02 November 2018—*American Mineralogist*—Revision 1

An evolutionary system of mineralogy: Proposal for a classification of planetary materials based on natural kind clustering

ROBERT M. HAZEN[1,*]

[1]Geophysical Laboratory, Carnegie Institution for Science,
5251 Broad Branch Road NW, Washington, DC 20015, U. S. A.

ABSTRACT

Minerals reveal the nature of the co-evolving geosphere and biosphere through billions of years of Earth history. Mineral classification systems have the potential to elucidate this rich evolutionary story; however, the present mineral taxonomy, based as it is on idealized major element chemistry and crystal structure, lacks a temporal aspect and thus cannot reflect planetary evolution. A complementary evolutionary system of mineralogy based on the quantitative recognition of "natural kind clustering" for a wide range of condensed planetary materials with different paragenetic origins has the potential to amplify, though not supersede, the present classification system.

***E-mail:** rhazen@ciw.edu

Keywords: philosophy of mineralogy; classification; mineral evolution; mineral ecology; data-driven discovery; cluster analysis; natural kinds

INTRODUCTION

For more than 2000 years, the classification of natural objects and phenomena into "kinds" has been a central pursuit of natural philosophers (Aristotle/Thompson 1910; Locke 1690; Linnaeus 1758). The modern mineral classification system, rooted in the chemical framework of James Dwight Dana (1850), is based on unique combinations of idealized major element composition and crystal structure (Strunz 1941; Palache et al. 1944, 1951; Liebau 1985; Mills et al. 2009). This robust and effective scheme not only allows for the unambiguous and reproducible categorization of most natural crystalline materials, but it also reflects the thermodynamic importance of end-member phases in characterizing the complex natural world. However, this system of mineralogy is but one of many potentially valid formalisms; natural condensed materials have also been successfully organized according to their importance to specialized fields, for example in gemology, ore geology, petrology, or the construction industry.

Effective scientific classification systems not only define and organize objects of nature, but they also reflect and elaborate current theory, for example in the context of an evolving natural world. Biological classification schemes from Linnaeus' *Systema Naturae* (1758), to those incorporating patterns of interbreeding (e.g., Mayr 1969), to modern genetic analyses (e.g., Pace 2009; Ruggiero et al. 2015) implicitly incorporate information on inherited similarities, coupled with differences that arise through Darwinian selection, and thus are effectively evolution-based (Richards 2016). Many other familiar classification systems incorporate evolutionary time series, either explicitly (i.e., the stages of cell division; embyogenesis) or implicitly (stellar classification; human technologies).

By contrast, mineralogical classification systems, which traditionally have been more deeply rooted in inorganic chemistry and materials science than planetary evolution, have long relied on a combination of physical and chemical attributes to distinguish mineral “species” (Burke 1969; Povarennykh 1972; Hazen 1984). This longstanding tradition does not incorporate a temporal or evolutionary framework, either implicitly or explicitly (however, see Heaney 2016). Here I propose a complementary classification method that exploits the inherent evolving “messiness” of planetary materials by grouping them according to “natural kind clusters” (Boyd 1999). Natural solids, including a variety of noncrystalline condensed materials not represented by the current formalism, can be categorized by distinct “kinds” according to their distinctive combinations of nonideal atomic structures, complex chemical compositions, variable physical properties, and diverse modes of origin. Cluster analysis based on the observed range of properties in natural specimens thus complements and amplifies, though not supercedes, the present mineral classification scheme as codified by the International Mineralogical Association (IMA). By recognizing natural kinds of planetary materials, this approach to mineral classification incorporates an evolutionary component in addition to chemistry and structure.

NATURAL VERSUS ARTIFICIAL CLASSIFICATION OF MINERALS

A longstanding philosophical debate considers the extent to which a basis exists for “natural” classification of kinds—a division of natural objects based on the organization of nature, as opposed to human-imposed “artificial” classification rules (Mill 1884; Dupré 1981; Kuhn 2000; Hawley and Bird 2011; Magnus 2012; Wilkins and Ebach 2013; Bird and Tobin 2018). Some natural systems would seem to provide unambiguous quantifiable categories on which to base a classification system [relativist claims that all human classifications are inherently artificial notwithstanding (e.g., Woolgar 1988; Kukla 2000)]. For example, a unique integral number of protons in the nucleus defines each chemical element. Further subdivision according to the integral number of neutrons defines each isotope. Thus, in the case of atoms nature has provided an unambiguous quantitative basis for classification of kinds.

In the more nuanced example of biological systems, because each new genetic characteristic arises at a specific time in a specific organism, a natural classification of living organisms based on an evolutionary sequence of genetic modifications seems plausible. [A significant caveat is the recognition of pervasive lateral gene transfer, especially among microbial communities—a mode of evolutionary change less amenable to a simple timeline and branching tree of life (e.g., Doolittle 2000; Ochman et al. 2000; Keeling and Palmer 2008).] By contrast, many other classification systems of the natural world, such as the segmentation of the continuous electromagnetic spectrum into partially overlapping ranges of radio, microwave, infrared, etc., or of visible light into colors, resort to the division of nature into more arbitrary kinds. The extent to which humans impose arbitrary classification rules to define kinds, however quantitative and reproducible that system may be, reflects the extent to which a classification system can be described as artificial as opposed to natural.

In this context, the present classification system of minerals incorporates both natural traits and artificial rules. The IMA chemical and structural rules for defining and approving new species are unambiguous, independently quantifiable characteristics of minerals. However, the idealized compositions and crystal structures of IMA mineral species are rarely observed in nature; therefore, rules defining minerals based on the dominant major elements and idealized crystal structures do not fully reflect natural mineralogical kinds. In response, this contribution proposes a modification and amplification of the present mineral classification schema—an evolutionary system of mineralogy that incorporates mineral modes of formation and thus essential aspects of planetary evolution.

SHORTCOMINGS OF THE PRESENT MINERAL CLASSIFICATION SYSTEM

What constitutes the most natural division of the mineral kingdom? The present system of mineral classification possesses the important advantage of establishing unambiguous criteria for the identification of the great majority of natural crystalline materials, both known and yet to be discovered and described. Following a rigorous IMA approval process, each valid mineral species is defined by a unique combination of idealized major element chemistry and crystal structure. This protocol satisfies the most basic requirement of any classification scheme—independently reproducible and verifiable criteria for assigning mineral names; as of 30 October 2018, a total of 5370 mineral species had been approved by the IMA (rruff.info/ima).

Longstanding questions in mineralogy ask how many different kinds of minerals occur on Earth? Does that number change through time? How does that number on Earth compare to other (typically less well endowed) planets and moons, both in our solar system and beyond? And by what natural physical, chemical, and biological processes do new minerals arise? Those questions have been explored recently in the contexts of "mineral evolution" and "mineral ecology," which analyze the temporal and spatial diversity and distribution of minerals, respectively (Zhabin 1981; Hazen et al. 2008, 2015, 2016; Hystad et al. 2015). Unfortunately, these questions of mineral diversity and planetary evolution cannot be fully resolved using the IMA criteria for differentiating mineral species.

This contribution introduces a complementary division of condensed planetary materials into natural kinds based on the observed range of chemical and physical characteristics of any natural condensed phase—properties that reflect not only a substance's major element chemistry and crystal structure, but also its paragenetic mode (i.e., the physical, chemical, and/or biological process by which it formed). Based on this genetic, evolutionary definition of natural mineral kinds, at least three categories of planetary materials are imperfectly catalogued by the present mineral classification system: (1) distinct natural kinds that have been lumped in the IMA classification; (2) individual natural kinds that have been split by the IMA classification; and (3) noncrystalline materials.

Natural kinds that have been lumped by the IMA classification: The IMA mineral species criteria of idealized major element composition and crystal structure in some instances lump together demonstrably distinct natural kinds of minerals. Diamond offers a dramatic example (Table 1). The first mineral in the cosmos was nanocrystalline diamond that condensed from incandescent, expanding and cooling gases ejected from the first generation of large stars more than 13 billion years ago (Hazen et al. 2008; Ott 2009). These vapor-deposited nanodiamonds, which still must form in vast numbers around energetic stars across the universe today and which are distinct from all other diamond populations in their origins, morphologies, isotopic compositions, and other properties [for example, anomalous microwave emissions (Greaves et al. 2018)], fall to Earth in chondrite meteorites and presolar grains.

Contrast these well-traveled nanodiamonds with two populations of mantle-derived macroscopic crystals, some formed from deep, high-pressure carbon-bearing aqueous solutions, including “Type I” diamonds with IR- and UV-absorbing nitrogen impurities (Davis 1984; Shirey et al. 2013; Sverjensky and Huang 2015), and others from deep, high-pressure, carbon-saturated Fe-Ni melts (including nitrogen-poor, IR-transparent “Type II” diamonds; Smith et al. 2016). Equally distinct is the enigmatic “carbonado” form of diamond, which typically consists of porous, black, superhard sintered masses (Heaney et al. 2005; Garai et al. 2006). In addition, microscopic diamond with a disordered structure (equivalent to the now discredited "lonsdaleite") can form from carbonaceous material subject to the shock of large impacts (Vishnevsky and Raitala 2000; Németh et al. 2014). Thus, from the standpoint of cosmic evolution, the mineral species "diamond" can be viewed as at least five different natural kinds of minerals, each with a distinct set of properties, mode of origin, and age range of formation (Table 1).

Similar arguments can be presented for many common minerals. Microscopic hydroxylapatite grains in chondrite meteorites differ in several respects from the coarser euhedral hydroxylapatite crystals in granitic pegmatite, which are in turn distinct from the hydroxylapatite/biopolymer composites of teeth and bones (Harlov and Rakovan 2015). Likewise, quartz displays multiple kinds: in granite and granite pegmatite, in hydrothermal veins, in quartzite, and in the biosilica of diatom skeletons (Heaney et al. 1994; Wysokowski et al. 2018). Pyrite differs in polymetallic veins, in black shales, and pyritized brachiopods (Rickard 2015); while calcite occurs in abiotic precipitates, biomineralized shells, and a dozen other contexts (Reeder 1983; Dove 2010).

Mineral solid solutions offer additional examples of the lumping of distinctive natural kinds. Of special note are the plagioclase feldspars, the most abundant minerals in Earth's crust (Rudnick and Gao 2005) and probably on Mars (Milam et al. 2010). The official division of plagioclase into two idealized end-member species, albite ($NaAlSi_3O_8$) and anorthite ($CaAl_2Si_2O_8$), does not reflect the varied paragenetic modes of intermediate compositions (Klein and Hurlbut 1980; Wenk and Bulakh 2004). Andesine, oligoclase, labradorite, and bytownite, though admittedly defined by somewhat arbitrary and overlapping criteria, long served petrologists as useful natural mineral categories (e.g., Tilley et al. 1964).

Therefore, in the planetary context of understanding mineral diversity and distribution through deep time, especially in enumerating the evolving numbers of mineral kinds and their global distributions, many IMA-approved mineral species should be split into two or more distinctive natural kinds, each with a quantifiable combination (i.e., clustering) of physical and chemical properties.

Natural kinds that have been artificially split by the IMA classification: In many instances, especially in mineral structure groups with great compositional plasticity, the division of minerals into numerous species according to ideal end-member compositions potentially results in the artificial splitting of natural kinds. By imposing compositional boundaries between species of minerals that occur in a continuous solid solution, the present mineral classification scheme does not adequately reflect natural kinds with wide ranges of solid solution.

The tourmaline supergroup is a case in point. The IMA now recognizes at least 32 approved species of tourmaline (with 8 more species pending), each with a different distribution of major elements among six of its crystallographic sites (Henry et al. 2011; Grew et al. 2017; rruff.info/ima, accessed October 30, 2018). Given natural compositional variations, this classification means that an individual thin section may hold two or more different tourmaline species (e.g., Henry et al. 2011; Grew et al. 2015), even if all tourmaline grains were formed in the same petrogenetic event. Indeed, individual grains that grow during a single magmatic or metamorphic event can display major element zoning that modulates among more than one tourmaline species. (Note that it is also possible for an individual mineral grain to represent two natural kinds—a core of igneous tourmaline or zircon, for example, with a hydrothermally deposited rim.) A division of tourmaline into natural kinds might thus provide a more parsimonious description of the supergroup and would facilitate a more accurate understanding of boron mineral diversity, distribution, and evolution (Grew et al. 2017).

The black mica known as "biotite," which is distinguished in hand specimen and thin section based on optical properties and morphology, has now been subdivided into several mica group mineral species, including annite, fluorannite, siderophyllite, and tetraferriphlogopite (Rieder et al. 1998). Similar splitting of natural kinds into many species occurs in the complex amphibole group with more than 100 approved species (Hawthorne et al. 2012; rruff.info/ima), the garnet group (Grew et al. 2013), oxide and sulfide spinels (Biagioni and Pasero 2014), and other rock-forming mineral groups.

Binary solid solutions, including ferromagnesian olivine, orthopyroxene, and many other examples, underscore the potentially artificial nature of classification based only on major element composition and crystal structure. Any rock that incorporates olivine grains with close to a 50:50 ratio of Mg:Fe will likely technically contain two species, both forsterite (Mg_2SiO_4) and fayalite (Fe_2SiO_4), even though all olivine grains arose from a single petrogenetic event.

Current conventions for recognizing rare earth element (REE) mineral species provide additional potential cases of splitting natural kinds. Under the current system, parisite-(Ce) and parasite-(La) are distinct species, based on differences in the most abundant REE, even though both species contain the full suite of REE in solid solution and are represented by the general formula $Ca(REE)_2(CO_3)_3F_2$ (Table 2). Similar arguments could be made for some of the multiplicity of species of almost 40 other REE mineral structures (including Ce-, La-, Nd-, and Sm-dominant variants of florencite, a REE aluminum phosphate; Table 2). In some cases, these split species represent a single natural kind with one stability field that incorporates yttrium and a range of light and heavy REE and thus one paragenetic mode.

In each of the above examples, the end-member compositions of diverse mineral structural groups are useful idealized thermodynamic constructs; the present IMA-approved mineral species should be retained as the primary systematic means to identify minerals. However, in studies of mineral evolution and mineral ecology, which are based on the diversity and distribution of minerals through time and space, this splitting of natural mineral kinds into multiple species obscures relationships that determine mineral co-occurrence in varied paragenetic environments. As in the case of splitting a single mineral species into two or more natural kinds, the lumping of several species into a single natural kind affects any estimates of total mineral diversity and distribution.

Natural kinds of non-crystalline planetary materials. The definition of a mineral as a naturally occurring crystalline material is deeply ingrained, yet it arbitrarily excludes significant volumes of condensed planetary materials from formal mineralogical consideration. Volcanic glass, solidified silica gel, shungite, amber, composite materials such as coal and mixed-layer clays, and natural nanomaterials such as carbon nanotubes and buckeyballs are among the many potentially important condensed solid phases that may play key roles in our understanding of planetary evolution, yet which lie outside the purview of modern mineralogy (Rogers 1917; Povarennykh 1996; Povarennykh et al. 2018).

This mineralogical requirement of crystallinity may lead to biases when attempting to understand deposits rich in amorphous and nanoscale materials. For example, recent data from NASA’s Mars Science Laboratory reveals that some martian soils contain greater than 50 weight percent amorphous material (e.g., Morrison et al. 2018). By expanding the classification of mineral kinds to consider a broader range of characteristic physical and chemical properties—i.e., beyond materials with a strictly periodic atomic structure—the potential exists to enrich mineralogy while better representing the actual materials that make up planets.

IMPLEMENTING AN EVOLUTIONARY SYSTEM OF MINERALOGY

Three significant challenges must be overcome to transform the concept of an evolutionary system of mineralogy into practical protocols for mineral classification: (1) creating extensive, reliable, and open-access mineral data resources; (2) applying diverse methods of cluster analysis to differentiate mineral natural kinds; and (3) developing a coherent and consistent nomenclature for mineral natural kinds.

1. *Creating data resources*: Quantitative identification of mineral natural kinds (e.g., the several kinds of diamond in Table 1) will emerge from analysis of extensive, reliable, and open-access data resources that are not yet generally available for most mineral species and groups. Consequently, the mineralogical community needs to create accurate and comprehensive tabulations of varied mineral attributes. The defining attributes will vary for different mineral species and groups, but will always include trace and minor elements. Additional parameters of interest might include isotopes of major, minor, and trace elements; crystal size, morphology, twinning, and defects; optical, electrical, magnetic, and elastic properties; the mineral's biological context, including local microbiota, fauna, and flora; age of formation; associated minerals, petrological context, and tectonic setting; and climate zone, local aqueous chemistry, and other environmental parameters. Each of these variables adds information that collectively have the potential to differentiate natural kinds through multi-dimensional analysis, and which might elucidate the origins and subsequent history of a mineral specimen in the context of planetary evolution.

Building robust data resources is thus the next step in implementing this proposed evolutionary system of mineralogy, both through "brute-force" compilations (i.e., transcription of literature data by hand), and through emerging machine learning methods that can rapidly scan pre-existing literature (e.g., https://geodeepdive.org; accessed 31 October 2018). A major ongoing challenge to the international mineralogy and petrology community is to promote a culture of data sharing, including the retrieval of "dark data" and the implementation of FAIR data policies by publications and societies (Downs 2006; Lehnert et al. 2007; Hazen 2014; Wilkinson et al. 2016).

2. Applying natural kind cluster analysis: "Cluster analysis" is a constellation of analytical methods that group objects into subsets (clusters) whose members are more alike than objects outside the cluster (e.g., Bailey 1994; Everitt 2011). Expanded mineral data resources on numerous specimens with many attributes are well suited for varied analytical approaches under the cluster analysis umbrella. Though there exists no single definition of a "cluster," two groups of minerals could be represented as distinct "kinds" if cluster analysis of any combination of attributes results in two non-overlapping groups in n-dimensional space.

In this endeavor mineralogists can learn important lessons from other scientific disciplines that have embraced classifications system based on natural kind clusters (Boyd 1991, 1999; Millikan 1999). Paleontologists and biologists have long employed the data-driven, cluster approach of morphometric analysis, for example to distinguish superficially similar species from ontonogenic sequences (Lohmann 1983; Bookstein 1991; Ashraf 2004; Turvey et al. 2018). In this formalism, the key to recognizing distinct natural kinds is the collection and analysis of numerous individual specimens to obtain statistically meaningful distributions of traits related to size and shape.

A revealing recent example is the application of cluster analysis to discern four major human personality types (Gerlach et al. 2018), based on analysis of more than 1.5 million individual results from the Five-Factor model of human personality traits (e.g., Widiger 2015). Their study reveals both the promise and potential pitfalls of cluster analysis. They initially employed an unsupervised Gaussian mixture model, which led to an unreasonably large number of discrete clusters—a difficulty that can arise in cluster analysis if groups differ significantly in size (Burnham and Anderson 2002; Lancichinetti et al. 2015). Gerlach et al. employed varied statistical tests to reveal that four major clusters provide an optimal fit to this large dataset. The authors thus emphasize "limitiations of unsupervised machine learning methods to the analysis of big data."

A similar strategy can be applied to implementation of an evolutionary system of mineralogy, which must be predicated on the analysis and comparison of numerous specimens from different mineral-forming environments. As with classifications in other domains, the recognition of mineral natural kinds will ultimately depend on the analytical comparison of large numbers of individual mineral descriptions, with richly varied information, data analysis, and visualization.

A significant challenge lies in determining what constitutes a mineral cluster. Ambiguity arises because no one algorithm or set of criteria can be universally applied to discern optimal clustering (Jain 2010). Experts in specific mineral species or groups must therefore supervise the application of cluster analysis, for example by selecting the most important attributes and constraining the total number of clusters. Each natural kind should be defined by continuous ranges of multiple attributes that arise from a well-defined paragenetic process—ideally a combination of characteristics that do not overlap with those of any other mineral kind. For example, vapor-deposited nanodiamonds from the expanding and cooling gaseous envelopes of energetic stars possess physical and chemical characteristics that are inherently different from those of high-pressure/temperature diamonds formed in Earth's mantle, and thus will form a separate cluster.

Identifications of natural kinds, including both the lumping and the splitting of existing IMA species, is context dependent and must be considered on a case-by-case basis. Depending on one's focus, the resulting number of clusters may differ significantly. For example, one researcher studying hydroxylapatite from the broad-brush perspective of billions of years of Earth history might choose to divide all specimens into three clusters: meteoritic, crustal, and biomineralized. By contrast, a biologist examining hydroxylapatite from a different evolutionary viewpoint might recognize multiple types of biomineralization with different kinds of bio-apatite in brachiopods, fish scales, cartilage, teeth, and bones (Roy 1974; Onozato 1979; Ohirta 1986; Sherman 2008).

The flexible, context-dependent nature of cluster analysis renders this approach ill-suited to be the primary classification system for minerals. Nevertheless, recognition of distinct mineral kinds is essential if we are to understand how the mineralogy of planets evolves through a succession of physical, chemical, and biological processes.

3. Developing a nomenclature for mineral natural kinds: Unambiguous, standardized mineralogical nomenclature is essential. In spite of attempts to introduce systematic and rational approaches to mineralogical nomenclature (e.g., Nickel and Grice 1998), relatively few of the more than 5300 approved mineral names provide useful clues regarding chemical or physical attributes of species, much less their varied modes of occurrence. The community of Earth scientists would be ill-served by any system that adds layers of taxonomic obscurity on the existing scheme.

A logical solution in the case of an evolutionary system is to employ descriptive paragenetic modifiers to the existing IMA mineral names. In the case of diamond, for example, names for several natural kinds already exist. "Presolar diamond" and "impact diamond" are self-explanatory, whereas "type I," "type II," and "carbonado" are well established varietal names for diamond. In each case the name "diamond" is retained, but with a familiar modifier. In the context of planetary evolution, recognizing and naming mineral natural kinds in this manner will enhance our ability to communicate stages of mineral evolution with clarity.

Finally, it is important to recognize that in the majority of instances, especially rare minerals with only one known mode of formation (Hazen and Ausubel 2016), natural mineral kinds will be exactly equivalent to IMA mineral species. Therefore, in most instances mineralogical nomenclature will require no modification.

IMPLICATIONS

An underlying assumption of this proposal is that complementary classification schemes of natural objects have the potential to reflect different aspects, and thus varied theories, of the natural world. The present IMA scheme focuses on idealized end-member compositions and structures of minerals, and thus is rooted in the principles of thermodynamics independent of a mineral's geological context. The proposed evolutionary system of mineralogy, based on the complex range of attributes stemming from the paragenetic modes of minerals, represents a complementary classification that is particularly suited to revealing a deeper understanding of planetary evolutionary processes. Different natural mineral kinds arise at different evolutionary stages. As we attempt to compare and contrast different terrestrial worlds, for example Earth and Mars, it is insufficient to know the identities of idealized end-member mineral species. We must also understand the natural kinds of minerals, with their attendant implications for the dynamic histories of planets and moons. This evolutionary system of mineralogy incorporates fundamental aspects of a mineral's chemical composition and atomic structure, but also recognizes that every natural condensed solid arises at a time, and in an environmental context, that are essential to defining its natural kind.

There is an appealing elegance in the existing system of classifying natural crystals as objects whose essence is captured in purely chemical and structural terms—whose idealized character is divorced from the sometime messy context of the natural world. Nevertheless, many ways exist to ascribe order to the universe and its objects; multiple classification schemes may serve parallel roles in science. When we consider the rich evolutionary history of our planetary home, as well as the growing inventory of thousands of other distant rocky planets and moons, each with its own unique evolutionary history, a complementary system of mineralogy beckons—one that acknowledges the information-rich complexity of natural minerals and the remarkable stories they tell of the changing physical, chemical, and biological environments that produced them.

ACKNOWLEDGEMENTS

I am grateful to Peter Burns, Carol Cleland, Robert Downs, Olivier Gagné, Allen Glazner, Joshua Golden, Edward Grew, Shaun Hardy, Peter Heaney, John Hughes, Morris Hindle, Daniel Hummer, Sergey Krivovichev, Chao Liu, Shaunna Morrison, Dietmar Mueller, Feifei Pan, Simone Runyon, Steven Shirey, and two anonymous reviewers for useful discussions and suggestions.

This publication is a contribution to the Deep Carbon Observatory. Studies of mineral evolution and mineral ecology are supported by the Deep Carbon Observatory, the Alfred P. Sloan Foundation, the W. M. Keck Foundation, the John Templeton Foundation, the NASA Astrobiology Institute, a private foundation, and the Carnegie Institution for Science.

REFERENCES CITED

Aristotle/Thompson, D'A. (1910) Historia Animalium. The Works of Aristotle Translated Into English. Oxford: Clarendon Press.

Ashraf, A.M.T. [Editor] (2004) Morphometrics: Applications in Biology and Paleontology. New York: Springer.

Bailey, K.D. (1994) Typologies and Taxonomies: An Introduction to Classification Techniques. Studies in Quantitative Applications in the Social Sciences, 102. New York: SAGE Publications.

Biagioni, C. and Pasero, M. (2014) The systematics of the spinel-type minerals: An overview. American Mineralogist, 99, 1254-1264.

Bird, A. and Tobin, E. (2018) Natural kinds. E. N. Zalta [Editor], The Stanford Encyclopedia of Philosophy (Spring 2018 Edition). https://plato.stanford.edu/archives/spr2018/entries/natural-kinds/

Bookstein, F.L. (1991) Morphometric Tools for Landmark Data: Geometry and Biology. Cambridge: Cambridge University Press.

Boyd, R. (1991) Realism, anti-foundationalism and the enthusiasm for natural kinds. Philosophical Studies, 61, 127-148.

Boyd, R. (1999) Homeostasis, species, and higher taxa. In R. Wilson [Editor], Species: New Interdisciplinary Essays. Cambridge, Massachusetts: Cambridge University Press, pp. 141-186.

Burke, J.G. (1969) Mineral classification in the early nineteenth century. In C.J. Schneer [Editor] Toward a History of Geology. Cambridge, Massachusetts: MIT Press, pp. 62-77.

Burnham, K.P., and Anderson, D.R. (2002) Model Selection and Multimodel Inference, 2^{nd} Edition. New York: Springer.

Christy, A.G. (2018) The diversity of mineral species: how many are there, why do some elements form many more than others, and how complex can they get? Australian Journal of Mineralogy19, 21-33.

Dana, J.D. (1850) A System of Mineralogy, Comprising the Most Recent Discoveries, Including Full Descriptions of Species and their Localities, Chemical Analyses and Formulas (Third Edition). New York and London: George P. Putnam.

Davis, G. (1984) Diamond. Bristol, United Kingdom: Adam Hilger Ltd.

Doolittle, W.F. (2000) Uprooting the tree of life. *Scientific American*, 282(2), 90-95.

Dove, P.M. (2010) The rise of skeletal biomineralization. Elements, 6, 37-42.

Downs, R.T. (2006) The RRUFF project: An integrated study of the chemistry, crystallography, Raman and infrared spectroscopy of minerals. Program and Abstracts of the 19th General Meeting of the International Mineralogical Association in Kobe, Japan, O03-13.

Dupré, J. (1981) Natural kinds and biological taxa. Philosophical Review, 90, 66-90.

Ellis, B. (2001) Scientific Essentialism. Cambridge Studies in Philosophy. Cambridge, UK: Cambridge Univesity Press.

Everitt, B. (2011) Cluster Analysis. Chichester, United Kingdom: Wiley.

Garai, J., Haggerty, S.E., Rekhi, S., and Chance, M. (2006) Infrared absorption investigations confirm the extraterrestrial origin of carbonado-diamonds. The Astrophysical Journal, 653, L153-L156.

Gerlach, M., Farb, B., Revelle, W., and Amaral, L.A.N. (2018) A robust data-driven approach identifies four personality types across four large data sets. Nature Human Behaviour, 2, 735-742.

Greaves, J.S., Scaife, A.M.M., Frayer, D.T., Green, D.A., Mason, B.S., and Smith, A.M.S. (2018) Anomalous microwave emission from spinning nanodiamonds around stars. Nature Astronomy. doi: 10.1038/s41550-018-0495-z

Greene, J.C. and Burke, J.G. (1978) The Science of Minerals in the Age of Jefferson. Philadelphia, Pennsylvania: American Philosophical Society.

Grew, E.S., Locock, A.J., Mills, S.J., Galuskina, I.O., Galuskin, E.V., and Hålenius, U. (2013) Nomenclature of the garnet supergroup. American Mineralogist, 98, 785-811.

Grew, E.S., Dymek, R.F., De Hoog, J.C.M., Harley, S.L., Boak, J.M., Hazen, R.M., and Yates, M.G. (2015) Boron isotopes in tourmaline from the 3.7-3.8 Ga Isua Belt, Greenland: Sources for boron in Eoarchean continental crust and seawater. Geochimica et Cosmochimica Acta, 163, 156-177.

Grew, E.S., G. Hystad, R.M. Hazen, S.V. Krivovichev, and L.A. Gorelova (2017) How many boron minerals occur in Earth’s upper crust? American Mineralogist, 102, 1573-1587.

Harlov, D.E. and Rakovan, J.F. [Editors] (2015) Apatite: A mineral for all seasons. Elements, 5, 165-200.

Hazen, R.M. (1984) Mineralogy: A historical review. Journal of Geological Education, 32, 288-298.

Hazen, R.M. (2014) Data-driven abductive discovery in mineralogy. American Mineralogist, 99, 2165-2170.

Hazen, R.M. and Ausubel, J. (2016) On the nature and significance of rarity in mineralogy. American Mineralogist 101 (2016): 1245-1251. Doi: 10.2138/am-2016-5601

Hazen, R.M., Papineau, D., Bleeker, W., Downs, R.T., Ferry, J., McCoy, T., Sverjensky, D.A., and Yang, H. (2008) Mineral evolution. American Mineralogist, 93, 1693-1720.

Hazen, R.M., Grew, E.S., Downs, R.T., Golden, J., and Hystad, G. (2015) Mineral ecology: Chance and necessity in the mineral diversity of terrestrial planets. Canadian Mineralogist, 53, 295-323. DOI: 10.3749/canmin.1400086

Hazen, R.M., Hummer, D.R., Hystad, G., Downs, R.T., and Golden, J.J. (2016) Carbon mineral ecology: Predicting the undiscovered minerals of carbon. American Mineralogist, 101, 889-906.

Hawley, K. and Bird, A. (2011) What are natural kinds? Philosophical Perspectives, 25, 205-221.

Hawthorne, F.C., Oberti, R., Harlow, G.E., Maresch, W.V., Martin, R.F., Schumacher, J.C., and Welch, M.D. (2012) Nomenclature of the amphibole supergroup. American Mineralogist, 97, 2031-2048.

Heaney, P.J. (2016) Time's arrow in trees of life and minerals. American Mineralogist, 101, 1027-1035.

Heaney, P.J., Prewitt, C.T., and Gibbs, G.V. (1994) Silica: Physical behavior, geochemistry, and materials applications. Reviews in Mineralogy and Geochemistry, 29, 606 p.

Heaney, P.J., Vincenzi, E.P., and De, S. (2005) Strange diamonds: The mysterious origns of carbonado and framesite. Elements, 1, 85-89.

Henry, D.J., Novák, M. Hawthorne, F.C., Ertl, A., Dutrow, B.I., Uber, P., and Pezzotta, F. (2011) Nomenclature of the tourmaline-supergroup minerals. American Mineralogist, 96, 895-913.

Hystad, G., Downs, R.T., and Hazen, R.M. (2015) Mineral frequency distribution data conform to a LNRE model: Prediction of Earth's "missing" minerals. Mathematical Geosciences, 47, 647-661.

Jain, A.K. (2010) Data clustering 50 years beyond k-means. Pattern Recognition Letters, 31, 651-666.

Keeling, P.J. and Palmer, J.D. (2008) Horizontal gene transfer in eukaryotic evolution. Nature Reviews Genetics, 9, 605-618.

Klein, C. and Hurlbut, C.S., Jr. (1980) Manual of Mineralogy, 20th Edition. New York: Wiley, pp. 454-456.

Kuhn, T. (2000) The Road Since Structure. Chicago: University of Chicago Press.

Kukla, A. (2000) Social Construction and the Philosophy of Science. London: Routledge.

Lancichinetti, A., Sirer, M.I., Wang, J.X., Acuna, D., Körding, K., and Amaral, L.A.N. (2015) A high-reproducibility and high-accuracy method for automated topic classification. Physical Review X, 5, 011007.

Lefebvre, J.-J. and Gasparrini, G. (1980) Florencite, an occurrence in the Zairan Copperbelt. Canadian Mineralogist, 18, 301-311.

Lehnert, K.A., Walker, D., and Sarbas, B. (2007) EarthChem: A geochemistry data network. Geochemica et Cosmochimica Acta, 71, A559.

Liebau, F. (1985) Structural Chemistry of Silicates: Structure, Bonding, and Classification. Berlin: Springer-Verlag.

Linneaus, C. (1758) Systema Naturae per Regna Tria Naturae. Stockholm: Laurentius Salvius.

Locke, J. (1690) An Essay Concerning Human Understanding. P.H. Nidditch [Editor], Oxford: Clarendon Press.

Lohman, G.P. (1983) Eigenshape analysis of microfossils: A general morphometric procedure for describing changes in shape. Mathematical Geology, 15, 659-672.

Magnus, P.D. (2012) Scientific Enquiry and Natural Kinds: From Mallards to Planets. London: Palgrave MacMillan.

Mayr, E. (1969) Principles of Systematic Zoology. New York: McGraw-Hill.

Menezes Filho, L.A.D., Chaves, M.L.S.C., Chukanov, N.V., Atencio, D., Scholz, R., Pekov, I., Magela da Costa, G., Morrison, S.M., Andrade, M.B., Freitas, E.T.F., Downs, R.T., and Belakovskiy, D.I. (2018) Parisite-(La), ideally $CaLa_2(CO_3)_3F_2$, a new mineral from Novo Horizonte, Bahia, Brazil. Mineralogical Magazine, 82, 133-144.

Milam, K.A., McSween, H.Y., Jr., Moersch, J., and Christensen, P.R. (2010) Distribution and variation of plagioclase compositions on Mars. Journal of Geophysical Research, 115, E09004.

Millikan, R.G. (1999) Historical kinds and the special sciences. Philosophical Studies, 95, 45-65.

Mill, J.S. (1884) A System of Logic. London: Longman.

Mills, S.J., Hatert, F., Nickel, E.H., and Ferrais, G. (2009) The standardization of mineral group hierarchies: Application to recent nomenclature proposals. European Journal of Mineralogy, 21, 1073-1080.

Milton, D.J. and Bastron, H. (1971) Churchite and florencite (Nd) from Sausalito, California. Mineralogical Record, 2, 166-168.

Morrison, S.M., Downs, R.T., Blake, D.F., Vaniman, D.T., Ming, D.W., Rampe, E.B., Bristow, T.F., Achilles, C.N., Chipera, S.J., Yen, A.S., Morris, R.V., Treiman, A.H., Hazen, R.M., Sarrazin, P.C., Fendrich, K.V., Morookian, J.M., Farmer, J.D., Des Marais, D.J., and Craig, P.I. (2018) Crystal chemistry of martian minerals from Bradbury Landing through Naukluft Plateau, Gale crater, Mars. American Mineralogist, 103, 857-871. DOI: 10.2138/am-2018-6124

Németh, P., Garvie, L.A.J., Aoki, T., Dubrovinskaia, N., Dubrovinsky, L., and Buseck, P.R. (2014) Lonsdaleite is faulted and twinned cubic diamond and does not exist as a discrete material. Nature Communications, 5, 5447-5451.

Ni, Y., Post, J.E., and Hughes, J.M. (2000) The crystal structure of parisite-(La), $CaCe_2(CO_3)_3F_2$. American Mineralogist, 85, 251-258.

Ochman, H., Lawrence, J.G., and Groisman, E.A. (2000) Lateral gene transfer and the nature of bacterial innovation. Nature, 405, 299-304.

Ohirta, T. (1986) Hydroxyapatite deposition in articular cartilage by intra-articular injections of methylprednisolone. A histological, ultrastructural, and x-ray-microprobe analysis in rabbits. The Journal of Bone and Joint Surgery, 68 (4), 509–520.

Onozato, H. (1979) Studies on fish scale formation and resorption. Cell and Tissue Research, 201 (3), 409–422.

Ott, H. (2009) Nanodiamonds in meteorites: Properties and astrophysical context. Journal of Achievements of Materials and Manufacturing Engineering, 37, 779-784.

Pace, N. (2009) Mapping the tree of life: Progress and prospects. Microbiology and Molecular Biology Reviews, 73, 565-576.

Palache, C., Berman, H., and Frondel, C. [Editors] (1944, 1951) The System of Mineralogy of James Dwight Dana and Edward Salisbury Dana, 2 volumes. New York: John Wiley and Sons.

Papike, J. J. [ed.], Planetary Materials. (Chantilly, Virginia: Mineralogical Society of America, 1998).

Pouliot, G. and Hofmann, H.J. (1981) Florencite: a first occurrence in Canada. Canadian Mineralogist, 19, 535-540.

Povarennykh, A.S. (1972) A short history of mineralogy and the classification of minerals. In Crystal Chemical Classification of Minerals. Monographs in Geoscience. Boston: Springer, pp. 3-26.

Povarennykh, M.Y. (1986) Fullerenes as protominerals. Proceedings of the Russian Mineralogical Society, 5, 97-103.

Povarennykh, M.Y., Matvienko, E.N., Pavlikov, A.V., and Shatalova, T.B. (2018) The first occurrence of carbon nanotubes in nature. Priroda, 5, 12-21.

Reeder, R.J. (ed) (1983) Carbonates: Mineralogy and Chemistry. Reviews in Mineralogy, 11. Mineralogical Society of America: Washington, DC.

Repina, S.A., Popova, V.I., Churin, E.I., Belogub, E.V., and Chiller, V.V. (2010) Florencite-(Sm), $(Sm,Nd)Al_3(PO_4)_2(OH)_6$—a new mineral of the alunite-jarosite group from the Subpolar Urals. Zapiski Rossiiskogo Mineralogicheskogo Obshchetstva, 139, 16-25.

Richards, R.A. (2016) Biological Classification: A Philosophical Introduction. Cambridge Introduction to Philosophy and Biology. Cambridge: Cambridge University Press.

Rickard, D. (2015) Pyrite: A Natural History of Fool's Gold. New York: Oxford University Press.

Rieder, M., Cavazzini, G., D'Yakonov, Y.S., Frank-Kamenetskii, V.A., Gottarsi, G., Guggenheim, S., Koval, P.V., Müller, G., Neiva, A.M.R., Radoslovich, E.W., Robert, J.-L., Sassi, F.P., Takeda, H., Weiss, Z., and Wones, D.R. (1998) Nomenclature of the micas. Mineralogist, 36, 905-912.

Rogers, A.F. (1917) A review of the amorphous minerals. The Journal of Geology, 25, 515-541.

Roy, D.M. (1974) Hydroxyapatite formed from coral skeletal carbonate by hydrothermal exchange. Nature, 247, 220–222.

Rudnick, R.L. and Gao, S. (2005) Composition of the continental crust. In The Crust: Treatise on Geochemistry, edited by Roberta L. Rudnick (New York: Elsevier), pp. 1-64.

Ruggiero, M.A., Gordon, D.P., Orrell, T.M., Bailly, N., Bourgoin, T., Brusca, R.C., Cavalier-Smith, T., Guiry, M.D., Kirk, P.M., and Thuesen, E.V. (2015) A higher level classification of all living organisms. PLOS ONE, 10, e0119248.

Sherman, V.R. (2008) The materials science of collagen. Journal of the Mechanical Behavior of Biomedical Materials, 61 (5), 529–534.

Shirey, S.B., Cartigny, P., Frost, D.J., Keshav, S., Nestola, F., Minis, P., Pearson, D.G., Sobolev, N.V., and Walter, M.J. (2013) Diamonds and the geology of mantle carbon. Reviews of Mineralogy and Geochemistry 75, 355-421.

Smith, E.M., Shirey, S.B., Nestola, F., Bullock, E.S., Wang, J., Richardson, S.H., and Wang, W. (2016) Large gem diamonds from metallic liquid in Earth's deep mantle. Science 354, no. 6318, 1403-1405.

Strunz, H. (1941) Mineralogische Tabellen. Leipzig: Akademische Verlagsgesellschaft.

Sverjensky, D.A. and Huang, F. (2015) Diamond formation due to a pH drop during fluid-rock interactions. Nature Communications 6, Article number 8702 (2015).

Tilley, C.E., Nockolds, S.R., and Black, M. (1964) Harker's Petrology for Students, 8th Edition. Cambridge, UK: Cambridge University Press.

Turvey, S.T., Bruun, K., Ortiz, A., Hansford, J., Hu, S., Ding, Y., Zhang, T., and Chatterjee, H.J. (2018) New genus of extinct Holocene gibbon associated with humans in Imperial China. Science, 360, 1346-1349.

Vishnevsky, S. and Raitala, J. (2000) Impact diamonds as indicators of shock metamorphism in strongly-reworked Pre-Cambrian impactites. In I. Gilmour and C. Koeberl [Editors]: Impacts and the Early Earth. Berlin: Springer, pp. 229-247.

Wenk, H.-R. and Bulakh, A. (2004) Minerals: Their Constitution and Origin. New York: Cambridge University Press.

Widiger, T.A. (2015) The Oxford Handbook of the Five Factor Model of Personality. Oxford, UK: Oxford University Press.

Wilkins, J.S. and Ebach, M.C. (2013) The Nature of Classification: Relationships and Kinds in the Natural Sciences. New York: Palgrave MacMillan.

Wilkinson, M.D. et al. (2016) The FAIR guiding principles for scientific data management and stewardship. Scientific Data, 3. Doi:10.1038/sdata.2016.18

Winchell, (1949)

Woolgar, S. (1988) Science: The Very Idea. London: Tavistock.

Wysokowski, M., Jesionowski, T., and Ehrlich, H. (2018) Biosilica as a source for inspiration in biological materials science. American Mineralogist, 103, 665-691.

Zhabin, A.G. (1981) Is there evolution of mineral speciation on Earth? Doklady Earth Science Sections, 247, 142-144.

Table 1. Selected natural kinds of diamond: The mineral species "diamond," which is defined as pure carbon in the cubic diamond structure, encompasses several natural kinds based on their different paragenetic modes. These differing modes of formation result in distinctive morphologies, trace element and isotopic compositions, and physical properties. Data from Davies (1984), Vishnevsky and Raitala (2000), Heaney et al. (2005), Garai et al. (2006), Ott (2009), Shirey et al. (2013), and Greaves et al. (2018).

Diamond kind	**Size/morphology**	**Distinctive properties**	**Paragenetic Mode**	**Maximum Age (Ga)**
Stellar vapor deposition	<5 nm/nanocrystalline	Anomalous microwave emission	Low-P, condensation	> 13
"Type I"	to 2 cm/euhedral	Absorbs 8 μm IR and 300 nm UV	High-P, aqueous fluid	> 3
"Type II"	to 10 cm/euhedral	IR/UV transparent	High-P, Fe-Ni melt	> 3
Carbonado	to >10 cm/polycrystalline	Black, porous, superhard	Unknown	Unknown
Impact diamond	<1 mm/euhedral/also in polycrystalline aggregates	Birefringent; hardness = 3	Shock transformation	> 4.5

Table 2. Rare earth element (REE) compositions (in atom percent) of IMA mineral species of florencite and parisite. The assignment of different mineral species to specimens that differ in the most abundant REE may lead to splitting of natural kinds.

IMA mineral species	Ideal formula	Ce	La	Nd	Sm	Y	Reference
Florencite-(Ce)	$CeAl_3(PO_4)_2(OH)_6$	0.56	0.28	0.12	0.04	-	Pouliot & Hofmann (1981)
Florencite-(La)	$LaAl_3(PO_4)_2(OH)_6$	0.34	0.61	0.02	-	-	Lefebvre & Gasparrini (1980)
Florencite-(Nd)	$NdAl_3(PO_4)_2(OH)_6$	0.05	0.19	0.28	0.10	0.15	Milton, D.J. and Bastron, H. (1971)
Florencite-(Sm)	$SmAl_3(PO_4)_2(OH)_6$	0.10	0.02	0.32	0.38	-	Repina et al. (2010)
Parisite-(Ce)	$CaCe_2(CO_3)_3F_2$	1.03	0.49	0.42	-	0.06	Ni et al. (2000)
Parisite-(La)	$CaLa_2(CO_3)_3F_2$	0.37	0.83	0.51	0.04	0.03	Menezes Filho et al. (2018)