PERSPECTIVE

Historical natural kinds and mineralogy: Systematizing contingency in the context of necessity

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The advancement of science depends upon developing classification protocols that systematize natural objects and phenomena into "natural kinds"—categorizations that are conjectured to represent genuine divisions in nature by virtue of playing central roles in the articulation of successful scientific theories. In the physical sciences, theoretically powerful classification systems, such as the periodic table, are typically time independent. Similarly, the standard classification of mineral species by the International Mineralogical Association's Commission on New Minerals, Nomenclature, and Classification relies on idealized chemical composition and crystal structure, which are time-independent attributes selected on the basis of theoretical considerations from chemical theory and solid-state physics. However, when considering mineral kinds in the historical context of planetary evolution, a different, time-dependent classification scheme is warranted. We propose an "evolutionary" system of mineral classification based on recognition of the role played by minerals in the origin and development of planetary systems. Lacking a comprehensive theory of chemical evolution capable of explaining the time-dependent pattern of chemical complexification exhibited by our universe, we recommend a bootstrapping approach to mineral classification based on observations of geological field studies, astronomical observations, laboratory experiments, and analyses of natural samples and their environments. This approach holds the potential to elucidate underlying universal principles of cosmic chemical complexification.

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Most scientific disciplines systematically carve the domains of phenomena that they investigate into kinds (categories). Characterizing a kind as "natural" amounts to conjecturing that it represents a genuine division in nature—a grouping that is, in an important sense, independent of human conventions, interests, and actions (1). Natural kind classification systems play central roles in the articulation of successful scientific theories. Theoretical generalizations, which are the source of inductive (predictive and explanatory) inferences, are formulated in terms of (allegedly) natural kinds (2–8). The inductive successes of a scientific classification scheme support the claim that its categories are genuinely natural. To the extent that the categories carved out by a scientific classification system fail to accommodate the discovery of inductively reliable, theoretical generalizations, it is inadequate and needs to be modified (augmented, revised, or even replaced).

In this contribution we consider the prospects for developing a system of historical natural kinds for the discipline of mineralogy. Geology and planetary science are inherently historical sciences. They garner many of their insights through the study of minerals, which are the most information-rich and persistent records of the past 5 billion years of planetary history. As Cleland (9–12) argues, historical reasoning in the natural sciences requires differentiating which of the many and diverse attributes of present-day material things provide empirically reliable records of past events and processes from those that do not. The former (but not the latter) supply a theoretically

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promising basis for scientifically reconstructing otherwise inaccessible past events and processes. Historically oriented geologists and planetary scientists could thus benefit from a concept of mineral kinds that groups solid materials into categories on the basis of historically informative properties about their etiology (causal history), in contrast to classifying them in terms of manifest similarities and differences among their chemical and structural attributes.

Formulating a scientifically fruitful, historical concept of mineral kinds is challenging, however. The classification schemes used in the natural sciences are almost all time independent, that is, designed to accommodate universal, timeless generalizations about the natural world. Some philosophers have rejected the scientific viability of historical natural kinds on the grounds that they represent contingent or "accidental" (nonlawlike) temporal patterns (13–17). The most promising candidates in the natural sciences for historical natural kinds are found in the biological sciences; see refs. 18–21 for defenses of biological species as historical natural kinds. Evolutionary species concepts have been developed to accommodate the historical distinction, central to Darwin's theory of evolution by natural selection, between those properties of organisms that arise from a shared common ancestor ("homologies") and those that do not ("analogies"). Mere inspection of the manifest characteristics of organisms cannot reveal which are homologous and which are analogous. Indeed, prior to Darwin's theory of evolution by natural selection, taxonomists based biological classification systems initially on external morphological and later on internal anatomical and physiological similarities and differences among organisms; they lacked a principled basis for distinguishing homologies from analogies. Planetary scientists are in a position uncomfortably similar to that of biologists before Darwin. They lack a unifying theory—dominated by comprehensive principles, subject to well-understood contingencies—for distinguishing solid materials arising under relevantly similar environmental conditions, and from the same kinds of causal processes, from those that do not.

This paper focuses on challenges and opportunities faced by the classification of minerals as currently systematized by the International Mineralogical Association's Commission on New Minerals, Nomenclature, and Classification (IMA). The IMA system is widely accepted as providing a universal framework of natural kinds for the geosciences, analogous to the theoretical framework provided by the periodic table of the elements for chemistry. Under the IMA mineral system, more than 5,600 distinct solid materials are grouped into "mineral species" on the basis of similarities and differences in "major" chemical element composition and the arrangement of chemical elements into crystalline structures. Other characteristics are usually, although not always (see below), ignored for purposes of classification.

We consider three aspects of mineral classification in relation to the question of historical natural kinds. First, we review the standard IMA classification protocols and the extent to which they provide a scientifically fruitful, theoretical framework for inductive reasoning throughout the geosciences. In this context, we consider briefly the central role that the IMA system has played in the articulation of successful scientific theories. In particular, the IMA system reflects and amplifies solid-state theory, which posits that the properties of materials are a consequence of their elemental compositions and the ways in which atoms are chemically bonded into higher-order (including crystalline) structures. This framework helps to explain the enduring appeal of the IMA system of mineralogy to many geoscientists.

Second, we outline potential shortcomings of the IMA system vis-à-vis the inductive needs of historical geoscientists. IMA classification protocols lump together into the same mineral species some solid materials originating under different physical and chemical conditions at different stages of planetary evolution. They also split some solid materials that originated under the same conditions into different mineral species. Such lumpings and splittings are potentially misleading from the perspective of geoscientists concerned with understanding the causal processes and conditions involved in the origins of solid materials and the planetary bodies they compose. In addition, a variety of natural solid materials do not qualify as minerals under the IMA protocols because they are amorphous. Significantly, differences among these unsystematized solid materials carry important historical information about how condensed solids form and the roles that they play in the formation and development of planetary bodies.

Third, we explore the prospects of devising mineral classification protocols based on the concept of an historical natural kind. Carlos Santana (22) has recently argued that the IMA system does not treat minerals as natural kinds. Indeed, he claims that pursuing a natural kind taxonomy for condensed materials is futile. We agree with Santana that the current IMA system does not provide a natural kind taxonomy. Unlike Santana, however, we do not reject the prospects for a natural kind classification system for condensed materials. Instead, we diagnose the time-invariant character of the IMA classification protocols as the source of the difficulty. In particular, we consider a newly emerging "evolutionary system of mineralogy," which attempts to categorize minerals according to their historical contexts, and consequent idiosyncratic combinations of attributes (23–26). One of the most serious challenges to the possibility of a taxonomy of historical mineral kinds is the highly contextual nature of our current understanding of the origin and development of solid materials and the planetary bodies they compose. In contrast to chemistry and physics, nonlawlike historical contingencies play an outsized role in the inductive reasoning of planetary geoscientists. To deal with this problem, we propose a bootstrapping approach based on the vast body of information acquired over the past two centuries from geological field studies, astronomical observations, laboratory experiments, and analyses of natural samples and their environments.

The IMA Classification System of Minerals

Founded upon the 19th-century chemical framework of James Dwight Dana (27), the modern IMA mineral system classifies solid materials into mineral kinds on the basis of unique combinations of idealized major element composition and geometrically idealized crystalline structure, independently of the temporally extended and complex conditions and processes that produce them. Thus, for example, "quartz" is defined by the IMA as pure silicon dioxide (SiO_2) in the idealized quartz atomic structure, without regard to its environment of formation. Quartz differs from other "polymorphs" of SiO_2, such as coesite and stishovite, which have different periodic crystalline arrangements of silicon and oxygen atoms as a consequence of different pressures and/or temperatures of formation. Quartz also differs from its "isomorph," berlinite ($AlPO_4$), which has the same crystal structure but different chemical composition. In this way, quartz is defined by its unique combination of chemical composition and crystal structure.

An underlying and usually unspoken concern regarding the IMA classification system is that this idealized vision of quartz is a fiction. Ideal quartz does not exist in nature (or in the laboratory), because every quartz specimen has myriad trace and minor elements, isotopic variations, fluid and solid inclusions, structural defects, crystal size and shape, and many other information-rich attributes that distinguish one sample from the next. The IMA system successfully categorizes the great majority of Earth's natural condensed solids, but it does not incorporate those nonideal attributes, which are the very characteristics that reveal details of each specimen's history.

In some instances, the IMA protocol's idealization of mineral chemistry and structure leads to challenges in classification. Consider the chemical composition of natural crystals. Natural solids typically contain a diversity of different elements—often scores of elements in varying concentrations. The decision to idealize a few of these elements as "essential," while labeling many others as "trace" elements or "contaminants," for purposes of classifying a given mineral specimen, reflects theoretical conjectures about which chemical elements will prove most fruitful for inductive reasoning about the structure and properties of that solid material. Hence, for example, the element beryllium is considered to be an essential, and thus defining, element in $\sim$100 IMA-approved mineral species, in each of which Be is posited to be critical to identifying the crystalline structure and properties of that species of mineral. Beryllium is also found as a trace or minor element in scores of other minerals, in which Be is not considered to be an essential element and thus is not incorporated into the mineral species' definitions.

Whether to include a specific element as essential is almost always based on its representing more than half of the atoms in one atomic position in a crystal (the so-called "dominant-occupancy rule"). However, there are important and, at times, confusing exceptions. For example, in the case of metal alloys, which can incorporate numerous elements in a single crystalline grain, the most abundant element usually defines the mineral name, even if that element represents significantly less than half of an atomic position. Thus, a natural metal grain of composition $(Os_{0.26}Ru_{0.25}Ir_{0.25}Pt_{0.24})$ would be called "osmium" because Os is the most abundant of several elements, whereas an almost identical grain of composition $(Os_{0.25}Ru_{0.26}Ir_{0.25},Pt_{0.24})$ is "ruthenium" because of the slight excess of Ru compared to other elements. Nevertheless, the IMA protocols for identifying mineral species have the virtue of being clearly defined and, with adequate analytical capabilities, those protocols lead to unambiguous classifications. As discussed in the next section, however, these sharply defined mineral species do not provide a satisfactory theoretical framework for inductive reasoning in all areas of the geosciences.

In a few other intriguing instances, a minor amount of one element appears to be essential to "fix" a particular crystal structure, and thus that minor element must be integral to the definition of the mineral species. For example, the presence of a small amount of the large atom barium in some minerals that otherwise contain the smaller element calcium can cause the structure of a solid to "expand"; thus, a collapsed and distorted crystal structure may shift into a higher-symmetry, "fully inflated" form. In the IMA system, that increase in symmetry to a different crystal structure requires the assignment of a different mineral species name. In such cases, even a few percent of barium atoms can be essential. Thus, the complexities of the natural world thwart attempts to define every mineral species in terms of an idealized end-member composition. IMA protocols are sufficient to categorize these interesting special cases of mineral species; however, such ad hoc rules, designed to preserve the scope and consistency of the IMA mineral system, are not necessarily useful for inductive reasoning throughout the geosciences.

A similar contrast exists between the idealized arrangements of chemical elements into crystalline structures employed for purposes of IMA classification and the actual crystalline structures of natural specimens, which almost always deviate from the idealized arrangements of chemical elements used by the IMA. These natural deviations are characterized variously as structural "disorder," "twinning," "stacking faults," "dislocations," "zoning," or even "defects" and are generally ignored for purposes of classification.

Dana's (27) choice of idealized compositional and structural properties for classifying solid materials into mineral kinds was fortuitous insofar as modern equilibrium chemistry and thermodynamics have established a close relationship between those attributes and certain geologically important physical properties of natural solids, such as hardness, melting point, density, brittleness, and optical and electrical properties. For areas of the geosciences, such as those aspects of petrology, geophysics, and Earth materials science concerned primarily with time-invariant physical properties of solids, the IMA system of mineral classification works very well. Geophysicists may not care about how a mineral originated or what modifications it has undergone in the past; they may care only about its manifest physical properties, such as the brittle failure that might lead to earthquakes.

Indeed, the IMA mineral classification system satisfies most of the inductive demands of some important areas of the geosciences, such as rock mechanics, seismology, and structural geology. The modern IMA system was firmly grounded in materials science and solid-state chemistry and physics and was thus designed to facilitate investigations into physical properties of solid materials and the geological contexts in which they occur for ahistorical theoretical purposes, such as discovering new chemical elements and compounds, while understanding the nature of crystalline solids, as well as practical pursuits (e.g., predicting the likelihood of earthquakes or building structurally sound dams).

Furthermore, the IMA classification of minerals based on idealized chemical composition and crystal structure has played an important role in the development of solid-state theory—the concept that a material's properties are a consequence of the identity of its constituent atoms and their structural arrangement. As such, mineralogy has contributed centrally to many advances in materials science, as manifest in Nobel prizes for the discovery of radioactive elements (Marie Sklodowska-Curie, Pierre Curie, and Antoine Becquerel, physics, 1903; Marie Curie, chemistry, 1913), the discovery of fluorine (Henri Moissan, chemistry, 1906), X-ray crystallography (Max von Laue, physics, 1914; William Henry Bragg and Lawrence Bragg, physics, 1915), electron diffraction by crystals (Clinton Davisson and George Thomson, physics, 1937), high-pressure phase transformations (Percy Bridgman, physics, 1946), and principles of chemical bonding (Linus Pauling, chemistry, 1954).

The IMA System and Planetary Evolution

The system of the International Mineralogical Association's Commission on New Minerals, Nomenclature, and Classification is successful in establishing unambiguous criteria for distinguishing among more than 5,600 different mineral species, with $\sim$100 new species discovered and approved by IMA each year. The system provides the essential nomenclature for most of the solid materials that comprise Earth and other planets, while exemplifying theoretical principles of solid-state physics and chemistry.

The IMA mineral classification scheme, by design, does not incorporate information regarding the causal contexts in which these materials arise and change over time and therefore is inadequate for applications by planetary scientists, geobiologists, paleontologists, and other historically oriented geoscientists, who want to know the temporal context of minerals. The IMA protocols cannot inform how the materials that make up terrestrial planets form in interstellar space; clump together; and are subsequently modified by physical, chemical, and/or biological processes to produce new varieties of solids that play important roles in the development and maintenance of varied planetary environments. In this historical approach, a given mineral such as diamond or quartz, with its idealized chemical composition and crystalline structure, may reappear in multiple historical contexts, with different trace elements, structural defects, and distinctive sizes and shapes.

The IMA mineral system was not designed to accommodate these "idiosyncrasies" that reflect different historical contexts for a given IMA mineral species. The inductive interests of the IMA system employ idealized properties for classifying solid materials into mineral kinds that do not preserve historical information. Not only does the IMA system lump together solid materials having very different causal histories, but also it splits some solid materials having essentially the same etiologies, rendering its categories inadequate for purposes of reasoning scientifically about how Earth and other terrestrial planets form and change through time.

Consider the example of diamond, defined by IMA protocols as pure carbon in the idealized diamond structure. The IMA system does not distinguish among vapor-deposited nanodiamonds formed 5 billion y ago in the expanding cooling atmospheres of aged stars, mantle-derived gem diamonds formed 500 million y ago at high temperature and pressure from carbon-bearing aqueous solutions, and impact diamond formed 5,000 y ago when a large meteor struck a carbon-rich sediment. The IMA system classifies all three as "diamond" because they all approximate pure carbon in the diamond crystalline structure, thus lumping together mineral kinds that have demonstrably different historical conditions of formation and resultant physical and chemical properties. Diamond might better be split into several kinds when considering these distinctive historical contexts. Similar situations occur for numerous minerals, notably common phases such as calcite, quartz, and apatite that form both in abiotic and in biological contexts with strikingly different morphologies, trace elements, and other physical and chemical attributes.

In other instances, the IMA protocols result in the splitting of solid materials into separate mineral species, despite their having basically the same etiology. Solid solution series, by which two or more elements substitute for each other, and thus offer a continuum of possible compositions, provide good illustrations of this problem. For example, iron and magnesium occur in solid solution in numerous common mineral structural groups, including olivine, pyroxene, mica, and garnet. In each instance (and many more), the iron and magnesium end-members are defined as different mineral species. For example, the olivine species forsterite (Mg_2SiO_4) and fayalite (Fe_2SiO_4) represent idealized end-members of a continuous chemical series, better represented in nature by $[(Mg,Fe)_2SiO_4]$. In nature, specimens with ∼50:50 mixtures of Fe and Mg are not uncommon, leading to ambiguity regarding which end-member species name should be assigned. Furthermore, many crystals are "zoned," with gradations in the ratio of element pairs like iron and magnesium. As a consequence, a given crystal grain may oscillate between similar compositions, some regions being slightly iron dominant and others slightly magnesium dominant. IMA protocols require defining that single zoned grain as two different end-member species, neither of which represents the crystal at hand. The same situation occurs with hundreds of IMA mineral species, including most of the common rock-forming minerals that form >99% of the volume and mass of Earth's crust.

The splitting and lumping of natural minerals into end-member IMA species are not only ad hoc, but at times may lead to confusion regarding the proper naming of intermediate compositional examples, thus obscuring information that points to very different modes of formation of individual specimens. Consider again the example of forsterite, which is a major mineral in Earth's upper mantle. In this context, forsterite erupts in volcanic rocks that originate deep in Earth's interior, usually with ∼10 atom % of Fe substituting for Mg. That iron-bearing forsterite is compositionally distinct from near end-member Mg_2SiO_4 that forms at much shallower depths in the crust when the Mg-bearing mineral dolomite is metamorphosed. Thus, by ignoring the essential differences in olivine Fe content—by splitting forsterite and fayalite into two species, yet lumping all specimens that approximate Mg_2SiO_4 into the one species "forsterite"—important information about the causal histories of each specimen is lost.

The complexities of mineral solid solutions, and the classification dilemmas they pose, cannot always be resolved with any simple modifications of the IMA system. Indeed, in a few instances IMA nomenclature appears to deviate significantly from their own guidelines. Consider the difficult example of the rock-forming clinopyroxene group of minerals, which are traditionally illustrated on a "quadrilateral diagram" (Fig. 1) that represents compositions intermediate among three idealized pyroxene end-members: enstatite (EN: $Mg_2Si_2O_6$), ferrosililite (FS: $Fe_2Si_2O_6$), and wollastonite (WO: $Ca_2Si_2O_6$). These three end-members can be represented on a triangle (a "ternary diagram" of compositions). However, pyroxenes are restricted to having no more than 50 atom % of the calcium end-member; consequently, the pyroxene quadrilateral is bounded by the four end-members EN, FS,

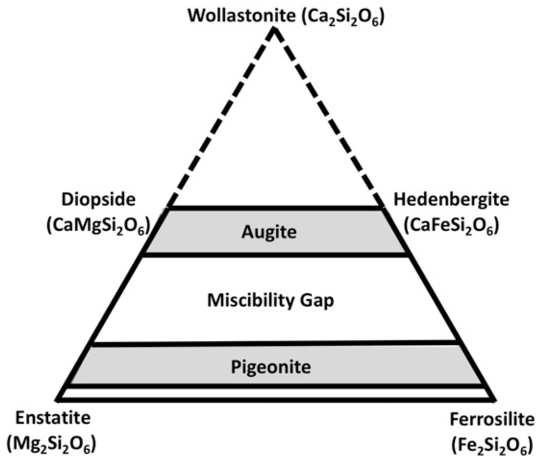

Fig. 1. **The "pyroxene quadrilateral," illustrating chemical compositions of pyroxenes with idealized compositions represented by $(Mg,Fe,Ca)_2Si_2O_6$. Most natural pyroxenes do not lie near one of the corners of this quadrilateral and are given the names "augite" or "pigeonite."**

diopside (DI: $CaMgSi_2O_6$), and hedenbergite (HD: $CaFeSi_2O_6$), as illustrated in Fig. 1.

Some natural occurrences of pyroxenes are close to one of the EN, FS, DI, or HD end-members and thus can be named unambiguously as one of those four end-member species. However, the vast majority of rock-forming clinopyroxenes have compositions lying somewhere in the middle of this quadrilateral—a situation recognized by IMA through the approval of two additional names. "Augite" is thus defined as a range of pyroxenes with from ∼35 to 50 atom % calcium. In addition, "pigeonite" is defined as a different range of pyroxenes with from 5 to ∼15 atom % calcium. (Note that pyroxenes with 15 to 35 atom % calcium are rarely observed.) Augite and pigeonite, defining as they do intermediate solid solutions with rather arbitrary chemical boundaries, are not consistent with most other IMA nomenclature protocols.

The situation becomes even more confused for an important group of pyroxene occurrences found primarily in the most primitive meteorites, where significant amounts of additional elements, notably aluminum and titanium, substitute for Mg, Fe, and Ca. Thus, these pyroxene compositions lie significantly outside of the quadrilateral in a higher-dimensional composition regime. The arcane details of pyroxene nomenclature aside (28), these pyroxenes, although most are technically augite, are universally called "fassaite" by the meteoritic research community, even though the IMA has discredited that name (unlike augite or pigeonite).

A third concern about the IMA protocols, in addition to problems with lumping and splitting, relates to natural condensed phases that are not typically included in the IMA system. In almost all instances, IMA does not recognize noncrystalline materials (liquid mercury and opal are exceptions, having been "grandfathered in"). However, a surprising number of condensed planetary materials, including different kinds of volcanic glass (e.g., "obsidian"); poorly crystallized clay-like phases in soils; and a range of biologically derived solids such as amber, coal, and kerogen, lack a well-defined crystalline structure and thus do not come under the purview of the IMA mineral system. However, these phases may be critical to interpreting the historical context of planetary deposits. For example, many Martian soils analyzed by the *Curiosity* rover contain more than 50 wt% noncrystalline materials. These components of the Martian soil are thought to have precipitated as gels in an ancient lake and thus have an important story to tell about the early history of the Martian surface (29). We conclude that, despite the essential role of the IMA classification system in many areas of geology and its firm theoretical grounding in chemistry and physics, the system was never intended to be used as a classification system in historical areas of geology such as planetary science.

Results

Planetary geoscientists need a more historical concept of mineral kind embedded in a classification scheme that categorizes solid materials in terms of similarities and differences in the causal processes and conditions that give rise to them. The very concept of an historical natural kind is problematic, however. The vast majority of classification systems used in science are time independent; they categorize physical entities into kinds solely on the basis of similarities and differences among manifest properties, regardless of etiology. The periodic table of the chemical elements provides a classic illustration. Whether an element is helium depends only upon its atomic number, equal to the number of protons in its nucleus. That helium is created by fusion reactions inside stars and also by radioactive decay of heavy elements, such as uranium and thorium, is irrelevant to its identity as the element helium. The justification for ignoring the conditions and processes that produce elemental helium is based on chemical theory. Helium's manifest chemical properties (being colorless, odorless, etc.) and its chemical behavior (lack of reactivity with other elements of the periodic table) do not depend upon how it originates; universal (timeless) principles of chemistry explain, for example, why there are no helium-bearing minerals in nature.

The most promising candidates for genuinely historical, natural kinds are found in evolutionary biology. Not all of the manifest similarities among organisms are relevant for purposes of understanding their evolutionary relatedness. It is thus a mistake to classify organisms into evolutionary kinds on the basis of similarities in form and structure alone. Evolutionary biologists need to distinguish similarities that are the product of shared common ancestry (homologies) from similarities that are not (analogies). Before the advent of Darwin's theory there was no need for a distinction between homologies and analogies. Biological species were viewed as separately created and unchanging—in essence, as eternal and timeless. A salient illustration is provided by the 17th-century debate over whether bats are birds. The debate centered on the fact that both have wings and revolved around the question of whether their wings were similar enough to categorize them as the same kind of animal. The philosopher–physician, John Locke (30), dismissed the debate as pointless and called for disputants to make an arbitrary decision; in his view, there was not a principled distinction on which to resolve the dispute. With the advent of Darwin's theory of evolution, however, it became clear that the debate is far from pointless. The wings of bats and birds are analogous, as opposed to homologous; bats and birds do not share a common winged ancestor. In contrast, the mammary glands of whales and zebras are now understood to be homologous in virtue of deriving from a unique, shared, common mammalian ancestor. As late as the mid-18th century, however, whales were still classified as fish because they more closely resemble fish in external morphology and lifestyle than mammals like zebras (31). Linnaeus classified whales as fish in the 1735 first edition of his *System of Nature*, and this convention persisted through the ninth edition of 1756 (32). However, by the 1770s most taxonomists, including Linnaeus, were classifying whales as mammals. The rationale for doing this, however, was still based on manifest similarities and differences among organisms, more specifically, the internal anatomical and physiological characteristics of whales, fish, and mammals; they deemed whales more like mammals than fish by virtue of, for example, having lungs and four-chambered hearts, being warm blooded, and suckling their young. The historical significance of this cluster of internal similarities among cetaceans and other mammals was not recognized until the advent of Darwin's theory. Darwin's theory explains why internal anatomical and physiological (and as we now know, genomic) similarities among organisms are of greater consequence for understanding historical interrelations among organisms than external morphology and lifestyle. The pre-Darwinian decision to classify organisms into biological kinds on the basis of their internal anatomy and physiology can be viewed in hindsight as auspicious—a lucky choice that was able to accommodate the later development of Darwin's theory of evolution by natural selection.

Unfortunately, evolutionary biology does not provide a good model for developing an historical concept of mineral kinds. The classification of organisms into historical–evolutionary kinds is based on differentiating clusters of properties (organismal traits) that are associated as a consequence of common descent. Planetary geoscientists are not typically interested in grouping minerals into kinds on the basis of whether they share an ancestral solid material having a unique spatiotemporal location [although, see Heaney (33), who introduces the concept of mineral evolutionary trees]. Rather, they are concerned with grouping minerals into categories on the basis of similarities and differences in the causal processes and physicochemical conditions that produced them—i.e., their "paragenetic modes." The notion of etiology required for accommodating inductive reasoning in the historical geosciences is thus very different from that required for inductive reasoning in evolutionary biology. Nevertheless, some instructive similarities occur for both the mineralogical and biological cases. As in evolutionary biology, mere resemblance among manifest characteristics of solid materials is not enough to systematically group them into historical natural kinds. The fact that the IMA system classifies a solid as diamond tells one very little about the conditions and processes involved in its formation, because the combination of properties (idealized major element composition and crystalline structure) used by the IMA system does not incorporate historical information.

The challenge for planetary scientists is identifying which idiosyncratic combinations of features of solid materials are most reliable for historical purposes—for understanding the origin and evolution of condensed planetary materials, as well as their role in the evolution of terrestrial planets. Many of the properties of solid materials currently treated by the IMA as insignificant deviations from idealized major element composition and crystalline structure can reveal a mineral's paragenetic mode. A minute amount of a carbon or nitrogen isotope can reveal mineral origins in an ancient exploding supernova; a morphological quirk can unambiguously point to microbially precipitated crystals. These information-rich, potentially historically informative attributes include trace and minor elements, ratios of isotopes, fluid and solid inclusions of other phases, sizes and shapes of crystals, associated minerals, structural defects, and many other physical and chemical properties.

Minerals classified as diamond by the IMA's time-independent protocols provide compelling illustrations. Diamonds formed as stardust differ from mantle-derived diamonds in, among other things, their carbon isotope compositions, their morphologies, and their geological context—all properties not considered by the IMA system. Mantle-derived diamonds, which form under high pressures from different types of carbon solutions, are further distinguished in terms of the presence of nitrogen impurities ("type I" diamonds) or diagnostic metal inclusions ("type II" diamonds). Indeed, the IMA mineral species diamond consists of at least five different historical mineral kinds, each characterized by a distinctive set of manifest properties supplying critical information about the conditions, processes, and time required to produce them (34).

The challenge facing mineralogists who would formulate an evolutionary classification of minerals is identifying which clusters of information-rich mineralogical properties are historically informative in the context of a planet's evolution. The idealized major element composition and crystal structure currently used by the IMA system for classifying mineral kinds are, by themselves, inadequate for this purpose.

By what process might such an historically informed system of mineral classification be devised? Ideally, geoscientists could appeal to emerging geological theories of the development of planetary materials analogous to Darwin's theory of biological evolution to discriminate what are, in essence, geological homologies from mere geological analogies. Many facets of this historical approach are in place. Separate groups of experts have studied and explained modes of mineral formation in stellar atmospheres, in cool molecular clouds in interstellar space, in the earliest stages of the stellar nebula that formed our solar system, and in the first generation of planetesimals that provided raw materials for emerging planets and moons. Likewise, scientists have focused on the earliest stages of Earth's evolution—the differentiation of core, mantle, and crust; the formation of oceans and atmospheres; the development of global-scale tectonic processes, with consequent emplacement of ore bodies; the origins of microbial life; and the emergence of a biosphere that came to dominate many near-surface mineral-forming processes. Qualitative explorations of the sweep of Earth's geological evolution have been forthcoming and suggest a framework for an evolutionary system of mineralogy (35, 36). What has been lacking is an integration of those separate phases of Earth evolution into an empirically powerful, general theoretical framework of mineral evolution that is grounded in the information-rich attributes of minerals.

Discussion

The scientific utility of taxonomic systems lies in their ability to reveal unity in the midst of diversity for purposes of inductive (explanatory and predictive) reasoning about a domain of natural phenomena. The IMA system of classifying solid materials into mineral species provides a good illustration. Resting on the twin pillars of idealized chemical composition and crystalline structure, it elaborates modern chemical theory and solid-state physics—specifically, the idea that the properties of material things are a consequence of their compositions and arrangements of their chemical elements. A knowledge of composition and crystal structure not only provides a basis for discriminating among solid materials as different mineral kinds, but also provides a principled foundation for understanding many important similarities and differences among their attributes.

However, the IMA system is concerned only with time-independent attributes of minerals. The evolution of natural mineral-forming environments through deep time and the consequent variations of minerals and their attributes play no role in its classification protocols. Yet the latter hold the key to successful inductive reasoning about the origin of condensed planetary materials and their roles in the development of Earth and other terrestrial planets.

In light of these considerations, the following questions arise: What might be the theoretical basis for classifying solid materials as historical mineral kinds? Is there an historical analogy to chemical theory that might guide the development of an etiological taxonomy of mineral kinds? Can we identify potentially unifying, general historical principles related to mineral origins and "evolution," as opposed to a collection of loosely related, highly contextual rules of thumb?

What is needed is a system of mineral classification able to discriminate those similarities and differences among natural phases of matter that are historically informative from those that are not, while at the same time exposing the more general etiological principles responsible for them. In this sense, our ambitions parallel those of Darwin's biological theory of evolution, through which empirical observations of manifest (morphological, anatomical, and physiological) variations among organisms acquired a theoretical foundation (via the principles of heritability and natural selection) for discriminating those similarities and differences among groups of organisms that have an historical explanation (in terms of unique common ancestry) from those that do not. As discussed earlier, however, nonliving solid materials do not possess a genetic system (physical source of heritable variation), nor are they subject to natural selection, except in the chemical sense of the "selection" of thermodynamically more stable phases over unstable arrangements of chemical elements (37). In short, historical geoscientists currently lack unifying etiological principles, analogous to those provided by Darwinian evolution for organisms, for classifying solid materials into mineral kinds.

What abiological, etiological principles could underlie the origin and temporally asymmetric development of condensed planetary materials and the planetary bodies that they compose? There are compelling reasons for thinking that such principles exist, although it is clear that our understanding of them is still embryonic. A widely accepted model posits that the universe began in the Big Bang ~13.8 billion y ago and subsequently went through an ordered sequence of many physicochemical stages, each of which added chemical and structural complexity to the cosmos, eventually producing planetary environments supporting the emergence of the first living things. In this context, mineral evolution is just one aspect of a larger theoretical framework, often called "cosmic chemical evolution" or simply "cosmic evolution" (34, 35, 38–40). Cosmic chemical evolution subsumes Darwin's theory as a special case, one among many facets of the increasing complexification (evolution in a broader sense of the term) of stellar and planetary materials. New chemical compounds, including the varied natural condensed solid phases we call minerals, emerged as a consequence of gradual complexifying changes in the characteristics of local environments, including such factors as pressure, temperature, chemical composition, and notably the temporal sequence and rates of change of those variables. In the fullness of time, some of these environments became chemically and structurally complex enough for the emergence of living things capable of Darwinian evolution.

The logical character of the general principles underlying cosmic chemical evolution—whether they are deterministic or probabilistic and whether they represent time-independent processes (operating on temporally asymmetric initial conditions of the universe, as determined by fine tuning and gravity) or are themselves (intrinsically) temporally asymmetric—is unclear. The only temporally asymmetrical law of nature that has thus far been widely endorsed by the scientific community is the second law of thermodynamics, but it has the wrong character insofar as the arrow of time and the direction of complexification run in opposite directions. In this context, a number of researchers (e.g., refs. 41–43) speculate that there may be additional laws of thermodynamics for open, self-constructing physicochemical systems, most conspicuously organisms and biospheres. We remain agnostic, however, about the ultimate source of the temporally asymmetrical pattern of increasing complexification exhibited by the universe.

What we are not agnostic about is the existence of a temporally asymmetrical pattern of increasing complexification that the cosmic evolutionary model aspires to explain: Shortly after the Big Bang's "moment of creation" 13.8 billion y ago, some atoms formed from newly condensed quarks and leptons. Molecules then formed from atoms; stars arose from gravitational clumping of those atoms and molecules; and stars, in turn, underwent nucleosynthesis, producing most of the chemical elements of the periodic table. From the turbulent, cooling atmosphere of stars the first minerals arose, which became building blocks of asteroids, planets, and moons. Planets became engines of mineral evolution, as a diversity of new chemical and physical processes selected and concentrated elements into new combinations that were subjected to new pressure–temperature regimes. On Earth, and perhaps countless other worlds across the universe, mineral-rich environments fostered the origin of life, which in turn led to new mineral-forming environments as life and rocks coevolved. Indeed, all cells today hold biochemical reminders of life's rocky start (44–48), while more than two-thirds of all mineral species arose, at least indirectly, through biological changes in Earth's near-surface environment (36).

In this context, we propose a bootstrapping approach to building a mineral classification system based on historically revelatory, information-rich chemical, physical, and biological attributes of solid materials, while remaining agnostic about the nature of the unifying theoretical principles underlying it. We explicitly accept the temporally asymmetrical pattern of increasing complexification exhibited by the universe as compelling evidence that such principles exist. The core idea is to search for historically revealing clusters of covarying attributes. As in evolutionary biology, clusters of covarying attributes should be treated as fallible indicators of historical natural kinds (18, 20). The mere fact that attributes covary is not enough to conclude that they represent historical natural kinds; as in evolutionary biology, and as underscored by the IMA system's utility in many geological applications, attributes often covary for ahistorical reasons. It is thus important to resist reading historical significance from mere covariance of manifest attributes. The key is to search for clusters of attributes whose covariance is best explained etiologically. This search can be accomplished by beginning with highly contextual rules of thumb. As more evidence accumulates, patterns of unity among what initially seem to be historically disparate clusters of attributes are likely to emerge. Classifications can be revised in light of these discoveries with the goal of improving the system's scope and reliability and hence its capacity to support increasingly powerful, inductive (explanatory and, especially in the case of history, retrodictive) inferences. In this manner, an evolving system of historical mineral kinds, initiated by highly contextual rules of thumb, may lead to the discovery of the precise nature of the as yet poorly understood unifying principles underlying the pattern of increasing complexification exhibited by the universe.

Three parallel (bootstrapping) approaches inform the development of the proposed evolutionary system of mineralogy. First, we catalog dozens of distinct mineral-forming environments, based on centuries of geological field studies, astronomical observations, laboratory experiments, and theoretical analysis of natural samples and their environments. A vast body of research, much of it derived from minerals themselves, documents stages of planetary evolution—many of them inferred from ancient deposits and others observed in action on dynamic Earth today. An evolutionary theory of mineralogy must build on that foundation.

Second, we rely on the exhaustive catalog of minerals represented by the IMA classification system. Among the numerous defining attributes of historical kinds of minerals, chemical composition and crystal structure must be included. In this sense, any historical classification system of minerals builds upon the IMA standard.

Third, we have begun to develop and expand mineralogical databases, which will provide the quantitative foundation for defining distinct historical natural kinds. Each mineral specimen is an information-rich object that has hundreds of quantifiable attributes. Our contention is that a specimen's attributes, taken collectively, preserve a record of that specimen's historical origins, as well as its subsequent alteration through a sequence of environments. Furthermore, given a large enough number of specimens with myriad carefully measured attributes, we can apply methods of cluster analysis to discriminate different populations for any given IMA mineral species. Thus, for example, such characteristics as size, shape, color, inclusions, isotopes, and trace elements should be sufficient to differentiate stellar diamond, mantle diamond, and impact diamond. Similarly, "idiosyncratic" (from an IMA perspective) combinations of attributes will be employed to identify biotic versus abiotic minerals.

Two parallel research efforts are necessary to accomplish this vision. First, we must review and synthesize the vast research literature of the past 200 y to document all known minerals in the contexts of their historical modes of formation. Such a synthesis will be, of necessity, incomplete and speculative, but the emerging historical framework will provide the theoretical context for the evolutionary system. At the same time, such a framework is vital to efforts to compare and contrast the mineral evolution of different planets and moons—Earth and Mars, for example.

At the same time, a crucial long-term effort must be to consolidate existing and new mineral data resources into an open-access, integrated, and "FAIR" (findable, accessible, interoperable, reusable) (49) repository that tabulates hundreds of attributes for millions of specimens. Quantitative rigor in defining historical natural kinds can only emerge from the multidimensional analysis of vast numbers of well-characterized specimens. Such an effort has begun, but the successful development, expansion, and curation of such a data resource will become a perpetual challenge for future generations of mineralogists.

It is important to keep in mind that we are not contending that an evolutionary (etiological) system of mineral kinds should replace the traditional IMA system of minerals. As philosopher John Dupré (50) famously counsels, any set of material objects can in principle be classified in a variety of different ways. The scientific value (or "naturalness") of a kind concept depends upon the extent to which the categories that it carves out support the formulation of inductively powerful generalizations. The IMA system is successful at supporting inductive generalizations in those time-independent areas of Earth, planetary, and solid-state sciences for which it was originally designed. However, the IMA system is unable to support inductively reliable generalizations in the historical geosciences, especially planetary science in the context of comparative planetary evolution. A more historically oriented system of mineral classification is thus needed in the latter areas of the Earth and planetary sciences.

Whether a taxonomy of historical mineral kinds should be viewed as complementing the standard, time-independent IMA system of mineralogy or (more pluralistically) replacing it in historical contexts is a philosophical question that we leave open. It is worth noting, however, that the concept of species in the biological sciences is treated in practice pluralistically, with structural biologists, for instance, using a typological (morphological/phenotypical) species concept and evolutionary biologists using an evolutionary (phylogenetic) species concept (51). Despite significant efforts, biologists have yet to formulate a concept of biological species applicable throughout the biosciences, and some biologists are beginning to question whether a univocal concept of species is even feasible (52). It is unclear whether the geosciences will ultimately be faced with the same predicament.

Data Availability. There are no data underlying this work.

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