

Packing schemes of cavities in selected clathrasils and zeolites and the analogous packings of atoms in crystal structures

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ABSTRACT

Sizes of cavities and their packing schemes in selected zeolites and clathrasils were studied by means of least squares fitting of circumscribed spheres to them. Resulting packing of spheres of different diameters was analyzed by the coordinates of their centers, their volumes and sphericity, and interpreted by comparison with analogous packings of atoms in inorganic compounds and alloys. The topology is described qualitatively as “negative” structures formed by the cavities.

Melanophlogite and dodecasils 3C and 1H are all clathrasils with isolated cavities. They all have pentagonal dodecahedral [5¹²] cages, associated with other cavity types. The packing of cavities in melanophlogite is analogous to the packing of atoms in the structure of Cr₃Si, where the Cr atoms form icosahedra around the Si sites. Dodecasil 3C has a cubic arrangement of [5¹²] cavities, which is described as ABC stacking of kagome nets and its cavity packing is an analog to the packing scheme of atoms in the cubic Laves phase MgCu₂. Dodecasil 1H has an arrangement of [5¹²] cavities in an AA stacking of kagome nets and is analogous to the alloy structure type CaZn₅. Edingtonite and natrolite are built from two types of cavities, tetragonal scalenohedra and [8⁶] cavities. The [8⁶] cavities have different shape and packing in the two structures. In paulingite, the largest cavity, a large rhombicuboctahedron [4¹²6⁸8⁶] with a diameter of 11.02 Å is in a body centered configuration. It is interspaced by six other types of cavities with diameters from 5.10 to 8.20 Å, arranged in a complex pattern. In this structure, there are three non-intersecting channel systems. Their cavity arrangements mimic sodalite and a modified ReO₃ structure. The cubic structure of sodalite has only one type of cavity, a truncated octahedron [4⁶6⁸] with a diameter of 6.41 Å, arranged in a body-centered packing analogous to α-Fe. Chabasite has a rhombohedral packing of elongate cavities [4¹²6²8⁶], whereas Linde Type A has [4⁶6⁸] and [4¹²6⁸8⁶] cavities in a CsCl-type arrangement. The cavity representation used here gives a clear picture of cavities and interconnections even for complicated cases.

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