Fractal distribution of mineral species among the crystallographic point groups

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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 threefold (or sixfold) symmetry elements (i.e., trigonal, hexagonal, isometric) have significantly lower fractal dimension (<2), while those with only one-, two-, or fourfold 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 $\bar{T}$ 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.

Keywords: Fractals, point groups, crystal systems, symmetry, crystallography, mineral species

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 (onefold axis), monoclinic (a single twofold axis), orthorhombic (three orthogonal twofold axes), trigonal/rhombohedral (a single threefold axis), tetragonal (a single fourfold axis), hexagonal (sixfold axis), and isometric/cubic (four threefold 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 toward 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$\bar{3}2/m$), $P\bar{T}$ (point group $\bar{T}$), and $C2/c$ (point group 2/m), representing the holohedral 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; Podberezskaja 2006), very little work has distinguished between synthetic materials and natural mineral species (Urusov and Nadezhina 2006), and no work the