

Preparation and Crystal Structures of the Isotypic Compounds $\text{CdXO}_4 \cdot 2 \text{HgO}$ ($X = \text{S}, \text{Se}$)

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Colourless single crystals of the compounds $\text{CdXO}_4 \cdot 2 \text{HgO}$ ($X = \text{S}, \text{Se}$) were obtained under hydrothermal conditions (250 °C, 5 d), starting from stoichiometric amounts of HgO , $\text{CdSO}_4 \cdot 7\text{H}_2\text{O}$ and $\text{CdSeO}_4 \cdot 2\text{H}_2\text{O}$, respectively. The crystal structures were determined from X-ray diffraction data sets. The $\text{CdXO}_4 \cdot 2\text{HgO}$ compounds crystallise isotypically with two formula units in space group $P\bar{1}$ (#2) [$\text{CdSO}_4 \cdot 2\text{HgO}$ ($\text{CdSeO}_4 \cdot 2\text{HgO}$): $a = 6.793(2)$ ($6.9097(5)$) Å, $b = 7.205(2)$ ($7.1786(6)$) Å, $c = 7.359(2)$ ($7.4556(6)$) Å, $\alpha = 73.224(6)$ ($74.586(2)$)°, $\beta = 66.505(6)$ ($68.229(1)$)°, $\gamma = 63.054(5)$ ($63.886(1)$)°, 1670 (1786) structure factors, 92 parameters, $R[F^2 > 2\sigma(F^2)] = 0.0379$ (0.0244)] and are made up from *zig-zag* $[\text{O}-\text{Hg}-\text{O}]_\infty$ chains with very short bonds of $\bar{d}(\text{Hg}-\text{O})$ 2.025 Å, distorted $[\text{CdO}_6]$ octahedra ($\bar{d}(\text{Cd}-\text{O}) = 2.297$ Å), and XO_4 tetrahedra ($\bar{d}(\text{S}-\text{O}) = 1.458$ Å, $\bar{d}(\text{Se}-\text{O}) = 1.633$ Å) as the main building blocks. The $\text{CdXO}_4 \cdot 2\text{HgO}$ compounds reveal no structural relationship with the corresponding $\text{HgXO}_4 \cdot 2\text{HgO}$ phases.

Key words: Mercury, Cadmium, Sulfate, Selenate, Hydrothermal Synthesis, Crystal Structure