




## Article

# Ontology, archetypes and the definition of ‘mineral species’

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### Abstract

*Ontology* deals with questions concerning what things exist, and how such things may be associated according to similarities and differences and related within a hierarchy. Ontology provides a rigorous way to develop a general definition of a mineral species. Properties may be divided into two principal groups: an *intrinsic property* is characteristic of the object and is independent of anything else; an *extrinsic property* depends on the relation between the object and other things. A *universal* is an entity that is common to all objects in a set. Here the objects are mineral samples, each entity is a specific property of these minerals, and the set of objects is all mineral samples of that mineral species. The key intrinsic properties of a mineral species are its name, its end-member formula and *Z* (the number of formula units in the unit cell), its space group and the bond topology of the end-member structure. These are also universals as they are common to all mineral samples belonging to that mineral species. An archetype is a pure form which embodies the fundamental characteristics of an object. Thus the archetype of a mineral species embodies the above set of universals. Real mineral samples of this mineral species are imperfect copies of that archetype, with a range of chemical composition defined by the boundaries between end-member formulae of this and other end members of the same bond topology. The result is a formal definition of a mineral species: A specific mineral species is the set of imperfect copies of the corresponding archetype and 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.

**Keywords:** mineral species, definition, intrinsic properties, extrinsic properties, universals, archetype

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### Introduction

Minerals *sensu lato* have been a key factor in the development of humanity and human society. One of the first scientific acts of our ancestors was to differentiate different rocks and use them as tools in accord with their properties (Hawthorne, 1993). As mining and trade developed, it became important to recognise minerals, and written descriptions of minerals and their properties were necessary to do this...it was the beginning of Mineralogy as an empirical scientific discipline. The expansion of smelting techniques to derive metals from ores led to ideas of chemical elements, which in turn led to the extensive chemical work in the late 18<sup>th</sup> and 19<sup>th</sup> Centuries, resulting in the development by Jöns Jacob Berzelius (Berzelius, 1814a,b) of the ‘anionic’ classification of minerals, and the construction of the Periodic Table by Dmitri Mendeleev (Mendeleev, 1897). In the first half of the 20<sup>th</sup> Century, the development of crystal-structure analysis (Bragg, 1913, 1937) gave an atomistic basis to our knowledge of minerals and mineral properties, and Goldschmidt (1937, 1954) used this atomistic basis to describe the behaviour of elements in

geochemical processes. The second half of the 20<sup>th</sup> Century brought numerous physical methods to the study of minerals: microbeam analytical methods, X-ray-, neutron- and electron-scattering methods, and many absorption and emission spectroscopies, both for elemental and isotopic analysis and for probing short-range structure in solids. These advances in mineral characterisation were accompanied by the use of standard theoretical and computational techniques from Physics and Chemistry to try and understand both stereochemical details of mineral structures and a wide array of physical and dynamic processes in bulk crystals and at the surface of minerals. Despite these advances in physical, chemical and computational techniques that are used for minerals, the principal thrust of this work is to apply the results to other disciplines: e.g. Petrology, Geochemistry and Environmental Sciences. Mineralogy is still an empirical science despite the sophistication of the various methods used to characterise minerals; we are still predominantly (to paraphrase Ernest Rutherford) “finding things and putting them in boxes”. This is not necessarily to denigrate putting things in boxes. Dmitri Mendeleev put elements in boxes and developed the Periodic Table which eventually led to a fundamental understanding of the atomic structure of the elements. However, it is necessary to understand what such boxes mean (among other things) if we are to develop a fundamental understanding of minerals and their behaviour.

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## The current state of Mineralogy

The justification for doing Mineralogy is almost always couched in terms of how useful it is to contiguous disciplines; mineralogists are rarely funded to look at issues that are fundamental to Mineralogy itself. Why do minerals have the chemical formulae that they do? Why do minerals have their particular bond topologies? Why are minerals stable over specific ranges of pH, Eh, temperature, pressure and activities of their various constituents? What are the relations between bond topology and both enthalpy and entropy of formation? What are the environmental controls on different crystal forms and habits? What mechanistic details control the sequence of crystallisation of minerals in specific parageneses? Many of these questions are fundamental to Mineralogy itself and yet have tended to be ignored in the past. Why is this the case? Crystal chemistry, thermodynamics and computational mineralogy are very powerful methods, but they have tended to dictate the questions that we ask about minerals. We ask questions to which standard theory can give us an answer. What about these other questions of scientific interest mentioned above, questions that are opaque to standard theoretical techniques? These questions tend to be neglected because they are viewed as both intractable and of no immediate practical use to other branches of Science. Moreover, most mineralogists do not seem interested in such matters, perhaps because the empirical basis of Mineralogy provides no way to consider these problems.

Recently there has been some work directed toward putting Mineralogy on a more rigorous basis and attempting to address some of the questions mentioned above. Hawthorne (1983, 2012, 2015) has provided a bond-topological basis for Mineralogy which can address many of these problems. Quantification of the Structure Hierarchy Hypothesis (Hawthorne, 1983, 1985, 1990, 2014) and the development of specific structure hierarchies: e.g. borates (Hawthorne *et al.*, 1996; Grice *et al.*, 1999), sulfates (Hawthorne *et al.*, 2000), uranyl oxysalts (Burns, 2005; Lussier *et al.*, 2016), arsenates (Majzlan *et al.*, 2014), tellurium oxycompounds (Christy *et al.*, 2016a), anion-centred polyhedra (Filatov *et al.*, 1992; Krivovichev and Filatov, 1999; Krivovichev *et al.*, 2013) and silicates (Hawthorne *et al.*, 2019; Day and Hawthorne, 2020) has led to a much greater understanding of the factors affecting the crystallisation of hydroxy-hydrated oxysalts (e.g. Schindler *et al.*, 2001a,b,c, 2006; Schindler and Hawthorne, 2004) and crystallisation sequences of such minerals (e.g. Christy *et al.*, 2016b, Missen *et al.*, 2020). Introduction of the idea of the complexity of an atomic arrangement (Krivovichev, 2013) has given a quantitative measure of what was hitherto only an intuitive idea, and there is the possibility of relating complexity (Shannon entropy) to thermodynamic entropy (Krivovichev, 2016) and questions of mineral diversity (Christy, 2018; Krivovichev *et al.*, 2018).

## Definition of a mineral species

In developing a fundamental theoretical basis for Mineralogy, it is of critical importance that we have a rigorous definition of a mineral species. The former IMA-CNMMN (International Mineralogical Association Commission on New Minerals and Mineral Names) formulated a definition of a mineral (Nickel, 1995a,b): *In general terms, a mineral is an element or chemical compound that is normally crystalline and that has been formed as a result of geological processes.* However, there is not a formal general definition of the meaning of the term *mineral species*. It may seem that there is from a casual inspection of the

approval process of the current IMA-CNMMNC (International Mineralogical Association Commission on New Minerals, Nomenclature and Classification) but this is not so. Definition, nomenclature and classification of a mineral are three distinct processes: first, a *specific* mineral species must be defined; subsequently, the issues of naming (nomenclature) and classification can be considered (Mills *et al.*, 2009; Hatert *et al.*, 2013, 2017).

The approval of a new mineral species amounts to the definition of that species and requires measurement of many properties of the type material. Some of these properties show the type mineral to be distinct from all other approved mineral species (Nickel, 1992; Nickel and Grice, 1998; Hatert and Burke, 2008; Bosi *et al.*, 2019) and allow a new mineral species to be defined. What are those properties? Chemical formula, space group, cell dimensions, powder X-ray diffraction pattern and crystal-structure refinement (in most cases). A mineralogist has to be able to recognise minerals, and other properties required for IMA-CNMMNC approval are important from this perspective: crystal size, forms present and habit, colour, streak, hardness, cleavage, density and optical properties, associated minerals, petrologic setting and mechanism of formation.

## Use of a mineral name

When we use the same name for two samples of mineral, for example, two diamonds, does this imply that the two samples are identical? No, it does not. For example, the two samples of diamond may be of different colour. So how do we decide that they are both to be named diamond? The straightforward answer is that they have the same properties. However, in our example of two diamonds, they do not have the same properties: they are of different colour. Thus the properties of a mineral do not have equal significance when assigning a name to that mineral; many properties of minerals are not relevant to the assignment of a mineral name. It is necessary to define a set of properties with which a mineral species in general may be defined.

## Ontology and its relation to the properties of an object

Ontology deals with issues pertaining to what things exist, how such things may be grouped, and how these things and sets of things may be related within a hierarchy (i.e. hierarchically classified), and provides a rigorous basis with which to deal with the issue that we will consider here. The things that we will consider are minerals, and minerals are material objects; herein we will refer to minerals as objects. To properly define a specific mineral species, we need to have a rigorous general definition of a mineral species: here, we address this issue.

## Properties of crystalline minerals

We may describe a specific mineral sample by its properties: chemical composition (including trace elements and isotopes), crystal structure (including defects of various sorts), colour, refractive index and hardness just to name a few. Are all of these properties important? The simple answer is 'yes'; they are all properties of a mineral and hence a complete description of that mineral will include them all. However, are all of these properties of equivalent importance? Can properties have different degrees of importance? The answers to these questions are a matter of context. For example: (1) not all properties are required for approval as a new mineral species by the IMA-CNMMNC (e.g. bulk modulus or thermal-expansion coefficients); (2) when using a

mineral as a filler for drilling mud, important properties are density, (lack of) cleavage, (lack of) toxicity and cost; (3) when using a mineral as a gemstone, critical properties are clarity, (attractive) colour, hardness, size and (lack of) cleavage. It is apparent that, from a pragmatic perspective, all mineral properties are important as they affect the usefulness of a mineral to human society, and all users of minerals will develop their own mineral classifications in order to facilitate these uses.

### Intrinsic and extrinsic properties

Properties may be divided into two principal groups: (1) an *intrinsic property* is a property that is characteristic of the object itself and is independent of anything else; (2) an *extrinsic property* is a property that depends on the relation between the object itself and other things. We will examine these definitions in a little more detail. Can a physical property be intrinsic? For example, is the space group of diamond an intrinsic property of diamond? The space group of diamond does not change with variation in temperature and pressure until diamond breaks down and transforms to something else. Thus the space group of diamond is an intrinsic property of diamond, because while diamond exists, its space group does not change. The unit-cell dimensions of a mineral are extrinsic properties of that mineral. Their magnitudes depend on both (1) the chemical composition and crystal structure of the mineral, and (2) on the ambient temperature and pressure, and hence they depend both on the mineral and on the ambient conditions. Note that related properties may be intrinsic and extrinsic: thus the mass of a crystal is an intrinsic property of that crystal whereas the weight of a crystal depends on both the mass and the magnitude of the surrounding gravitational acceleration and is hence an extrinsic property.

There are other classifications of properties. For example, the properties of an object may be *intensive* or *extensive*. Intensive properties are independent of the size of the object whereas extensive properties are dependent on size of the object, and this classification is familiar to us from Chemical Thermodynamics (e.g. Spear, 1993; Anderson, 2005). One may divide properties into other types: (1) *categorical property*: an intrinsic property of an object that is independent of its form; (2) *dispositional property*: an intrinsic property of an object that is influenced by its form. For example, an arborescent crystal can be very fragile whereas a massive crystal of the same mineral may not be fragile. There are many metaphysical complications concerning categorical and dispositional properties (Choi and Fara, 2018) and we will avoid use of this classification. Note that the existence of these other classifications does not affect the validity of the classification used here.

### Intrinsic properties of a mineral

#### Space group

Space-group symmetry is a discrete property and does not change within a single phase; hence it is an intrinsic property of a mineral. Note that this includes space groups for minerals with periodic structures (Guinier *et al.*, 1984; International Union of Crystallography, 1987), quasicrystal structures (Rabson *et al.*, 1991; Mermin, 1992), polytypic and disordered (OD) structures (Guinier *et al.*, 1984) and superspace groups for modulated structures (Janssen *et al.*, 1999, 2002). Many minerals show magnetic behaviour that is governed by their magnetic space groups (Litvin, 2014). Traditionally the magnetic behaviour of minerals

has not been a factor in terms of defining separate mineral species. However, minerals with the same atomic arrangement but different magnetic structures are formally different phases and the magnetic phase transitions between these phases may be treated in the same way as phase transitions between diamagnetic phases.

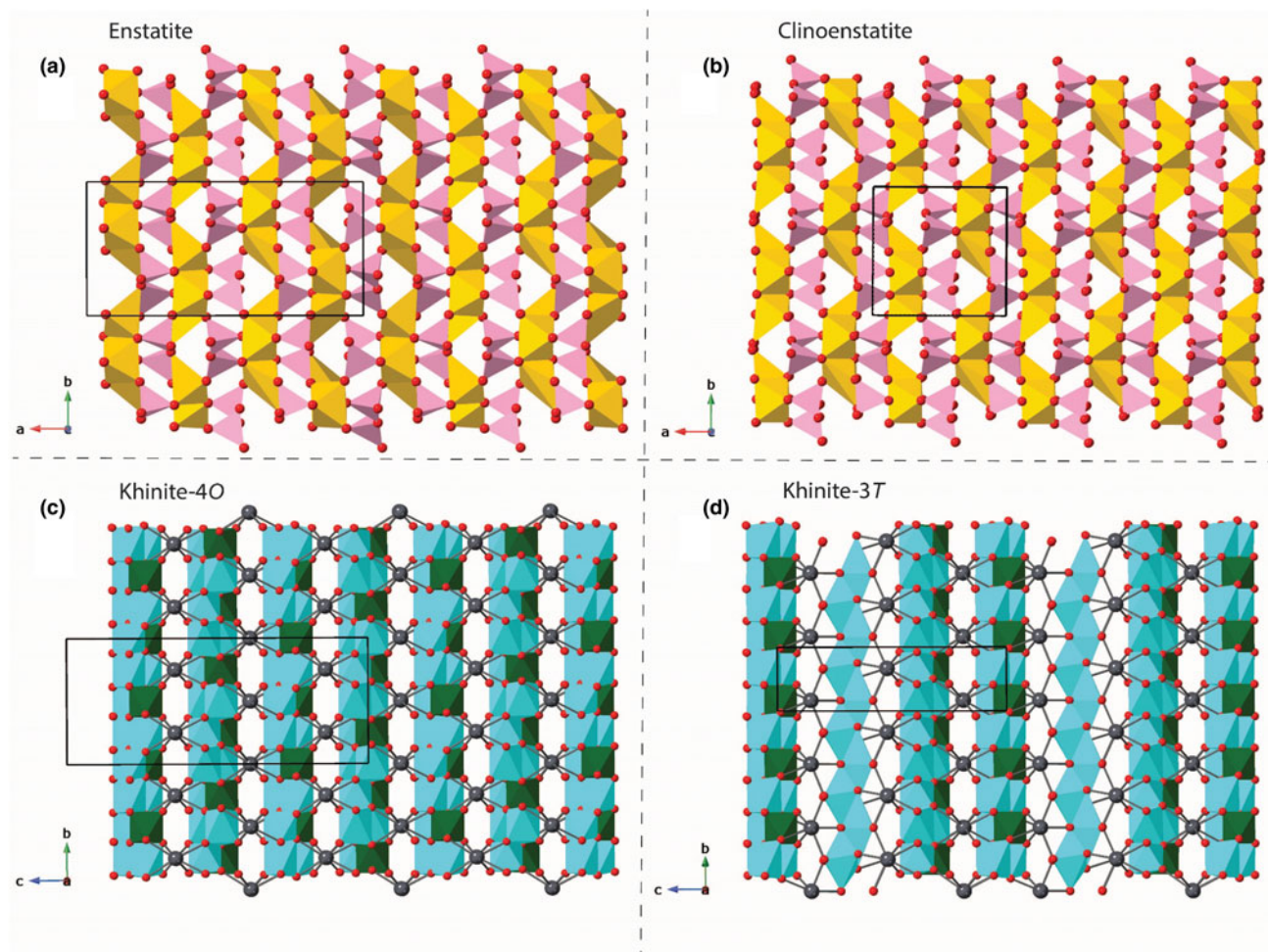
Enstatite, ideally  $\text{MgSiO}_3$  with  $Z=8$ , has the space group  $Pbca$  whereas clinoenstatite, ideally  $\text{MgSiO}_3$  with  $Z=4$ , has the space group  $P2_1/c$  (Figs 1a,b). Muscovite-1M, ideally  $\text{KAl}_2(\text{Si}_3\text{Al})\text{O}_{10}(\text{OH})_2$  with  $Z=2$ , has the space group  $C2/m$  whereas muscovite-2M<sub>1</sub>, ideally  $\text{KAl}_2(\text{Si}_3\text{Al})\text{O}_{10}(\text{OH})_2$  with  $Z=4$ , has the space group  $C2/c$ . Each of these examples are polytypes; the IMA–CNMNC considers enstatite and clinoenstatite as separate species but does not consider muscovite-1M and muscovite-2M<sub>1</sub> as separate species. Polytypes have different bond topologies and are different mineral species, and thus for example muscovite-1M and muscovite-2M<sub>1</sub> should be regarded as different mineral species.

There are many currently accepted mineral species where each species has different space groups for the same chemical formula, a common situation for minerals that undergo ferro-elastic phase transitions. For example,  $\text{Pb}^{2+}\text{Cu}_3^{2+}\text{Te}^{6+}\text{O}_6(\text{OH})_2$  occurs as khinite-4O and khinite-3T (Hawthorne *et al.*, 2009) (Figs 1c,d) and Burns *et al.* (1995) suggest that this composition may crystallise with  $P6_2$  or  $P3_2$  symmetry and transform to khinite-4O and khinite-3T on cooling. Here, two minerals separated by a ferro-elastic phase transition should be considered discrete mineral species. Many minerals show such behaviour, e.g. garnet (Cesare *et al.*, 2019). Others may change space group as a function of chemical composition. For example, titanites with compositions close to end member,  $\text{CaTi}^{4+}\text{SiO}_4\text{O}$ , have the space group  $P2_1/a$  (e.g. Taylor and Brown, 1976), compositions with small to medium amounts of additional ions have the space group  $A2/a$  (e.g. Riva di Sanseverino, 1968), and compositions with large amounts of additional ( $\text{Ta}^{5+}, \text{Nb}^{5+}$ ) and  $\text{Al}^{3+}$  ions have the space group  $P\bar{1}$  (Lussier *et al.*, 2009). Again, these are separate species and could be named by adding the space group after the root name: e.g. titanite- $P2_1/a$ . This approach has been used to great effect in the hydrotalcite supergroup (Mills *et al.*, 2012), especially in the differentiation of quintinite polytypes such as quintinite-2H-3c, quintinite-1M and quintinite-2H (Krivovichev *et al.*, 2010a,b; Zhitova *et al.*, 2010, 2018).

#### Dominant end-member formula

The chemical composition of a specific sample of a mineral is fixed if it is in equilibrium with its environment. However, different samples of the same mineral can have different chemical compositions, also in equilibrium with their environment. Consider the chemical composition of tremolite. It is highly variable; what we may call the end-member composition is  $\square\text{Ca}_2\text{Mg}_5\text{Si}_8\text{O}_{22}(\text{OH})_2$  (Hawthorne *et al.*, 2012), but tremolite samples show extensive incorporation of major amounts of  $\text{Na}^+$ ,  $\text{Fe}^{2+}$ ,  $\text{Al}^{3+}$  and  $\text{F}^-$  and minor amounts of many other ions. So can we define the property called ‘chemical formula’ as an intrinsic property for all tremolite as distinct from a specific specimen of tremolite? The simple answer is no. However, if we define an end-member formula for tremolite, all amphiboles with chemical compositions which have that end-member tremolite formula as their dominant end-member constituent have the same intrinsic property: their dominant end-member formula and  $Z$  (the number of formula units in the unit cell). If a tremolite sample is reacting with its environment and its chemical composition changes,





**Fig. 1.** The crystal structures of (a) enstatite (Gatta *et al.*, 2007); (b) clinoenstatite (Tribaudino *et al.*, 2002); (c) khinite-4O (Cooper *et al.*, 2008); (d) khinite-3T (Burns *et al.*, 1995). Fe/Mg polyhedra (orange), Si tetrahedra (pink), Cu polyhedra (blue), Te polyhedra (green), Pb (grey) and O (red). Unit cells are outlined in black.

then chemical composition cannot be an intrinsic property. However, provided its space group and value of  $Z$  do not change, its dominant end-member formula does not change and it remains tremolite; thus its dominant end-member formula is an intrinsic property even though its chemical composition is not.

### Bond topology of the end-member structure

Bond topology may differ from place to place (locally) in a structure with the incorporation of defects and/or vacancies and the occurrence of short-range order (local structure). Again, how do we define bond topology as an intrinsic property for all tremolite? We define it as the bond-topology of the long-range structure of end-member tremolite in which there are no vacancies (except those intrinsic to the end-member formula) and no defects. The structures of samples of tremolite will have the same long-range bond topology which we derive from crystal-structure refinement because defects and short-range atom arrangements are averaged out in the diffraction process.

### Extrinsic properties of a mineral

What are extrinsic properties of a mineral? Refractive index (dependent on the wavelength of light illuminating the crystal), density (dependent on the value of gravitational acceleration at

the location of the mineral), unit-cell volume (dependent on ambient temperature and pressure). There are many more extrinsic properties of a mineral, but those listed here give a flavour of the differences between intrinsic and extrinsic properties.

### Universals

A *universal* is an entity that is common to all objects in a particular set. Let us consider the entity to be a specific property of those objects, and let those objects be minerals. Can we define a set of universals that is common to all minerals? It seems logical to consider only intrinsic properties of these minerals as capable of belonging to this set, as extrinsic properties will vary with changes in ambient environment. From the above discussion, the intrinsic properties that are characteristic of a mineral species are: dominant end-member chemical formula and  $Z$ , space group, and bond topology of the end-member structure. All that remains to add is the mineral name, another intrinsic property that is common to all minerals of this species. These properties, in combination, are *sufficient to uniquely identify the mineral and distinguish it from all other mineral species*.

### The archetype of a mineral

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: mineral name, end-member chemical formula and Z, space group, and bond topology of the end-member structure. 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, with compositional boundaries that limit the range of its chemical composition and arise automatically from the set of end-member compositions consistent with the space-group symmetry, Z and the bond topology of the end-member structure.

### The IMA–CNMNC

First, we emphasise that this paper is not an official publication of IMA–CNMNC; it expresses the views only of the authors. The intent is to rigorously define the meaning of the term *mineral species*. Up until now, the IMA–CNMNC has operated without such a formal definition and hence all of its decisions have necessarily been made on an ad hoc basis. However, we do not suggest that the IMA–CNMNC immediately change all of its procedures in response to this new definition. Such changes need careful consideration with regard to their practical application.

Polytypes, polytypoids and topologically similar polymorphs have different bond topologies and are characterised by different space groups. As space groups are intrinsic properties defining the archetypes of minerals, these phases are distinct mineral species. However, the IMA–CNMNC does not define polytypes, polytypoids or topologically similar polymorphs as distinct mineral species (Nickel and Grice, 1998). Polytypes, polytypoids and topologically similar polymorphs are difficult to distinguish without characterisation by crystal-structure solution and refinement. Thirty years ago, approval of a mineral species did not require crystal-structure solution/refinement, practically excluding polytypes, polytypoids and topologically similar polymorphs as distinct minerals. Since then, current practice has changed and crystal-structure solution and refinement is generally required for approval of a new mineral species, suggesting that the mineralogical community has the instrumental capability to characterise polytypes, polytypoids and topologically similar polymorphs as new minerals.

Above, we have shown that minerals with the same chemical formula and space group but different magnetic space groups are distinct mineral species. However, magnetic structure is commonly very sensitive to grain size and minor-to-trace constituents, and defining distinct minerals on the basis of magnetic space group may not currently be a practical proposition. However, this is something that the IMA–CNMNC could investigate in more detail in the future, particularly as Earth Sciences expands its activities to non-terrestrial environments.

### Summary

- (1) An *intrinsic* property is a property that is characteristic of an object itself and is independent of anything else.
- (2) An *extrinsic* property is a property that depends on the relation between an object and other things.
- (3) A *universal* is an entity that is common to all objects in a particular set.
- (4) An *archetype* is a pure form which embodies the fundamental characteristics of a thing.

- (5) Key intrinsic properties of a mineral species are its name, its dominant end-member formula and Z (the number of formula units in the unit cell), its space group, and the bond topology of the end-member structure.
- (6) The intrinsic properties in (5) constitute a set of universals that are associated with the archetype of a mineral species.
- (7) Real mineral samples corresponding to this archetype are imperfect copies of that archetype, with structural defects, short-range order and a range of chemical compositions defined by the boundaries between end-member compositions of this and other end members with the same bond topology.
- (8) From the above points (1)–(7), we have a formal definition of a mineral species: A specific mineral species is the set of imperfect copies of the corresponding archetype and is defined by the following set of universals: mineral 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.

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