American Mineralogist, Volume 99, pages 1761–1766, 2014

A new biogenic, struvite-related phosphate, the ammonium-analog of hazenite, $(NH_4)NaMg_2(PO_4)_2 \cdot 14H_2O$

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Abstract

A new biogenic, struvite-related phosphate, the ammonium analog of hazenite (AAH), ideally $(NH_4)NaMg_2(PO_4)_2 \cdot 14H_2O$, has been found in cultures containing the bacterial strain *Virgibacillus* sp.NOT1 (GenBank Accession Number: JX417495.1) isolated from an XVII Century document made of parchment. The chemical composition of AAH, determined from the combination of electron microprobe and X-ray structural analyses, is $[(NH_4)_{0.78}K_{0.22}]NaMg_2(PO_4)_2 \cdot 14H_2O$. Single-crystal X-ray diffraction shows that AAH is orthorhombic with space group *Pmnb* and unit-cell parameters $a = 6.9661(6)$, $b = 25.236(3)$, $c = 11.292(1)$ Å, and $V = 1985.0(3)$ Å^3. Compared with hazenite, the substitution of NH_4^+ for K^+ results in a noticeable increase of the average *A*-O ($A = NH_4^+ + K^+$) bond length and the unit-cell volume for AAH, as also observed for struvite vs. struvite-K. Both infrared and Raman spectra of AAH resemble those of hazenite, as well as struvite. Our study reveals that AAH forms only in cultures with Na-bearing solutions and pH below 10.0. No AAH or hazenite was found in experiments with the K-bearing solutions, suggesting the necessity of a Na-bearing solution for AAH formation.

Keywords: Ammonium phosphate, hazenite, struvite-type materials, biomineral, crystal structure, X-ray diffraction, infrared and Raman spectra