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Which minerals are the most complex? Shannon-information-based study

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Which minerals are the most complex and how to quantify structural complexity of minerals? At present, there is no accepted measure that would provide quantitative evaluation of structural complexity. Recently, we proposed to use information-based measures to estimate complexity of a crystal structure [1]. It is based upon structural information content, Ig, or Shannon entropy of the quotient graph of the crystal structure considered as a network of atoms and bonds. The more information content of the structure is, the more complex it is. The total information content is measured in bits. Analysis of 19587 mineral-related structure reports stored in the Inorganic Crystal Structure Database using the software package TOPOS 4.0 [2] allowed to calculate information contents for all structurally characterized minerals and their polymorphs. The average information content of a mineral crystal structure can be estimated as 143(2) bits, whereas 20 most complex structures are (in bits): paulingite [7079.643], fantappieite [5948.330], mendeleevite-(Y) [3398.878], bouazzerrite [3035.201], megacyclite [2950.928], vandenrisscheite [2835.307], giuseppettite [2723.097], bijvoetite-(Y) [2607.924], stavelotite [2411.498], rogermitchellite [2320.653], parsettensite [for theoretical model; 2309.820], apjohnite [2305.361], antigorite [polysome with n = 17; 2187.799], tschoertnerite [2132.228], natrophosphate [2109.177], farneseite [2094.012], bannisterite [2075.685], mutinaite [2025.067], charoite [1991.599], and vonbezingite [1899.370]. The most complex mineral structures are silicates (in particular, zeolites and Mn silicates), and minerals based upon nanoscale units (bouazzerite and charoite). Some other applications of the information-based complexity measures will be discussed.

[1] Krivovichev S.V. Acta Crystallogr. A68 (2012) 393-398.
[2] Blatov V.A. IUCr CompComm Newsletter. 2006, 4-38.