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# Acentric structure (*P*3) of bechererite, $Zn_7Cu(OH)_{13}[SiO(OH)_3SO_4]$

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## Abstract

The crystal structure of bechererite from the Tonopah-Belmont mine, Arizona, was reinvestigated using a single-crystal X-ray diffractometer (Mo$K\alpha$ radiation) equipped with a CCD area detector. The structure was refined in space group *P*3 ($a$ = 8.319(2), $c$ = 7.377(1) Å) with 1247 unique reflections up to $(\sin\theta)/\lambda$ = 0.65 leading to $R1$ = 2.7%, w$R2$ = 6.4%. In agreement with the previously reported centric structure (*P*3), bechererite is composed of (001) brucite-like sheets formed by edge-sharing $(Zn,Cu)O_6$ octahedra and $\frac{1}{7}$ ordered octahedral vacancies. The layers are connected parallel to $c$ by ditetrahedral $(Zn,Cu)_2(OH)_7$ units. Due to the attractive force of a weak hydrogen bond, the bridging O atom of the ditetrahedral unit is displaced from the threefold axis. A characteristic feature of the structure is isolated tetrahedra, which connect only with one apex to the octahedral sheet. The acentric structure (*P*3) reveals ordering between $SiO(OH)_3$ and $SO_4$ tetrahedra yielding characteristic distortions of the neighboring $(Zn,Cu)O_6$ octahedra caused by bond-valence requirements of the shared O atoms. The $[SiO(OH)_3]^{1-}$ tetrahedron is only 70(1)% occupied and is partly substituted by tetrahedral $[O_4H_7]^{1-}$ clusters. The existence of $H_2O$ molecules in the $[O_4H_7]^{1-}$ cluster is supported by FTIR spectroscopy.