Revision 1

Fractal distribution of mineral species among the crystallographic point groups

Daniel R. Hummer

School of Earth Systems and Sustainability, Southern Illinois University, Carbondale, IL 62901

Key words: fractals, point groups, crystal systems, symmetry, crystallography, mineral species

Abstract

Crystallographic data from 5289 IMA-approved mineral species in the RRUFF database were used to examine the distribution of species among the 32 crystallographic point groups. It is found that within each crystal system, minerals strongly prefer point groups with higher group orders. Within a crystal system, the abundance of minerals belonging to each point group approximately obeys a power law with respect to group order, the same mathematical formalism that describes objects with fractal geometry. In this framework, each crystal system has its own fractal dimension; crystal systems possessing 3 (or 6)-fold symmetry elements (i.e., trigonal, hexagonal, isometric) have significantly lower fractal dimension (< 2), while those with only 1, 2, or 4-fold symmetry elements (triclinic, monoclinic, orthorhombic, tetragonal) have higher fractal dimension (> 2). While higher symmetry is preferred within a crystal system, the opposite trend is observed when comparing between crystal systems, with more species preferring crystals systems with lower order symmetry elements than those with higher order symmetry elements at constant group order. The combination of these two competing trends leads to a complex distribution of minerals among the crystal systems, and to the monoclinic group 2/m, the orthorhombic group 2/m2/m2/m, and the triclinic group $\bar{1}$ being the three most popular point groups, respectively. The fractal behavior of symmetry distribution among minerals points toward universal scaling patterns not just in physical, geometric objects, but also in the way that symmetry is incorporated into natural periodic structures.

Introduction

Students of crystallography will recall that rotational symmetry elements can be combined in 32 unique, self-consistent ways (that are also consistent with the translational symmetry of a periodic structure), and these distinct ways comprise the 32 crystallographic point groups. These point groups can be further grouped according to their highest order symmetry axis into seven distinct crystal systems (Fig. 1): Triclinic (1-fold axis), monoclinic (a single 2-fold axis), orthorhombic (three orthogonal 2-fold axes), trigonal/rhombohedral (a single 3-fold axis), tetragonal (a single 4-fold axis), hexagonal (6-fold axis), and isometric/cubic (four 3-fold axes). Although the trigonal system is sometimes consolidated into the hexagonal system due to the similar construction of their crystallographic axes, in this contribution we will consider them as separate crystal systems for reasons that will later become apparent.

It has long been known that some symmetry groups are greatly more populated than others, and that crystal structures have a strong preference for the so-called holohedral group (i.e., the group with highest symmetry) within each crystal system (Novatskii 1949; Mackay 1967; Urusov 2007). In contrast, the most sparsely populated groups among inorganic crystal structures tend to have low symmetry (Urusov and Nadezhina 2006). The tendency towards higher symmetry point groups and space groups is so pervasive that many of the most common mistakes in the analysis of new crystal structures involve erroneously assigning a structure to a lower symmetry subgroup of the structure’s true symmetry (Baur and Tillmanns 1986; Baur and Kassner 1992; Marsh 1994, 1999; Marsh and Herbstein 1988; Herbstein and Marsh 1998; Marsh et al. 2002; and many others). Especially common is the mistake of assigning a structure to a non-centrosymmetric space group when the true space group is centrosymmetric (Baur and Tillmanns 1986; Hu 2000, 2001; Marsh 1994,1999; Marsh et al. 2002).

An extensive analysis of space group frequencies for 164,146 natural and synthetic inorganic crystal structure records by Urusov and Nadezhina (2009) yielded only 24 space groups with populations >1%, and 20 of these space groups belonged to holohedral point groups. The five most populous space groups in descending order were *Pnma* (point group 2/m2/m2/m), $P2_1/c$ (point group 2/m), $Fm\bar{3}m$ (point group 4/m-32/m), $P\bar{1}$ (point group $\bar{1}$), and *C*2/*c* (point group 2/m), representing the holohodral point groups of the triclinic, monoclinic, orthorhombic, and isometric systems. These results reinforce the idea that within a crystal system, crystal structures strongly prefer the point group of highest symmetry. However, beyond this qualitative trend, there has been very little work quantifying the entire distribution of known crystal structures across symmetry groups (a notable exception being Mackay 1967). In particular, although there has been some attention to inorganic vs. organic materials (Novatskii 1949; Mackay 1967; Podbereszkaya 2006), very little work has distinguished between synthetic materials and natural mineral species (Urusov and Nadezhina 2006), and no work the author is aware of has examined the distribution of structures at the point group level.

Since grouping data into higher organizational levels provides enhanced counting statistics, and very often reveals trends that are not visible at more particulate levels of analysis, it is worthwhile to examine the distribution of symmetry in minerals when organized by point group symmetry. In this contribution, the complete distribution of natural mineral phases as of 18 May, 2020 is quantitatively examined at the level of the 32 crystallographic point groups. The quantitative trends of point group symmetries within and between the seven crystal systems are examined and discussed, particularly in the context of fractal behavior. The implications of these results for the distribution of symmetry in natural crystalline materials, the discovery and characterization of new crystal structures, and extrapolating the behavior of mineral symmetry in the universe as a whole, is also discussed.

Methods

The database of IMA-approved mineral species at www.rruff.info maintained at the University of Arizona (Downs 2006; Hazen et al. 2019) was searched as of 18 May, 2020. At the time of data acquisition, a total of 5564 species were listed in the database. However, only 5289 of these species had crystal structures that were characterized well enough to unambiguously identify the point group to which they belong, and therefore only these species were used in the following analysis. The reason for focusing on mineral species as opposed to other possible sets of crystalline compounds is that minerals, by definition, include nearly all naturally occurring crystalline materials. Since the goal of this study is to examine symmetry distributions in nature, the complete set of known mineral species comprises the ideal data set. Although a wide variety of other organic and inorganic synthetic crystalline compounds could certainly be included in such a study, including such materials would skew the results away from the symmetry that is naturally generated in geologic settings, and towards some unknown subset of the physically feasible crystal structures.

For each of the 32 crystallographic point groups, the number of mineral species belonging to that group was tallied. Each group was also categorized as belonging to one of the seven crystal systems (triclinic, monoclinic, orthorhombic, tetragonal, trigonal, hexagonal, or isometric) according to its highest order symmetry elements (Fig. 1). To avoid confusion, throughout this text we use the full, unabbreviated Hermann-Mauguin notation (Burzlaff and Zimmermann 2006) for each point group (i.e., 2/m2/m2/m rather than 2/mmm). The group order (i.e., the complete number of unique symmetry operators in each point group) was also tabulated, and the base 2 logarithm of each group order was calculated. The number 2 is a convenient and natural choice of base since many point groups have orders that are an integral power of 2.

To examine fractal behavior, the abundance of mineral species in each point group within a crystal system was considered a function of the group order. Each crystal system was fit to the following power law equation:

$$N = 2^{b} G^{D} \qquad (1)$$

or in logarithmic format,

$$\log_2 N = D \log_2 G + b \qquad (2)$$

in which N is the number of mineral species in a point group, G is the group order, *D* is the fractal dimension (also known as the Hausdorff dimension), and *b* is a dimensionless constant representing the number of minerals belonging to a hypothetical point group of order 1 (Hausdorff 1918; Duvall et al. 2000). It can be easily seen from Eq. 2 that a log-log plot of group order (G) vs. number of species (N) should yield a linear relationship if fractal behavior is obeyed, with a slope of *D* and a y-intercept of *b*.

Results

Analysis of mineral totals for each crystal system confirmed the well-established observation that the monoclinic system is by far the most populated crystal system, with 1784 mineral representatives (about 34% of the mineral kingdom). Following that are orthorhombic, trigonal, triclinic, isometric, hexagonal, and tetragonal, respectively (Table 1, Fig. 2). One reason for including trigonal as its own crystal system is apparent in these results: The trigonal system contains an impressive 666 mineral representatives, even surpassing the total for the fully hexagonal point groups.

When the crystal systems are broken down by individual point groups, another well-known trend is apparent: Minerals have a strong preference for the holohedral point group within each crystal system ($\bar{1}$, 2/m, 2/m2/m2/m, $\bar{3}2/m$, 4/m2/m2/m, 6/m2/m2/m, and $4/m\bar{3}2/m$). Point group 2/m leads the pack with 1534 minerals, followed by 2/m2/m2/m and $\bar{1}$ (Table 2), in reasonably good agreement with the most frequent space groups found by Urusov and Nadezhina (2009). However, a previously unobserved trend is seen when point group populations are considered as a function of group order: there is an approximate log-log linear relationship within each crystal system, equivalent to the power law expressed in Eq. 1. A least squares regression was therefore performed for each crystal system fitting Eq. 2, the logarithmic form of the power law, to the data in Table 2. The parameters of the best fit lines are shown in Table 3 and plotted in Fig. 3. In general, as the symmetry and the number of point groups increases, the R^2 value of the regression decreases from near perfect values to more modest values, and finally to 0.35 for the isometric system. However, it should be noted that the very high R^2 values for the triclinic, monoclinic, and orthorhombic systems are not particularly meaningful since these systems have only 2 or 3 data points. Thus, while there is evidence that the power law relationship is clearly observed in every crystal system, it is only approximate and certainly not a strictly quantitative relationship.

While higher symmetry is preferred within a crystal system, the opposite trend appears when comparing between crystal systems, but only when comparing along constant group order. The power law relationships for the seven crystal systems are vertically stratified such that at constant group order, minerals prefer crystal systems in the order triclinic > monoclinic > orthorhombic > trigonal > tetragonal > hexagonal > isometric (Fig. 3). Note that this ordering strictly adheres to a sequence from least symmetry to most symmetry, and is somewhat different than the ordering obtained from the raw totals shown in Table 1 and Fig. 2. This is due to the fact that although high symmetry crystal systems (such as hexagonal and isometric) may be the least preferred at *constant* group order, they contain point groups that reach *higher* group order than lower symmetry crystal systems.

Thus, an alternative way to interpret the trend between crystal systems in Fig. 3 is to compare crystal systems horizontally, across group order. Higher symmetry systems contain higher order symmetry elements, and therefore contain higher order point groups. These higher order point groups (with exponentially higher populations) help counteract the overall lower popularity of these high symmetry crystal systems. It is the tight competition between these two clear but opposing trends that leads to the enigmatic and seemingly random distribution of minerals among the seven crystal systems observed in Fig. 2. So while it’s accurate to say that lower symmetry systems are preferred at constant group order, it is equally accurate to say that each crystal system has a similar (fractal) distribution of minerals among its point groups, but that higher symmetry systems are shifted toward higher group order (Fig. 3). The alternative ways of viewing this trend makes the physical interpretation unclear, but it is inarguable that the two opposing trends apparent in these data creates competition between the seven crystal systems.

It should be noted that although tetragonal symmetry is listed as being preferable to hexagonal symmetry (when comparing at constant group order), there is ambiguity in this ordering. The trend lines for the tetragonal and hexagonal systems cross each other at a value within the range of group orders for both systems (Fig. 3), such that hexagonal symmetry is actually preferred at low group order but tetragonal symmetry is preferred at higher group order. Interestingly, the combination of lower vertical position, stronger slope, and degree of scatter for the tetragonal trend leads to all three of the least populous point groups being low order tetragonal groups (4, 4mm, and $\bar{4}$, respectively). Point group 4 contains only four mineral representatives (gwihabaite, percleveite-(Ce), pinnoite, piypite), point group 4mm contains only eight representatives (including the common sorosilicate vesuvianite), and point group $\bar{4}$ contains only nine representatives, among them the rare fluorescent and phosphorescent species tugtupite (whose popularity among mineral collectors apparently makes up for the lack of popularity of its structure's symmetry).

It is apparent from the trends in Fig. 3 that the slopes for the trigonal, hexagonal, and isometric systems are substantially smaller than those for the other four crystal systems. Indeed, the regressions in Table 3 show that the trigonal, hexagonal, and isometric systems have lower fractal dimension (1.19, 1.25, 1.43, respectively) than the triclinic, monoclinic, orthorhombic, and tetragonal systems (2.75, 3.62, 2.31, 2.48, respectively). It is likely not a coincidence that the crystal systems that include 3- or 6-fold symmetry elements all have fractal dimension $D < 2$, while those that lack these symmetry elements all have $D > 2$. Apparently, having these higher order non-binary symmetry elements actually reduces a crystal system's ability to scale up its structural abundance with respect to group order.

Implications

Self-similar geometric objects with fractal geometry look the same at different spatial scales (Mandelbrot 1982), and obey a scaling law of the form $N = M^D$, where N is the number of smaller object copies within a larger copy, M is the spatial magnification factor between smaller and larger copies, and D is the fractal dimension (Hausdorff 1918; Duvall et al. 2000). In such an object, we can therefore think of this power law as the object "copying" itself by a factor N using a special kind of symmetry operation, which in fractal objects happens to be magnification by a factor of M, and *D* is the number of "dimensions" through which this magnification factor is applied (Duvall et al. 2000).

Similarly, applying this analogy to types of crystalline symmetry via Eq. 1, we can envision that each point group "copies" or "populates" itself with a number of minerals "N" representing the variety of possible structures that conform to that type of symmetry. This variety of minerals is achieved by utilizing a symmetry operator G (which is itself the number of actual, spatial symmetry operations contained in the group), and applying this "symmetry richness" operator across *D* "symmetry dimensions". Apparently, there is a trade-off between the types of physical symmetry elements a point group contains, and the number of "symmetry dimensions" through which those symmetry elements allow a point group to accommodate physically feasible crystalline structures. Thus, the crystal systems containing 3- or 6-fold symmetry elements having non-binary order (trigonal, hexagonal, isometric) have a fractal "symmetry dimension" restricted to $D < 2$. In contrast, the crystal systems containing physical symmetry elements with orders based on the binary numbers 1, 2, and 4, whose geometries are perhaps more naturally suited to our universe's three orthogonal spatial dimensions (triclinic, monoclinic, orthorhombic, tetragonal), seem to have room for a fractal "symmetry dimension" of $D > 2$, allowing them to leverage their tool kit of symmetry operators to accommodate greater structural variety. It should be noted that symmetry groups are mathematical constructs and obviously don't play an active role in "creating" crystal structures - rather, the structures of lowest free energy form in nature and possess a particular symmetry. However, viewing the populations of each point group as being generated in the fashion described above helps us make sense of the fractal patterns observed in this study.

It is intriguing that nature apparently prefers higher symmetry when we focus within one crystal system, and yet simultaneously prefers lower symmetry when we compare different crystal systems. Evidently, nature is able to produce a greater variety of physically feasible crystalline structures using an abundance of simple symmetry elements as opposed to a few complex symmetry elements. One practical consequence of these trends is that when analyzing new crystal structures, it is a better strategy to specifically search for and then rule out symmetry elements rather than assume their absence. Crystallographers should be using diffraction data to specifically test for particular symmetry elements, similar to approaches advocated by Baur and Tillamns (1986). The results in this work indicate this is likely a good rule of thumb for many types of symmetry, though crystallographers know it is particularly true for the center of symmetry (Hu 2000, 2001; Marsh 1994,1999; Marsh et al. 2002). According to an analysis of published structures, about 3% of new structures are misclassified as belonging to a lower symmetry space group than their true symmetry, and a majority of these were placed in a non-centrosymmetric space group when they are in fact centrosymmetric (Baur and Tillmanns 1986).

An important caveat in considering these results is that we are not necessarily counting the population of each point group properly for the purpose at hand, which is to examine the symmetry distribution of natural crystalline structures. Two important factors influence the way in which materials are counted. First, our sampling is obviously biased towards crystalline structures that occur on Earth. While the > 5000 recognized mineral species are certainly a statistically healthy sample size, the great majority of these are native to Earth. It is always possible that other places in the cosmos are populated with mineral species that follow a somewhat different distribution of symmetry for any number of reasons, including different chemical compositions and ranges of pressure/temperature conditions that could favor different structure types. Additionally, consideration of other sets of crystalline compounds (such as protein crystals or synthetic inorganic compounds) could obviously yield a substantially different distribution of symmetry. For example, organic structures tend to have fewer mirror planes and proper rotation axes (Wilson 1988), which would likely produce a distribution with far less emphasis on holohedral point groups.

We also know that even symmetry distributions restricted to Earth are very likely time-dependent. Krivovichev et al. (2018) recently analyzed the chemical and structural complexity of mineral groups from four different stages of mineral evolution (Hazen et al. 2008), and found that both increased over geologic time. Since chemical complexity strongly correlates with lower symmetry (Krivovichev and Krivovichev 2020), this indicates that Earth started out with mostly higher symmetry minerals, and added lower symmetry minerals over time without replacing the early high symmetry structures. Thus, the fractal dimension of each crystal system (as calculated from the slopes in Fig. 3) likely started at a higher value and decreased over time as lower order point groups became more populated relative to higher order groups. The present distribution of mineral symmetries therefore represents a snapshot in time, and is capable of evolving on a geologically active planet.

Second, the very definition of the mineral “species” we are counting influences the results. The IMA defines a mineral species in terms of a unique combination of nominal chemical composition and crystalline structure (Nickel and Grice 1998), but this means we are counting chemically unique substances rather than crystalline structures. For example, the garnet group contains 14 different mineral species according to the IMA definition (Grew et al. 2013), but because all garnets are isostructural, this group represents only one unique arrangement of atoms in the mathematical sense. A method based on counting IMA-approved mineral species therefore biases the data set in favor of structures that happen to accommodate a wide range of end-member compositions within Earth's bulk composition. In contrast, alternative mineral classification systems have already been proposed that cluster minerals based on "natural kinds" using parameters such as mode of occurrence, morphology, size, chemical and isotope signatures, etc. in addition to chemistry and structure (Hazen 2019; Hazen and Morrison 2020; Morrison and Hazen 2020). Such systems could result in either grouping or splitting of the traditional IMA-defined species depending on circumstances (Hazen 2019), altering the way in which natural materials are counted toward each symmetry group.

However minerals are counted, the competing trends observed in this study clearly highlight an important role for both the nature and number of symmetry elements in a point group in creating the variety of physically possible periodic structures in our universe. The underlying fractal behavior of the mineral kingdom's structural variety reveals to us that dimensional scaling laws apply not only to the actual symmetry of physical objects, but also in a more abstract sense to the very way in which physical symmetry generates such a rich variety of naturally occurring materials. Future work should focus on further exploring and quantifying these trends in other sets or subsets of crystalline materials to determine how universal these trends truly are.

Acknowledgments

This work was made possible by the searchable RRUFF mineral database at www.rruff.info maintained by Robert T. Downs at the University of Arizona, which includes the IMA database of mineral species. The author also thanks Patrick J. Hummer, whom I bribed with a cookie, for assistance with the statistics utilized in this study.

References

Baur, W.H., and Kassner, D. (1992) The perils of *Cc*: Comparing the frequencies of falsely assigned space groups with their general population. Acta Crystallographica B, 48, 356-369.

Baur, W.H., and Tillmanns, E. (1986) How to avoid unnecessarily low symmetry in crystal-structure determinations. Acta Crystallographica B, 42, 95-111.

Brown, T.L., LeMay, H.E., Bursten, B.E., Murphy, C., Woodward, P., Stoltzfus, M.E. (2015) *Chemistry: The Central Science, 13th Ed*., xxx p. (Chapter 12) Pearson Education, London.

Burzlaff, H., and Zimmermann, H. (2006) Space-group symbols. In: Hahn, Th. (Ed.), International Tables for Crystallography Volume A: Space-group symmetry. Springer, Netherlands, pp. 821–822. (Chapter 12.2).

Downs, R.T. (2006) The RRUFF project: an integrated study of the chemistry, crystallography, Raman and infrared spectroscopy of minerals. In: Proceedings of the 19th General Meeting of the International Mineralogical Association; 2006 July 23–28; Kobe, Japan.

Duvall, P., Keesling, J., Vince, A. (2000) The Hausdorff dimension of the boundary of a self-similar tile. Journal of the London Mathematical Society, 61, 649-760.

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

Hausdorff, F. (1918) Dimension und äußeres Maß. Mathematische Annalen, 79, 157-179.

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

Hazen, R.M. (2019) An evolutionary system of mineralogy: Proposal for a classification of planetary materials based on natural kind clustering. American Mineralogist, 104, 810-816.

Hazen, R.M., and Morrison, S.M. (2020) Anevolutionary system of mineralogy. Part I: Stellar mineralogy (>13 to 4.6 Ga). American Mineralogist, 105, 627-651.

Hazen, R.M., Downs, R.T., Eleish, A., Fox, P., Gagné, O.C., Golden, J.J., Grew, E.S., Hummer, D.R., Hystad, G., Krivovichev, S.V., Li, C., Liu, C., Ma, X., Morrison, S.M., Pan, F., Pires, A.J., Prabhu, A., Ralph, J., Runyon, S.E., Zhong, H. (2019) Data-driven discovery in mineralogy: Recent advances in data resources, analysis, and visualization. Engineering, 5, 397-405.

Herbstein, F.H., and Marsh, R.E. (1998) More space group corrections: From triclinic to centered monoclinic, and to rhombohedral; Also from $P1$ to $P\bar{1}$ and from Cc to $C2/c$. Acta Crystallographica B, 54, 677-686.

Hu, S.Z. (2000) On the incorrect assignment of space groups – IV. Monoclinic system: From non-centrosymmetric to centrosymmetric. Chinese Journal of Structural Chemistry, 19, 234-238.

Hu, S.Z. (2001) On the incorrect assignment of space groups V. Revisions of non-centrosymmetric to centrosymmetric structure without changing crystal system. Chinese Journal of Structural Chemistry, 20, 151-156.

Krivovichev, S.V., Krivovichev, V.G., Hazen, R.M. (2018) Structural and chemical complexity of minerals: correlations and time evolution. European Journal of Mineralogy, 30, 231-236.

Krivovichev, S.V., Krivovichev, V.G. (2020) The Fedorov-Groth law revisited: complexity analysis using mineralogical data. Acta Crystalloraphica A, 76, 429-431.

Mackay, A.L. (1967) The statistics of the distribution of crystalline substances among the space groups. Acta Crystallographica, 22, 329-330.

Mandelbrot, B.B. (1983) *The Fractal Geometry of Nature*, 18-19 p., Freeman, New York.

Marsh, R.E. (1994) The centrosymmetric-noncentrosymmetric ambiguity – some more examples. Acta Crystallographica A, 50, 450-455.

Marsh, R.E. (1999) $P1$ or $P\bar{1}$? Or something else? Acta Crystallographica B, 55, 931-936.

Marsh, R.E. and Herbstein, F.H. (1988) More space group changes. Acta Crystallographica B, 44, 77-88.

Marsh, R.E., Kapon, M., Hu, S.Z., Herbstein, F.H. (2002) Some 60 new space-group corrections. Acta Crystallographica B, 58, 62-77.

Morrison, S.M., and Hazen, R.M. (2020) An evolutionary system of mineralogy. Part II: Interstellar and solar nebula primary condensation mineralogy (> 4.565 Ga). American Mineralogist, 105, in press.

Novatskii, N. (1949) Supplement to the Translation of *“Stereochemistry”by P. Niggli*, IL, Moscow [in Russian].

Nickel, E.H., and Grice, J.D. (1998) The IMA commission on new minerals and mineral names: Procedures and guidelines on mineral nomenclature, 1998. The Canadian Mineralogist, 36, 3-16.

Podberezskaya, N.V. (2006) *Chemistry, Symmetry, Geometry of Crystals*. In: Vestnik Nizhegorodskogo Universiteta, Ser. Fiz. Tverd. Tela, 1(9), 24 [in Russian].

Urusov, V.S., and Nadezhina T.N. (2006) Empty and sparse spatial groups in structural mineralogy. Vest. Mosk. Gos. Univ., Ser. Geol., 6, 52–59.

Urusov, V.S. (2007) Symmetry statistics of mineral species and the evolutionary dissymmetrization of mineral matter. Geology of Ore Deposits, 49, 497-504.

Urusov, V.S., and Nadezhina, T.N. (2009) Frequency distribution and selection of space groups in inorganic crystal chemistry. Journal of Structural Chemistry, 50 (Supplement), S22-S37.

Wilson, A.J.C. (1988) Space groups rare for organic structures. I. Triclinic, monoclinic, and orthorhombic crystal classes. Acta Crystallographica A, 44, 715-724.

Table 1: Number of mineral species and percentage of mineral species belonging to each of the seven crystal systems for 5289 minerals with determined crystal structures in the RRUFF mineral database as of 18 May, 2020.

Crystal System	**Number of species**	**%**
Triclinic	571	10.8
Monoclinic	1784	33.7
Orthorhombic	1020	19.3
Tetragonal	375	7.1
Trigonal	666	12.6
Hexagonal	384	7.3
Isometric	489	9.2
Total	**5289**	**100.0**

Table 2: Hermann-Mauguin designation, crystal system, group order, and number of mineral species of the 32 crystallographic point groups for 5289 minerals with determined crystal structures in the RRUFF mineral database as of 18 May, 2020. (A standard $\sqrt{N}$ error from counting statistics was used for the number of species.)

Point group (H-M)	Crystal System	Group order	Number of Species
1	Triclinic	1	74
-1	Triclinic	2	497
2	Monoclinic	2	120
m	Monoclinic	2	130
2/m	Monoclinic	4	1534
222	Orthorhombic	4	100
2mm	Orthorhombic	4	206
2/m2/m2/m	Orthorhombic	8	714
4	Tetragonal	4	4
-4	Tetragonal	4	9
4/m	Tetragonal	8	75
422	Tetragonal	8	24
4mm	Tetragonal	8	8
-42m	Tetragonal	8	61
4/m2/m2/m	Tetragonal	16	194
3	Trigonal	3	53
-3	Trigonal	6	124
3m	Trigonal	6	150
32	Trigonal	6	62
-32/m	Trigonal	12	277
6	Hexagonal	6	48
-6	Hexagonal	6	10
6/m	Hexagonal	12	72
6mm	Hexagonal	12	59
622	Hexagonal	12	26
-62m	Hexagonal	12	33
6/m2/m2/m	Hexagonal	24	136
23	Isometric	12	38
432	Isometric	24	11
-43m	Isometric	24	97
2/m-3	Isometric	24	69
4/m-32/m	Isometric	48	274

Table 3: Fit parameters for the least squares regression of point group population/order data to the power law N = 2^b G^D, where N = number of species, 2^b is the scaling constant, G is the group order, and *D* is the fractal dimension. (Numbers in parentheses indicate 1σ errors in the final digits of the parameter value – no error estimates were possible for the triclinic regression since there were only two data points)

Crystal System	No. groups	R^2	*b*	*D*
Triclinic	2	1.000	6.21	2.75
Monoclinic	3	0.999	3.35 (14)	3.62 (10)
Orthorhombic	3	0.868	2.54 (215)	2.31 (90)
Tetragonal	7	0.707	-2.43 (209)	2.48 (71)
Trigonal	5	0.749	3.71 (106)	1.19 (40)
Hexagonal	7	0.519	1.09 (189)	1.25 (54)
Isometric	5	0.346	-0.63 (524)	1.43 (113)

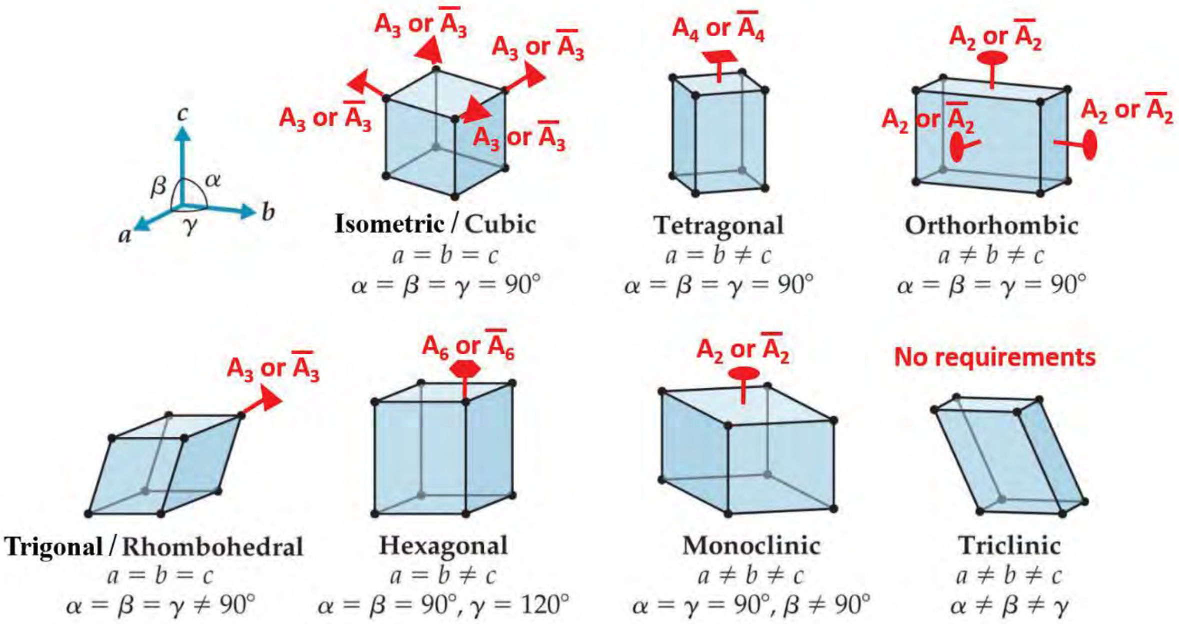
Figure Captions

Figure 1: Illustration of the seven crystal systems, the relationships between their crystallographic axes (below each name), and their minimum symmetry requirements (in red). a, b, and c refer to the lengths of the crystallographic axes; α, β, and γ refer to the interaxial angles (as shown in upper left); A_n and $-A_n$ refer to n-fold rotation axes and n-fold axes of rotoinversion, respectively. Note that in the axes descriptions, the "$\neq$" sign does not necessarily mean "unequal to", but instead means "not constrained to be equal to". (modified from Brown et al. 2015)

Figure 2: Bar chart of the number of mineral species belonging to each of the seven crystal systems for 5289 minerals with determined crystal structures in the RRUFF mineral database as of 18 May, 2020.

Figure 3: Log-log plot of group order vs. number of mineral species for the 32 crystallographic point groups. Symbols represent the crystal system to which each point group belongs (red right triangles = triclinic; orange parallelograms = monoclinic; yellow rectangles = orthorhombic; blue equilateral triangles = trigonal; green squares = tetragonal; purple hexagons = hexagonal; black circles = isometric). Correspondingly colored lines represent the best fit power law for each crystal system using a least squares regression. Each point group is labeled with its Hermann-Mauguin notation. Vertical error bars represent a standard $\sqrt{N}$ error from counting statistics plotted in log-space; error bars not shown are smaller than the symbol. No horizontal error bars are shown since the group order is a fixed, errorless parameter unique to each group.

Figure 1



c
β
α
a
γ
b
A_3 or $\overline{A}_3$
A_3 or $\overline{A}_3$
A_3 or $\overline{A}_3$
A_3 or $\overline{A}_3$
Isometric / Cubic
$a = b = c$
$\alpha = \beta = \gamma = 90°$
A_4 or $\overline{A}_4$
Tetragonal
$a = b \neq c$
$\alpha = \beta = \gamma = 90°$
A_2 or $\overline{A}_2$
A_2 or $\overline{A}_2$
A_2 or $\overline{A}_2$
Orthorhombic
$a \neq b \neq c$
$\alpha = \beta = \gamma = 90°$
A_3 or $\overline{A}_3$
Trigonal / Rhombohedral
$a = b = c$
$\alpha = \beta = \gamma \neq 90°$
A_6 or $\overline{A}_6$
Hexagonal
$a = b \neq c$
$\alpha = \beta = 90°, \gamma = 120°$
A_2 or $\overline{A}_2$
Monoclinic
$a \neq b \neq c$
$\alpha = \gamma = 90°, \beta \neq 90°$
No requirements
Triclinic
$a \neq b \neq c$
$\alpha \neq \beta \neq \gamma$

Figure 2

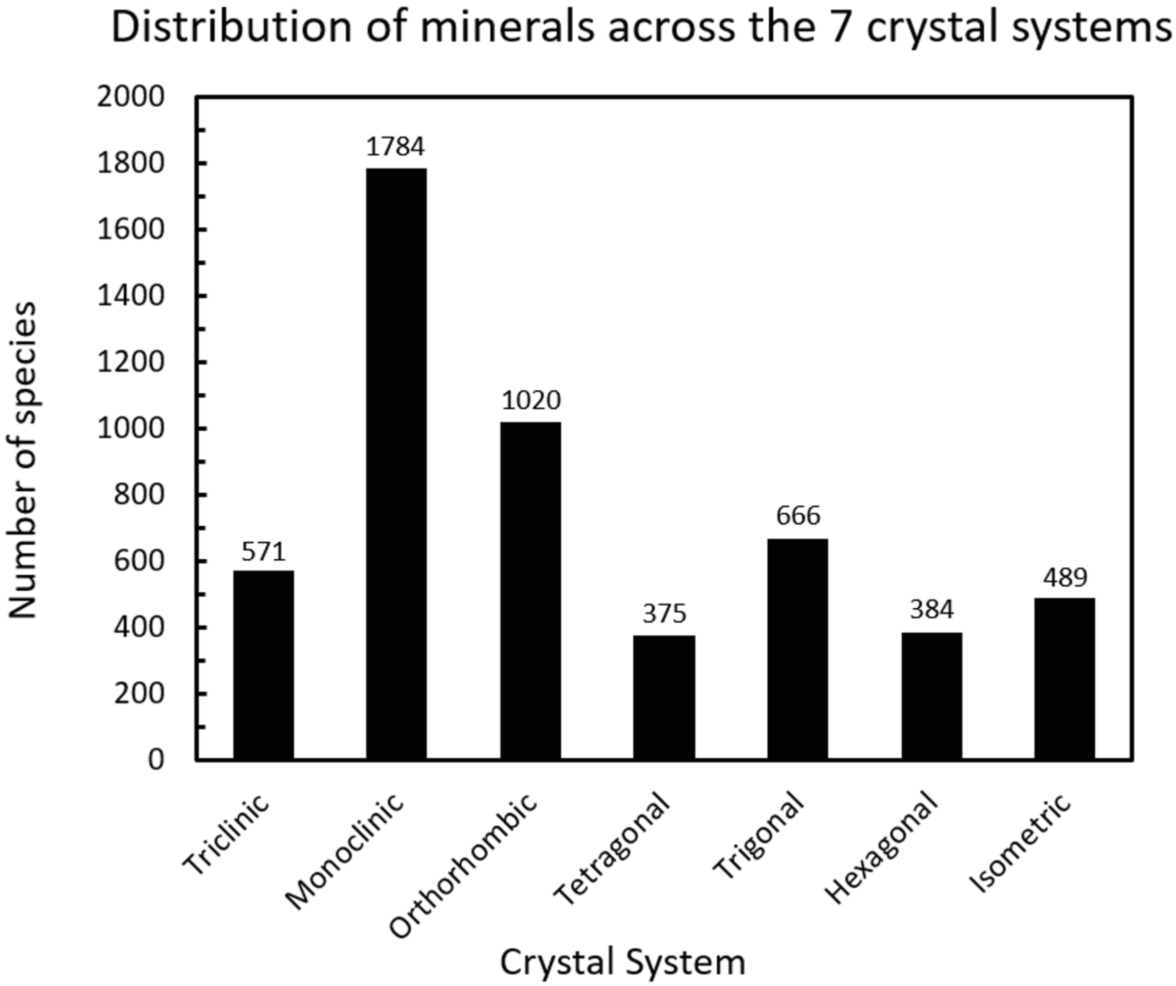
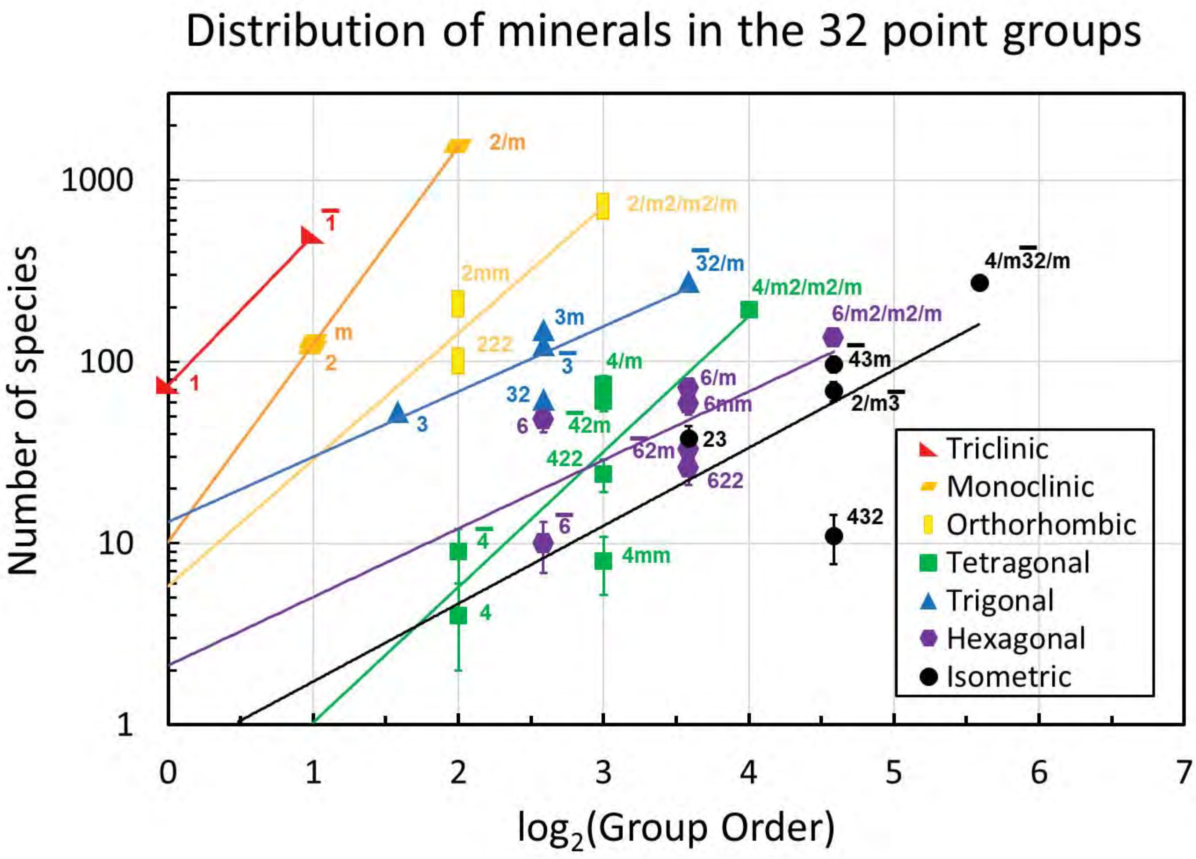
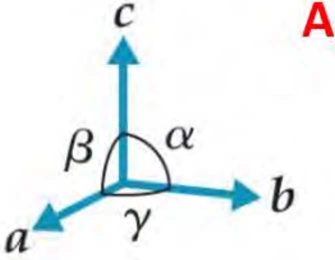
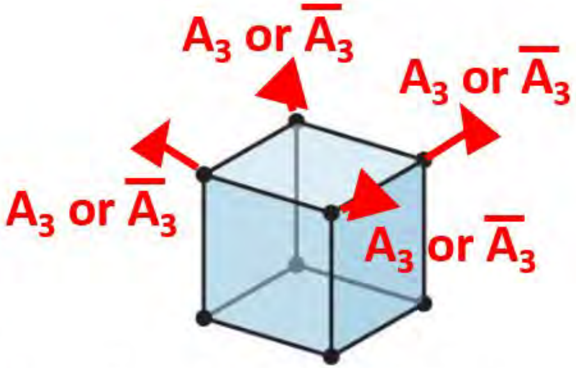

Distribution of minerals across the 7 crystal systems
Number of species
2000
1800
1600
1400
1200
1000
800
600
400
200
0
571
1784
1020
375
666
384
489
Triclinic
Monoclinic
Orthorhombic
Tetragonal
Trigonal
Hexagonal
Isometric
Crystal System

Figure 3


Distribution of minerals in the 32 point groups
Number of species
log$_2$(Group Order)
1000
100
10
1
0
1
2
3
4
5
6
7
2/m
2/m2/m2/m
$\bar{1}$
2mm
m
2
222
1
$\bar{3}$2/m
3m
$\bar{3}$
4/m
32
3
6
$\bar{4}$2m
422
4/m2/m2/m
6/m2/m2/m
6/m
6mm
$\bar{6}$2m
23
622
4/m$\bar{3}$2/m
$\bar{4}$3m
2/m$\bar{3}$
432
$\bar{4}$
$\bar{6}$
4
4mm
Triclinic
Monoclinic
Orthorhombic
Tetragonal
Trigonal
Hexagonal
Isometric

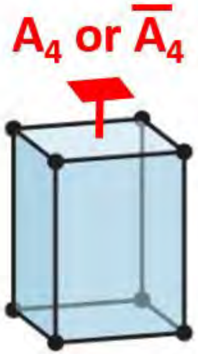




Isometric / Cubic

$a = b = c$

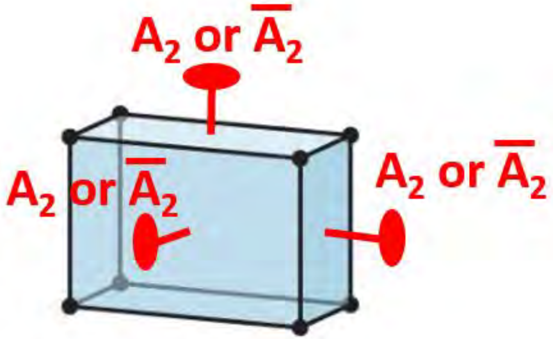
$\alpha = \beta = \gamma = 90^\circ$



Tetragonal

$a = b \neq c$

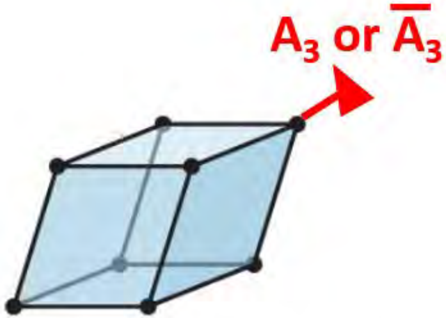
$\alpha = \beta = \gamma = 90^\circ$



Orthorhombic

$a \neq b \neq c$

$\alpha = \beta = \gamma = 90^\circ$



Trigonal / Rhombohedral

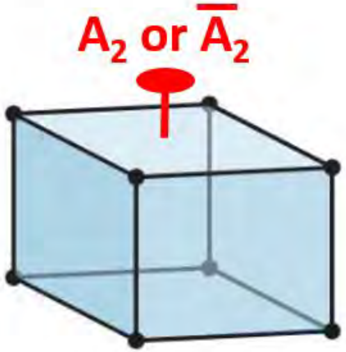
$a = b = c$

$\alpha = \beta = \gamma \neq 90^\circ$

Hexagonal

$a = b \neq c$

$\alpha = \beta = 90^\circ, \gamma = 120^\circ$



Monoclinic

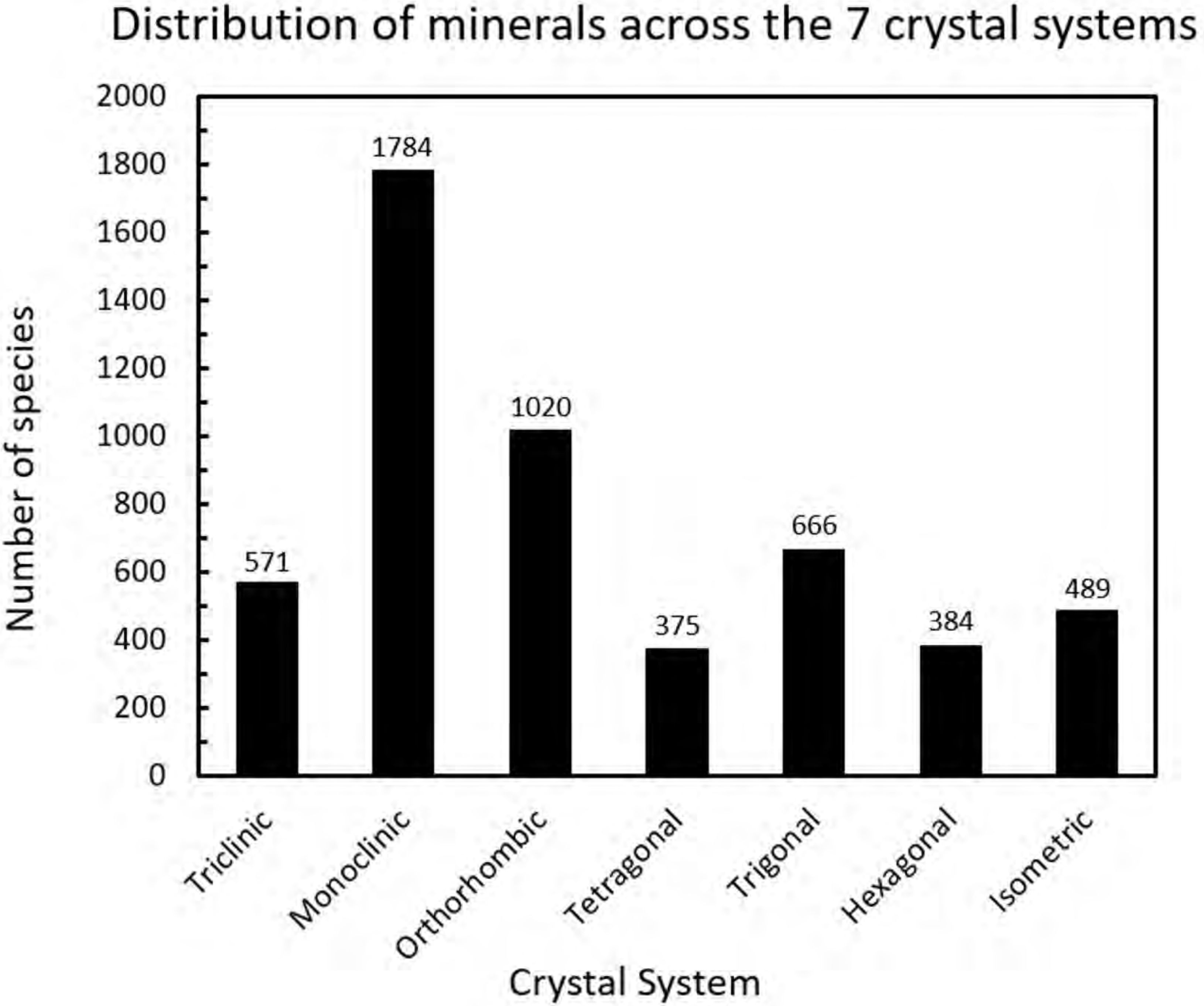
$a \neq b \neq c$

$\alpha = \gamma = 90^\circ, \beta \neq 90^\circ$

Triclinic

$a \neq b \neq c$

$\alpha \neq \beta \neq \gamma$


Distribution of minerals across the 7 crystal systems
Number of species
2000
1800
1600
1400
1200
1000
800
600
400
200
0
571
1784
1020
375
666
384
489
Triclinic
Monoclinic
Orthorhombic
Tetragonal
Trigonal
Hexagonal
Isometric
Crystal System

Distribution of minerals in the 32 point groups