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 \(\text{I}\) along the \(a\) axis.

Fig. S3. The molecular structure of \(\text{I}\) with the 30\% thermal ellipsoids.