Synthesis, crystal and band structures, and optical properties of a novel quaternary mercury and cadmium chalcogenide: $(Hg_2Cd_2S_2Br)Br$

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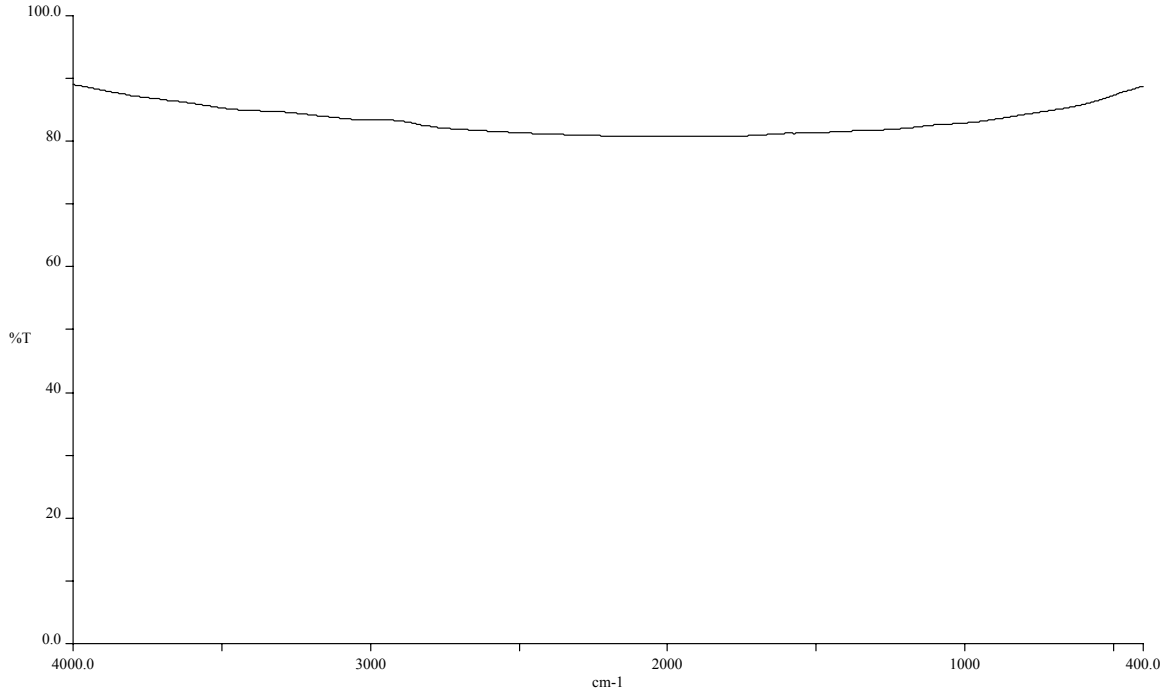

Fig. S1. FTIR spectrum of **1** on transparent pellets (1% samples mixed with KBr).

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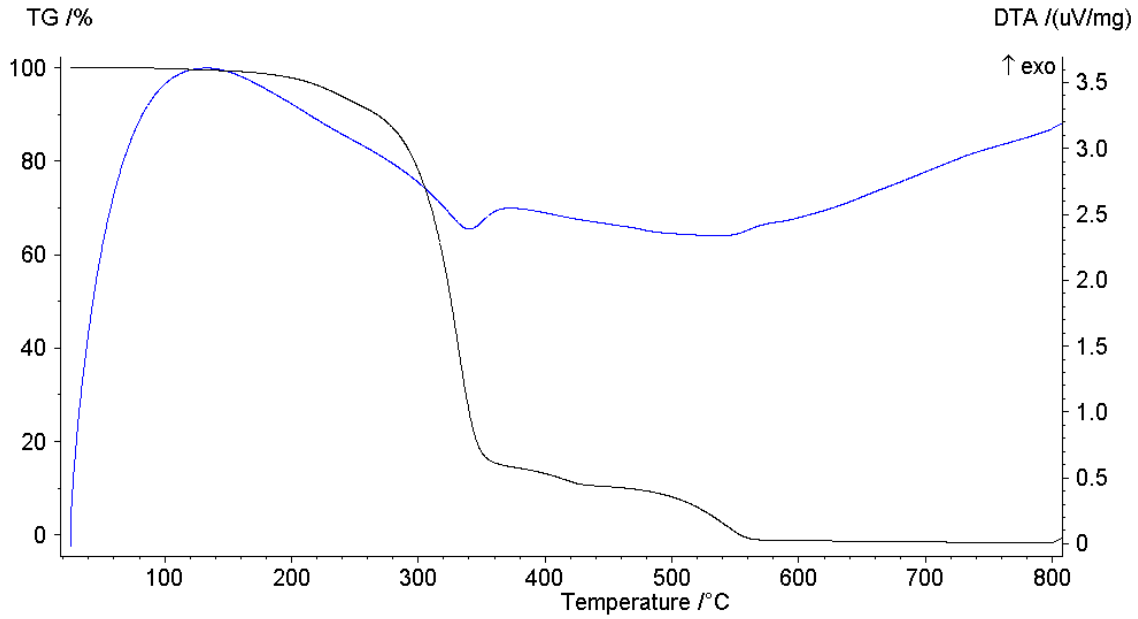
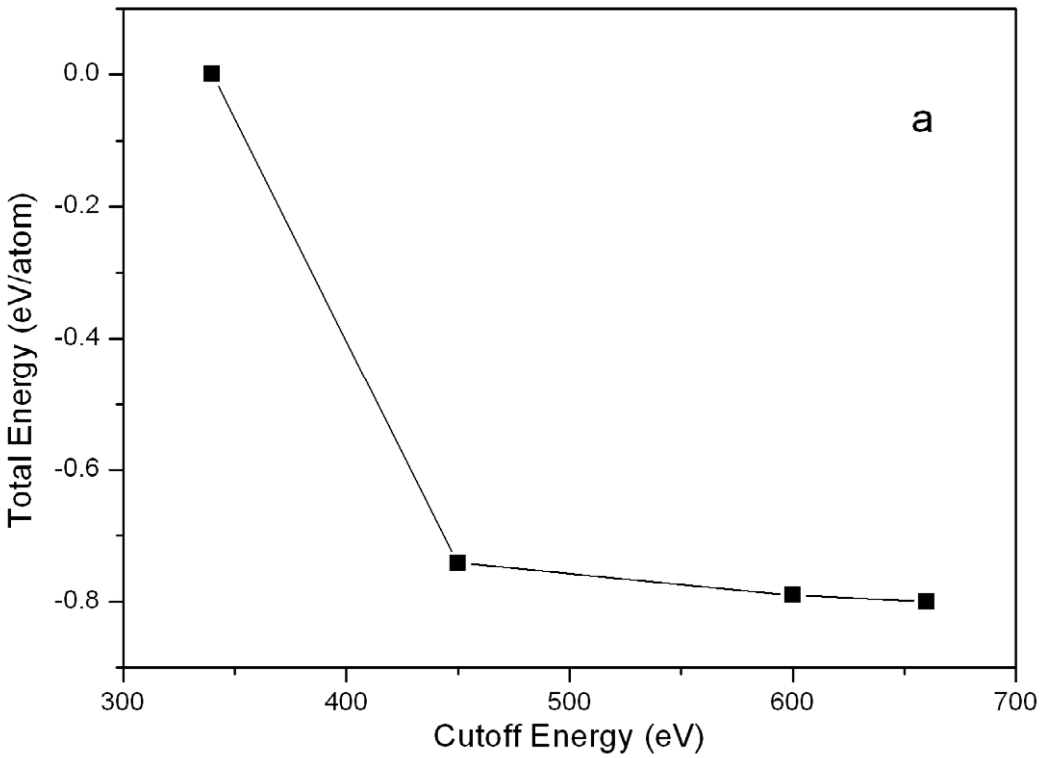


Fig. S2. TG-DTA curves of **1**.



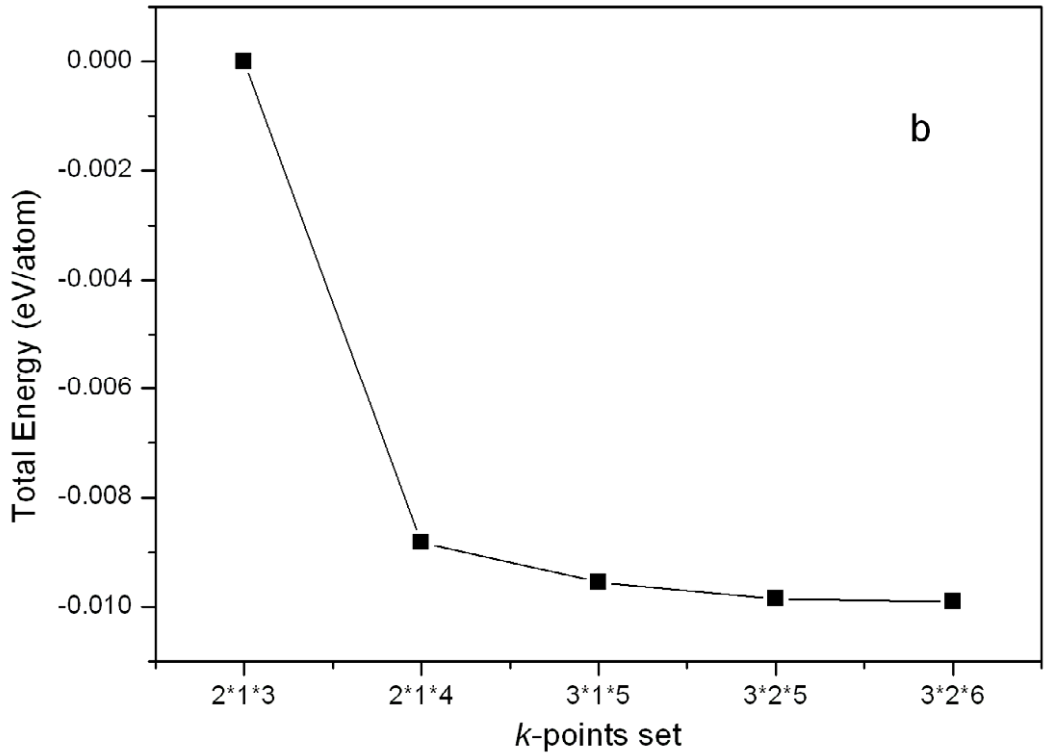


Fig. S3. Convergence of the total energy of **1** at different computational parameters. (a) Total energy versus the cutoff energy for the *k*-point mesh of 3 × 1 × 5. (b) Total energy versus the *k*-point mesh for the cutoff energy of 450 eV.

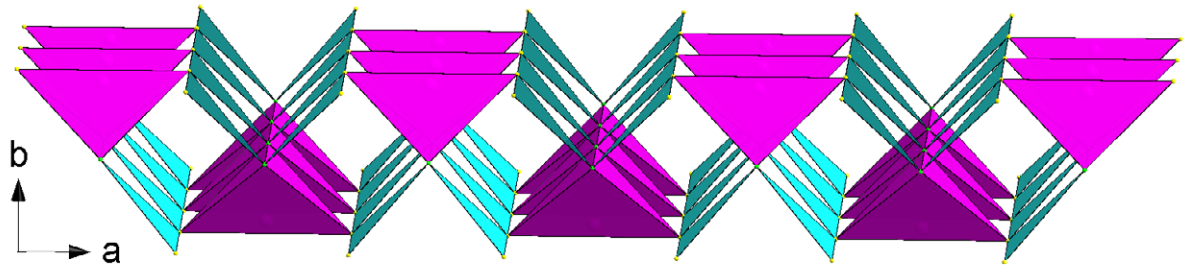
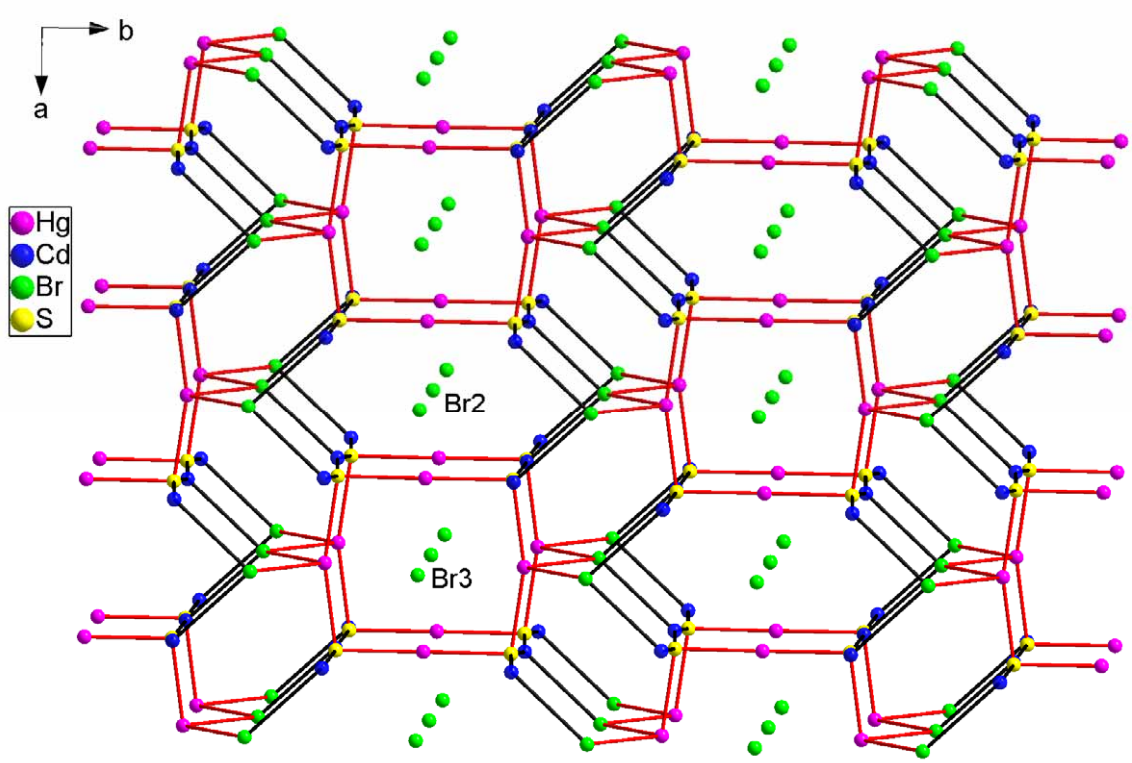


Fig. S4. A view of linear Hg tetrahedral chains and V-shape Cd trigonal chains extending along the *c* direction.



(a)

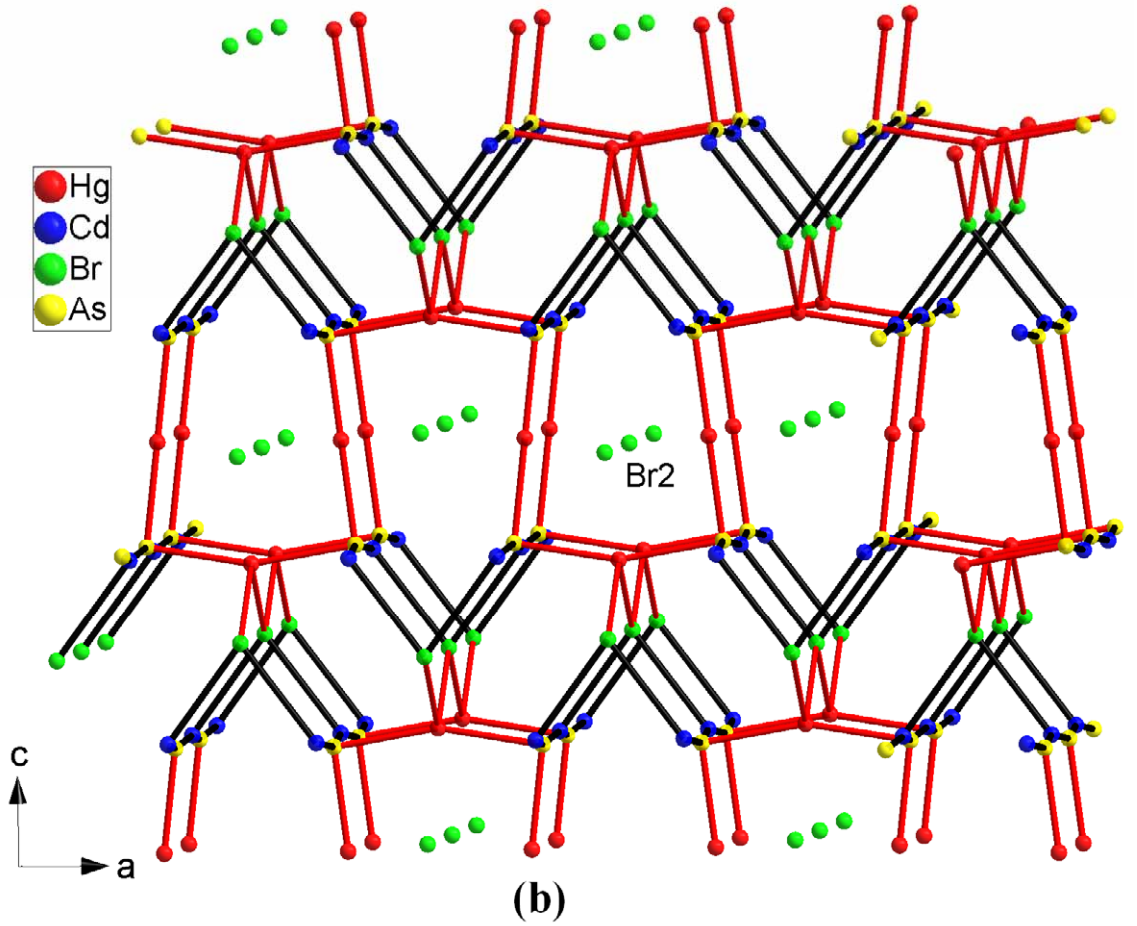


Fig. S5. (a) Crystal structure of **1**; (b) Crystal structure of the reported compound HgCdAsBr.

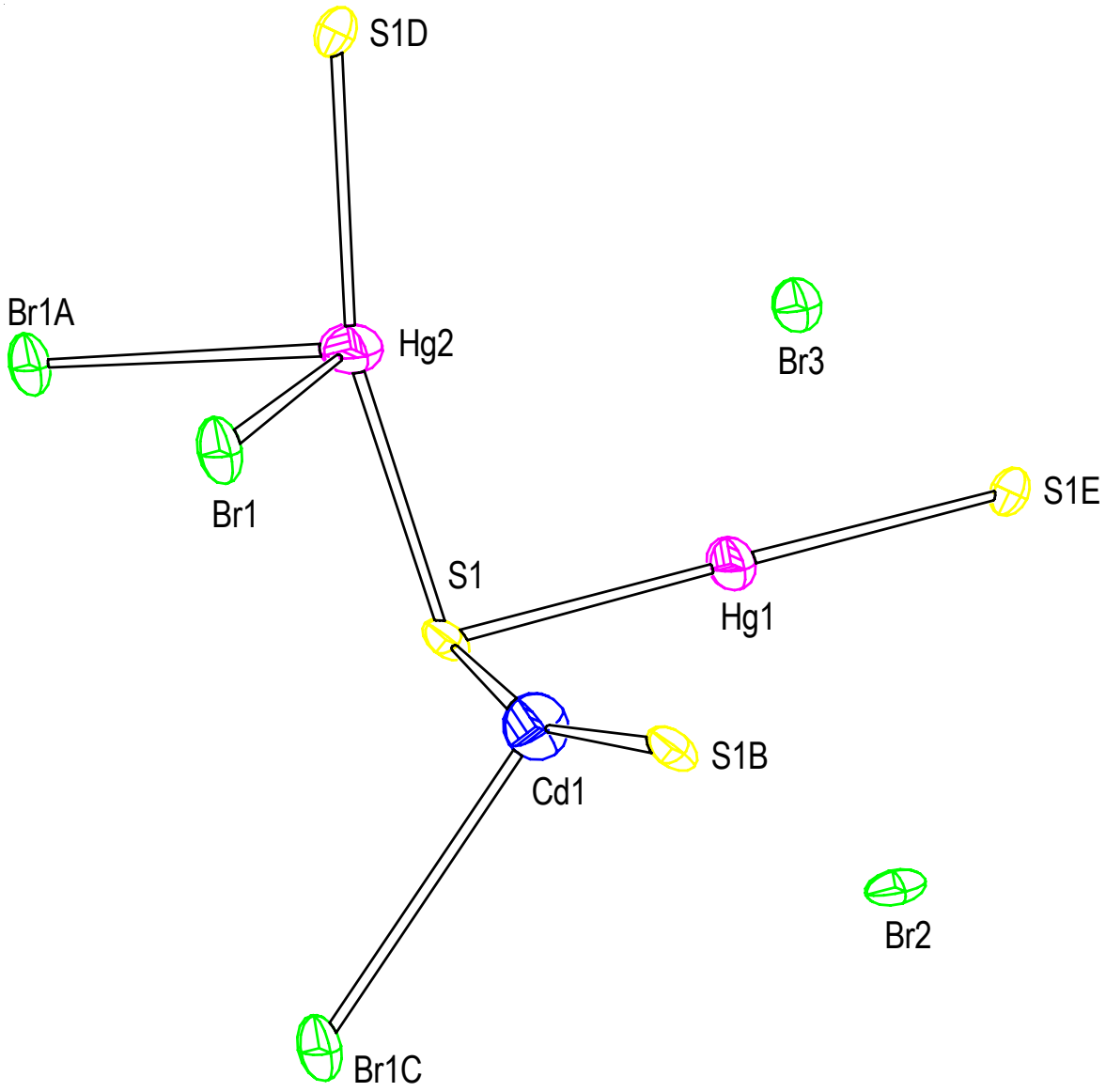


Fig. S6. Molecular structure of **1**. (Symmetric codes: A: x, y, 1 + z; B: x, y, -1 + z; C: 0.5 - x, 0.5 – y, z; D: 1 – x, y, 1 – z; E: x, 1 - y, 1 – z)

Fig. S7. The picture of a single crystal of **1**.