MINERALS IN THE HUMAN BODY

Weddellite from renal stones: Structure refinement and dependence of crystal chemical features on H2O content†

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ABSTRACT

The refinement of the structures of 17 weddellite crystals [Ca(C\textsubscript{2}O\textsubscript{4})\textsubscript{2}(2+x)H\textsubscript{2}O, \textit{I}4\textit{m}, \textit{a} = 12.329–12.378 Å, \textit{c} = 7.345–7.366 Å, \textit{V} = 1117.8–1128.6 Å\textsuperscript{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 (\textit{R} = 0.024–0.057). According to the results of the study, the amount of “zeolitic” water molecules (\textit{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 \textit{a} parameter and the average distance of <Ca1-O> in Ca polyhedron. Obtained linear regression equation: \textit{x} = 5.43\textit{a} – 66.80, can be used for determination of the “zeolitic” water amount using the known unit-cell \textit{a} parameter with mean-root-square error ±0.03 pfu. It was found that the \textit{x} value for the crystals selected from the “mono-weddellite” stones (\textit{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

INTRODUCTION

The first samples of weddellite CaC\textsubscript{2}O\textsubscript{4}(2+x)H\textsubscript{2}O (\textit{x} \leq 0.5) were found in the sediments of the Weddell Sea (Antarctica) in 1936 (Bannister and Hey 1936). The classic form of weddellite crystals is a tetragonal bipyramid, flattened on [001], but sometimes the combination of the tetragonal bipyramid and pinacoid also occurs. Quite often, weddellite dehydrates to more stable whewellite-calcium oxalate monohydrate (CaC\textsubscript{2}O\textsubscript{4}⋅H\textsubscript{2}O), forming excellent pseudomorphs of granular whewellite after weddellite tetragonal dipyramids.

In nature, weddellite occurs in peat and calcareous lake sediments, in biofilms on the surface of limestone, and in plants (Graustein et al. 1977; Frank-Kamenetskaya et al. 2012). As well, most of the human urinary system stones consists of calcium oxalates both mono- and dihydrates (the amount of calcium oxalate stones is up to 75% depending on the region) (Korago 1992; Izatulina and Yelnikov 2008). Although the results of thermodynamic calculations show that whewellite is the stable calcium oxalate phase under physiological conditions (Yelnikov et al. 2007), the frequency of weddellite occurrence in oxalate uroliths is significant. According to our collection (more than 1000 renal stones), 46% of samples contain weddellite and 5% are mono-weddellite. Quite often a rhythmic alternation of whewellite and weddellite (Fig. 1) is detected in renal stones that indicate a sudden and periodic change

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FIGURE 1. Biomineral renal stone: central part = whewellite, outer part = weddellite. Picture taken in polarized light. (Color online.)