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Characteristics of the distribution of minerals among the space groups

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Abstract

The RRUFF online database (a project by Robert Downs, University of Arizona) catalogs the occurrence of point and space group symmetries of over 4800 of the nearly 6000 currently accepted mineral species. Of these, over 90% are monomorphic, while the remaining species have been recognized to be polymorphic. To avoid issues of reliability and inconsistency of characterization, the 4499 monomorphic minerals are the subject of this analysis. It has long been recognized that minerals are non-uniformly distributed among the space groups as well as their corresponding point groups and crystal systems. However, this non-uniformity is not non-systematic. A random distribution of minerals among the space groups would result in an average of about 20 species per group. In fact, the observed distribution of minerals is highly skewed. Analysis of the frequency distribution of minerals among the space groups reveals three distinct populations: those without currently known monomorphic species (52), those sparsely populated by minerals that exhibit an exponential distribution of species abundances (170), and those most populous space groups (8) that are differentiated from the others by an inflection in the slope of the species frequency distribution. Additionally, a series of relationships have been identified, and they collectively characterize crystallographic controls on and resultant distributions of mineral occurrence. First, there is a strong preference across all crystal systems for minerals to exhibit structures associated with the holohedral space groups relative to those pedial groups of the lowest symmetry. Second, mineral species exhibit a strong preference for the Laue class space groups over their paired Sohncke groups. Furthermore, it is recognized that the space groups that make up the 11 enantiomorphic pairs are either sparsely populated or devoid of known mineral species. Third, the centering types of the Bravais lattices and structures defined by the Wyckoff multiplicities of the various space groups are recognized to strongly influence the distribution of mineral species such that more structurally and symmetrically complex space groups (those with non-primitive lattice structures) tend to be represented by more minerals. Fourth, when considering the 73 arithmetic space group classes, in most cases non-symmorphic space groups are more richly populated than their linked symmorphic space groups, and in those cases where both hemisymmorphic and asymmorphic space groups are present in the same arithmetic class, the asymmorphic space groups typically contain more species. Together, these observations and interpretations augment and advance previously achieved understandings of mineral frequency distributions among the point groups and imply four future lines of inquiry: extending consideration to polymorphic species as well as relating distributions among the space groups to terrestrial mineral species abundance, mineral chemistry, as well as the evolution of mineral chemistry and paragenesis.

Keywords: Space groups, point groups, crystal systems, mineral frequency, crystallography