

JOANNEUMITE, $\text{Cu}(\text{C}_3\text{N}_3\text{O}_3\text{H}_2)_2(\text{NH}_3)_2$, A NEW MINERAL SPECIES WITH AMMINE AND ISOCYANURATE GROUPS

Walter, F¹ & Bojar, H.-P²

¹Institute of Earth Sciences, University of Graz, Universitätsplatz 2, 8010 Graz, Austria

²Department of Geosciences, Universalmuseum Joanneum, Weinzöttlstraße 16, 8045 Graz, Austria

e-mail: franz.walter@uni-graz.at

The new mineral joanneumite was found at Calleta Pabellon de Pica, Tarapaca region, Chile. Joanneumite occurs as spherical aggregates of hypidiomorphic, mm-sized violet crystals associated with salammoniac, dittmarite, apthitalite and brushite. The mineral (IMA 2012-001) is named for the 200th anniversary of the foundation of the Universalmuseum Joanneum. Joanneumite is triclinic, space group $P\bar{1}$, $a = 4.982(1)$, $b = 6.896(1)$, $c = 9.115(2)$ Å, $\alpha = 90.53(3)$, $\beta = 97.85(3)$, $\gamma = 110.08(3)$ °, $V = 290.8(1)$ Å³, $Z = 1$ (at 100 K).

The chemical composition, X-ray powder- and FTIR-data of joanneumite and the synthetic bis(isocyanurato)diammine-copper(II) are identical. Due to the lack of suitable natural crystals, single crystal structure refinement was done with synthetic joanneumite, which crystallized from the melt of Cu(II) chloride dihydrate and urea. The crystal structure was solved with direct methods (program SHELXS). Least-squares refinement using anisotropic displacement parameters for all non-hydrogen atoms was carried out with the program SHELXL97 (SHELDRICK, 2008) and yielded $R1 = 0.024$ for 1153 unique reflections with $F_o > 4\sigma(F_o)$.

The basic structural unit in the joanneumite structure is similar to that of ammineite, $\text{CuCl}_2(\text{NH}_3)_2$, (BOJAR et al., 2010). The two chlorine atoms of ammineite are replaced by two isocyanurate groups in the joanneumite structure (Fig. 1a-c). The copper centre has distorted square-planar coordination and the $\text{Cu}(\text{C}_3\text{N}_3\text{O}_3\text{H}_2)_2(\text{NH}_3)_2$ molecules are cross-linked by hydrogen bonds from 1.92 to 2.31 Å, forming a three dimensional network (Fig. 1d) with good cleavage parallel (010).

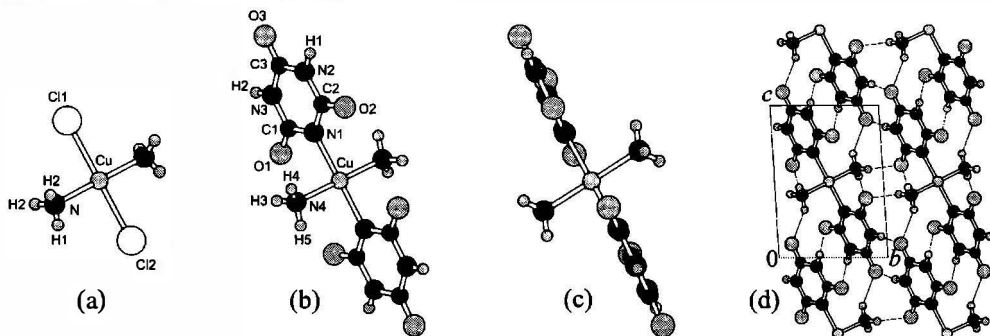


Figure 1. The basic structural units of ammineite (a), joanneumite (b, c) and the crystal structure of joanneumite with outlined hydrogen bonds (single lines), view along [100] (d).

BOJAR, H.-P., WALTER, F., BAUMGARTNER, J., FÄRBER, G. (2010): Can. Mineral., 48, 1359-1371.
 SHELDRICK, G. M. (2008): Acta Cryst., A64, 112-122.