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Weddellite from renal stones: Structure refinement and dependence of crystal chemical features on H_2O content†

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Abstract

The refinement of the structures of 17 weddellite crystals [$Ca(C_2O_4)\cdot(2+x)H_2O$, $I4/m$, a = 12.329–12.378 Å, c = 7.345–7.366 Å, V = 1117.8–1128.6 Å^3], which were taken from the oxalic renal stones of the St. Petersburg (Russian Federation) citizens of both sexes aged from 24 to 65 years, has been carried out by the means of single-crystal X-ray diffraction (R_1 = 0.024–0.057). According to the results of the study, the amount of "zeolitic" water molecules (x) in the structure of weddellite varies from 0.13 to 0.37 pfu. A significant positive correlation between the amount of "zeolitic" water in the structure of weddellite and the closest interatomic distance between coordination water molecules in the large channels (OW1-OW1) was found as well as positive correlation between the value of the a parameter and the average distance of <Ca1-O> in Ca polyhedron. Obtained linear regression equation: $x = 5.43a - 66.80$, can be used for determination of the "zeolitic" water amount using the known unit-cell a parameter with mean-root-square error ±0.03 pfu. It was found that the x value for the crystals selected from the "mono-weddellite" stones (x = 0.13–0.24) are at the bottom of the range, thus we can assume that weddellite crystals with fewer "zeolitic" water amounts would be relatively stable. This work expands the knowledge of pathogenic crystal growth processes in living organisms and the development of the theory of oxalate stone formation in humans and animals, and may provide a building block for biomolecular technologies that approach the prevention and treatment of diseases associated with lithiasis.

Keywords: Weddellite, calcium oxalate, crystal structure, renal stones, biomineralogy