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Lumping and Splitting:
Toward a Classification of Mineral Natural Kinds

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"I am got ***extremely*** *interested in tabulating ... the species having any varieties marked by Greek letters or otherwise: the result (as far as I have yet gone) seems to me one of the most important arguments I have yet met with, that varieties are only small species—or species only strongly marked varieties. The subject is in many ways so very important for me. ... It is good to have hair-splitters & lumpers."*

Charles Darwin to Joseph Hooker, 1 August 1857

ABSTRACT

How does one best subdivide nature into kinds? All classification systems require rules for lumping similar objects into the same category, while splitting differing objects into separate categories. Mineralogical classification systems are no exception. Our work in placing mineral species within their evolutionary contexts necessitates this lumping and splitting, because we classify "mineral natural kinds" based on unique combinations of formational environments and continuous temperature-pressure-composition phase space. Consequently, we lump two minerals into a single natural kind only if they: (1) are part of a continuous solid solution; (2) are isostructural or members of a homologous series; and (3) form by the same process. A systematic survey based on these criteria suggests that 2310 (~41 %) of 5659 IMA-approved mineral species can be lumped with one or more other mineral species, corresponding to 667 "root mineral kinds," of which 353 lump pairs of mineral species, while 129 lump three species. Eight mineral groups, including cancrinite, eudialyte, hornblende, jahnsite, labuntsovite, satorite, tetradymite, and tourmaline, are represented by 20 or more lumped IMA-approved mineral species. A list of 5659 IMA-approved mineral species correspond to 4016 root mineral kinds according to these lumping criteria.

The evolutionary system of mineral classification assigns an IMA-approved mineral species to two or more mineral natural kinds under either of two splitting criteria: (1) if it forms in two or more distinct paragenetic environments, or (2) if cluster analysis of the attributes of numerous specimens reveals more than one discrete combination of chemical and physical attributes. A total of 2310 IMA-approved species are known to form by two or more paragenetic processes and thus correspond to multiple mineral natural kinds; however, adequate data resources are not yet in hand to perform cluster analysis on more than a handful of mineral species.

We find that 1623 IMA-approved species (~29 %) correspond exactly to mineral natural kinds; i.e., they are known from only one paragenetic environment and are not lumped with another species in our evolutionary classification. Greater complexity is associated with 587 IMA-approved species that are both lumped with one or more other species and occur in two or more paragenetic environments. In these instances, identification of mineral natural kinds may involve both lumping and splitting of the corresponding IMA-approved species on the basis of multiple criteria.

Based on the numbers of root mineral kinds, their known varied modes of formation, and predictions of minerals that occur on Earth but are as yet undiscovered and described, we estimate that Earth holds more than 10,000 mineral natural kinds.

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INTRODUCTION

For Charles Darwin in 1857, soon to publish his revolutionary thesis *On the Origin of Species by Means of Natural Selection* (Darwin 1859), the distinction between biological "varieties" and "species" was crucial. His original hypothesis rested on four carefully argued propositions: (1) individual organisms exhibit variations in their traits; (2) more individuals are born than can survive; (3) individuals with advantageous traits will preferentially survive to pass those traits on to the next generation; and (4) over many generations, small variations can accumulate to produce new species under the influence of natural selection.

A persistent challenge faced biological taxonomists: How, in this grand evolutionary view of life, does one distinguish between varieties and species? One can imagine Darwin perplexed, recalling the diverse finches of the Galapagos Islands, trying to decide if he was seeing variations on one avian theme (lumping), or more than a dozen separate species (splitting). That he found no rigorous answer to the dilemma is a characteristic inherent in many messy natural systems.

The tension between "lumping" and "splitting" (the felicitous terms coined by Darwin in that 1857 missive; Endersby 2009) has played a role in virtually every domain where classification holds sway, including extant biology (Simpson 1945; Avise and Johns 1999), paleobiology (Horner and Goodwin 2009; Hublin 2014), sociology (Zerubavel 1996; Berg 2018), history (Hochschild 2000; Stearns 2017), psychiatry (Solomon et al. 2011; Marquand et al. 2016), linguistics (Michalove et al. 2003; Rowe and Levine 2015), philosophy (Piccinini and Scott 2006; Dyson 2015), and musical genres (Bickerstaffe and Makalic 2003; Goulart et al. 2012). In each discipline, rival camps advocate competing philosophies: either grouping similar things in the same category unless compelling reasons exist to divide them (lumping), or dividing two things into separate categories unless compelling reasons exist to combine them (splitting). At a deeper level, one's tendency to lump or to split may reflect a philosophical mindset regarding the extent to which the world can be characterized with broad simplifying generalizations, as opposed to infinite complexity.

But what of mineralogy? Does lumping and splitting play a role in the classification of natural solids? For more than four centuries, naturalists have attempted to systematize the diversity of minerals on the basis of some combination of physical and chemical attributes (Hazen 1984; Heaney 2016), culminating in the standard classification of "mineral species" (Table 1) by the International Mineralogical Association's Commission on New Minerals, Nomenclature and Classification (IMA-CNMNC). The IMA-CNMNC classification relies primarily on idealized chemical compositions and crystal structures, which are quantifiable attributes selected on the basis of theoretical considerations from solid-state physics and crystal chemistry (e.g., Burke 2006; Mills et al. 2009; Schertl et al. 2018; Hawthorne et al. 2021). The inherent advantage of this system – one that largely bypasses any lumping/splitting debates – is that each unique combination of end-member composition and crystal structure represents a distinct mineral species. Therefore, any mineral specimen can be classified based on rigorous quantitative criteria. With but few exceptions, such as the use of "augite" or "pigeonite" as designations of intermediate phase regions not associated with specific compositional end-members (Morimoto et al.1988), classification of minerals by the IMA-CNMNC system provides unambiguous rules for lumping or splitting any pair of mineral specimens (Heaney 2016; Cleland et al. 2020; Hatert et al. 2021).

Hawthorne et al. (2021) state that there is not yet a formal general definition of the term “mineral species.” They propose that, in addition to idealized end-member composition and crystal structure, the definition of a mineral species should include “the range of chemical composition limited by the compositional boundaries between end members with the same bond topology.” Rigorous IMA-CNMNC guidelines defining such compositional ranges, notably the “dominant-constituent rule” (Nickel and Grice 1998; Hatert and Burke 2008; Bosi et al. 2019a)) and “dominant valency rule” (Bosi et al. 2019b), as well as associated nomenclature conventions (Hatert et al. 2012), have been approved. Those guidelines have been applied explicitly to the major-element chemical ranges for several important “mineral groups” (Mills et al. 2009) that display significant compositional plasticity, including the pyrochlore supergroup (Atencio et al. 2010), the tourmaline supergroup (Henry et al. 2011), the amphibole supergroup (Hawthorne et al. 2012), the garnet supergroup (Grew et al. 2013), and the perovskite supergroup (Mitchell et al. 2017). In addition, even if information on compositional ranges is not explicitly included in the formal definitions of some new mineral species, such ranges are implied by IMA approval and implicit application of the dominant-constituent and dominant-valency rules.

Hawthorne et al. (2021) also suggest that each unique combination of idealized end-member composition and *Z*, space group, and bond topology be termed a “mineral archetype.” According to Hawthorne et al.’s proposal:

> “An archetype is a pure form, which embodies the fundamental characteristics of a thing. We may define a set of intrinsic properties that

> are common to all mineral samples of a specific mineral species, and consider these as the set of universals for that mineral species. … This set of universals may be considered to define an archetype, and all mineral samples of the same name are imperfect copies of that archetype."

In most instances, an IMA-approved mineral species can be matched unambiguously to a mineral archetype.

Such certainty has important advantages in cataloguing the diversity of natural crystalline compounds, but it may also come at a price. In particular, IMA-approved mineral species, or their corresponding mineral archetypes, cannot be considered to be "natural kinds," because they are defined by idealized chemical and physical attributes. According to Hawthorne et al. (2021), "A specific mineral species … is defined by the following set of universals: name, end-member formula and *Z*, space group, and bond topology of the end-member structure, with the range of chemical composition limited by the compositional boundaries between end members with the same bond topology". However, mineral species as thus defined do not represent "genuine divisions in nature" – i.e., groups that are "independent of human conventions, interests, and actions" (Bird and Tobin 2018; see also: Quine 1969; Laporte 2004; Santana 2019; Cleland et al. 2020; Hatert et al. 2021; Hazen 2021). Rather, the dominant-constituent and dominant-valency rules of the IMA-CNMNC result in discrete entities that are rigorously defined, simplified versions of complex natural objects. In this respect, the IMA-CNMNC classification of minerals differs from that, for example, of elements in the periodic table, each of which is characterized by a unique integral atomic number that reflects its true natural identity.

Table 1: Glossary of terms related to mineral classification

Term	Definition
Mineral Archetype	Hawthorne et al. (2021) state: “An archetype is a pure form” that “embodies the fundamental characteristics of an object.” A mineral archetype is characterized by four intrinsic properties: “its name, its end-member formula and *Z*, its space group, and the bond topology of the end-member structure.”
Mineral Species	A mineral with a unique combination of (1) chemical composition range, and (2) crystal structure, as approved by the IMA-CNMNC. In this contribution we consider 5659 IMA-approved mineral species.*
Root Mineral Kind	A grouping of one or more IMA-approved mineral species that have been lumped by virtue of their shared temperature-pressure-composition (*T*-*P*-*X*) phase space and cannot be further lumped. In this contribution we identify 4016 root mineral kinds.
Paragenetic Mode	A natural process by which a collection of atoms in solid and/or fluid form are reconfigured into one or more new solid forms. Hazen and Morrison (2021a) describe a chronological sequence of 57 mineral paragenetic modes.
Mineral Natural Kinds	A natural kind represents a “genuine division of nature” (e.g., Bird and Tobin 2018). Our preliminary list includes 7816 unique combinations of a root mineral kind and a paragenetic mode, each of which we propose is a discrete mineral natural kind. Cluster analysis has the potential to reveal many more mineral natural kinds.

*Hawthorne et al. (2021) suggest that the formal definition of “mineral species” should include “the complete range of chemical composition limited by the compositional boundaries between end members,” as defined by IMA’s dominant-constituent and dominant-valency rules (Hatert and Burke 2008; Bosi et al. 2019a, 2019b).

Mineral natural kinds: Hazen, Morrison, and colleagues have proposed an evolutionary system of mineralogy that builds on, and is complementary to, the IMA-CNMNC classification (Hazen 2019; Hazen and Morrison 2020, 2021b; Morrison and Hazen 2020, 2021; Hazen et al. 2021). This effort attempts to classify "mineral natural kinds" (Table 1; Boyd 1991, 1999; Hawley and Bird 2011; Magnus 2012; Khalidi 2013; Ereshefsky 2014; Godman 2019; Cleland et al. 2020) that are based on a temporal sequence of "paragenetic modes" (Table 2) in the context of planetary evolution (Hazen and Morrison 2021a), as manifest in distinctive combinations of physical and chemical attributes (e.g., trace elements, isotope ratios, inclusions, and other characteristics).

This new mineral classification scheme seeks to identify "genuine divisions in nature" (Bird and Tobin 2018) that arose by historical processes – an effort that depends on the enumeration of diagnostic suites of mineral attributes that are linked to historical planetary processes by which those distinctive properties arose. In this context, some IMA-approved species are lumped in the evolutionary system on the basis of their shared *T-P-X* phase space and paragenetic mode, whereas other species are split based on having two or more modes of formation, each of which imparts a distinctive suite of chemical and physical attributes.

Lumping mineral species

We adopt three rules for lumping two IMA-approved species into one natural kind:

1) The two species must be compositionally similar, forming a continuous solid solution with no miscibility gaps at their temperatures of equilibration. This criterion introduces a potential complication, as two species that form a continuous solid solution

under one high-temperature paragenetic process may be separated by a miscibility gap under a lower-temperature process.

2) The two species must form by the same paragenetic process. Hazen and Morrison (2021a) have proposed a list of 57 paragenetic modes organized in a roughly chronological sequence (Table 1).

3) The two minerals must be isostructural or, in some cases, members of a homologous series of minerals.

We have applied these three criteria to an examination of the chemical compositions, crystal structures, and paragenetic modes of 5659 IMA-approved mineral species (https://rruff.info/ima; accessed 7 April 2021). Our survey reveals that 2310 minerals – approximately 41 % of all species – bear close compositional, structural, and paragenetic relationships to at least one other species (whereas 3349 species are not lumped with another species). We combine these 2310 species into 667 separate "root mineral kinds" (Table 1), which we define as an IMA-approved species or group of species that cannot be further lumped (Supplemental Table 1). Of these 667 root mineral kinds, 353 lump pairs of IMA-approved mineral species, whereas 129 lump triplets of mineral species. Eight root mineral kinds, each with 20 or more lumped species, are especially diverse. Three of these groups, *eudialyte* (with 30 species; Johnsen et al. 2003), *labuntsovite* (28 species; Chukanov et al. 2002), and *cancrinite* (22 species; Gatta and Lotti 2016), are associated primarily with agpaitic and other peralkaline Si-poor lithologies. We lump 20 species from the jahnsite and whiteite groups (Moore and Ito 1978), which are most often associated with granite pegmatites, into *jahnsite*. In addition, *sartorite* (23 species) and *tetradymite* (24 species) groups combine homologous suites of hydrothermal sulfosalts

(Moélo et al. 2008). "*Hornblende*" with 26 lumped species (Deer et al. 1997a; Hawthorne et al. 2012) and a subset of 20 lumped tourmaline group mineral species (Henry et al. 2011) are special cases complicated by the existence of multiple paragenetic modes and are treated in more detail below.

The nomenclature of root mineral kinds is an important consideration. In the case of the 3349 species that are not lumped with another mineral, we retain the IMA-approved names for those mineral species. We distinguish root mineral kinds by italicizing the corresponding IMA-approved species name. For the 667 root mineral kinds with two or more lumped species, whenever possible we employ the italicized IMA-approved name of the earliest reported member in that group. Accordingly, we employ italicized IMA-approved species names for 544 root mineral kinds (representing 1721 IMA species). In an additional 101 instances, representing a total of 423 IMA-approved species, we adopt a simplified name for the group by eliminating compositional suffixes; for example, we lump arisite-(Ce) and arisite-(La) under "*arisite*," and demicheleite-Cl, demicheleite-Br, and demicheleite-I under "*demicheleite*." Finally, we lump 166 IMA species into 22 root mineral kinds with names that do not correspond to valid IMA species names, though in most cases we employ a familiar group name (Table 3), including such useful petrologic terms as *biotite*, *fassaite*, *hornblende*, *lepidolite*, *phengite*, *plagioclase*, and *tourmaline*.

The net result of this lumping exercise is that 5659 IMA-approved mineral species correspond to 4016 root natural kinds – a reduction of 29 %. In the following two sections we review some of our lumping decisions based on compositional and structural relationships, respectively.

Lumping based on compositions: The majority of decisions to lump minerals are based on well-documented solid-solution series. Of the 2310 IMA-approved species that we identify as candidates for lumping, more than 90 % are grouped entirely on the basis of solid solutions between isomorphous endmembers. Thus, for example, of the 353 lumped pairs of IMA-approved mineral species, 300 are related by one of 86 different simple element substitutions, the most frequently encountered of which are Al-Fe^{3+} (28 pairs), Mg-Fe^{2+} (23), F-OH (20), rare-earth elements and Y (19), and Fe^{2+}-Mn^{2+} (15). Divalent iron participates in the greatest number of simple solid solutions (50 pairs), followed by Mg (41), and Mn (38).

For example, we lump four pairs of meteorite impact minerals that display continuous Mg-Fe^{2+} solid solution. We group asimowite (ideally Fe_2SiO_4, but reported with composition Fe_{55}) with wadsleyite (ideally Mg_2SiO_4, but typically with compositions of Fe_{30-45}; Bindi et al. 2019). We apply the group name "*wadsleyite*" (the earlier described of the two related species) to all specimens of the asimowite—wadsleyite solid solution. Likewise, we combine meteoritic impact ahrensite (ideally Fe_2SiO_4, but with reported composition ~Fe_{54}) with ringwoodite (formally Mg_2SiO_4, but typically close to Fe_{45}; Ma et al. 2016). Other examples include akimotoite—hemleyite [$(Mg,Fe)SiO_3$; Bindi et al. 2017, their Figure 5] and bridgmanite—hiroseite [$(Mg,Fe)SiO_3$; Bindi et al. 2020].

The isomorphous phosphides barringerite (ideally Fe_2P; Buseck 1969) and transjordanite (Ni_2P; Britvin et al. 2020) both form by two different paragenetic modes –

in achondrite meteorites (Morrison and Hazen 2021) and in the pyrometamorphic Hatrurim Formation in the Middle East (Sokol et al. 2019). Britvin and colleagues (2020, their Figure 4) summarize dozens of analyses from both terrestrial and meteoritic occurrences and demonstrate a continuous barringerite—transjordanite Fe-Ni solid solution, as well as modest substitution (to ~20 mol %) of S for P. Accordingly, we lump transjordanite with barringerite and assign the earlier name "*barringerite*" to all such occurrences. A similar situation obtains for meteoritic nickelphosphide (ideally Ni_3P; Ma and Rubin 2019), which forms a solid solution with schreibersite (Fe_3P) – minerals that we lump into "*schreibersite*."

Volcanic fumaroles feature a number of lumped species, including aluminoedtoilite and edtoilite [$K_2NaCu_5(Al,Fe^{3+})O_2(AsO_4)_4$] with Al-$Fe^{3+}$ solid solution (Pekov et al. 2019a), and three species of the rhabdoborite group (Hålenius et al. 2018), rhabdoborite-Mo, -V, and -W [$Mg_{12}(Mo,V,W)^{6+}{}_{1.33}O_6(BO_3)_6F_2$], all of which are known only from the Tolbachik Volcano, Kamchatka, Russia. Two adranosite group minerals, also representing Al-Fe^{3+} solid solution [$(NH_4)_4Na(Al,Fe)_2(SO_4)_4Cl(OH)_2$] (Mitolo et al. 2013), occur as sublimates both at volcanic fumaroles and in coal fires. We lump these species into the root natural kinds "*edtoilite*," "*rhabdoborite*," and "*adranosite*," respectively.

In many other cases, persuasive evidence exists that the three lumping criteria are met. For example, the linnaeite group mineral carrollite [$Cu(Co,Ni)_2S_4$], which occurs in hydrothermal systems, forms a solid solution with the less common isomorph fletcherite

[$Cu(Ni,Co)_2S_4$]. In their original description of fletcherite, Craig and Carpenter (1977) report a range of compositions from ($Cu_{1.13}Ni_{1.04}Co_{0.84}Fe_{0.06}S_4$) to ($Cu_{0.67}Ni_{2.11}Co_{0.61}Fe_{0.01}S_4$). Subsequently, Anthony et al. (1990-2003) recorded 8 representative carrollite-fletcherite compositions, spanning the range from $Co_{99}Ni_{01}$ through ~$Co_{50}Ni_{50}$ to $Co_{10}Ni_{90}$. Of 12 known fletcherite localities (https://mindat.com; accessed 31 March 2021), five also have recorded specimens of carrollite. It seems likely, therefore, that fletcherite and carrollite represent a single root natural kind, "*carrollite*".

In addition to the 300 mineral pairs related by simple element substitution, we document 29 lumped pairs of mineral species that display a wide variety of more than two dozen different coupled substitutions. Examples include alcaparosaite—magnanelliite [$K3(Fe^{3+},Ti^{4+})Fe^{3+}(SO_4)_4(OH,O)(H_2O)_2$] with $Fe^{3+}(OH) \leftarrow\rightarrow Ti^{4+}O$ substitution (Biagioni et al. 2019); norrishite—balestraite [$KLi(Li,Mn^{3+},V^{5+})_2Si_4O_{12}$] with $LiV^{5+} \leftarrow\rightarrow 2Mn^{3+}$ (Lepore et al. 2015); yurmarinite—anatolyite [$Na_6(Ca,Na)(Mg,Al,Fe^{3+})_4(AsO_4)_6$] with $CaMg \leftarrow\rightarrow Na(Al,Fe^{3+})$ (Pekov et al. 2019b); and lindsleyite—mathiasite [$(K,Ba)(Zr^{4+},Fe^{3+})(Mg,Fe^{3+})2(Ti^{4+},Cr^{3+},Fe^{3+})_{18}O_{38}$] with both $KZr^{4+} \leftarrow\rightarrow BaFe^{3+}$ and $MgTi^{4+} \leftarrow\rightarrow 2Fe^{3+}$ coupled substitutions (Haggerty et al. 1983).

Members of large mineral groups with multiple lumped species often display both simple and coupled element substitutions. The eudialyte group, which now boasts a profusion of at least 30 IMA-approved species found in agpaitic rocks, represents an important test case (Johnsen et al. 2003). These minerals, with the complex general formula $[(N1—N5)_3(M1)_3(M2)_3(M3)(M4)(Z)_3(\mathrm{Si}_{24}\mathrm{O}_{72})\mathrm{O}_4(\mathrm{Cl,F,OH,CO}_3)_2]$ incorporating 10 different *N*, *M*, and *Z* cation sites, share a trigonal structure with $a \sim 14$ Å and $c \sim 30$ Å (in 3 instances doubled to ~60 Å). Collectively, these 10 crystallographic sites can accommodate more than a dozen essential elements (Na, K, H_3O^+, Ca, Fe^{2+}, Mn, Fe^{3+}, REE, Si, Ti, Zr, W, Nb) with oxidation states ranging from +1 to +5 in varied solid solutions – a circumstance that leads to the group's diversity. We lump these closely-related phases into one root natural kind, "*eudialyte*".

The labuntsovite group, with a general formula $\{(A1)_4(A2)_4(A3)_{4-2x}[(M2)_x(\mathrm{H_2O})_{2x}][(M1)_8(\mathrm{O,OH})_8][\mathrm{Si_4O_{12}}]_4{}^{\cdot}n\mathrm{H_2O}\}$, also has at least 30 closely-related mineral species from agpaitic pegmatites (Chukanov et al. 1999, 2002). We lump 28 labuntsovite group species that are monoclinic (space group *Bm* or *B*2/*m*) with similar unit cells. However, we distinguish two orthorhombic (*Pbam*) members of the group, korobitsynite and nenadkevchite (Pekov et al. 1999), pending more information on their conditions of formation.

Lumping of modular structures: In most instances of lumped species, the grouped minerals are strictly isostructural with the same atomic topology and space group. However, we also lump more than 200 mineral species that are members of homologous or polysomatic structural series based on stacking of two or more modules, which may result in incremental compositional variations and different space groups (Thompson 1970, 1978; Ferraris et al. 2008). It should be noted, however, that consideration of these structural variants often leads to a significant degree of subjectivity regarding what constitutes structural equivalents.

In some cases, lumping structural variants is unambiguous. Polytypes, defined as structural modifications of a compound arising from different arrangements of the same module (consequently, not resulting in significant chemical variations), are not generally given separate species names (Nickel and Grice 1998). Thus, for example, IMA-CNMNC protocols do not define species based on varied stacking arrangements of layered minerals, such as the 3R and 4H polytypes of graphite (C; Trubkin and Novgorodova 1996), the 6H and 15R polytypes of moissanite (SiC; Shiryaev et al. 2011), and the 1M and 3T polytypes of mica group minerals (Fleet 2003). A similar situation related to orientations of adjacent glycolate molecules was observed by Yang et al. (2021) in lazaraskeite [$Cu(C_2H_3O_3)_2$], which occurs in two topologically equivalent polytypes – slightly different structural variants designated M_1 and M_2 but not separate species.

In a few specific cases, such as domeykite/domeykite-β (Michejev 1949), fergusonite/fergusonite-β (Kuo et al. 1973), roselite/roselite-β (Frondel 1955), and three variants of gersdorffite (space groups $P2_13$, $Pa3$, and $Pca2_1$; Bayliss 1986) the IMA-CNMNC assigns species names to different mineral polymorphs with similar or identical compositions that appear to bear supergroup-subgroup relationships, perhaps owing to slight variations in cation ordering. In other cases of pairs of related minerals, including andorite-IV/andorite-VI (Donnay and Donnay 1954) and joséite-A/joséite-B (Moélo et al. 2008; Ciobanu et al. 2009), the relationship between mineral pairs is close but uncertain.

In each of these examples we lump the minerals in question into a single root natural kind.

Members of polysomatic series of minerals display systematic compositional variations as two or more structural modules are arranged in different ratios. The resulting polysomes are given different species names by IMA-CNMNC conventions. For example, the högbomite group of hydrous Mg-Fe-Zn-Al-Ti oxide minerals features various stacking arrangements of nolanite (*N*) and spinel (*S*) modules (McKie 1963; Armbruster 2002), resulting in distinctions among the structures of ferronigerite-2*N*1*S*, magnesiohögbomite-2*N*2*S*, magnesiobeltrandoite-2*N*3*S*, zincohögbomite-2*N*6*S*, and zincovelesite-6*N*6*S*. However, we lump these compositionally and structurally related polysomes as "*högbomite*." Similarly, we lump members of the taaffeite polysomatic series (Armbruster 2002).

The biopyribole group of chain and sheet silicates provides an important example of polysomatic relationships (Thompson 1970, 1978; Deer et al. 1997a, 1997b; Fleet 2003), while underscoring the difficulty in lumping and splitting minerals that bear structural similarities. We follow IMA conventions and distinguish among single-chain pyroxene, double-chain amphibole, and mica group minerals. However, we lump several multiple-chain biopyriboles, including jimthompsonite, clinojimthompsonite, and chesterite, because high-resolution transmission electron microscope images reveal pervasive chain-width disorder within these phases (Veblen and Buseck 1979; Veblen and Burnham 1988). On the other hand, we split members of the polysomatic humite group [$Mg(OH,F)_2 \cdot n(Mg_2SiO_4)$], with n = 1 to 4 corresponding to norbergite, chondrodite, humite, and clinohumite, respectively (Deer et al. 1982). These minerals (as well as their

Mn analogs alleghanyite, leucophoenicite, and sonolite with *n* = 2 to 4, respectively) typically form discrete, well-ordered crystals without intermediate compositional variants.

Perhaps most problematic in terms of whether to lump closely related species are homologous series of sulfosalt minerals, which display related structures with modules that adapt to almost continuous variations of complex multi-element compositions (Ferraris et al. 2008; Moélo et al. 2008). For example, the *sartorite* group of hydrothermal Pb sulfosalts (variously with Ag, Tl, As, and/or Sb) includes at least 24 species, all of which have pseudo-orthogonal unit cells and a pair of cell edges of ~8 Å and ~4.2 Å (or multiples thereof). The close similarities among these species are underscored by the observation that at least 14 of the 24 have been recorded from one locality, the famed Lengenbach Quarry, Valais, Switzerland (Raber and Roth 2018; https://mindat.org; accessed 6 April 2021).

Similarly, we lump 11 members of the homologous *aikinite* series (Cu-Pb-Bi-S), which have orthorhombic unit cells with two cell edges of ~4 Å and ~11.5 Å. The principal differences among structures within these groups lies in the stacking of modules. Based on these criteria, we lump members of several other homologous series of sulfosalts, including the root mineral kinds *cylindrite* [Pb-Sn-(Sb,As)-S], *fizelyite* (Ag-Pb-Sb-S), *germanite* [Cu-(Fe,Mg)-Ge-S], *pavonite* [Ag-Bi-S], and *tetradymite* [Pb-Bi-Te-Se-S] (Moélo et al. 2008).

Complexities and counterexamples: In many instances, we separate two mineral species that might at first examination appear to be strong candidates for lumping because important differences occur. For example, osbornite (TiN), carlsbergite (CrN), and uakitite (VN) are rare cubic nitrides with the NaCl structure that are known almost exclusively from meteorites (Hazen et al. 2020; Morrison and Hazen 2021). Solid solutions among these and other compositions may occur, but reported meteoritic examples lie close to their respective Ti, Cr, and V end-members. Therefore, until examples of intermediate compositions are described, we recognize meteoritic *osbornite*, *carlsbergite*, and *uakitite* as distinct root natural kinds.

The sapphirine group of single-chain silicates provides other examples of similar species that should not be lumped into root natural kinds (Jensen 1996; Deer et al. 1997b; Kunzmann 1999). For example, aenigmatite and rhönite, $[Na_2Fe^{2+}{}_{10}Ti_2O_4(Si_{12}O_{36})]$ and $[Ca_4(Mg_8Fe^{3+}{}_2Ti_2)O_4(Si_6Al_6O_{36})]$, respectively, are compositionally and structurally similar but they display limited solid solution (Yagi 1953; Deer et al. 1997b). Serendibite $Ca_4[Mg_6Al_6]O_4[Si_6B_3Al_3O_{36}]$ is also isostructural with and compositionally similar to rhönite, but it appears to require at least some B substitution for Al and Si (Grice et al. 2014). Furthermore, serendibite only occurs in B-rich skarns and thus has a different formational environment (Deer et al. 1997b).

More subjective and borderline examples occur with some groups of minerals related by structure and paragenesis. For example, the gyrolite group has 11 members, all of which are hydrous layer Ca silicates that form in relatively low-temperature hydrothermal environments (Mamedov and Belov 1958; Merlino 1988; Ferraris et al. 1995). Each of these 11 species forms from a combination of modules – tetrahedral, octahedral, and large cation layers – but they have significantly different layer arrangements and cation types; therefore, until more clarity on the phase relationships among these minerals is available, we provisionally treat these structures as distinct root mineral kinds.

The structures of uranyl $(U^{6+}O_2)^{2+}$ minerals are particularly complex, displaying a variety of structural modules and motifs typically linked in topologies that are not easily reduced to homologous series (Burns et al. 1996; Burns 2005; Lussier et al. 2016). The phosphuranylite group of 17 related uranyl phosphates and arsenates is a case in point. All of these closely-related minerals form through near-surface weathering/oxidation of prior U-bearing phases and thus might seem likely candidates for lumping. However, we divide this group into 9 different root mineral kinds based on their distinct structures. Althupite (Piret and Deliens 1987), bergenite (Locock and Burns 2003a), metavanmeersscheite (Christ and Clark 1960; Piret and Deliens 1982), mundite (Deliens and Piret 1981), and phurcalite (Plášil et al. 2020) have unique structures and are not lumped with other species. We lump arsenovanmeersscheite with isostructural vammeersscheite (Piret and Deliens 1982). Similarly, we combine hugelite and dumontite (Locock and Burns 2003b); phuralumite, francoisite-Ce, francoisite-Nd, and upalite (Deliens and Piret 1979; Piret et al. 1988); and phosphuranaylite, arsenuranylite, dewindite, and yingjiangite (Hogarth and Nuffield 1954; Belova 1958; Chen et al. 1990) on the basis of solid solutions among isostructural species.

Splitting mineral species

We suggest two circumstances that might justify the splitting of an IMA-approved mineral species or a root mineral kind into two or more natural kinds:

1) If the species/kind forms by two or more different paragenetic modes; and/or,
2) If cluster analysis of numerous chemical and/or physical attributes of one species/kind reveals two or more distinct multi-dimensional combinations of attributes.

Multiple paragenetic modes: The case of multiple paragenetic modes is the easier to demonstrate, because geological context is often sufficient to distinguish very different formation environments. Hazen and Morison (2021a) propose that each mineral species can be assigned to one or more of 57 paragenetic modes. Of 5659 IMA-approved species, 3349 are known from only one paragenetic context and thus cannot be split by this criterion. However, 2310 species arise from two or more processes, and thus appear to be candidates for splitting. Of these species, 1372 have been reported to form in two different ways and 458 have three known paragenetic modes, whereas in the most diverse examples, 42 species are associated with 10 or more paragenetic modes Hazen and Morrison 2021a). These varied formational environments typically lead to distinctive combinations of chemical and physical attributes, including trace and minor elements, isotopes, external morphology, color, structural defects, solid and fluid inclusions, petrologic context, and many other characteristics. In the evolutionary classification system of minerals, each distinct paragenetic mode (and resulting combination of physical and chemical attributes) for a root mineral kind is treated as a different mineral natural kind.

Diamond provides one straightforward example (Hazen 2019). Hazen and Morrison (2021a) attribute 7 paragenetic modes to diamond, including condensation in stellar atmospheres, meteorite and terrestrial impact formation, mantle-derived from varied lithologies, and via ultra-high-pressure (UHP) metamorphism in subduction zones. These processes lead to morphologically distinct *stellar diamond*, *impact diamond*, *mantle diamond*, and *UHP diamond* – at least four variants that can be viewed as different natural kinds.

Pyrite (FeS_2) displays the most diverse range of formation environments, with more than 20 reported paragenetic modes spanning 4.56 billion years (Hazen and Morrison 2021a). Pyrite is known from: meteorites, as an alteration phase that formed in planetesimals; volcanic fumaroles; hydrothermal deposits; authigenic marine and terrestrial sediments; varied igneous lithologies, including granite, layered intrusions, and carbonatites; regional metamorphic rocks; near-surface weathering environments; microbially-precipitated deposits; coal measures and sublimates from coal fires; and a variety of anthropogenic processes associated with mining. Pyrite thus displays a wide range of morphologies, petrologic contexts, and chemical attributes – idiosyncratic combinations of characteristics that represent more than a dozen natural kinds (Bowles et al. 2011; Gregory et al. 2019).

Similar analyses apply to all minerals with multiple modes of origin. Special attention might be paid to species such as calcite, hydroxylapatite, magnetite, and quartz that are known to form both abiotically and via directed biomineralization (Lowenstam and Weiner 1989; Weiner and Wagner 1998; Dove et al. 2003; Aparicio and Ginebra 2016). Those species and others formed by cellular processes hold special promise in the search for mineralogical biosignatures (Chan et al. 2019).

Cluster analysis: The second criterion for splitting mineral species into two or more natural kinds relies on cluster analysis, which is a statistical method that provides a quantitative approach to defining similarities and differences among populations of minerals (Scrucca et al. 2016; Fop and Murphy 2017; Boujibar et al. 2021). Ewing (1976) was well ahead of his time in an effort to apply compositional data to sorting out relationships among AB_2O_6-type orthorhombic rare-earth Nb-Ta-Ti oxides. His multivariate analysis of 91 specimens with 58 chemical and physical attributes suggested a "three-fold chemical classification – aeschynite, euxenite, and polycrase."

In spite of the power of this method, one must fast-forward more than four decades to find significant applications of multivariate analysis to mineral classification. A significant challenge in applying cluster analysis is its dependence on the availability of large databases of mineral properties with multiple attributes. In spite of significant efforts to develop such data resources (Hazen et al. 2019; Chiama et al. 2020; Golden et al. 2020; Prabhu et al. 2020), only a few such studies have been attempted. Gregory et al. (2019) assembled a database of 3,579 analyses of pyrite trace elements and applied a random forest machine-learning classifier to group the analyses into probable ore-forming environments, including iron oxide copper-gold (IOGG), sedimentary exhalative (SEDEX), and volcanic-hosted massive sulfide (VHMS) deposits. Ongoing work will apply cluster analysis to an expanded pyrite database (Zhang et al. 2019).

Boujibar and colleagues (2021) expanded a database of the Si, C, and N isotopic compositions of ~17,000 pre-solar moissanite (SiC) grains (Hynes and Gyngard 2009) – individual crystals formed in the atmospheres of stars prior to the formation of the solar nebula at ~4.567 Ga and now identified by their extreme isotopic anomalies (Nittler and Ciesla 2016). Analyses by Boujibar et al. (2021) and Hystad et al. (2021) point to 7 or more moissanite clusters that represent different stellar environments of formation (and possibly as many moissanite mineral natural kinds). If confirmed, this result would modify the division of stellar moissanite proposed by previous investigators (Davis 2011; Zinner 2014; see Hazen and Morrison 2020).

Many examples of minerals that might be split into multiple natural kinds on the basis of idiosyncratic combinations of chemical and physical attributes are familiar to mineralogists and petrologists. Mantle diamonds display at least two contrasting types of optical absorption spectra, coupled with different suites of inclusions, that distinguish deep-formed diamonds of Type I from Type II, as well as several subtypes (Walker 1979; Smith et al. 2016). The grain morphologies, trace elements, and associations of muscovite from complex pegmatites differ from those in metasediments (Fleet 2003). Similarly, plagioclase from basalt differs in morphology, chemical zoning, compositional range, trace elements, twinning and other microstructures, inclusions, and many other attributes from regional metamorphic plagioclase (Deer et al. 2001). Especially dramatic contrasts occur between abiotic forms of calcite, aragonite, and hydroxylapatite and the exquisitely sculpted examples formed by directed biomineralization. In these and many other minerals, distinctive combinations of chemical and physical attributes point to different mineral natural kinds. Data-driven approaches to classification of mineral natural kinds thus represent a new and emerging opportunity. However, advances in mineral classification by cluster analysis must await the assembly, curation, and expansion of robust open-access mineral data resources, which are the key to future advances (e.g., Chiama et al. 2020).

Both Lumping and Splitting

In the cases of 587 IMA-approved mineral species, strong arguments exist both for lumping with one or more other species based on composition and structure, while splitting into two or more paragenetic modes. In these instances, IMA-approved mineral species do not bear a simple relationship to natural kinds. A relatively straightforward example is provided by two isostructural pyroxenoids, pyroxmangite (ideally $MnSiO_3$; Pinckney and Burnham 1988) and pyroxferroite ($FeSiO_3$; Chao et al. 1970). Pyroxmangite almost always has significant Fe content and therefore might be lumped with pyroxferroite. However, lunar and Martian pyroxferroite specimens invariably have only minor Mn content. Therefore, we use *extraterrestrial pyroxferroite* exclusively for the extraterrestrial Mn-poor mineral, whereas the root mineral kind "*pyroxmangite*" includes all occurrences of terrestrial [$(Mn,Fe)SiO_3$], including *pegmatite pyroxmangite* and *metamorphic pyroxmangite*, even in the less common circumstances when Fe > Mn.

The hornblende group of calcic amphiboles, with a general formula [$(\square,Na,K)Ca_2(Mg,Fe^{2+},Al,Fe^{3+})_5(Si,Al)_8O_{22}(OH,F,Cl)_2$], presents a far more formidable challenge (Deer et al 1997a; Hawthorne et al. 2011). With at least 34 species and more than a dozen modes of formation in diverse igneous and metamorphic environments, there is no simple way to convert IMA-approved species of calcic amphiboles to natural kinds. However, important clues emerge from graphs of compositional ranges of 200 samples, as plotted by Deer et al. (1997a; their figures 115 through 126, 279, 281, 286, 290, 292, 295, and 342). These graphs clearly demonstrate a wide range of continuous solid solutions amongst members of the hornblende, tschermakite, edenite, pargasite, hastingsite, and sadanagaite subgroups of calcic amphiboles, as well as significant clustering associated with groups of species and different paragenetic contexts. Our long-term ambition is to assemble a database of hundreds of thousands of amphibole chemical analyses and physical attributes and to apply cluster analysis. Prior to that major effort, we lump 26 calcic amphibole species, including those with (Mg,Fe^{2+},Fe^{3+},Al,Si) as the essential tetrahedral and octahedral cations, as well as Na- and K-bearing species and OH, F, and Cl varieties, into "*hornblende*." Calcic amphiboles excluded from the hornblende group include 4 species of the compositionally distinct Si-poor sadanagaite group (Shimazaki et al. 1984; Nikondrov et al. 2001), which come from sub-silicic skarns, and oxo-magnesio-hastingsite (Zaitsev et al. 2013), which is a product of prior amphibole dehydration and oxidation. We acknowledge that the lumping of most calcic amphiboles into one root mineral kind, "*hornblende*," is a preliminary decision, as a number of compositional attributes point to specific paragenetic modes. For example, Fe^{3+}-rich calcic amphiboles are often associated with secondary dehydration oxidation; K-rich hornblendes are found in kimberlites, carbonatites, pyroxenites; some Na-rich examples occur in skarns; Crbearing amphiboles are found in ultramafic lithologies; F-rich amphiboles, typically with appreciable OH, often occur in Mg-rich skarns; and some Cl-rich calcic amphiboles are associated with magnetite skarns. Each of these distinctive relationships between composition and paragenesis may eventually warrant separate natural kinds.

A similar situation obtains for tourmaline group minerals. Compositional considerations suggest that 20 (of 37 approved) tourmaline species form a continuous solid solution with the general formula $[(\square,Na,Ca)(Mg,Fe,Al)_3(Mg,Al)_6(Si_6O_{18})(BO_3)_3(OH,F)_3(OH,O)]$. Accordingly, we lump these 20 species into one root mineral kind, "*tourmaline*." However, those species are known from varied igneous and metamorphic environments. Thus, splitting of the root mineral kind into tourmaline natural kinds will also be required.

In contrast to the hornblende and tourmaline groups, in which we provisionally lumped numerous isostructural species into a single root mineral kind, many of the almost 50 species of the seidozerite group of titanium silicates cannot be lumped for two reasons (Christiansen et al. 2003; Ferreris et al. 2008; Sokolova and Cámara 2017). First, this group is structurally varied. The only topological feature in common is a Ti-heterophyllosilicate layer; otherwise crystal chemical details vary significantly. Second, seidozerite group minerals form in a variety of geological settings, including alkaline rocks (nepheline syenites) of the Kola peninsula (e.g., bafertisite, murmanite, lamprophyllite, etc.); paleovolcanic region in Eifel, Southern Germany (schullerite, lileyite, etc.); syenites of the Magnet Cove quarry, Arkansas (delindeite); and metamorphosed Mn deposits (ericssonite). Consequently, we have subdivided seidozerite group minerals into 17 different root mineral kinds. In two cases – 12 species of the rinkite group and 9 species of the lamprophyllite group (e.g., lamprophyllite, barytolamprophyllite, nabalamprophyllite, and their polytypes) that are only known from agpaitic rocks – lumping into root mineral kinds is easily justified. However, 9 species of the seidozerite group are not lumped with other species and must be considered to be separate root mineral kinds. For example, betalomonosovite bears a close structural relationship to lomonosovite; however, betalomonosovite forms from lomonosovite by secondary aqueous solutions and therefore represents a distinct mineral evolution event (Lykova et al. 2018).

The milarite cyclosilicate group of 25 mineral species (Gagné and Hawthorne 2016), which we divide into 9 kinds, provides another example of simultaneous lumping of related compositions and splitting of paragenetic modes. We recognize five species as separate root mineral kinds: *yagiite* is found only as a minor phase in silicate inclusions of iron meteorites (Bunch and Fuchs 1969); *agakhanovite*-(Y) (Hawthorne et al. 2014) and *poudretteite* (B-bearing; Grice et al. 1987) ari compositionally distinct; and *almarudite* (Mihailovic et al. 2004) and *armenite* (Armbruster and Czank 1992) are structurally distinct, with unique space groups and unit cells, as well as differing modes of origin. *Armenite* must also be split, as it forms in both metamorphosed Ba deposits and as an aqueous alteration phase. We lump four compositionally-related Be-bearing species (friedrichbeckite, laurenthomsonite, milarite, and oftedahlite) under the root mineral kind "*milarite*," which is split into natural kinds from intrusive and extrusive igneous rocks, as well as aqueous alteration environments. Five Mg-Fe-Al species (chayesite, eifelite, osumilite, osumilite-(Mg), and trattnerite) are compositionally lumped into the root mineral kind *osumilite*, which also should be split owing to formation in a range of igneous, metamorphic, and coal environments. And nine Li-Zn-Mn-bearing species (aluminosugilite, berezanskite, brannockite, daripiosite, dusmatovite, klochite, shibkovite, sogdianite, and sugilite) are lumped into the root mineral kind *sugilite*, but the root mineral *sugilite* must be split according to distinct igneous and metamorphic paragenetic modes. Finally, merrihueite and roedderite, which form a solid solution in thermally metamorphosed enstatite chondrite meteorites (Fuchs et al. 1966; Dodd et al. 1965; Hazen and Morrison 2021b), are lumped into *roedderite*, a single root mineral kind and natural kind.

One additional example, plagioclase feldspars, represent a challenging example of a common mineral group where both end-members, as well as ranges of intermediate compositions, appear to be valid root mineral kinds (Deer et al. 2001). Consider meteorite occurrences. On the one hand, near end-member anorthite ($CaAl_2Si_2O_8$) is an important primary condensate phase in meteorite chondrules and in achondrite meteorites, and end-member albite ($NaAlSi_3O_8$) is a common, if volumetrically minor, phase in silicate-rich clasts in iron meteorites (Hazen et al. 2021; Morrison and Hazen 2021). On the other hand, intermediate plagioclase with compositions from An < 20 to An > 90 occur both as primary and secondary phases in a range achondrite meteorites (Morrison and Hazen 2021; Hazen and Morrison 2021b). Occurrences of end-member albite and anorthite, and ranges of intermediate plagioclase, are also associated with varied igneous and metamorphic lithologies (Deer et al. 2001; Hazen and Morrison 2021a). We conclude that end-member *albite* and *anorthite* are root mineral kinds, likely with multiple natural kinds based on different formational environments, but *plagioclase* should also be considered a root mineral kind, also with multiple natural kinds.

IMPLICATIONS

Mineral species versus *root mineral kinds*: We define each mineral natural kind on the basis of its unique combination of structural, chemical, and paragenetic attributes. Hazen and Morrison (2021a; their Table 1 and Supplement 1) investigated 5659 IMA-approved mineral species and their modes of formation by one or more of 57 different paragenetic processes, tabulating 10,556 unique combinations of mineral species and paragenetic mode. However, because of the lumping criteria outlined above, not all of these 10,556 combinations correspond to different mineral natural kinds.

In the present study, we demonstrate that those 5659 IMA-approved species correspond by lumping criteria to 4016 root natural kinds, which are associated with 7816 unique combinations of root mineral kinds and the 57 paragenetic modes (Table 2; Supplemental Table 1). Lumping thus reduces 10,556 combinations of mineral species and their paragenetic modes by 26 %, to 7816 combinations that conform to our definition of mineral natural kinds.

This 26 % reduction is not equally distributed across all paragenetic modes (Table 2; column "% reduced"). Lumping of meteorite minerals (Table 2; paragenetic modes #1 to #6) results in a ~10 % decrease in the number of combinations of mineral and paragenetic mode – a value similar to that for Phanerozoic minerals associated with biological and anthropogenic processes (modes #48 to #57). Lumping of weathered/oxidized minerals associated with the Great Oxidation Event (modes #45 to #47) leads to a ~19 % reduction. Thus, it appears that minerals formed by processes in meteorites, or those directly or indirectly associated with biological activities, are more likely than average to have unique combinations of structure and composition.

By contrast, lumping of minerals from complex granite pegmatites and agpaitic rocks (paragenetic modes #34 and #35) leads to an almost 50 % decrease in the number of unique combinations. This significant reduction results in part from a number of mineral groups with 20 or more lumped species, including cancrinite, eudialyte, jahnsite, labuntsovite, and tourmaline, that are associated with these compositionally distinctive environments. The greater "lumpability" of these species reflects their chemically adaptable structures with numerous cation sites, coupled with more complex solid solution behavior available for minerals that have crystallized under sustained high-temperature conditions (Andrew Christy, personal communication, July 2, 2021).

Machine learning and classification: The greatest to challenge to any classification system that aspires to define natural kinds is the inherent subjectivity of lumping and splitting. Our preliminary efforts have focused on employing the benchmark list of mineral species approved by the IMA-CNMNC as a starting point for classifying mineral natural kinds in their evolutionary context. We have attempted to identify continuous *T-P-X* phase regions (as a basis for lumping) and distinctive paragenetic processes (as a basis for splitting). Neither effort – lumping or splitting minerals in the context of IMA-approved species – yields unambiguous results, at least not yet. However, a more rigorous quantitative approach based on machine learning applied to large and growing mineral data resources offers promise.

Data-driven methods, especially those coupled to multi-dimensional analysis and applications of machine learning, represent rapidly evolving opportunities for developing rigorous lumping and splitting criteria in many classification efforts. Large and growing data resources in fields from medical diagnoses to musical genres to geomaterials are the key to significant advances (Bickerstaffe and Makalic 2003; Goulart et al. 2012; Marquand et al. 2016; Prabhu et al. 2020).

In this regard, the mineral sciences have lagged behind many other disciplines. A critical need is the development, expansion, and curation of open-access mineral databases that record scores of chemical and physical attributes for millions of samples. Pioneering work has been made in petrology databases (e.g., Lehnert et al. 2007), while important mineral data resources document properties and localities of all known species (https://rruff.info/ima; https://mindat.org; Downs 2006; Lafuente et al. 2015; Golden 2020). A few concerted efforts to tabulate multiple attributes for thousands of specimens for specific mineral species and groups represent encouraging progress (Gregory et al. 2019; Chiama et al. 2020; Boujibar et al. 2021; Cheng et al. 2021). However, a more unified and widespread international mineral informatics program is necessary to collect and preserve vast amounts of "dark data" and make those data available in *F*indable, *A*ccessible, *I*nteroperable, and *R*eusable ("*FAIR*"; Wilkinson et al. 2016) platforms.

How many mineral natural kinds? This analysis of lumping and splitting criteria applied to 5659 IMA-approved mineral species facilitates preliminary estimates of the possible total number of mineral natural kinds, based on the proposition that each natural kind represents a distinct combination of continuous solid solution (often in multi-dimensional *T*-*P*-*X* phase space), shared crystal structure (including homologous series), and paragenetic mode (with the acknowledgement that a significant degree of subjectivity will exist in any enumeration of paragenetic modes; Hazen and Morrison 2021a).

We suggest that 5659 IMA-approved species correspond by lumping criteria to 4016 root mineral kinds (a reduction of ~29 %), of which 1623 species have only one known paragenetic mode and thus may be directly equated to 1623 natural kinds. However, each of the remaining 2393 root mineral kinds forms by two or more processes, and thus likely represents multiple natural kinds. Hazen and Morrison (2021a) identified 6193 paragenetic modes linked to those 2393 root natural kinds. Accordingly, we estimate that the 5649 IMA-approved species correspond to approximately 1623 + 6193 = 7816 known mineral natural kinds.

What of mineral natural kinds not yet described? Hystad et al. (2019) used statistical methods to estimate that ~4000 additional mineral species (based on IMA-CNMNC criteria) exist on Earth but have yet to be discovered and described using currently available methods. If we assume that approximately 70 % of those “missing” minerals cannot be lumped with previously approved species into root mineral kinds (the same percentage as for the 5659 known mineral species considered here), and that most undescribed species are extremely rare and therefore likely form by only one paragenetic process, then it is reasonable to conclude that an additional 2800 natural kinds await discovery. We conclude that Earth holds more than 10,000 mineral natural kinds.

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Table 2. Division of 4016 "root mineral kinds" among 57 paragenetic modes of minerals; compare with Hazen and Morrison (2021a, their Table 1)

Paragenetic Mode[a]	Age (Ga)	#Kinds[b]	% Reduced[c]	#Unique[d]
Pre-terrestrial "Ur-minerals"	*> 4.57*	*28*	7	*7*
1. Stellar atmosphere condensates		20	0	0
2. Interstellar condensates[e]		8	0	7
Stage 1: Primary nebular phases	*4.567—4.561*	*76*	12	*13*
3. Solar nebular condensates (CAIs, AOAs, URIs)	> 4.565	42	12	13
4. Primary chondrule phases	4.566—4.561	43	9	0
Stage 2: Planetesimal differentiation & alteration	*4.566—4.550*	*230*	12	*56*
5. Primary asteroid phases	4.566—4.560	87	7	21
6. Secondary asteroid phases	4.565—4.550	178	13	35
Stage 3a: Earth's earliest Hadean crust	*> 4.50*	*285*	29	*35*
7. Ultramafic igneous rocks		100	22	7
8. Mafic igneous rocks		53	43	3
9. Lava/xenolith minerals		90	29	1
10. Basalt-hosted zeolite minerals		70	35	19
11. Volcanic fumarole minerals; reduced phases		32	11	5
Stage 3b: Earth's earliest hydrosphere	*> 4.45*	*256*	27	*34*
12. Hadean hydrothermal subsurface sulfide deposits		87	33	20
13. Hadean serpentinization		56	16	6
14. Hot springs, geysers, and other subaerial geothermal minerals		53	13	1
15. Black/white smoker minerals; seafloor hydrothermal minerals		29	9	0
16. Low-T aqueous alteration of Hadean subaerial lithologies		57	31	3
17. Marine authigenic Hadean minerals		35	31	1

18. Minerals formed by freezing		4	0	3
Stage 4a: Earth's earliest continental crust	*> 4.4—3.0*	*1731*	27	*664*
Igneous rocks		96	40	8
19. Granitic intrusive rocks		82	43	7
20. Acidic volcanic rocks		27	40	1
Near-surface Processes		882	21	190
21. Chemically precipitated carbonate, phosphate, iron formations		69	13	1
22. Hydration and low-T subsurface aqueous alteration		182	26	65
23. Subaerial aqueous alteration by non-redox-sensitive fluids		314	21	60
24. Authigenic minerals in terrestrial sediments		58	22	0
25. Evaporites (prebiotic)		183	13	55
26. Hadean detrital minerals		171	32	4
27. Radioactive decay; auto-oxidation		9	0	0
28. Photo-alteration, pre-biotic		10	0	0
29. Lightning-generated minerals		9	0	0
30. Terrestrial impact minerals		16	0	5
High-T alteration and/or metamorphism		1049	30	466
31. Thermally altered carbonate, phosphate, and iron formations		224	37	37
32. Ba/Mn/Pb/Zn deposits, including metamorphic deposits		272	34	97
33. Minerals deposited by hydrothermal metal-rich fluids		598	25	332
Stage 4b: Highly evolved igneous rocks	*> 3.0*	*843*	43	*252*
34. Complex granite pegmatites		291	48	77
35. Ultra-alkali and agpaitic igneous rocks		383	47	150
36. Carbonatites, kimberlites, and related igneous rocks		220	24	22
37. Layered igneous intrusions and related PGE minerals		102	24	3
Stage 5: Initiation of plate tectonics	*< 3.5—2.5*	*318*	31	*27*
38. Ophiolites		95	12	5

39. High-P metamorphism		50	29	7
40. Regional metamorphism		201	37	15
41. Mantle metasomatism		14	12	0
42. Sea-floor Mn nodules		15	0	0
43. Shear-induced minerals		8	11	0
Stage 6: Anoxic biosphere	*< 4.0*			
44. Anoxic microbially-mediated minerals		11	0	0
Stage 7: Great Oxidation Event	*< 2.4*	*1887*	19	*946*
45. Oxidized fumarolic minerals		350	17	88
a. [Sulfates, arsenates, selenates, antimonates]		[198]	22	[83]
b. [Other oxidized fumarolic minerals]		[230]	83	[46]
46. Near-surface hydrothermal alteration of minerals		43	17	9
47. Low-T subaerial oxidative hydration, weathering		1619	19	849
a. [Near-surface hydration of prior minerals]		[1303]	21	[701]
b. [Sulfates and sulfites]		[352]	11	[153]
c. [Carbonates, phosphates, borates, nitrates]		[438]	24	[229]
d. [Arsenates, antimonates, selenates, bismuthinates]		[356]	30	[241]
e. [Vanadates, chromates, manganates]		[307]	17	[175]
f. [Uranyl (U^{6+}) minerals]		[211]	11	[150]
g. [Halogen-bearing surface weathering minerals]		[201]	15	[101]
h. [Near-surface oxidized, dehydrated minerals]		[285]	10	[149]
i. [Terrestrial weathering of meteorites]		[27]	4	[9]
Stage 8: "Intermediate Ocean"	1.9—0.9	0		0
Stage 9: "Snowball Earth"	0.9—0.6	0		0
Stage 10a: Neoproterozoic oxygenation/terrestrial biosphere	< 0.6	*532*	11	*57*
48. Soil leaching zone minerals	< 0.6	57	20	3

49. Oxic cellular biomineralization	< 0.54	76	1	1
50. Coal and/or oil shale minerals	< 0.36	255	7	3
51. Pyrometamorphic minerals	< 0.36	101	21	22
52. Guano- and urine-derived minerals	< 0.4	67	7	15
53. Other minerals with taphonomic origins	< 0.4	111	5	13
Stage 10b: Anthropogenic minerals	< 10 Ka	*544*	10	*8*
54. Coal and other mine fire minerals		212	9	4
55. Anthropogenic mine minerals		234	13	4
56. Slag and smelter minerals		130	9	0
57. Other minerals formed by human processes		49	0	0

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a The 10 stages of mineral evolution refer to temporal divisions, as outlined in Table 1 of Hazen et al. (2008). The 57 paragenetic modes, designated [*#1*] to [*#57*], are detailed by Hazen and Morrison (2021b).

b Numbers of root mineral kinds are based on paragenetic modes identified by Hazen and Morrison (2021a; see their Table 1).

c "% reduced" is the percentage reduction from the number of IMA-approved mineral species, as recorded in Table 1 of (Hazen and Morrison 2021a), to the number of root mineral kinds recorded here for each of 57 paragenetic modes and 11 compositional subsets.

d Numbers of root mineral kinds known to form only by that paragenetic mode.

e Includes 7 interstellar ice phases that are not IMA-approved mineral species.

Table 3. Names, formulas, and representative species for 22 root mineral kinds with names that do not correspond to mineral species' names approved by IMA-CNMNC

Group Name	Formula	Representative Species	Group Size	Ref.*
Androsite	$(Ca.Mn)(REE)(Fe,Mn,Al,V)_3(Si_2O_7)(SiO_4)O(OH)$	Ferriakasakaite-(Ce)	10	1
		Ferribushmakininte		
		Manganiandrosite-(La)		
		Vanadoallanite-(La)		
Apophyllite	$(Na,K,NH_4)Ca_4Si_8O_{20}(F,OH)\cdot 8H_2O$	Fluorapophyllite-(Na)	5	2
		Fluorapophyllite-(NH_4)		
		Hydroxyapophyllite-(K)		
Biotite	$K_2(Mg,Fe^{2+},Fe^{3+},Al,Ti)_6(Si,Al)_8O_{20}(OH,F)_4$	Annite	6	3
		Meifuite		
		Montdorite		
		Siderophyllite		
Clinoholmquistite	$\square Li_2(Mg,Fe^{2+})_3Fe^{3+}{}_2)Si_8O_{22}(OH,F)_2$	Clino-ferri-holmquistite	7	4
		Ferro-ferri-pedrizite		
		Fluoro-pedrizite		
Ellestadite	$Ca_5(SiO_4)_{1.5}(SO_4)_{1.5}(Cl,F,OH)$	Chlorellestadite	3	5
		Hydroxylellestadite		
Fassaite	$Ca(Mg,Al,Ti^{3+},Ti^{4+})(Al,Si)SiO_6$	Grossmanite	2	6,7
Fe-Mo Alloy	(Fe,Mo)	Hexamolybdenum	2	7
Högbomite	$(Zn,Al,Fe^{2+},Mg,Ti)_3(Al,Fe^{3+},Ti^{4+},Mn)_8O_{15}(OH)$	Ferrohögbomite-2N2S	15	8,9
		Magnesiohögbomite-2N3S		
		Zinconigerite-6N6S		

Hornblende	$(Na,K)Ca_2(Mg,Fe^{2+},Al,Fe^{3+})_5(Si,Al)_8O_{22}(OH,F,Cl)_2$	Ferro-ferri-hornblende Fluoro-edenite Magnesio-hastingsite Potassic-pargasite Tschermakite	26	4
Leakite	$NaNa_2(Mg,Fe,Mn^{3+},Al,Li,Ti^{4+})_5Si_8O_{22}(O,OH,F)_2$	Ferro-ferri-fluoro-leakeite Potassic-ferri-leakeite Oxo-mangani-leakeite Mangani-dellaventuraite	7	4
Lepidolite	$(K,Cs,Rb)(\square,Li,Mg,Mn,Fe,Al,Ti)_3(Al,Si)_4O_{10}(F,OH,O)_2$	Fluorluanshiweiite Garmite Orlovite Polylithionite Voloshinite	11	3
Mayenite	$Ca_{12}(Al,Fe^{3+},Si)_{14}O_{32}[H_2O,F,Cl]_6$	Chlormayenite Fluorkyuygenite Wadalite	6	10
Microlite	$(Na,Ca,Bi,Sn,Sb)_2Ta_2O_6(O,OH,F)$	Fluorcalciomicrolite Hydroxykenomicrolite Oxystannomicrolite	10	11
Obertite	$NaNa_2(Mg,Mn,Fe^{3+},Ti^{4+})_5Si_8O_{22}O_2$	Ferro-ferri-obertite Mangani-obertite	3	4
Os-Ru Alloy	(Os,Ru,Ir)	Osmium Rutheniridosmine Hexaferum	5	7,12
Phengite	$K(Mg,Fe,Al,Mn)_{2.5\text{-}3}(Si,Al)_4O_{10}(OH)_2$	Aluminoceladonite Manganiceladonite	6	3

Pyrochlore	$(Na,Ca,Pb,Mn)_2Nb_2O_6(O,F,OH)$	Fluorcalciopyrochlore Hydroxykenopyrochlore Jixianite	7	11
Roméite	$(Ca,Fe,Mn)_2Sb_2O_6(O,OH,F)$	Fluorcalcioroméite Hydroxyferroroméite Oxyplumboroméite	7	11
Scapolite	$(Na,Ca)_4(Al,Si)_{12}O_{24}(CO_3,SO_4,Cl)$	Marialite Meionite Silvialite	3	2
Taaffeite	$(Fe,Mg,Zn)_3Al_8BeO_{17}$	Magnesiotaaffeite-2N2S Ferrotaaffeite-6N3S	4	8
Tourmaline	$(\square,Na,Ca)(Mg,Fe,Al)_3(Mg,Al)_6(Si_6O_{18})(BO_3)_3(OH,F)_3(OH,O)$	Dravite Magnesio-foitite Oxy-schorl Fluor-uvite Olenite Povondraite Lucchesiite	20	13,14
Wolframite	$(Fe,Mn,Mg)(WO_4)$	Ferberite Hübnerite Huanzalaite	3	15

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* Numbered references: 1. Armbruster et al. (2006); 2. Deer et al. (2004); 3. Fleet (2003); 4. Deer et al. (1997a); 5. Pasero et al. (2010); 6. Deer et al. (1997b); 7. Hazen et al. (2021); 8. Armbruster (2002); 9. Hejny et al. 2002; 10. Bailau et al. (2010); 11. Christy & Atencio (2013); 12. Hazen & Morrison (2020); 13. Deer et al. (1986); 14. Henry et al. (2011); 15. Anthony et al. (2003)