

Supporting Information

Synthesis, crystal and band structures, and optical properties of a new mixed-framework mercury selenide diselenite, $(\text{Hg}_3\text{Se}_2)(\text{Se}_2\text{O}_5)$

Jian-Ping Zou, Guo-Cong Guo, Sheng-Ping Guo, Ying-Bing Lu, Ke-Jun Wu, Ming-Sheng
Wang, Jin-Shun Huang

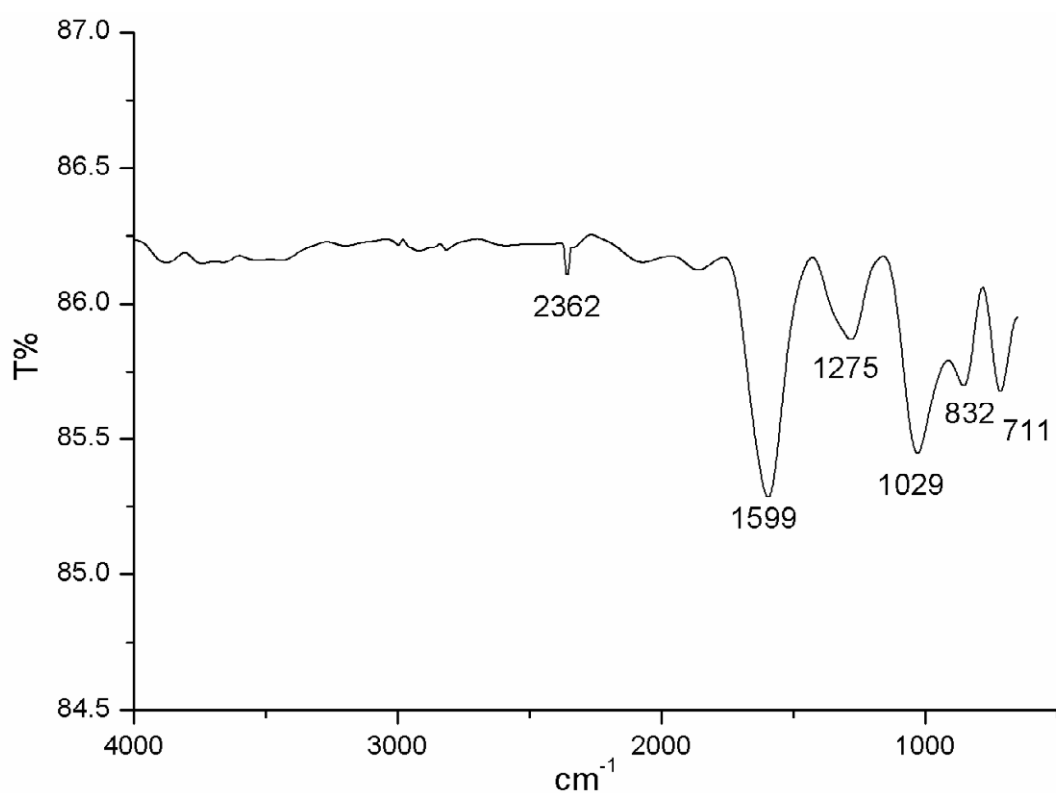


Fig. S1. Microscopic IR spectrum of single crystal of **1**. The vibrational spectra at 2362 and 1275 cm^{-1} due to the presence of CO_2 from atmosphere, the absorption band at 1599 cm^{-1} can be assigned to the antisymmetric H-O-H bending due to the water molecule from atmosphere.

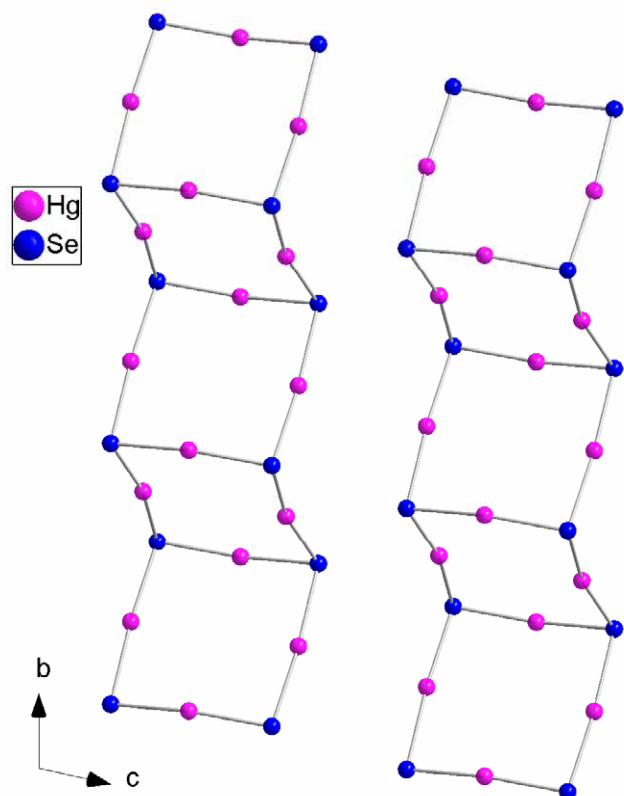


Fig. S2. View of the stair-like structure of $(\text{Hg}_3\text{Se}_2)^{2+}$ in **1** along the a axis.

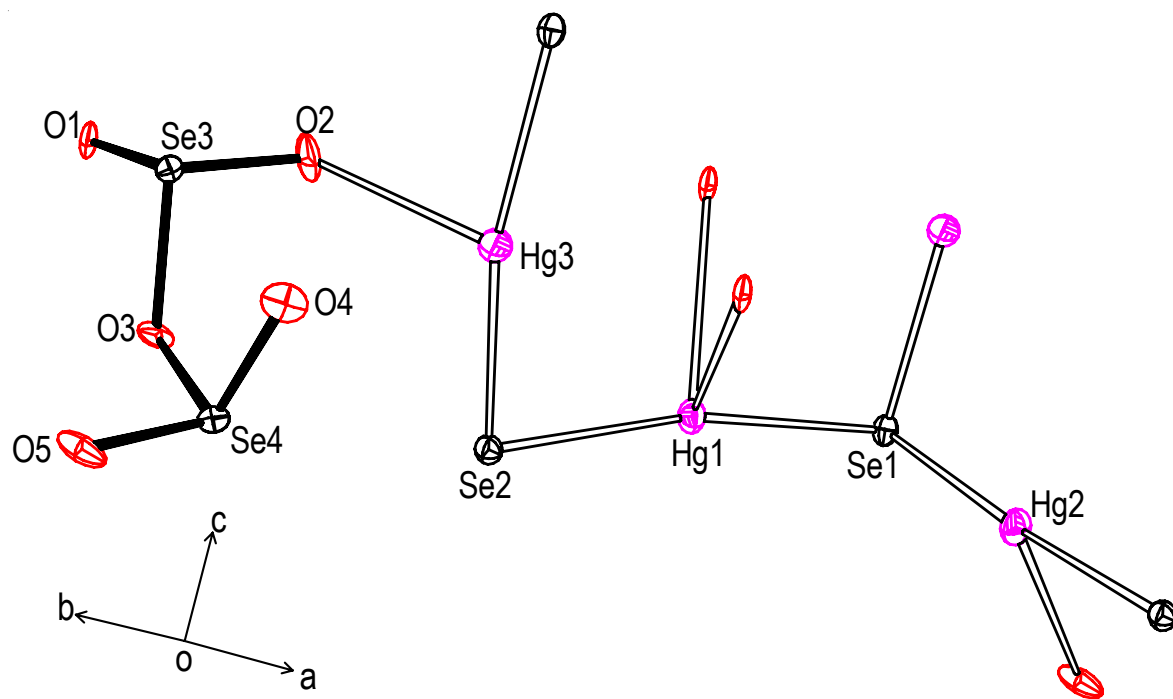


Fig. S3. The molecular structure of **1** with the 30% thermal ellipsoids.