

Structural and Magnetic Studies on Three New Mixed Metal Copper(II) Selenites and Tellurites

Xue-Li Cao, Fang Kong, Zhang-Zhen He, and Jiang-Gao Mao*

Supporting Information

Table S1. IR data for $\text{CdCu}(\text{SeO}_3)_2$, $\text{HgCu}(\text{SeO}_3)_2$ and $\text{Hg}_2\text{Cu}_3(\text{Te}_3\text{O}_8)_2$.

Figure S1. Simulated and experimental XRD powder patterns of $\text{CdCu}(\text{SeO}_3)_2$ (a), $\text{HgCu}(\text{SeO}_3)_2$ (b) and $\text{Hg}_2\text{Cu}_3(\text{Te}_3\text{O}_8)_2$ (c).

Figure S2. A 1D $[\text{Cu}_2\text{O}_4(\text{SeO}_3)_2]^{8-}$ anionic chain along the a axis (a), a 2D $[\text{Cu}_2\text{O}_6(\text{SeO}_3)]^{10-}$ layer parallels to the bc plane (b), and the coordination geometries around Cu (c), Hg (d), Se(1) (e) and Se(2) (f) atoms in $\text{Hg}_2\text{Cu}_3(\text{Te}_3\text{O}_8)_2$.

Figure S3. TGA and DSC curves of $\text{CdCu}(\text{SeO}_3)_2$ (a), $\text{HgCu}(\text{SeO}_3)_2$ (b) and $\text{Hg}_2\text{Cu}_3(\text{Te}_3\text{O}_8)_2$ (c).

Figure S4. IR spectra of $\text{CdCu}(\text{SeO}_3)_2$ (a), $\text{HgCu}(\text{SeO}_3)_2$ (b) and $\text{Hg}_2\text{Cu}_3(\text{Te}_3\text{O}_8)_2$ (c).

Figure S5. UV-Vis absorption spectra of $\text{CdCu}(\text{SeO}_3)_2$ (a), $\text{HgCu}(\text{SeO}_3)_2$ (b) and $\text{Hg}_2\text{Cu}_3(\text{Te}_3\text{O}_8)_2$ (c).

Figure S6. Optical diffuse reflectance spectra of $\text{CdCu}(\text{SeO}_3)_2$ (a), $\text{HgCu}(\text{SeO}_3)_2$ (b) and $\text{Hg}_2\text{Cu}_3(\text{Te}_3\text{O}_8)_2$ (c).

Figure S7. Plot of χT versus T for $\text{HgCu}(\text{SeO}_3)_2$.

Figure S8. Plot of χT versus T (a), and magnetization versus applied field at 2 K (b) as

well as heat capacity measured in zero magnetic fields (the inset) for $\text{CdCu}(\text{SeO}_3)_2$.

Figure S9. Plot of χT versus T for $\text{Hg}_2\text{Cu}_3(\text{Te}_3\text{O}_8)_2$.

Table S1. IR data for $\text{CdCu}(\text{SeO}_3)_2$, $\text{HgCu}(\text{SeO}_3)_2$ and $\text{Hg}_2\text{Cu}_3(\text{Te}_3\text{O}_8)_2$.

	$\nu(\text{Te/Se-O})$	$\nu(\text{Te/Se-O-Te/Se})$
$\text{Hg}_2\text{Cu}_3(\text{Te}_3\text{O}_8)_2$	755, 681, 647	509, 443
$\text{HgCu}(\text{SeO}_3)_2$	796, 717, 671	522, 492, 432
$\text{CdCu}(\text{SeO}_3)_2$	809, 750, 706	538, 496, 405

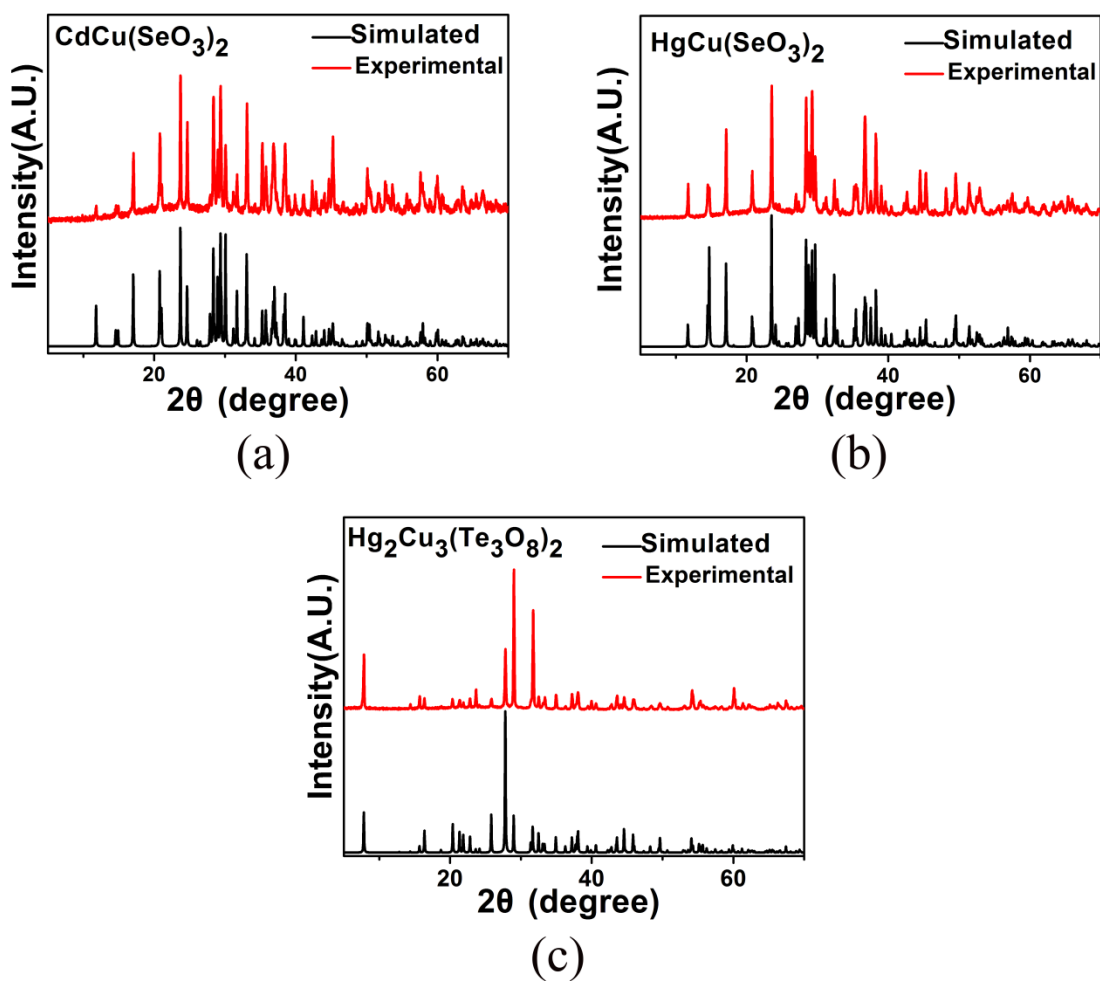


Figure S1. Simulated and experimental XRD powder patterns of $\text{CdCu}(\text{SeO}_3)_2$ (a), $\text{HgCu}(\text{SeO}_3)_2$ (b) and $\text{Hg}_2\text{Cu}_3(\text{Te}_3\text{O}_8)_2$ (c).

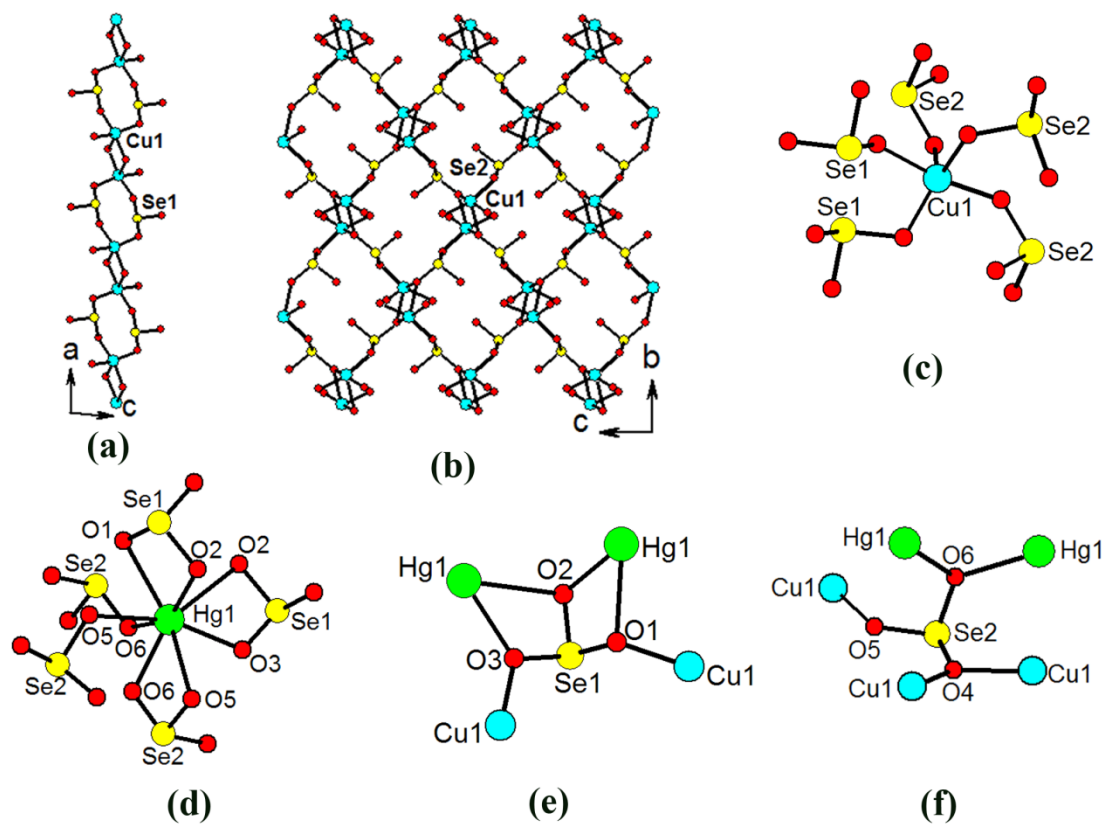


Figure S2. A 1D $[\text{Cu}_2\text{O}_4(\text{SeO}_3)_2]^{8-}$ anionic chain along the a axis (a), a 2D $[\text{Cu}_2\text{O}_6(\text{SeO}_3)]^{10-}$ layer parallels to the bc plane (b), and the coordination geometries around Cu (c), Hg (d), Se(1) (e) and Se(2) (f) atoms in $\text{Hg}_2\text{Cu}_3(\text{Te}_3\text{O}_8)_2$.

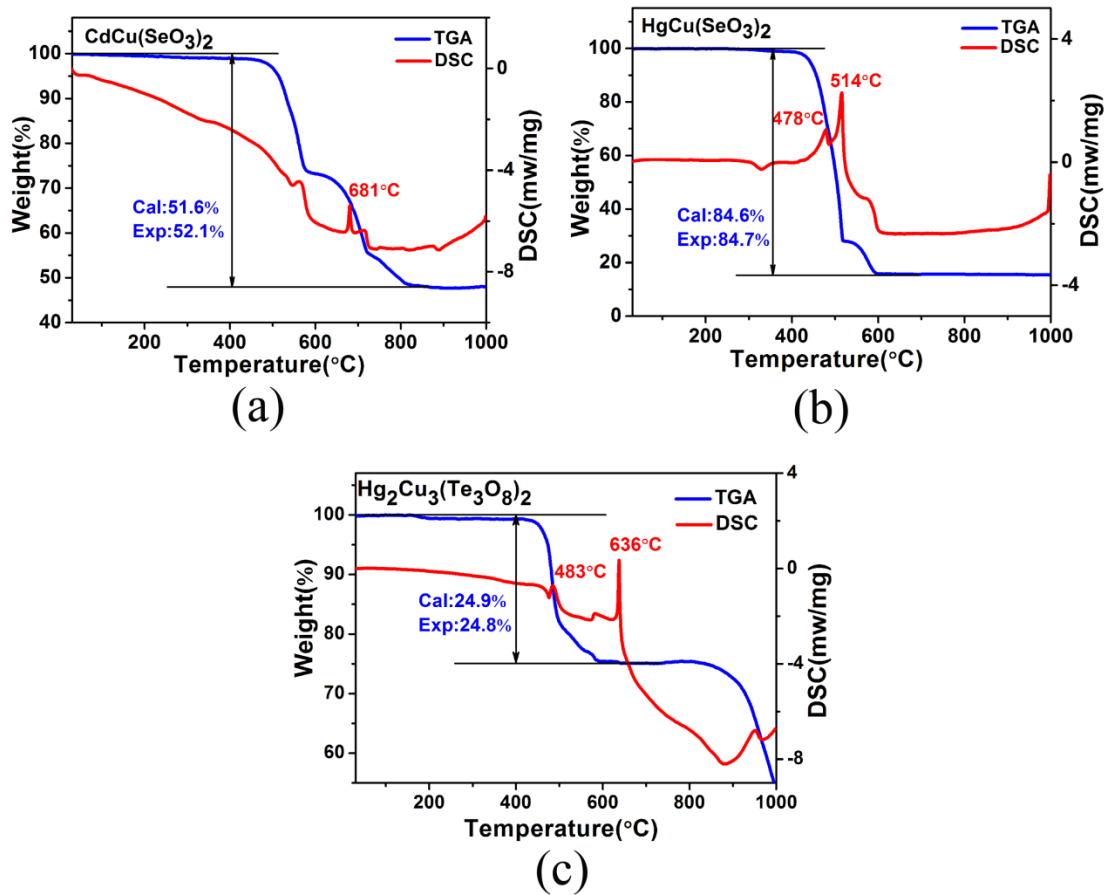


Figure S3. TGA and DSC curves of $\text{CdCu}(\text{SeO}_3)_2$ (a), $\text{HgCu}(\text{SeO}_3)_2$ (b) and $\text{Hg}_2\text{Cu}_3(\text{Te}_3\text{O}_8)_2$ (c).

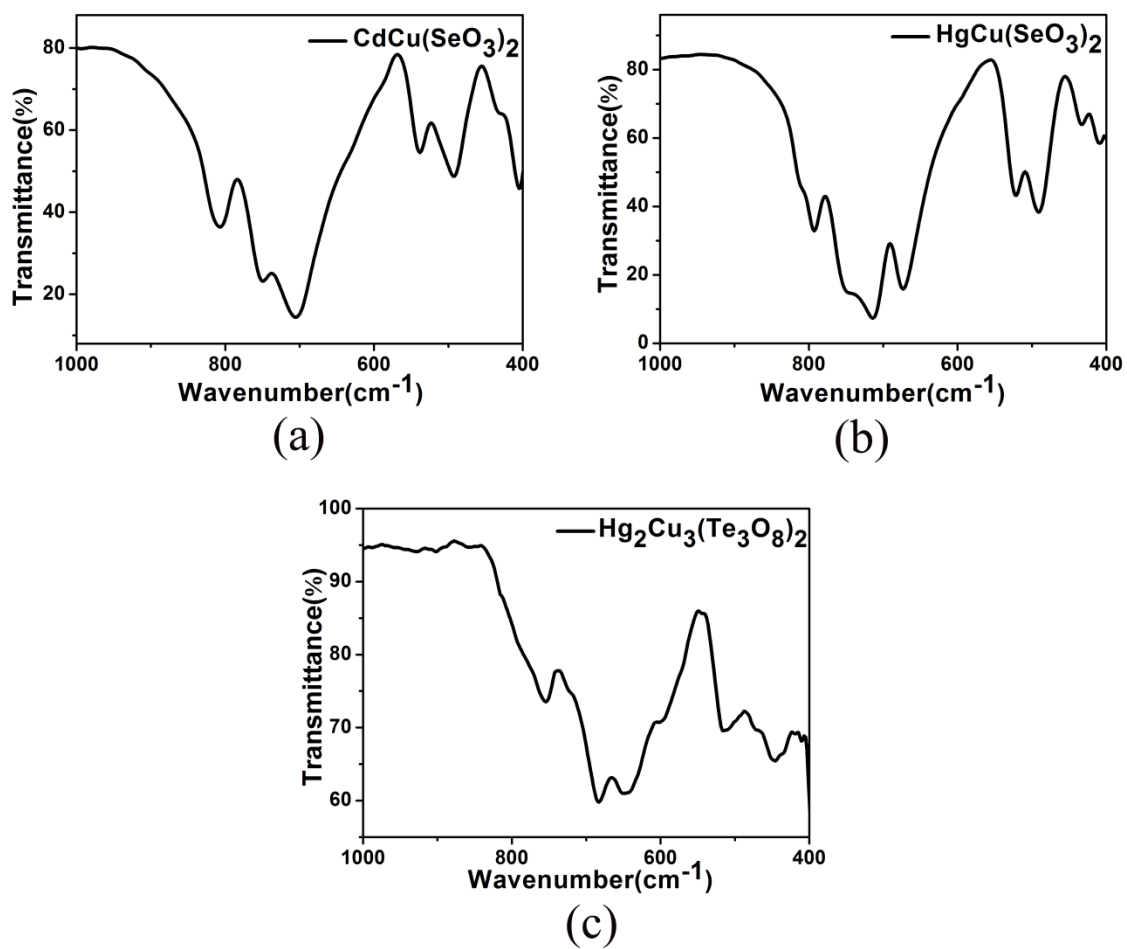


Figure S4. IR spectra of CdCu(SeO₃)₂ (a), HgCu(SeO₃)₂ (b) and Hg₂Cu₃(Te₃O₈)₂ (c).

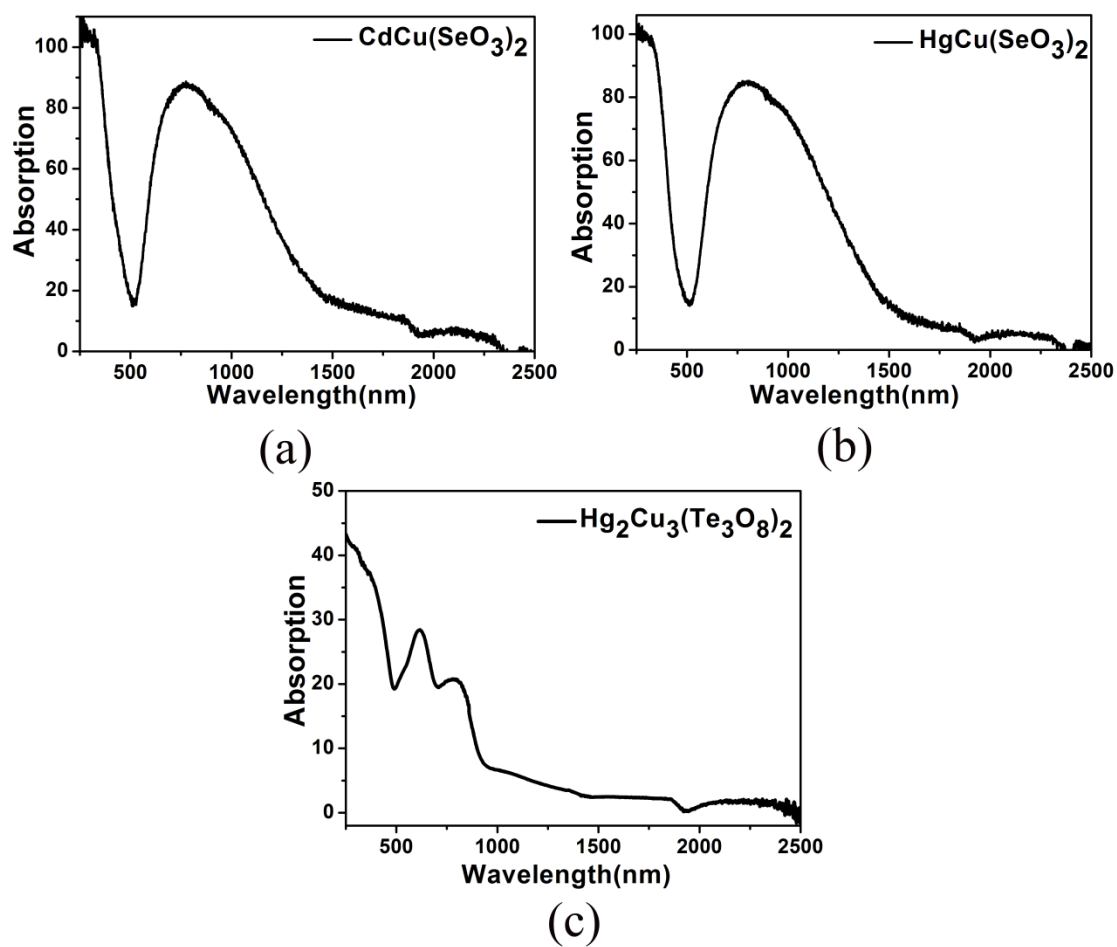


Figure S5. UV-Vis absorption spectra of $\text{CdCu}(\text{SeO}_3)_2$ (a), $\text{HgCu}(\text{SeO}_3)_2$ (b), and $\text{Hg}_2\text{Cu}_3(\text{Te}_3\text{O}_8)_2$ (c).

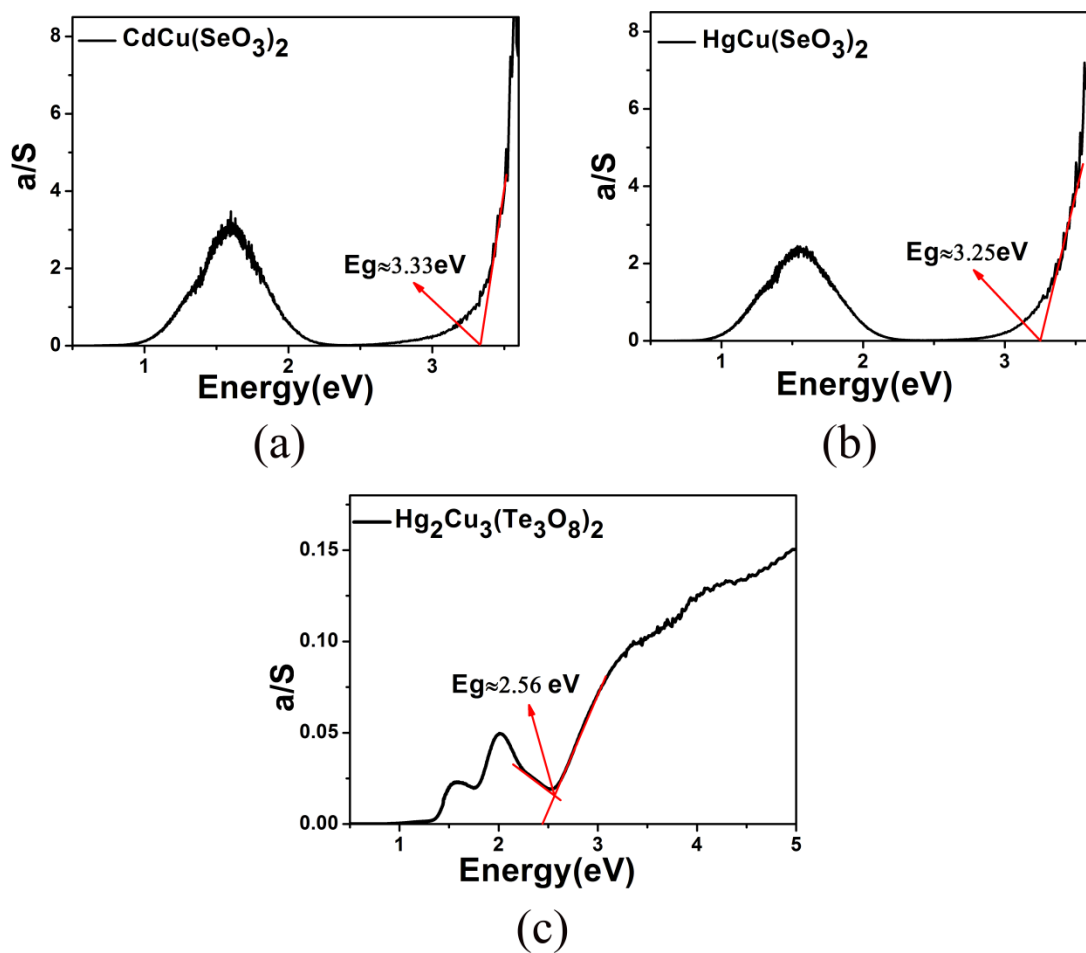


Figure S6. Optical diffuse reflectance spectra of $\text{CdCu}(\text{SeO}_3)_2$ (a), $\text{HgCu}(\text{SeO}_3)_2$ (b) and $\text{Hg}_2\text{Cu}_3(\text{Te}_3\text{O}_8)_2$ (c).

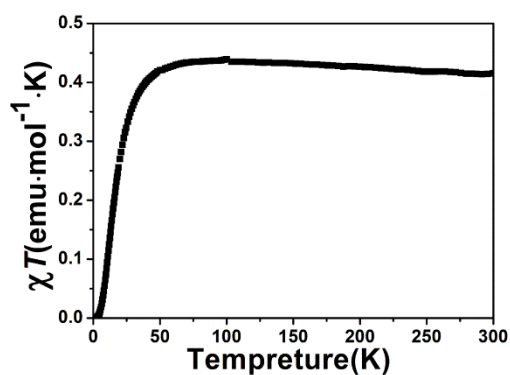


Figure S7. Plot of χT versus T for $\text{HgCu}(\text{SeO}_3)_2$.

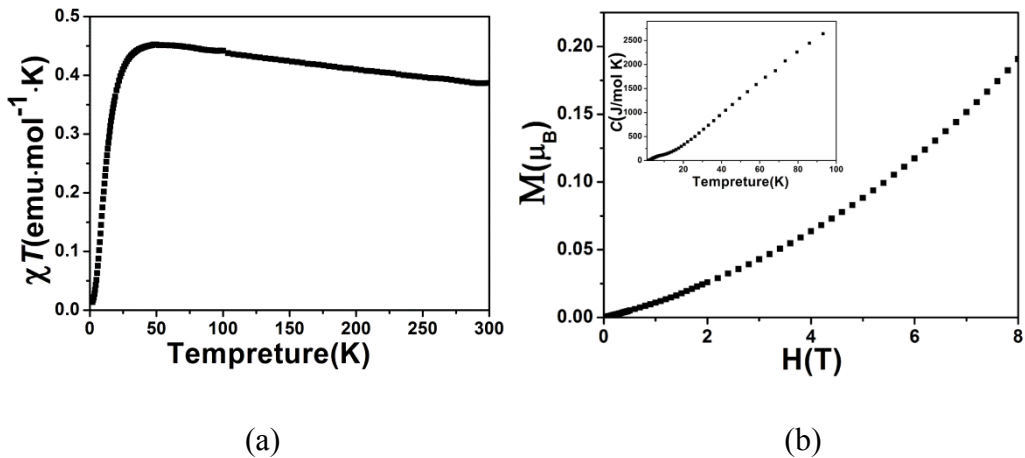


Figure S8. Plot of χT versus T (a), and magnetization versus applied field at 2 K (b) as well as heat capacity measured in zero magnetic fields (the inset) for $\text{CdCu}(\text{SeO}_3)_2$.

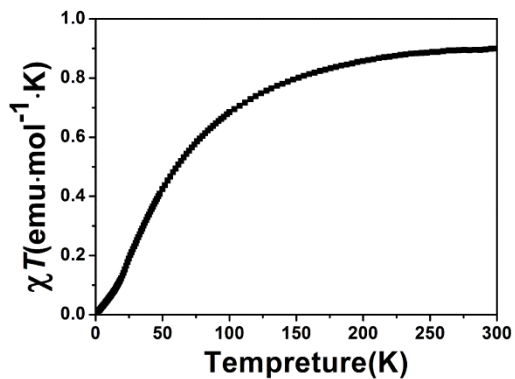


Figure S9. Plot of χT versus T for $\text{Hg}_2\text{Cu}_3(\text{Te}_3\text{O}_8)_2$.