Analysis of Microporous Crystal Structures with Voronoi-Dirichlet Polyhedra

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The methods for computer characterization of voids in crystal structures by means of Voronoi-Dirichlet polyhedra are extended to microporous mineral phases and synthetic ionic conductors. It is shown that these methods allow one to appropriately visualize cavities, cages, and channels, and estimate their geometrical properties, such as size and shape. Some typical minerals (sodalite, olivine, pyroxene, sheelite, anortite, *etc*) are considered to analyze the systems of pores, and the methods are found to be an effective tool for predicting type and positions of interstitial cations. Moreover, the absence of some phases with large alkali cations (e.g. Sc-containing olivines or pyroxenes with Na, K, Rb, or Cs cations) is successfully explained by comparing typical cation sizes and shapes with those for crystal structure cavities. In addition, several ionic conductors are tested, such as Nasicon, Liphos, $Na_{15}Y_3[Si_{12}O_{36}]$, *etc*, to visualize the conductive channels, assess their size, and find possible paths of ion migration. Special attention is paid to framework rare-earth silicates and germanates, possessing high conductivity and/or ion-exchange properties. The principal advantage of the proposed methods is their independence of any empirical parameters (such as ionic or van der Waals radii) and, hence, the possibility of being used for hosts and guest atoms or molecules of any chemical composition and geometry.

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