Synthesis, crystal and band structures, and optical properties of a novel quaternary mercury and cadmium chalcogenide: (Hg$_2$Cd$_2$S$_2$Br)Br

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Fig. S1. FTIR spectrum of 1 on transparent pellets (1% samples mixed with KBr).

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Fig. S2. TG-DTA curves of 1.
**Fig. S3.** Convergence of the total energy of 1 at different computational parameters. (a) Total energy versus the cutoff energy for the $k$-point mesh of $3 \times 1 \times 5$. (b) Total energy versus the $k$-point mesh for the cutoff energy of 450 eV.

**Fig. S4.** A view of linear Hg tetrahedral chains and V-shape Cd trigonal chains extending along the $c$ direction.
Fig. S5. (a) Crystal structure of 1; (b) Crystal structure of the reported compound HgCdAsBr.
Fig. S6. Molecular structure of 1. (Symmetric codes: A: x, y, 1 + z; B: x, y, -1 + z; C: 0.5 - x, 0.5 - y, z; D: 1 - x, y, 1 - z; E: x, 1 - y, 1 - z)
Fig. S7. The picture of a single crystal of 1.