

**SrHAsO<sub>4</sub>: STRUCTURAL RELATIONS TO MONETITE, WEILITE, α-SrHPO<sub>4</sub>,  
α-NaHSO<sub>4</sub>, AND HgHPO<sub>4</sub>**

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From an indexed X-ray powder spectrum NABAR & DALVI (1977) found a triclinic unit cell for SrHAsO<sub>4</sub>:  $a = 7.34(1)$ ,  $b = 6.97(1)$ ,  $c = 7.40(2)$  Å,  $\alpha = 96.0(2)$ ,  $\beta = 103.5(2)$ ,  $\gamma = 86.9(2)^\circ$ ,  $Z = 4$ ; it is called 'average cell' hereafter. In analogy to weilite, CaHAsO<sub>4</sub> (FERRARIS & CHIARI, 1970), a centrosymmetric space-group symmetry  $P\bar{1}$  was assumed. During the present work SrHAsO<sub>4</sub> was synthesized under hydrothermal conditions. The strong reflections of a single-crystal X-ray structure investigation correspond to the former description. 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,  $\alpha = 95.20(3)$ ,  $\beta = 104.78(3)$ ,  $\gamma = 88.11(3)^\circ$ ,  $Z = 64$ ) was chosen to facilitate the comparison with the related compounds: The unit cells of weilite, monetite (CaHPO<sub>4</sub>; CATTI et al., 1977, 1980), α-SrHPO<sub>4</sub> (BOUDJADA et al., 1978), α-NaHSO<sub>4</sub> (WERNER et al., 1996), and HgHPO<sub>4</sub> (DUBLER et al., 1981) agree with the 'average cell' of SrHAsO<sub>4</sub>. The arrangements of the *M* and *X* atoms ( $M = \text{Na, Ca, Sr, Hg}$ ;  $X = \text{S, P, As}$ ) compare well; their coordination figures are qualitatively maintained. Despite the 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 H bonds. Only half of the H atoms pfu forms conventional H bonds (donor and acceptor atoms are not related by symmetry). At least on the average, the H2 and H3 atoms form H bonds restricted by  $\bar{1}$  symmetry ( $\text{O}\cdots\text{O} \geq 2.40$  Å). They link the XO<sub>4</sub> tetrahedra in [101]. In the low-T modification of monetite, H2 and H3 become ordered (space group  $P1$ ). In SrHAsO<sub>4</sub> the formation of a *superstructure* violates these inversion centres and all H bonds have distinct donor and acceptor atoms. However, short  $\text{O}\cdots\text{O}$ ' contacts (2.47 to 2.50 Å) are maintained. In both cases polar chains of (XO<sub>3</sub>OH) groups are formed parallel to [101]; in the low-T modification of monetite they are oriented parallel to each other, in SrHAsO<sub>4</sub> neighbouring chains point in different directions. In HgHPO<sub>4</sub> the position of the H3 atom is principally different; the phosphate tetrahedra are linked to chains by both symmetry restricted and non-restricted H bonds in [100]. [PO<sub>2</sub>(OH)<sub>2</sub>] groups are necessarily formed besides [PO<sub>3</sub>(OH)] and [PO<sub>4</sub>].

Financial support of the Austrian science foundation (FWF) is gratefully acknowledged (Grant P15875-N03).

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