Hydrogen Bonds in Triclinic MH(XO$_4$) Compounds

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The crystal structure of triclinic $SrHAsO_4$ was re-investigated from single crystal X-ray data. The strong reflections of the present investigation are in agreement with a former description [1]. However, additional weak superstructure reflections are responsible for a unit cell with four-fold cell volume. The non-standard space-group setting $F\bar{1}$ (a = 14.697(3), b = 28.230(5), c = 14.920(3) Å, α = 95.20(3), β = 104.78(3), γ = 88.11(3)°, Z = 64) was chosen to facilitate the comparison with $CaHPO_4$ (monetite), $CaHAsO_4$ (weilite), α-$SrHPO_4$, $NaHSO_4$, and $HgHAsO_4$. Their unit cells correspond with the average cell of $SrHAsO_4$. The arrangements of the M and X atoms (M = Na, Ca, Sr, Hg; X = S, P, As) compare well; their coordination figures are qualitatively maintained. Despite a structural analogy, isotypy is not verified. Essential differences are evident for the hydrogen bonds. The parental structure has space group $P\bar{1}$ (Z = 4) and exhibits three crystallographically different hydrogen bonds. Only half of the H atoms p.f.u. forms conventional hydrogen bonds. Two hydrogen bonds are restricted by $\bar{1}$ symmetry (O···O ≥ 2.40 Å). Distinct order phenomena in the structurally related compounds are observed. In $SrHAsO_4$ the formation of a superstructure violates these inversion centres and all hydrogen bonds have distinct donor and acceptor atoms. However, some short contacts O···O' ≥ 2.47 Å are maintained.

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[1] Nabar M.A., Dalvi A.P., *Bull. Soc. fr. Min. Crist.*, 1977, **100**, 353.

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