American Mineralogist, Volume 96, pages 869–877, 2011

Cranswickite $MgSO_4 \cdot 4H_2O$, a new mineral from Calingasta, Argentina

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ABSTRACT

Cranswickite is a newly recognized mineral of composition $MgSO_4 \cdot 4H_2O$ from Calingasta, San Juan Province, Argentina (IMA2010-016). Cranswickite is monoclinic, space group $C2/c$, $a = 11.9236(3)$, $b = 5.1736(1)$, $c = 12.1958(3)$ Å, $\beta = 117.548(2)°$, $V = 667.0(1)$ Å^3, $Z = 4$, $d_{obs} = 1.917$ g/cm^3, and $d_{calc} = 1.918$ g/cm^3. The mineral occurs0 as a soft white vein filling in a metasedimentary rock. The atomic structure has been determined by direct methods and refined by Rietveld analysis of powder diffraction data. The atomic structure consists of chains of corner-sharing magnesium-containing octahedra and sulfate tetrahedra similar to the structure of pentahydrite. All the water molecules directly coordinate magnesium in the structure. The five strongest lines in the powder X-ray diffraction data are [d_{obs} in angstroms (*I*) (*hkl*)]: 5.259 (100) (200), 3.927 (46) (11$\bar{2}$), 3.168 (45) (11$\bar{3}$), 4.603 (29) (11$\bar{1}$), 2.570 (23) (311). Infrared and Raman spectra are very similar to the spectra measured from starkeyite. The chemical composition of cranswickite is the same as starkeyite $MgSO_4 \cdot 4H_2O$, but starkeyite has an atomic structure where two sulfate tetrahedra and two $Mg(H_2O)_6$ octahedra share corners to form a four-membered ring and not a chain as in cranswickite. The new mineral is named in honor of Lachlan M.D. Cranswick (1968–2010), an Australian crystallographer who helped to developed and maintain the Collaborative Computational Project No. 14 in Powder and Small Molecule Single Crystal Diffraction (CCP14).

Keywords: Cranswickite, starkeyite, pentahydrite, epsomite, meridianiite, chalcanthite, powder diffraction, atomic structure, magnesium sulfate, Argentina