	14.8403	13.3782	14.7529	14.4017	14.3912	11.2921	10.6612	12.3506	13.8045	9.3497	9.3515
H28Z	1.7644	1.7702	0	3.0962	3.7081	2.439	3.0972	2.5403	3.7695	16.7469	16.8173	16.105	14.8316	14.0229	13.18	15.8346	14.33	15.7748	15.7078	15.5503	12.3625	11.8897	13.6821	15.0665	10.3009	10.3927
H27X	3.7961	2.5805	3.0962	0	1.7723	1.7704	4.351	3.7497	3.8076	17.3384	17.1994	16.4083	15.6979	14.5987	14.0362	16.748	15.2402	16.4696	15.7484	15.825	13.0721	12.2014	13.4971	14.8634	11.0802	10.7225
H27Y	4.3558	3.7879	3.7081	1.7723	0	1.7666	3.7972	3.0395	2.6053	18.1606	17.9024	17.2575	16.5893	15.5466	14.8764	17.4161	15.8232	17.0126	16.3758	16.325	13.7141	12.8552	14.0448	15.272	11.5713	11.0813
H27Z	3.7051	3.0441	2.439	1.7704	1.7666	0	3.7637	2.528	3.1863	18.3446	18.253	17.5377	16.5948	15.6322	14.9125	17.5557	16.0074	17.3243	16.9013	16.8348	13.9366	13.2299	14.6872	16.011	11.8293	11.5973
H26X	2.5656	3.775	3.0972	4.351	3.7972	3.7637	0	1.7674	1.771	16.3397	16.1585	15.7474	14.6256	13.9163	12.8839	15.1533	13.493	14.8267	14.9211	14.5157	11.6456	11.1879	12.7882	13.9145	9.3236	9.1564
H26Y	3.111	3.7632	2.5403	3.7497	3.0395	2.528	1.7674	0	1.766	17.8465	17.7214	17.2177	16.07	15.3153	14.3469	16.7361	15.1076	16.4695	16.4754	16.1502	13.2173	12.7238	14.3196	15.5052	10.9439	10.7991
H26Z	3.7902	4.3536	3.7695	3.8076	2.6053	3.1863	1.771	1.766	0	17.5109	17.2156	16.7919	15.9175	15.0872	14.1632	16.4375	14.7605	15.9911	15.7989	15.4752	12.8355	12.1945	13.53	14.6104	10.5179	10.1035
H18X	15.1224	15.5476	16.7469	17.3384	18.1606	18.3446	16.3397	17.8465	17.5109	0	1.7657	1.7703	2.4424	3.0052	3.7037	2.5347	3.7697	3.1731	3.8101	4.0028	4.7901	5.5093	5.8287	6.1199	7.1984	7.8778
H18Y	15.1546	15.5918	16.8173	17.1994	17.9024	18.253	16.1585	17.7214	17.2156	1.7657	0	1.7729	3.7115	3.7774	4.3566	3.0302	3.7824	2.5723	2.3499	2.5506	4.6631	5.0552	4.6789	6.008	6.9492	7.2614
H18Z	14.513	14.7857	16.105	16.4083	17.2575	17.5377	15.7474	17.2177	16.7919	1.7703	1.7729	0	3.1296	2.573	3.796	3.7526	4.3537	3.7877	2.6807	3.5894	4.5542	4.6906	4.5763	5.073	6.8389	7.2178
H20X	13.243	12.7613	14.8316	15.6979	16.5893	16.5948	14.6256	16.07	15.9175	2.4424	3.7115	3.1296	0	1.771	1.765	2.5134	3.0944	3.7534	4.9799	4.9397	3.6319	4.7184	6.1198	6.9206	5.8582	6.9692
H20Y	12.4685	12.0752	14.0229	14.5987	15.5466	15.6322	13.9163	15.3153	15.0872	3.0052	3.7774	2.573	1.771	0	1.7708	3.7465	3.7979	4.3519	4.2616	4.7072	3.2885	3.7198	5.0031	6.1131	5.3904	6.2285
H20Z	11.5613	12.0752	13.18	14.0362	14.8764	14.9125	12.8839	14.3469	14.1632	3.7037	4.3566	3.796	1.765	1.7708	0	3.1246	2.6074	3.8143	4.8373	4.6526	2.1096	3.2693	5.23	6.2768	4.1527	5.3463
H19X	14.1458	14.8403	15.8346	16.748	17.4161	17.5557	15.1533	16.7361	16.4375	2.5347	3.0302	3.7526	2.5134	3.7465	3.1246	0	1.7655	1.7644	4.6191	3.8011	3.7526	5.1093	6.0773	6.2796	5.951	6.9055
H19Y	12.6123	13.3782	14.33	15.2402	15.8232	16.0074	13.493	15.1076	14.7605	3.7697	3.7824	4.3537	3.0944	3.7979	2.6074	1.7655	0	1.7729	4.4697	3.3802	2.2598	2.2054	3.8342	5.1957	5.5537	5.2595
H19Z	14.0475	14.7529	15.7748	16.4696	17.0126	17.3243	14.8267	16.4695	15.9911	3.1731	2.5723	3.7877	3.7534	4.3519	3.8143	1.7644	1.7729	0	3.5307	2.2598	3.495	4.5189	4.9296	4.7926	5.5337	6.0836
H15A	14.063	14.4017	15.7078	15.7484	16.3758	16.9013	14.9211	16.4754	15.7989	3.8101	2.3499	2.6807	4.9799	4.2616	4.8373	4.6191	4.4697	3.5307	0	1.7518	4.3198	3.8979	2.5229	2.4417	6.1428	5.9114
H15B	13.8419	14.3912	15.5503	15.825	16.325	16.8348	14.5157	16.1502	15.4752	4.0028	2.5506	3.5894	4.9397	4.7072	4.6526	3.8011	3.3802	2.2598	1.7518	0	3.7456	3.8213	3.0541	2.5766	5.4879	5.3775
H13A	10.6602	11.2921	12.3625	13.0721	13.7141	13.9366	11.6456	13.2173	12.8355	4.7901	4.6631	4.5542	3.6319	3.2885	2.1096	3.7526	2.2054	3.495	4.3198	3.7456	0	1.7494	3.9563	4.9479	2.4087	3.3825
H13B	10.2231	10.6612	11.8897	12.2014	12.8552	13.2299	11.1879	12.7238	12.1945	5.5093	5.0552	4.6906	4.7184	3.7198	3.2693	5.1093	3.8342	4.5189	3.8979	3.8213	1.7494	0	2.6514	4.0524	2.551	2.629
H16A	12.0653	12.3506	13.6821	13.4971	14.0448	14.6872	12.7882	14.3196	13.53	5.8287	4.6789	4.5763	6.1198	5.0031	5.23	6.0773	5.1957	4.9296	2.5229	3.0541	3.9563	2.6514	0	1.7567	4.8324	4.0301
H16B	13.4213	13.8045	15.0665	14.8634	15.272	16.011	13.9145	15.5052	14.6104	6.1199	6.008	5.073	6.9206	6.1131	6.2768	6.2796	5.5537	4.7926	2.4417	2.5766	4.9479	4.0524	1.7567	0	5.8995	5.0124
H11A	8.5573	9.3497	10.3009	11.0802	11.5713	11.8293	9.3236	10.9439	10.5179	7.1984	6.9492	6.8389	5.8582	5.3904	4.1527	5.951	5.5537	5.5337	6.1428	5.4879	2.4087	2.551	4.8324	5.8995	0	1.7731
H11B	8.6728	9.3515	10.3927	10.7225	11.0813	11.5973	9.1564	10.7991	10.1035	7.8778	7.2614	7.2178	6.9692	6.2285	5.3463	6.9055	5.2595	6.0836	5.9114	5.3775	3.3825	2.629	4.0301	5.0124	1.7731	0
H10A	8.7834	9.8452	10.5132	11.1679	11.1833	11.7235	8.6691	10.4233	9.6695	9.4124	8.7538	9.0867	8.4981	8.1703	6.9414	7.8745	6.1247	6.9746	7.6489	6.6342	4.9415	4.8599	6.0466	6.4892	3.0647	2.5177
H10B	8.6466	9.8158	10.3995	11.1458	11.6481	11.9307	8.8323	10.5582	10.0885	8.8411	8.494	8.773	7.5288	6.5015	7.051	5.3041	6.504	7.8187	6.7224	4.3519	4.7964		6.9535	7.1907	2.4789	3.0632
H2A	9.6184	9.9556	11.2348	11.0502	11.518	12.1818	10.2295	11.7594	10.9428	7.6272	6.8017	6.5492	7.1361	5.9956	5.7089	7.3138	5.9471	6.3506	4.9636	5.0007	4.0082	2.4455	2.5879	3.8539	3.4439	2.0826
H2B	11.0833	11.3147	12.6409	12.1388	12.5318	13.3636	11.5401	13.041	12.0679	7.9421	6.8044	6.6866	7.9751	6.7826	6.8042	7.9497	6.7893	6.7379	4.6126	4.8985	5.2024	3.6473	2.1468	2.917	5.0749	3.6371
H3A	10.4728	10.8121	11.9744	11.2954	11.3665	12.4143	10.4165	11.9271	10.7234	8.9164	8.9838	9.9633	8.9029	8.6148	9.706	8.3176	8.3942		6.7994	6.7007	6.7371	5.3734	4.4374	4.7186	5.8083	4.0049
H3B	9.2582	9.8192	10.8569	10.5879	10.6518	11.5456	9.1995	10.8098	9.7277	9.7371	8.7517	8.845	9.2633	8.3695	7.7617	8.9797	7.4153	7.8036	6.9129	6.5093	5.7693	4.6585	4.6208	5.1283	4.3886	2.6398
H9A	7.002	7.7305	8.6759	8.8556	9.0248	9.6622	7.152	8.7998	7.9618	10.0756	9.4824	9.3482	9.0074	8.1915	7.3027	9.0743	7.3871	8.2942	8.0005	7.5462	5.4831	4.6779	5.84	6.7947	3.3545	2.2416
H9B	6.9016	7.9328	8.5455	8.9689	8.8313	9.4933	6.4854	8.2207	7.3129	11.2953	10.6839	10.741	10.1939	9.5916	8.4981	9.9859	8.2339	9.1755	9.3175	8.611	6.6237	6.1309	7.2771	7.9763	4.3539	3.5327
H8A	4.4933	5.7091	6.189	7.123	7.1613	7.4695	6.1579	5.6408		12.1578	11.874	11.644	10.6223	10.0039	8.8651	10.8764	9.1702	10.4318	10.7035	10.1487	7.3852	7.0233	8.7145	9.7553	4.9969	4.841
H8B	4.7128	5.4915	6.4313	7.0399	7.4537	7.7427	5.4219	6.9669	6.51	11.0018	10.7677	10.343	9.4639	8.648	7.7023	10.011	8.3827	9.6264	9.5432	9.2223	6.3513	5.7695	7.5231	8.7773	4.1266	3.965
H4A	8.9592	9.0712	10.2473	9.11	9.0935	10.3037	8.7688	10.0834	8.7577	12.0677	11.0904	10.8745	11.5898	10.3761	10.0785	11.7085	10.2304	10.5966	8.9931	9.0505	8.3216	6.8809	6.4881	7.1525	6.8937	5.2492
H4B	7.8306	8.2424	9.2664	8.6283	8.5655	9.5677	7.5617	9.0444	7.8108	11.6292	10.736	10.684	10.906	9.8696	9.2888	10.937	9.3326	9.9134	8.8918	8.673	7.4417	6.2451	6.4491	7.1843	5.6643	4.1273
H5A	6.3933	6.4412	7.7766	7.055	7.4671	8.2805	6.8837	8.1821	7.2558	13.3356	10.7807	10.2474	10.2952	9.067	8.645	10.8999	9.3868	10.2018	9.0243	9.1154	7.1886	6.8951	6.6149	7.856	5.4761	4.3874
H5B	7.5519	7.2842	8.7037	7.3527	7.7302	8.7723	7.9269	9.028	7.9418	12.1617	11.4757	10.8881	11.3646	9.984	9.8163	12.003	10.5838	11.1938	9.5088	9.8224	8.4031	6.9051	7.0315	8.1762	6.9642	5.6852
H21A	3.4276	4.3198	4.6241	4.8249	4.4547	5.0997	2.4318	3.9556	2.9717	14.6389	14.2809	13.9217	13.1529	12.3225	11.3894	13.5742	11.8861	13.0589	12.8601	12.5053	9.9487	9.2814	10.6179	11.6851	7.6277	7.1344
H21B	2.1351	3.1425	3.7205	4.5358	4.7805	4.9077	2.6774	4.0588	3.7896	13.8495	13.6846	13.1759	12.1753	11.3521	10.4324	12.8487	11.2317	12.5399	12.4324	12.1564	9.2403	8.6713	10.321	11.5724	7.0122	6.85
H23A	4.6316	4.6534	4.8705	3.5007	2.4096	3.8752	3.3841	3.7186	2.1984	16.905	16.4663	15.9997	15.5207	14.5038	13.7755	16.0096	14.4122	15.4777	14.8328	14.6728	13.2609	11.4514	12.4372	13.4988	10.1451	9.4215
H23B	4.877	4.2916	5.0333	2.7714	2.4431	3.9057	4.5262	4.6969	3.606	16.5694	16.1587	15.5347	15.2236	14.0558	13.5222	15.9867	14.4075	15.4306	14.4624	14.5089	12.2362	11.1703	12.0499	13.228	10.1922	9.4299
H24A	5.5016	5.8247	6.3814	5.3626	4.6978	6.015	4.3827	5.4579	3.9099	15.2369	14.6343	14.3169	14.0672	13.0603	12.3307	14.3836	12.7044	13.3816	12.908	12.6817	10.7132	9.7323	10.4814	11.698	8.525	7.5451
H24B	6.2838	6.1071	6.9168	5.1021	4.5912	6.1208	5.549	6.2632	4.7666	15.7297	15.0907	14.6457	14.6612	13.4847	12.9681	15.1396	13.5301	14.3516	13.2261	13.2179	11.4308	10.0462	10.7338	11.698	9.4201	8.32
H14Q	12.2163	12.5055	13.8283	14.0394	14.8158	15.1678	13.3455	14.8284	14.3304	3.7149	3.2575	2.521	3.6461	2.4073	3.0039	4.2981	3.8053	3.8598	2.3463	3.0425	2.7705	2.2602	2.6117	3.7815	4.6612	4.826
H12Q	12.0692	12.8298	13.8175	14.3754	14.7684	15.2089	12.5998	14.2825	13.6656	5.2322	4.3786	5.1145	5.1024	5.0499	4.1712	3.9064	2.4937	2.6037	3.7878	2.384	2.4934	3.045	3.6572	3.7038	3.5787	3.7115
H1Q	12.5182	13.1868	14.2344	14.3795	14.6235	15.3115	12.7687	14.456	13.5874	6.2263	5.3099	6.0901	6.496	6.5366	6.0339	5.8268	4.6515	4.2336	3.857	4.2373	3.8627	3.0397	2.7697	4.2373	4.6809	3.8806
H6Q	5.2066	4.7962	6.1146	4.6188	4.9917	5.9949	5.5471	6.4045	5.4197	13.8833	13.4272	12.78	12.6743	11.4241	10.0085	13.454	11.9326	12.8571	11.6897	11.8324	9.7094	8.5042	9.2825	10.5258	7.8525	6.9704
H7Q	4.0542	4.2116	5.4772	5.2384	5.7766	6.2701	4.8627	6.0968	5.4828	12.4148	12.1266	11.5182	10.9694	9.8982	9.2497	11.7463	10.1893	11.3128	10.6609	10.618	8.0084	7.08	8.4263	9.7608	6.0008	5.4942
H22Q	3.0197	2.396	3.6385	2.5376	3.2495	3.7275	3.7924	4.297	3.8478	14.9714	14.7563	14.0453	13.4212	12.3237	11.7281	14.3495	12.8151	13.9929	13.281	13.3105	10.6375	9.7313	11.0197	12.3649	8.6292	8.194

(cont.) Table H.2: Hydrogen Distances for the Optimized Structure of 4e,4'e *cis-anti-cis* DtBuCH18C6

H10A	H10B	H2A	H2B	H3A	H3B	H9A	H9B	H8A	H8B	H4A	H4B	H5A	H5B	H21A	H21B	H23A	H23B	H24A	H24B	H14Q	H12Q	H1Q	H6Q	H7Q	H22Q	
8.7834	8.6466	9.6184	11.0833	10.4728	9.2582	7.002	6.9016	4.4933	4.7128	8.9592	7.8306	6.3933	7.5519	3.4276	2.1351	4.6316	4.877	5.5016	6.2838	12.2163	12.0692	12.5182	5.2066	4.0542	3.0197	H28X
9.8452	9.8158	9.9556	11.3147	10.8121	9.8192	7.7305	7.9328	5.7091	5.4915	9.0712	8.2424	6.4412	7.2842	4.3198	3.1425	4.6534	4.2916	5.8247	6.1071	12.5055	12.8298	13.1868	4.7962	4.2116	2.396	H28Y
10.5132	10.3995	11.2348	12.6409	11.9744	10.8569	8.6759	8.5455	6.189	6.4313	10.2473	9.2664	7.7766	8.7037	4.6241	3.7205	4.8705	5.0333	6.3814	6.9168	13.8283	13.8175	14.2344	6.1146	5.4772	3.6385	H28Z
11.1679	11.4858	11.0502	12.1388	11.2954	10.5879	8.8556	8.9689	7.123	7.0399	9.11	8.6283	7.055	7.3527	4.8249	5.4358	3.5007	2.7714	5.3626	5.1021	14.0394	14.3754	14.3795	4.6188	5.2384	2.5376	H27X
11.1833	11.6481	11.518	12.5318	11.3665	10.6518	9.0248	8.8313	7.1613	7.4537	9.0935	8.5655	7.4671	7.3302	4.4547	4.7805	2.4096	2.4431	4.6978	4.5912	14.8158	14.7684	14.6235	4.9917	5.7766	3.2495	H27Y
11.7235	11.9307	12.1818	13.3636	12.4143	11.5456	9.6622	9.4933	7.4695	7.7427	10.3037	9.6189	8.2805	8.7723	5.0997	4.9077	3.8752	3.9057	6.015	6.1208	15.1678	15.2089	15.3115	5.9949	6.2701	3.7275	H27Z
8.6691	8.8323	10.2295	11.5401	10.4165	9.1995	7.152	6.4854	5.4219		8.7688	7.5617	6.8837	7.9269	2.4318	2.6774	3.3841	4.5262	4.3827	5.549	13.3455	12.5998	12.7687	5.5471	4.8627	3.7924	H26X
10.4233	10.5582	11.7594	13.041	11.9271	10.8098	7.8998	8.2207	6.1579	6.9669	10.0834	9.0444	8.1821	9.028	3.9556	4.0588	3.7186	4.6969	5.4579	6.2632	14.2824	14.2825	14.456	6.4045	6.0968	4.297	H26Y
9.6695	10.0885	10.9428	12.0679	10.7234	9.7277	7.9618	7.3129	5.6408	6.51	8.7577	7.8108	7.2558	7.9418	2.9717	3.7896	2.1984	3.606	3.9099	4.7666	14.3304	13.6656	13.5874	5.4197	5.4828	3.8478	H26Z
9.4124	8.8411	7.6272	7.9421	10.0912	9.7371	10.0756	11.2953	12.1578	11.0018	12.0677	11.6292	11.3356	12.1617	14.6389	13.8495	16.905	16.5694	15.2369	15.7297	3.7149	5.2322	6.6263	13.8833	12.4148	14.9714	H18X
8.7538	8.4894	6.8017	6.8044	8.9164	8.7517	9.4824	10.6839	11.8724	10.7677	11.0904	10.7736	10.7807	11.4757	14.2809	13.6846	16.4663	16.1587	14.6343	15.0907	3.2575	4.3786	5.3099	13.3272	12.1266	14.7563	H18Y
9.0867	8.773	6.5492	6.6866	8.9838	8.845	9.3482	10.741	11.644	10.343	10.8745	10.6384	10.2474	10.8881	13.9217	13.1759	15.9997	15.5347	14.3169	14.6457	2.521	5.1145	6.0901	12.78	11.5182	14.0453	H18Z
8.4981	7.5983	7.1361	7.9751	9.9633	9.2633	9.0074	10.1939	10.6223	9.4639	11.5898	10.906	10.2952	11.3646	13.1529	12.1753	15.5207	15.2236	14.0672	14.6612	3.6461	5.1024	6.9496	12.6743	10.9694	13.4212	H20X
8.1703	7.5288	5.9956	6.7826	8.9029	8.3695	8.1915	9.5916	10.0039	8.648	10.3761	9.067	9.984		12.3225	11.3521	15.5348	14.0558	13.0603	13.4847	2.4073	5.0499	6.5366	11.4241	9.8982	12.3237	H20Y
6.9414	6.0515	5.7089	6.8042	6.6148	7.7617	7.3027	8.4981	8.8651	7.7023	10.0785	9.2888	8.645	9.8163	11.3894	10.4324	13.7755	13.5222	12.3307	12.9681	3.0039	4.1712	6.0339	11.0085	9.2497	11.7281	H20Z
7.8745	7.051	7.3138	7.9497	9.706	8.9797	9.0743	9.9859	10.8764	10.011	11.7085	10.937	10.8999	12.003	13.5742	12.8487	16.0696	15.9867	14.3836	15.1396	4.2981	3.9064	5.8268	13.454	11.7463	14.3495	H19X
6.1247	5.3041	5.9471	6.7893	8.3176	7.4153	7.3871	8.2339	9.1702	8.3827	10.2304	9.3326	9.3868	10.5838	11.8861	11.2317	14.412	14.4075	12.7044	13.5301	3.8053	2.4937	4.6515	11.9326	10.193	12.8151	H19Y
6.9746	6.5034	6.3506	6.7379	8.3942	7.8036	8.2942	9.1755	10.4318	9.9264	10.5966	9.9134	10.2018	11.1938	13.0589	12.5399	14.5777	15.4306	13.6198	14.3516	3.8598	2.6037	4.2336	12.8571	11.3128	13.9929	H19Z
7.6489	7.8187	4.9636	4.6126	6.7994	6.9129	8.0005	9.3175	10.7035	9.5432	8.9931	8.8918	9.0243	9.5088	12.8601	12.4324	14.8328	14.4624	12.908	13.2261	2.3463	3.7878	3.854	11.6897	10.6609	13.281	H15A
6.6342	6.7224	5.0007	4.8985	6.7007	6.5093	7.5462	8.611	10.1487	9.2223	9.0505	8.673	9.1154	9.8224	12.5053	12.1564	14.6728	14.5089	12.6817	13.2179	3.0425	2.384	2.7697	11.8324	10.618	13.3105	H15B
4.9415	4.3184	4.0082	5.2024	6.7371	5.7693	5.4831	6.6237	7.3852	6.3513	8.3216	7.4417	7.1886	8.4031	9.9487	9.2403	12.3609	12.2362	10.7132	11.4308	2.7705	2.4934	2.4373	9.7094	8.0084	10.6375	H13A
4.8599	4.7964	2.4455	3.6473	5.3734	4.6585	4.6779	6.1309	7.0233	5.7695	6.8809	6.2451	5.8951	6.9051	9.2814	8.6713	11.4514	11.1703	9.7323	10.0462	2.2602	3.045	3.8627	8.5042	7.08	9.7313	H16A
6.0466	6.5935	2.5879	2.1468	4.4374	4.6208	5.84	7.2771	8.7145	7.5231	6.4881	6.4491	6.6149	7.0315	10.6179	10.321	12.4372	12.0499	10.4814	10.7338	2.6117	3.6572	3.0397	9.2825	8.4263	11.0197	H16B
6.4892	7.1907	3.8539	2.917	4.7186	5.1283	6.7947	7.9763	9.7553	8.7773	7.1525	7.1843	7.856	8.1762	11.6851	11.5724	13.4988	13.228	11.3946	11.688	3.7815	3.7038	2.3704	10.5258	9.7608	12.3649	H11A
3.0647	2.4789	3.4439	5.0749	5.8083	4.3886	3.3545	4.3539	4.9969	4.1266	6.8937	5.6643	5.4761	6.9642	6.6277	7.0122	10.1451	10.1922	8.525	9.4201	4.6612	5.3787	4.6809	7.8525	6.0008	8.6292	H11B
2.5177	3.0632	2.0826	3.6371	4.0449	2.6398	2.2416	3.5327	4.841	3.965	5.2492	4.1273	4.3874	5.6852	7.1344	6.8508	9.4215	9.4299	7.5451	8.32	4.826	3.7115	3.8806	6.9704	5.4942	8.194	H11B
0	1.7747	4.3539	5.4992	4.9796	3.2796	2.7067	2.4545	4.3547	4.4668	6.0659	4.5433	5.6349	7.0241	6.8181	6.9026	9.3176	9.7841	7.3788	8.5665	6.932	4.491	4.5795	7.8049	6.2742	8.7416	H10A
1.7747	0	5.1256	6.5244	4.7944	3.6659	3.5364	4.5144	4.854	7.5194	5.9619	6.4921	6.921	8.0685	7.3181	7.0416	10.0321	10.4984	8.3647	9.6205	6.7986	4.3872	5.2813	8.5756	6.6946	9.1243	H10B
4.3539	5.1256	0	1.7747	3.0492	2.6101	3.3659	4.9563	6.2629	5.0703	4.4874	4.0945	4.1453	4.8706	8.034	7.7949	9.8822	9.5737	7.9548	8.3102	4.09	4.2635	3.7732	6.6607	5.9182	5.5415	H2A
5.4992	6.5244	1.7747	0	2.419	3.0434	4.713	6.1276	7.7313	6.6369	4.4048	4.6099	5.0988	5.2655	9.2286	9.1948	10.7857	10.4047	8.7331	8.8771	4.5233	4.8433	3.6049	7.6943	7.1976	9.6819	H2B
4.9796	4.7944	3.0492	2.419	0	1.7752	4.0399	4.9763	6.9291	6.2635	2.6345	2.9132	4.739	4.498	8.0068	8.4153	9.3517	9.1953	7.1071	7.324	6.7529	6.0833	6.6339	6.7756	6.6167	8.8978	H3A
3.2796	4.7944	2.6101	3.0434	1.7752	0	2.4431	3.3288	5.3786	4.851	3.1363	2.2898	3.8937	4.6043	6.8687	8.6499	8.6968	7.0294	7.0294	6.4829	6.4829	5.2917	6.3339	6.3339	5.6504	8.1098	H3B
2.7067	3.6659	3.3659	4.713	4.0399	2.4431	0	1.7773	3.0605	2.4734	4.1094	2.5353	2.9464	4.4578	4.9938	4.9922	7.2435	7.3973	5.3392	6.2607	6.8816	5.8527	5.1737	5.1737	3.7714	6.3482	H9A
2.4545	3.5364	4.9563	6.1276	4.9763	3.3288	1.7773	0	2.5211	3.0698	4.8949	3.1217	4.175	5.5992	4.4703	4.8707	6.8869	7.4586	4.9676	6.2785	8.3544	6.6679	5.7794	5.7794	4.4333	6.6194	H9B
4.3547	4.5144	6.2629	7.7313	6.9291	5.3786	3.0605	2.5211	0	1.7778	6.2218	4.5741	4.2884	5.9306	2.8841	2.6527	5.6928	6.2823	4.5357	6.2785	9.2597	8.1669	5.0343	5.0343	3.1543	4.9245	H8A
4.4668	4.854	5.0703	6.6369	6.2635	4.851	2.4734	3.0698	1.7778	0	5.6174	4.1872	3.1237	4.8812	3.6944	2.9423	6.166	6.2587	4.9725	5.9448	9.4818	8.2281	4.3696	4.3696	2.1965	4.6166	H8B
6.0659	7.5194	4.4874	4.4048	2.6345	3.1363	4.1094	4.8949	6.2218	5.6174	0	1.7798	3.0559	2.4876	6.3549	6.9711	7.105	6.8031	4.9657	4.8299	8.4818	7.42	7.0074	4.5756	5.1328	6.899	H4A
4.5433	5.9619	4.0945	4.6099	2.9132	2.2898	2.5353	3.1217	4.5741	4.1872	1.7798	0	2.5189	3.0574	6.4453	6.5218	5.9355	6.5218	4.609	4.7455	7.42	7.9732	4.5756	3.4474	4.1898	6.2625	H4B
5.6349	6.4921	4.1453	5.0988	4.739	3.8937	2.9464	4.175	4.2884	3.1237	3.0559	2.5189	0	1.7768	6.6453	5.4654	9.3555	5.4422	3.4173	4.4321	7.7468	9.0195	5.5646	2.345	2.345	4.5997	H5A
7.0241	8.0685	4.8706	5.2655	4.498	4.6043	4.4578	5.5992	5.9306	4.8812	2.4876	3.0574	1.7768	0	5.7088	5.8636	6.2274	5.4209	4.6684	4.1311	8.4644	8.2775	7.9732	3.6667	3.6667	5.1845	H5B
6.8181	7.3181	8.034	9.2286	8.0068	6.8687	4.9938	4.4703	2.8841	3.6944	6.3549	6.4453	6.6453	5.7088	0	1.7585	2.8481	3.7475	2.4313	3.8372	11.4488	10.7118	10.6391	3.7143	3.0237	3.0514	H21A
6.9026	7.0416	7.7949	9.1948	8.4153	8.6499	4.9922	4.8707	2.6527	2.9423	6.9711	6.5218	5.4654	5.8636	1.7585	0	3.9419	4.3032	3.885	4.9156	10.7723	10.3825	10.385	3.0237	2.3694	2.5839	H21B
9.3176	10.0321	9.8822	10.7857	9.3517	8.6968	7.2435	6.8869	5.6928	6.166	7.105	5.9355	9.3555	6.2274	2.8481	3.9419	0	1.7533	2.3694	2.6585	13.4968	13.0926	12.7388	4.6421	4.6421	3.0315	H23A
9.7841	10.4984	9.5737	10.4047	9.1953	7.0294	7.3973	7.4586	6.2823	6.2587	6.8031	6.5218	5.4422	5.4209	3.7475	4.3032	1.7533	0	1.796	1.796	13.0635	13.1387	12.7647	4.301	4.301	2.3317	H23B
7.3788	8.3647	7.9548	8.7331	7.1071	7.0294	5.3392	4.9676	4.5357	4.9725	4.9657	4.609	3.4173	4.6684	2.4313	3.885	2.3694	1.796	0	1.7567	11.796	11.146	10.2425	5.2567	3.7843	3.7446	H24A
8.5665	9.6205	8.3102	8.8771	7.324	6.4829	6.2607	6.2785	6.2785	5.9448	4.8299	4.7455	4.4321	4.1311	3.8372	4.9156	2.6585	1.796	1.7567	0	12.1429	11.9338	11.2307	4.2667	4.2667	3.7851	H24B
6.932	6.7986	4.09	4.5233	6.7529	6.4829	6.8816	8.3544	9.2597	9.4818	8.4818	7.42	7.7468	8.4644	11.4488	10.7723	13.4968	13.0635	11.796	12.1429	0	3.7181	4.5427	10.3141	9.0607	11.6293	H14Q
4.491	4.3872	4.2635	4.8433	6.0833	5.2917	5.8527	6.6679	8.1669	8.2281	7.42	7.9732	9.0195	8.2775	10.7118	10.3825	13.0926	13.1387	11.146	11.9338	3.7181	0	2.2183	10.6331	9.1575	11.86	H12Q
4.5795	5.2813	3.7732	3.6049	6.6339	6.3339	5.1737	5.7794	5.0343	4.3696	7.0074	4.5756	5.5646	7.9732	10.6391	10.385	12.7388	12.7647	10.2425	11.2307	4.5427	2.2183	0	10.2425	9.1771	11.8441	H1Q
7.8049	8.5756	6.6607	7.6943	6.7756	6.3339	5.1737	5.7794	5.0343	4.3696	4.5756	3.4474	2.345	3.6667	3.7143	3.0237	4.6421	4.301	5.2567	4.2667	10.3141	10.6331	10.2425	0	2.3004	2.5027	H6Q
6.2742	6.6946	5.9182	7.1976	6.6167	5.6504	3.7714	4.4333	3.1543	2.1965	5.1328	4.1898	2.345	3.6667	3.0237	2.3694	4.6421	4.301	3.7843	4.2667	9.0607	9.1575	9.1771	2.3004	0	2.7085	H7Q
8.7416	9.1243	5.5415	9.6819	8.8978	8.1098	6.3482	6.6194	4.9245	4.6166	6.899	6.2625	4.5997	5.1845	3.0514	2.5839	3.0315	2.3317	3.7446	3.7851	11.6293	11.86	11.8441	2.5027	2.7085	0	H22Q

Figure H.5: Optimized Structure of 4z,4'z *cis-anti-cis* DtBuCH18C6 with Hydrogen Labels

Figure H.6: Optimized Structure of 4z,4'z *cis-anti-cis* DtBuCH18C6 with Carbon and Oxygen Labels

Table H.3: Hydrogen Distances for the Optimized Structure of 4z,4'z *cis-anti-cis* DtBuCH18C6

	H27X	H27Y	H27Z	H26X	H26Y	H26Z	H28X	H28Y	H28Z	H20X	H20Y	H20Z	H19X	H19Y	H19Z	H18X	H18Y	H18Z	H15A	H15B	H13A	H13B	H16A	H16B	H11A	H11B
H27X	0	1.7721	1.7648	3.7972	4.3551	3.7019	2.5704	3.1163	3.7923	15.3179	14.0901	13.7995	16.6963	15.3299	16.5555	17.1214	16.9728	16.114	13.8079	14.894	13.4752	12.3556	11.865	13.0492	10.8479	10.0649
H27Y	1.7721	0	1.7704	2.5811	3.7869	3.0373	3.7779	3.7624	4.353	15.9943	14.638	14.5008	17.3665	16.0163	17.105	17.6205	17.3411	16.4761	14.1061	15.0743	14.0757	12.8816	12.0725	13.0619	11.5186	10.51
H27Z	1.7648	1.7704	0	3.0996	3.7055	2.4345	3.0953	2.5396	3.769	17.0557	15.7991	15.5358	18.4168	17.0333	18.228	18.8184	18.6206	17.7698	15.4369	16.4698	15.1449	14.0337	13.4442	14.5415	12.5203	11.6944
H26X	3.7972	2.5811	3.0996	0	1.7724	1.7706	4.3516	3.7454	3.8046	17.3985	16.0366	15.8217	18.4977	17.0357	18.0172	18.8459	18.36	17.685	15.2913	16.0307	14.9937	13.959	13.0851	13.9108	12.4833	11.4667
H26Y	4.3551	3.7869	3.7055	1.7724	0	1.7666	3.7939	3.0283	2.6001	17.7781	16.5254	16.1279	18.7039	17.1544	18.189	19.2682	18.7685	18.2191	15.8648	16.569	15.1256	14.2639	13.6288	14.5302	12.5885	11.7663
H26Z	3.7019	3.0373	2.4345	1.7706	1.7666	0	3.7615	2.5227	3.1878	18.3324	17.0544	16.7349	19.4584	17.9741	19.0696	19.9318	19.5449	18.8554	16.4867	17.321	15.9852	15.0006	14.3294	15.2829	13.3948	12.539
H28X	2.5704	3.7779	3.0953	4.3516	3.7939	3.7615	0	1.7671	1.7708	15.7935	14.7423	14.157	16.8725	15.3637	16.6649	17.6389	17.4513	16.8044	14.5658	15.5684	13.5263	12.6937	13.2091	14.3611	11.5285	11.0273
H28Y	3.1163	3.7624	2.5396	3.7454	3.0283	2.5227	1.7671	0	1.7658	17.4808	16.3776	15.8519	18.5752	17.0635	18.3252	19.2847	19.051	18.3899	16.1093	17.0723	15.1893	14.3284	14.0582	15.2419	12.5331	11.9746
H28Z	3.7923	4.353	3.769	3.8046	2.6001	3.1878	1.7708	1.7658	0	16.7442	15.6739	15.0581	17.637	16.0559	17.2693	18.4498	18.1136	17.5915	15.3299	16.1747	14.1443	13.4132	13.2091	14.3611	11.5285	11.0273
H20X	15.3179	15.9943	17.0557	17.3985	17.7781	18.3324	15.7935	17.4808	16.7442	0	1.7654	1.7667	2.5417	3.1068	3.7633	2.5276	3.7497	3.0405	3.7153	4.6991	4.0468	3.9344	5.448	6.2595	5.673	6.3089
H20Y	14.0901	14.638	15.7991	16.0366	16.5254	17.0544	14.7423	16.3776	15.6739	1.7654	0	1.7718	3.7711	3.7896	4.3541	3.1859	3.809	2.6069	2.1958	3.607	3.7841	2.9521	3.8969	4.7638	4.929	5.1061
H20Z	13.7995	14.5008	15.5358	15.8217	16.1279	16.7349	14.157	15.8519	15.0581	1.7667	1.7718	0	3.0997	2.5625	3.7726	3.7629	4.3512	3.7982	3.3797	4.5249	2.6629	2.4155	4.3778	5.5471	3.9225	4.6952
H19X	16.6963	17.3665	18.4168	18.4977	18.7039	19.4584	16.8725	18.5752	17.637	2.5417	3.7711	3.0997	0	1.7643	1.7702	2.4357	3.0924	3.7063	4.8681	5.0358	3.7149	4.6071	6.3827	6.9147	6.1393	7.08
H19Y	15.3299	16.0163	17.0333	17.0357	17.1544	17.9741	15.3637	17.0635	16.0559	3.1068	3.7896	2.5625	1.7643	0	1.772	3.7036	3.7981	4.3568	4.6299	4.8807	2.1291	3.416	5.5105	6.287	4.5812	5.7016
H19Z	16.5555	17.105	18.228	18.0172	18.189	19.0696	16.6649	18.3252	17.2693	3.7633	4.3541	3.7726	1.7702	1.772	0	3.0473	2.5834	3.79	4.6511	4.2947	3.1394	4.2994	5.829	6.1049	5.8046	6.608
H18X	17.1214	17.6205	18.8184	18.8459	19.2682	19.9318	17.6389	19.2847	18.4498	2.5276	3.1859	3.7629	2.4357	3.7036	3.0473	0	1.7699	1.7664	3.8748	3.9128	4.9048	5.0755	6.0077	6.117	7.129	7.5342
H18Y	16.9728	17.3411	18.6206	18.36	18.7685	19.5449	17.4513	19.051	18.1136	3.7497	3.809	4.3512	3.0924	3.7981	2.5834	1.7699	0	1.7723	3.5031	2.781	4.5415	4.8039	5.3624	5.1008	6.8768	7.0925
H18Z	16.114	16.4761	17.7698	17.685	18.2191	18.8554	16.8044	18.3899	17.5915	3.0405	2.6069	3.7982	3.7063	4.3568	3.79	1.7664	1.7723	0	2.4119	2.4504	4.7831	4.4323	4.6882	4.5871	6.6534	6.6473
H15A	13.8079	14.1061	15.4369	15.2913	15.8648	16.4867	14.5658	16.1093	15.3299	3.7153	2.1958	3.3797	4.8681	4.6299	4.6511	3.8748	3.5031	2.4119	0	1.7532	3.9426	2.8254	2.3531	2.6559	4.9707	4.5209
H15B	14.894	15.0743	16.4698	16.0307	16.569	17.321	15.5684	17.0723	16.1747	4.6991	3.607	4.5249	5.0358	4.8807	4.2947	3.9128	2.781	2.4504	1.7532	0	4.3103	3.7245	3.0322	2.3566	5.7905	5.332
H13A	13.4752	14.0757	15.1449	14.9937	15.1256	15.9852	13.5263	15.1893	14.1443	4.0468	3.7841	2.6629	3.7149	2.1291	3.1394	4.9048	4.5415	4.7831	3.9426	4.3103	0	1.756	3.905	4.9301	2.6701	3.6739
H13B	12.3556	12.8816	14.0337	13.959	14.2639	15.0006	12.6937	14.3284	13.4132	3.9344	2.9521	2.4155	4.6071	3.416	4.2994	5.0755	4.8039	4.4323	2.8254	3.7245	1.756	0	2.4386	3.833	2.2349	2.5206
H16A	11.865	12.0725	13.4442	13.0851	13.6288	14.3294	12.567	14.0582	13.2091	5.448	3.8969	4.3778	6.3827	5.5105	5.829	6.0077	5.3624	4.6882	2.3531	3.0322	3.905	2.4386	0	1.7583	3.768	2.6406
H16B	13.0492	13.0619	14.5415	13.9108	14.5302	15.2829	13.8385	15.2419	14.3611	6.2595	4.7638	5.5471	6.9147	6.287	6.1049	6.117	5.1008	4.5871	2.6559	2.3566	4.9301	3.833	1.7583	0	5.3198	4.1971
H11A	10.8479	11.5186	12.5203	12.4833	12.5885	13.3948	10.8627	12.5331	11.5285	5.673	4.929	3.9225	6.1393	4.5812	5.8046	7.129	6.8768	6.6534	4.9707	5.7905	2.6701	2.2349	3.768	5.3198	0	1.7759
H11B	10.0649	10.51	11.6944	11.4667	11.7663	12.539	10.3942	11.9746	11.0273	6.3089	5.1061	4.6952	7.08	5.7016	6.608	7.5342	7.0925	6.6473	4.5209	5.332	3.6739	2.5206	2.6406	4.1971	1.7759	0
H10A	9.4803	9.8689	10.9647	10.3074	10.3137	11.3691	9.32	10.825	9.5959	8.5012	7.4967	6.8189	8.7564	7.1418	7.978	9.5578	8.8746	7.8869	6.7886	7.1805	5.0473	4.6315	4.7454	5.8406	3.0534	2.5611
H10B	10	10.6638	11.5503	11.2193	11.0487	12.0717	9.5531	11.1692	9.8353	7.3518	6.2934	8.1251	6.4131	7.5164	9.3296	8.8535	8.8667	7.1313	7.6521	4.514	4.5149	5.4819	6.7883	2.4467	3.0585
H2A	10.416	10.5195	11.9045	11.2095	11.6436	12.505	10.9236	12.3424	11.348	7.4223	6.0172	6.0397	8.0416	6.7968	7.2421	8.092	7.2736	6.902	4.6645	4.9787	4.7763	3.6819	2.3408	3.137	3.633	2.0485
H2B	11.1553	10.991	12.5203	11.5458	12.1424	12.9979	11.8824	13.1595	12.2048	8.3171	6.7966	7.1818	8.9243	7.8868	7.9938	8.5705	7.5459	7.1583	5.0016	4.9363	6.0286	4.9383	2.9111	2.6751	5.3385	3.7662
H3A	11.2056	10.9481	12.4111	10.9541	11.2994	12.4348	11.53	12.694	11.4976	10.0696	8.7517	8.7691	10.0216	8.9377	9.0158	10.2573	9.0482	9.0486	7.0808	6.7371	6.9746	6.3734	4.9871	4.796	6.1264	4.463
H3B	10.661	10.6767	11.9885	10.8089	10.9663	12.1247	10.723	12.0372	10.7727	9.2319	8.0663	7.761	9.2988	7.8459	8.1859	9.7157	8.6612	8.7149	6.7455	6.6333	5.7925	5.3619	4.6095	4.9766	4.6646	3.6821
H9A	7.4759	7.9624	8.9118	8.3501	8.2303	9.2719	7.1097	8.6084	7.363	10.1399	9.1082	8.4082	10.6447	9.0194	10.0429	11.487	10.9542	10.6984	8.5763	9.1845	6.9872	6.4273	6.4599	7.653	4.5672	4.0868
H9B	7.575	8.4264	9.0944	9.0371	8.744	9.6678	6.8936	8.5429	7.3576	9.9273	9.1242	8.1666	10.4348	8.7851	10.0471	11.5482	10.9808	9.0161	9.8018	6.9454	6.563	7.1668	8.5852	4.4229	4.5549
H8A	5.8652	6.847	7.5612	8.0929	8.1634	8.6725	5.8556	7.5576	6.8215	9.9598	8.9619	8.3047	11.0429	9.5899	10.9214	11.8115	11.7107	11.078	8.9589	10.063	7.8042	6.9186	7.169	8.6946	5.1412	4.8289
H8B	5.9297	6.464	7.547	7.5488	7.8595	8.4659	6.3335	7.8649	7.0738	9.9239	8.6933	8.2996	11.0106	9.5858	10.699	11.5072	11.2063	10.5535	8.2738	9.2365	7.6285	6.5558	6.2351	7.5685	5.0592	4.1679
H4A	8.984	8.6361	10.0143	8.3096	8.5325	9.7686	9.1249	10.1314	8.8789	11.8175	10.4878	10.3025	12.1688	10.7111	11.145	12.4616	11.4559	11.3035	9.1252	9.1623	8.6054	7.9231	6.8071	7.1122	6.9464	5.7298
H4B	8.7555	8.7636	9.9884	8.7198	8.7634	9.9778	8.6509	9.892	8.5791	10.6591	9.4669	9.0458	10.9557	9.4007	10.0224	11.5098	10.637	10.5207	8.382	8.575	7.2864	6.7298	6.0983	6.7632	5.4368	4.4786
H5A	6.8044	6.7912	8.1641	7.342	7.7831	8.6195	7.3249	8.5938	7.6469	10.5036	9.1153	9.8364	11.3897	9.9748	10.7784	11.669	11.0583	10.5236	8.1692	8.7866	7.8828	6.8142	5.8756	6.7848	5.6485	4.3218
H5B	6.8631	6.4162	7.9206	6.4889	7.0547	7.987	7.4847	8.4521	7.4988	12.0402	10.5835	10.5258	12.8623	11.4684	12.1197	13.0141	12.2583	11.7631	9.4044	9.8304	9.3561	8.3158	7.0762	7.6508	7.2858	5.8903
H21A	3.3746	4.2821	4.5683	4.799	4.4325	5.0585	2.3763	3.9021	2.9338	13.8185	12.7418	12.1409	14.7683	13.2234	14.4511	15.5369	15.2482	14.6906	12.4489	13.3568	11.3174	10.5211	10.384	11.6335	8.6761	8.1632
H21B	2.1364	3.1333	3.7255	4.534	4.7924	4.9149	2.7167	4.0875	3.8121	13.5544	12.3665	11.9664	14.777	13.349	14.5678	15.3149	15.1101	14.3634	12.1623	10.4319	10.0752	11.3187	8.8203	8.101		
H23A	4.628	4.6673	4.8858	3.5404	2.4641	3.9186	3.3692	3.726	2.1953	15.9458	14.8015	14.2409	16.6771	15.0651	16.1205	17.4237	16.9045	16.4922	14.2079	14.8649	13.0555	12.3604	11.9723	12.9592	10.5442	9.8968
H23B	4.8663	4.2846	5.0098	2.7432	2.3994	3.867	4.5033	4.6535	3.5638	16.0068	14.7241	14.3517	16.7949	15.2361	16.1535	17.3227	16.701	16.2462	13.903	14.4706	13.1581	12.3349	11.607	12.4091	10.7309	9.819
H24A	5.5662	5.86	6.4435	5.374	4.7337	6.0632	4.4901	5.5478	4.0017	13.8789	12.7995	12.1493	14.4527	12.807	13.8419	15.2887	14.7328	14.4425	12.2137	12.8079	10.8002	10.2209	9.9938	11.0227	8.3507	7.8025
H24B	6.2798	6.0676	6.9076	5.0507	4.5917	6.1112	5.5067	6.3013	4.8273	14.5337	13.3386	12.8427	15.0516	13.4344	14.2838	15.5178	14.995	14.7296	12.4732	12.8908	11.3531	10.7284	10.1595	10.0393	9.062	8.268
H14Q	15.0657	15.424	16.6814	16.2531	16.5477	17.4349	15.3607	16.9429	15.8958	4.2968	3.8499	3.7936	3.6368	3.0253	2.3929	3.7255	2.5359	3.2482	3.0315	2.3306	2.6003	3.039	3.7569	3.7865	4.8094	5.0143
H12Q	13.5496	13.9095	15.1021	14.4635	14.5741	15.6153	13.5518	15.1009	13.9006	6.0424	5.4435	4.8417	5.393	4.0009	4.0979	6.1663	5.1157	5.68	4.5879	4.2034	2.3838	3.0484	3.8205	4.2412	3.536	3.8049
H1Q	13.9967	14.1248	15.498	14.7008	15.0446	16.0191	14.3511	15.8107	14.7032	6.3205	5.344	5.4766	5.1414	4.715	5.9018	4.5285	4.9018	3.6969	2.7372	3.8102	3.6663	3.047	2.5168	4.876	4.3928	
H6Q	5.0119	4.5877	5.9213	4.4625	4.8911	5.8413	5.425	6.2646	5.3255	13.4215	12.0531	11.824	14.3163	12.8423	13.6981	14.6664	14.0519	13.5169	11.1484	11.7466	10.7486	9.7666	8.8583	9.6583	8.3836	7.251
H7Q	4.1588	4.4252	5.6316	5.471	5.9527	6.4551	4.884	6.1798	5.535	11.9404	10.6284	10.3582	13.0924	11.681	12.7386	13.4778	13.1231	12.4164	10.0679	10.9742	9.6946	8.583	7.9531	9.0838	7.1562	6.1489
H22Q	3.0199	2.3931	3.6364	2.5288	3.249	3.7206	3.8006	4.2959	3.8482	14.8743	13.527	13.2931	15.978	14.5305	15.5302	16.3393	15.8885	15.2111	12.8293	13.6158	12.5	11.4431	10.6391	11.5631	9.9842	8.9603

(cont.) Table H.3: Hydrogen Distances for the Optimized Structure of 4z,4'z *cis-anti-cis* DtBuCH18C6

	H10A	H10B	H2A	H2B	H3A	H3B	H9A	H9B	H8A	H8B	H4A	H4B	H5A	H5B	H21A	H21B	H23A	H23B	H24A	H24B	H14Q	H12Q	H1Q	H6Q	H7Q	H22Q
H27X	9.4803	10	10.416	11.1553	11.2056	10.661	7.4759	7.575	5.8652	5.9297	8.984	8.7555	6.8044	6.8631	3.3746	2.1364	4.628	4.8663	5.5662	6.2798	15.0657	13.5496	13.9967	5.0119	4.1588	3.0199
H27Y	9.8689	10.6638	10.5195	10.991	10.9481	10.6767	7.9624	8.4264	6.847	6.464	8.6361	8.7636	6.7912	6.4162	4.2821	3.1333	4.6673	4.2846	5.86	6.0676	15.424	13.9095	14.1248	4.5877	4.4252	2.3931
H27Z	10.9647	11.5503	11.9045	12.5203	12.4111	11.9885	8.9118	9.0944	7.5612	7.547	10.0143	9.9884	8.1641	7.9206	4.5683	3.7255	4.8858	5.0098	6.4435	6.9076	16.6814	15.1021	15.498	5.9213	5.6316	3.6364
H26X	10.3074	11.2193	11.2095	11.5458	10.9541	10.8089	8.3501	9.0371	8.0929	7.5488	8.3096	8.7198	7.342	6.4889	4.799	4.534	3.5404	2.7432	5.374	5.0507	16.2531	14.4635	14.7008	4.4625	5.471	2.5288
H26Y	10.3137	11.0487	11.6436	12.1424	11.2994	10.9663	8.2303	8.744	8.1634	7.8595	8.5325	8.7634	7.7831	7.0547	4.4325	4.7924	2.4641	2.3994	4.7337	4.5917	16.5477	14.5741	15.0446	4.8911	5.9527	3.249
H26Z	11.3691	12.0717	12.505	12.9979	12.4348	12.1247	9.2719	9.6678	8.6725	8.4659	9.7686	9.9778	8.6195	7.987	5.0585	4.9149	3.9186	3.867	6.0632	6.1112	17.4349	15.6153	16.0191	5.8413	6.4551	3.7206
H28X	9.32	9.5531	10.9236	11.8824	11.53	10.723	7.1097	6.8936	5.8556	6.3335	9.1249	8.6509	7.3249	7.4847	2.3763	2.7167	3.3692	4.5033	4.4901	5.6067	15.3607	13.5518	14.3511	5.425	4.884	3.8006
H28Y	10.825	11.1692	12.3424	13.1595	12.694	12.0372	8.6084	8.5429	7.5576	7.8649	10.1314	9.892	8.5938	8.4521	3.9021	4.0875	3.726	4.6535	5.5478	6.3013	16.9429	15.1009	15.8107	6.2646	6.1798	4.2959
H28Z	9.5959	9.9332	11.348	12.2048	11.4976	10.7727	7.363	7.3576	6.8218	7.0738	8.8789	8.5791	7.6469	7.4988	2.9338	3.8181	2.1953	3.5638	4.0017	4.8273	15.8958	13.9006	14.7032	5.3255	5.535	3.8482
H20X	8.5012	8.0353	7.4223	8.3171	10.096	10.1399	9.9273	9.9598	9.9239	11.8175	10.6591	10.5036	12.0402	13.8185	13.5544	15.9458	16.0068	13.8789	14.5337		4.2968	6.0424	6.3205	13.4215	11.9404	14.8743
H20Y	7.4967	7.3518	6.0172	6.7966	8.7517	8.0663	9.1082	9.1242	8.9619	10.4878	9.4669	9.1153	10.5835	12.7418	12.3665	14.8015	14.7241	12.7995	13.3386		3.8499	5.4435	5.344	12.0531	10.6284	13.527
H20Z	6.8189	6.2934	6.0397	7.1818	8.7691	7.761	8.4082	8.1666	8.3047	8.2996	10.3025	9.0458	8.9364	10.5258	12.1409	11.9664	14.2409	14.3517	12.1493	12.8427	3.7936	4.8417	5.4766	11.824	10.3582	13.2931
H19X	8.7564	8.1251	8.0416	8.9243	10.2116	9.2988	10.6447	10.4348	11.0429	11.0106	12.1688	10.9557	11.3897	12.8623	14.7683	14.777	16.6771	16.7949	14.4527	15.0516	3.6368	5.393	6.0303	14.3163	13.0924	15.978
H19Y	7.1418	6.4131	6.7968	7.8868	8.9377	7.8459	9.0194	8.7851	9.5899	9.5858	10.7111	9.4007	9.9748	11.4684	13.2234	13.349	15.0651	15.2361	12.8097	13.4344	3.0253	4.0009	5.1414	12.8423	11.681	14.5305
H19Z	7.978	7.5164	7.2421	7.9938	9.0158	8.1859	10.0429	10.0471	10.9214	10.699	11.145	10.0224	10.7784	12.1197	14.4511	14.5678	16.1205	16.1535	13.8419	14.2838	2.3929	4.0979	4.715	13.6981	12.7386	15.5302
H18X	9.5578	9.3296	8.092	8.5705	10.2573	9.7157	11.487	11.5482	11.8115	11.5072	12.4616	11.5098	11.669	13.0141	15.5369	15.3149	17.4237	17.3227	15.2887	15.7178	3.7255	6.1663	5.9018	14.6664	13.4778	16.3393
H18Y	8.8746	8.8535	7.2736	7.5459	9.0482	8.6612	10.9542	11.2369	11.7107	11.2063	11.4559	10.6337	11.0583	12.2583	15.2482	15.1101	16.9045	16.701	14.7328	14.995	2.5359	5.1157	4.5285	14.0519	13.1231	15.8885
H18Z	8.7869	8.8667	6.902	7.1583	9.0486	8.7149	10.6984	10.9808	11.078	11.0535	11.3035	10.5207	10.5236	11.7631	14.6906	14.3634	16.4922	16.2462	14.4295	14.7296	3.2482	5.68	4.9018	13.5169	12.4164	15.2111
H15A	6.7886	7.1313	4.6645	5.0016	7.0808	6.7455	8.5763	9.0161	8.9589	8.2738	9.1252	8.382	8.1692	9.4044	12.4489	12.0719	14.2079	13.903	12.2137	12.4732	3.0315	4.5879	3.6969	11.1484	10.0679	12.8293
H15B	7.1805	7.6521	4.9787	4.9363	6.7371	6.6333	9.1845	9.8018	10.063	9.2365	9.1623	8.575	8.7866	9.8304	13.3568	13.1027	14.8649	14.4706	12.8079	12.8908	2.3306	4.2034	2.7372	11.7466	10.9742	13.6158
H13A	5.0473	4.514	4.7763	6.0286	6.9746	5.7925	6.9872	6.9454	7.8042	7.6285	8.6054	7.2864	7.8828	9.3561	11.3174	11.4623	13.0555	13.1581	10.8002	11.3531	2.6003	2.3838	3.8102	10.7486	9.6946	12.5
H13B	4.6315	4.5149	3.6819	4.9383	6.3734	5.3619	6.4273	6.563	6.9186	6.5558	7.9231	6.7298	8.8142	9.3158	10.5211	10.4319	12.3604	12.3349	10.2209	10.7284	3.039	3.0484	3.6663	9.7666	8.583	11.4431
H16A	4.7454	5.4819	2.3408	2.9111	4.9871	4.6095	6.4599	7.1668	7.169	6.2351	6.8071	6.0983	5.8756	7.0762	10.384	10.0752	11.9723	11.607	9.9938	10.1595	3.7569	3.8205	3.047	8.8583	7.9531	10.6391
H16B	5.8406	6.7883	3.137	2.6751	4.796	4.9766	7.653	8.5852	8.6946	7.5685	7.1122	6.7632	6.7848	7.6508	11.6335	11.3187	12.091	11.0227	10.9393		3.7865	4.2412	2.5168	9.6583	9.0838	11.5631
H11A	3.0534	2.4467	3.633	5.3385	6.1264	4.6646	5.4672	4.4229	5.1412	5.0592	6.9464	5.4368	5.6485	7.2858	8.6761	8.8203	10.5442	10.7309	8.3507	9.062	4.8094	3.536	4.8876	8.3836	7.1562	9.9842
H11B	2.5611	3.0585	2.0485	3.7662	4.8621	3.6821	4.0868	4.5549	4.8289	4.1679	5.7298	4.4786	4.3218	5.8903	8.1632	8.101	9.8968	9.819	7.8025	8.268	5.0143	3.8049	4.3928	7.251	6.1489	8.9603
H10A	0	1.7742	2.9147	4.4164	4.05	2.3719	2.2439	3.1713	4.5224	3.8219	4.1006	2.4487	3.5251	4.858	6.9581	7.3876	8.2097	8.2267	5.9331	6.3184	6.4628	4.3117	5.3312	6.0005	5.5017	7.93
H10B	1.7742	0	4.2389	5.9008	5.6919	2.8857	2.7178	4.5079	4.994	4.4994	5.753	4.0101	4.928	6.3952	7.2869	7.8699	8.0058	9.1476	7.2454	6.5027	4.3809	5.9834	6.3505	7.1734	6.3505	8.8491
H2A	2.9147	4.2389	0	1.7696	3.0561	2.4845	5.5438	5.6494	4.7464	4.4985	3.7842	3.8889	4.9936	4.9936	8.6449	8.5391	9.921	9.507	7.911	7.9302	5.1568	3.9079	3.6114	6.8313	6.3036	8.8097
H2B	4.4164	5.9008	1.7696	0	2.5042	3.0595	5.8678	7.1995	7.3767	5.9316	4.5276	4.4955	4.5785	5.1356	9.6592	9.4366	10.6341	9.9443	8.7969	8.4861	5.6781	4.811	3.681	7.2534	7.1058	9.2955
H3A	4.05	5.6919	3.0561	2.5042	0	1.7799	3.9714	5.3671	6.4928	5.3109	2.846	3.106	4.4956	4.566	9.2494	9.0566	9.6536	8.9436	7.7065	7.1715	6.8447	5.1626	4.5862	6.6202	7.1577	8.8963
H3B	2.3719	2.8857	2.4845	3.0595	1.7799	0	3.065	2.4867	3.065	2.5163	2.9994	2.2444	3.9853	4.6165	8.3656	8.0051	8.6609	6.9313	7.0002	6.2518	8.6161	6.5378	7.5028	3.6664	6.5507	8.5947
H9A	2.2439	2.7178	5.5438	5.8678	3.9714	3.065	0	1.7759	3.0571	2.5163	4.0391	2.4744	2.7241	4.0118	4.7445	4.7106	6.0789	6.2941	3.824	4.5408	8.9874	7.0007	8.3192	5.5575	3.7727	6.0106
H9B	3.1713	4.5079	5.6494	7.1995	5.3671	2.4867	1.7759	0	2.4867	3.065	5.8044	4.1846	4.2216	5.6303	4.7106	5.4615	6.5166	7.1444	4.3693	5.586	9.7327	8.2122	9.1225	5.0598	4.479	6.7516
H8A	4.5224	4.994	4.7464	7.3767	6.4928	3.065	3.0571	2.4867	0	1.7707	6.515	5.2592	3.8883	5.3869	3.9161	3.8725	6.3996	6.8833	4.8134	6.0502	9.7327	8.2122	9.1225	5.0598	3.0801	5.7006
H8B	3.8219	4.4994	4.4985	5.9316	5.3109	2.5163	2.5163	3.065	1.7707	0	5.0479	4.4955	2.186	3.7486	4.1952	3.9939	5.8084	6.2383	4.6502	6.0502	9.1431	7.6424	9.1225	4.097	2.1182	5.0273
H4A	4.1006	5.753	4.4985	4.5276	2.846	2.9994	4.0391	5.8044	6.515	5.0479	0	1.775	3.0472	2.4394	6.9508	7.2904	6.9254	6.1504	5.2338	4.3886	9.1431	7.1506	7.1286	4.097	5.2497	6.4076
H4B	2.4487	4.0101	3.8889	4.4955	3.106	2.2444	2.4744	4.1846	5.2592	4.4955	1.775	0	2.6014	3.0551	6.3217	6.1181	6.8167	6.4705	6.8195	4.792	8.9193	7.2587	7.4191	3.0029	4.8225	6.564
H5A	3.5251	3.8889	4.9936	4.5785	4.4956	3.9853	2.7241	4.2216	3.8883	2.186	3.0472	2.6014	0	1.7774	5.1249	4.9855	6.225	5.7369	4.5517	4.5544	10.1177	8.4165	8.327	2.2261	2.6815	4.9326
H5B	4.858	6.3952	4.9936	5.1356	4.566	4.6165	4.0118	5.6303	5.3869	3.7486	2.4394	3.0551	1.7774	0	5.4876	5.3596	5.8084	4.8689	4.5498	3.8968	13.1117	11.4977	8.327	3.2602	3.2602	4.3939
H21A	6.9581	7.2869	8.6449	9.6592	9.2494	8.3656	4.7445	4.7106	3.9161	4.1952	6.9508	6.3217	5.1249	5.4876	0	1.7536	2.8083	3.7595	2.578	3.9401	13.0884	11.2158	12.0222	3.6721	2.9871	3.0529
H21B	7.3876	7.8699	8.5391	9.4366	9.0566	8.0051	4.7106	5.4615	3.8725	3.9939	7.2904	6.1181	4.9855	5.3596	1.7536	0	3.9306	4.3106	3.9547	3.9401	11.2158	11.4977	12.0222	3.6693	2.3458	2.5782
H23A	8.2097	8.0058	9.921	10.6341	9.6536	8.6609	6.0789	6.5166	6.3996	5.8084	6.9254	6.8167	6.225	5.8084	2.8083	3.9306	0	1.7537	2.3635	2.6936	14.5984	12.4965	13.1876	3.7195	4.6943	3.0386
H23B	8.2267	9.1476	9.507	9.9443	8.9436	6.9313	6.2941	7.1444	6.8833	6.2383	6.1504	6.4705	5.7369	4.8689	3.7595	4.3106	1.7537	0	2.3559	2.4909	12.4965	12.8127	11.0305	2.8287	4.5049	2.3449
H24A	5.9331	7.2454	7.911	8.7969	7.7065	7.0002	3.824	4.3693	4.8134	4.6502	6.9327	6.8195	6.225	5.7369	2.578	3.9547	2.3635	2.3559	0	1.7594	12.3765	10.253	11.0305	3.0442	3.7373	3.755
H24B	6.3184	6.5027	7.9302	8.4861	7.1715	6.2518	4.5408	5.586	6.0502	6.0502	4.3886	4.792	4.5544	3.8968	3.9401	3.9547	2.6936	2.4909	1.7594	0	12.617	10.4285	10.9863	2.5604	4.2909	3.7367
H14Q	6.4628	4.3809	5.1568	5.6781	6.8447	8.6161	8.9874	9.7327	9.7327	9.1431	9.1431	8.9193	10.1177	13.1117	13.0884	11.2158	14.5984	12.4965	12.3765	12.617	0	2.5896	2.4176	11.8716	11.0937	13.7987
H12Q	4.3117	5.9834	3.9079	4.811	5.1626	6.5378	7.0007	8.2122	8.2122	7.6424	7.1506	7.2587	8.4165	11.4977	11.2158	11.4977	12.4965	12.8127	10.253	10.4285	2.5896	0	2.2253	10.0446	9.5084	12.0668
H1Q	5.3312	6.3505	3.6114	3.681	4.5862	7.5028	8.3192	9.1225	9.1225	9.1225	7.1286	7.4191	8.327	8.327	12.0222	12.0222	13.1876	11.0305	11.0305	10.9863	2.4176	2.2253	0	10.2631	9.8786	12.3474
H6Q	6.0005	7.1734	6.8313	7.2534	6.6202	3.6664	5.5575	5.0598	5.0598	4.097	4.097	3.0029	2.2261	3.2602	3.6721	3.6693	3.7195	2.8287	3.0442	2.5604	11.8716	10.0446	10.2631	0	2.3608	2.3141
H7Q	5.5017	6.3505	6.3036	7.1058	7.1577	6.5507	3.7727	4.479	3.0801	2.1182	5.2497	4.8225	2.6815	3.2602	2.9871	2.3458	4.6943	4.5049	3.7373	4.2909	11.0937	9.5084	9.8786	2.3608	0	2.9492
H22Q	7.93	8.8491	8.8097	9.2955	8.8963	8.5947	6.0106	6.7516	5.7006	5.0273	6.4076	6.564	4.9326	4.3939	3.0529	2.5782	3.0386	2.3449	3.755	3.7367	13.7987	12.0668	12.3474	2.3141	2.9492	0

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Figure H.7: Optimized Structure of 4e,4'e *cis-syn-cis* DtBuCH18C6 with Hydrogen Labels

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Figure H.8: Optimized Structure of 4e,4'e *cis-syn-cis* DtBuCH18C6 with Carbon and Oxygen Labels

Table H.4: Hydrogen Distances for the Optimized Structure of 4e,4'e *cis-syn-cis* DtBuCH18C6

	H27X	H27Y	H27Z	H26X	H26Y	H26Z	H28X	H28Y	H28Z	H20X	H20Y	H20Z	H19X	H19Y	H19Z	H18X	H18Y	H18Z	H23A	H23B	H21A	H21B	H24A	H24B	H8A	H8B
H27X	0	1.7716	1.7658	3.1887	3.8066	2.6051	3.7726	4.3518	3.7863	14.2769	15.3069	16.03	16.4755	16.1692	14.8147	17.7182	17.0656	17.3682	2.1892	3.582	3.877	2.9687	3.933	4.762	7.4275	7.2778
H27Y	1.7716	0	1.7667	3.7629	4.3502	3.7973	3.0987	3.7705	2.5598	13.814	14.7209	15.5402	16.2409	16.0535	14.654	17.3223	16.5915	17.0696	3.3703	4.5134	2.788	2.3786	4.4018	5.5521	6.6588	6.8838
H27Z	1.7658	1.7667	0	2.5256	3.7467	3.0345	2.5447	3.7647	3.1086	14.3095	15.3752	16.0207	16.6031	16.4823	15.0095	17.8986	17.3237	17.721	3.7178	4.678	4.1413	3.9132	5.4767	6.2583	8.1066	8.0979
H26X	3.1887	3.7629	2.5256	0	1.771	1.7669	2.4363	3.0501	3.704	13.0209	14.2943	14.7038	15.0443	14.9558	13.4416	16.6025	16.2409	16.4754	3.9031	3.9001	4.9307	5.0707	6.0304	6.1163	8.5119	8.0393
H26Y	3.8066	4.3502	3.7467	1.771	0	1.7723	3.0935	2.5854	3.7975	11.5082	12.8077	13.2124	13.445	13.2746	11.8041	15.0119	14.6559	14.8165	3.5305	2.775	4.5191	4.8062	5.3663	5.094	7.4905	6.7459
H26Z	2.6051	3.7973	3.0345	1.7669	1.7723	0	3.7066	3.7912	4.3554	13.0632	14.3131	14.7923	14.9627	14.6672	13.279	16.4873	16.0568	16.1743	2.4461	2.4318	4.8083	4.4604	4.7165	4.5865	7.989	7.3166
H28X	3.7726	3.0987	2.5447	2.4363	3.0935	3.7066	0	1.772	1.7655	12.3321	13.429	13.9818	14.709	14.7919	13.2139	16.0254	15.5476	16.0375	4.8801	5.0301	3.7364	4.5542	6.3883	6.9133	7.5247	7.4918
H28Y	4.3518	3.7705	3.7647	3.0501	2.5854	3.7912	1.772	0	1.7705	10.6508	11.7541	12.3302	13.0226	13.0599	11.5062	14.313	13.8214	14.2837	4.6608	4.2966	3.0886	4.2469	5.8139	6.0983	6.286	6.0524
H28Z	3.7863	2.5598	3.1086	3.704	3.7975	4.3554	1.7655	1.7705	0	11.7385	12.6602	13.4134	14.2841	14.2987	12.7943	15.3647	14.7138	15.3013	4.6268	4.8775	2.1425	3.3374	5.5001	6.2833	5.9332	6.1542
H20X	14.2769	13.814	14.3095	13.0209	11.5082	13.0632	12.3321	10.6508	11.7385	0	1.7701	1.772	3.0598	3.7947	2.5887	3.766	3.7703	4.3528	13.2124	11.8092	11.3924	12.6558	12.8766	12.2395	9.6535	8.908
H20Y	15.3069	14.7209	15.3752	14.2943	12.8077	14.3131	13.429	11.7541	12.6602	1.7701	0	1.7653	3.7033	4.3552	3.7977	3.0996	2.5583	3.7851	14.2573	12.9528	12.156	13.4288	13.689	13.1733	9.9649	9.4293
H20Z	16.03	15.5402	16.0207	14.7038	13.2124	14.7923	13.9818	12.3302	13.4134	1.772	1.7653	0	2.4344	3.705	3.0852	2.5475	3.1087	3.7753	14.9823	13.5688	13.1111	14.4021	14.6351	13.9882	11.2808	10.5986
H19X	16.4755	16.2409	16.6031	15.0443	13.445	14.9627	14.709	13.0226	14.2841	3.0598	3.7033	2.4344	0	1.7667	1.7712	2.5267	3.7631	3.1829	15.2071	13.6457	13.9408	15.056	14.9346	14.0234	12.1886	11.1901
H19Y	16.1692	16.0535	16.4823	14.9558	13.2746	14.6672	14.7919	13.0599	14.2987	3.7947	4.3552	3.705	1.7667	0	1.7723	3.0407	3.7969	2.6036	14.7144	13.1353	13.7422	14.6897	14.2897	13.2749	11.7478	10.6097
H19Z	14.8147	14.654	15.0095	13.4416	11.8041	13.279	13.2139	11.5062	12.7943	2.5887	3.7977	3.0852	1.7712	1.7723	0	3.7481	4.3495	3.8055	13.4893	11.9108	12.4018	13.4452	13.2396	12.285	10.7619	9.6461
H18X	17.7182	17.3223	17.8986	16.6025	15.0119	16.4873	16.0254	14.313	15.3647	3.766	3.0996	2.5475	2.5267	3.0407	3.7481	0	1.7667	1.7658	16.4556	15.0095	14.8127	15.9491	15.8756	15.1185	12.4988	11.7307
H18Y	17.0656	16.5915	17.3237	16.2409	14.6559	16.0568	15.5476	13.8214	14.7138	3.7703	2.5583	3.1087	3.7631	3.7969	4.3495	1.7667	0	1.7716	15.7951	14.4513	13.9748	15.0747	15.0037	14.3624	11.3239	10.6828
H18Z	17.3682	17.0696	17.721	16.4754	14.8165	16.1743	16.0375	14.2837	15.3013	4.3528	3.7851	3.7753	3.1829	2.6036	3.8055	1.7658	1.7716	0	15.9428	14.4985	14.5403	15.521	15.1989	14.3701	11.9649	11.0899
H23A	2.1892	3.3703	3.7178	3.9031	3.5305	2.4461	4.8801	4.6608	4.6268	13.2124	14.2573	14.9823	15.2071	14.7144	13.4893	16.4556	15.7951	15.9428	0	1.7545	3.9691	2.8697	2.3607	2.6474	6.5519	5.9713
H23B	3.582	4.5134	4.678	3.9001	2.775	2.4318	5.0301	4.2966	4.8775	11.8092	12.9528	13.5688	13.6457	13.1353	11.9108	15.0095	14.4513	14.4985	1.7545	0	4.2973	3.7787	3.0371	2.3588	6.337	5.3559
H21A	3.877	2.788	4.1413	4.9307	4.5191	4.8083	3.7364	3.0886	2.1425	11.3924	12.156	13.1111	13.9408	13.7422	12.4018	14.8127	13.9748	14.5403	3.9691	4.2973	0	1.7589	3.9062	4.9167	4.0438	4.3862
H21B	2.9687	2.3786	3.9132	5.0707	4.8062	4.4604	4.5542	4.2469	3.3374	12.6558	13.4288	14.4021	15.056	14.6897	13.4452	15.9491	15.0747	15.521	2.8697	3.7787	1.7589	0	2.5288	3.9228	4.5934	4.7878
H24A	3.933	4.4018	5.4767	6.0304	5.3663	4.7165	6.3883	5.8139	5.5001	12.8766	13.689	14.6351	14.9346	14.2897	13.2396	15.8756	15.0037	15.1989	2.3607	3.0371	3.9062	2.5288	0	1.7541	5.0381	4.5681
H24B	4.762	5.5521	6.2583	6.1163	5.094	4.5865	6.9133	6.0983	6.2833	12.2395	13.1733	13.9882	14.0234	13.2749	12.285	15.1185	14.3624	14.3701	2.6474	2.3588	4.9167	3.9228	1.7541	0	5.6408	4.6115
H8A	7.4275	6.6588	8.1066	8.5119	7.4905	7.989	7.5247	6.286	5.9332	9.6535	9.9649	11.2808	12.1886	11.7478	10.7619	12.4988	11.3239	11.9649	6.5519	6.337	4.0438	4.5934	5.0381	5.6408	0	1.7773
H8B	7.2778	6.8838	8.0979	8.0393	6.7459	7.3166	7.4918	6.0524	6.1542	8.908	9.4293	10.5986	11.1901	10.6097	9.6461	11.7307	10.6828	11.0899	5.9713	5.3559	4.3862	4.7878	4.5681	4.6115	1.7773	0
H9A	7.8203	7.191	8.1347	7.6845	6.3436	7.4555	6.764	5.1072	5.5827	7.0735	7.7378	8.7902	9.6466	9.4174	8.1789	10.3247	9.4449	10.0246	6.8857	6.0008	4.5378	5.695	6.2348	6.1949	3.0668	2.5099
H9B	8.2307	7.2663	8.4424	8.4586	7.3814	7.1092	5.6754	5.6532		7.8305	8.1753	9.4278	10.0537	9.3215	10.9741	9.9207	10.752		7.6166	7.0866	4.4929	5.7743	6.7474	7.1235	2.4958	3.0571
H5A	7.4818	7.6618	8.5689	8.0584	6.5521	6.9573	8.2368	6.7933	7.2838	9.2619	10.0188	10.9515	11.0054	10.1548	9.329	11.8411	10.9776	10.9927	6.5322	4.6186	5.7159	6.6535	4.3878	3.5254	4.1476	2.4397
H5B	6.7875	7.3481	7.9493	7.1446	5.6151	5.8507	7.8281	6.518	7.213	10.0673	11.0533	11.7713	11.5904	10.7404	9.844	12.7371	12.0697	11.9242	4.742	3.4763	5.9448	5.658	4.0727	2.6378	5.5233	3.8942
H4A	7.632	8.0071	8.3415	6.967	5.212	6.1222	7.5122	5.953	7.1303	8.133	9.3535	9.8333	9.5905	8.9297	7.8261	11.0103	10.5784	10.409	5.9188	4.2756	6.3825	6.7093	5.8889	4.6568	6.1491	4.4895
H4B	7.6629	7.6492	8.2689	7.2493	5.5773	6.6134	7.2104	5.517	6.4806	7.283	8.3097	9.0371	9.1976	8.6547	7.4993	10.3181	9.6834	9.7835	6.1642	4.7758	5.5249	6.1476	7.5559	4.9645	4.6637	3.0998
H10A	10.0223	9.4463	10.3273	9.648	8.1829	9.4231	8.7961	7.0832	7.7306	5.0944	5.5868	6.7567	7.6843	7.4541	6.3425	8.1322	7.1895	7.8252	8.9396	7.8581	6.7933	7.9153	8.1834	7.8969	4.5662	3.9275
H10B	10.7547	9.9288	10.9858	10.6355	9.3336	10.5152	9.4441	7.8527	8.1793	5.661	5.6545	7.1024	8.4563	8.3654	7.3782	8.4355	7.2611	8.2318	9.9803	9.0327	7.1677	8.3775	8.9288	8.9398	4.4904	4.5214
H11A	11.9575	11.3268	12.501	12.1868	10.7596	11.7458	11.2883	9.6664	9.963	6.2708	5.9355	7.5205	8.5072	7.9818	7.4844	8.1014	6.6537	7.4294	10.7452	9.8756	9.4164	9.3835	9.2307		5.0603	4.8462
H11B	11.0791	10.6815	11.7261	11.1806	9.636	10.6023	10.5978	8.9112	9.4196	6.0362	6.1565	7.4846	8.0341	7.3096	6.7393	8.0946	6.88	7.2815	9.6598	8.6182	8.0432	8.7545	8.4097	7.9838	4.8525	4.023
H3A	10.4126	10.5872	11.0143	9.5918	7.8277	8.9358	9.8437	8.1412	9.3523	5.9589	7.1441	7.5139	6.9718	6.1194	5.2176	8.3458	8.007	7.6336	8.7459	7.1477	8.5709	9.146	8.3976	7.227	7.2471	5.6436
H3B	9.7891	9.6947	10.3255	9.2009	7.5031	8.6631	9.0486	7.2944	8.3102	5.5068	6.4841	7.2002	7.2423	6.6011	5.5693	8.2623	7.6612	7.658	8.2865	6.8607	7.3976	8.1474	7.7244	6.8747	5.7142	4.275
H2A	10.9929	9.9858	11.8441	11.005	9.3279	10.1583	10.9584	9.2706	10.0159	6.7835	7.2849	8.2301	8.0567	6.9529	6.5524	8.5653	7.6521	7.481	9.2383	7.9855	8.655	9.0486	9.0998	7.2082	6.0114	5.5844
H2B	11.9254	12.0782	12.74	11.5906	9.8438	10.7448	11.78	10.0759	11.0512	6.5205	7.2226	7.8304	7.1511	5.8528	5.6249	7.954	7.3449	6.791	10.0974	8.6595	9.8979	10.2954	9.2339	8.0946	7.6538	6.1238
H13A	14.541	13.9798	14.8192	13.9458	12.4089	13.7505	13.1226	11.4058	12.1538	3.0785	2.1426	3.7355	4.9296	4.8077	4.5188	4.1361	2.7838	3.8805	13.3462	12.1241	11.3072	12.4167	12.4721	11.9932	8.5782	8.0492
H13B	15.5179	15.0775	15.9517	15.0564	13.447	14.6932	14.4101	12.6656	13.4238	4.2409	3.338	4.5577	5.0715	4.4621	4.803	3.913	2.3742	2.9762	14.1421	12.8863	12.4143	13.3588	13.1252	12.5179	9.418	8.7581
H15A	14.4953	14.4522	15.0076	13.6419	11.9082	13.1371	13.5721	11.8109	12.9429	4.2985	4.8812	5.0306	3.9047	2.4342	2.7837	4.6823	4.5088	3.5827	12.8907	11.3614	12.1191	12.254	11.2146	9.8811	6.6268	
H15B	15.9431	15.8004	16.458	15.2065	13.49	14.7193	14.9895	13.2189	14.2519	4.6604	4.6271	4.8801	3.9016	2.4458	3.5341	3.7185	3.3632	2.1883	14.3588	12.8942	13.346	14.1461	13.5562	12.6091	10.7551	9.672
H16A	14.3807	14.3793	15.1316	14.0341	12.2959	13.2902	14.006	12.2577	13.1793	6.0997	6.2861	6.9143	6.12	4.5891	5.1055	6.2568	5.5396	4.7587	12.6191	11.229	12.0033	12.5321	11.6032	10.5936	9.2501	8.004
H16B	15.2016	15.0126	15.8816	14.938	13.2436	14.2978	14.6448	12.8879	13.6869	5.5044	5.4929	5.3827	6.028	4.7173	5.3701	5.47	4.3842	3.9308	13.5592	12.2616	12.4744	13.1252	12.4128	11.5979	9.3941	8.4212
H22Q	3.8517	3.8082	4.3073	3.7322	2.5337	3.247	3.6535	2.4061	3.0437	10.4471	11.5024	12.2076	12.6498	12.3651	11.0009	13.8684	13.2505	13.5466	3.0322	2.3272	2.5472	3.0437	3.728	3.7668	4.9656	4.3133
H7Q	5.1727	4.6255	6.1406	6.8821	6.1262	6.1374	6.2499	5.3834	4.772	11.4613	12.0308	13.1759	13.8652	13.3749	12.2966	14.4922	13.4574	13.9323	4.3384	4.6221	2.6412	2.3037	2.7482	3.8679	5.2577	2.8756
H6Q	5.9422	6.0159	7.1781	7.2758	6.1178	6.137	7.2911	6.1501	6.1501	10.8604	11.5415	12.5833	12.8933	12.1688	11.2403	13.6478	12.6888	12.8898	4.2819	3.9457	4.2807	3.7891	2.4858	2.462	3.348	2.3624
H1Q	12.8874	12.695	13.6501	12.892	11.2387	12.1705	12.5902	10.8701	11.5383	6.1476	6.1518	7.2882	7.2751	6.1353	6.1194	7.1764	6.0082	5.9453	10.1242	10.0555	10.1726	10.7229	9.9803	9.2588	7.0261	5.9945
H12Q	13.9253	13.4579	14.4917	13.8621	12.2943	13.3743	13.1801	11.4693	12.0237	5.371	4.7716	6.2485	6.8822	6.1384	6.127	6.1396	4.6213	5.181	12.5295	11.4329	10.7602	11.5711	11.267	10.8062	7.422	6.856
H14Q	13.5451	13.2525	13.8701	12.65	11.0032	12.3701	12.2147	10.4534	11.4952	2.404	3.0508	3.6523	3.7335	3.2439	2.5347	4.3074	3.8056	3.8524	12.1901	10.7589	10.7822	11.7891	11.5912	10.8132	8.59	7.596

(cont.)Table H.4: Hydrogen Distances for the Optimized Structure of 4e,4'e *cis-syn-cis* DtBuCH18C6

| H9A	H9B	H5A	H5B	H4A	H4B	H10A	H10B	H11A	H11B	H3A	H3B	H2A	H2B	H13A	H13B	H15A	H15B	H16A	H16B	H22Q	H7Q	H6Q	H1Q	H12Q	H14Q	
7.8203	8.2307	7.4818	6.7875	7.632	7.6629	10.0223	10.7547	11.9575	11.0791	10.4126	9.7891	10.9929	11.9254	14.541	15.5179	14.4953	15.9431	14.3807	15.2016	3.8517	5.1727	5.9422	12.8874	13.9253	13.5451	H27X
7.191	7.2663	7.6618	7.3481	8.0071	7.6492	9.4463	9.9288	11.3268	10.6815	10.5872	9.6947	10.9858	12.0782	13.9798	15.0775	14.4522	15.8004	14.3793	15.0126	3.8082	4.6255	6.0159	12.695	13.4579	13.2525	H27Y
8.1347	8.4424	8.5689	7.9493	8.3415	8.2689	10.3273	10.9858	12.501	11.7261	11.0143	10.3255	11.8441	12.74	14.8192	15.9517	15.0076	16.458	15.1316	15.8816	4.3073	6.1406	7.1781	13.6501	14.4917	13.8701	H27Z
7.6845	8.4586	8.0584	7.1446	6.967	7.2493	9.648	10.6355	12.1868	11.1806	9.5918	9.2009	11.005	11.5906	13.9458	15.0564	13.6419	15.2065	14.0341	14.938	7.3722	6.6821	7.2758	12.892	13.8621	12.65	H26X
6.3436	7.3814	6.5521	5.6151	5.212	5.5773	8.1829	9.3336	10.7596	9.636	7.8277	7.5031	9.3279	9.8438	12.4089	13.447	11.9082	13.49	12.2959	13.2436	2.5337	6.1262	6.1178	11.2387	12.2943	11.0032	H26Y
7.4555	8.3695	6.9573	5.8507	6.1222	6.6134	9.4231	10.5152	11.7458	10.6023	8.9358	8.6631	10.1583	10.7448	13.7505	14.6932	13.1371	14.7193	13.2902	14.2978	3.247	6.1374	6.1371	12.1705	13.3743	12.3701	H26Z
6.764	7.1092	8.2368	7.8281	7.5122	7.2104	8.7961	9.4441	11.2883	10.5978	9.8437	9.0486	10.9584	11.78	13.1226	14.4101	13.5721	14.9895	14.006	14.6448	3.6535	6.2499	7.2911	12.5902	13.1801	12.2147	H28X
5.1072	5.6754	6.7933	6.518	5.953	5.517	7.0832	7.8527	9.6664	8.9112	8.1412	7.2944	9.2706	10.0759	11.4058	12.6656	11.8109	13.2189	12.2577	12.8879	2.4061	5.5834	6.1568	10.8701	11.4693	10.4534	H28Y
5.5827	5.6532	7.2838	7.213	7.1303	6.4806	7.7306	8.1793	9.963	9.4196	9.3523	8.3102	10.0159	11.0512	12.1538	13.4238	12.9429	14.2519	13.1793	13.6869	3.0437	4.772	6.1501	11.5383	12.0237	11.4952	H28Z
7.0735	7.8305	9.2619	10.0673	8.133	7.283	5.0944	5.661	6.2708	6.0362	5.9589	5.5068	6.7835	6.5205	3.0785	4.2409	4.2985	4.6604	6.0997	5.8044	10.4471	11.4613	10.8604	6.1476	5.371	2.404	H20X
7.7378	8.1753	10.0188	11.0533	9.3535	8.3097	5.5868	5.6545	5.9355	6.1565	7.1441	6.4841	7.2849	7.2226	2.1426	3.338	4.8812	4.6271	6.2861	5.4929	11.5024	12.0308	11.5415	6.1518	4.7716	3.0508	H20Y
8.7902	9.4278	10.9515	11.7713	9.8333	9.0371	6.7567	7.1024	7.5205	7.4846	7.5139	7.2002	8.2301	7.8304	3.7355	4.5577	5.0306	4.8801	6.9143	6.3827	12.2076	13.1759	12.5833	7.2882	6.2485	3.6523	H20Z
9.6466	10.6251	11.0054	11.5904	9.5905	9.1976	7.6843	8.4563	8.5072	8.0341	6.9718	7.2423	8.0567	7.1511	4.9296	5.0715	3.9047	3.9016	6.12	6.028	12.6498	13.8652	12.8933	7.2751	6.8822	3.7335	H19X
9.4174	10.5037	10.1548	10.7404	8.9297	8.6547	7.4541	8.3654	7.9818	7.3096	6.1194	6.6011	6.9529	5.8528	4.8077	4.4621	2.4342	2.4458	4.5891	4.7173	12.3651	13.3749	12.1688	6.1353	6.1384	3.2439	H19Y
8.1789	9.3215	9.329	9.844	7.8261	7.4993	6.3425	7.3782	7.4844	6.7393	5.2176	5.5693	5.6524	6.2249	4.5188	4.8083	2.7837	5.3341	5.1055	5.3701	11.0009	12.2966	11.2403	6.1194	6.127	2.5347	H19Z
10.3247	10.9741	11.8411	12.7371	11.0103	10.3181	8.1322	8.4355	8.1014	8.0946	8.3458	8.2623	8.5653	7.954	4.1361	3.913	4.6823	3.7185	6.2568	5.47	13.8684	14.4922	13.6478	7.1764	6.1396	4.3074	H18X
9.4449	9.9207	10.9776	12.0697	10.5784	9.6834	7.1895	7.2611	6.6537	6.88	8.007	7.6412	7.6521	7.3449	2.7838	2.3742	4.5088	3.3632	5.5396	4.3842	13.2505	13.454	12.6888	6.0082	4.6213	3.8056	H18Y
10.0246	10.752	10.9927	11.9242	10.409	9.7835	8.2252	8.2318	7.4294	7.2815	7.6336	7.658	7.481	6.791	3.8805	2.9762	5.5827	2.1883	4.7587	3.9308	13.5466	13.9323	12.8898	5.9453	5.181	3.8524	H18Z
6.8857	7.6166	5.6322	4.742	5.9188	6.1642	8.9396	9.8803	10.7452	9.6598	8.7459	8.2865	9.2383	10.0974	13.3462	14.1421	12.8907	14.3588	12.6191	13.5592	3.0322	4.3384	4.2819	11.2442	12.5295	12.1901	H23A
6.0008	7.0866	4.6186	3.4763	4.2756	4.7758	7.8581	9.0327	9.8756	8.6182	7.1477	6.8607	7.9855	8.6595	12.1241	12.8863	11.3614	12.8942	11.229	12.2616	2.3272	4.6221	3.9457	10.0555	11.4329	10.7589	H23B
4.5378	4.4929	5.7159	5.9448	6.3825	5.5249	6.7933	7.1677	8.5768	8.0432	8.5709	7.3976	8.655	9.8979	11.3072	12.4143	12.1191	13.346	12.0033	12.4744	2.5472	2.6412	4.2807	10.1726	10.7602	10.7822	H21A
5.695	5.7743	5.6535	5.658	6.7093	6.1476	7.9153	8.3775	9.4164	7.8545	9.146	8.1474	9.0486	10.2954	12.4167	13.3588	12.8856	14.1461	12.5321	13.1252	3.0437	2.3037	3.7891	10.7229	11.5711	11.7891	H21B
6.2348	6.7474	4.3878	4.0727	5.8889	5.7559	8.1834	8.9288	9.3835	8.4097	8.3976	7.7244	8.0998	9.2339	12.4721	13.1184	12.254	13.5562	11.6032	12.4128	3.728	2.7482	2.4858	9.9803	11.267	11.5912	H24A
6.1949	7.1235	3.5254	2.6378	4.6568	4.9645	7.8969	8.9398	9.2307	7.9838	7.227	6.8747	7.2082	8.0946	11.9932	12.5179	11.2146	12.6091	10.5936	11.5979	3.7668	3.8679	2.462	9.2588	10.802	10.8132	H24B
3.0668	2.4958	4.1476	5.5233	6.1491	6.6637	4.5662	4.4904	5.0603	4.8525	5.7471	5.7142	6.0114	7.6538	8.5782	9.418	9.8811	10.7551	9.2501	9.3941	4.9656	5.2277	3.348	7.0261	7.422	8.59	H8A
2.5099	3.0571	2.4397	3.8942	4.4895	3.0998	3.9275	4.5214	4.8462	4.023	5.6436	4.275	4.5844	6.1238	8.0492	8.7581	8.6268	9.672	8.004	8.4212	4.3133	2.8756	2.3628	5.9945	6.856	7.596	H8B
0	1.7781	4.0685	5.1223	4.4204	2.6942	2.2613	3.0702	4.5656	3.9201	5.1147	3.4848	5.0015	6.2309	6.7972	7.9156	7.8538	8.9406	7.9052	8.1845	4.2475	4.4557	4.4942	6.1039	6.45	6.3249	H9A
1.7781	0	5.2595	6.4971	6.1428	4.4212	3.0603	2.7568	4.4939	4.52	6.7675	5.0505	6.1615	7.5846	7.1642	8.3735	9.0253	9.8782	8.9467	8.9278	5.1496	4.39	5.1498	6.8768	6.7635	7.2961	H9B
4.0685	5.2595	0	1.7796	3.0494	2.6019	5.0039	6.1603	5.996	4.5707	4.4822	3.8433	3.735	4.8822	8.6533	9.0427	7.9818	9.2387	7.2172	8.1028	4.6062	4.2172	2.1998	5.7387	7.325	7.5788	H5A
5.1223	6.4971	1.7796	0	2.4466	3.0415	6.2296	7.5816	7.6375	6.1078	4.685	4.5901	4.8819	5.5335	9.8954	10.2894	8.6558	10.0974	8.1054	9.2384	4.2355	4.8927	2.8275	7.0447	8.7828	8.4646	H5B
4.4204	6.1428	3.0494	2.4466	0	1.777	5.1098	6.7627	7.2293	5.628	2.886	3.05	4.4792	4.6865	8.5669	9.1389	7.1433	8.7441	7.238	8.3998	4.2743	6.108	4.5679	6.5233	8.0634	6.8025	H4A
2.6942	4.4212	2.6019	3.0415	1.777	0	3.4788	5.0451	5.6946	4.2514	3.056	2.1354	3.8369	4.5898	7.3912	8.1372	6.8533	8.2818	7.721	9.3656	3.9656	5.1667	5.6625	6.866	6.866	6.0326	H4B
2.2613	3.0603	5.0039	6.2296	5.1098	3.4788	0	1.7782	3.0667	2.5096	4.4359	2.7072	4.0754	5.135	4.541	5.6974	6.0033	6.892	6.2101	6.2405	6.3258	6.4533	6.1043	4.5017	4.4557	4.2499	H10A
3.0702	2.7568	6.1603	7.5816	6.7627	5.0451	1.7782	0	2.496	3.0572	6.1552	4.4317	5.259	6.5026	4.4913	5.7706	7.084	7.6171	7.1282	6.7427	7.3032	6.7683	6.8749	5.1493	4.382	5.149	H10B
4.5656	4.4939	5.996	7.6375	7.2293	5.6946	3.0667	2.496	0	1.7771	6.1451	4.6603	4.1336	5.514	4.0045	4.59	6.3263	6.5337	5.0291	5.7421	8.587	7.4221	3.3391	2.5198	2.5198	4.959	H11A
3.9201	4.52	4.5707	6.1078	5.6228	4.2514	2.5096	3.0572	1.7771	0	4.482	3.0919	4.2299	3.8882	4.3894	4.7893	5.3475	5.9725	4.6154	4.5717	7.5881	8.6568	5.986	2.3651	2.8791	4.3063	H11B
5.1147	6.7675	4.4822	4.685	2.886	3.056	4.4359	6.1552	6.1451	4.482	0	2.6021	3.0489	2.4468	6.3913	6.7117	4.273	5.9194	4.6677	5.8948	6.8081	8.0736	6.5296	4.5671	6.1094	4.2785	H3A
3.4848	5.0505	3.8433	4.5901	3.05	2.1354	2.7072	4.4317	4.6603	3.0919	2.6021	0	2.6021	3.0417	5.5262	6.144	4.7652	6.159	4.9715	5.7565	6.0399	6.8803	5.6722	4.0043	5.1642	3.9592	H3B
5.0015	6.1615	3.735	4.8819	4.4792	3.8369	4.0754	5.259	4.1336	4.2299	3.0489	2.6021	0	1.7794	5.7142	5.6477	6.4128	6.5319	3.5332	3.3916	7.5819	7.3337	7.5429	2.1961	4.2116	4.6011	H2A
6.2309	7.5846	4.8822	5.5335	4.6865	4.5898	5.135	6.5026	5.514	3.8882	2.4468	3.0417	1.7794	0	5.9505	5.658	3.4766	4.7455	2.6498	4.0811	8.4689	8.7913	7.049	2.8255	4.893	4.2387	H2B
6.7972	7.1642	8.6533	9.8954	8.5669	7.3912	4.541	4.4913	4.0045	4.3894	6.3913	5.5262	5.7142	5.9505	0	1.759	4.2976	3.9708	4.9169	3.8983	10.7856	10.765	10.1719	4.2815	2.6405	2.5497	H13A
7.9156	8.3735	9.0427	10.2894	9.1389	8.1372	5.6974	5.7706	4.59	4.7893	6.7117	6.144	5.6477	5.658	1.759	0	3.7769	2.8715	3.9152	2.516	11.7891	11.5735	10.7192	3.7861	2.3041	3.0432	H13B
7.8538	9.0253	7.9818	8.6558	7.1433	6.8533	6.0033	7.084	6.3263	5.3475	4.273	4.7652	6.4128	3.4766	4.2976	3.7769	0	1.755	2.3618	3.0384	10.757	11.4352	10.0546	3.9409	4.6205	2.3247	H15A
8.9406	9.8782	9.2387	10.0974	8.7441	8.2818	6.892	7.6171	6.5337	5.9725	5.9194	6.159	6.5319	4.7455	3.9708	2.8715	1.755	0	2.6458	2.363	12.192	12.5371	11.2476	4.284	4.3441	3.0315	H15B
7.9052	8.9467	7.2172	8.1054	7.238	7.721	6.2101	7.1282	5.0291	4.6154	4.6677	4.9715	3.5332	2.6498	4.9169	3.9152	2.3618	2.6458	0	1.7541	10.8265	10.8221	9.2709	2.4631	3.867	3.7701	H16A
8.1845	8.9278	8.1028	9.2384	8.3998	9.3656	6.2405	6.7427	5.7421	4.5717	5.8948	5.7565	3.3916	4.0811	3.8983	2.516	3.0384	2.363	1.7541	0	11.5965	11.2763	9.9858	2.4897	2.7461	3.7243	H16B
4.2475	5.1496	4.6062	4.2355	4.2743	3.9656	6.3258	7.3032	8.587	7.5881	6.8081	6.0399	7.5819	8.4689	10.7856	11.7891	10.757	12.192	10.8265	11.5965	0	3.7328	3.9054	9.4007	10.3625	9.7104	H22Q
4.4557	4.39	4.2172	4.8927	6.108	5.1667	6.4533	6.7683	7.4221	8.6568	8.0736	6.8803	7.3337	8.7913	10.765	11.5735	11.4352	12.5371	10.8221	11.2763	3.7328	0	2.3102	8.8257	9.6274	10.3654	H7Q
4.9942	5.1498	2.1998	2.8275	4.5679	5.6625	6.8749	7.0146	3.3391	2.3651	4.5671	4.0043	2.1961	8.2255	4.2815	3.7861	3.9409	4.284	2.4631	2.4897	3.9054	2.3102	0	2.3104	8.8191	9.3994	H6Q
6.1039	6.8768	5.7387	7.0447	6.5233	5.6625	5.1493	3.3391	2.5198	2.3651	4.5671	4.0043	2.1961	4.2116	4.2815	3.7861	3.9409	4.284	2.4631	2.4897	9.4007	8.8257	8.8191	0	2.3104	3.902	H1Q
6.45	6.7635	7.325	8.7828	8.0634	6.866	4.4557	4.382	2.8791	2.8791	6.1094	5.1642	4.893	4.893	2.6405	2.3041	4.6205	4.3441	3.867	2.7461	10.3625	9.6274	8.8191	2.3104	0	3.7304	H12Q
6.3249	7.2961	7.5788	8.4646	6.8025	6.0326	4.2499	5.149	4.959	4.3063	4.2785	3.9592	4.6011	4.2387	2.5497	3.0432	2.3247	3.0315	3.7701	3.7243	9.7104	10.3654	9.3994	3.902	3.7304	0	H14Q

Figure H.9: Optimized Structure of 4z,4'e *cis-syn-cis* DtBuCH18C6 with Hydrogen Labels
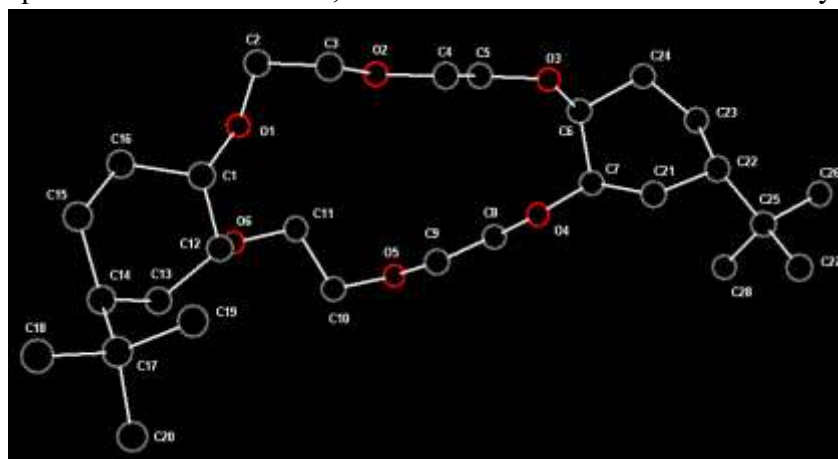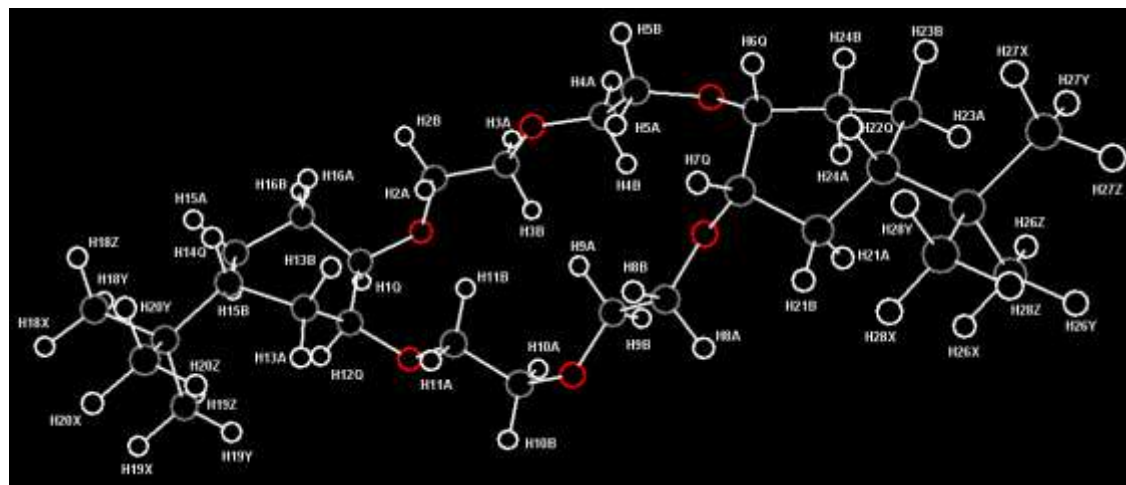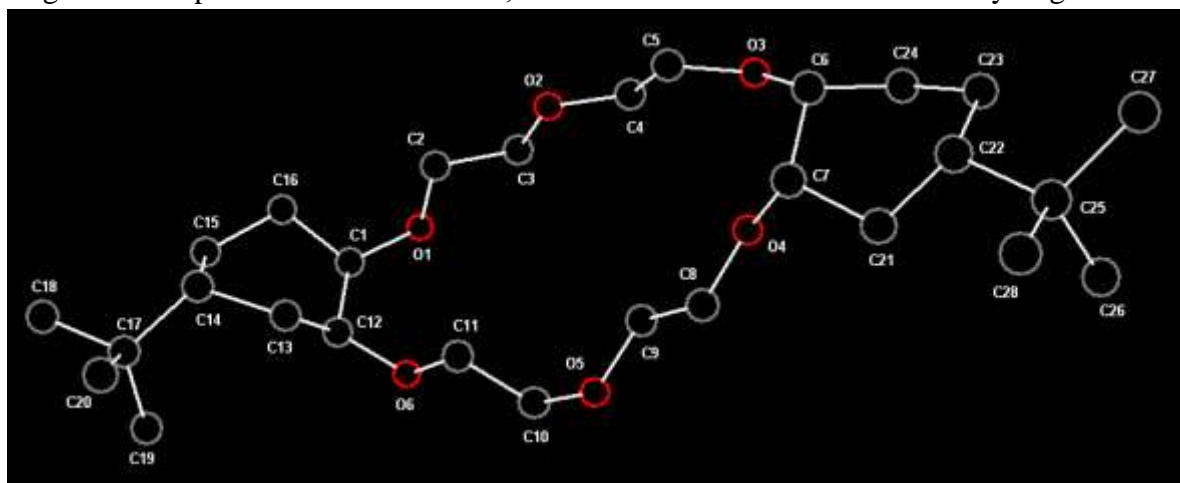
Figure H.10: Optimized Structure of 4z,4'e *cis-syn-cis* DtBuCH18C6 with Carbon and Oxygen Labels

Table H.5: Hydrogen Distances for the Optimized Structure of 4z,4'e *cis-syn-cis* DtBuCH18C6

	H26X	H26Y	H26Z	H28X	H28Y	H28Z	H27X	H27Y	H27Z	H20X	H20Y	H20Z	H19X	H19Y	H19Z	H18X	H18Y	H18Z	H23A	H23B	H21A	H21B	H24A	H24B	H8A	H8B
H26X	0	1.7729	1.7641	3.0345	3.7786	2.5634	3.6757	3.816	4.3519	15.0388	16.1552	16.8009	16.8915	16.4282	15.166	18.3063	17.7459	17.8123	2.1557	3.0501	4.5635	4.8533	4.4428	4.6246	7.7543	8.0442
H26Y	1.7729	0	1.7704	3.7589	4.353	3.78	3.0745	2.6255	3.8177	15.1075	16.1019	16.8719	17.2119	16.8341	15.5267	18.4659	17.7951	18.0324	2.8225	3.9878	4.7997	4.4303	4.3011	5.1277	7.2071	7.8808
H26Z	1.7641	1.7704	0	2.5447	3.7753	3.1705	2.3886	3.0592	3.6744	15.3457	16.4864	17.0903	17.3348	17.0432	15.6589	18.7868	18.2704	18.4473	3.7137	4.3682	5.0546	4.921	5.6607	6.1408	8.3167	8.8464
H28X	3.0345	3.7589	2.5447	0	1.7665	1.7667	2.5436	3.7601	3.0485	13.6028	14.9066	15.3085	15.3962	15.1785	13.7403	17.0504	16.7224	16.7992	4.3112	3.8654	3.8733	4.2883	6.1681	6.237	8.0586	8.2463
H28Y	3.7786	4.353	3.7753	1.7665	0	1.7715	3.1596	3.7821	2.5668	11.8862	13.1764	13.6053	13.7032	13.4668	12.037	15.3111	14.9624	15.0441	4.1554	3.1554	2.2892	3.0461	5.4549	5.4717	6.6797	6.7112
H28Z	2.5634	3.78	3.1705	1.7667	1.7715	0	3.7742	4.3528	3.7815	13.1537	14.4303	14.8834	14.8077	14.4003	13.0902	16.4203	16.0416	16.0022	3.0911	2.2788	3.1245	4.1164	5.0216	4.7241	7.366	7.2749
H27X	3.6757	3.0745	2.3886	2.5436	3.1596	3.7742	0	1.7705	1.7637	13.8725	14.9954	15.5789	16.0535	15.9705	14.4644	17.4685	16.9816	17.316	4.9151	5.0435	4.4026	3.721	6.1734	6.9209	7.489	8.216
H27Y	3.816	2.6255	3.0592	3.7601	3.7821	4.3528	1.7705	0	1.7725	13.4611	14.4207	15.1887	15.7986	15.6474	14.208	16.995	16.3422	16.7653	4.4031	4.7916	4.0412	2.8733	5.0206	6.1297	6.134	7.0993
H27Z	4.3519	3.8177	3.6744	3.0485	2.5668	3.7815	1.7637	1.7725	0	12.1604	13.2495	13.8733	14.4092	14.3385	12.8326	15.7545	15.2387	15.6109	4.8471	4.5727	3.1015	2.1499	5.5385	6.3163	6.012	6.7099
H20X	15.0388	15.1075	15.3457	13.6028	11.8862	13.1537	13.8725	13.4611	12.1604	0	1.7699	1.7721	3.0359	3.7864	2.5815	3.7632	3.775	4.352	13.9499	12.5577	10.4799	10.7596	12.9009	12.8237	9.4921	8.6732
H20Y	16.1552	16.1019	16.4864	14.9066	13.1764	14.4303	14.9954	14.4207	13.2495	1.7699	0	1.766	3.7053	4.3555	3.7972	3.1208	2.5703	3.7935	14.9538	13.6685	11.6046	11.7387	13.6653	13.6957	9.9627	9.2433
H20Z	16.8009	16.8719	17.0903	15.3085	13.6053	14.8834	15.5789	15.1887	13.8733	1.7721	1.766	0	2.4393	3.7085	3.1063	2.5397	3.0914	3.7685	15.7162	14.3117	12.2442	12.5128	14.6481	14.554	11.1749	10.367
H19X	16.8915	17.2119	17.3348	15.3962	13.7032	14.8077	16.0535	15.7986	14.4092	3.0359	3.7053	2.4393	0	1.7672	1.7709	2.529	3.7642	3.1913	15.7663	14.2303	12.4381	13.0353	14.8755	14.4905	11.9088	10.7954
H19Y	16.4282	16.8341	17.0432	15.1785	13.4668	14.4003	15.9705	15.6474	14.3385	3.7864	4.3555	3.7085	1.7672	0	1.7726	3.0298	3.7927	2.5994	15.1474	13.6188	12.0713	12.831	14.1866	13.6666	11.4575	10.1602
H19Z	15.166	15.5267	15.6589	13.7403	12.037	13.0902	14.4644	14.208	12.8326	2.5815	3.7972	3.1063	1.7709	1.7726	0	3.7491	4.3502	3.8042	14.0221	12.4756	10.7418	11.4191	13.1762	12.7501	10.3939	9.2074
H18X	18.3063	18.4659	18.7868	17.0504	15.3111	16.4203	17.4685	16.995	15.7545	3.7632	3.1208	2.5397	2.529	3.0298	3.7491	0	1.767	1.7659	17.0197	15.612	13.7983	14.2133	15.8067	15.5612	12.4528	11.4408
H18Y	17.7459	17.7951	18.2704	16.7224	14.9624	16.0416	16.9816	16.3422	15.2387	3.775	2.5703	3.0914	3.7642	3.7927	4.3502	1.767	0	1.7712	16.3468	15.0534	13.2635	13.5658	14.9264	14.7875	11.4008	10.4563
H18Z	17.8123	18.0324	18.4473	16.7992	15.0441	16.0022	17.316	16.7653	15.6109	4.352	3.7935	3.7685	3.1913	2.5994	3.8042	1.7659	1.7712	0	16.3769	14.9965	13.3004	13.9248	15.0731	14.7263	11.9109	10.7461
H23A	2.1557	2.8225	3.7137	4.3112	4.1554	3.0911	4.9151	4.4031	4.8471	13.9499	14.9538	15.7162	15.7663	15.1474	14.0221	17.0197	16.3468	16.3769	0	1.7623	3.8055	4.3413	2.4811	2.4891	6.2688	6.3556
H23B	3.0501	3.9878	4.3682	3.8654	3.1554	2.2788	5.0435	4.7916	4.5727	12.5577	13.6685	14.3117	14.2303	13.6188	12.4756	15.612	15.0534	14.9965	1.7623	0	2.6215	3.8078	3.0631	2.4695	5.9026	5.624
H21A	4.5635	4.7997	5.0546	3.8733	2.2892	3.1245	4.4026	4.0412	3.1015	10.4799	11.6046	12.2442	12.4381	12.0713	10.7418	13.7983	13.2635	13.3004	3.8055	2.6215	0	1.765	3.9992	4.1387	4.5116	4.4238
H21B	4.8533	4.4303	4.921	4.2883	3.0461	4.1164	3.721	2.8733	2.1499	10.7596	11.7387	12.5128	13.0353	12.831	11.4191	14.2133	13.5658	13.9248	4.3413	3.8078	1.765	0	4.1596	4.9667	3.9558	4.5613
H24A	4.4428	4.3011	5.6607	6.1681	5.4549	5.0216	6.1734	5.0206	5.5385	12.9009	13.6653	14.6481	14.8755	14.1866	13.1762	15.8067	14.9264	15.0731	2.4811	3.0631	3.9992	4.1596	0	1.7652	4.3428	4.5373
H24B	4.6246	5.1277	6.1408	6.237	5.4717	4.7241	6.9209	6.1297	6.3163	12.8237	13.6957	14.554	14.4905	13.6666	12.7501	15.5612	14.7875	14.7263	2.4891	2.4695	4.1387	4.9667	1.7652	0	5.2796	4.8631
H8A	7.7543	7.2071	8.3167	8.0586	6.6797	7.366	7.489	6.134	6.012	9.4921	9.9627	11.1749	11.9088	11.4575	10.3939	12.4528	11.4008	11.9109	6.2688	5.9026	4.5116	3.9558	4.3428	5.2796	0	1.7791
H8B	8.0442	7.8808	8.8464	8.2463	6.7112	7.2749	8.216	7.0993	6.7099	8.6732	9.2433	10.367	10.7954	10.1602	9.2074	11.4408	10.4563	10.7461	6.3556	5.624	4.4238	4.5613	4.5373	4.8631	1.7791	0
H9A	8.8829	8.6939	9.2882	8.1747	6.4839	7.5986	8.061	7.2322	6.3315	6.7079	7.4734	8.4514	9.1245	8.86	7.5971	9.9553	9.1648	9.6196	7.6632	6.6263	4.5033	4.4589	6.4053	6.7535	3.0506	2.6102
H9B	9.1095	8.5724	9.3502	8.6158	7.0804	8.2346	7.9686	6.8749	6.2677	7.6087	8.094	9.0293	10.0479	9.907	8.0391	9.8816	10.5889	7.9638	7.2698	5.141	4.4688	6.4706	7.2479	2.4378	3.0479
H5A	7.4962	7.9056	8.706	7.9481	6.5146	6.5297	6.8816	7.8862	7.4437	9.7045	10.5011	11.368	11.207	10.2729	9.5015	12.1515	13.1677	11.2296	5.5969	5.4878	4.4972	5.5074	4.2783	3.5402	4.247	7.2385
H5B	7.1523	7.9406	8.4443	7.3991	6.0518	5.8387	8.6345	8.1735	7.559	10.1769	11.1916	11.8202	11.3555	10.3903	9.6049	12.6022	12.0393	11.6966	5.4411	4.1165	4.4848	5.9273	4.9018	3.6506	5.7187	4.2943
H4A	7.3361	8.3965	8.6127	7.0144	5.3779	5.8418	8.1847	7.9241	6.8461	8.2155	9.4388	9.8935	9.5095	8.8103	7.7399	10.0884	10.075	10.3511	6.457	4.8424	3.8935	5.3071	6.0968	5.3269	5.5779	4.2169
H4B	7.7355	8.0267	8.5174	7.2365	5.5322	6.2073	7.8556	7.2579	6.3351	7.7787	8.787	9.5201	9.5454	8.9325	7.8238	10.7093	10.0891	10.1017	6.3119	4.9667	5.3271	4.4557	5.3854	5.0811	3.8938	2.5576
H10A	11.0697	10.9066	11.5089	10.3004	8.5751	9.6933	10.2344	9.4161	8.4868	4.8878	5.3903	6.5515	7.4096	7.174	6.053	7.9092	6.9991	7.5865	9.7544	8.6632	6.6527	6.6761	8.3297	8.5566	4.6281	3.9625
H10B	11.7043	11.2786	12.0329	11.0988	9.4561	10.6201	10.6364	9.6201	8.9002	5.677	5.7221	7.1462	8.4418	8.3505	7.3205	8.5185	7.3826	8.3023	10.4079	9.5553	7.5002	7.1236	8.7557	9.2912	4.5665	4.4873
H11A	12.8257	12.502	13.4334	12.6284	10.9676	11.8618	12.3589	11.2256	10.671	6.2678	5.9035	7.5058	8.525	8.0358	7.5	8.8143	6.703	7.494	11.2154	10.417	8.8132	8.6817	9.2699	9.6149	5.3808	4.8663
H11B	11.8478	11.7463	12.5923	11.6381	9.9427	10.7183	11.6943	10.6865	10.028	6.0523	6.1092	7.4672	8.0139	7.2911	6.7327	8.0515	6.8254	7.2226	10.1751	9.2207	7.7854	7.9824	8.3766	8.4431	4.9727	3.9152
H3A	10.4127	10.8794	11.1741	9.5215	7.7982	8.5347	10.4126	10.0268	8.8658	5.7221	6.886	7.3165	6.8584	6.0859	5.1027	8.2144	7.8568	7.5496	9.0652	7.5491	6.1975	7.194	8.2486	7.671	6.3512	4.8483
H3B	9.9346	10.1383	10.6581	9.3023	7.5558	8.3667	9.7979	9.1456	8.1655	5.8795	6.7519	7.5684	7.6355	6.9735	5.9766	8.586	7.8988	7.9349	8.4725	7.1671	5.622	6.2804	7.2771	7.0216	4.7455	3.311
H2A	11.2744	11.5546	12.2722	11.1453	9.4743	9.9464	11.7478	10.9501	10.2064	6.8384	7.312	8.2552	8.0173	6.8862	6.5135	8.5349	7.6424	7.4182	9.5024	8.3477	7.4353	8.187	8.0024	7.5196	5.8594	4.2094
H2B	11.9126	12.3953	12.9037	11.4903	9.8139	10.2863	12.3871	11.8138	10.8719	6.3924	7.1056	7.6977	6.9771	5.6933	5.4339	7.8284	7.2628	6.6835	10.2675	8.9078	8.0211	9.0059	9.1084	8.3902	7.2803	5.5911
H13A	15.4076	15.3214	15.9044	14.5445	12.7903	13.8871	14.6027	13.8333	12.8469	3.1297	2.1442	3.738	4.9307	4.8051	4.5349	4.1179	2.75	3.8467	13.9925	12.8192	10.9595	11.1007	12.4567	12.4945	8.7374	7.9339
H13B	16.1719	16.192	16.8279	15.4861	13.7229	14.6631	15.7129	14.9201	13.98	4.2793	3.3651	4.5669	5.0707	4.4475	4.8064	3.9107	2.3792	2.9496	14.6139	13.4303	11.824	12.1313	13.0158	12.8894	9.566	8.552
H15A	14.6327	15.0431	15.4029	13.7264	11.9964	12.7711	14.5282	14.0663	12.9064	4.2799	4.8651	5.025	3.8959	2.44	2.752	4.687	4.5222	3.5991	13.1786	11.7233	10.3873	11.196	12.0779	11.5108	9.5464	8.1047
H15B	16.173	16.5015	16.9506	15.3547	13.6105	14.4011	16.035	15.4748	14.3762	4.6593	4.6338	4.8839	3.9017	2.4363	3.5115	3.7332	3.3897	2.2098	14.6451	13.2616	11.9097	12.6036	13.3678	12.8747	10.5861	9.2241
H16A	14.4002	14.7813	15.3683	13.9868	12.2813	12.8298	14.741	14.0736	13.1544	6.0918	6.2773	6.9127	6.1155	4.5903	5.0755	6.2727	5.5681	4.7825	12.6975	11.4138	10.0479	11.2379	11.3214	10.7145	9.0031	7.4593
H16B	14.4744	15.6882	16.3652	15.0715	13.3368	14.003	15.5867	14.8023	13.9344	5.822	5.5079	6.3931	6.0297	4.7104	5.3525	5.4888	4.4193	3.9444	13.7553	12.5621	11.3884	11.978	12.1808	11.7797	9.3762	8.0321
H22Q	3.1866	2.4557	3.6798	4.3069	3.836	3.8382	3.6754	2.4471	3.1625	12.942	13.8373	14.7083	15.1251	14.7149	13.4552	16.2269	15.4703	15.7571	2.4884	3.0601	3.0666	2.5043	2.5798	3.7607	4.7656	5.4585
H7Q	5.4839	4.955	6.1106	6.119	4.9853	5.3984	5.6127	4.2628	4.3955	11.0408	11.7586	12.7876	13.3108	12.8423	11.6841	14.1668	13.2716	13.6299	4.0824	3.9704	3.0518	2.4855	2.4925	3.6994	2.2921	3.0832
H6Q	6.2554	6.3188	7.3891	7.121	5.8674	5.8574	7.3852	6.3216	6.2406	10.7356	11.4553	12.4532	12.6096	11.8423	10.9262	13.4623	12.5692	12.6623	4.308	3.7671	4.2875	2.454	2.4898	3.0625	2.3986
H1Q	13.2398	13.3684	14.1526	13.0546	11.3477	11.9598	13.3462	12.5519	11.8215	6.1628	6.1358	7.2878	7.276	6.143	6.1154	7.177	6.0113	5.942	11.4674	10.3896	9.2684	9.7836	9.7745	9.4841	6.9885	5.6257
H12Q	14.637	14.5511	15.3614	14.2878	12.5573	13.3949	14.3668	13.3974	12.6611	5.4053	4.7697	6.2502	6.8826	6.1371	6.1298	6.1344	4.6158	5.1626	12.9648	11.9544	10.4799	10.6809	11.1583	11.1549	7.6796	6.728
H14Q	14.0674	14.2394	14.6318	13.0201	11.2583	12.2831	13.4646	12.9229	11.7579	2.4047	3.0185	3.6512	3.7399	3.2663	2.5481	4.3077	3.7996	3.8539	12.7229	11.3472	9.5972	10.0848	11.5161	11.2728	8.3649	7.2287

(cont.) Table H.5: Hydrogen Distances for the Optimized Structure of 4z,4'e *cis-syn-cis* DtBuCH18C6

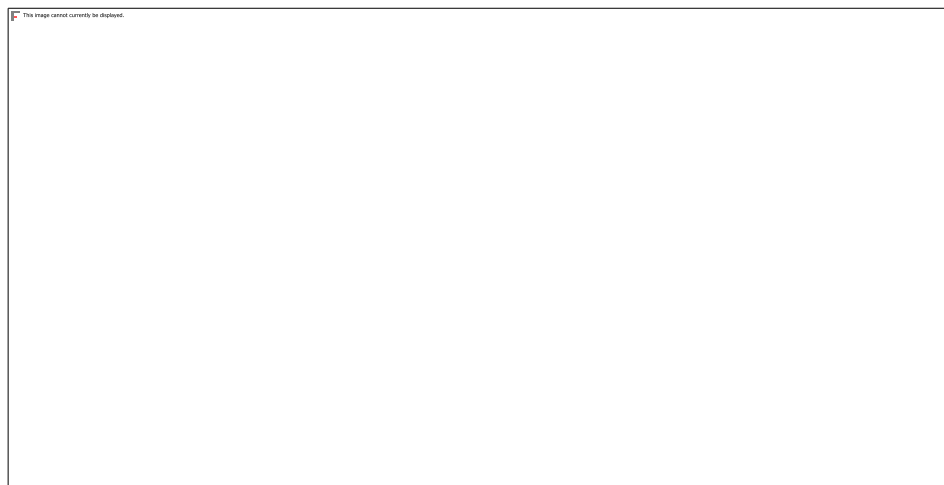| H9A	H9B	H5A	H5B	H4A	H4B	H10A	H10B	H11A	H11B	H3A	H3B	H2A	H2B	H13A	H13B	H15A	H15B	H16A	H16B	H22Q	H7Q	H6Q	H1Q	H12Q	H14Q	
8.8829	9.1095	7.4962	7.1523	7.7361	7.7355	11.0697	11.7043	12.8257	11.8478	10.4127	9.9346	11.2744	11.9126	15.4076	16.1719	14.6327	16.173	14.4002	15.4744	3.1866	5.4839	6.2554	13.2398	14.637	14.0674	H26X
8.6939	8.5724	7.9056	7.9406	8.3965	8.0267	10.9066	11.2786	12.502	11.7463	10.8794	10.1383	11.5546	12.3953	15.3214	16.192	15.0431	16.5015	14.7813	15.6882	2.4557	4.955	6.3188	13.3684	14.5511	14.2394	H26Y
9.2882	9.3502	8.706	8.4443	8.6127	8.5174	11.5089	12.0329	13.4334	12.5923	11.1741	10.6581	12.2722	12.9037	15.9044	16.8279	15.4029	16.9506	15.3683	16.3652	3.6798	6.1106	7.3891	14.1526	15.3614	14.6318	H26Z
8.1747	8.6158	7.9481	7.3991	7.0144	7.2365	10.3004	11.0988	12.6284	11.6381	9.5215	9.3023	11.1453	11.4903	14.5445	15.4861	13.7264	15.3547	13.9868	15.0715	4.3069	6.119	7.121	13.0546	14.2878	13.0201	H28X
6.4839	7.0804	6.5146	6.0518	5.3779	5.5322	8.5751	9.4561	10.9676	9.9427	7.7982	7.5558	9.4743	9.8139	12.7903	13.7229	11.9964	13.6105	12.2813	13.3368	3.836	4.9853	5.8606	11.3477	12.5573	11.2583	H28Y
7.5986	8.2346	6.5297	5.8387	5.8418	6.2073	9.6933	10.6201	11.8618	10.7183	8.5347	8.3667	9.9464	10.2863	13.8871	14.6631	12.7711	14.4011	12.8298	14.003	3.8382	5.3984	5.8574	11.9598	13.3949	12.2831	H28Z
8.061	7.9686	8.6816	8.6345	8.1847	7.8556	10.2344	10.6364	12.3589	11.6943	10.4126	9.7979	11.7478	12.3871	14.6027	15.7129	14.5282	16.035	14.741	15.5867	3.6754	5.6127	7.3852	13.4462	14.3668	13.4646	H27X
7.2322	6.8749	7.8862	8.1735	7.9241	7.2579	9.4161	9.6201	11.2256	10.6865	10.0268	9.1456	10.9501	11.8138	13.8333	14.9201	14.0663	15.4748	14.0736	14.8023	2.4471	4.2628	6.3216	12.5519	13.3974	12.9229	H27Y
6.3315	6.2677	7.4437	7.559	6.8461	6.3351	8.4868	8.9002	10.671	10.028	8.8658	8.1655	10.2064	10.8719	12.8469	13.98	12.9064	14.3762	13.1544	13.9344	3.1625	4.3955	6.2406	11.8215	12.6611	11.7579	H27Z
6.7079	7.6087	9.7045	10.1769	8.2155	7.7787	4.8878	5.677	6.2678	6.0523	5.7221	5.8795	6.8384	6.3924	3.1297	4.2793	4.2799	4.6593	6.0918	5.822	12.942	11.0408	10.7356	6.1628	5.4053	2.4047	H20X
7.4734	8.094	10.5011	11.1916	9.4388	8.787	5.3903	5.7221	5.9035	6.1092	6.886	6.7519	7.312	7.1056	2.1442	3.3651	4.8651	6.4338	6.2773	5.5079	13.8373	11.7586	11.4553	6.1358	4.7697	3.0185	H20Y
8.4514	9.2638	11.368	11.8202	9.8935	9.5201	6.5515	7.1462	7.5058	7.4672	7.3165	7.5684	8.2552	7.6977	3.738	4.5669	5.025	4.8839	6.9127	6.3931	14.7083	12.7876	12.4532	7.2878	6.2502	3.6512	H20Z
9.1245	10.2923	11.207	11.3555	9.5095	9.5454	7.4096	8.4418	8.525	8.0139	6.8584	7.6355	8.0173	6.9771	4.9307	5.0707	3.8959	3.9017	6.1155	6.0297	15.1251	13.3108	12.6096	7.276	6.8826	3.7399	H19X
8.86	10.1479	10.2729	10.3903	8.8103	8.9325	7.174	8.3505	8.0358	7.2911	6.0859	6.9735	6.8862	5.6933	4.8051	4.4475	2.44	2.4363	4.5903	4.7104	14.7149	12.8423	11.8423	6.143	6.1371	3.2663	H19Y
7.5971	8.907	9.5015	9.6049	7.7399	7.8238	6.053	7.3205	7.5	6.7327	5.1027	5.9766	6.5135	5.4339	5.4349	4.8064	2.752	3.5115	5.0755	3.5525	13.4552	11.6841	10.9262	6.1154	6.1298	2.5481	H19Z
9.9553	10.8391	12.1515	12.6022	10.9884	10.7093	7.9092	8.5185	8.1413	8.0515	8.2144	8.586	8.5349	7.8284	4.1179	3.9107	4.687	3.7332	6.2727	5.4888	16.2269	14.1668	13.4623	7.177	6.1344	4.3077	H18X
9.1648	9.8816	11.3677	12.0393	10.6075	10.0891	6.991	7.3826	6.703	6.8254	7.8568	7.8988	7.6424	7.2628	2.75	2.3792	4.5222	3.3897	5.5681	4.4193	15.4703	13.271	12.5692	6.0113	4.6158	3.7996	H18Y
9.6196	10.5889	11.2296	11.6966	10.3511	10.1017	7.5865	8.3023	7.494	7.2226	7.5496	7.9349	7.4182	6.6835	3.8467	2.9496	5.3991	2.2098	4.7825	3.9444	15.7571	13.6299	12.6623	5.942	5.1626	3.8539	H18Z
7.6632	7.9638	5.5969	5.4411	6.457	6.3119	9.7544	10.4079	11.2154	10.1751	9.0652	8.4725	9.5024	10.2675	13.9925	14.6139	13.1786	14.6451	12.6975	13.7553	2.4884	4.0824	4.3026	11.4674	12.9648	12.7229	H23A
6.6263	7.2698	4.5878	4.1165	4.8424	4.9667	8.6632	9.5553	10.417	9.2207	7.5491	7.1671	8.3477	8.9078	12.8192	13.4303	11.7233	13.2616	11.4138	12.5621	3.0601	3.9704	3.8025	10.3896	11.9544	11.3472	H23B
4.5033	5.141	4.4972	4.4848	3.8935	3.5271	6.6527	7.5002	8.8132	7.7854	6.1975	5.622	7.4353	8.0211	10.9595	11.824	10.3873	11.9097	10.4279	11.3884	3.0666	3.0518	3.7671	9.2684	10.4799	9.5972	H21B
4.4589	4.4688	5.5074	5.9273	5.3071	4.4557	6.6761	7.1236	8.6817	7.9824	7.194	6.2804	8.187	9.0059	11.1007	12.1313	11.196	12.6036	11.2379	11.978	2.5043	2.4855	4.2875	9.7836	10.6809	10.0848	H24A
6.4053	6.4706	4.2783	4.9018	6.0968	5.3854	8.3297	8.7557	9.2699	8.3766	8.2486	7.2771	8.0024	9.1084	12.4567	13.0158	12.0779	13.3678	11.3214	12.1808	2.5798	2.4925	2.454	9.7745	11.1583	11.5161	H8A
6.7535	7.2479	3.5402	3.6506	5.0811	5.566	9.2912	9.6149	8.4431	7.671	7.0216	7.5196	8.3902		12.4945	12.8894	11.5108	12.8747	10.7145	11.7797	3.7607	3.6694	2.4898	9.4841	11.1549	11.2728	H8B
0	1.7748	4.5537	5.5466	4.1563	2.5693	2.2263	3.0725	4.5992	3.8722	4.0615	2.5917	4.7249	5.6309	6.6534	7.6953	7.2454	8.4409	7.3624	7.8066	6.373	4.3446	4.586	5.7812	6.3506	5.8415	H9A
1.7748	0	5.5917	6.8281	5.7671	4.0837	3.0251	2.757	4.5685	4.471	5.7892	4.1973	5.9495	7.1142	7.2106	8.3826	8.6085	9.6032	8.5904	8.765	6.2326	4.1144	5.035	6.6833	6.8437	6.9751	H9B
4.5537	5.5917	0	1.7714	3.0635	2.55	5.7403	6.7873	6.7413	5.2764	4.5123	3.8341	3.9954	4.8999	9.2114	9.4572	8.0382	9.3484	7.1889	8.2651	5.847	4.2473	2.043	6.0336	7.8457	7.9171	H5A
5.5466	6.8281	1.7714	0	2.466	3.0572	6.7752	8.0669	8.1726	6.5772	4.5515	4.5359	4.8446	5.1559	10.1122	10.3081	8.2609	9.737	7.6423	8.9771	6.2372	5.2478	3.2689	7.0136	8.9752	8.4401	H5B
4.1563	5.7671	3.0635	2.466	0	1.7742	5.3095	6.8392	7.4712	5.9179	2.8036	3.1292	4.5547	4.515	8.7278	9.1996	8.6866	8.6153	7.0541	8.2326	6.6715	5.4525	5.5623	5.8224	8.2059	6.8336	H4A
2.5693	4.0837	2.55	3.0572	1.7742	0	3.9906	5.3115	6.042	6.4554	2.9792	2.2111	3.9754	5.4648	7.8861	8.51	7.0235	8.4855	6.9081	7.8803	5.8702	4.216	3.3465	3.3496	7.2203	6.4147	H4B
2.2263	3.0251	5.7403	6.7752	5.3095	3.9906	0	1.7802	3.0546	2.544	3.8752	2.4913	4.1023	4.9035	4.4337	5.5542	5.6964	6.6229	5.9428	6.0382	8.5553	6.38	6.2382	5.1399	4.3912	3.9613	H10A
3.0725	2.757	6.7873	8.0669	6.8392	5.3115	1.7802	0	2.4748	3.0471	5.6327	4.1218	5.3206	6.3957	4.6557	5.9266	7.0205	7.633	7.08	6.8002	8.8977	6.6238	6.8699	3.4623	4.5401	5.0994	H10B
4.5992	4.5685	6.7413	8.1726	7.4712	6.042	3.0546	2.4748	0	1.777	5.9375	4.4906	4.3616	5.6722	4.0827	4.6955	6.394	6.6382	5.7434	5.1698	9.3183	7.5818	7.1422	2.2971	4.2826	4.1044	H11A
3.8722	4.471	5.2764	6.5772	5.9179	6.4554	2.544	3.0471	1.777	0	4.3564	2.973	2.617	3.9889	4.3629	4.7342	5.3176	5.9144	4.5472	4.4939	8.8163	6.9177	6.0548	4.5181	2.8148	4.2826	H11B
4.0615	5.7892	4.5123	4.5515	2.8036	2.9792	3.8752	5.6327	5.9375	4.3564	0	1.7776	3.0653	2.4834	6.2033	6.5737	4.2453	5.8726	4.6715	5.8407	8.8163	7.1512	6.0337	3.9353	5.9742	4.1044	H3A
2.5917	4.1973	3.8341	4.5359	3.1292	2.2111	2.4913	4.1218	4.4906	2.973	1.7776	0	2.5296	3.0612	5.7464	6.312	5.0326	6.3833	5.0189	5.8193	7.8827	5.9023	4.9812	2.1751	5.1857	4.2789	H3B
4.7249	5.9495	3.9954	4.8446	4.5547	3.9754	4.1023	5.3206	4.3616	2.617	3.0653	2.5296	0	1.7786	5.5827	6.6416	5.4112	5.5191	3.3413	4.2724	9.2851	7.1667	5.5514	2.9324	4.2675	4.6141	H2A
5.6309	7.1142	4.8999	5.1559	4.515	5.4648	4.9035	6.3957	5.6722	3.9889	2.4834	3.0612	1.7786	0	5.9178	5.6175	3.3181	4.621	2.5779	4.0472	10.253	8.3553	6.7136	4.2812	4.9458	4.1313	H2B
6.6534	7.2106	9.2114	10.1122	8.7278	7.8861	4.4337	4.6557	4.0827	4.3629	6.2033	5.7464	5.5827	5.9178	0	1.7581	4.2991	3.9612	4.9161	3.9023	12.9534	10.6917	10.1671	2.6396	2.6396	2.5531	H13A
7.6953	8.3826	9.4572	10.3081	9.1996	8.51	4.6557	5.9266	4.6955	4.7342	6.5737	6.312	6.6416	5.6175	1.7581	0	3.7738	2.8582	3.916	3.9023	13.8086	11.5015	10.63	3.7796	2.3037	3.0438	H13B
7.2454	8.6085	8.0382	8.2609	8.6866	7.0235	5.6964	7.0205	6.394	5.3176	4.2453	5.0326	5.4112	3.3181	4.2991	3.7738	0	1.7548	2.3608	3.0366	12.8693	10.9158	9.6804	3.9509	4.6263	2.3282	H15A
8.4409	9.6032	9.3484	9.737	8.6153	8.4855	6.6229	7.633	6.6382	5.9144	5.8726	6.3833	5.5191	4.621	3.9612	2.8582	1.7548	0	2.6508	2.3598	14.2534	11.1627	10.931	4.2781	4.3367	3.0321	H15B
7.3624	8.5904	7.1889	7.6423	7.0541	6.9081	5.9428	7.08	5.7434	4.5472	4.6715	5.0189	3.3413	2.5779	4.9161	3.916	2.3608	2.6508	0	1.7529	12.5439	10.4486	8.8772	2.4586	3.87	3.7611	H16A
7.8066	8.765	8.2651	8.9771	8.2326	7.8803	6.0382	6.8002	5.1698	4.4939	5.8407	5.8193	4.2724	4.0472	3.9023	3.9023	3.0366	2.3598	1.7529	0	13.3544	10.931	9.7331	2.475	2.7493	3.7226	H16B
6.373	6.2326	5.847	6.2372	6.6715	5.8702	8.5553	8.8977	9.3183	8.8163	8.8163	7.8827	9.2851	10.253	12.9534	13.8086	12.8693	14.2534	12.5439	13.3544	0	2.5068	4.1365	11.0077	12.1214	11.9881	H22Q
4.3446	4.1144	4.2473	5.2478	5.4525	4.216	6.38	6.6238	7.5818	6.9177	7.1512	5.9023	7.1667	8.3553	10.6917	11.5015	10.9158	11.1627	10.4486	10.931	2.5068	0	2.4538	8.7073	9.7119	9.9438	H7Q
4.586	5.035	2.043	3.2689	5.5623	3.3465	6.2382	6.8699	7.1422	6.0548	6.0337	4.9812	5.5514	6.7136	10.1671	10.63	9.6804	10.931	8.8772	9.7331	4.1365	2.4538	0	7.3426	8.8161	9.1853	H6Q
5.7812	6.6833	6.0336	7.0136	5.8224	3.3496	5.1399	3.4623	2.2971	4.5181	3.9353	2.1751	2.9324	4.2812	2.6396	3.7796	3.9509	4.2781	2.4586	2.475	11.0077	8.7073	7.3426	0	2.3071	3.9011	H1Q
6.3506	6.8437	7.8457	8.9752	8.2059	7.2203	4.3912	4.5401	4.2826	2.8148	5.9742	5.1857	4.2675	4.9458	2.6396	2.3037	4.6263	4.3367	3.87	2.7493	12.1214	9.7119	8.8161	2.3071	0	3.7286	H12Q
5.8415	6.9751	7.9171	8.4401	6.8336	6.4147	3.9613	5.0994	4.1044	4.2826	4.1044	4.2789	4.6141	4.1313	2.5531	3.0438	2.3282	3.0321	3.7611	3.7226	11.9881	9.9438	9.1853	3.9011	3.7286	0	H14Q

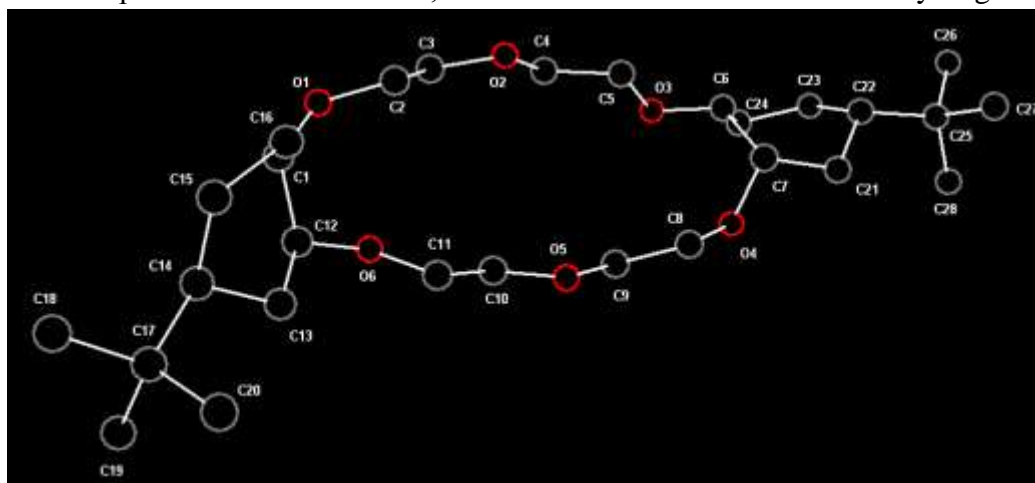Figure H.11: Optimized Structure of 4z,4'z *cis-syn-cis* DtBuCH18C6 with Hydrogen Labels

Figure H.12: Optimized Structure of 4z,4'z *cis-syn-cis* DtBuCH18C6 with Carbon and Hydrogen Labels

Table H.6: Hydrogen Distances for the Optimized Structure of 4z,4'z *cis-syn-cis* DtBuCH18C6

	H26X	H26Y	H26Z	H28X	H28Y	H28Z	H27X	H27Y	H27Z	H20X	H20Y	H20Z	H19X	H19Y	H19Z	H18X	H18Y	H18Z	H23A	H23B	H21A	H21B	H24A	H24B	H8A	H8B
H26X	0	1.7727	1.764	3.0401	3.7789	2.5647	3.6746	3.818	4.3513	16.2041	17.3978	17.7217	16.5669	15.4815	14.9251	18.3594	18.099	17.4444	2.1548	3.0855	4.5705	4.8518	4.4228	4.621	7.8369	7.9159
H26Y	1.7727	0	1.7705	3.7602	4.3525	3.7815	3.0717	2.6283	3.8184	16.4188	17.5265	18.009	17.0721	15.9968	15.375	18.7296	18.3273	17.824	2.853	4.0176	4.7995	4.4217	4.2844	5.1237	7.3974	7.8729
H26Z	1.764	1.7705	0	2.5454	3.7753	3.167	2.3884	3.0642	3.6752	16.8948	18.132	18.4775	17.4762	16.5078	15.7953	19.3039	19.0445	18.4975	3.7196	4.391	5.0573	4.9193	5.6434	6.1378	8.4962	8.7606
H28X	3.0401	3.7602	2.5454	0	1.7669	1.7665	2.5389	3.7574	3.0408	15.3354	16.7195	16.8859	15.8392	15.0345	14.1933	17.8457	17.7716	17.1962	4.2945	3.8685	3.8804	4.2956	6.1581	6.2424	8.1733	8.0401
H28Y	3.7789	4.3525	3.7753	1.7669	0	1.7715	3.1597	3.7795	2.5624	13.5743	14.9558	15.135	14.1408	13.3597	12.4766	16.1242	16.0423	15.5058	4.1281	3.1312	2.2952	3.0604	5.4456	5.473	6.7538	6.469
H28Z	2.5647	3.7815	3.167	1.7665	1.7715	0	3.7713	4.3534	3.779	14.4799	15.825	15.9681	14.7562	13.8281	13.1409	16.738	16.6659	15.9789	3.0605	2.2856	3.1444	4.1318	5.0165	4.7343	7.3854	7.0171
H27X	3.6746	3.0717	2.3884	2.5389	3.1597	3.7713	0	1.7708	1.7643	15.8461	17.1065	17.5037	16.7726	15.9761	15.0481	18.5835	17.4876	17.9442	4.9189	5.0437	4.3966	3.718	6.1598	6.9174	7.758	8.1725
H27Y	3.818	2.6283	3.0642	3.7574	3.7795	4.3534	1.7708	0	1.7723	15.232	16.3598	16.9122	16.2851	15.3993	14.5348	17.9175	17.4876	17.198	4.4231	4.7926	4.0266	2.8559	5.0092	6.1245	6.4477	7.1492
H27Z	4.3513	3.8184	3.6752	3.0408	2.5624	3.779	1.7643	1.7723	0	14.1457	15.3915	15.8216	15.1886	14.4331	13.4493	16.9537	16.6554	16.3598	4.848	4.557	3.0882	2.15	5.532	6.3146	6.2838	6.6705
H20X	16.2041	16.4188	16.8948	15.3354	13.5743	14.4799	15.8461	15.232	14.1457	0	1.7729	1.7639	3.0436	3.7805	2.5658	3.6725	3.8177	4.3514	14.6903	13.3235	11.8375	12.3945	13.3753	13.0188	9.9498	8.8845
H20Y	17.3978	17.5265	18.132	16.7195	14.9558	15.825	17.1065	16.3598	15.3915	1.7729	0	1.7703	3.7588	4.3531	3.7818	3.0589	2.626	3.8163	15.7815	14.5201	13.0936	13.5493	14.2647	13.9778	10.7028	9.7877
H20Z	17.7217	18.009	18.4775	16.8859	15.135	15.9681	17.5037	16.9122	15.8216	1.7639	1.7703	0	2.5408	3.772	3.1612	2.3847	3.0718	3.6726	16.1628	14.7794	13.4264	14.0647	14.8587	14.398	11.5591	10.4378
H19X	16.5669	17.0721	17.4762	15.8392	14.1408	14.7562	16.7726	16.2851	15.1886	3.0436	3.7588	2.5408	0	1.7667	1.767	2.5466	3.7607	3.0376	14.9714	13.5306	12.5236	13.4402	13.8648	13.1365	11.1515	9.7497
H19Y	15.4815	15.9968	16.5078	15.0345	13.3597	13.8281	15.9761	15.3993	14.4331	3.7805	4.3531	3.772	1.7667	0	1.771	3.1696	3.7805	2.5643	13.7686	12.4143	11.631	12.5873	12.5715	11.7913	10.0803	8.6384
H19Z	14.9251	15.375	15.7953	14.1933	12.4766	13.1409	15.0481	14.5348	13.4493	2.5658	3.7818	3.1612	1.767	1.771	0	3.776	4.3527	3.7789	13.3493	11.9145	10.8106	11.6864	12.2279	11.5746	9.4459	8.0416
H18X	18.3594	18.7296	19.3039	17.8457	16.1242	16.738	18.5835	17.9175	16.9537	3.6725	3.0589	2.3847	2.5466	3.1696	3.776	0	1.7705	1.7637	16.6358	15.3297	14.3255	15.08	15.245	14.6387	12.2626	11.0654
H18Y	18.099	18.3273	19.0445	17.7716	16.0423	16.6659	17.4876	17.4876	16.6554	3.8177	2.626	3.0718	3.7607	3.7805	4.3527	1.7705	0	1.7727	16.3013	15.1229	14.0925	14.692	14.6947	14.2379	11.5228	10.5088
H18Z	17.4444	17.824	18.4975	17.1962	15.5058	15.9789	17.9442	17.198	16.3598	4.3514	3.8163	3.6726	3.0376	2.5643	3.7789	1.7637	1.7727	0	15.6174	14.4055	13.6191	14.4049	14.1425	13.4936	11.3835	10.174
H23A	2.1548	2.853	3.7196	4.2945	4.1281	3.0605	4.9189	4.4231	4.848	14.6903	15.7815	16.1628	14.9714	13.7686	13.3493	16.6358	16.3013	15.6174	0	1.7624	3.7943	4.3409	2.4862	2.4772	6.263	6.2194
H23B	3.0855	4.0176	4.391	3.8685	3.1312	2.2856	5.0437	4.7926	4.557	13.3235	14.5201	14.7794	13.5306	12.4143	11.9145	15.3297	15.1229	14.4055	1.7624	0	2.5967	3.7899	3.0662	2.4846	5.7881	5.331
H21A	4.5705	4.7995	5.0573	3.8804	2.2952	3.1444	4.3966	4.0266	3.0882	11.8375	13.0936	13.4264	12.5236	11.631	10.8106	14.3255	14.0925	13.6191	3.7943	2.5967	0	1.7635	3.9992	4.1501	4.515	4.1887
H21B	4.8518	4.4217	4.9193	4.2956	3.0604	4.1318	3.718	2.8559	2.15	12.3945	13.5493	14.0647	13.4402	12.5873	11.6864	15.08	14.692	14.4049	4.3409	3.7899	1.7635	0	4.1522	4.9665	4.1726	4.5423
H24A	4.4228	4.2844	5.6434	6.1581	5.4456	5.0165	6.1598	5.0092	5.532	13.3753	14.2647	14.8587	13.8648	12.5715	12.2279	15.245	14.6947	14.1425	2.4862	3.0662	3.9992	4.1522	0	1.7565	4.3042	4.5689
H24B	4.621	5.1237	6.1378	6.2424	5.473	4.7343	6.9174	6.1245	6.3146	13.0188	13.9778	14.398	13.1365	11.7913	11.5746	14.6387	14.2379	13.4936	2.4772	2.4846	4.1501	4.9665	1.7565	0	5.0716	4.6931
H8A	7.8369	7.3974	8.4962	8.1733	6.7538	7.3854	7.758	6.4477	6.2838	9.9498	10.7028	11.5591	11.1515	10.0803	9.4459	12.2626	11.5228	11.3835	6.263	5.7881	4.515	4.1726	4.3042	5.0716	0	1.7848
H8B	7.9159	7.8729	8.7606	8.0401	6.469	7.0171	8.1725	7.1492	6.6705	8.8845	9.7877	10.4378	9.7497	8.6384	8.0416	11.0654	10.5088	10.174	6.2194	5.331	4.1887	4.5423	4.5689	4.6931	1.7848	0
H9A	8.9926	8.848	9.4338	8.2844	6.5788	7.675	8.2414	7.4287	6.517	7.8541	8.9418	9.5624	9.2785	8.5861	7.5171	10.7095	10.2654	10.202	7.7338	6.6276	4.5817	4.6453	6.4991	6.7723	3.0671	2.5283
H9B	9.0541	8.5627	9.3445	8.584	7.0272	8.0132	6.9247	6.3111	8.9363	8.9057	9.8057	10.0644	10.6438	9.9276	9.8114	11.1542	11.275	11.275	7.8656	7.1034	5.0286	4.4593	6.3674	7.0806	2.4718	3.0672
H5A	6.633	7.239	8.0565	7.5403	6.3574	5.953	8.462	7.7378	7.4971	10.9817	11.9332	12.2589	10.8708	9.48	9.3704	12.378	12.0552	11.2155	4.6144	3.7941	4.6536	5.7923	6.3307	2.3689	4.7582	6.6442
H5B	6.1864	7.1374	7.5703	6.6284	5.4683	4.9695	8.0177	7.6633	7.1437	11.2079	12.3632	12.4659	10.9156	9.6694	9.4359	12.7115	12.6228	11.6905	4.5	3.1955	4.2212	5.749	4.4523	2.9919	5.7916	4.5074
H4A	8.4988	9.303	9.8171	8.7231	7.3447	7.1664	9.9902	9.5113	8.8625	9.2899	10.3658	10.4038	8.7318	7.3902	7.3437	10.455	10.41	9.3838	6.721	5.4485	5.7806	7.1808	6.0674	4.7936	6.004	4.3514
H4B	8.002	8.6913	9.0757	7.7161	6.1593	6.3631	8.8807	8.4746	7.5979	8.7251	9.9703	10.0322	8.6139	7.518	7.0461	10.49	10.4643	9.6479	6.4354	4.9362	4.5365	5.9337	5.8775	4.9215	5.198	4.3885
H10A	11.3413	11.11	11.7543	10.6102	8.9021	10.043	10.4412	9.5639	8.69	6.1685	7.0521	7.913	8.1809	7.7158	6.5231	9.2475	8.6506	8.9368	10.0173	8.9514	6.956	6.8884	8.5434	8.8358	4.535	4.1962
H10B	11.5937	11.1091	11.949	11.1437	9.5324	10.6486	10.6038	9.4927	8.8926	7.3277	7.8757	9.0122	9.4989	8.9408	7.9136	10.2247	9.3594	9.8159	10.2523	9.4554	7.5053	7.0702	8.5075	9.1015	4.2232	4.5583
H11A	13.3953	13.0884	13.9247	12.975	11.287	12.2974	12.7196	11.666	10.9947	5.4057	5.6461	6.9637	7.7299	7.2679	6.3501	8.0815	7.095	7.7476	11.871	10.0468	8.5449	8.4539	10.0589	10.359	5.8921	5.7257
H11B	12.4378	12.1249	13.1152	12.3963	10.7577	11.5697	12.1491	10.9667	10.4955	6.4119	6.6068	7.8857	8.2205	7.3815	6.781	8.5812	7.4945	7.8816	10.761	9.9842	8.5449	8.4539	7.8665	9.083	4.7469	6.6555
H3A	10.4906	11.031	11.7123	10.6482	9.109	9.224	11.5883	10.8935	10.2387	7.326	8.1852	8.3674	6.8473	5.358	5.481	8.2655	8.0585	7.1033	8.6133	7.4458	7.2286	8.3123	7.3928	6.4852	5.9734	4.3395
H3B	10.1282	10.5741	11.1362	9.8536	8.193	8.6235	10.6865	10.0582	9.2062	6.5257	7.6293	7.824	6.5871	5.4252	4.9622	8.2333	8.0785	7.3799	8.434	7.1013	6.3036	7.3111	7.3049	6.2244	5.2495	5.3388
H2A	10.4914	10.5494	11.4222	10.543	8.8976	9.4342	10.8259	9.2671	8.0396	6.6694	7.3571	8.0941	7.4854	6.2919	5.8754	8.5085	7.8452	7.5514	6.6835	7.7051	6.698	7.1675	6.9484	6.7791	3.8607	2.7124
H2B	10.653	10.8041	11.7987	11.1364	9.6051	9.8327	11.5433	10.5025	10.1289	7.6291	8.1146	8.815	7.9174	6.4382	6.5058	8.7516	8.0279	7.4936	8.6611	7.8522	7.4211	8.0162	6.8177	6.4414	4.6031	3.5221
H13A	13.5109	13.769	14.3634	12.998	11.2582	11.9614	13.5733	12.8641	11.9323	3.0981	4.0374	4.4025	3.8784	3.137	2.2922	5.0589	4.8025	4.5716	11.8541	10.5643	9.3564	10.029	10.4677	10.0339	7.3575	6.1085
H13B	14.5698	14.666	15.2809	13.9276	12.166	13.0468	14.2659	13.501	12.5569	2.1517	2.868	3.7212	4.2914	4.1244	3.0517	4.921	4.4283	4.8557	12.9841	10.5259	10.6886	11.4923	11.2725	7.92	6.9702	
H15A	14.4407	14.8122	15.5352	14.3592	12.6985	13.0893	15.0897	14.3039	13.5542	4.5703	4.7948	5.044	3.8663	2.2802	3.1455	4.3766	3.9989	3.0634	12.5782	11.4179	10.7441	11.5585	11.088	10.4366	8.5413	7.2457
H15B	15.9596	16.2408	17.0556	15.9756	14.3104	14.7174	16.5809	15.6976	15.021	4.8472	4.4097	4.9142	4.3052	3.0795	4.1433	3.7156	2.8325	2.1565	14.0461	12.9787	12.2859	12.9787	12.3928	11.8397	9.6638	8.5643
H16A	14.1723	14.3541	15.3297	14.5381	12.9445	13.2291	14.9984	13.9703	13.5098	6.3168	6.1223	6.9198	6.2351	4.7219	5.4639	6.1314	5.1314	4.2266	12.168	11.304	10.8029	11.3978	10.3265	9.8769	7.8083	6.8602
H16B	15.0614	15.0929	16.0795	15.2573	13.6071	14.0873	15.5122	14.431	13.9336	5.5448	5.0237	6.1723	6.1656	5.0187	5.4527	6.6538	4.2943	4.4334	13.1246	12.2536	11.4233	11.8228	11.1864	10.9512	8.0936	7.3673
H22Q	3.1735	2.4486	3.6761	4.3079	3.8382	3.8381	3.6815	2.4578	3.1771	14.1314	15.1736	15.7372	14.9186	13.8413	13.2001	16.4672	15.9924	15.5714	2.4979	3.0576	3.0659	2.5069	2.5581	3.7428	4.9532	5.4923
H7Q	5.5009	4.9685	6.1253	6.1345	4.9985	5.424	5.6198	4.2639	4.4023	11.9677	12.8829	13.5821	12.9408	11.8507	11.2142	14.2955	13.6957	13.3962	4.118	3.9769	3.0539	2.4794	2.5192	3.7159	4.2291	3.2371
H6Q	6.2571	6.3012	7.3868	7.1457	5.8896	5.8974	6.2976	6.239	6.239	10.9757	11.4811	10.1962	9.8423	12.275	11.747	13.797	12.8422	12.275	3.797	4.2844	2.4342	2.5046	2.7004	3.2108		
H1Q	12.7165	12.676	13.6946	12.975	11.3556	11.8433	13.1264	12.0024	11.5711	6.2421	6.3141	7.3837	7.1299	5.8725	5.869	7.3885	6.3121	6.2579	8.0064	9.996	9.1219	9.4418	8.8238	8.7203	5.6517	4.9873
H12Q	14.2479	14.1524	15.0311	14.0609	12.3514	13.1182	14.1282	13.095	12.4499	4.3906	4.2647	5.6162	6.1312	5.4224	4.989	6.1321	4.9819	5.5171	12.5048	11.5325	10.2097	10.4217	10.6474	10.6335	6.9271	6.3374
H14Q	16.0653	16.164	16.9434	15.7829	14.0502	14.7415	16.1311	15.2289	14.462	3.171	2.4544	3.6793	4.308	3.8377	3.8358	3.679	2.4536	3.1825	14.2865	13.1771	12.0121	12.4672	12.5788	12.2943	9.1794	8.296

(cont.) Table H.6: Hydrogen Distances for the Optimized Structure of 4z,4'z *cis-syn-cis* DtBuCH18C6

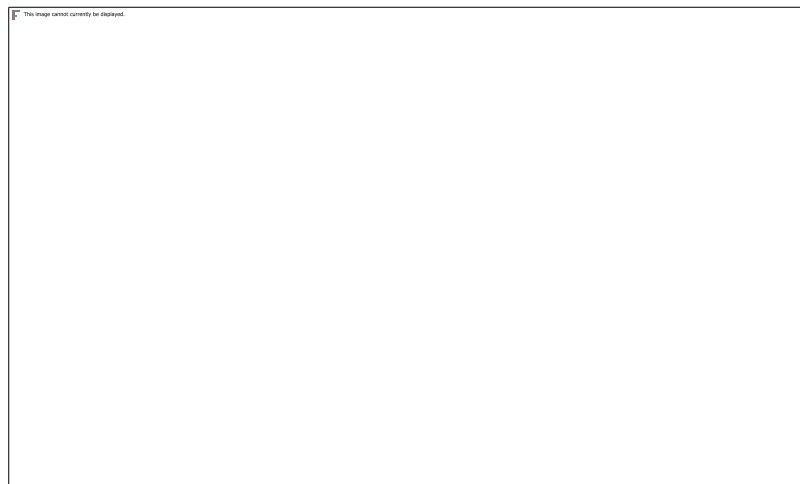| H9A	H9B	H5A	H5B	H4A	H4B	H10A	H10B	H11A	H11B	H3A	H3B	H2A	H2B	H13A	H13B	H15A	H15B	H16A	H16B	H22Q	H7Q	H6Q	H1Q	H12Q	H14Q	
8.9926	9.0541	6.633	6.1864	8.4988	8.002	11.3413	11.5937	13.3953	12.4378	10.4906	10.1282	10.4914	10.653	13.5109	14.5698	14.4407	15.9596	14.1723	15.0614	3.1735	5.5009	6.2571	12.7165	14.2479	16.0653	H26X
8.848	8.5627	7.239	7.1374	9.303	8.6913	11.11	11.1091	13.0884	12.1249	11.031	10.5741	10.5494	10.8041	13.769	14.666	14.8122	16.2408	14.3341	15.0929	2.4486	4.9685	6.3012	12.676	14.1524	16.164	H26Y
9.4338	9.3445	8.0565	7.5703	9.8171	9.0757	11.7543	11.949	13.9247	13.1152	11.7123	11.1362	11.4222	11.7987	14.3634	15.2809	15.5352	17.0556	15.3297	16.0795	3.6761	6.1253	7.3868	13.6946	15.0311	16.9434	H26Z
8.2844	8.584	7.5403	6.6284	8.7231	7.7161	10.6102	11.1437	12.9775	12.3963	10.6482	9.8536	10.543	11.1364	12.998	13.9276	14.3592	15.9756	14.5381	15.2573	4.3079	6.1345	7.1457	12.975	14.0609	15.7829	H28X
6.5788	7.0272	6.3574	5.4683	7.3447	6.1593	8.9021	9.5324	11.287	10.7577	9.109	8.193	8.8976	9.6051	11.2582	12.166	12.6985	14.3104	12.9445	13.6071	3.8382	4.9985	5.8896	11.3556	12.3514	14.0502	H28Y
7.675	8.1573	5.953	4.9695	7.1664	6.3631	10.043	10.6486	12.2974	11.5697	9.224	8.6235	9.4342	9.8327	11.9614	13.0468	13.0893	14.7174	13.2291	14.0873	3.8381	5.424	5.8974	11.8433	13.1182	14.7415	H28Z
8.2414	8.0132	8.462	8.0177	9.9902	8.8807	10.4412	10.6038	12.7196	12.1491	11.5883	10.6865	10.8259	11.5433	13.5733	14.2659	15.0897	16.5809	14.9984	15.5122	3.6815	5.6198	7.3799	13.1264	14.1282	16.1311	H27X
7.4287	6.9247	7.7378	7.6633	9.5113	8.4746	9.5639	9.4927	11.666	10.9667	10.8935	10.0582	9.8396	10.5025	12.8641	13.501	14.3039	15.6976	13.9703	14.431	2.4578	4.2639	6.2976	12.0024	13.095	15.2289	H27Y
6.517	6.3111	7.4971	7.1437	8.8625	7.5979	8.69	8.8926	10.9947	10.4955	10.2387	9.2062	9.2671	10.1289	11.9323	12.5569	13.5542	15.021	13.5098	13.9336	3.1771	4.4023	6.239	11.5711	12.4499	14.462	H27Z
7.8541	8.9363	10.9817	11.2079	9.2899	8.7251	6.1685	7.3277	5.4057	6.4119	7.326	6.5257	6.6694	7.6291	3.0981	2.1517	4.5703	4.8472	6.3168	5.5448	14.1314	11.9677	10.9757	6.2421	4.3906	3.171	H20X
8.9418	9.8057	11.9332	12.3632	10.3658	9.9703	7.0521	7.8757	5.6461	6.6068	8.1852	7.6293	7.3571	8.1146	4.0374	2.868	4.7948	4.4097	6.1323	6.0237	15.1736	12.8829	11.8478	6.3141	4.2647	2.4544	H20Y
9.5624	10.6644	12.2589	12.4659	10.4038	10.0322	7.913	9.0122	6.9637	7.8857	8.3674	7.824	8.0941	8.815	4.4025	3.7212	5.044	4.9142	6.9198	6.1723	15.7372	13.5821	12.439	7.3837	5.6162	3.6793	H20Z
9.2785	10.6438	10.8708	10.9156	8.7318	8.6139	8.1809	9.4989	7.7299	8.2205	6.8473	6.5871	7.4854	7.9174	3.8784	4.2914	3.8663	4.3052	6.2351	6.1656	14.9186	12.9408	11.4811	7.1299	6.1312	4.308	H19X
8.5861	9.9276	9.48	9.6694	7.3902	7.518	7.7158	8.9408	7.2679	7.3815	5.358	5.4252	6.2919	6.4382	3.137	2.2802	3.0795	4.7219	5.0187	4.6187	13.8413	11.8507	10.1962	5.8725	5.4224	3.8377	H19Y
7.5171	8.9114	9.3704	9.4359	7.3437	7.0461	6.5231	7.9136	6.3501	6.781	5.481	4.9622	5.8754	6.5058	2.2922	3.0517	3.1455	4.1433	5.4639	4.4527	13.2001	11.2142	9.8423	5.869	4.989	3.8358	H19Z
10.7095	11.8139	12.378	12.7115	10.455	10.49	9.2475	10.2247	8.0815	8.5812	8.2655	8.2333	8.5085	8.7516	5.0589	4.921	4.3766	3.7156	6.142	5.6538	16.4672	14.2955	12.822	7.3885	6.1321	3.679	H18X
10.2654	11.1542	12.0552	12.6228	10.41	10.4643	8.6506	9.3594	7.095	7.4945	8.0585	8.0785	7.8452	8.0279	4.8025	4.4283	3.9989	2.8325	5.1314	4.2943	15.9924	13.6957	12.2775	6.3121	4.9819	2.4536	H18Y
10.202	11.2705	11.2155	11.6905	9.3838	9.6479	9.9368	9.8159	7.7476	7.8816	7.1033	7.3799	7.5514	7.4936	4.5716	4.8557	3.0634	2.1565	4.6266	4.4334	15.5714	13.3962	11.7487	6.2579	5.5171	3.1825	H18Z
7.7338	7.8656	4.6144	4.5	6.721	6.4354	10.0173	10.2523	11.871	10.761	8.6133	8.434	8.6835	8.6611	11.8541	12.9841	12.5782	14.0461	12.168	13.1246	2.4979	4.118	4.3032	10.8064	12.5048	14.2865	H23A
6.6276	7.1034	3.7941	3.1955	5.4485	4.9362	8.9514	9.4554	10.9468	9.9842	7.4458	7.1013	7.7051	7.8522	10.5643	11.7399	11.4179	12.9787	11.304	12.2536	3.0576	3.9769	3.8176	9.996	11.5325	13.1771	H23B
4.5817	5.0286	4.6536	4.2212	5.7806	4.5365	6.956	7.5053	9.2091	8.5449	7.2286	6.3036	6.698	7.4211	9.3564	10.2539	10.7441	12.2859	10.8029	11.4233	3.0659	3.0539	3.797	9.1219	10.297	12.0121	H21A
4.6453	4.4593	5.7923	5.749	7.1808	5.9337	6.6884	7.0702	9.0894	8.4539	8.3123	7.3111	7.1675	8.0162	10.029	10.6886	11.5585	12.9787	11.3978	11.8228	2.5069	2.4794	2.4844	9.4418	10.4217	12.4672	H21B
6.4991	6.3674	3.6307	4.4523	6.0674	5.8775	8.5434	8.5075	10.0589	8.7665	7.3928	7.3049	6.9484	6.8177	10.4677	11.4923	11.088	12.3928	10.3265	11.1864	2.5581	2.5192	2.4342	8.8238	10.6474	12.5788	H24A
6.7723	7.0806	2.3689	2.9919	4.7936	4.9215	8.8358	9.1015	10.3659	9.083	6.8452	6.6244	6.7791	6.4414	10.0339	11.2725	10.4366	11.8397	9.8769	10.9512	3.7428	3.7159	2.5046	8.7203	10.635	12.2943	H24B
3.0671	2.4718	4.7582	5.7916	6.004	5.198	4.535	4.2232	5.8921	7.4469	5.9734	5.2495	3.8607	4.6031	7.3575	7.92	5.5413	9.6638	7.8083	8.0936	4.9532	4.2291	2.7004	6.6517	6.9271	9.1794	H8A
2.5283	3.0672	3.6442	4.5074	4.3514	3.4885	4.1962	4.5583	5.7257	4.6555	4.3395	3.5388	2.7124	3.5221	6.1085	6.9702	7.2457	8.5643	6.8602	7.3673	5.4923	3.2371	2.3108	4.9873	6.3374	8.296	H8B
0	1.7794	5.8364	6.155	5.8948	4.4587	2.3761	3.2348	4.7149	4.4525	5.6245	4.1293	3.5638	5.1411	5.6947	6.0971	7.6329	8.926	7.7688	7.8192	6.5369	4.4837	4.6123	5.6967	6.0371	8.0168	H9A
1.7794	0	6.589	7.1843	7.1836	5.9057	2.8478	2.6126	4.7644	4.3736	6.8862	5.6064	4.3782	5.8108	6.9056	7.0416	8.7408	9.8355	8.4603	8.3367	6.2144	4.0248	4.8275	6.1215	6.4903	8.7757	H9B
5.8364	6.589	0	1.7755	2.5405	3.0519	7.6168	8.1628	8.9651	7.7207	4.1525	4.5041	5.013	4.5288	7.9496	9.338	8.1772	9.6372	7.8204	9.0045	5.5009	4.5135	2.2849	6.94	8.8542	10.2472	H5A
6.155	7.1843	1.7755	0	2.3705	2.5563	8.1033	8.9293	9.7626	8.7564	4.6565	4.7356	5.9343	5.7467	8.3261	9.7806	8.7495	10.36	8.8547	10.0379	5.7024	5.2241	3.5088	8.0763	9.7239	10.9378	H5B
5.8948	7.1836	2.5405	2.3705	0	1.7826	7.2818	8.2836	8.5451	7.5912	2.4429	2.9551	4.5833	4.215	6.3735	7.9797	6.4904	8.1217	6.8154	8.0884	7.5562	6.378	4.2863	6.4397	8.0339	8.9004	H4A
4.4587	5.9057	3.0519	2.5563	1.7826	0	6.0591	7.2044	7.7296	7.0109	3.0828	2.4375	4.1763	4.5225	5.9583	6.7924	6.7924	8.4808	7.3222	8.2831	6.8225	5.5721	3.9914	4.4477	7.667	8.7661	H4B
2.3761	2.8478	7.6168	8.1033	7.2818	6.0591	0	1.7828	2.5604	3.0465	6.2151	4.7523	3.6467	5.4065	4.5954	4.3576	6.8159	7.793	7.0119	6.5578	8.753	6.5139	6.4832	4.8682	4.3077	6.348	H10A
3.2348	2.6126	8.1628	8.9293	8.2836	7.2044	1.7828	0	2.3937	2.5658	7.1924	5.9784	4.2373	5.778	5.8183	5.3921	7.7263	8.4573	7.3847	6.7585	8.7212	6.3653	6.6445	4.9828	4.5666	6.9477	H10B
4.7149	4.7644	8.9651	9.7626	8.5451	7.7296	2.5604	2.3937	0	1.7817	6.8514	5.8398	4.1374	5.512	4.323	3.4646	6.1055	6.523	5.9029	4.8967	10.659	8.2216	7.8991	3.8456	2.452	4.7141	H11A
4.4525	4.3736	7.7207	8.7564	7.5912	7.0109	3.0465	2.5658	1.7817	0	5.9209	5.2165	3.0116	4.1074	4.5256	4.1167	5.7661	6.2585	4.4487	4.3012	9.6764	7.1671	6.6126	2.5846	2.5226	5.046	H11B
5.6245	6.8862	4.1525	4.6565	2.4429	3.0828	6.2151	7.1924	6.8514	5.9209	0	1.7794	3.0646	2.5417	4.3098	3.5924	4.1167	5.7089	4.4487	5.6996	8.9767	7.2078	5.1499	4.3298	5.8697	6.5415	H3A
4.1293	5.6064	4.5041	4.7356	2.9551	2.4375	4.7523	5.9784	5.8398	5.2165	1.7794	0	2.4557	3.0659	3.5924	5.0841	4.5101	6.1664	4.3155	5.981	8.43	6.5809	4.9726	4.3807	5.3708	6.3392	H3B
3.5638	4.3782	5.013	5.9343	4.5833	4.1763	3.6467	4.2373	4.1374	3.0116	3.0646	2.4557	0	1.785	3.7617	4.6849	4.6849	6.8885	4.3155	4.536	8.1847	5.8778	4.2958	2.4958	3.8917	5.6547	H2A
5.1411	5.8108	4.5288	5.7467	4.215	4.5225	5.4065	5.778	5.512	4.1074	2.5417	3.0659	1.785	0	4.6161	5.7763	4.5115	5.6085	3.5503	4.5164	8.5416	6.3635	4.5101	2.4799	4.6719	6.0725	H2B
5.6947	6.9056	7.9496	8.3261	6.3735	5.9583	4.5954	5.8183	4.323	4.5256	4.3098	3.5924	3.7617	4.6161	0	1.764	2.6206	3.805	4.1398	4.007	11.4781	9.313	8.0426	3.7776	3.0469	3.0671	H13A
6.0971	7.0416	9.338	9.7806	7.9797	6.7924	4.3576	5.3921	3.4646	4.1167	3.5924	5.0841	4.6849	5.7763	1.764	0	3.8076	4.3429	4.9686	4.1686	12.3142	10.0444	9.0952	3.811	2.467	2.5076	H13B
7.6329	8.7408	8.1772	8.7495	6.4904	6.7924	6.8159	7.7263	6.1055	5.7661	4.1167	4.5101	4.6849	4.5115	2.6206	3.8076	0	1.7618	2.4685	3.0637	12.5776	10.445	8.7052	4.0014	4.0014	3.0598	H15A
8.926	9.8355	9.6372	10.36	8.1217	8.4808	7.793	8.4573	6.523	6.2585	5.7089	6.1664	6.8885	5.6085	3.805	4.3429	1.7618	0	2.4879	2.4767	13.9575	11.7198	10.03	4.129	4.129	2.4889	H15B
7.7688	8.4603	7.8204	8.8547	6.8154	7.3222	7.0119	7.3847	5.9029	4.4487	4.4487	4.3155	4.3155	3.5503	4.1398	4.9686	2.4685	2.4879	0	1.7655	12.0779	9.8254	8.058	4.3027	3.7461	3.7569	H16A
7.8192	8.3367	9.0045	10.0379	8.0884	8.2831	6.5578	6.7585	4.8967	4.3012	5.6996	5.981	4.536	4.5164	4.007	4.1686	3.0637	2.4767	1.7655	0	12.7249	10.0314	8.8832	2.557	2.557	2.5754	H16B
6.5369	6.2144	5.5009	5.7024	7.5562	6.8225	8.753	8.7212	10.659	9.6764	8.9767	8.43	8.1847	8.5416	11.4781	12.3142	12.5776	13.9575	12.0779	12.7249	0	2.5269	4.1088	10.2935	11.7238	13.7837	H22Q
4.4837	4.0248	4.5135	5.2241	6.378	5.5721	6.5139	6.3653	8.2216	7.1671	7.2078	6.5809	5.8778	6.3635	9.313	10.0444	10.445	11.7198	9.8254	10.0314	2.5269	0	2.4209	7.8835	9.2739	11.4213	H7Q
4.6123	4.8275	2.2849	3.5088	4.2863	3.9914	6.4832	6.6445	7.8991	6.6126	5.1499	4.9726	4.2958	4.5101	8.0426	9.0952	8.7052	10.03	8.058	8.8832	4.1088	2.4209	0	6.5257	8.3099	10.1699	H6Q
5.6967	6.1215	6.94	8.0763	6.4397	4.4477	4.8682	4.9828	3.8456	2.5846	4.3298	4.3807	2.4958	2.4799	3.7776	3.811	4.0014	4.129	4.3027	2.557	10.2935	7.8835	6.5257	0	2.4606	4.1243	H1Q
6.0371	6.4903	8.8542	9.7239	8.0339	7.667	4.3077	4.5666	2.452	2.5226	5.8697	5.3708	3.8917	4.6719	3.0469	2.467	4.0014	4.129	3.7461	2.557	11.7238	9.2739	8.3099	2.4606	0	2.5344	H12Q
8.0168	8.7757	10.2472	10.9378	8.9004	8.7661	6.348	6.9477	4.7141	5.046	6.5415	6.3392	5.6547	6.0725	3.0671	2.5076	3.0598	2.4889	3.7569	2.5754	13.7837	11.4213	10.1699	4.1243	2.5344	0	H14Q

Figure H.13: Optimized Structure of 4e,5'e *cis-anti-cis* DtBuCH18C6 with Hydrogen Labels
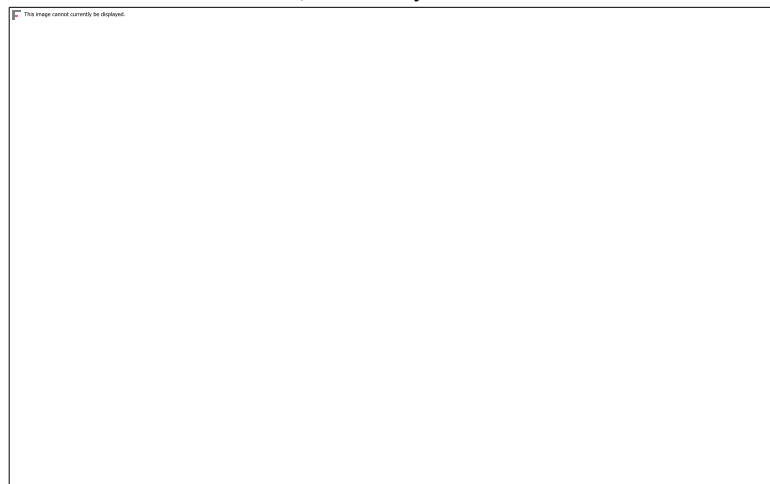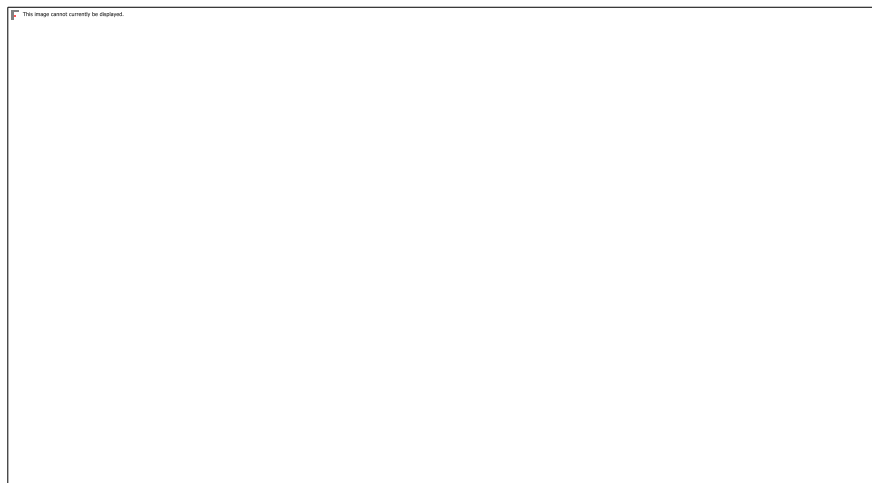

Figure H.14: Optimized Structure of 4e,5'e *cis-anti-cis* DtBuCH18C6 with Carbon and Oxygen Labels

Table H.7: Hydrogen Distances for the Optimized Structure of 4e,5'e *cis-anti-cis* DtBuCH18C6

	H18X	H18Y	H18Z	H19X	H19Y	H19Z	H20X	H20Y	H20Z	H27X	H27Y	H27Z	H28X	H28Y	H28Z	H26X	H26Y	H26Z	H14A	H14B	H13A	H13B	H16A	H16B	H11A	H11B
H18X	0	1.7646	1.7659	3.134	3.7435	2.5075	2.5465	3.7581	3.0239	16.8473	18.0443	17.6348	16.6682	15.328	15.0785	17.8512	16.4216	17.3126	3.8001	4.6037	6.2572	6.1073	5.102	3.7393	8.1817	8.2381
H18Y	1.7646	0	1.7728	3.8202	4.3508	3.7489	3.1802	3.7813	2.5623	16.085	17.3888	16.9766	16.1292	14.6772	14.626	17.4285	16.1055	16.9048	2.2517	3.5048	4.7631	4.9571	4.5205	3.4854	6.6558	6.8892
H18Z	1.7659	1.7728	0	2.6179	3.8029	3.0886	3.7772	4.3537	3.7764	15.3144	16.5536	16.0598	15.3088	13.9291	13.7255	16.4132	14.9995	15.796	3.3575	4.4489	5.5237	5.2312	3.8255	2.2886	6.9465	7.1083
H19X	3.134	3.8202	2.6179	0	1.7707	1.7654	3.7044	3.7981	4.3568	14.5244	15.553	15.2243	14.0238	12.8333	12.3683	15.1219	13.6271	14.6487	4.6418	4.8288	6.2608	5.256	3.2414	2.1049	7.7986	7.3773
H19Y	3.7435	4.3508	3.8029	1.7707	0	1.7715	2.9864	2.574	3.7747	14.8661	15.827	15.6927	14.1	12.9582	12.4975	15.4096	13.9748	15.1347	4.714	4.2691	6.1193	5.0338	3.7194	3.3055	8.1103	7.3841
H19Z	2.5075	3.7489	3.0886	1.7654	1.7715	0	2.4471	3.1507	3.7144	16.1712	17.1778	16.914	15.5565	14.3925	13.9148	16.7262	15.2331	16.3172	4.9427	4.982	6.9132	6.1493	4.7025	3.6223	8.9038	8.4825
H20X	2.5465	3.1802	3.7772	3.7044	2.9864	2.4471	0	1.7702	1.7658	17.1865	18.2881	18.1229	16.6559	15.3852	15.122	18.0876	16.7172	17.7917	4.0281	3.8059	6.1127	5.8405	5.5028	4.7877	8.6381	8.2559
H20Y	3.7581	3.7813	4.3537	3.7981	2.574	3.1507	1.7702	0	1.7731	15.9604	17.0371	16.9942	15.3345	14.0669	13.8676	16.9165	15.6281	16.7481	3.6024	2.6741	5.0612	4.5687	4.6844	4.5562	7.6965	7.0259
H20Z	3.0239	2.5623	3.7764	4.3568	3.7747	3.7144	1.7658	1.7731	0	16.5697	17.7763	17.6157	16.2531	14.8696	14.8078	17.8102	16.5463	17.5328	2.5825	2.3493	4.5976	4.6948	5.0628	4.6621	7.2635	6.9838
H27X	16.8473	16.085	15.3144	14.5244	14.8661	16.1712	17.1865	15.9604	16.5697	0	1.7661	1.7702	3.1404	2.604	3.8134	3.7078	4.3564	3.7933	14.7959	14.6209	13.1473	12.1216	11.8236	13.1497	11.1693	10.5528
H27Y	18.0443	17.3888	16.5536	15.553	15.827	17.1778	18.2881	17.0371	17.7763	1.7661	0	1.7713	2.5167	3.0787	3.7538	2.4518	3.7179	3.1397	16.1468	15.8765	13.4146	13.4146	13.0139	14.335	12.736	11.9963
H27Z	17.6348	16.9766	16.0598	15.2243	15.6927	16.914	18.1229	16.9942	17.6157	1.7702	1.7713	0	3.749	3.7933	4.3505	2.9989	3.7741	2.5688	15.8625	15.7828	13.3136	12.7145	12.7145	13.9004	12.3961	11.8689
H28X	16.6682	16.1292	15.3088	14.0238	14.1	15.5565	16.6559	15.3345	16.2531	3.1404	2.5167	3.749	0	1.7659	1.7654	2.5335	3.0246	3.7514	14.8885	14.4162	13.3654	12.057	11.643	13.0354	11.9833	10.9561
H28Y	15.328	14.6772	13.9291	12.8333	12.9582	14.3925	15.3852	14.0669	14.8696	2.604	3.0787	3.7933	1.7659	0	1.7731	3.7674	3.4517	3.7903	13.5132	13.0811	12.9612	11.7676	10.2506	11.6851	10.2638	9.2973
H28Z	15.0785	14.626	13.7255	12.3683	12.4975	13.9148	15.122	13.8676	14.8078	3.8134	3.7538	4.3505	1.7654	1.7731	0	3.1815	2.5777	3.7903	13.5132	13.0811	12.178	10.7761	10.1174	11.443	10.9492	9.9049
H26X	17.8512	17.4285	16.4132	15.1219	15.4096	16.7262	18.0876	16.9165	17.8102	3.7078	2.4518	2.9989	2.5335	3.7674	3.1815	0	1.7656	1.7703	16.4166	16.116	15.1078	13.7719	12.967	14.1583	13.5898	12.7437
H26Y	16.4216	16.1055	15.796	13.6271	13.9748	15.2331	16.7172	15.6281	16.5463	4.3564	3.7179	3.7741	3.0246	3.4517	2.5777	1.7656	0	1.7728	15.2439	14.9855	14.1406	12.7237	11.6639	12.7546	12.7805	12.5544
H26Z	17.3126	16.9048	15.796	14.6487	15.1347	16.3172	17.7917	16.7481	17.5328	3.7933	3.1397	2.5688	3.7514	4.3517	3.7903	1.7703	1.7728	0	16.0356	15.9185	14.8729	13.5778	12.5518	13.5979	13.2118	12.5544
H14A	3.8001	2.2517	3.3575	4.6418	4.714	4.9427	4.0281	3.6024	2.5825	14.7959	16.1468	15.8625	14.8885	13.3654	13.5132	16.4166	15.2439	16.0356	0	1.7509	2.5469	3.0646	3.8122	3.7197	4.8325	4.9141
H14B	4.6037	3.5048	4.4489	4.8288	4.2691	4.982	3.8059	2.6741	2.3493	14.6209	15.8765	15.7828	14.4162	12.9612	13.0811	16.116	14.9855	15.9185	1.7509	0	2.437	2.5244	3.9096	4.3162	5.2408	4.7388
H13A	6.2572	4.7631	5.5237	6.2608	6.1193	6.9132	6.1127	5.0612	4.5976	14.5494	13.4146	13.3136	12.057	11.7676	10.5401	15.1078	14.1406	14.8729	2.5469	2.437	0	1.7617	4.0704	4.9386	2.9279	2.6951
H13B	6.1073	4.9571	5.2312	5.256	5.0338	6.1493	5.8405	4.5687	4.6948	12.1216	13.4146	12.7145	12.057	10.5401	10.7761	13.7719	12.7237	13.5778	3.0646	2.5244	1.7617	0	2.7156	4.0124	3.4378	2.4745
H16A	5.102	4.5205	3.8255	3.2414	3.7194	4.7025	5.5028	4.6844	5.0628	11.8236	13.0139	12.7145	11.643	10.2506	10.1174	12.967	11.6639	12.5518	3.8122	3.9096	4.0704	2.7156	0	1.7527	4.9008	4.3206
H16B	3.7393	3.4854	2.2886	2.1049	3.3055	3.6223	4.7877	4.5562	4.6621	13.1497	14.335	13.9004	13.0354	11.6851	11.443	14.1583	12.7546	13.5979	3.7197	4.3162	4.9386	4.0124	1.7527	0	5.9298	5.742
H11A	8.1817	6.6558	6.9465	7.7986	8.1103	8.9038	8.6381	7.6965	7.2635	11.1693	12.736	12.3961	11.9833	10.2638	10.9492	13.5898	12.7805	13.2118	4.8325	5.2408	2.9279	3.4378	4.9008	5.9298	0	1.7811
H11B	8.2381	6.8892	7.1083	7.3773	7.3841	8.4825	8.2559	7.0259	6.9838	10.5528	11.9963	11.8689	10.9561	9.2973	9.9049	12.7437	11.9299	12.5544	4.9141	4.7388	2.6951	2.4745	4.3206	5.742	1.7811	0
H10A	9.3446	8.0552	7.8174	8.3403	8.9267	9.7784	10.0871	9.1772	8.9878	9.0749	10.6915	10.1624	10.1997	8.4662	9.1788	11.5541	10.765	11.0159	6.614	7.0734	5.0768	4.8601	5.2559	6.3375	2.4883	3.0622
H10B	10.1888	8.8042	8.8301	9.2393	9.5201	10.5556	10.4323	9.3054	9.0047	10.6119	10.3288	10.0511	8.2964	9.2285	11.7073	11.1079	11.4111		7.0163	7.1464	4.9398	4.8785	6.046	7.3692	2.3977	2.4983
H2A	6.839	6.0397	5.2031	5.228	6.114	6.8567	7.7823	7.1033	7.185	10.194	11.5354	10.9854	10.5726	9.0646	9.1146	10.6775	10.4462	11.0378	5.3	5.8292	4.9713	3.9972	2.5067	3.2971	4.203	4.138
H2B	5.973	5.5741	4.2958	4.1728	5.4467	5.8763	7.2435	6.896	7.0077	11.3005	12.5253	11.8932	11.5013	10.1352	9.9162	12.3673	10.9669	11.615	5.5203	6.21	5.9647	4.9642	2.622	2.4559	5.7267	5.7207
H3A	7.2089	6.6269	5.4565	6.1963	7.7452	7.7452	8.9748	8.8642	8.5859	11.5616	12.9222	11.9941	12.3613	10.9351	10.8956	12.9504	11.9343	11.877	6.7363	7.8437	7.1379	6.6167	4.8251	4.4225	6.1313	6.7543
H3B	7.9387	7.0168	6.1918	6.9649	8.1671	8.5245	9.4233	9.0415	7.369	10.512	11.9971	11.122	11.5406	9.9879	10.2111	13.3285	11.1877	11.4045	6.5571	7.5566	6.3385	5.9443	4.7853	4.9497	4.74	4.4956
H9A	10.8892	9.8276	9.3058	9.2846	9.8408	10.8805	11.5307	10.5022	10.6381	6.7412	8.3455	7.8033	7.9606	6.2375	7.0071	9.2221	8.5131	8.6923	8.4879	8.7049	6.947	6.2655	6.2073	7.4477	4.6658	4.5437
H9B	11.6349	10.4795	10.1857	10.0776	10.352	11.5592	11.9431	10.7188	10.9235	6.551	8.1377	7.9265	7.6395	5.876	6.9353	9.2919	8.8172	9.0772	8.841	8.7828	6.893	6.2906	6.8726	8.3368	4.7042	4.2277
H8A	11.4121	10.5526	10.0572	9.3095	9.3911	10.8015	11.443	10.1061	10.7052	6.0117	7.2569	7.3412	6.0698	4.257	5.074	7.9066	7.23	7.9206	9.0514	8.6769	7.346	6.1967	6.3369	7.9324	5.9904	4.8918
H8B	10.3906	9.6387	8.916	8.2001	8.564	9.8173	10.7331	9.5915	10.1273	6.4931	7.7602	7.4965	6.6997	5.3102	5.3906	8.0851	7.1023	7.7506	8.4277	8.3083	5.884	5.3388	6.7445	5.7448	9.217	
H4A	10.1765	9.3796	8.4304	8.6017	9.6754	10.3084	11.4307	10.8262	10.8266	8.146	9.6059	8.596	9.4186	7.9377	8.1942	9.9611	8.9115	8.9309	8.7341	9.4103	8.0582	7.3559	6.1968	6.7601	6.0529	6.4157
H4B	9.0517	8.2329	7.3705	7.3182	8.1973	9.0105	10.0259	9.2692	9.3969	8.2648	9.6857	8.9684	9.0715	7.5252	7.7351	9.9881	8.775	9.2165	7.3919	7.8652	6.6029	5.7134	4.6295	5.486	4.9133	4.9377
H5A	9.6565	9.2545	8.0593	7.2854	8.1591	9.042	10.525	9.7943	10.2759	7.8244	8.9118	8.2157	8.0457	6.8134	6.4721	8.6278	7.2367	7.7986	8.7307	8.994	8.2549	6.9777	5.2338	5.5984	7.1055	6.7262
H5B	10.7322	10.3098	9.0542	8.5745	9.6432	10.338	11.8824	11.2902	11.6163	7.6833	8.8014	7.7834	8.4064	7.2455	6.98	8.5577	7.2314	7.4166	9.9192	10.3943	9.4897	8.398	6.6711	7.1586	7.9743	7.9052
H21A	14.1393	13.3881	12.5105	11.9684	12.5849	13.6855	14.8122	13.7895	14.2204	3.3022	4.7564	3.7763	5.1274	3.8418	4.504	5.5341	5.0627	4.7144	12.3183	12.4275	10.9667	9.9789	9.3183	10.4393	8.8782	8.5433
H21B	14.7659	13.9816	13.2241	12.5175	12.9037	14.1712	15.1578	13.9709	14.5214	2.1122	3.6423	3.3019	3.7843	2.3314	3.5113	4.8117	4.6834	4.5679	12.7134	12.5961	11.1306	10.0989	9.7579	11.0785	9.1766	8.5787
H23A	14.7969	14.4899	13.2857	12.1113	12.7067	13.7938	15.3847	14.4589	15.2244	4.833	4.9922	4.2661	4.625	4.4776	3.5351	3.8232	2.3652	2.6905	13.8056	13.7761	12.9158	11.5517	10.2075	11.1153	11.4561	10.8284
H23B	13.9072	13.5624	12.4691	11.1712	11.5735	12.8071	14.2598	13.2059	14.0595	4.6416	4.9343	4.7018	3.7917	3.3816	2.25	3.9985	2.5478	3.5841	12.7255	12.5259	11.7162	10.2857	9.1342	10.2228	10.4497	9.6147
H24A	13.2848	12.8186	11.6532	10.9082	11.7214	12.6594	14.1517	13.3335	13.8408	5.2325	6.1462	5.0376	6.0931	5.2028	4.9319	5.8653	4.7158	4.6201	12.1539	12.1539	11.304	10.101	8.7841	9.5555	9.5678	9.2513
H24B	12.4812	12.2129	10.9421	9.8702	10.6272	11.5863	13.2366	12.4439	13.1128	6.2577	6.9161	6.1177	6.2592	5.5361	4.7629	6.1199	4.6015	5.0819	11.6942	11.8095	10.9659	9.7089	8.0791	8.8267	9.7525	9.2402
H15Q	4.2992	3.8579	3.8041	2.9959	2.4174	3.6524	3.7111	2.5154	3.2643	13.5243	14.6446	14.5323	13.0537	11.7251	11.5742	14.5814	13.3095	14.349	3.0427	2.353	3.7834	2.6291	2.2611	2.7822	5.8311	5.0385
H12Q	6.0449	4.4837	4.818	6.1138	6.6345	7.0902	6.8373	6.2382	5.5384	12.6772	14.1814	13.741	13.2898	11.6373	12.0405	14.7312	13.6997	14.2281	2.9769	3.9879	2.3718	3.0093	3.8221	4.2715	2.2735	3.1795
H1Q	9.3701	2.6578	2.5592	4.2204	5.0946	5.1525	5.2874	5.1324	4.4053	13.7098	15.0995	14.054	12.5188	12.6121	15.3006	14.059	14.7023		2.3401	3.7562	3.619	3.6558	3.0451	2.519	4.4666	4.9336
H6Q	11.2064	10.76	9.7141	8.6487	9.169	10.3367	11.6886	10.6956	11.3897	6.0723	7.0148	6.5939	5.912	4.7276	4.3199	6.7189	5.4094	6.1693	9.9275	9.8639	9.0272	7.6341	6.3836	7.4811	7.825	7.0865
H7Q	12.927	12.3188	11.4867	10.4454	10.7145	12.0581	13.1482	11.9426	12.6811	4.1988	5.1492	5.1208	3.9501	2.5152	2.6574	5.3217	4.4866	5.2193	11.1536	10.885	9.7909	8.4876	7.8867	9.2428	8.3791	7.4713
H22Q	15.5707	15.0095	13.9718	13.1397	13.7496	14.8607	16.2149	15.2148	15.8078	2.9869	3.6471	2.4092	4.2991	3.8012	3.8551	3.7194	3.2647	2.5279	14.0924	14.1322	12.8891	11.7384	10.7978	11.8372	10.9989	10.5375

(cont.) Table H.7: Hydrogen Distances for the Optimized Structure of 4e,5'e *cis-anti-cis* DtBuCH18C6

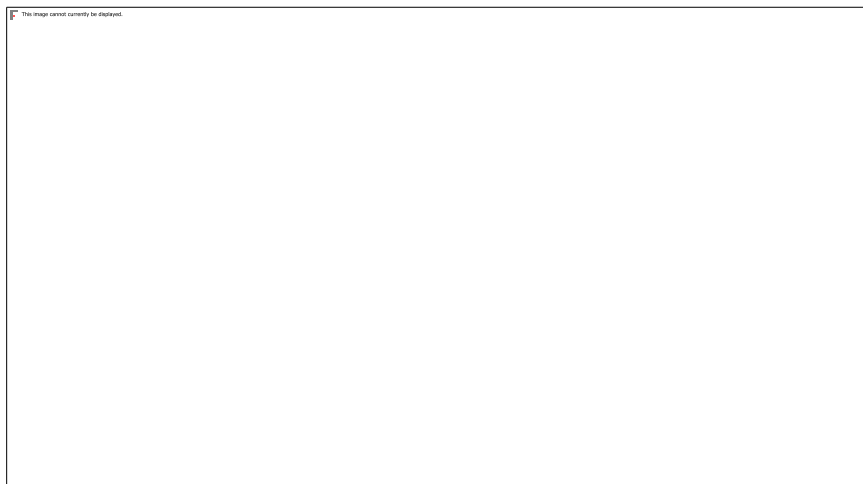| H10A	H10B	H2A	H2B	H3A	H3B	H9A	H9B	H8A	H8B	H4A	H4B	H5A	H5B	H21A	H21B	H23A	H23B	H24A	H24B	H15Q	H12Q	H1Q	H6Q	H7Q	H22Q	
9.3446	10.1888	6.839	5.973	7.2089	7.9387	10.8892	11.6349	11.4121	10.3906	10.1765	9.0517	9.6565	10.7322	14.1393	14.7659	14.7969	13.9072	13.2848	12.4812	4.2992	6.0449	3.9701	11.2064	12.927	15.5707	H18X
8.0552	8.8042	6.0397	5.5741	6.6269	7.0168	9.8276	10.4795	10.5526	9.6387	9.3796	8.2329	9.2545	10.3098	13.3881	13.9816	14.4899	13.5624	12.8186	12.2129	3.8579	4.4837	2.6578	10.76	12.3188	15.0095	H18Y
7.8174	8.8301	5.2031	4.2958	5.4565	6.1918	9.3058	10.1857	10.0572	8.916	8.4304	7.3705	8.0593	9.0542	12.5105	13.2241	13.2857	12.4691	11.6532	10.9421	3.8041	4.818	2.5592	9.7141	11.4867	13.9718	H18Z
8.3403	9.2393	5.228	4.1728	6.1963	6.9649	9.2846	10.0776	9.3095	8.2001	8.6017	7.3182	7.2854	8.5745	11.9684	12.5175	12.1113	11.1712	10.9082	9.8702	2.9959	6.1138	4.2204	8.6487	10.4454	13.1397	H19X
8.9267	9.5201	6.114	5.4467	7.6591	8.1671	9.8408	10.352	9.3911	8.564	9.6754	8.1973	8.1591	9.6432	12.5849	12.9037	12.7067	11.5735	11.7214	10.6272	2.4174	6.6345	5.0946	9.169	10.7145	13.7496	H19Y
9.7784	10.5478	6.8567	5.8763	7.7452	8.5245	10.8805	11.5592	10.8015	9.8173	10.3084	9.0105	9.042	10.338	13.6855	14.1712	13.7938	12.8071	12.6594	11.5863	3.6524	7.0902	5.1525	10.3367	12.0581	14.8607	H19Z
10.0871	10.5556	7.7823	7.2435	8.9748	9.4233	11.5307	11.9431	11.443	10.7331	11.4307	10.0259	10.525	11.8824	14.8122	15.1578	15.3847	14.2598	14.1517	13.2366	3.7111	6.8373	5.2818	11.6886	13.1482	16.2149	H20X
9.1772	9.4323	7.1033	6.896	8.8642	9.0415	10.5022	10.7188	10.1061	9.5915	10.8262	9.2692	9.7943	11.2902	13.7895	13.9709	14.4589	13.2059	13.3335	12.4439	2.5154	6.2382	5.1324	10.6956	11.9426	15.2148	H20Y
8.9878	9.3054	7.185	7.0077	8.5859	8.7369	10.6381	10.9235	10.7052	10.1273	10.8266	9.3969	10.2759	11.6163	14.2204	14.5214	15.2244	14.0595	13.8408	13.1128	3.2643	5.5384	4.4053	11.3897	12.6811	15.8078	H20Z
9.0749	9.0047	10.194	11.3005	11.5616	10.512	6.7412	6.551	6.0117	6.4931	8.146	8.2648	7.8244	7.6833	3.3022	2.1122	4.833	4.6416	5.2325	6.2577	13.5243	12.6772	13.7098	6.0723	4.1988	2.9869	H27X
10.6915	10.6119	11.5354	12.5253	12.9222	11.9971	8.3455	8.1377	7.2569	7.7602	9.6059	9.6857	8.9118	8.8014	4.7564	3.6423	4.9922	4.9343	6.1462	9.161	14.6446	14.1814	15.0995	7.0148	5.1492	3.6471	H27Y
10.1624	10.3288	10.9854	11.8932	11.9941	11.122	7.8033	7.9265	7.3412	7.4965	8.596	8.9684	8.2157	7.7834	3.7763	3.3019	4.2661	4.7018	5.0376	6.1177	14.5323	13.741	14.594	6.5939	5.1208	2.4092	H27Z
10.1997	10.0511	10.5726	11.5013	12.3613	11.5406	7.9606	7.6395	6.0698	6.6997	9.4186	9.0715	8.0457	8.4064	5.1274	3.7843	4.625	3.7917	6.0931	6.2592	13.0537	13.2898	14.054	5.912	3.9501	4.2991	H28X
9.1788	9.2285	9.1146	9.9162	10.8956	10.2111	7.0071	6.9353	5.074	5.3906	8.1942	7.7351	6.4721	6.98	4.504	3.5113	5.3351	2.25	4.9319	4.7629	11.5742	12.0405	12.6121	4.3199	2.6574	3.8551	H28Y
11.5541	11.7073	11.6775	12.3673	12.9504	12.3285	9.2221	9.2919	7.9066	8.0851	9.9611	9.9881	8.6278	8.5577	5.5341	4.8117	3.8232	3.9985	5.8653	6.1199	14.5814	14.7312	15.3006	6.7189	5.3217	3.7194	H28Z
10.765	11.1079	10.4462	10.9669	11.6409	11.1877	8.5131	8.8172	7.23	7.1023	8.9115	8.8775	7.2367	7.2314	5.0627	4.6834	2.3652	2.5478	4.7158	4.6015	13.3095	13.6997	14.059	5.4094	4.4866	3.2647	H26X
11.0159	11.4111	11.0378	11.615	11.9343	11.4045	8.6923	9.0772	7.9206	7.7506	9.2165	9.165	7.7986	7.4166	4.7144	4.5679	2.6905	3.5841	4.6201	5.0819	14.349	14.2281	14.7023	6.1693	5.2193	2.5279	H26Y
6.614	7.0163	5.3	5.5203	6.7363	6.5571	8.4879	8.841	9.0514	8.4277	8.7341	7.3919	8.7307	9.9192	12.3183	12.7134	13.8056	12.7255	12.1539	11.6942	3.0427	2.9769	2.3401	9.9275	11.1536	14.0924	H14A
7.0734	7.1464	5.8292	6.21	7.8437	7.5566	8.7049	8.7828	8.6769	8.3083	9.4103	7.8652	8.994	10.3943	12.4275	12.5961	13.7761	12.5259	12.3755	11.8095	2.353	3.9879	3.7562	9.8639	10.885	14.1322	H14B
5.0768	4.9398	4.9713	5.9647	7.1379	6.3385	6.947	6.893	7.346	7.1228	8.0582	6.6029	8.2549	9.4897	10.9667	11.306	12.9158	11.7162	11.3034	10.659	3.7834	2.3718	3.619	9.0272	7.7909	12.8891	H13A
4.8601	4.8785	3.9972	4.9642	6.6167	5.9443	6.2655	6.2906	6.1967	5.884	7.3559	5.7134	6.9777	8.398	9.9789	10.0989	11.5517	10.2857	10.1301	9.7089	2.6291	3.0093	3.6558	6.6341	8.4876	11.7384	H13B
5.2559	6.046	2.5067	2.622	4.8251	4.7853	6.2073	6.8726	6.3369	5.3388	6.1968	4.6295	5.2338	6.6711	9.3183	9.7579	10.2075	9.1342	8.7841	8.0791	2.2611	3.8221	3.0451	6.3836	7.8867	10.7978	H16A
6.3375	7.3692	3.2971	2.4559	4.4225	4.9497	7.4477	8.3368	7.9324	6.7445	6.7601	5.486	5.9584	7.1586	10.0439	11.0785	11.1153	10.2228	9.5955	8.8267	2.7822	4.2715	2.519	7.4811	9.2428	11.872	H16B
2.4883	2.3977	4.203	5.7267	6.1313	4.74	4.6658	4.7042	5.9904	5.7448	6.0529	4.9133	7.1055	9.743	8.8782	9.1766	11.4561	10.4497	9.5678	9.7525	5.8311	2.2735	4.4666	7.825	8.3791	10.9989	H11A
3.0622	2.4983	4.138	5.7207	6.7543	5.4956	4.5437	4.2277	4.8918	4.9217	6.4157	4.9377	6.7262	7.9052	8.5433	8.5787	10.8284	9.6147	9.2513	9.2402	5.0385	3.1795	4.9336	7.0865	7.4713	10.5375	H11B
0	1.7813	3.4493	5.1398	5.1384	3.452	2.3704	3.0496	4.6133	4.0561	3.8355	2.9556	5.3201	5.8921	6.5406	7.0604	9.3142	8.5012	7.7258	7.7001	6.9127	3.883	5.4929	5.9825	6.5367	8.6956	H10A
1.7813	0	4.7785	6.5452	6.8606	2.963	2.4783	4.3372	4.923	4.4923	5.4039	4.4203	6.5339	7.2711	7.0105	7.1149	9.9852	8.9826	8.2073	8.6618	7.2977	4.5077	6.4566	6.7033	6.7172	9.1994	H10B
3.4493	4.7785	0	1.7813	3.0697	2.5209	4.2197	5.3582	3.9658	3.9658	3.7237	2.2558	3.5625	4.6521	7.364	8.0904	8.7417	7.9181	6.5701	5.6701	4.7069	3.6673	5.045	5.045	6.6311	9.0087	H2A
5.1398	6.5452	1.7813	0	2.4773	3.0637	5.7878	7.0532	6.7603	5.2368	4.4645	3.4289	3.8206	4.7795	8.3682	9.2455	9.1153	8.4481	7.365	6.7551	4.7322	4.6384	3.6284	5.6779	7.6282	9.7339	H2B
5.1384	6.8606	3.0697	2.4773	0	1.7738	5.9134	5.93	7.842	6.2472	3.6045	3.5793	4.5367	4.5776	8.3494	9.5644	9.5385	9.2496	7.358	7.2077	6.858	5.1336	4.4685	6.6169	8.5093	9.8131	H3A
3.452	2.963	2.5209	3.0637	1.7738	0	4.4111	5.93	6.8422	5.2647	2.6342	2.5019	3.4532	4.4638	7.3674	8.4829	9.2141	8.8053	7.0655	6.858	6.8606	4.3014	6.12	6.12	7.6661	9.1214	H3B
2.3704	2.4783	4.2197	5.7878	5.9134	4.4111	0	1.7793	2.4938	2.504	3.1927	2.561	2.4387	4.6729	4.2171	4.6843	7.1692	6.3887	5.2657	5.8936	8.0558	6.0359	6.0359	2.4333	4.4005	6.3843	H9A
3.0496	4.3372	5.3582	7.0532	5.93	5.93	1.7793	0	1.7775	3.0578	4.9718	4.154	5.62	6.2724	4.8348	4.6843	7.9101	6.8904	6.4091	7.0061	8.3742	6.5193	8.0775	3.5539	4.5303	6.9599	H9B
4.6133	4.923	3.9658	6.7603	7.842	6.8422	2.4938	1.7775	0	1.7775	5.5638	4.3831	4.7592	5.868	4.636	4.1286	5.182	4.7272	4.6252	4.5414	7.7345	7.3459	8.4041	2.3023	2.7786	6.2331	H8A
4.0561	4.4923	3.9658	5.2368	6.2472	5.2647	2.504	3.0578	1.7775	0	4.0775	2.8312	3.0125	4.2045	4.2703	4.4298	5.5742	5.5742	4.8041	4.4459	7.1048	6.6756	7.3987	3.2023	2.8053	5.8704	H8B
3.8355	5.4039	3.7237	4.4645	3.6045	2.6342	3.1927	4.9718	5.5638	4.0775	0	1.7772	3.0685	2.5274	4.8936	6.2227	6.9023	6.7128	4.4661	5.0097	8.4172	6.3985	6.8373	4.4198	5.7768	6.5814	H4A
2.9556	4.4203	2.2558	3.4289	3.5793	2.5019	2.561	4.154	4.3831	2.8312	1.7772	0	2.4693	3.0631	5.254	6.1882	7.0845	6.4636	4.9816	5.0925	6.8061	5.2571	7.3328	3.7508	5.1715	7.0069	H4B
5.3201	6.5339	3.5625	3.8206	4.5367	3.4532	2.4387	5.62	4.7592	3.0125	3.0685	2.4693	0	1.7771	4.9589	5.9143	3.6493	4.769	3.0275	3.617	7.3617	7.1078	2.1784	2.1784	5.0382	5.9864	H5A
5.8921	7.2711	4.6521	4.7795	4.5776	4.4638	4.6729	6.2724	5.868	4.2045	2.5274	3.0631	1.7771	0	4.5621	5.939	5.0196	5.0532	2.8533	2.8119	8.8833	8.107	8.052	3.1562	5.0382	5.4488	H5B
6.5406	7.0105	7.364	8.3682	8.3494	7.3674	4.2171	4.8348	4.636	4.2703	4.8936	5.254	4.9589	4.5621	0	1.7484	3.879	3.7937	2.6059	3.9995	11.2804	10.0817	10.9265	3.8045	3.0448	2.2752	H21A
7.0604	7.1149	8.0904	9.2455	9.5644	8.4829	4.6843	4.6843	4.1286	4.4298	6.2227	6.1882	5.9143	5.939	1.7484	0	4.3266	3.7552	3.9446	4.9303	11.5091	10.5982	11.5977	4.2635	2.5132	2.764	H21B
9.3142	9.9852	8.7417	9.1153	9.5385	9.2141	7.1692	7.9101	5.182	5.5742	6.9023	7.0845	3.6493	5.0196	3.879	4.3266	0	1.7521	2.5487	2.4396	12.0723	12.1611	12.3733	3.9226	3.9044	2.351	H23A
8.5012	8.9826	7.9181	8.4481	9.2496	8.8053	6.3887	6.8904	4.7272	5.5742	6.7128	6.4636	4.769	5.0532	3.7937	3.7552	1.7521	0	3.0667	2.5613	10.8443	11.226	11.5171	2.8741	2.4991	3.0404	H23B
7.7258	8.2073	6.5701	7.365	7.358	7.0655	5.2657	6.4091	4.6252	4.8041	4.4661	4.9816	3.0275	2.8533	2.6059	3.9446	2.5487	3.0667	0	1.7619	10.8647	10.222	10.1323	3.615	3.723	2.6451	H24A
7.7001	8.6618	5.6701	6.7551	7.2077	6.858	5.8936	7.0061	4.5414	4.4459	5.0097	5.0925	3.617	2.8119	3.9995	4.9303	2.4396	2.5613	1.7619	0	10.0564	10.143	10.1323	3.2615	3.7597	3.789	H24B
6.9127	7.2977	4.7069	4.7322	6.858	6.8606	8.0558	8.3742	7.7345	7.1048	8.4172	6.8061	7.3617	8.8833	11.2804	11.5091	12.0723	10.8443	10.8647	10.0564	0	4.5994	3.7234	8.2506	9.5255	12.7359	H15Q
3.883	4.5077	3.6673	4.6384	5.1336	4.3014	6.0359	6.5193	7.3459	6.6756	6.3985	5.2571	7.1078	8.107	10.0817	10.5982	12.1611	11.226	10.222	10.143	4.5994	0	2.2962	8.4035	9.4728	12.0549	H12Q
5.4929	6.4566	5.045	3.6284	4.4685	6.12	6.0359	8.0775	8.4041	7.3987	6.8373	7.3328	2.1784	8.052	10.9265	11.5977	12.3733	11.5171	10.1323	10.1323	3.7234	2.2962	0	8.6505	10.1545	12.6607	H1Q
5.9825	6.7033	5.045	5.6779	6.6169	6.12	2.4333	3.5539	2.3023	3.2023	4.4198	3.7508	2.1784	3.1562	3.8045	4.2635	3.9226	2.8741	3.615	3.2615	8.2506	8.4035	8.6505	0	2.2991	4.5867	H6Q
6.5367	6.7172	6.6311	7.6282	8.5093	7.6661	4.4005	4.5303	2.7786	2.8053	5.7768	5.1715	5.0382	5.0382	3.0448	2.5132	3.9044	2.4991	3.723	3.7597	9.5255	9.4728	10.1545	2.2991	0	3.8065	H7Q
8.6956	9.1994	9.0087	9.7339	9.8131	9.1214	6.3843	6.9599	6.2331	5.8704	6.5814	7.0069	5.9864	5.4488	2.2752	2.764	2.351	3.0404	2.6451	3.789	12.7359	12.0549	12.6607	4.5867	3.8065	0	H22Q

Figure H.15: Optimized Structure of 4z,5'e *cis-anti-cis* DtBuCH18C6 with Hydrogen Labels
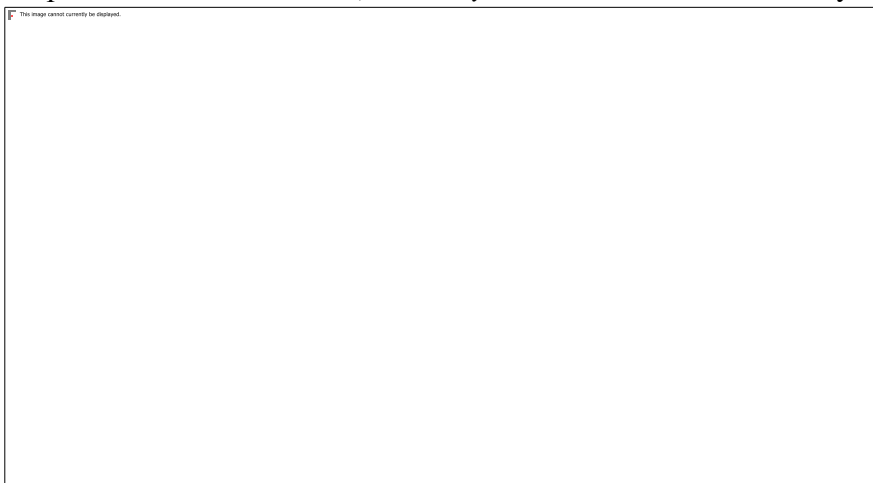

Figure H.16: Optimized Structure of 4z,5'e *cis-anti-cis* DtBuCH18C6 with Carbon and Oxygen Labels

Table H.8: Hydrogen Distances for the Optimized Structure of 4z,5'e *cis-anti-cis* DtBuCH18C6

	H27X	H27Y	H27Z	H26X	H26Y	H26Z	H28X	H28Y	H28Z	H18X	H18Y	H18Z	H20X	H20Y	H20Z	H19X	H19Y	H19Z	H15A	H15B	H16A	H16B	H13A	H13B	H2A	H2B
H27X	0	1.7656	1.7706	3.1223	2.6096	3.8159	3.704	4.3561	3.7989	12.5013	13.634	13.9776	16.0259	16.5866	16.2541	15.2262	13.6015	15.0313	14.8013	14.6332	13.0105	12.1133	12.0014	13.1908	11.1312	10.5065
H27Y	1.7656	0	1.7713	2.508	3.0946	3.7504	2.4449	3.7131	3.1426	13.5447	14.7215	14.9186	17.1738	17.7286	17.2737	16.3008	14.6184	15.9737	16.1825	15.903	14.4071	13.4058	13.2216	14.4221	12.6944	11.9396
H27Z	1.7706	1.7713	0	3.7432	3.7984	4.3512	2.9967	3.7781	2.5773	13.5019	14.7693	14.9803	17.1083	17.5255	17.2295	15.9633	14.3386	15.8104	15.8958	15.7944	14.2729	13.2917	12.9014	13.9427	12.3971	11.8394
H26X	3.1223	2.508	3.7432	0	1.766	1.765	2.5471	3.0316	3.7595	11.8626	13.0236	13.0759	15.5462	16.1579	15.5146	14.7955	13.0572	14.2534	14.96	14.4577	13.1992	12.0413	11.8841	13.1957	11.9149	10.8649
H26Y	2.6096	3.0946	3.7984	1.766	0	1.7733	3.7762	3.777	4.3521	10.5762	11.6981	11.9056	14.193	14.8273	14.2921	13.5401	11.8414	13.1151	13.3967	12.9785	11.5967	10.5148	10.4489	11.7862	10.1899	9.2066
H26Z	3.8159	3.7504	4.3512	1.765	1.7733	0	3.1756	2.5639	3.7825	10.3883	11.6626	11.6049	14.1378	14.6456	14.0179	13.1726	11.4267	12.6362	13.6424	13.1463	12.0528	10.7697	10.3906	11.6395	10.9457	9.8541
H28X	3.704	2.4449	2.9967	2.5471	3.7762	3.1756	0	1.7661	1.7704	13.4152	14.7585	14.6647	17.1853	17.0361	15.9446	14.2211	15.5019	16.5285	16.1633	14.9816	13.757	13.2212	14.315	13.5906	12.6959	11.8951
H28Y	4.3561	3.7131	3.7781	3.0316	3.777	2.5639	1.7661	0	1.773	12.1426	13.5867	13.369	15.9422	16.2322	15.6921	14.4697	12.7534	14.0318	15.393	15.035	14.0298	12.6892	11.9306	12.9328	12.818	11.8951
H28Z	3.7989	3.1426	2.5773	3.7595	4.3521	3.7825	1.7704	1.773	0	13.2431	14.6848	14.5901	16.9951	17.2527	16.8527	15.4591	13.7916	15.1854	16.1471	15.948	14.7667	13.5395	12.7829	13.7098	13.256	12.5319
H18X	12.5013	13.5447	13.5019	11.8626	10.5762	10.3883	13.4152	12.1426	13.2431	0	1.7723	1.7658	3.8138	4.351	3.7537	3.7882	2.574	3.1805	4.5098	3.499	4.3109	2.6925	2.2456	3.5181	6.0439	4.8893
H18Y	13.634	14.7215	14.7693	13.0236	11.6981	11.6626	14.7585	13.5867	14.6848	1.7723	0	1.7653	2.6062	3.7957	2.515	4.3525	3.7818	3.7695	3.8353	2.3168	3.6244	2.549	3.3654	4.465	6.0096	4.8951
H18Z	13.9776	14.9186	14.9803	13.0759	11.9056	11.6049	14.6647	13.369	14.5901	1.7658	1.7653	0	3.1342	3.7479	2.515	3.7519	3.025	2.5354	5.1127	3.7646	5.2961	3.9865	3.7938	4.6121	7.486	6.3164
H20X	16.0259	17.1738	17.1083	15.5462	14.193	14.1378	17.1853	15.9422	16.9951	3.8138	2.6062	3.1342	0	1.7706	1.7653	3.7957	4.3565	3.7062	3.2698	2.1039	4.5277	4.2256	4.6412	4.8353	7.2621	6.6661
H20Y	16.5866	17.7286	17.5255	16.1579	14.8273	14.6456	17.0361	16.2322	17.2527	4.351	3.7957	3.7479	1.7706	0	1.7713	2.5722	3.7758	3.0003	3.7329	3.289	3.6294	5.5898	5.1397	4.2694	8.0557	7.6494
H20Z	16.2541	17.2737	17.2295	15.5146	14.2921	14.0179	15.9446	15.6921	16.8527	3.7537	2.515	2.515	1.7653	1.7713	0	3.1375	3.148	2.4476	4.723	3.6294	5.181	4.9406	4.986	8.4974	7.7249	
H19X	15.2262	16.3008	15.9633	14.7955	13.5401	13.1726	14.2211	14.4697	15.4591	3.7882	4.3525	3.7519	3.7957	2.5722	3.1375	0	1.7725	1.7702	4.6938	4.5549	6.247	5.2353	3.6077	2.6877	8.0798	7.6322
H19Y	13.6015	14.6184	14.3386	13.0572	11.8414	11.4267	15.5019	12.7534	13.7916	2.574	3.7818	3.025	4.3565	3.7758	3.148	1.7725	0	1.7663	5.0563	4.6682	5.9066	4.5051	2.5747	2.3515	7.4465	6.7366
H19Z	15.0313	15.9737	15.8104	14.2534	13.1151	12.6362	16.5285	14.0318	15.1854	3.1805	3.7695	2.5354	3.7062	3.0003	2.4476	1.7702	1.7663	0	5.5134	4.7953	6.5937	5.3497	4.02	3.8142	8.6077	8.031
H15A	14.8013	16.1825	15.8958	14.96	13.3967	13.6424	16.1633	15.393	16.1471	4.5098	3.8353	5.1127	3.2698	3.7329	4.723	4.6938	5.0563	5.5134	0	1.7432	2.5127	3.0651	3.7994	3.8948	4.7191	4.8606
H15B	14.6332	15.903	15.7944	14.4577	12.9785	13.1463	16.1633	15.035	15.948	3.499	2.3168	3.7646	2.1039	3.289	3.6294	4.5549	4.6682	4.7953	1.7432	0	2.4371	2.5247	3.7308	4.3186	5.2023	4.7406
H16A	13.0105	14.4071	14.2729	13.1992	11.5967	12.0528	14.9816	14.0298	14.7667	4.3109	3.6244	5.2961	4.5277	3.6294	5.5898	6.247	5.9066	6.5937	2.5127	2.4371	0	1.7597	3.898	4.9226	2.873	2.6027
H16B	12.1133	13.4058	13.2917	12.0413	10.5148	10.7697	13.757	12.6892	13.5395	2.6925	2.549	3.9865	4.2256	5.1397	5.181	5.2353	4.5051	5.3497	3.0651	2.5247	1.7597	0	2.4709	3.8953	3.5063	2.568
H13A	12.0014	13.2216	12.9014	11.8841	10.4489	10.3906	13.2212	11.9306	12.7829	2.2456	3.3654	3.7938	4.6412	4.7109	4.9406	3.6077	2.5747	4.02	3.7994	3.7308	3.898	2.4709	0	1.7619	4.9211	4.3212
H13B	13.1908	14.4221	13.9427	13.1957	11.7862	11.6395	14.315	12.9328	13.7098	3.5181	4.465	4.6121	4.8353	4.2694	4.986	2.6877	2.3515	3.8142	3.8948	4.3186	4.9226	3.8953	1.7619	0	5.9462	5.7585
H2A	11.1312	12.6944	12.3971	11.9149	10.1899	10.9457	13.5906	12.818	13.256	6.0439	6.0096	7.486	7.2621	8.0557	8.4974	8.0798	7.4465	8.6077	4.7191	5.2023	2.873	3.5063	4.9211	5.9462	0	1.7811
H2B	10.5065	11.9396	11.8394	10.8649	9.2066	9.8541	12.6959	11.8951	12.5319	4.8893	4.8951	6.3164	6.6661	7.6494	7.7249	7.6322	6.7366	8.031	4.8606	4.7406	2.6027	2.568	4.3212	5.7585	1.7811	0
H3A	9.0381	10.6651	10.1736	10.1694	8.419	9.2268	11.5961	10.858	11.1003	6.8151	7.3702	8.5053	8.9537	9.4993	9.8776	8.8641	7.9163	9.3922	6.5704	7.0646	5.0108	4.8981	5.3912	6.3746	2.4948	3.061
H3B	8.9596	10.553	10.3264	9.9468	8.1972	9.1928	11.6814	11.1184	11.4407	7.0684	7.3385	8.6343	9.1058	9.956	10.1358	9.6549	8.6611	9.9552	6.9434	7.1408	4.8648	4.9592	6.1381	7.4043	2.4008	2.5022
H11A	10.0907	11.4672	10.9032	10.5528	8.9976	9.1512	10.846	10.493	11.0359	4.6299	5.7736	6.3481	7.1989	7.2539	7.647	5.9345	4.8752	6.5479	5.4325	5.859	4.9216	3.9141	2.7122	3.3858	4.2177	4.0972
H11B	11.2464	12.5101	11.8687	11.5247	10.0999	9.9847	12.4311	11.0672	11.6724	4.6228	5.9486	6.1312	6.9725	6.6073	7.1243	4.8202	3.8984	5.6449	5.577	6.0714	5.8093	4.6838	2.5898	2.3665	5.7032	5.6002
H10A	11.5036	12.8894	11.9497	12.3654	10.8985	10.949	12.9772	11.7018	11.9542	7.0069	8.1593	8.5121	8.8941	8.3934	9.2279	6.7051	6.1336	7.8476	8.6573	7.8117	7.1926	6.5166	4.8332	4.2465	6.3368	6.8353
H10B	10.4171	11.9245	11.0294	11.5193	9.9379	10.2458	12.3138	11.2119	11.3779	7.0529	8.0676	8.71	9.0926	9.9253	9.6635	5.5642	6.8548	8.5515	7.405	7.6642	6.5101	6.0154	4.9299	4.9011	5.0444	5.6951
H4A	6.7263	8.3434	7.8226	7.9608	6.2213	7.0745	9.2741	8.6044	8.7709	7.5428	8.4448	9.2718	10.3999	10.9065	11.0384	9.8881	8.6197	10.1816	8.4656	8.7008	6.8515	6.2735	6.3579	7.4571	4.6671	4.5372
H4B	6.4795	8.0536	7.8826	7.5146	5.7548	6.8665	9.2247	8.7739	9.0491	7.7654	8.4333	9.3836	10.5695	11.3408	11.2874	10.6135	9.3	10.6972	8.8294	8.8169	6.8204	6.361	7.0133	8.3734	4.7224	4.2473
H5A	5.9973	7.2333	7.3043	6.0199	4.376	5.0491	7.8485	7.146	7.8473	6.7311	7.6894	8.2366	10.099	10.8217	10.4556	9.8413	8.2804	9.589	9.07	8.7034	7.2251	6.2037	6.4578	7.9522	5.9795	4.8722
H5B	6.5195	7.8081	7.5104	6.7836	5.1911	5.5045	8.1521	7.1702	7.7843	6.2146	7.4338	7.8572	9.6504	10.104	9.9262	8.8183	7.2788	8.7749	8.4529	8.3127	6.9934	5.8418	5.4851	6.7504	5.7274	4.8911
H9A	8.0906	9.56	8.5289	9.4119	7.9156	8.2329	9.9469	8.9256	8.9026	8.1485	9.4031	9.8774	10.9144	10.8712	11.3045	9.2745	8.1788	9.933	8.8961	9.5042	8.1784	7.4216	6.3819	6.7331	6.3603	6.6237
H9B	8.1647	9.6072	8.8705	9.0375	7.4626	7.753	9.9588	8.8806	9.1742	6.4836	7.7135	8.2328	9.3844	9.4943	9.787	8.0387	6.8262	8.5365	7.5591	7.966	6.6679	5.7659	4.8617	5.5388	5.1203	5.0735
H8A	7.8065	8.9152	8.2054	8.0768	6.8021	6.5319	8.6714	7.3	8.7276	6.5989	8.1759	8.1806	9.9822	9.9226	9.9512	8.0319	6.5715	8.2373	8.8623	9.9812	8.183	6.8661	5.408	5.9978	7.2157	6.73
H8B	7.7158	8.8432	7.8135	8.4669	7.277	7.0622	8.6213	7.3101	7.4677	8.2431	9.7952	9.8335	11.4453	11.2573	11.4515	9.2702	7.9638	9.6725	10.0529	10.39	9.4823	8.3249	6.8175	7.1255	8.1791	7.9917
H24A	3.2864	4.7395	3.7491	5.1183	3.8341	4.5265	5.5248	5.0677	4.7033	10.4321	11.7	12.0566	13.8641	14.1994	14.1152	12.6738	11.1609	12.7494	12.3738	12.4567	10.9072	9.9823	9.4992	10.4536	8.9608	8.5831
H24B	2.108	3.6371	3.2932	3.7657	2.3186	3.519	4.8043	4.6787	4.5371	10.5371	11.6875	12.0764	14.01	14.5454	14.2856	13.198	11.607	13.078	12.7292	12.6099	11.011	10.0912	9.9291	11.1086	9.1685	8.553
H22A	4.8366	4.9877	4.2742	4.616	4.4519	3.5154	3.8156	2.3561	2.6859	11.0021	12.5552	13.2562	14.7367	14.8481	15.5136	12.9302	11.2939	12.7192	13.9595	13.8041	12.834	11.4952	10.445	11.2418	11.5545	10.8282
H22B	4.6383	4.937	4.7081	3.7967	3.3515	2.2495	4.0177	2.572	3.5985	9.6931	11.1756	11.0053	13.4729	13.7284	13.2711	11.9752	10.2724	11.6202	12.8569	12.5463	11.5924	10.2184	9.3722	10.3699	10.4863	9.5681
H21A	5.2551	6.1529	5.0394	6.1043	5.2099	4.9529	5.852	4.709	4.5979	10.0117	11.5373	11.5577	13.5386	13.5742	13.5312	11.6768	10.1742	11.7801	12.3113	12.4234	11.2986	10.1164	9.0012	9.6517	9.7604	9.3426
H21B	6.2626	6.9151	6.1206	6.2585	5.5137	4.7638	6.1189	4.6022	5.0754	9.9054	10.724	10.5081	12.7221	12.6878	12.4962	10.6767	9.1106	10.6226	11.8797	11.8385	10.0227	9.6449	8.3104	8.9407	9.9126	9.2792
H14Q	14.9679	16.2375	15.8759	14.917	13.4665	13.4299	16.2596	14.9442	15.7792	3.8553	3.8052	4.2984	2.9979	2.4099	3.6477	2.5198	3.2582	3.7144	2.2644	2.7671	4.2399	3.8153	3.045	2.3527	6.1677	6.0711
H1Q	12.6397	14.1591	13.7361	13.2767	11.5996	12.0897	14.7704	13.7781	14.2878	5.3096	5.2681	6.6243	5.8618	6.305	7.1024	6.0905	7.2031		2.8933	3.9469	2.3912	3.0221	3.7982	4.2744	2.272	3.1838
H12Q	13.6464	15.0753	14.5464	14.0924	12.5095	12.7046	15.3588	14.151	14.7422	4.8776	5.1179	6.0135	4.9239	6.0395	4.546	4.667	5.7898		2.5261	3.6153	3.7155	3.6577	5.0433	2.542	4.4501	4.9511
H7Q	6.0879	7.0475	6.6053	5.9732	4.7533	4.4049	6.7738	5.4699	6.198	7.2303	8.736	8.7283	10.8993	11.1032	10.8409	9.3936	7.7553	9.2543	10.0393	9.8721	8.9198	7.5569	5.6867	5.7637	7.8802	7.0652
H6Q	4.2093	5.1694	5.1252	3.9797	2.5256	2.7073	5.3459	4.5033	5.2249	8.4255	9.6946	9.8683	12.0829	12.5684	12.1583	11.1531	9.4785	10.8557	11.2152	10.9005	9.6482	8.4464	8.0841	9.3312	8.3628	7.4134
H23Q	3.0016	3.6505	2.4132	4.2991	3.8	3.8603	3.7126	3.2615	2.517	11.7505	13.1529	13.2607	15.3715	15.6209	15.4097	13.895	12.3041	13.8318	14.176	14.1526	12.8081	11.71	10.9956	11.8855	11.075	10.5497

(cont.) Table H.8: Hydrogen Distances for the Optimized Structure of 4z,5'e *cis-anti-cis* DtBuCH18C6

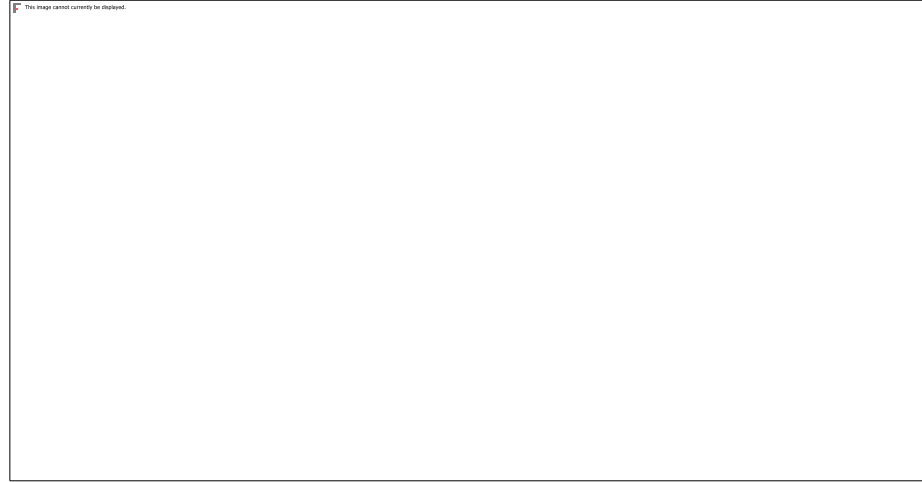| H3A	H3B	H11A	H11B	H10A	H10B	H4A	H4B	H5A	H5B	H9A	H9B	H8A	H8B	H24A	H24B	H22A	H22B	H21A	H21B	H14Q	H1Q	H12Q	H7Q	H6Q	H23Q	
9.0381	8.9596	10.0907	11.2464	11.5036	10.4171	6.7263	6.4795	5.9973	6.5195	8.0906	8.1647	7.8065	7.7158	3.2864	2.108	4.8366	4.6383	5.2551	6.2626	14.9679	12.6397	13.6464	6.0879	4.2093	3.0016	H27X
10.6651	10.553	11.4672	12.5101	12.8894	11.9245	8.3434	8.0536	7.2333	7.8081	9.56	9.6072	8.9152	8.8432	4.7395	3.6371	4.9877	4.937	6.1529	6.9151	16.2375	14.1591	15.0753	7.0475	5.1694	3.6505	H27Y
10.1736	10.3264	10.9032	11.8687	11.9497	11.0294	7.8226	7.8826	7.3043	7.5104	8.5289	8.8705	8.2054	7.8135	3.7491	3.2932	4.2742	4.7081	5.0394	6.1206	15.8759	13.7361	14.5464	6.6053	5.1252	2.4132	H27Z
10.1694	9.9468	10.5528	11.5247	12.3654	11.5193	7.9608	7.5146	6.0199	6.7836	9.4119	9.0375	8.0768	8.4669	5.1183	3.7657	4.616	3.7967	6.2585	6.1043	14.917	13.2767	14.0924	5.9732	3.9797	4.2991	H26X
8.419	8.1972	8.9976	10.0999	10.8985	9.9379	6.2213	5.7548	4.376	5.1911	7.9156	7.4626	6.8021	7.277	3.8341	2.3186	4.4519	3.3515	5.2099	5.5137	13.4665	11.5996	12.5095	4.7533	2.5256	3.8	H26Y
9.2268	9.1928	9.1512	9.9847	10.9439	10.2458	7.0745	6.8665	5.0186	5.5045	8.2329	7.753	6.5319	7.0622	4.5265	3.519	3.5154	2.2495	4.9529	4.7638	13.4299	12.0897	12.7084	4.4049	2.7073	3.8603	H26Z
11.5961	11.6814	11.6846	12.4311	12.9772	12.3138	9.2741	9.2247	7.8485	8.1521	9.9469	9.9588	8.6714	8.6213	5.5248	4.8043	3.8156	4.0177	5.8572	6.1189	16.2596	14.7704	15.3588	6.7738	5.3459	3.7126	H28X
10.858	11.1184	10.493	11.0672	11.7018	11.2119	8.6044	8.7739	7.146	7.1702	9.9256	8.8806	7.3	7.3101	5.0677	4.6787	2.3561	2.572	4.709	4.6022	14.9442	13.7781	14.1571	5.4699	4.5033	3.2615	H28Y
11.1003	11.4407	11.0359	11.6724	11.9542	11.3779	8.7709	9.0491	7.8473	7.7843	8.9026	9.1742	7.8276	7.4677	4.7033	4.5625	2.6859	3.5985	4.5979	5.0754	15.7792	14.2878	14.7422	6.198	5.2249	2.517	H28Z
6.8151	7.0684	4.6299	4.6228	7.0069	7.0529	7.5428	7.7654	6.7311	6.2146	8.1485	6.4836	6.5989	8.2431	10.4321	10.5371	11.0021	10.0117	9.0954	3.8553	5.3096	4.8776	7.2303	8.4255	11.7505	H18X
7.3702	7.3385	5.7736	5.9486	8.1593	8.0676	8.4448	8.4333	7.6894	7.4338	9.4031	7.7135	8.1759	7.9952	11.7	11.6875	12.5552	11.1756	11.5373	10.724	3.8052	5.2681	5.1179	8.736	6.6946	13.1529	H18Y
8.5053	8.6343	6.3481	6.1312	8.5121	8.71	9.2718	9.3836	8.2366	7.8572	9.8774	8.2328	8.1806	9.8335	12.0566	12.0764	12.3562	11.0053	11.5577	10.5081	4.2984	6.6243	6.0135	8.7283	9.8683	13.2607	H18Z
8.9537	9.1058	7.1989	6.9725	8.8941	9.0926	10.3999	10.5695	10.099	9.6504	10.9144	9.3844	9.9822	11.4453	13.8641	14.021	14.7367	13.4729	13.5386	12.7221	2.9979	5.8618	5.1222	10.8993	12.0829	15.3715	H20X
9.4993	9.956	7.2539	6.6073	8.3934	8.9253	10.9065	11.3408	10.8217	10.104	10.8712	9.4943	9.9226	11.2573	14.1994	14.5454	14.8481	13.7284	13.5742	12.6878	2.4099	6.305	4.9239	11.1032	12.5684	15.6209	H20Y
9.8776	10.1358	7.647	7.1243	9.2279	9.6635	11.0384	11.2874	10.4556	9.9262	11.3045	9.787	9.9512	11.4515	14.1152	14.2856	14.5136	13.2711	13.5132	12.4962	3.6477	7.1024	6.0395	10.8409	12.1583	15.4097	H20Z
8.8641	9.6549	5.9345	4.8202	6.7051	7.5642	9.8881	10.6135	9.8413	8.8183	9.2745	8.0387	8.0319	9.2702	12.6738	13.198	12.9302	11.9752	11.6768	10.6767	2.5198	6.3431	4.546	9.3936	11.1531	13.895	H19X
7.9163	8.6611	4.8752	3.8984	6.1636	6.8548	8.6197	9.3	8.2804	7.2788	8.1788	6.8262	6.5715	7.9638	11.1609	11.6077	11.2939	10.2724	10.1742	9.1106	3.2582	6.0905	4.667	7.7553	9.4785	12.3041	H19Y
9.3922	9.9552	6.5479	5.6449	7.8476	8.5515	10.1816	10.6972	9.589	8.7749	9.933	8.5365	8.2373	9.6725	12.7494	13.078	12.7192	11.6202	11.7801	10.6226	3.7144	7.2031	5.7898	9.2543	10.8557	13.8318	H19Z
6.5704	6.9434	5.4325	5.577	6.8573	6.7405	8.4656	8.8294	9.07	8.4529	8.8961	7.5591	8.8623	10.0529	12.3738	12.7292	13.9595	12.8569	12.3113	11.8797	2.2644	2.8933	2.5261	10.0393	11.2152	14.176	H15A
7.0646	7.1408	5.859	6.0714	7.8117	7.6642	8.7008	8.8169	8.7034	8.3127	9.5042	7.966	8.9812	10.39	12.4567	12.6099	13.8041	12.5463	12.4234	11.8385	2.7671	3.9469	3.8435	9.8721	10.9005	14.1526	H15B
5.0108	4.8648	4.9216	5.8093	7.1926	6.5101	6.8515	6.8204	7.2251	6.9934	8.1784	6.6679	6.6661	9.4823	10.972	11.011	11.4952	10.2184	10.1164	9.6449	3.8153	3.0221	3.6577	7.5569	8.4464	12.8081	H16A
4.8981	4.9592	3.9141	4.6838	6.5166	6.0154	6.2735	6.361	6.2037	5.8418	7.4216	5.7659	6.8661	8.3249	9.9823	10.0912	11.4952	10.2184	10.1164	6.6449	3.8153	3.0221	3.6577	7.5569	8.4464	11.71	H16B
5.3912	6.1381	2.7122	2.5898	4.8332	4.9299	6.3579	7.0133	6.4578	5.4851	6.3819	4.8617	5.408	6.8175	9.4992	9.9291	10.445	9.3722	9.0012	8.3104	3.045	3.7982	3.0433	6.5867	8.0841	10.9956	H13A
6.3746	7.4043	3.3858	2.3665	4.2465	4.9011	7.4571	8.3734	7.9522	6.7504	6.7331	5.5388	5.9978	7.1255	10.4536	11.1086	11.2418	10.3699	9.6517	8.9407	2.3527	4.2744	2.542	7.5637	9.3312	11.8855	H13B
2.4948	2.4008	4.2177	5.7032	6.3368	5.0444	4.6671	4.7224	5.9795	5.7274	5.1203	7.2157	8.1791	8.9608	9.1685	11.5545	10.4863	9.7604	9.9126	6.1677	2.272	4.4501	7.8802	8.3628	11.075	H2A
3.061	2.5022	4.0972	5.6002	6.8353	5.6951	4.5372	4.2473	4.8722	4.8911	6.6237	5.0735	6.73	7.9917	8.5831	8.553	10.8282	9.5681	9.3426	9.2792	6.0711	3.1838	4.9511	7.0652	7.4134	10.5497	H2B
0	1.7822	3.443	5.1642	5.3361	3.7024	2.3622	3.0422	4.6033	4.0489	4.1783	3.1804	5.4962	6.1646	6.6321	7.055	9.4741	8.6019	7.5219	7.9349	7.4138	3.8775	5.4391	6.0968	6.5572	8.8004	H3A
1.7822	0	4.7513	6.515	7.0371	5.462	2.9833	2.5014	4.3387	4.496	4.6092	4.6414	7.497	7.1142	7.109	10.071	8.9989	8.4154	8.1167	4.5061	6.4314	6.7589	6.6901	9.2808	H3B
3.443	4.7513	0	1.7809	3.0724	2.5328	4.1231	5.2729	5.1973	3.8207	3.7195	2.2601	3.5897	4.6683	7.2836	7.9864	8.79	9.7529	6.9312	6.6577	5.1774	3.7601	3.707	5.0409	6.5792	8.9677	H11A
5.1642	6.515	1.7809	0	2.4697	3.0636	5.7403	6.9798	6.596	5.0842	4.4643	3.434	3.8551	4.8042	8.329	9.1795	9.2139	8.5216	7.4246	6.8756	4.6093	4.6319	3.5961	5.6766	7.592	9.742	H11B
5.3361	7.0371	3.0724	2.4697	0	1.7733	5.9528	7.5334	7.7474	6.1097	3.5986	3.5855	4.54	4.5714	8.3097	9.5075	9.0668	9.3263	7.3995	7.303	6.1595	5.3033	4.4005	6.5912	8.474	9.8013	H10A
3.7024	5.462	2.5328	3.0636	1.7733	0	4.4422	6.0197	6.6498	5.1588	2.6196	2.5164	3.4629	4.4567	7.296	8.403	9.2473	8.8314	6.9407	7.1436	6.6006	4.4512	4.4766	6.1063	7.6339	9.0706	H10B
2.3622	2.9833	4.1231	5.7403	5.9528	4.4422	0	1.7791	3.0654	2.5013	3.3849	2.6154	4.347	4.875	4.3064	4.7154	7.3075	6.4841	5.481	6.0864	8.9376	6.011	7.2073	4.3357	4.437	6.4804	H4A
3.0422	2.5014	5.2729	6.9798	7.5334	6.0197	1.7791	0	2.4978	3.0576	5.1561	4.2121	5.6456	6.4038	4.8878	4.6447	7.9217	6.8485	6.5343	7.0721	9.5726	6.5223	8.0457	5.097	4.4673	6.9803	H4B
4.6033	4.3387	5.1973	6.596	7.7474	6.6498	3.0654	2.4978	0	1.7778	5.3644	4.3209	4.6218	5.804	4.6198	4.1101	6.472	5.0553	5.6622	5.6578	9.3607	7.3257	8.373	3.4355	2.6819	6.1767	H5A
4.0489	4.496	3.8207	5.0842	6.1097	5.1588	2.5013	3.0576	1.7778	0	4.0112	2.7151	2.9088	4.1446	4.2674	4.4483	5.9383	4.7658	4.5423	4.8548	8.4548	6.6406	7.3363	2.3007	2.8575	5.8775	H5B
4.1783	5.73	3.7195	4.4643	3.5986	2.6196	3.3849	5.1561	5.3644	4.0112	0	1.7766	3.0683	2.5279	4.8544	6.185	6.9255	6.7341	4.4925	5.0751	8.706	6.6121	6.8444	4.4063	5.7664	6.5426	H9A
3.1804	4.6092	2.2601	3.434	3.5855	2.5164	2.6154	4.2121	4.3209	2.7151	1.7766	0	2.4702	3.0638	5.1691	6.0952	7.0915	6.4665	4.9885	5.1447	7.4336	5.4249	5.7777	3.7282	5.1236	6.9416	H9B
5.4962	6.6414	3.5897	3.8551	4.54	3.4629	4.347	5.6456	4.6218	2.9088	3.0683	2.4702	0	1.7767	4.941	5.8849	5.3742	4.8149	3.6715	3.0973	8.196	7.3049	7.1512	2.1479	4.4314	5.9846	H8A
6.1646	7.497	4.6683	4.8042	4.5714	4.4567	4.875	6.4038	5.8034	4.1446	2.5279	3.0638	1.7767	0	4.6	5.9683	5.1002	5.1224	2.9115	2.9086	9.3816	8.2594	8.0646	3.144	5.054	5.4859	H8B
6.6321	7.1142	7.2836	8.329	8.3097	7.296	4.3064	4.8878	4.6198	4.2674	4.8544	5.1691	4.941	4.6	0	1.7488	3.8974	3.8002	2.6596	4.0305	12.3769	10.1252	10.8835	3.8045	3.0459	2.2756	H24A
7.055	7.109	7.9864	9.1795	9.5075	8.403	4.7154	4.6447	4.1101	4.4483	6.185	6.0952	5.8849	5.9683	1.7488	0	4.3241	3.7973	3.4933	2.8712	12.2743	11.5408	4.2656	2.5109	2.7734	H24B
9.4741	10.071	8.79	9.2139	9.6068	9.2473	7.3075	7.9217	6.472	5.9383	6.9255	7.0915	5.3742	5.1002	3.8974	4.3241	0	1.7522	2.5407	2.4398	13.387	12.2743	12.4604	3.9454	3.8872	2.3539	H22A
8.6019	8.9989	7.9529	8.5216	9.2963	8.8314	6.4841	6.8485	5.0553	4.7658	6.7341	6.4665	4.8149	5.1224	3.8002	3.7379	1.7522	0	3.067	2.553	12.3826	11.2966	11.5993	2.9142	2.4759	3.0413	H22B
7.5219	8.4154	6.9312	7.4246	7.3995	6.9407	5.481	6.5343	5.6622	4.6349	4.4925	4.9885	3.6715	2.9115	2.6596	3.9793	2.5407	3.067	0	1.7618	10.396	10.5729	3.0026	3.7273	2.6422	H21A
7.9349	8.8155	6.6577	6.8756	7.303	7.1436	6.0864	7.0721	5.6578	5.4423	5.0751	5.1447	3.0973	2.9086	4.0305	3.7379	2.4398	2.553	1.7618	0	11.1574	10.306	10.2462	2.3533	3.7315	3.7884	H21B
7.4138	8.1167	5.1774	4.6093	6.1595	6.6006	8.9376	9.5726	9.3607	8.4548	8.706	7.4336	8.196	9.3816	12.3769	12.8783	13.387	12.3826	11.8323	11.1574	0	4.2035	2.5371	9.5837	11.1181	13.9403	H14Q
3.8775	4.5061	3.7601	4.6319	5.3033	4.5512	6.011	6.5223	7.3257	6.6406	6.6121	5.4249	7.3049	8.2594	10.1252	10.5799	12.2743	11.2966	10.3796	10.306	4.2035	0	2.2817	8.4641	9.4755	12.1138	H1Q
5.4391	6.4314	3.707	3.5961	4.4005	4.4766	7.2073	8.0457	8.373	7.3363	6.8444	5.7777	7.1512	8.0646	10.8835	11.5408	12.4604	11.5993	10.5729	10.2462	2.5371	2.2817	0	8.6902	10.1621	12.655	H12Q
6.0968	6.7589	5.0409	5.6766	6.5912	6.1063	4.3357	5.097	3.4355	2.3007	4.4063	3.7282	2.1479	3.144	3.8045	4.2656	3.9454	2.9142	3.0026	2.3533	9.5837	8.4641	8.6902	0	2.3092	4.5885	H7Q
6.5572	6.6901	6.5792	7.592	8.474	7.6339	4.437	4.4673	2.6819	2.8575	5.7664	5.1236	4.3314	5.054	3.0459	2.5109	3.8872	2.4759	3.7273	3.7315	11.1181	9.4755	10.1621	2.3092	0	3.8029	H6Q
8.8004	9.2808	8.9677	9.742	9.8013	9.0706	6.4804	6.9803	6.1767	5.8775	6.5426	6.9416	5.9846	5.4859	2.2756	2.7734	2.3539	3.0413	2.6422	3.7884	13.9403	12.1138	12.655	4.5885	3.8029	0	H23Q

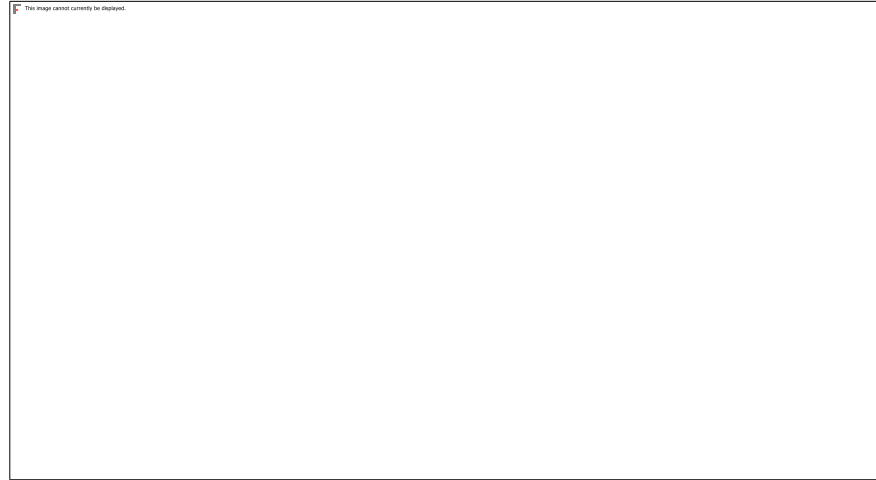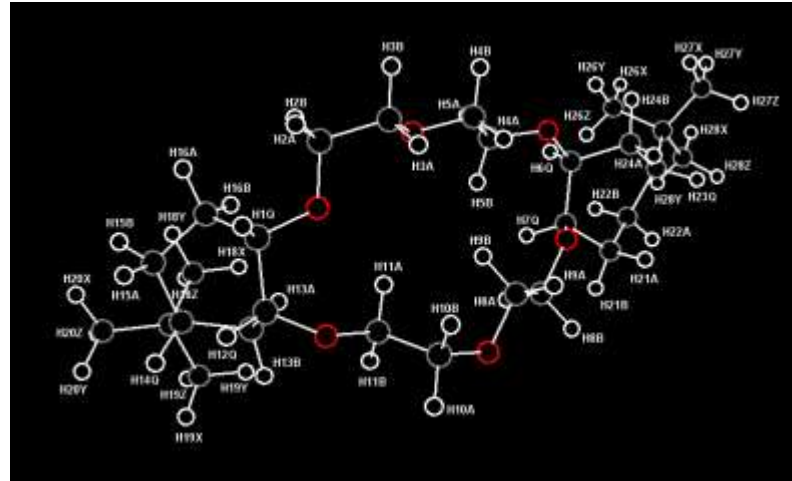Figure H.17: Optimized Structure of 4z,5'z *cis-anti-cis* DtBuCH18C6 with Hydrogen Labels

Figure H.18: Optimized Structure of 4z,5'z *cis-anti-cis* DtBuCH18C6 with Carbon and Oxygen Labels

Table H.9: Hydrogen Distances for the Optimized Structure of 4z,5'z *cis-anti-cis* DtBuCH18C6

	H18X	H18Y	H18Z	H20X	H20Y	H20Z	H19X	H19Y	H19Z	H26X	H26Y	H26Z	H27X	H27Y	H27Z	H28X	H28Y	H28Z	H15A	H15B	H16A	H16B	H13A	H13B	H2A	H2B
H18X	0	1.7725	1.7658	3.8109	4.3518	3.7579	3.7908	2.5773	3.1797	12.9595	14.1179	12.7596	12.4119	12.2892	13.7649	13.1332	12.8893	14.2017	4.5046	3.4911	4.3054	2.6886	2.2434	3.5221	6.0668	4.919
H18Y	1.7725	0	1.7654	2.6004	3.793	3.0887	4.3527	3.7833	3.767	14.1315	15.3676	13.9423	13.9174	13.6696	15.1847	14.4829	14.3721	15.611	3.8345	2.3128	3.6265	2.5552	3.3707	4.4705	6.0394	4.921
H18Z	1.7658	1.7654	0	3.1313	3.752	2.5217	3.7503	3.0255	2.5314	14.3952	15.6154	14.316	13.9068	13.8839	15.2997	14.432	14.2059	15.5821	5.1124	3.7628	5.2964	3.9881	3.79	4.6138	7.5122	6.3459
H20X	3.8109	2.6004	3.1313	0	1.7709	1.7649	3.7971	4.3566	3.7065	16.5413	17.6907	16.2302	16.0177	15.7722	17.3345	16.8856	16.6539	17.9252	3.2778	2.1096	4.5323	4.2317	4.6442	4.8407	7.28	6.6747
H20Y	4.3518	3.793	3.752	1.7709	0	1.7711	2.5747	3.7783	3.0105	17.0845	18.1145	16.694	16.1066	15.9664	17.5136	17.2805	16.8693	18.2113	3.7274	3.2846	5.5847	5.1399	4.7076	4.2683	8.0584	7.6526
H20Z	3.7579	3.0887	2.5217	1.7649	1.7711	0	3.1289	3.7132	2.4458	16.7092	17.8535	16.501	15.9663	15.9164	17.3912	16.7838	16.4585	17.8471	4.7253	3.6338	5.9313	5.1889	4.9386	4.9846	8.518	7.7459
H19X	3.7908	4.3527	3.7503	3.7971	2.5747	3.1289	0	1.7724	1.7706	15.6761	16.5712	15.2584	14.2075	14.2441	15.7172	15.6346	15.0277	16.45	4.6956	4.5543	6.2481	5.2394	3.6039	2.6907	8.0908	7.6521
H19Y	2.5773	3.7833	3.0255	4.3566	3.7783	3.7132	1.7724	0	1.7665	14.0223	14.9608	13.6893	12.6635	12.7424	14.1782	13.9247	13.3579	14.7937	5.0518	4.6631	5.9026	4.5038	2.563	2.3486	7.4582	7.7615
H19Z	3.1797	3.767	2.5314	3.7065	3.0105	2.4458	1.7706	1.7665	0	15.4237	16.4471	15.2054	14.216	14.3523	15.7471	15.2456	14.7309	16.2114	5.514	4.7935	6.592	5.3494	4.0107	3.8145	8.6226	7.8261
H26X	12.9595	14.1315	14.3952	16.5413	17.0845	16.7092	15.6761	14.0223	15.4237	0	1.7706	1.7726	4.3527	3.7889	3.75	2.5704	3.7951	3.1321	15.4105	15.2016	13.6442	12.6902	12.5238	13.7054	11.8591	11.1942
H26Y	14.1179	15.3676	15.6154	17.6907	18.1145	17.8535	16.5712	14.9608	16.4471	1.7706	0	1.7668	3.7667	3.1774	2.5308	3.004	3.7063	2.4463	16.3906	16.3272	14.7465	13.8177	13.4709	14.5007	12.7993	12.3187
H26Z	12.7596	13.9423	14.316	16.2302	16.694	16.501	15.2584	13.6893	15.2054	1.7726	1.7668	0	3.7823	2.5746	3.0256	3.7751	4.3566	3.7138	14.7915	14.7778	13.1076	12.2619	12.0304	13.0929	11.0771	10.6576
H27X	12.4119	13.9174	13.9068	16.0177	16.1066	15.9663	14.2075	12.6635	14.216	4.3527	3.7667	3.7823	0	1.7726	1.7654	3.7958	2.6065	3.0861	14.8162	14.8796	13.6582	12.5107	11.5323	12.2324	11.9814	11.5666
H27Y	12.2892	13.6696	13.8839	15.7722	15.9664	15.9164	14.2441	12.7424	14.3523	3.7889	3.1774	2.5746	1.7726	0	1.7662	4.3509	3.8143	2.5164	14.2879	14.4393	12.9765	12.0092	11.2867	12.0616	11.0239	10.7535
H27Z	13.7649	15.1847	15.2997	17.3345	17.5136	17.3912	15.7172	14.1782	15.7471	3.75	2.5308	3.0256	1.7654	1.7662	0	3.7489	3.1344	2.5164	15.9753	16.0697	14.6591	13.6371	12.8678	13.6341	12.756	12.4201
H28X	13.1332	14.4829	14.432	16.8856	17.2805	16.7838	15.6346	13.9247	15.2456	2.5704	3.004	3.7751	3.7958	4.3509	3.7489	0	1.7707	1.7711	16.1238	15.8106	14.5821	13.3793	12.8502	13.93	13.1418	12.318
H28Y	12.8893	14.3721	14.2059	16.6539	16.8693	16.4585	15.0277	13.3579	14.7309	3.7951	3.7063	4.3566	2.6065	3.8143	3.1344	1.7707	0	1.7651	15.8786	15.6645	14.5171	13.2909	12.446	13.3411	13.1787	12.444
H28Z	14.2017	15.611	15.5821	17.9252	18.2113	17.8471	16.45	14.7937	16.2114	3.1321	2.4463	3.7138	3.0861	2.5164	2.5164	1.7711	1.7651	0	16.9541	16.7978	15.511	14.356	13.6825	14.6173	13.8759	13.2413
H15A	4.5046	3.8345	5.1124	3.2778	3.7274	4.7253	4.6956	5.0518	5.514	15.4105	16.3906	14.7915	14.8162	14.2879	15.9753	16.1238	15.8786	16.9541	0	1.7438	2.5102	3.0656	3.8017	3.8936	4.7145	4.8439
H15B	3.4911	2.3128	3.7628	2.1096	3.2846	3.6338	4.5543	4.6631	4.7935	15.2016	16.3272	14.7778	14.8796	14.4393	16.0697	15.8106	15.6645	16.7978	1.7438	0	2.436	2.5245	3.731	4.3174	5.2128	4.7358
H16A	4.3054	3.6265	5.2964	4.5323	5.5847	5.9313	6.2481	5.9026	6.592	13.6442	14.7465	13.1076	13.6582	12.9765	14.6591	14.5821	14.5171	15.511	2.5102	2.436	0	1.7596	3.9043	4.923	2.887	2.5826
H16B	2.6886	2.5552	3.9881	4.2317	5.1399	5.1889	5.2394	4.5038	5.3494	12.6902	13.8177	12.2619	12.5107	12.0092	13.6371	13.3793	13.2909	14.356	3.0656	2.5245	1.7596	0	2.4783	3.8992	3.5303	2.5811
H13A	2.2434	3.3707	3.79	4.6442	4.7076	4.9386	3.6039	2.563	4.0107	12.5238	13.4709	12.0304	11.5323	11.2867	12.8678	12.8502	12.446	13.6825	3.8017	3.731	3.9043	2.4783	0	1.7611	4.9451	4.3543
H13B	3.5221	4.4705	4.6138	4.8407	4.2683	4.9846	2.6907	2.3486	3.8145	13.7054	14.5007	13.0929	12.2324	12.0616	13.6341	13.93	13.3411	14.6173	3.8936	4.3174	4.923	3.8992	1.7611	0	5.9518	5.7765
H2A	6.0668	6.0394	7.5122	7.28	8.0584	8.518	8.0908	7.4582	8.6226	11.8591	12.7993	11.0771	11.9814	11.0239	12.756	13.1418	13.1787	13.8759	4.7145	5.2128	2.887	3.5303	4.9451	5.9518	0	1.7813
H2B	4.919	4.921	6.3459	6.6747	7.6526	7.7459	7.6521	7.7615	7.8261	11.1942	12.3187	10.6576	11.5666	10.7535	12.4201	12.318	12.444	13.2413	4.8439	4.7358	2.5826	2.5811	4.3543	5.7765	1.7813	0
H3A	6.8221	7.383	8.5138	8.9652	9.5036	9.8894	8.8762	7.9228	9.399	9.7555	10.5312	8.8085	9.6454	8.6096	10.3578	11.077	11.0339	11.6433	6.5732	7.0683	5.014	4.9028	5.4079	6.3854	2.4976	3.061
H3B	7.0951	7.3637	8.6618	9.1173	9.9605	10.1569	9.6748	8.6843	9.977	9.7312	10.7102	8.9705	10.394	9.266	10.9484	11.2471	11.9869		6.933	7.141	4.8587	4.9712	6.1687	7.4217	2.3951	2.5045
H11A	4.5613	5.7163	6.2803	7.1528	7.2078	7.5919	5.8943	4.8174	6.4885	10.669	11.4184	9.9165	9.4814	9.0366	10.7	11.2211	10.7651	11.8307	5.4044	5.8121	4.4895	3.8628	2.6576	3.3558	4.2289	4.0954
H11B	4.6282	5.9616	6.1341	6.9888	6.6181	7.1313	4.8296	3.8962	5.6451	11.745	12.3884	11.0108	9.9934	9.8012	11.3773	11.9846	11.3042	12.5172	5.5936	6.0835	5.8238	4.6957	2.5978	2.3797	5.7215	5.633
H10A	7.0059	8.1704	8.5228	8.94	8.4509	9.2687	6.7682	6.1915	7.8859	11.9321	12.2629	10.8766	9.7543	9.3874	10.9893	12.3509	11.549	12.5651	6.8947	7.8349	7.1882	6.5053	4.8377	4.292	6.2879	6.7982
H10B	7.0009	8.0205	8.6656	9.0746	8.9201	9.6442	7.5749	6.8379	8.5374	10.9417	11.3432	9.8253	9.2923	8.6416	10.3441	11.6963	11.097	11.9512	6.7206	7.6261	6.4505	5.9496	4.8944	4.904	4.9534	5.5066
H4A	7.5436	8.4476	9.27	10.4125	10.9241	11.0513	9.918	8.6383	10.1934	7.3896	8.1741	6.4717	7.4189	6.3624	8.0794	8.7059	8.7134	9.2666	8.4851	8.7069	6.8556	6.2741	6.3854	7.4952	4.6925	4.5466
H4B	7.8002	8.4507	9.4157	10.5747	11.3531	11.313	10.6563	9.3498	10.7389	7.2765	8.3279	6.6151	8.2819	7.1586	8.7543	8.84	9.1886	9.6172	8.8113	8.8032	6.7875	6.3568	7.0571	8.4152	4.6923	4.2304
H5A	6.8078	7.7174	8.2986	10.0315	10.8921	10.5227	9.9719	8.4204	9.7034	6.587	7.9071	6.4304	7.5549	6.8993	8.3217	7.5615	7.9042	8.6569	9.092	8.7085	7.1933	6.2126	6.5749	8.0922	5.9673	4.8508
H5B	6.2145	7.4071	7.8414	9.6545	10.1466	9.9427	9.8085	7.3578	8.8236	7.0034	8.0498	5.5843	6.8798	6.3645	7.9084	7.6815	7.6204	8.5601	8.4827	8.3037	6.967	5.8212	5.5608	6.8704	5.7423	4.8679
H9A	8.0645	9.3133	9.7986	10.8575	10.8414	11.256	9.2769	8.1551	9.904	8.5402	8.8103	7.3597	6.7509	6.0428	7.7454	9.2839	8.6638	9.4158	8.8386	9.4223	8.068	7.3104	6.3277	6.7311	6.2293	6.4864
H9B	6.3865	7.6133	8.1377	9.3109	9.4421	9.7174	8.015	6.7815	8.4819	8.7094	9.319	7.8011	7.4673	6.8622	8.2552	9.4096	8.957	9.8632	7.4974	8.7872	6.5665	6.6547	4.8	5.5246	5.0356	4.9672
H8A	6.5546	8.1287	8.1364	9.9653	9.9323	9.9393	8.0681	6.5856	8.2398	8.691	8.4919	6.207	6.1912	7.6569	8.1318	7.4039	8.6311	8.8543	8.948	8.1332	6.8101	5.3989	6.0396	7.1787		6.6848
H8B	8.2004	9.7483	9.7967	11.436	11.2801	11.4518	9.3228	7.988	9.6915	7.9106	8.1313	7.0228	5.2842	5.2478	6.7008	7.9523	7.003	8.0822	10.0409	10.3542	9.4158	8.2567	6.8028	7.1684	8.0989	7.909
H24A	10.4558	11.7227	12.0659	13.9104	14.2642	14.1547	12.754	11.2208	12.7906	3.6173	4.0253	2.578	3.373	2.2502	3.8004	4.7184	4.651	4.9486	12.454	12.5045	10.9596	10.0224	9.5736	10.5575	9.0538	8.6493
H24B	10.5461	11.6778	12.0735	14.0245	14.5751	14.3014	13.2627	11.6647	13.1153	2.7004	3.8192	2.3486	4.4693	3.5163	4.614	4.2805	4.8469	4.9934	12.6029		10.9943	10.0824	9.9793	11.187	9.1847	8.5542
H22A	10.9767	12.5187	13.2279	14.7162	14.853	14.5061	12.9604	11.3133	12.7284	4.5574	4.7964	4.6665	2.3161	3.4958	3.7654	3.2927	2.1113	3.6346	13.9379	13.7667	12.7806	11.4465	10.4391	11.2682	11.517	10.7954
H22B	9.6347	11.1166	10.9292	13.4183	13.6842	13.2098	11.9401	10.2293	11.5568	4.7004	5.5176	5.0517	3.8331	4.5017	5.1127	3.7451	3.2839	4.7331	12.8325	12.5004	11.5641	10.1792	9.3457	10.36	10.5161	9.5933
H21A	9.9904	11.4972	11.5402	13.5296	13.6044	13.5296	11.7501	10.294	11.8265	5.2316	5.3368	4.4907	2.5426	2.6727	3.9735	5.1418	4.3221	5.1792	12.7	11.1285	10.0485	9.0078	9.7111	9.6675	9.8389	9.2509
H21B	9.0866	10.704	10.5074	12.7197	12.7111	12.5148	10.7273	9.1512	10.6622	6.2481	6.5867	5.8952	3.615	4.2924	5.2854	5.5975	4.5379	5.9295	11.8534	11.8062	10.959	9.5919	8.3034	9.8684	9.8389	9.2233
H14Q	3.8542	3.8062	4.2989	3.0053	2.4064	3.6459	2.5217	3.2543	3.7162	15.5134	16.422	14.9384	14.4	14.1237	15.7385	15.884	15.4316	16.673	2.2651	2.7673	4.2396	3.8184	3.044	2.351	6.1689	6.0739
H1Q	5.3053	5.2691	6.6219	5.862	6.2925	7.0993	6.3406	6.0833	7.1981	13.3174	14.1723	12.5033	12.8037	12.0476	13.7886	14.3097	14.1071	14.9889	2.8832	3.9405	2.3894	3.023	3.8051	4.2714	2.2637	3.165
H12Q	4.8777	5.1276	6.018	5.1404	4.629	6.0469	4.5507	4.6609	5.7923	14.281	15.0118	12.6018	14.2962	14.8991	14.4527	15.5171			2.5396	3.8545	3.7233	3.664	0.0439	2.5353	4.4392	9.443
H7Q	7.2132	8.7043	8.7022	10.8936	11.1292	10.8447	9.454	8.7023	9.2804	6.3369	7.1876	6.0741	5.2464	5.2865	6.603	6.293	5.8489	7.0868	10.0485	9.8531	8.8867	7.5241	6.6166	7.6374	7.876	7.0477
H6Q	8.3998	9.6438	9.829	12.0482	12.5668	12.1397	11.1941	9.5144	10.8671	4.5816	5.8299	4.6789	5.1891	4.9154	6.0699	5.0016	5.2178	6.1149	11.196	10.8539	9.5904	8.3972	8.106	9.3885	8.3482	7.3818
H23Q	10.896	12.1914	12.2583	14.6018	15.0619	14.5996	13.5423	11.8409	13.1855	2.5247	3.7175	3.2577	3.8046	3.8546	4.2982	2.4082	2.9981	3.6462	13.7737	13.4558	12.1818	11.0045	10.5985	11.7693	10.7798	9.9143

(cont.) Table H.9: Hydrogen Distances for the Optimized Structure of 4z,5'z *cis-anti-cis* DtBuCH18C6

H3A	H3B	H11A	H11B	H10A	H10B	H4A	H4B	H5A	H5B	H9A	H9B	H8A	H8B	H24A	H24B	H22A	H22B	H21A	H21B	H14Q	H1Q	H12Q	H7Q	H6Q	H23Q	
6.8221	7.0951	4.5613	4.6282	7.0059	7.0009	7.5436	7.8002	6.8078	6.2145	8.0645	6.3865	6.5546	8.2004	10.4558	10.5461	10.9767	9.6347	9.9904	9.0866	3.8542	5.3053	4.8777	7.2132	8.3998	10.896	H18X
7.383	7.3637	5.7163	5.9616	8.1704	8.0205	8.4476	8.4507	7.7174	7.4071	9.3133	7.6133	8.1287	9.7483	11.7227	11.6778	12.5187	11.1166	11.4972	10.704	3.8062	5.2691	5.1276	8.7043	9.6438	12.1914	H18Y
8.5138	8.6618	6.2803	6.1341	8.5228	8.6656	9.27	9.4157	8.2986	7.8414	9.7986	8.1377	8.1364	9.7967	12.0659	12.0735	12.3279	10.9292	11.5402	10.5074	4.2989	6.6219	6.018	8.7022	9.829	12.2583	H18Z
8.9652	9.1173	7.1528	6.9888	8.94	9.0746	10.4125	10.5747	10.1315	9.6545	10.8575	9.3109	9.9653	11.436	13.9104	14.0245	14.7162	13.4183	13.5296	12.7197	3.0053	5.862	5.1404	10.8936	12.0482	14.6018	H20X
9.5036	9.9605	7.2078	6.6181	8.4509	8.9201	10.9241	11.3531	10.8921	10.1466	10.8414	9.4421	9.9323	11.2801	14.2642	14.5751	14.853	13.6842	13.6044	12.7111	2.4064	6.2925	4.9284	11.1292	12.5668	15.0619	H20Y
9.8894	10.1569	7.5919	7.1313	9.2687	9.6442	11.0513	11.313	10.5227	9.9427	11.256	9.7174	9.9393	11.4518	14.1547	14.3014	14.5061	13.2098	13.5269	12.5148	3.6459	7.0993	6.0469	10.8447	12.1397	14.5996	H20Z
8.8762	9.6748	5.8943	4.8296	6.7682	7.5749	9.918	10.6563	9.9719	8.9085	9.2769	8.015	8.0681	9.3228	12.754	13.2627	12.9604	11.9401	11.7501	10.7273	2.5217	6.3406	4.5507	9.454	11.1941	13.5423	H19X
7.9228	8.6843	4.8174	3.8962	6.1915	6.8379	8.6383	9.3498	8.4204	7.3578	8.1551	6.7815	6.5856	7.988	11.2208	11.6647	11.3133	10.2293	10.2294	9.1512	3.2543	6.0833	4.6609	7.8023	9.5144	11.8409	H19Y
9.399	9.977	6.4885	5.6451	7.8859	8.5374	10.1934	10.7389	9.7034	8.8236	9.904	8.4819	8.2398	9.6915	12.7906	13.1153	12.7284	11.5568	11.8265	10.6622	3.7162	7.1981	5.7923	9.2804	10.8671	13.1855	H19Z
9.7555	9.7312	10.669	11.745	11.9321	10.9417	7.3896	7.2765	6.5867	7.0034	8.5402	8.7094	8.1081	7.9106	3.6173	2.7004	4.5574	4.7004	5.2316	6.2481	15.5134	13.3174	14.2481	6.3369	4.5816	2.5247	H26X
10.5312	10.7102	11.4184	12.3884	12.2629	11.3432	8.1741	8.3279	7.9071	8.0498	8.8103	9.3149	8.691	8.1313	4.0253	3.8192	4.7964	5.5176	5.3368	5.5867	16.422	14.1723	15.0118	7.1876	5.8299	3.7175	H26Y
8.8085	8.9705	9.9165	11.0108	10.8766	9.8253	6.4717	6.6151	6.4304	6.5843	7.3597	7.8011	7.4919	7.0228	2.578	2.3486	4.6665	5.0517	4.4907	5.8952	14.9384	12.5033	13.443	6.0741	4.6789	3.2577	H26Z
9.6454	10.3794	9.4814	9.9934	9.7543	9.2923	7.4189	8.2819	7.5549	6.8798	6.7509	7.4673	6.207	5.2842	3.373	4.4693	2.3161	3.8331	2.5426	3.615	14.4	12.8037	13.1055	5.2464	5.1891	3.8046	H27X
8.6096	9.266	9.0366	9.8012	9.3874	8.6416	6.3624	7.1586	6.8993	6.0428	6.8622	6.1912	5.2478	2.2502	3.5163	3.4958	4.5017	2.6727	4.2924		14.1237	12.0476	12.6018	5.2865	4.9154	3.8546	H27Y
10.3578	10.9484	10.7	11.3773	10.9893	10.3441	8.0794	8.7543	8.3217	7.9084	7.7454	8.5652	7.6569	6.7008	3.8004	4.614	3.7654	5.1127	3.9735	5.2854	15.7385	13.7886	14.2962	6.603	6.0699	4.2982	H27Z
11.077	11.2471	11.2211	11.9846	12.3589	11.6963	8.7059	8.84	7.5603	7.6815	9.2839	9.4096	8.1318	7.9523	4.7184	4.2805	3.2927	3.7451	5.1418	5.5975	15.884	14.3097	14.8991	6.293	5.0016	2.4082	H28X
11.0339	11.4755	10.7651	11.3042	11.549	11.097	8.7134	9.1886	7.9042	7.6204	8.6638	8.957	7.4039	7.003	4.651	4.8469	2.1113	3.289	4.2321	4.5379	15.4316	14.101	14.4527	5.8489	5.2178	2.9981	H28Y
11.6433	11.9869	11.8307	12.5172	12.5651	11.9512	9.2666	9.6172	8.6569	8.5601	9.8632	9.6311	8.0822	9.4486	4.9934	5.346	6.3346	4.7331	5.1792	5.9295	16.673	14.9889	15.5171	7.0868	6.1149	3.6462	H28Z
6.5732	6.9333	5.4044	5.5936	6.8947	6.7206	8.4851	8.8113	9.092	8.4827	8.8386	7.4974	8.8543	10.0409	12.454	12.7458	13.9379	12.8325	12.29	11.8534	2.2651	2.8832	2.5396	10.0485	11.196	13.7737	H15A
7.0683	7.141	5.8121	6.0835	7.8349	7.6261	8.7069	8.8032	8.7085	8.3037	9.4223	7.8772	8.948	10.3542	12.5045	12.6029	13.7667	12.5004	12.3818	11.8062	2.7673	3.9405	3.8546	9.8531	10.8539	13.4558	H15B
5.014	4.8587	4.8895	5.8238	7.1882	6.4505	6.8556	6.7875	7.1933	6.967	8.068	6.5665	8.1332	9.4158	10.9596	10.9943	12.806	11.5641	11.2185	10.959	4.2396	2.3894	3.7233	8.8867	9.5904	12.1818	H16A
4.9028	4.9712	3.8628	4.6957	6.5053	5.9496	6.2741	6.3568	6.2126	5.8212	7.3104	5.6547	6.8101	8.2567	10.0224	10.0824	11.4465	10.1792	10.0485	9.5919	4.3184	3.023	3.664	7.5241	8.3972	11.0045	H16B
5.4079	6.1687	2.6576	2.5978	4.8377	4.8944	6.3854	7.0571	6.5749	5.5608	6.3277	4.8	5.3989	6.8028	9.5736	9.9793	10.4391	9.3457	9.0078	8.3034	3.044	3.8051	3.0439	6.6166	8.106	10.5985	H13A
6.3854	7.4217	3.3558	2.3797	4.292	4.904	7.4952	8.4152	8.0922	6.8704	6.7311	5.5246	6.0396	7.1684	10.5575	11.187	10.36	9.7111	8.9684		2.351	4.2714	2.5353	7.6374	9.3885	11.7693	H13B
2.4976	2.3951	4.2289	5.7215	6.2879	4.9534	4.6925	4.6923	5.9673	5.7423	6.2293	5.0356	7.1787	8.0989	9.1847	11.517	10.5161	9.6675	8.8389		6.1689	2.2637	4.4392	7.876	8.3482	10.7798	H2A
3.061	2.5045	4.0954	5.633	6.7982	5.6066	4.5466	4.2304	4.8508	4.8679	6.4864	4.9672	6.6848	7.909	8.6493	8.5542	10.7954	9.5933	9.2509	9.2233	6.0739	3.165	4.9443	7.0477	7.3818	9.9143	H2B
0	1.7815	3.4806	5.1819	5.2647	3.6032	2.3934	3.0195	4.6154	4.0912	4.0266	3.1058	5.451	6.0619	6.7354	7.0847	9.426	8.6372	7.4115	7.8356	7.4211	3.8905	5.4392	6.0932	6.5589	8.7984	H3A
1.7815	0	4.7826	6.5456	6.9725	5.3629	3.053	2.467	4.3012	4.487	5.5741	4.5255	6.5972	7.3927	7.2052	7.123	10.0354	9.0644	8.2925	8.7352	8.1212	4.4996	6.424	6.7481	6.6787	8.9292	H3B
3.4806	4.7826	0	1.7809	3.0711	5.2334	5.3274	5.3236	3.9524	3.7078	2.2544	3.5946	4.6646	7.4116	7.4116	8.0724	7.8888	7.9531	6.9471	6.6288	5.1444	3.7663	3.6938	5.0896	6.6275	8.9951	H11A
5.1819	6.5456	1.7809	0	2.4672	3.0629	5.7854	7.0405	6.7719	5.2508	4.4705	3.4491	3.903	4.8358	8.4417	9.2761	9.2317	8.5177	7.481	6.88	4.6238	4.6517	3.6038	5.7668	7.6751	9.8978	H11B
5.2647	6.9725	3.0711	2.4672	0	1.7737	5.9116	7.4852	7.83	6.2213	3.5849	3.5862	4.5557	4.5732	8.3692	9.5328	9.5614	9.2453	7.2295	7.2295	6.2172	5.3082	4.4342	6.6318	8.4981	10.4282	H10A
3.6032	5.3629	5.2334	3.0629	1.7737	0	4.399	5.9435	6.6844	5.244	2.6012	2.514	3.4683	4.4514	7.3903	8.4317	8.102	6.9232	7.0662	7.0662	6.6018	4.5172	4.4687	6.1329	7.6434	9.6526	H10B
2.3934	3.053	5.3274	5.7854	5.9116	4.399	0	1.7796	3.0637	2.5111	3.2442	2.5747	4.2845	4.7457	4.3765	4.7171	7.2279	6.5046	5.3244	5.9565	8.9663	6.0496	7.2395	4.2965	4.4114	6.4651	H4A
3.0195	2.467	5.3236	7.0405	7.4852	5.9435	1.7796	0	2.489	3.0569	5.0228	4.166	5.6345	6.321	4.9944	4.6885	7.933	6.9862	6.431	7.0374	9.5862	6.5068	8.0446	5.1215	4.5043	6.5583	H4B
4.6154	4.3012	3.9524	6.7719	7.83	6.6844	3.0637	2.489	0	1.7772	2.792	2.9843	4.7219	5.8463	4.3216	4.087	5.929	5.666	5.7573	4.5576	9.4445	7.353	5.3366	5.3366	2.7129	5.1622	H5A
4.0912	4.487	3.7078	5.2508	6.2213	5.244	2.5111	3.0569	1.7772	0	4.0495	1.7771	5.2913	4.1863	4.9318	4.314	6.5514	4.6216	4.5576	4.4917	8.527	6.6958	7.4271	3.2223	2.7969	5.3172	H5B
4.0266	5.5741	2.2544	4.4705	3.5849	2.6012	3.2442	5.0228	2.792	4.0495	0	1.7771	3.0687	2.5285	5.2913	6.192	6.8961	6.723	4.4766	4.9917	8.685	6.546	6.8155	4.4162	5.7592	7.3869	H9A
3.1058	4.5255	3.5946	3.4491	3.5862	2.514	2.5747	4.166	2.9843	1.7771	1.7771	0	2.4697	3.0641	4.9552	6.1507	6.473	4.4766	4.9935	5.097	7.3969	8.2328	9.408	3.1466	5.1399	7.2579	H9B
5.451	6.5972	4.6646	3.903	4.5557	3.4683	4.2845	5.6345	4.7219	5.2913	3.0687	2.4697	0	1.7772	4.5595	5.9059	5.0391	3.6977	2.9153	2.8064	8.2164	8.2164	9.408	1.7725	4.3467	6.178	H8A
6.0619	7.3927	7.4116	4.8358	4.5732	4.4514	4.7457	6.321	5.8463	4.1863	2.5285	3.0641	1.7772	0	5.9425	5.9425	5.0369	5.0369	2.9153	2.8064	9.408	8.2328	8.0747	3.1466	5.0455	6.3013	H8B
6.7354	7.2052	7.4116	8.4417	8.3692	7.3903	4.3765	4.9944	4.3216	4.9318	5.2913	4.9552	4.5595	5.9425	0	1.7577	3.7335	3.7914	2.4598	3.8844	12.4666	10.2363	10.9925	3.78	3.0473	3.0518	H24A
7.0847	7.123	8.0724	9.2761	9.5328	8.4317	4.7171	4.6885	4.087	4.314	6.192	6.1507	5.9059	5.9425	1.7577	0	4.3246	3.8969	4.9194	2.4417	12.9257	10.6174	12.456	3.9248	2.532	2.3677	H24B
9.426	10.0354	7.8888	9.2317	9.5614	8.102	7.2279	7.933	5.929	6.5514	6.8961	6.473	5.0391	5.0391	3.7335	4.3246	0	3.0673	2.5159	2.5159	13.3943	12.2546	12.456	3.9382	3.9382	2.7654	H22A
8.6372	9.0644	7.9531	8.5177	9.2453	6.9232	6.5046	6.9862	5.666	4.6216	6.723	4.4766	3.6977	5.0369	3.7914	3.8969	3.0673	0	1.7596	1.7596	12.3581	10.3429	11.5922	2.8655	2.6209	2.2666	H22B
7.4115	8.2925	6.9471	7.481	7.2295	7.0662	5.3244	6.431	5.7573	4.5576	4.4766	4.9935	2.9153	2.9153	2.4598	4.9194	2.5159	1.7596	0	1.7596	11.8629	10.2603	10.2258	3.0128	3.7174	3.819	H21A
7.8356	8.7352	6.6288	6.88	7.2295	7.0662	5.9565	7.0374	4.5576	4.4917	4.9917	5.097	2.8064	2.8064	3.8844	2.4417	2.5159	1.7596	1.7596	0	11.1691	10.2603	10.0258	2.3717	3.7897	4.2448	H21B
7.4211	8.1212	5.1444	4.6238	6.2172	6.6018	8.9663	9.5862	9.4445	8.527	8.685	7.3969	8.2164	9.408	12.4666	12.9257	13.3943	12.3581	11.8629	11.1691	0	4.1963	2.5447	9.6259	11.1356	13.6356	H14Q
3.8905	4.4996	3.6938	4.6517	5.3082	4.5172	6.0496	6.5068	7.353	6.6958	6.546	8.2328	8.2164	8.2328	10.2363	10.6174	12.2546	10.3429	10.2603	10.2603	4.1963	0	2.2783	8.4852	9.4781	11.9678	H1Q
5.4392	6.424	3.6938	3.6038	4.4342	4.4687	7.2395	8.0446	5.3366	7.4271	6.8155	9.408	9.408	8.0747	10.9925	12.456	12.456	11.5922	10.2258	10.0258	2.5447	2.2783	0	8.7358	10.1876	12.6381	H12Q
6.0932	6.7481	5.0896	5.7668	6.6318	6.1329	4.2965	5.1215	5.3366	3.2223	4.4162	3.1466	1.7725	3.1466	3.78	3.9248	3.9382	2.8655	3.0128	2.3717	9.6259	8.4852	8.7358	0	2.3053	4.1951	H7Q
6.5589	6.6787	6.6275	7.6751	8.4981	7.6434	4.4114	4.5043	2.7129	2.7969	5.7592	5.1399	4.3467	5.0455	3.0473	2.532	3.9382	2.6209	3.7174	3.7897	11.1356	9.4781	10.1876	2.3053	0	2.6096	H6Q
8.7984	8.9292	8.9951	9.8978	10.4282	9.6526	6.4651	6.5583	5.1622	5.3172	7.3869	7.2579	6.178	6.3013	3.0518	2.3677	2.7654	2.2666	3.819	4.2448	13.6356	11.9678	12.6381	4.1951	2.6096	0	H23Q

Figure H.19: Optimized Structure of 4e,5'e *cis-syn-cis* DtBuCH18C6 with Hydrogen Labels
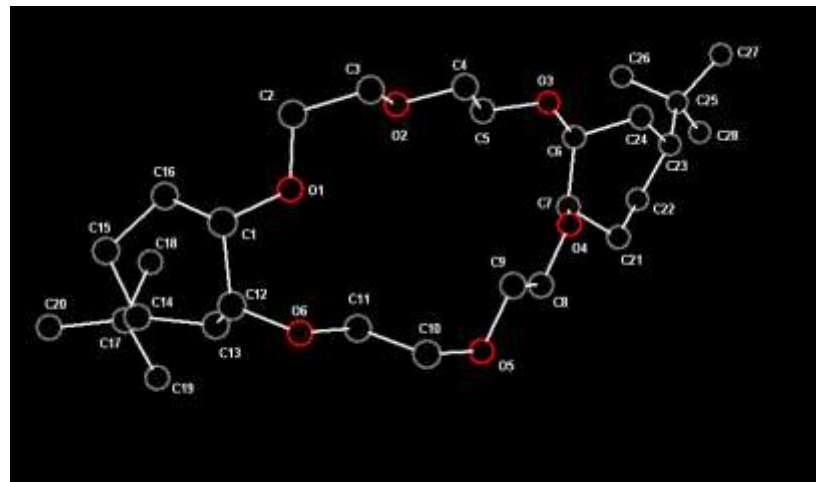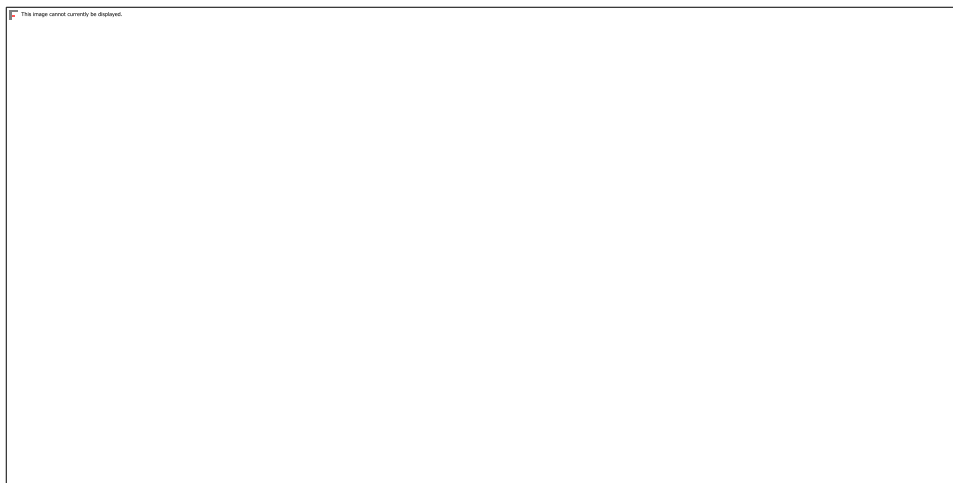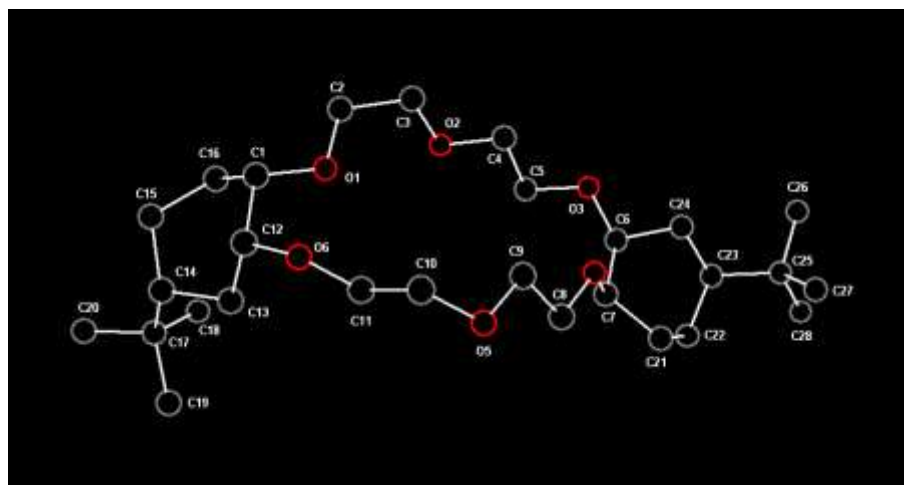

Figure H.20: Optimized Structure of 4e,5'e *cis-syn-cis* DtBuCH18C6 with Carbon and Oxygen Labels

Table H.10: Hydrogen Distances for the Optimized Structure of 4e,5'e *cis-syn-cis* DtBuCH18C6

	H18X	H18Y	H18Z	H19X	H19Y	H19Z	H20X	H20Y	H20Z	H27X	H27Y	H27Z	H26X	H26Y	H26Z	H28X	H28Y	H28Z	H15A	H15B	H13A	H13B	H16A	H16B	H11A	H11B
H18X	0	1.7664	1.773	3.0322	3.7813	2.5711	3.712	3.7786	4.3562	14.674	15.9369	16.1498	13.9406	13.4213	15.0615	16.627	15.8066	16.7288	2.3487	2.5541	4.6611	5.0522	4.6943	4.5888	6.9979	7.203
H18Y	1.7664	0	1.7702	2.5341	3.7695	3.1706	2.4448	3.0119	3.7066	15.1597	16.3954	16.5241	13.9816	13.6539	15.2036	16.8433	15.8606	16.8651	3.813	4.0068	4.7934	5.5151	5.8506	6.1122	7.2574	7.8356
H18Z	1.773	1.7702	0	3.7524	4.3537	3.7879	3.127	2.575	3.7973	13.8831	15.2199	15.2628	12.8902	12.4082	13.984	15.8354	14.9058	15.7737	2.6878	3.5961	4.5587	4.6977	4.5993	5.0752	6.8894	7.1634
H19X	3.0322	2.5341	3.7524	0	1.7655	1.7646	2.5142	3.7469	3.1223	15.0386	16.0595	16.4267	13.8652	13.6913	15.2438	16.3436	15.4165	16.6042	4.6201	3.8038	3.7505	5.1094	6.0978	6.2646	6.0128	6.8832
H19Y	3.7813	3.7695	4.3537	1.7655	0	1.7729	3.096	3.7967	2.6055	13.6258	14.5586	15.036	12.5867	12.4178	13.9858	14.8437	13.9971	15.2151	4.4679	3.3777	2.3007	3.8313	5.2132	5.5357	4.3372	5.245
H19Z	2.5711	3.1706	3.7879	1.7646	1.7729	0	3.754	4.3518	3.8132	14.4332	15.4711	15.9313	13.7038	13.3435	14.9838	15.9948	15.2353	16.3414	3.5295	2.2617	3.4915	4.515	4.948	4.7743	5.5896	6.0506
H20X	3.712	2.4448	3.127	2.5142	3.096	3.754	0	1.771	1.7653	14.0793	15.1815	15.3154	12.4507	12.3912	13.8334	15.3061	14.1916	15.3376	4.9816	4.9414	3.6363	4.726	6.1408	6.9128	5.9189	6.947
H20Y	3.7786	3.0119	2.575	3.7469	3.7967	4.3518	1.771	0	1.7706	12.6581	13.8667	13.8954	11.1238	10.936	12.4032	14.1278	13.0356	14.0546	4.2642	4.7074	3.2918	3.7274	5.0217	6.1101	5.4377	6.1902
H20Z	4.3562	3.7066	3.7973	3.1223	2.6055	3.8132	1.7653	1.7706	0	12.5129	13.5437	13.7623	10.9473	10.9074	12.3704	13.6503	12.5858	13.7684	4.839	4.6512	2.1145	3.2786	5.2508	6.2699	4.2107	5.3314
H27X	14.674	15.1597	13.8831	15.0386	13.6258	14.4332	14.0793	12.6581	12.5129	0	1.7728	1.7655	3.7993	2.6055	3.1179	3.7827	4.3537	3.7729	12.8193	13.2104	11.3596	9.9845	10.4077	11.6859	9.6947	8.7942
H27Y	15.9369	16.3954	15.2199	16.0595	14.5586	15.4711	15.1815	13.8667	13.5437	1.7728	0	1.7644	4.3521	3.8109	3.756	5.2681	3.784	3.1601	14.1366	14.369	12.3234	11.0823	11.6985	12.9289	10.4208	9.6133
H27Z	16.1498	16.5241	15.2628	16.4267	15.036	15.9313	15.3154	13.8954	13.7623	1.7655	1.7644	0	3.7473	3.1018	2.5162	3.0463	3.7578	2.5407	14.3718	14.7979	12.7504	11.4435	12.0144	13.3572	11.0683	10.3259
H26X	13.9406	13.9816	12.8902	13.8652	12.5867	13.7038	12.4507	11.1238	10.9473	3.7993	4.3521	3.7473	0	1.7712	1.771	3.784	2.5787	3.0232	12.5422	12.958	10.32	9.2683	10.4776	12.0723	8.83	8.6104
H26Y	13.4213	13.6539	12.4082	13.6913	12.4178	13.3435	12.3912	10.936	10.9074	2.6055	3.8109	3.1018	1.7712	0	1.7647	4.3573	3.798	3.7021	11.803	12.327	10.1176	8.8316	9.6174	11.1436	8.7245	8.1749
H26Z	15.0615	15.2036	13.984	15.2438	13.9858	14.9838	13.8334	12.4032	12.3704	3.1179	3.756	2.5162	1.771	1.7647	0	3.707	3.1126	2.436	13.5068	14.0424	11.6936	10.4871	11.3626	12.9037	10.254	9.8186
H28X	16.627	16.8433	15.8354	16.3436	14.8437	15.9948	15.3061	14.1278	13.6503	3.7827	5.2681	3.0463	3.784	4.3573	3.707	0	1.7729	1.7654	15.0863	15.2211	12.637	11.6539	12.7829	14.15	10.6364	10.2372
H28Y	15.8066	15.8606	14.9058	15.4165	13.9971	15.2353	14.1916	13.0356	12.5858	4.3537	3.784	3.7578	2.5787	3.798	3.1126	1.7729	0	1.7704	14.4314	14.6146	11.794	10.9086	12.2746	13.7652	9.9316	9.7704
H28Z	16.7288	16.8651	15.7737	16.6042	15.2151	16.3414	15.3376	14.0546	13.7684	3.7729	3.1601	2.5407	3.0232	3.7021	2.436	1.7654	1.7704	0	15.2079	15.5292	12.9582	11.9029	12.9791	14.45	11.1844	10.8244
H15A	2.3487	3.813	2.6878	4.6201	4.4679	3.5295	4.9816	4.2642	4.839	12.8193	14.1366	14.3718	12.5422	11.803	13.5068	15.0863	14.4314	15.2079	0	1.7511	4.3185	3.8934	2.5361	2.436	6.1758	5.8356
H15B	2.5541	4.0068	3.5961	3.8038	3.3777	2.2617	4.9414	4.7074	4.6512	13.2104	14.369	14.7979	12.958	12.327	14.0424	15.2211	14.6146	15.5292	1.7511	0	3.7377	3.8084	3.0645	2.5553	5.5208	5.3098
H13A	4.6611	4.7934	4.5587	3.7505	2.3007	3.4915	3.6363	3.2918	2.1145	11.3596	12.3234	12.7504	10.32	10.1176	11.6936	12.637	11.794	12.9582	4.3185	3.7377	0	1.7524	3.9726	4.9353	2.4649	3.3633
H13B	5.0522	5.5151	4.6977	5.1094	3.8313	4.515	4.726	3.7274	3.2786	9.9845	11.0823	11.4435	9.2683	8.8316	10.4871	11.6539	10.9086	11.9029	3.8934	3.8084	1.7524	0	2.6571	4.0396	2.5728	2.5676
H16A	4.6943	5.8506	4.5993	6.0978	5.2132	4.948	6.1408	5.0217	5.2508	10.4077	11.6985	12.0144	10.4776	9.6174	11.3626	12.7829	12.2746	12.9791	2.5361	3.0645	3.9726	2.6571	0	1.7621	4.8513	3.9446
H16B	4.5888	6.1122	5.0752	6.2646	5.5357	4.7743	6.9128	6.1101	6.2699	11.6859	12.9289	13.3572	12.0723	11.1436	12.9037	14.15	13.7652	14.45	2.436	2.5553	4.9353	4.0396	1.7621	0	5.9049	4.9255
H11A	6.9979	7.2574	6.8894	6.0128	4.3372	5.5896	5.9189	5.4377	4.2107	9.6947	10.4208	11.0683	8.83	8.7245	10.254	10.6364	9.9316	11.1844	6.1758	5.5208	2.4649	2.5728	4.8513	5.9049	0	1.7802
H11B	7.203	7.8356	7.1634	6.8832	5.245	6.0506	6.947	6.1902	5.3314	8.7942	9.6133	10.3259	8.6104	8.1749	9.8186	10.2372	9.7704	10.8244	5.8356	5.3098	3.3633	2.5676	3.9446	4.9255	1.7802	0
H10A	8.6663	9.3528	9.0228	7.8242	6.0797	6.8962	8.4773	8.1433	6.9322	9.9295	10.3725	11.4273	10.043	9.7522	11.2726	10.8766	10.6381	11.8129	7.5456	6.519	4.9118	4.8103	5.9502	6.3517	3.0604	2.5521
H10B	8.5963	8.9596	8.8603	7.2002	5.4495	6.6451	7.7102	7.5984	6.1413	10.537	10.9206	11.8925	10.0145	10.0116	11.4381	11.033	10.5611	11.6917	7.8818	6.8085	4.3925	4.8039	6.0054	7.2066	2.4515	3.0683
H2A	6.9722	8.2659	7.0637	8.2279	7.0967	8.8674	8.4974	7.4033	7.4046	9.3206	10.5289	10.0448	10.2587	9.1583	9.9153	11.9745	11.8091	12.3471	7.4388	4.9006	5.7344	4.3103	2.4895	2.666	5.6275	4.0628
H2B	7.2213	8.6177	7.7079	8.1582	6.9386	6.6166	8.9153	8.1272	7.8334	10.3433	11.3507	12.0888	11.3835	10.3866	12.125	12.7402	12.6709	13.3213	5.2228	4.8045	5.952	4.9235	3.4529	2.8989	5.709	4.1741
H3A	9.2803	10.5549	9.4583	10.1759	8.8231	8.7759	10.568	9.5416	9.2769	8.4447	9.3967	10.2086	10.1232	9.8536	10.6204	11.0608	11.2456	11.6891	7.1338	6.9998	7.3379	6.0541	4.8762	4.9074	6.4849	4.7109
H3B	8.9834	10.1168	9.2434	9.3496	7.8302	8.029	9.8513	9.0123	8.4362	8.5925	9.3481	10.3127	9.8418	9.8402	10.5928	10.6716	10.7624	11.4554	7.0891	6.6068	6.4012	5.3405	4.8919	5.055	5.16	4.4535
H9A	9.3905	10.0901	9.3404	9.1013	7.4185	8.2127	9.1584	8.3384	7.4903	7.3777	7.9408	8.9289	7.8273	7.3323	8.8881	8.7003	8.5567	9.5397	7.8282	7.3432	5.5866	4.7196	5.626	6.4656	3.5217	2.264
H9B	10.6491	11.3359	10.7657	10.0374	8.29	9.1503	10.3307	9.7198	8.6576	8.0698	8.2675	9.5136	8.6627	8.3419	9.7307	8.8513	8.8918	9.9656	9.2291	8.5002	6.7248	6.1859	7.1696	7.781	4.476	3.6255
H8A	11.7965	12.1799	11.5893	10.9665	9.0216	10.0421	10.754	10.0586	8.994	6.8951	6.8377	8.0373	6.8059	6.9043	8.0357	6.8187	6.6852	7.9694	10.5066	9.9823	7.4192	6.9139	8.4203	9.4259	4.9805	4.7019
H8B	10.7479	11.1296	10.3593	10.2333	8.5943	9.6984	9.7659	8.8475	8.0137	5.958	6.3277	7.243	5.7094	5.6008	6.9557	5.6714	6.2289	7.3911	9.3404	9.0674	6.523	5.7226	7.1644	8.3703	4.2787	3.8132
H4A	10.8516	11.8983	10.6828	11.5934	10.1523	10.4252	11.5346	10.3135	10.0724	6.0265	6.9698	7.7846	8.1436	6.8705	8.4348	8.8053	9.1438	9.4049	8.7078	8.7875	8.3029	6.8274	6.2084	6.8048	6.9578	5.2809
H4B	10.7255	11.6688	10.6601	11.0044	9.4212	9.9002	11.0673	10.0297	9.491	6.3355	6.9676	8.0311	7.9984	7.0502	8.5855	8.4132	8.6959	9.2544	8.7842	8.5576	7.601	6.3702	6.3331	6.9594	5.8796	4.304
H5A	10.254	10.8897	9.8159	10.4139	8.8862	9.6371	9.9424	8.7443	8.303	5.0486	5.9349	6.6644	5.7986	4.9797	6.6128	7.0095	6.8834	7.5673	8.4638	8.4936	6.7379	5.4196	6.0238	7.2108	4.9971	3.8079
H5B	10.3989	11.1419	9.8475	11.0411	9.6635	10.1883	10.4576	9.0641	8.9568	4.6113	5.8976	6.3215	5.9434	4.6675	6.3647	7.4305	7.3917	7.7023	8.4015	8.7436	7.5207	5.951	5.9098	7.0875	6.2238	4.8868
H21A	14.4321	14.8411	14.0876	13.8049	12.113	13.243	13.4073	12.5409	11.6443	5.5215	4.7777	6.2699	6.1175	6.2861	6.9204	4.5969	5.092	6.1207	12.9528	12.6115	10.1645	9.4368	10.6643	11.7112	7.7922	7.3192
H21B	13.0807	13.379	12.6194	12.4441	10.8049	12.0002	11.8606	10.955	10.106	5.2228	4.9505	6.0935	4.9987	5.2769	6.1285	4.6431	4.5445	5.8085	11.6892	11.4369	8.7663	8.0413	9.4766	10.6845	6.4736	6.1653
H22A	15.2758	15.7033	14.7134	15.0429	13.4416	14.4738	14.3562	13.2315	12.6391	3.3204	2.2383	3.7959	4.7213	4.6394	4.9479	2.6143	6.6551	4.0446	13.6095	13.583	11.2992	10.2713	11.2009	12.377	9.1492	8.4835
H22B	15.2563	15.4998	14.6381	14.7309	13.1451	14.349	13.9257	12.9069	12.2049	4.416	3.4672	4.5814	4.2842	4.8445	4.9715	2.313	2.7092	3.7964	13.7999	13.7121	11.0335	10.2084	11.5243	12.8075	8.8459	8.5215
H24A	12.5117	12.9469	11.7351	12.7677	11.3592	12.211	11.8166	10.4342	10.2324	2.2893	3.5002	3.7335	3.2717	2.105	3.603	4.6637	4.5556	4.7863	10.753	11.0911	9.0844	7.742	8.3869	9.7638	7.4685	6.6449
H24B	11.6382	11.9918	10.9539	11.5507	10.0638	11.0646	10.6888	9.464	9.0218	3.8259	4.5439	5.0933	3.6455	3.2299	4.6745	5.0543	4.6695	5.4884	10.0512	10.1777	8.7142	6.67	7.7557	9.1542	5.9834	5.369
H14Q	3.2562	3.7186	2.5252	4.299	3.8047	3.8605	3.6463	2.4066	3.0055	11.5143	12.7919	12.9411	10.6945	10.1727	11.8067	13.4466	12.6099	13.489	2.3483	3.0417	2.7736	2.264	2.6313	3.7819	4.6981	4.7638
H12Q	4.3847	5.2515	5.1299	3.9342	2.5271	2.6213	5.1344	5.074	4.2033	12.3144	13.2465	13.8726	11.9623	11.5249	13.1985	13.8802	13.3021	14.3859	3.7785	2.368	2.5159	3.0451	3.6557	3.6579	3.6338	3.6775
H1Q	5.4665	6.7754	6.2132	5.9851	4.4066	7.0605	6.6124	6.1059		11.5978	12.5751	13.2753	11.9526	11.2202	12.9568	13.6009	13.286	14.1625	3.9611	9.2288	4.2702	3.3878	3.0168	2.3786	4.6344	3.7012
H6Q	13.819	14.4328	13.3038	13.9622	12.403	12.2114	13.3807	12.1387	11.7157	2.5439	2.6917	3.9767	5.055	4.194	5.1516	4.4198	5.1396	5.2793	10.9582	10.0425	10.0463	8.9845	9.4661	10.5541	8.2963	7.2654
H7Q	13.7446	14.4037	13.4765	13.5624	11.8868	12.7456	13.3143	12.3027	11.5911	4.7417	4.4191	5.9746	6.5676	6.0733	7.0374	5.4679	6.1974	6.7644	11.9916	11.7493	9.9128	8.8943	9.5528	10.4423	7.7019	6.7167
H23Q	13.4853	13.6438	12.6994	13.1277	11.6569	12.8393	12.0774	10.9316	10.4158	3.8081	3.8572	4.2995	2.4148	3.0396	3.6532	3.235	2.5077	3.7089	12.0686	12.1736	9.4412	8.5142	9.8806	11.3336	7.5268	7.2709

(cont.) Table H.10: Hydrogen Distances for the Optimized Structure of 4e,5'e *cis-syn-cis* DtBuCH18C6

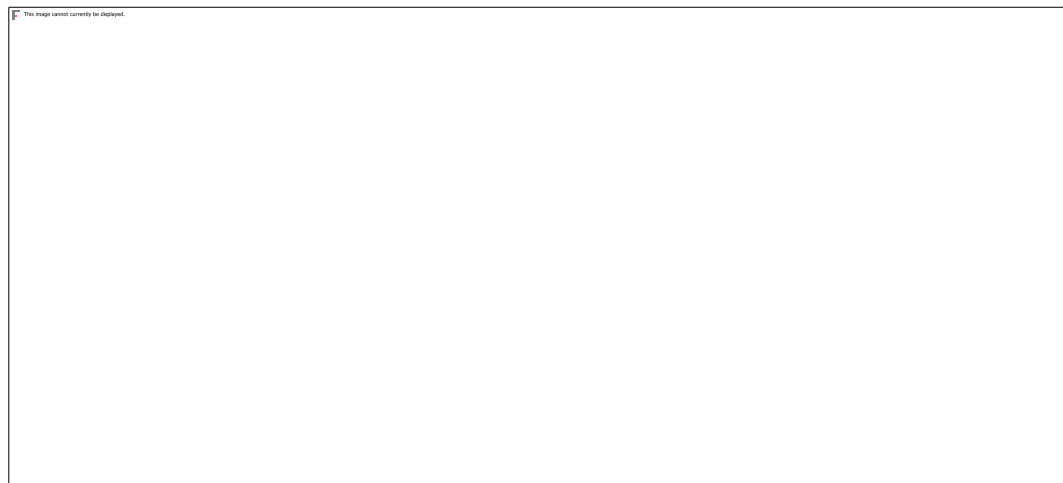|	H10A	H10B	H2A	H2B	H3A	H3B	H9A	H9B	H8A	H8B	H4A	H4B	H5A	H5B	H21A	H21B	H22A	H22B	H24A	H24B	H14Q	H12Q	H1Q	H6Q	H7Q	H23Q
H18X	8.6663	8.5963	6.9722	7.2213	9.2803	8.9834	9.3905	10.6491	11.7965	10.7479	10.8516	10.7255	10.254	10.3989	14.4321	13.0807	15.2758	15.2563	12.5117	11.6382	3.2562	4.3847	5.4665	13.819	13.7446	13.4853
H18Y	9.3528	8.9596	8.2659	8.6177	10.5549	10.1168	10.0901	11.3359	12.1799	11.1296	11.8983	11.6688	10.8897	11.1419	14.8411	13.379	15.7033	15.4998	12.9469	11.9918	3.7186	5.2515	6.7754	14.4328	14.4037	13.6438
H18Z	9.0228	8.8603	7.0637	7.7079	9.4583	9.2434	9.3404	10.7657	11.5893	10.3593	10.6828	10.6601	9.8159	9.8475	14.0876	12.6194	14.7134	14.6381	11.7351	10.9539	2.5252	5.1299	6.2132	13.3038	13.4765	12.6994
H19X	7.8242	7.2002	8.2279	8.1582	10.1759	9.3496	9.1013	10.0374	10.9665	10.2333	11.5934	11.0044	10.4139	11.0411	13.8049	12.4441	15.0429	14.7309	12.7677	11.5507	4.299	9.3942	5.9815	13.9622	13.5624	13.1277
H19Y	6.0797	5.4495	7.0967	6.9386	8.8231	7.8302	7.4185	8.29	9.2499	8.5943	10.1523	9.4212	8.8862	9.6635	12.113	10.8049	13.4416	13.1451	11.3592	10.0638	3.8047	2.5271	4.7741	12.403	11.8868	11.6569
H19Z	6.8962	6.6451	6.8674	6.6166	8.7759	8.029	8.2127	9.1503	10.4216	9.6984	10.4252	9.9002	9.6371	10.1883	13.243	12.0002	14.4738	14.349	12.211	11.0646	3.8605	2.6213	4.4066	13.2114	12.7456	12.8393
H20X	8.4773	7.7102	8.4974	8.9153	10.568	9.8513	9.1584	10.3307	10.7546	9.7659	11.5346	11.0673	9.9424	10.4576	13.4073	11.8606	14.3562	13.9257	11.8166	10.6888	3.6463	5.1344	7.0605	13.3807	13.3143	12.0774
H20Y	8.1433	7.5984	7.4033	8.1272	9.5416	9.0123	8.3384	9.7198	10.0586	8.8475	10.3135	10.0297	8.7443	9.0641	12.5409	10.955	13.2315	12.9069	10.4342	9.464	2.4066	5.074	6.6124	12.1387	12.3027	10.9316
H20Z	6.9322	6.1413	7.4046	7.8334	9.2769	8.4362	7.4903	8.6576	8.994	8.0137	10.0724	9.491	8.303	8.9568	11.6443	10.106	12.6391	12.2049	10.2324	9.0218	3.0055	4.2033	6.1059	11.7157	11.5911	10.4158
H27X	9.9295	10.537	9.3206	10.3433	8.4447	8.5925	7.3777	8.0698	6.8951	5.958	6.0265	6.3355	5.0486	4.6113	5.5215	5.2228	3.3204	4.416	2.2893	3.8259	11.5143	12.3144	11.5978	2.5439	4.7417	3.8081
H27Y	10.3725	10.9206	10.5289	11.3507	9.3967	9.3481	9.7408	8.2675	6.8377	6.3277	6.9698	6.9676	9.9349	5.8976	4.7777	4.9505	2.2383	3.4672	3.5002	4.5439	12.7919	13.2465	12.5751	6.2917	4.4191	3.8572
H27Z	11.4273	11.8925	11.0448	12.0888	10.2086	10.3127	8.9289	9.5136	8.0373	7.243	7.7846	8.0311	6.6644	6.3215	6.2699	6.0935	3.7959	4.5814	3.7335	5.0933	12.9411	13.8726	13.2753	3.9767	5.9746	4.2995
H26X	10.043	10.0145	10.2587	11.3835	10.1232	9.8418	7.8273	8.6627	6.8059	5.7094	8.1436	7.9984	5.7986	5.9434	6.1175	4.9987	4.7213	4.2842	3.2717	3.6455	10.6945	11.9623	11.9526	5.055	6.5676	2.4148
H26Y	9.7522	10.0116	9.1583	10.3866	8.9536	8.9402	7.3323	8.3419	6.9043	5.6008	6.8705	7.0502	4.9797	4.6675	6.2861	5.2769	4.8445	2.105	3.2299		10.1727	11.5249	11.2202	4.194	6.0733	3.0396
H26Z	11.2726	11.4381	10.9153	12.125	10.6204	10.5928	8.8881	9.7307	8.0357	6.9557	8.4348	8.5855	6.6128	6.3647	6.9204	6.1285	4.9479	4.9715	3.6303	4.6745	11.8067	13.1985	12.9568	5.1516	7.0374	3.6532
H28X	10.8766	11.033	11.9745	12.7402	11.0608	10.6716	8.7003	8.8513	6.8187	6.5714	8.8053	8.4132	7.0095	7.4305	4.5969	4.6431	2.6143	2.313	4.6637	5.0543	13.4466	13.8802	13.6009	4.4198	5.4679	3.235
H28Y	10.6381	10.5611	11.8091	12.6709	11.2456	10.7624	8.5567	8.8918	6.852	6.2289	9.1438	8.6959	5.092	4.5445	3.6551	2.7092	4.5556	4.6695			12.3069	13.3021	13.2806	5.1396	6.1974	2.5077
H28Z	11.8129	11.9197	12.3471	13.3213	11.6891	11.4554	9.5397	9.9656	7.9694	7.3911	9.4049	9.2544	7.5673	7.7023	6.1207	5.8085	4.0446	3.7964	4.7863	5.4884	13.489	14.3859	14.1625	5.2793	6.7644	3.7089
H15A	7.5456	7.8818	4.7388	5.2228	7.1338	7.0891	7.8282	9.2291	10.5066	9.3404	8.7078	8.7842	8.4638	8.4015	12.9528	11.6892	13.6095	13.7999	10.753	10.0512	2.3483	3.7785	3.9611	11.9582	11.9916	12.0686
H15B	6.519	6.8085	4.906	4.8045	6.9998	6.6068	7.3432	8.5002	9.9823	9.0674	8.7875	8.5576	8.4936	8.7436	12.6115	11.4369	13.583	13.7121	11.0911	10.1777	3.0417	2.368	2.9288	12.0425	11.7493	12.1736
H13A	4.9118	4.3925	5.7344	5.952	7.3779	6.4012	5.5866	6.7248	7.4192	6.523	8.3029	7.601	6.7379	7.5207	10.145	8.7663	11.0335	10.2713	9.0844	7.8142	2.7736	2.5159	4.2702	10.2463	9.9128	9.4412
H13B	4.8103	4.8039	4.3103	4.9235	6.0541	5.3405	4.7196	6.1859	6.9139	5.7226	6.8274	6.3702	5.4196	5.951	9.4368	8.0413	10.2713	10.2084	7.742	6.67	2.264	3.0451	3.8278	9.845	8.8943	8.5142
H16A	5.9502	6.6054	2.4895	3.4529	4.8762	4.8919	5.626	7.1696	8.4203	7.1644	6.2084	6.3331	6.0238	5.9098	10.6643	9.4766	11.2009	11.5243	8.3869	7.7557	2.6313	3.6557	3.0168	9.4661	9.5528	9.8806
H16B	6.3517	7.2066	2.666	2.8989	4.9074	5.055	4.6656	7.781	9.4259	8.3703	6.8048	6.9594	7.2108	7.0875	11.7112	10.6845	12.377	12.8075	9.7638	9.1542	3.7819	3.6579	2.3786	10.5541	10.4423	11.3336
H11A	3.0604	2.4515	5.6275	5.709	6.4849	5.16	5.3217	4.476	4.9805	4.2787	6.9578	5.8796	5.9971	6.2238	7.7922	6.4736	9.1492	8.8459	7.4685	5.9834	4.6981	6.3338	4.6344	8.2963	7.7019	7.5268
H11B	2.5521	3.0683	4.0628	4.1741	4.7109	3.4535	2.264	3.6255	4.7019	3.8132	5.2809	4.304	3.8079	4.8868	7.3192	6.1653	8.4835	8.5215	6.6449	5.369	4.7638	3.6775	3.7012	7.2654	6.7167	7.2709
H10A	0	1.774	5.5562	4.8363	5.3485	3.5995	2.5919	2.4577	3.4189	4.4423	6.1312	4.6539	5.1022	6.4848	7.059	6.3618	8.8307	8.8408	8.0115	6.6066	6.8725	4.3917	4.3204	7.9057	6.6298	8.222
H10B	1.774	0	6.7867	6.2637	6.9433	5.2511	3.609	3.5042	4.4374	4.6542	7.5287	6.0424	5.8849	7.4015	7.3586	6.4546	9.269	8.9399	8.5125	6.9151	6.8466	4.5032	5.2599	8.6788	7.4604	8.2303
H2A	5.5562	6.7867	0	1.7815	2.4781	3.0648	4.7571	6.1655	7.7592	6.6435	4.1576	4.5486	5.0492	4.7294	9.6415	8.779	10.0798	10.731	7.5752	7.1679	5.0693	4.9396	3.2013	8.1101	8.1026	9.4212
H2B	4.8363	6.2637	1.7815	0	2.4213	2.4805	4.7438	5.7424	7.7796	7.025	4.7305	4.6886	5.7959	5.8618	9.8266	9.1466	10.6289	11.2656	8.6273	8.0221	5.8598	4.4864	2.3063	8.7677	8.3098	10.2278
H3A	5.3485	6.9433	2.4781	2.4213	0	1.7822	4.1879	5.1364	6.9595	6.1859	2.4928	2.8924	4.5151	4.3046	8.3894	7.9464	8.8534	9.7669	7.0552	7.679	7.3259	6.4713	4.5514	6.8232	5.9234	8.9438
H3B	3.5995	5.2511	3.0648	2.4805	1.7822	0	2.7857	3.5517	5.6317	5.1034	3.1629	2.528	4.0444	5.5488	7.4667	6.985	8.4049	9.0795	6.7679	6.2703	6.999	5.5067	3.9037	6.6803	6.0957	8.3603
H9A	2.5919	3.6309	4.7571	4.7438	4.1879	2.7857	0	1.7782	3.0575	2.4625	4.0087	2.528	2.5418	4.0157	5.371	4.5458	6.6357	6.883	5.4864	4.2362	6.8817	5.7016	5.1624	5.4416	4.2547	6.0957
H9B	2.4577	3.5042	6.1655	5.7424	5.1364	3.5517	1.7782	0	2.525	3.0612	4.9692	3.2081	3.8622	5.4141	4.8077	4.4515	6.6121	6.7986	6.4536	5.151	8.3844	6.5966	6.104	5.8104	3.5625	6.5954
H8A	3.4189	4.4374	7.7592	7.7796	6.9595	5.6317	3.0575	2.525	0	1.7764	6.0098	4.4423	2.336	4.0558	6.7041	6.3586	4.9438	4.6314	5.3453	3.8113	9.1558	8.0767	8.0186	4.9066	3.763	4.5435
H8B	4.4423	4.6542	6.6435	7.025	6.1859	5.1034	2.4625	3.0612	1.7764	0	5.0967	3.8396	2.336	4.0558	6.3586	6.0892	4.8776	4.7198	4.0388	2.3942	7.8767	7.4338	7.3376	4.3164	4.6396	3.7836
H4A	6.1312	7.5287	4.1576	4.7305	2.4928	3.1629	4.0087	4.9692	6.0098	5.0967	0	1.7815	3.0621	2.5131	6.7041	6.3586	6.6587	7.7657	4.9157	4.9974	8.3347	8.0688	6.5538	4.4815	3.6717	7.0363
H4B	4.6539	6.0424	4.5486	4.6886	2.8924	2.528	2.528	3.2081	4.4423	3.8396	1.7815	0	2.4734	3.0596	6.3586	5.1925	6.0892	6.9644	4.9729	4.834	8.2209	7.3836	6.1204	4.2847	3.8147	6.4444
H5A	5.1022	5.8849	5.0492	5.7959	4.5151	4.0444	2.5418	3.8622	2.336	2.336	3.0621	2.4734	0	1.7698	4.9157	4.834	5.1865	5.6951	4.9543	5.1865	7.3009	7.3515	6.6892	5.3912	4.7338	4.4847
H5B	6.4848	7.4015	4.7294	5.8618	4.3046	5.5488	4.0157	5.4141	4.0558	4.0558	2.5131	3.0596	1.7698	0	4.9974	5.3508	5.8069	6.6094	4.0336	3.118	7.4334	8.0533	7.112	3.7892	5.2496	5.2496
H21A	7.059	7.3586	9.6415	9.8266	8.3894	7.4667	5.371	4.8077	6.7041	6.3586	6.6587	7.7657	4.9157	4.9974	0	1.7537	2.5646	2.4416	4.9543	4.1168	11.5956	10.8616	10.5267	3.6294	2.3582	3.7777
H21B	6.3618	6.4546	8.779	9.1466	7.9464	6.985	4.5458	4.4515	6.3586	6.0892	6.9644	4.9729	4.834	5.3508	1.7537	0	3.0543	2.5005	4.0336	2.7696	10.1555	9.7491	9.6321	6.6555	3.0299	2.599
H22A	8.8307	9.269	10.0798	10.6289	8.8534	8.4049	6.6357	6.6121	4.9438	4.8776	6.6587	6.0892	5.1865	5.8069	2.5646	3.0543	0	1.7514	3.7045	3.8283	12.2218	12.1571	11.6371	2.3138	2.8753	3.0451
H22B	8.8408	8.9399	10.731	11.2656	9.7669	9.0795	6.883	6.7986	4.6314	4.7198	7.7657	6.9644	5.6951	6.6094	2.4416	2.5005	1.7514	0	4.3166	3.9345	12.195	12.1495	11.9563	2.491	3.9158	2.3547
H24A	8.0115	8.5125	7.5752	8.6273	7.0552	6.7679	5.4864	6.4536	5.3453	4.0388	4.9157	4.9729	4.9543	4.0336	4.9543	4.0336	3.7045	4.3166	0	1.7496	9.3336	10.1463	9.6163	3.046	4.2423	2.8003
H24B	6.6066	6.9151	7.1679	8.0221	7.679	6.2703	4.2362	5.151	3.8113	2.3942	4.9974	4.834	5.1865	3.118	4.1168	2.7696	3.8283	3.9345	1.7496	0	8.4973	8.9633	6.8872	3.6608	3.8608	2.2592
H14Q	6.8725	6.8466	5.0693	5.8598	7.3259	6.999	6.8817	8.3844	9.1558	7.8767	8.3347	8.2209	7.3009	7.4334	11.5956	10.1555	12.2218	12.195	9.3336	8.4973	0	3.7291	4.5994	10.8117	10.9533	10.3223
H12Q	4.3917	4.5032	4.9396	4.4864	6.4713	5.5067	5.7016	6.5966	8.0767	7.4338	8.0688	7.3836	7.3515	8.0533	10.8616	9.7491	12.1571	12.1495	10.1463	8.9633	3.7291	0	2.8887	10.8638	10.2467	10.8317
H1Q	4.3204	5.2599	3.2013	2.3063	4.5514	3.9037	5.1624	6.104	8.0186	7.3376	6.5538	6.1204	6.6892	7.112	10.5267	9.6321	11.6371	11.9563	9.6163	6.8872	4.5994	2.8887	0	10.0407	9.4468	10.7771
H6Q	7.9057	8.6788	8.1101	8.7677	6.8232	6.6803	5.4416	5.8104	4.9066	4.3164	4.4815	4.2847	5.3912	3.7892	3.6294	6.6555	2.3138	2.491	3.046	3.6608	10.8117	10.8638	10.0407	0	2.2427	3.7036
H7Q	6.6298	7.4604	8.1026	8.3098	5.9234	6.0957	4.2547	3.5625	3.763	4.6396	3.6717	3.8147	4.7338	5.2496	2.3582	3.0299	2.8753	3.9158	4.2423	3.8608	10.9533	10.2467	9.4468	2.2427	0	4.5547
H23Q	8.222	8.2303	9.4212	10.2278	8.9438	8.3603	6.0957	6.5954	4.5435	3.7836	7.0363	6.4444	4.4847	5.2496	3.7777	2.599	3.0451	2.3547	2.8003	2.2592	10.3223	10.8317	10.7771	3.7036	4.5547	0

Figure H.21: Optimized Structure of 4z,5'e *cis-syn-cis* DtBuCH18C6 with Hydrogen Labels
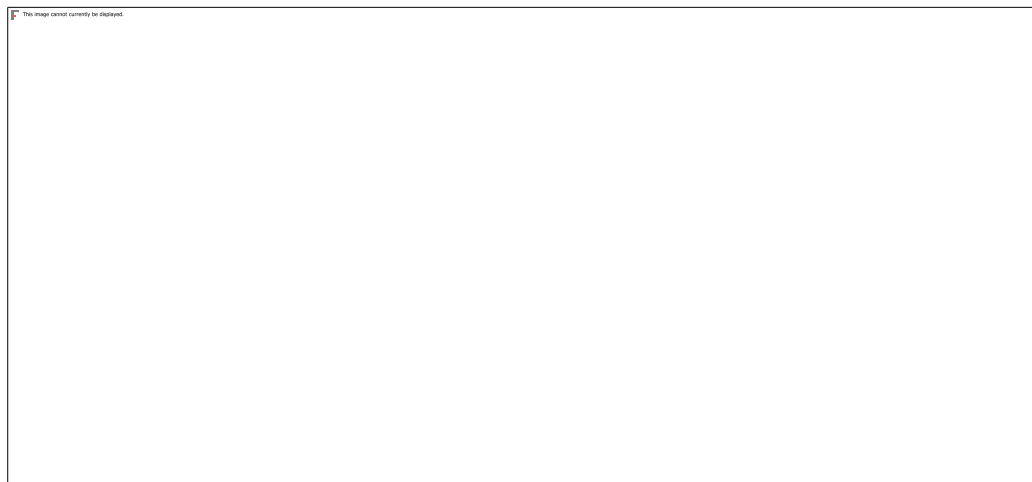

Figure H.22: Optimized Structure of 4z,5'e *cis-syn-cis* DtBuCH18C6 with Carbon and Oxygen Labels

Table H.11: Hydrogen Distances for the Optimized Structure of 4z,5'e *cis-syn-cis* DtBuCH18C6

	H20X	H20Y	H20Z	H18X	H18Y	H18Z	H19X	H19Y	H19Z	H26X	H26Y	H26Z	H27X	H27Y	H27Z	H28X	H28Y	H28Z	H15A	H15B	H16A	H16B	H13A	H13B	H2A	H2B
H20X	0	1.7729	1.765	3.1699	3.7828	2.565	3.7543	3.8131	4.3516	16.4087	16.0032	17.5098	15.6828	15.8525	17.2138	17.8308	16.6465	16.7301	2.2457	3.5124	4.7586	4.9487	4.523	3.5063	6.6631	6.8799
H20Y	1.7729	0	1.7657	3.7746	4.3533	3.779	3.1046	2.6075	3.7989	15.6107	15.2928	16.7038	14.8499	14.8452	16.2949	16.8121	15.5231	15.689	3.3504	4.4508	5.5128	5.211	3.8302	2.3062	6.9498	7.0879
H20Z	1.765	1.7657	0	2.5436	3.7583	3.0361	2.5139	3.1153	3.7466	17.2679	16.876	18.3107	16.3431	16.3518	17.8175	18.4392	17.3659	17.3659	4.0118	4.6145	6.2549	6.102	5.1086	3.7522	8.1928	8.2332
H18X	3.1699	3.7746	2.5436	0	1.7701	1.7662	2.4423	3.7037	3.0096	17.9756	17.3423	18.8433	16.6168	16.7469	18.1783	19.1241	17.8859	18.2382	4.0118	3.8138	6.1125	5.8527	5.5114	4.7951	8.6635	8.2747
H18Y	3.7828	4.3533	3.7583	1.7701	0	1.7728	3.1308	3.7994	2.5799	16.9184	16.1558	17.6937	15.3843	15.6245	16.9948	18.1033	16.945	17.3231	3.602	2.692	5.0776	4.5978	4.6907	4.5577	7.7459	7.0672
H18Z	2.565	3.779	3.0361	1.7662	1.7728	0	3.7116	4.3564	3.7817	17.2582	16.6016	18.1766	16.082	16.3771	17.7035	18.6529	17.5296	17.7447	2.5657	2.3489	4.5905	4.6964	5.0551	4.6682	7.2804	6.9912
H19X	3.7543	3.1046	2.5139	2.4423	3.1308	3.7116	0	1.7652	1.7713	16.949	16.4227	17.7939	15.5241	15.4206	16.9679	17.7951	16.4233	16.897	4.937	4.9843	6.9139	6.1522	4.7239	3.6351	8.9388	8.4973
H19Y	3.8131	2.6075	3.1153	3.7037	3.7994	4.3564	1.7652	0	1.7704	15.243	14.7703	16.1129	13.907	13.7725	15.3245	16.0762	14.6993	15.1493	4.6415	4.8409	6.2707	5.2663	3.2774	2.1084	7.8416	7.3988
H19Z	4.3516	3.7989	3.7466	3.0096	2.5799	3.7817	1.7713	1.7704	0	15.8213	15.161	16.5596	14.1659	14.1444	15.6556	16.6605	15.3489	15.8793	4.7073	4.2737	6.118	5.0349	3.719	3.2834	8.1433	7.3988
H26X	16.4087	15.6107	17.2679	17.9756	16.9184	17.2582	16.949	15.243	15.8213	0	1.7725	1.7703	3.7711	4.3541	3.7633	3.0319	3.7942	2.5949	15.2362	15.3506	12.8443	12.4772	13.6071	11.2889	11.0748
H26Y	16.0032	15.2928	16.876	17.3423	16.1558	16.6016	16.4227	14.7703	15.161	1.7725	0	1.7643	2.5581	3.7858	3.1141	3.6929	4.3547	3.8055	14.6802	14.6048	12.9536	12.0761	11.9135	13.206	10.76	10.3074
H26Z	17.5098	16.7038	18.3107	18.8433	17.6937	18.1766	17.7939	16.1129	16.5596	1.7703	1.7643	0	3.0881	3.7701	2.5407	2.4207	3.6973	3.104	16.2817	16.2362	14.6383	13.7162	13.3841	14.6023	12.4377	12.0155
H27X	15.6828	14.8499	16.3431	16.6168	15.3843	16.082	15.5241	13.907	14.1659	3.7711	2.5581	3.0881	0	1.7706	1.767	3.7594	3.7917	4.3516	14.4594	14.1962	12.8972	11.7316	11.3081	12.6221	11.1601	10.3743
H27Y	15.8525	14.8452	16.3518	16.7469	15.6245	16.3771	15.4206	13.7725	14.1444	4.3541	3.7858	3.7701	1.7706	0	1.766	3.2022	2.6019	3.8066	14.8505	14.6609	13.5446	12.2666	11.458	12.6092	11.9112	11.1591
H27Z	17.2138	16.2949	17.8175	18.1783	16.9948	17.7035	16.9679	15.3245	15.6556	3.7633	3.1141	2.5407	1.767	1.766	0	2.5193	3.0096	3.7414	16.0811	15.8709	14.5883	13.4154	12.8476	14.0736	12.7824	12.0737
H28X	17.8308	16.8121	18.4392	19.1241	18.1033	18.6529	17.7951	16.0762	16.6605	3.0319	3.6929	2.4207	3.7594	3.2022	2.5193	0	1.766	1.7705	16.867	16.9066	15.5217	14.4525	13.6728	14.7024	13.445	13.0384
H28Y	16.6465	15.5231	17.3659	17.8859	16.945	17.5296	16.4233	14.6993	15.3489	3.7942	4.3547	3.6973	3.7917	2.6019	3.0096	1.766	0	1.7726	15.8383	15.9166	14.4525	13.5354	12.4938	13.4156	12.7802	12.353
H28Z	16.7301	15.689	17.3659	18.2382	17.3231	17.7447	16.897	15.1493	15.8793	2.5949	3.8055	3.104	4.3516	3.8066	3.7414	1.7705	1.7726	0	15.8594	16.0594	14.6242	13.6359	12.7594	13.6743	12.4323	12.2131
H15A	2.2457	3.3504	3.7939	4.0118	3.602	2.5657	4.937	4.6415	4.7073	15.2362	14.6802	16.2817	14.4594	14.8505	16.0811	16.867	15.8383	15.8594	0	1.7513	2.5511	3.065	3.8062	3.733	4.859	4.921
H15B	3.5124	4.4508	4.6145	3.8138	2.692	2.3489	4.9843	4.8409	4.2737	15.3506	14.6048	16.2362	14.1962	14.6609	15.8709	16.9066	15.9166	16.0594	1.7513	0	2.4347	2.532	3.8943	4.3194	5.2692	4.7542
H16A	4.7586	5.5128	6.2549	6.1125	5.0776	4.5905	6.9139	6.2707	6.118	12.8443	12.9536	13.7162	12.8972	13.5446	14.5883	15.5217	14.4525	14.6242	2.5511	2.4347	0	1.7618	4.0479	4.9372	2.9544	2.7028
H16B	4.9487	5.211	6.102	5.8527	4.5978	4.6964	6.1522	5.2663	5.0349	12.4772	12.0761	13.7162	11.7316	12.2666	13.4154	14.4525	13.5354	13.6359	3.065	2.532	1.7618	0	2.6756	3.9883	3.4667	2.4876
H13A	4.523	3.8302	5.1086	5.5114	4.6907	5.0551	4.7239	3.2774	3.719	12.4772	11.9135	13.3841	11.3081	11.458	12.8476	13.6728	12.4938	12.7594	3.8062	3.8943	4.0479	2.6756	0	1.7523	4.9206	4.2997
H13B	3.5063	2.3062	3.7522	4.7951	4.5577	4.6682	3.6351	2.1084	3.2834	13.6071	13.206	14.6023	12.6221	12.6092	14.0736	14.7024	13.4156	13.6743	3.733	4.3194	4.9372	3.9883	1.7523	0	5.9568	5.7279
H2A	6.6631	6.9498	8.1928	8.6635	7.7459	7.2804	8.9388	7.8416	8.1433	11.2889	10.76	12.4377	11.1601	11.9112	12.7824	13.445	12.7802	12.4323	4.859	5.2692	2.9544	3.4667	4.9206	5.9568	0	1.7821
H2B	6.8799	7.0879	8.2332	8.2747	7.0672	6.9912	8.4973	7.3988	7.3988	11.0748	10.3074	12.0155	10.3743	11.1591	12.0737	13.0384	12.353	12.2131	4.921	4.7542	2.7028	2.4876	4.2997	5.7279	1.7821	0
H3A	8.0284	7.7872	9.3228	10.0563	9.2152	8.9847	9.7999	8.3703	8.9507	9.0101	8.6616	10.2627	9.1875	9.8386	10.7051	11.1385	10.4619	10.0344	6.6127	7.0867	5.0834	4.877	5.2766	6.3407	2.4741	3.0647
H3B	8.8033	8.8051	10.1789	10.563	9.4568	9.3136	10.541	9.2323	9.5009	9.0824	8.4527	10.163	9.0223	9.9523	10.6397	11.367	10.4717	10.4903	7.1626	4.9703	4.8732	6.0027	7.3367	2.4383	2.4857
H11A	5.985	5.148	6.7735	7.6908	7.002	7.0903	6.7793	5.1564	5.993	10.5001	10.1491	11.581	9.8588	9.9995	11.3235	11.8496	10.712	10.7739	5.2389	5.7296	4.898	3.868	3.2861	3.2149	4.2243	4.0601
H11B	5.6958	4.4116	6.099	7.4024	7.0633	7.1539	6.0452	4.3387	5.5991	11.4092	11.222	12.5076	10.7864	10.653	12.1127	12.457	11.1429	11.3065	5.6454	6.3465	6.0515	5.0459	2.7806	2.6083	5.7598	5.7384
H10A	6.7812	5.6996	7.4586	9.1751	9.007	8.7	8.0522	6.4876	7.8742	10.846	10.9947	12.2097	11.0805	10.9793	12.2766	12.1728	10.968	10.7708	6.7539	7.844	6.9816	6.4813	4.8901	4.6336	5.7966	6.4354
H10B	7.0004	6.2597	7.9896	9.3712	9.8179	8.6133	8.5771	7.0212	8.115	9.9071	9.9103	11.273	10.1796	10.3453	11.5015	11.5638	10.5403	10.2297	6.3917	7.3202	5.9868	5.5811	6.4383	4.9652	4.276	4.9815
H4A	9.6927	9.1561	10.7584	11.4617	10.4761	10.5572	10.8121	9.2196	9.7902	6.8854	6.5074	8.0744	6.9575	7.5813	8.437	8.8872	8.2246	7.8566	8.395	8.6512	6.8875	6.2198	6.1333	7.3291	4.5845	4.5058
H4B	10.4049	10.0307	11.5023	11.8368	10.6314	10.8649	11.3672	9.8664	10.1358	6.8101	6.0009	7.7107	6.3362	7.2912	7.9756	8.8683	8.4101	8.1503	8.8378	8.7628	9.6661	6.2433	6.6573	8.12	4.8864	4.3115
H5A	9.7106	9.0764	10.479	10.6524	9.4161	10.0009	9.8481	8.3088	8.4829	7.6662	6.7659	8.2926	6.1044	6.6355	7.7672	8.9358	8.0955	8.3592	8.3883	8.1054	9.6426	5.6557	5.377	6.8915	5.7618	4.6941
H5B	9.2343	8.3908	9.9535	10.5423	9.5492	9.9682	9.5076	7.8355	8.3781	7.4681	6.9675	8.3705	6.5261	6.7383	8.0057	8.6976	7.6636	7.8155	8.278	7.1201	5.9171	5.0414	6.2478	5.6852	5.0811
H9A	9.3369	8.1816	9.9385	11.5591	11.2534	11.1271	10.241	8.5637	9.893	8.9027	9.3529	10.332	9.5904	9.3126	10.5341	10.0514	8.8472	8.529	9.1615	10.075	8.9851	8.3306	6.7784	6.8323	7.2454	7.7694
H9B	9.2645	8.37	10.1274	11.5137	10.9972	10.844	10.4883	8.8207	9.9375	8.0053	8.2982	9.4761	8.7777	8.8208	9.8869	9.6018	8.6129	8.6145	8.6714	9.4722	8.0368	7.4865	6.4546	6.8922	5.9194	6.4788
H8A	10.4177	9.1466	10.8443	12.1014	11.5677	11.8191	10.5647	8.8041	9.914	7.5826	7.8863	8.742	7.6223	7.1002	8.4943	8.2012	6.8055	6.8731	10.0891	10.6329	9.6939	8.6474	9.9464	7.3313	8.124	8.1191
H8B	11.2637	10.1438	11.8917	13.2317	12.6799	12.7645	11.8854	10.1387	11.2569	6.6097	7.1902	8.0116	7.4997	7.1651	8.2768	7.6421	6.494	6.1058	10.7877	11.4331	10.163	9.344	8.0077	8.4611	8.1394	8.3868
H24A	13.8791	13.1731	14.7451	15.2135	14.0489	14.4815	14.3095	12.6631	13.0617	3.0838	2.1367	3.728	2.7971	3.8747	4.1454	4.9177	4.8092	4.5127	12.5763	12.5155	10.9207	9.993	9.7788	11.0821	8.8194	8.3176
H24B	13.423	12.5886	14.1114	14.491	13.3238	13.9326	13.4132	11.769	12.1173	4.2179	3.2849	4.4907	2.308	2.9062	3.8434	5.0206	4.4344	4.7792	12.2453	12.083	10.7809	9.6158	9.1002	10.375	9.0462	8.3169
H22A	14.5015	13.3382	14.9887	15.8967	15.0688	15.5493	14.4086	12.6594	13.4488	4.2768	4.8545	4.9756	4.4756	3.515	4.5971	3.8192	3.3525	2.7021	13.8154	14.0366	12.8569	11.7244	10.5062	11.3028	10.9608	10.6645
H22B	14.3655	13.2365	14.8025	15.4473	14.4905	15.1442	13.9807	12.2757	12.8636	4.6806	4.6226	4.8968	3.3591	2.1912	3.7286	3.9619	2.52	3.5727	13.5757	13.5827	12.533	11.2565	10.1128	11.0681	10.8878	10.3109
H21A	12.3345	11.0961	12.7334	13.7063	12.974	13.4449	12.1437	10.3902	11.2627	6.023	6.2802	6.8845	5.6618	4.8667	6.3176	6.0756	4.568	4.9695	11.8052	12.0589	11.1083	9.9096	8.4093	9.0772	9.482	9.1826
H21B	12.0202	10.9037	12.4664	13.1285	12.2053	12.8173	11.6996	9.9845	10.6036	5.907	5.6529	6.5141	4.6131	4.0823	5.6349	6.1062	4.7609	5.3751	11.2617	11.3053	10.3429	9.0333	7.7753	8.7259	8.8766	8.2843
H14Q	3.8591	3.8022	4.2996	3.7146	2.5191	3.2558	3.6498	3.0121	2.4105	14.4141	13.6905	15.2149	12.9695	13.209	14.5714	15.6145	14.4728	14.8132	3.0418	2.3515	3.7883	2.6406	2.2622	2.7756	5.8795	5.0666
H1Q	4.4245	4.7657	5.9908	6.7937	6.2253	5.4914	7.0675	6.1042	6.6161	12.8314	12.4218	14.0253	12.5854	13.0793	14.1661	14.7279	13.8344	13.6121	2.943	3.9685	2.3751	3.0145	3.8267	4.2715	2.3341	3.2071
H12Q	2.6442	2.5147	3.9398	5.269	5.1381	4.092	5.1381	4.1965	5.0755	13.8729	13.5455	15.046	13.4126	14.9215	15.4182	14.3094	14.263	2.3744	3.8886	3.6572	3.667	3.0455	2.5144	4.5117	4.9469
H7Q	12.4363	11.4628	13.1709	14.1737	13.3593	13.5954	12.9687	11.2221	12.0645	4.4696	4.9001	5.812	5.3526	5.275	6.1873	5.7686	4.8673	4.3927	11.6021	11.9715	10.5199	9.627	8.7043	9.5505	8.3432	8.3068
H6Q	11.8528	11.1587	12.7861	13.4667	12.4357	12.6831	12.6026	10.9387	11.504	4.6033	4.2806	5.7703	4.9046	5.5514	6.243	6.5864	6.0698	5.6336	10.6329	10.7882	9.1213	9.8	8.3057	8.0022	9.1898	6.867	6.6297
H23Q	14.4372	13.5095	15.1847	16.0132	15.0658	15.4128	14.836	13.1015	13.7956	2.3952	3.0327	3.6373	3.8083	3.8479	4.2957	3.7129	3.2546	2.52	13.4547	13.6591	12.1411	11.2153	10.5042	11.5047	9.9169	9.7154

(cont.) Table H.11: Hydrogen Distances for the Optimized Structure of 4z,5'e *cis-syn-cis* DtBuCH18C6

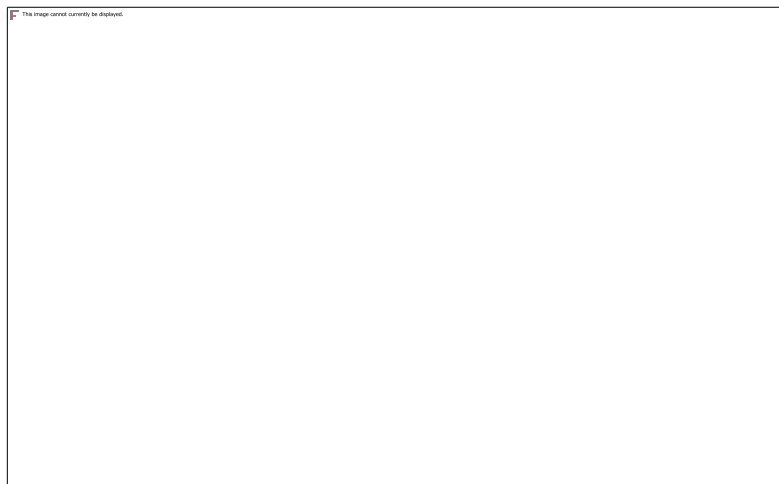| H3A	H3B	H11A	H11B	H10A	H10B	H4A	H4B	H5A	H5B	H9A	H9B	H8A	H8B	H24A	H24B	H22A	H22B	H21A	H21B	H14Q	H1Q	H12Q	H7Q	H6Q	H23Q	
8.0284	8.8033	5.985	5.6958	6.7812	7.0004	9.6927	10.4049	9.7106	9.2343	9.3369	9.2645	10.4177	11.2637	13.8791	13.423	14.5015	14.3655	12.3345	12.0202	3.8591	4.4245	2.6442	12.4363	11.8528	14.4372	H20X
7.7872	8.8051	5.148	4.4116	5.6996	6.2597	9.1561	10.0307	9.0764	8.3908	8.1816	8.37	9.1466	10.1438	13.1731	12.5886	13.3382	13.2365	11.0961	10.9037	3.8022	4.7657	2.5147	11.4628	11.1587	13.5095	H20Y
9.3228	10.1789	6.7735	6.099	7.4586	7.9896	10.7584	11.5023	10.479	9.9535	9.9385	10.1274	10.8443	11.8917	14.7451	14.1114	14.9887	14.8025	12.7334	12.4664	4.2996	5.9908	3.9398	13.1709	12.7861	15.1847	H20Z
10.0954	10.563	7.6908	7.4024	9.1751	9.3712	11.4617	11.8368	10.6524	10.5423	11.5591	11.5137	12.1014	13.2317	15.2135	14.491	15.8967	15.4473	13.7063	13.1285	3.7146	6.7937	5.269	14.1737	13.4667	16.0132	H18X
9.2152	9.4568	7.002	7.0633	9.007	8.9179	10.4761	10.6314	9.4161	9.5492	11.2534	10.9972	11.5677	12.6799	14.0489	13.3238	15.0688	14.4905	12.974	12.2053	2.5191	6.2253	5.1435	13.3593	12.4357	15.0658	H18Y
8.9847	9.3136	7.0903	7.1539	8.7	8.6133	10.5572	10.8649	10.0009	9.9682	11.1271	10.844	11.8191	12.7645	14.4815	13.9326	15.5493	15.1442	13.4449	12.8173	3.2558	5.4914	4.4092	13.5954	12.6831	15.4128	H18Z
9.7999	10.541	6.7793	6.0452	8.0522	8.5771	11.3672	11.367	9.8481	9.5076	10.241	10.4883	10.5647	11.8854	14.3095	13.4132	14.4086	13.9807	12.1437	11.6996	3.6498	7.0675	5.1381	12.9687	12.6026	14.836	H19X
8.3703	9.2323	5.1564	4.3387	6.4876	7.0212	9.2196	9.8664	8.3088	7.8355	8.5637	8.8207	8.8041	10.1387	12.6631	11.769	12.6594	12.2757	10.3902	9.9845	3.0121	6.1042	4.1965	11.2221	10.9387	13.1015	H19Y
8.9507	9.5009	5.993	5.5991	7.8742	8.115	9.7902	10.1358	8.4829	8.3781	9.893	9.9375	9.914	11.2569	13.0617	12.1173	13.4488	12.8636	11.2627	10.6036	2.4105	6.6161	5.0755	12.0645	11.504	13.7956	H19Z
9.0101	9.0824	10.5001	11.4092	10.8466	9.9071	6.8854	6.8101	7.6662	7.4681	8.9027	8.0053	7.5826	6.6097	3.0838	4.2179	4.2768	4.6806	6.023	5.907	14.4141	12.8314	13.8729	4.4696	4.6033	2.3952	H26X
8.6616	8.4527	10.1491	11.222	10.9947	9.9103	6.5074	6.0009	6.7659	9.675	9.3529	8.2982	7.8863	7.1902	2.1367	3.2849	3.8545	4.6226	6.2802	6.6529	13.6905	12.4218	13.5455	4.9001	4.2806	3.0327	H26Y
10.2627	10.163	11.581	12.5076	12.2097	11.273	8.0744	7.7107	8.2926	8.3705	10.332	9.4761	8.742	8.0116	3.728	4.4907	4.9756	4.8968	6.8845	6.5141	15.2149	14.0253	15.046	5.812	5.7703	3.6373	H26Z
9.1875	9.0223	9.8588	10.7864	11.0805	10.1796	6.9575	6.3362	6.1044	6.5261	9.5904	8.7777	7.6223	7.4997	2.7971	2.308	4.4756	3.3591	5.6618	4.6131	12.9695	12.5854	13.4126	5.3526	4.9046	3.8083	H27X
9.8386	9.9523	9.9995	10.653	10.9793	10.3453	7.5813	7.2912	6.6355	6.7383	9.3126	8.8208	7.1002	7.1651	3.8747	2.9062	3.515	2.1912	4.8667	4.0823	13.209	13.0793	13.6312	5.275	5.5514	3.8479	H27Y
10.7051	10.6397	11.3235	12.1127	12.2766	11.5015	8.437	7.9756	7.7672	8.0057	10.5341	9.8869	8.4943	8.2768	4.1454	3.8434	4.5971	7.3286	6.3176	5.6349	14.5714	14.1661	14.9215	6.1873	6.243	4.2957	H27Z
11.1385	11.367	11.8496	12.457	12.1728	11.5638	8.8872	8.8683	8.9358	8.6976	10.0514	9.6018	8.2012	7.6421	4.9177	5.0206	3.8192	3.9619	6.0756	6.1062	15.6145	14.7279	15.4182	5.7686	6.5864	3.7129	H28X
10.4619	10.8894	10.712	11.1429	10.968	10.5403	8.2246	8.4101	8.0955	7.6636	8.8472	8.6129	6.494	4.8092	4.4344	2.3252	2.52	4.568	4.7609	14.7218	13.8344	14.3034	4.8673	6.0698	3.2546	H28Y
10.0344	10.4717	10.7739	11.3065	10.7708	10.2297	7.8566	8.1503	8.3592	7.8155	8.529	8.1425	6.8731	6.1058	4.5127	4.7792	7.2021	3.5727	4.9695	3.5751	14.8132	13.6121	14.263	4.3927	5.6336	2.52	H28Z
6.6127	7.0403	5.2389	5.6454	6.7539	6.3917	8.395	8.8378	8.3883	8.2076	9.1615	8.6714	10.0891	10.7877	12.5763	12.2453	13.8154	13.5757	11.8052	11.2617	3.0418	2.943	2.3744	11.6021	10.6329	13.4547	H15A
7.0867	7.1626	5.7296	6.3465	7.844	7.3202	8.6512	8.7628	8.1054	8.278	10.075	9.4722	10.6329	11.4331	12.5155	12.083	14.0366	13.5827	12.0869	11.3053	2.3515	3.9685	3.7864	11.9715	10.7882	13.6591	H15B
5.0834	4.9703	4.898	6.0515	6.9816	5.9868	6.8875	6.9661	6.9426	7.1201	8.9851	8.0368	9.6939	10.163	10.9207	10.7809	12.8569	12.533	11.1083	10.3429	3.7883	2.3751	3.6572	10.5199	9.1213	12.1411	H16A
4.877	4.8732	3.868	5.0459	6.4813	5.5811	6.2198	6.2433	5.6557	5.9171	8.3306	7.4865	8.6474	9.344	9.993	9.6158	11.7244	11.2565	9.9096	9.0333	2.6406	3.0145	3.667	9.627	8.3057	11.2153	H16B
5.2766	6.0027	2.3861	2.7806	4.8901	4.6383	6.1333	6.6573	5.377	5.0414	6.7784	6.4546	6.9464	8.0077	9.7788	9.1002	10.5062	10.1128	8.4093	7.7753	2.2622	3.8267	3.0455	8.7043	8.0022	10.5042	H13A
6.3407	7.3367	3.2149	2.6083	4.636	4.9652	7.3291	8.12	6.8915	6.2478	6.8323	6.8922	7.3313	8.4611	11.0821	10.3875	11.3028	11.0681	9.0772	8.7259	2.756	4.2715	2.5144	9.5505	9.1898	11.5047	H13B
2.4741	2.4383	4.2243	5.7598	5.7966	4.276	5.4845	4.8864	5.7618	5.6852	7.2454	5.9194	8.124	8.1394	8.8194	9.0462	10.9608	10.8878	9.482	8.8766	5.8795	2.3341	4.5117	8.3432	6.867	9.9169	H2A
3.0647	2.4857	4.0601	5.7384	6.4354	4.9815	4.5058	4.3115	4.6941	5.0811	7.7694	6.4788	8.1191	8.3868	8.3176	8.3169	10.6645	10.3109	9.1826	8.2843	5.0666	3.2071	4.9469	8.3068	6.6297	9.7154	H2B
0	1.7828	3.521	5.0926	4.6697	2.8988	2.284	3.2063	4.3893	3.872	5.3221	3.7535	6.0206	5.8091	6.7162	7.0312	8.6089	8.7002	7.2597	6.8083	6.9561	3.9118	5.4853	5.9083	4.5779	7.533	H3A
1.7828	0	4.7391	6.4715	6.4018	4.6516	2.8745	2.6956	4.3679	4.5576	6.9963	5.3627	7.3636	7.1382	6.604	7.0511	9.3077	9.1795	8.2111	7.7405	7.3018	4.5841	6.4782	6.7319	4.8594	7.9616	H3B
3.521	4.7391	0	1.7849	3.0596	2.4601	4.1441	5.1391	4.2872	3.3332	4.5796	4.0769	4.9281	5.7451	8.0338	7.5618	8.6127	8.4925	6.5751	6.1788	4.5953	3.7337	6.6404	6.5414	6.0235	8.4778	H11A
5.0926	6.4715	1.7849	0	2.5161	3.0616	5.5713	6.7374	5.6234	4.4275	4.2981	4.5156	4.7778	5.8874	9.1564	8.5226	8.932	8.9216	6.6987	6.6228	4.8961	4.7014	3.6953	7.1565	7.178	9.2083	H11B
4.6697	6.4018	3.0596	2.5161	0	1.7801	5.2965	6.891	6.5975	5.0674	2.5922	2.9785	3.3494	4.7859	9.0703	8.326	8.6522	9.1121	6.6347	7.0397	6.9502	4.9554	4.4629	6.4998	6.8555	8.7018	H10A
2.8988	4.6516	2.4601	3.0616	1.7801	0	3.7839	5.342	5.4854	4.1362	3.0826	3.2225	4.5284	6.6438	7.9453	7.909	8.3348	8.6942	6.5169	6.2004	7.0044	4.0414	4.3985	5.8399	5.6523	7.9446	H10B
2.284	2.8745	4.1441	5.5713	5.2965	3.7839	0	1.7853	3.0547	2.4379	4.934	3.3289	4.7608	4.4597	4.5027	4.8	6.4861	6.5101	5.3941	4.8125	8.0283	5.9614	7.1523	3.8981	2.3333	5.342	H4A
3.2063	2.6956	5.1391	6.7374	6.891	5.342	1.7853	0	2.5548	0	6.6628	5.1073	6.1373	5.9576	4.0424	4.3873	7.0524	6.7117	6.2659	5.2423	8.2415	6.6303	8.0253	4.8549	2.6458	5.691	H4B
4.3893	4.3679	4.2872	5.6234	6.5975	5.4854	3.0547	2.5548	0	1.7795	4.5806	3.8719	3.6927	4.325	4.6892	3.9933	6.8315	5.8773	5.3723	3.9891	6.9682	6.8217	7.5757	5.1113	3.6418	6.0972	H5A
3.872	4.5576	3.3332	4.4275	5.0674	4.1362	2.4379	3.0674	1.7795	0	4.7766	3.8719	3.6927	4.325	4.8545	4.2295	5.8115	5.5409	4.1721	3.253	7.0311	6.4136	6.9208	3.9952	3.2087	5.5178	H5B
5.3221	6.9963	4.5796	4.2981	2.5922	3.0826	4.934	6.6628	6.5348	4.7766	0	1.782	2.513	2.4235	7.6728	7.5289	6.517	7.325	4.7505	5.6464	9.0054	7.083	6.9649	4.5261	5.6382	6.7098	H9A
3.7535	5.3627	4.0769	4.5156	2.9785	3.3289	3.3289	5.1073	4.5806	3.8719	1.782	0	3.0605	2.491	6.5343	6.503	6.6503	6.3991	7.0773	4.8693	5.3559	8.6514	6.2485	6.694	3.8396	4.3079	5.9936	H9B
6.0206	7.3636	4.9281	4.7778	4.3494	4.5284	4.7608	6.1373	5.3821	3.6927	2.513	3.0605	0	1.7828	6.2368	6.2368	6.6655	4.467	5.0259	2.3645	3.3413	9.1789	8.2519	8.1303	2.3189	6.4844	5.2037	H8A
5.8091	7.1382	5.7451	5.8874	4.7859	4.6438	4.4597	5.9576	5.9461	4.325	2.4235	2.491	1.7828	0	5.7353	5.6647	4.21	5.2194	2.9012	4.0241	10.2617	8.567	8.802	2.2961	4.0924	4.3751	H8B
6.7162	6.604	8.0338	9.1564	9.0703	7.9453	4.5027	4.0424	4.6892	4.8545	7.6728	6.5343	6.2368	5.7353	0	1.7545	4.3078	3.9355	4.9469	4.0694	11.573	10.3804	11.4435	3.5097	2.3329	2.539	H24A
7.0312	7.0511	7.5618	8.5226	8.326	7.909	4.3873	3.9933	4.2295	4.3873	7.5289	6.503	6.5655	5.6647	1.7545	0	3.8025	2.8146	4.0969	2.8012	10.8615	11.1216	11.216	3.663	2.9506	3.0559	H24B
8.6089	9.3077	8.6127	8.932	8.6522	8.3348	6.4861	7.0524	6.6375	5.8115	6.517	6.3991	4.467	4.21	4.3078	3.8025	0	1.7526	2.3314	3.0219	12.5891	11.8049	12.1466	2.893	4.6327	2.3546	H22A
8.7002	9.1795	8.4925	8.9216	9.1121	8.6942	6.5101	6.7117	5.8773	5.4409	7.325	7.0773	5.0259	5.2194	3.9355	2.8146	1.7526	0	2.7154	0	1.7611	12.0412	11.783	12.1213	3.7056	4.6862	3.0425	H22B
7.2597	8.2111	6.5751	6.6987	6.6347	6.5169	5.3941	6.2659	5.3723	4.1721	4.7505	4.8693	2.3645	2.9012	4.9469	4.0969	2.3314	2.7154	0	1.7611	10.5294	9.9903	10.0696	2.5902	4.2956	3.6828	H21A
6.8083	7.4505	6.1788	6.6228	7.0397	6.6202	4.8125	5.2423	3.9891	3.253	5.6464	5.3559	3.3413	4.0241	4.0694	2.8012	3.0219	2.3491	1.7611	0	9.7445	9.5736	9.807	3.0432	3.6969	3.7741	H21B
6.9561	7.3018	4.5953	4.8961	6.9502	6.7004	8.0283	8.2415	6.9682	7.0311	9.0054	8.6514	9.1789	10.2617	11.573	10.8615	12.5891	12.0412	10.5294	9.7445	0	4.6038	3.7368	10.8519	9.9386	12.547	H14Q
3.9118	4.5841	3.7337	4.7014	4.9554	4.0414	5.9614	6.6303	6.8217	6.4136	7.083	6.2485	8.2519	8.567	10.3804	10.3463	11.8049	11.783	9.9903	9.5736	4.6038	0	2.2956	9.303	8.2831	11.1559	H1Q
5.4853	6.4782	6.5414	3.6953	4.4629	4.3985	7.1523	8.0253	7.5757	6.9208	6.9649	6.694	8.1303	8.802	11.4435	11.1216	12.1466	12.1213	10.0696	9.807	3.7368	2.2956	0	9.9204	9.3324	11.9332	H12Q
5.9083	6.7319	6.5414	7.1565	6.4998	5.8399	3.8981	4.8549	5.1113	3.9952	4.5261	3.8396	2.3189	2.2961	3.5097	3.663	2.893	3.7056	2.5902	3.0432	10.8519	9.303	9.9204	0	2.3836	2.2126	H7Q
4.5779	4.8594	6.0235	7.178	6.8555	5.6523	2.3333	2.6458	3.6418	3.2087	5.6382	4.3079	4.6844	4.0924	2.3329	2.9506	4.6327	4.6862	4.2956	3.6969	9.9386	8.2831	9.3324	2.3836	0	3.1225	H6Q
7.533	7.9616	8.4778	9.2083	8.7018	7.9446	5.342	5.691	6.0972	5.5178	6.7098	5.9936	5.2037	4.3751	2.539	3.0559	2.3546	3.0425	3.6828	3.7741	12.547	11.1559	11.9332	2.2126	3.1225	0	H23Q

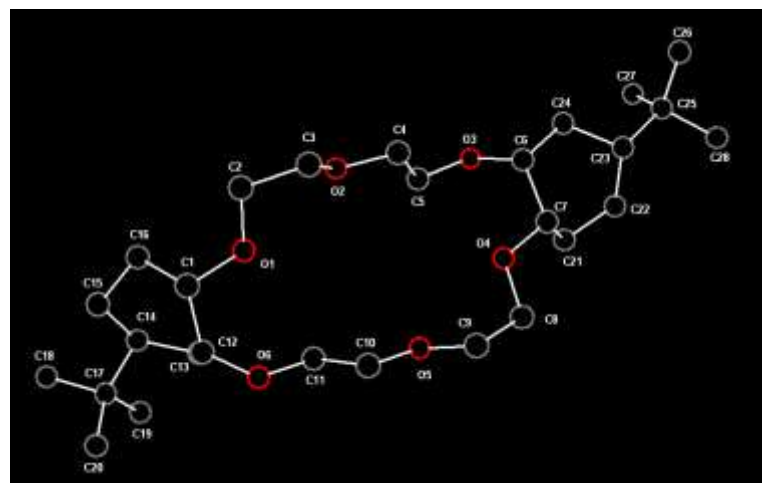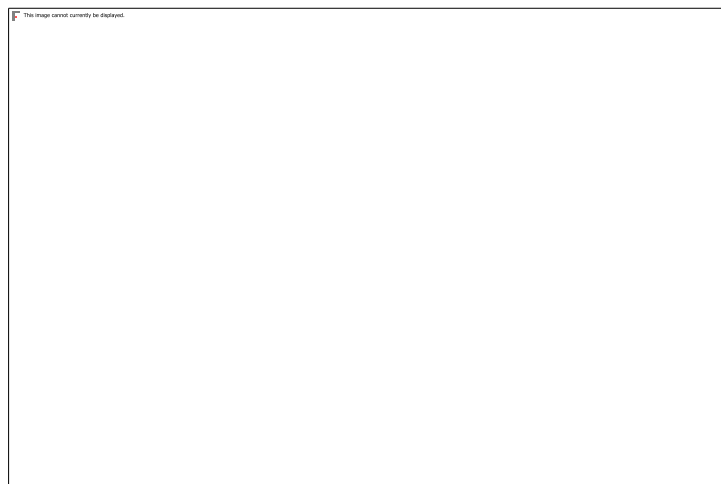Figure H.23: Optimized Structure of 4z,5'z *cis-syn-cis* DtBuCH18C6 with Hydrogen Labels
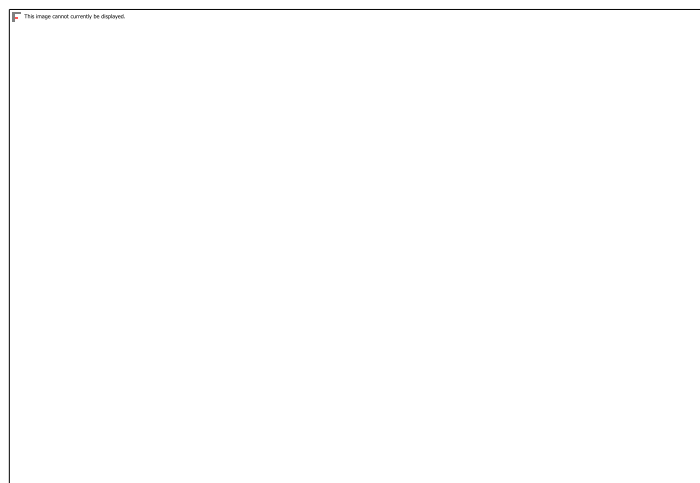

Figure H.24: Optimized Structure of 4z,5'z *cis-syn-cis* DtBuCH18C6 with Carbon and Oxygen Labels

Table H.12: Hydrogen Distances for the Optimized Structure of 4z,5'z *cis-syn-cis* DtBuCH18C6

	H18X	H18Y	H18Z	H19X	H19Y	H19Z	H20X	H20Y	H20Z	H27X	H27Y	H27Z	H26X	H26Y	H26Z	H28X	H28Y	H28Z	H15A	H15B	H16A	H16B	H13A	H13B	H2A	H2B
H18X	0	1.7718	1.7671	3.0431	3.799	2.6079	3.7105	3.7854	4.3553	16.4177	15.6778	17.2348	14.9822	15.2791	16.6111	17.6877	16.5534	16.8848	2.4734	2.3748	4.5713	4.67	4.4457	4.7909	7.3259	6.4487
H18Y	1.7718	0	1.7708	3.7479	4.3508	3.8089	3.0938	2.5763	3.7932	17.0493	16.3808	17.9851	15.9337	16.3181	17.5833	18.5474	17.4723	17.6447	2.8023	3.4786	5.1302	5.359	4.8135	4.5373	7.1069	6.6441
H18Z	1.7671	1.7708	0	2.5247	3.7623	3.1829	2.4435	3.0474	3.7083	17.8027	17.1631	18.6978	16.513	16.7307	18.1087	19.0612	17.8652	18.1705	3.9378	3.8464	6.112	5.9813	5.0812	4.9202	8.5424	7.8995
H19X	3.0431	3.7479	2.5247	0	1.7674	1.7662	2.5393	3.7621	3.1121	16.8236	16.3352	17.7411	15.5604	15.5331	17.0368	17.809	16.4676	16.8598	4.7234	3.7088	6.218	5.3946	3.9339	4.0836	8.9165	8.152
H19Y	3.799	4.3508	3.7623	1.7674	0	1.771	3.0959	3.7749	2.566	15.3726	14.9996	16.3772	14.3571	14.3006	15.7959	16.4065	15.0634	15.3679	4.5422	3.3912	5.5003	4.314	2.4074	2.7083	7.9434	7.2773
H19Z	2.6079	3.8089	3.1829	1.7662	1.771	0	3.7692	4.3531	3.7903	15.2726	14.7041	16.1266	13.8803	13.9083	15.3861	16.2599	14.9623	15.3823	3.629	2.1955	4.7033	3.842	2.9623	3.8163	7.7069	6.7247
H20X	3.7105	3.0938	2.4435	2.5393	3.0959	3.7692	0	1.7702	1.7647	17.8257	17.4193	18.9001	16.9728	17.0849	18.493	19.1346	18.6671	18.0549	5.0554	4.8586	6.9148	6.3425	4.5943	3.7271	8.7845	8.4915
H20Y	3.7854	2.5763	3.0474	3.7621	3.7749	4.3531	1.7702	0	1.7719	17.1121	16.7	18.2446	16.473	16.74	18.039	18.6671	17.5319	17.559	4.3035	4.6431	6.133	5.8088	4.2949	3.1362	7.4288	7.395
H20Z	4.3553	3.7932	3.7083	3.1121	2.566	3.7903	1.7647	1.7719	0	16.4736	16.1838	17.6376	15.8907	15.9887	17.3712	17.8512	16.6149	16.6842	4.8863	4.6305	6.2816	5.4632	3.3944	2.1372	7.7895	7.6555
H27X	16.4177	17.0493	17.8027	16.8236	15.3726	15.2726	17.8257	17.1121	16.4736	0	1.7723	1.7704	3.7761	4.3538	3.763	3.0422	3.7961	2.5967	14.4413	14.0708	12.1169	11.8228	13.2625	14.3694	11.264	11.0168
H27Y	15.6778	16.3808	17.1631	16.3352	14.9996	14.7041	17.4193	16.7	16.1838	1.7723	0	1.7645	2.564	3.7874	3.1067	3.6958	4.3543	3.8056	13.6798	13.3608	11.3197	11.2161	12.9068	14.1184	10.6265	10.2095
H27Z	17.2348	17.9851	18.6978	17.7411	16.3772	16.1266	18.9001	18.2446	17.6376	1.7704	1.7645	0	3.1004	3.7705	2.541	2.4239	3.6988	3.0984	15.3067	14.8954	12.9542	12.7485	14.344	15.5692	12.3411	11.9216
H26X	14.9822	15.9337	16.513	15.5604	14.3571	13.8803	16.9728	16.473	15.8907	3.7761	2.564	3.1004	0	1.7709	1.7665	3.7606	3.7892	4.3525	13.2342	12.678	10.918	10.7369	12.5094	13.9384	11.0375	10.2198
H26Y	15.2791	16.3181	16.7307	15.5331	14.3006	13.9083	17.0849	16.74	15.9887	4.3538	3.7874	3.7705	1.7709	0	1.7655	3.1893	2.5929	3.801	13.7217	12.9586	11.4777	11.0474	12.6067	14.0751	11.9191	11.0357
H26Z	16.6111	17.5833	18.1087	17.0368	15.7959	15.3861	18.493	18.039	17.3712	3.763	3.1067	2.541	1.7665	1.7655	0	2.5197	3.0175	3.7425	14.9145	14.2924	12.6091	12.2334	13.9906	15.4073	12.695	11.932
H28X	17.6877	18.5474	19.0612	17.809	16.4065	16.2599	19.1346	18.6671	17.8512	3.0422	3.6958	2.4239	3.7606	3.1893	2.5197	0	1.7668	1.7707	15.9775	15.3199	13.6907	13.1988	14.5523	15.8257	13.4897	12.9595
H28Y	16.5534	17.4723	17.8652	16.4676	15.0634	14.9623	18.6671	17.5319	16.6149	3.7961	4.3543	3.6988	3.7892	2.5929	3.0175	1.7668	0	1.7726	15.1021	14.1922	13.3306	13.4682	13.3306	14.6405	12.9072	12.2767
H28Z	16.8848	17.6447	18.1705	16.8598	15.3679	15.3823	18.0549	17.559	16.6842	2.5967	3.8056	3.0984	4.3525	3.801	3.7425	1.7707	1.7726	0	15.1617	14.5108	13.2801	13.2039	13.4682	16.342	12.5701	12.1765
H15A	2.4734	2.8023	3.9378	4.7234	4.5422	3.629	5.0554	4.3035	4.8863	14.4413	13.6798	15.3067	13.2342	13.7217	14.9145	15.9775	15.1021	15.1617	0	1.7524	2.3647	3.0456	3.7503	4.3029	4.886	4.0175
H15B	2.3748	3.4786	3.8464	3.7088	3.3912	2.1955	4.8586	4.6431	4.6305	14.0708	13.3608	14.8954	12.678	12.9586	14.2924	15.3199	14.1922	14.5108	1.7524	0	2.6188	2.369	2.8829	3.9723	5.8147	4.6874
H16A	4.5713	5.1302	6.112	6.218	5.5003	4.7033	6.9148	6.133	6.2816	12.1169	11.3197	12.9542	10.918	11.4777	12.6091	13.6907	13.3306	13.2801	2.3647	2.6188	0	1.7505	3.8216	4.915	3.5409	2.1172
H16B	4.67	5.359	5.9813	5.3946	4.314	3.842	6.3425	5.8088	5.4632	11.8228	11.2161	12.7485	10.7369	11.0474	12.2334	13.1988	13.4682	13.2039	3.0456	2.369	1.7505	0	2.4075	3.8637	4.4206	3.2932
H13A	4.4457	4.8135	5.0812	3.9339	2.4074	2.9623	4.5943	4.2949	3.3944	13.2625	12.9068	14.344	12.5094	12.6067	13.9906	14.5523	13.3306	13.4682	3.7503	2.8829	3.8216	2.4075	0	1.7541	5.8043	5.244
H13B	4.7909	4.5373	4.9202	4.0836	2.7083	3.8163	3.7271	3.1362	2.1372	14.3694	14.1184	15.5692	13.9384	14.0751	15.4073	15.8257	14.6405	16.342	4.3029	3.9723	4.915	3.8637	1.7541	0	6.1551	6.0511
H2A	7.3259	7.1069	8.5424	8.9165	7.9434	7.7069	8.7845	7.4288	7.7895	11.264	10.6265	12.3411	11.0375	11.9191	12.695	13.4897	12.9072	12.5701	4.886	5.8147	3.5409	4.4206	5.8043	6.1551	0	1.7806
H2B	6.4487	6.6441	7.8995	8.152	7.2773	6.7247	8.4915	7.395	7.6555	11.0168	10.2095	11.9216	10.2198	11.0357	11.932	12.9595	12.2767	12.1765	4.0175	4.6874	2.1172	3.2932	5.244	6.0511	1.7806	0
H3A	8.9221	8.9662	10.1554	9.9486	8.6521	8.6083	10.136	8.9695	8.8671	8.8891	8.4411	10.0958	9.0711	9.8914	10.6247	11.166	10.6114	10.1464	6.5957	6.959	4.6783	4.8742	6.2703	6.8791	2.5401	3.0527
H3B	8.9511	9.0853	10.3633	10.4461	9.3653	8.996	10.7393	9.5585	9.6908	9.1046	8.3325	10.0743	8.8414	9.8882	10.4974	10.981	10.6182	10.6243	6.5243	7.0755	5.2578	7.1043	7.854	4.2262	2.5193	3.8445
H11A	6.7615	7.1546	7.8168	6.9033	5.4025	5.5834	7.5607	6.891	6.23	10.2774	9.958	11.4231	9.8304	10.0745	11.3131	11.7946	11.1021	10.7246	5.0798	4.59	3.5408	2.3345	3.0711	4.1665	4.3439	3.8445
H11B	6.5683	6.9948	7.3142	5.9301	4.2478	4.8625	6.686	6.331	5.2658	11.3731	11.203	12.5414	10.9272	10.9172	12.2974	12.6161	11.3715	11.4292	5.4778	4.6166	4.5744	2.9469	2.2434	3.3051	5.8558	5.3973
H10A	8.7659	8.8673	9.3419	8.2029	7.2076	7.2076	8.2814	7.7085	6.6116	10.6847	10.8719	12.0976	11.072	11.072	12.2796	12.1329	10.9801	10.7049	7.4811	6.9415	6.4474	5.1021	4.3769	4.6354	6.4453	6.5742
H10B	8.8514	8.9199	9.6733	8.7123	7.0574	7.6686	8.9299	8.0928	7.3296	9.6006	9.6671	10.0228	10.0796	10.3048	11.3825	11.3738	10.4083	10.0083	7.1348	6.8777	5.7219	4.7436	4.8042	5.2142	5.0625	5.3392
H4A	10.0741	10.456	11.4067	10.8134	9.4288	9.3193	11.4477	10.5354	10.1559	6.7717	6.326	7.937	6.8524	7.598	8.36	8.8814	8.2998	7.907	7.9171	7.8432	5.6931	5.5505	7.1058	8.0779	4.6647	4.4711
H4B	10.1416	10.6563	11.6446	11.2612	10.0678	9.6463	12.0472	11.149	10.946	6.826	5.9317	7.6561	6.2047	7.2298	7.8697	8.8674	8.4381	8.2227	7.9392	7.9507	5.6043	5.8747	7.8518	8.9782	4.8543	4.2812
H5A	8.9352	9.8029	10.454	9.7248	8.5865	8.0286	10.9655	10.4093	9.9818	7.6698	6.7949	8.3191	6.1386	6.6701	7.7987	8.9456	8.3552	7.1224	6.6171		4.8241	4.6453	6.6557	8.1218	5.7283	4.5246
H5B	9.1331	9.8596	10.4639	9.4707	8.0932	7.9038	10.5741	10.0188	9.3728	7.3791	6.9086	8.3342	6.5739	6.8491	8.0619	8.7134	7.7109	7.8018	7.3699	6.7666	5.1931	4.5207	6.0318	7.3752	5.7507	4.9166
H9A	10.8915	11.225	11.6138	10.081	8.3363	9.1109	10.6938	10.2516	9.0799	8.8365	9.3147	10.2791	9.5718	9.304	10.5088	9.9995	8.798	8.4689	9.5496	8.836	8.0906	6.7656	6.5424	7.133	8.0176	8.0004
H9B	10.7582	11.02	11.6555	10.4481	8.7506	9.3161	10.9476	10.2609	9.3502	7.8191	8.1748	9.3193	8.7102	8.757	9.7871	9.4387	8.4637	7.9556	9.0751	8.6181	7.3715	6.3533	6.6324	7.261	6.7468	6.8661
H8A	11.0011	11.6992	11.9539	10.3147	8.7035	9.0885	11.4586	11.2034	10.0495	6.7818	7.9645	8.8377	7.6723	7.1736	8.5759	8.3162	7.0051	7.7232	7.9915	8.7622	6.6947	7.0368	8.1344	8.5775	8.0749	
H8B	12.2299	12.7635	13.1908	11.6982	10.0312	10.4903	12.5952	12.1508	10.7777	6.6109	7.1952	7.9907	7.445	7.0795	8.2124	7.5772	6.3912	6.0529	10.723	9.9795	8.8799	7.7586	8.1636	9.0656	8.7726	8.5594
H24A	13.5716	14.2765	15.0401	14.2124	12.8822	12.5854	15.2915	14.5916	14.0742	3.0729	2.1328	3.724	2.7985	3.8829	4.1403	4.9163	4.8048	4.5105	11.5943	11.2457	9.2416	9.0865	10.7865	12.0233	8.7398	8.2274
H24B	12.8902	13.7815	14.3708	13.3953	12.1345	11.7396	14.7241	14.2067	13.6005	4.2154	3.29	4.5008	2.3187	2.9307	3.8568	5.0287	4.4375	4.7834	11.1223	10.557	8.8105	8.5171	10.0276	11.6305	9.0002	8.178
H22A	14.6566	15.506	15.8735	14.4022	12.9257	12.966	15.73	15.3914	14.4066	4.283	4.8604	4.9822	4.4729	3.5156	4.6061	3.8279	2.3551	2.7164	13.141	12.2998	11.0131	10.1767	11.185	12.432	11.2049	10.6244
H22B	14.1272	15.1191	15.4508	14.0592	12.7176	12.5256	15.5687	15.2862	14.3859	4.6787	4.6206	4.8956	3.3474	2.1887	3.7288	3.9578	2.5152	3.576	12.6627	11.781	10.5023	9.7924	11.0582	12.4693	11.0465	10.2252
H21A	12.5701	13.4422	13.7069	12.1342	10.6504	10.7481	13.505	13.265	12.2067	6.0301	6.2827	6.8887	5.6447	4.8601	6.3158	4.569	4.9886		11.217	10.247	9.2356	8.1924	9.0126	10.298	9.8385	9.1555
H21B	11.8221	12.7923	13.1183	11.7439	10.392	10.2094	13.2202	12.9417	12.0522	5.8935	5.6356	6.5027	4.5854	4.0797	5.6251	6.1031	5.3813		10.3874	9.472	8.2898	7.4733	8.712	10.1517	9.0929	8.1952
H14Q	3.2405	2.5339	3.7267	4.2975	3.7961	3.8481	3.6401	2.3976	3.0222	15.0245	14.5089	16.1021	14.3165	14.7127	15.931	16.6747	15.6382	15.645	2.3234	3.0269	3.8225	3.7526	3.0466	2.5815	5.171	5.0008
H1Q	4.9859	4.6492	6.0169	6.4153	5.5567	5.4103	6.1567	4.8523	5.2499	12.97	12.4004	14.055	12.4497	13.0542	14.0991	14.8707	14.0179	13.8791	2.77	3.7483	2.5413	3.0534	3.7227	3.8595	2.6315	2.7053
H12Q	5.6968	5.1492	6.2033	6.0708	4.8636	5.4558	5.4374	4.1531	4.0377	13.3392	13.055	14.6036	13.2207	13.6148	14.7503	15.1778	14.205	13.9807	4.1919	4.6061	4.2573	3.7936	3.0415	2.3656	4.1395	4.5743
H7Q	12.8818	13.4898	14.0699	12.8234	11.2604	11.4122	13.057	13.237	13.3797	4.4699	4.9128	5.8148	5.3563	5.2789	5.7657	4.8529	4.3886		11.1316	10.5357	8.9988	8.2374	9.2333	10.2997	8.6521	8.3444
H6Q	11.9451	12.4998	13.2967	12.44	11.0058	10.9047	13.3215	12.5632	12.0024	4.5713	4.2728	5.7554	4.9145	5.5683	6.2432	6.5737	6.0549	5.6128	9.9355	9.62	7.6525	7.3245	8.8053	9.9069	6.9657	6.6358
H23Q	14.5958	15.2767	15.8993	14.7378	13.2467	13.2375	15.8139	15.2215	14.4466	2.392	3.0388	3.6354	3.8104	3.8489	4.2951	3.2444	2.5156		12.7707	12.2276	10.5148	9.9692	11.2231	12.3661	10.0553	9.6928

H3A	H3B	H11A	H11B	H10A	H10B	H4A	H4B	H5A	H5B	H9A	H9B	H8A	H8B	H24A	H24B	H22A	H22B	H21A	H21B	H14Q	H1Q	H12Q	H7Q	H6Q	H23Q	
8.9221	8.9511	6.7615	6.5683	8.7659	8.8514	10.0741	10.1416	8.9352	9.1331	10.8915	10.7582	11.0011	12.2299	13.5716	12.8902	14.6566	14.1272	12.5701	11.8221	3.2405	4.9859	5.6968	12.8818	11.9451	14.5958	H18X
8.9662	9.0853	7.1546	6.9948	8.8673	8.9199	10.456	10.6563	9.8029	9.8596	11.225	11.02	11.6992	12.7635	14.2765	13.7815	15.506	15.1191	13.4422	12.7923	2.5339	4.6492	5.1492	13.4898	12.4998	15.2767	H18Y
10.1554	10.3633	7.8168	7.3142	9.3419	9.6733	11.4067	11.6446	10.454	10.4639	11.6138	11.6555	11.9539	13.1908	15.0401	14.3708	15.8735	15.4508	13.7069	13.1183	3.7267	6.0169	6.2033	14.0699	13.2967	15.8993	H18Z
9.9486	10.4461	6.9033	5.9301	8.0209	8.7123	10.8134	11.2612	9.7248	9.4707	10.081	10.4481	10.3147	11.6982	14.2124	13.3953	14.4022	14.0592	12.1342	11.7439	4.2975	6.4153	6.0708	12.8234	12.44	14.7378	H19X
8.6521	9.3653	5.4025	4.2478	6.2729	7.0574	9.4288	10.0678	8.5865	8.0932	8.3363	8.7506	8.7035	10.0312	12.8822	12.1345	12.9257	12.7176	10.6504	10.392	3.7961	5.5567	4.8636	11.2604	11.0058	13.2467	H19Y
8.6083	8.996	5.5834	4.8625	7.2076	7.6686	9.3193	9.6463	8.0286	7.9038	9.1109	9.3161	9.0885	10.4903	12.5854	11.7396	12.966	12.5256	10.7481	10.2094	3.8481	5.4103	4.4558	11.4122	10.9047	13.2375	H19Z
10.136	10.7393	7.5607	6.686	8.2814	8.9299	11.4477	12.0472	10.9655	10.5741	10.6938	10.9476	11.4586	12.5952	15.2915	14.7241	15.73	15.5687	13.505	13.2202	3.6401	6.1567	5.4374	13.8057	13.3215	15.8139	H20X
8.9695	9.5585	6.891	6.331	7.7085	8.0928	10.5354	11.149	10.4093	10.0188	10.2516	10.2609	11.2034	12.1508	14.5916	14.2067	15.3914	15.2862	13.265	12.9417	2.3976	4.8523	4.1531	13.237	12.5632	15.2215	H20Y
8.8671	9.6908	6.23	5.2658	6.6116	7.3296	10.1559	10.946	9.9818	9.3728	9.0799	9.3502	10.0495	11.0777	14.0742	13.6005	14.4066	14.3859	12.2067	12.0522	3.0222	5.2499	4.0377	12.3797	12.0024	14.4466	H20Z
8.8891	9.1046	10.2774	11.3731	10.6847	9.6006	6.7717	6.826	7.6698	7.3791	8.8365	7.8191	7.6818	6.6109	3.0729	4.2154	4.283	4.6787	6.0301	5.8935	15.0245	12.97	13.3392	4.4699	4.5713	2.392	H27X
8.4411	8.3325	9.958	11.203	10.8719	9.6671	6.326	5.9317	6.7949	6.9086	9.3147	8.1748	7.9645	7.1952	2.1328	3.29	4.8604	4.6206	6.2827	6.6356	14.5089	12.4004	13.0556	4.9128	4.2728	3.0388	H27Y
10.0958	10.0743	11.4231	12.5414	12.0976	11.0228	7.937	7.6561	8.3191	8.3342	10.2791	9.3193	8.8377	7.9907	3.724	4.5008	4.9822	4.8956	6.8887	6.5027	16.1021	14.055	14.6036	5.8148	5.7554	3.6354	H27Z
9.0711	8.8414	9.8304	10.9272	11.0772	10.0796	6.8524	6.2047	6.1386	6.5739	9.5718	8.7102	7.6723	7.445	2.7985	2.3187	4.4729	3.3474	5.6447	4.5854	14.3165	12.4497	13.2207	5.3563	4.9145	3.8104	H26X
9.8914	9.8882	10.0745	10.9172	11.0472	10.3048	7.598	7.2298	6.6701	6.8491	9.304	8.757	7.1736	7.0795	3.8829	2.9307	3.5156	2.1887	4.8601	4.0797	14.7127	13.0542	13.6187	5.2789	5.5683	3.8489	H26Y
10.6247	10.4974	11.3131	12.2974	12.2796	11.3825	8.36	7.8697	7.7987	8.0619	10.5088	9.7871	8.5759	8.2124	4.1403	3.8568	4.6061	3.7288	6.3158	5.6251	15.931	14.0991	14.7503	6.1897	6.2432	4.2951	H26Z
11.166	11.3946	11.7946	12.6161	12.1329	11.3738	8.8814	8.8674	8.9456	8.7134	9.9995	9.4387	8.3162	7.5772	4.9163	5.0287	3.8279	3.9578	6.0823	6.1031	16.6747	14.8707	15.1778	5.7657	6.5737	3.7108	H28X
10.6114	10.981	10.7246	11.3715	10.981	10.4083	8.2998	8.4381	8.0897	7.7109	8.798	8.4637	6.9135	6.3912	4.8048	4.4375	2.3551	2.5152	4.569	4.7603	15.0382	14.0179	14.2065	4.8529	6.0549	3.2444	H28Y
10.1464	10.6182	10.6863	11.4292	10.7049	10.0083	7.907	8.2227	8.3552	7.8018	8.4689	7.9556	7.0051	6.6529	4.5105	4.7834	2.7164	3.576	4.9886	5.3813	15.645	13.8791	13.9807	4.3886	5.6128	2.5156	H28Z
6.5957	6.5243	5.0798	5.4778	7.4811	7.1348	7.9171	7.9392	7.1224	7.3699	9.5496	9.0751	9.7232	10.723	11.5943	11.1223	13.141	12.6627	11.2147	10.3874	2.3234	2.77	4.1919	11.1316	9.9355	12.7707	H15A
6.959	7.0755	4.59	4.6166	6.9415	6.8777	7.8432	7.9507	6.6171	6.7666	8.836	8.6181	8.7622	9.9795	11.2457	10.5507	12.2998	11.781	10.247	9.472	3.0269	3.7483	4.6061	10.5357	9.62	12.2276	H15B
4.6783	4.5079	3.5408	4.5744	6.4474	5.7219	5.6931	5.6043	4.8241	5.1931	8.0096	7.3715	7.9915	8.8799	9.2416	8.8105	11.0131	10.503	9.2356	8.2898	3.8225	2.5413	4.2573	8.9988	7.6525	10.5148	H16A
4.8742	5.2578	2.3345	2.9469	5.1021	7.4436	5.5505	5.8747	4.6453	4.5207	6.7656	6.3533	6.6947	7.7586	9.0865	8.5171	10.1767	9.9924	8.1924	7.4733	3.7526	3.0534	3.7936	8.2374	7.3245	9.9692	H16B
6.2703	7.1043	3.0711	2.2434	4.3769	4.8042	7.1058	7.8518	6.6557	6.0318	6.5424	6.6324	7.0368	8.1636	10.7865	10.2276	11.185	11.0582	9.0126	8.712	3.0466	3.7227	3.0415	9.2333	8.8053	11.2231	H13A
6.8791	7.8534	4.1665	3.3051	4.6354	5.2142	8.0779	8.9782	8.1218	7.3752	7.133	7.261	8.1344	9.0656	12.0233	11.6305	12.432	12.4693	10.2938	10.1517	2.5815	3.8595	2.3656	10.2997	9.9069	12.3661	H13B
2.5401	2.4262	4.3439	5.8558	6.4453	5.0625	4.6647	4.8543	5.7283	5.7507	8.0176	6.7468	5.8775	8.7726	8.7398	9.0002	11.2049	11.0465	9.8385	9.0929	5.171	2.6315	4.1395	8.6521	9.9657	10.0553	H2A
3.0527	2.5193	3.8445	5.3973	6.5742	5.3392	4.4711	4.2812	4.5246	4.9166	8.0004	6.8661	8.0749	8.5594	8.2274	8.178	10.6244	10.2252	9.1555	8.1952	5.0008	2.7053	4.5743	8.3444	6.6358	9.6928	H2B
0	1.7835	3.6741	5.365	5.3256	3.6133	2.3259	3.1366	4.4323	4.0109	6.1754	4.6415	6.6453	6.5343	6.5658	7.0015	8.9009	8.9303	7.7303	7.1402	6.7771	4.3991	5.0872	6.2379	4.6016	7.6376	H3A
1.7835	0	4.7641	6.5394	6.9412	5.2967	2.9804	2.662	4.3007	4.5998	7.7388	6.2096	7.8121	7.8026	6.5357	6.926	9.5313	9.2789	8.527	7.6043	7.2219	4.7295	6.0759	7.1047	5.0564	8.1384	H3B
3.6741	4.7641	0	1.7878	3.0603	2.4749	4.084	5.0613	4.2265	3.2634	4.572	4.0496	4.9017	5.6953	7.8578	7.5166	8.6282	8.5921	6.6836	6.3184	5.0018	3.7916	3.6386	6.3978	5.7805	8.3342	H11A
5.365	6.5394	1.7878	0	2.5006	3.0604	5.669	6.7386	5.5648	4.4534	4.3354	4.5215	4.8738	5.9414	9.1322	8.6248	9.1492	9.2149	6.9894	6.923	4.961	4.6466	3.7798	7.1671	7.0649	9.2457	H11B
5.3256	6.9412	3.0603	2.5006	0	1.7795	5.5568	7.1008	6.5803	5.0247	2.9556	3.4954	4.8028	8.9739	8.8245	8.6745	9.2037	6.7565	7.1801	6.5368	5.8612	4.4611	6.4089	6.7154	8.606	10.9A	H10A
3.6133	5.2967	2.4749	3.0604	1.7795	0	3.9813	5.5751	5.5412	4.0743	3.0939	2.2826	4.524	6.4032	7.754	7.8266	8.2252	6.752	6.539	6.6886	6.4901	5.1384	4.2566	6.5387	5.4308	7.7162	H10B
2.3259	2.9804	4.084	5.669	5.5568	3.9813	0	1.7839	3.0611	2.4657	5.4154	3.8378	5.1714	4.9496	4.3537	4.7464	6.6648	6.6497	5.7051	5.0319	8.3588	6.2043	6.7614	4.1341	2.3156	5.3917	H4A
3.1366	2.662	5.0613	6.7386	7.1008	5.5751	1.7839	0	2.5387	3.0708	7.0332	5.5559	6.3672	6.3302	4.0059	4.3094	7.1622	6.7446	6.424	5.3045	8.8368	6.6026	7.6684	5.0977	2.8586	5.8025	H4B
4.4323	4.3007	4.2265	5.5648	6.5803	5.5412	3.0611	2.5387	0	1.7784	6.5044	5.5535	5.2308	5.8814	4.7162	4.0053	6.6056	5.8703	5.3024	3.9349	8.2215	6.5134	7.4676	5.0828	3.3687	6.0909	H5A
4.0109	4.5998	3.2634	4.4534	5.0247	4.0743	2.4657	3.0708	1.7784	0	4.7292	3.8343	6.3398	4.2529	4.7933	4.2597	5.846	5.5506	4.2451	3.391	7.978	6.3617	6.778	3.9139	3.0694	5.463	H5B
6.1754	7.7388	4.572	4.3354	2.6253	3.0939	5.4154	7.0332	6.5044	4.7292	0	1.7825	2.5143	2.429	7.6528	7.5122	6.4705	7.3163	4.7571	5.6782	8.9646	8.0073	6.9572	4.4755	5.612	6.6587	H9A
4.6415	6.2096	4.0496	4.5215	2.9556	2.2826	3.8378	5.5559	5.5535	3.8343	1.7825	0	3.0615	2.4776	6.4591	6.6063	6.2601	7.0109	4.8281	5.3715	8.6663	7.2447	6.5319	3.6938	4.4221	5.834	H9B
6.6453	7.8121	4.9017	4.8738	4.3954	4.524	5.1714	6.3672	5.2308	6.3398	2.5143	3.0615	0	1.7824	6.29	6.6857	4.5765	5.1073	2.458	3.382	9.7013	8.6753	8.1548	3.3049	4.7117	5.3083	H8A
6.5343	7.8026	5.6953	5.9414	4.8028	4.6032	4.9496	6.3302	5.8814	4.2529	2.429	2.4776	1.7824	0	5.7471	5.6128	4.0921	5.1092	2.7703	3.9344	10.5831	9.2778	8.7107	2.2883	4.1331	4.3563	H8B
6.5658	6.5357	7.8578	9.1322	8.9739	7.754	4.3537	4.0059	4.7162	4.7933	7.6528	6.4591	6.29	5.7471	0	1.7541	4.3081	3.9355	4.9455	4.0507	12.4092	10.3588	11.0164	3.5264	2.339	2.5443	H24A
7.0015	6.9626	7.5166	8.6248	8.8245	7.8266	4.7464	4.3094	4.0053	4.2597	7.5122	6.6063	6.6857	5.6128	1.7541	0	3.7973	2.8153	4.0742	2.7665	12.0792	10.9348	10.9386	3.6601	2.9572	3.0556	H24B
8.9009	9.5313	8.6282	9.1492	8.6745	8.2252	6.6648	7.1622	6.6056	5.846	6.4705	6.2601	4.5765	4.0921	4.3081	3.7973	0	1.7527	2.3343	3.0254	13.5929	12.0937	12.0842	2.8747	4.6182	2.3524	H22A
8.9303	9.2789	8.5921	9.2149	9.2037	8.6752	6.6497	6.7446	5.8703	5.5506	7.3163	7.0109	5.1073	5.1092	3.9355	2.8153	1.7527	0	2.7106	2.3539	13.4001	11.9109	12.1781	3.7018	4.6922	3.0411	H22B
7.7303	8.527	6.6836	6.9894	6.7565	6.539	5.7051	6.424	5.3024	4.2451	4.7571	4.8281	2.458	2.7703	4.9455	4.0742	2.3343	2.7106	0	1.7611	11.5782	10.342	10.187	2.5911	4.2959	3.6928	H21A
7.1402	7.6043	6.3184	6.923	7.1801	6.6886	5.0319	5.3045	3.9349	3.391	5.6782	5.3715	3.382	3.9344	4.0507	2.7665	3.0254	2.3539	1.7611	0	11.0777	9.6979	9.9401	3.0432	3.698	3.7707	H21B
6.7771	7.2219	5.0018	4.961	6.5368	6.4901	8.3588	8.8368	8.2215	7.978	8.9646	8.6663	9.7013	10.5831	12.4092	12.0792	13.5929	13.4001	11.5782	11.0777	0	2.5459	2.6231	11.3746	10.4537	13.2435	H14Q
4.3991	4.7295	3.7916	4.6466	5.8612	5.1384	6.2043	6.6026	6.5134	6.3617	8.0073	7.2447	8.6753	9.2778	10.3588	10.2584	12.0937	11.9109	10.3242	9.6979	2.5459	0	2.261	9.6896	8.4369	11.3994	H1Q
5.0872	6.0759	3.6386	3.7798	4.2566	6.7614	6.7684	7.4676	6.9572	6.5319	8.1548	8.7107	11.0164	10.94	10.94	10.94	10.0842	12.1781	10.187	9.9401	2.6231	2.261	0	9.618	8.8495	11.577	H12Q
6.2379	7.1047	6.3978	7.1671	6.4089	6.5387	4.1341	5.0977	5.0828	3.9139	4.4755	3.6938	3.3049	2.2883	3.5264	3.6601	2.8747	3.7018	2.5911	3.0432	11.3746	9.6896	9.618	0	2.382	2.2159	H7Q
4.6016	5.0564	5.7805	7.0649	6.7154	5.4308	2.3156	2.8586	3.6687	3.0694	5.612	4.2421	4.7117	4.1331	2.339	2.9572	4.6182	4.6922	4.2959	3.698	10.4537	8.4369	8.8495	2.382	0	3.1055	H6Q
7.6376	8.1384	8.3342	9.2457	8.606	7.7162	5.3917	5.8025	6.0909	5.463	6.6587	5.834	5.3083	4.3563	2.5443	3.0556	2.3524	3.0411	3.6928	3.7707	13.2435	11.3994	11.577	2.2159	3.1055	0	H23Q

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EDUCATION:

- **Ph.D. Analytical Chemistry**   Aug 2007- Present
  University of Wisconsin – Milwaukee (Milwaukee, WI)
  Dissertation:" Stereochemical Effects in Crown Ethers: Implications for Metal Ion Extraction and Ionic Liquids Design"
  Advisor: Dr. Mark Dietz
  Expected Graduation Date: May 2014

- **B.S. Chemistry**   Aug 2002 – May 2007
  University of Alaska – Anchorage (Anchorage, AK)

EXPERIENCE:

- **Graduate Research Assistant**
  University of Wisconsin-Milwaukee   August 2008 – Present
  Separation and characterization of crown ether isomers that are used for the complexation for strontium. Separation of crown ethers was achieved by utilizing HPLC-ELSD and preparative LC-ELSD in combination with selective precipitation. Characterization of these crown ethers was achieved by radioactive work, TGA/DSC, ITC, IR, NMR, and X-ray crystallography

- **Chemistry Teaching Assistant**
  University of Wisconsin-Milwaukee   August 2007 – Present
  CHEM 100 (non-science majors), 102 (1st semester general chemistry for science majors), 104 (2nd semester general chemistry for science majors) 221 (quantitative analysis), and tutoring for all 100 level classes

- **Undergraduate Research Assistant**
  University of Alaska - Anchorage   August 2006 – August 2007
  Helped in the determination of the relative π acidity of N-heterocyclic carbenes under the supervision of Dr. Marc C. Perry.

MEMBERSHIPS AND EXTRACURRICULAR:

- Society for Applied Spectroscopy, University of Wisconsin-Milwaukee Student Chapter Member (2009-Present)
- American Chemical Society, Member (2011-Present)
- New Graduate Student Mentor, University of Wisconsin-Milwaukee Department of Chemistry and Biochemistry (August 2011-December 2012)

PUBLICATIONS:

- <u>A.J. Pawlak</u>, M.L. Dietz, "Investigations of the Thermal Properties of Macrocyclic Polyethers", Separation Science and Technology, **2014** (In Preparation)
- <u>A.J. Pawlak</u>, W.Shadrick, D.N. Frick, B.P. Hay, M.L. Dietz, "Formation Constants of Metal Ion-Crown Ether Complexes for Dicyclohexano-18-crown-6 and Divalent Metals Cations", Journal of Inclusion Phenomena and Macrocyclic Chemistry, **2014** (In Preparation)
- <u>A.J. Pawlak</u>, M.L. Dietz, "Formation of New Ternary Ionic Liquids" **2014**, (In Preparation)
- M. M. McCallum, <u>A. J. Pawlak</u>, W.R. Shadrick, A. Simeonov, A. Jadhav, A. Yasgar, D. Maloney, L. A. Arnold, "A Fluorescence-Based High Throughput Assay for the Determination of Small Molecule-Serum Albumin Protein Binding", Analytical and Bioanalytical Chemistry, **2014** (Accepted, In Press)
- P. Nandhikonda, A. Yasgar, A. M. Baranowski, K. Teske, B. Feleke, M. M. McCallum, <u>A.J. Pawlak</u> N. Y. Yuan, C. Kevin, D. D. Bikle, S. D. Ayers, P. Webb, G. Bantukallu, A. Simeonov, A. Jadhav, D. Maloney, L. A. Arnold, "PPAR δ agonist GW0742 interacts with multiple nuclear receptors including the vitamin D receptor", Biochemistry, **2013**, 52 (24), 4193-4203

ORAL PRESENTATION:

- <u>A.J. Pawlak</u>, W.R. Shadrick, G. Shahmohammadi, M.J. Corby, D.N. Frick, B.P. Hay, M.L. Dietz, "Separation and Characterization of Crown Ether Stereoisomers", 245th ACS National Meeting & Exposition, New Orleans, LA, April 7-11, 2013

POSTER PRESENTATIONS:

- <u>A.J. Pawlak</u>, W.R. Shadrick, G. Shahmohammadi, M.J. Corby, D.N. Frick, B.P. Hay, M.L. Dietz, "Separation and Characterization of Crown Ether Stereoisomers", 245th ACS National Meeting & Exposition, New Orleans, LA, April 7-11, 2013
- <u>A.J. Pawlak</u>, M.L. Dietz, "Investigation of the Thermal Properties of Macrocyclic Polyethers", 16th Symposium on Separation Science and Technology for Energy Applications, Gatlinburg, TN, October 18-22, 2009 and Chemistry in Southeastern Wisconsin Poster Mixer, Milwaukee, WI October 29, 2009