# Supporting Information

# Novel mercury selenidoantimonates with structures ranging from one-dimensional ribbon to three-dimensional open-framework

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**Table S1.** Selected hydrogen bonds data for **1**-**5**[a].

| D-H···A | d(D-H) | d(H···A) | d(D···A) | <(DHA) |
|---|---|---|---|---|
| $[Ni(1,2\text{-pda})_3]HgSb_2Se_5$ (**1**) | | | | |
| N(1)-H(1C)···Se(1)#3 | 0.90 | 2.68 | 3.561(6) | 166.5 |
| N(1)-H(1D)···Se(1) | 0.90 | 2.77 | 3.668(6) | 176.8 |
| N(2)-H(2B)···Se(3)#4 | 0.90 | 2.96 | 3.772(7) | 150.4 |
| N(3)-H(3D)···Se(4)#4 | 0.90 | 2.71 | 3.543(7) | 155.1 |
| N(3)-H(3E)···Se(1) | 0.90 | 2.94 | 3.780(6) | 155.0 |
| N(4)-H(4C)···Se(1)#3 | 0.90 | 2.95 | 3.799(7) | 157.6 |
| N(5)-H(5B)···Se(2)#3 | 0.90 | 2.78 | 3.547(5) | 144.3 |
| N(5)-H(5C)···Se(5)#5 | 0.90 | 2.85 | 3.560(6) | 136.7 |
| N(6)-H(6D)···Se(5)#4 | 0.90 | 2.79 | 3.651(6) | 159.8 |
| C(4)-H(4A)···Se(4)#6 | 0.97 | 2.88 | 3.805(8) | 160.0 |
| $[Mn(dien)_2]HgSb_2Se_5$ (**2**) | | | | |
| N(1)-H(1A)···Se(5)#3 | 0.90 | 2.79 | 3.651(6) | 159.5 |
| N(1)-H(1B)···Se(5)#4 | 0.90 | 2.70 | 3.584(6) | 166.1 |
| N(2)-H(2A)···Se(1) | 0.91 | 2.79 | 3.592(7) | 147.7 |
| N(3)-H(3A)···Se(3)#4 | 0.90 | 2.82 | 3.673(8) | 158.9 |
| N(3)-H(3B)···Se(3)#5 | 0.90 | 2.68 | 3.548(8) | 163.3 |
| N(4)-H(4A)···Se(1) | 0.90 | 2.84 | 3.702(8) | 160.5 |
| N(6A)-H(6C)···Se(4)#5 | 0.90 | 2.80 | 3.61(4) | 151.2 |
| N(6B)-H(6E)···Se(4)#5 | 0.90 | 2.68 | 3.57(4) | 171.7 |

| | | | | |
|---|---|---|---|---|
| C(8B)-H(8D)···Se(5)#3 | 0.97 | 2.97 | 3.93(2) | 177.2 |
| $[Ni(en)_3]Hg_2Sb_2Se_6$ (**3**) | | | | |
| N(1)-H(1C)···Se(3)#3 | 0.90 | 2.85 | 3.653(7) | 148.7 |
| N(1)-H(1D)···Se(2) | 0.90 | 2.72 | 3.492(7) | 144.1 |
| C(2)-H(2A)···Se(1)#6 | 0.97 | 2.78 | 3.648(9) | 149.6 |
| N(2)-H(2C)···Se(2)#7 | 0.90 | 3.00 | 3.747(8) | 141.0 |
| N(3)-H(3C)···Se(2) | 0.90 | 3.01 | 3.777(9) | 144.5 |
| $[Ni(en)(teta)]Hg_2Sb_2Se_6$ (**4**) | | | | |
| N(1)-H(1C)···Se(5) | 0.90 | 2.66 | 3.46(2) | 147.4 |
| N(1)-H(1D)···Se(1) | 0.90 | 2.89 | 3.74(2) | 157.2 |
| N(2)-H(2C)···Se(4)#7 | 0.91 | 2.65 | 3.551(19) | 171.8 |
| N(3)-H(3C)···Se(2)#8 | 0.91 | 3.02 | 3.77(2) | 141.3 |
| N(4)-H(4D)···Se(5) | 0.90 | 2.93 | 3.70(2) | 145.6 |
| N(4)-H(4C)···Se(1)#2 | 0.90 | 3.06 | 3.71(2) | 130.7 |
| N(5)-H(5C)···Se(2)#8 | 0.90 | 2.62 | 3.48(2) | 160.8 |
| N(5)-H(5D)···Se(4)#7 | 0.90 | 3.06 | 3.50(2) | 112.5 |
| N(6)-H(6D)···Se(5)#3 | 0.90 | 2.88 | 3.591(19) | 137.4 |
| C(1)-H(1B)···Se(3) | 0.97 | 2.91 | 3.67(2) | 135.3 |
| C(6)-H(6B)···Se(1)#2 | 0.97 | 2.77 | 3.54(3) | 136.4 |
| C(8)-H(8B)···Se(3)#5 | 0.97 | 2.93 | 3.71(3) | 138.3 |
| $[(Me)_2NH_2][Hg_3Sb_3Se_8]$ (**5**) | | | | |
| N(1)-H(1B)···Se(2) | 0.90 | 2.65 | 3.38(4) | 139.1 |
| N(1)-H(1A)···Se(2)#7 | 0.90 | 2.65 | 3.38(4) | 139.1 |
| C(2)-H(2C)···Se(2)#9 | 0.96 | 2.96 | 3.79(5) | 144.4 |

[a]Symmetry transformations used to generate equivalent atoms:

For **1**: #1 -*x*+2, -*y*, -*z*; #2 -*x*+1, -*y*, -*z*; #3 -*x*+1, -*y*, -*z*+1; #4 -*x*+2, -*y*+1, -*z*+1; #5 *x*, *y*, *z*+1; #6 *x*-1, *y*, *z*.

For **2**: #1 *x*+1/2, *y*, -*z*+3/2; #2 *x*-1/2, *y*, -*z*+3/2; #3 -*x*+1, *y*+1/2, -*z*+3/2; #4 -*x*+1/2, *y*+1/2, *z*; #5 *x*-1/2, -*y*+3/2, -*z*+1.

For **3**: #1 -*x*+3/2, -*y*+3/2, -*z*+1; #2 -*x*+3/2, *y*-1/2, -*z*+3/2; #3 -*x*+3/2, -*y*+1/2, -*z*+1; #4 -*x*+3/2, *y*+1/2, -*z*+3/2; #5 -*x*+1, *y*, -*z*+1/2; #6 *x*-1/2, *y*-1/2, *z*; #7 -*x*+1, -*y*+1, -*z*+1.

For **4**: #1 *x*, *y*-1, *z*; #2 *x*, *y*+1, *z*; #3 *x*+1/2, -*y*+3/2, *z*; #4 *x*-1/2, -*y*+1/2, *z*; #5 *x*+1/2, -*y*+1/2, *z*; #6 *x*-1/2, -*y*+3/2, *z*; #7 -*x*+1/2, *y*-1/2, *z*+1/2; #8 -*x*+1, -*y*+1, *z*+1/2.

For **5**: #1 -*x*+2, -*y*+1, *z*; #2 -*x*+2, *y*+0, *z*-1/2; #3 *x*, -*y*+1, *z*-1/2; #4 -*x*+2, -*y*+1/2, *z*-1/2; #5 *x*, -*y*+1, *z*+1/2; #6 -*x*+2, -*y*+1/2, *z*+1/2; #7 *x*, -*y*+1/2, *z*; #8 -*x*+1, -*y*+1, z; #9 -*x*+1, *y*+0, *z*+1/2.

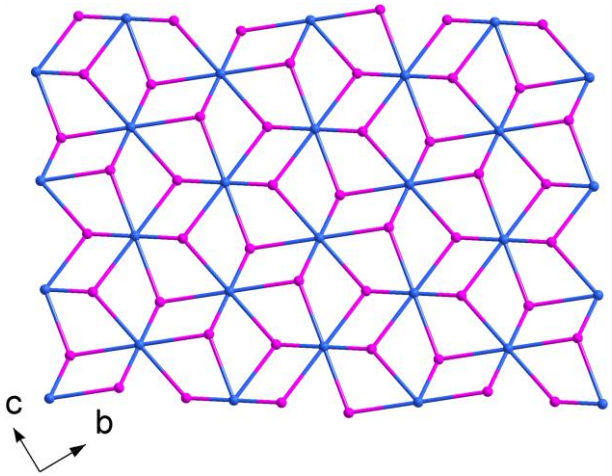


**Fig. S1** Topology of the $[Hg_2Sb_2Se_6]_n^{2n-}$ layer in compounds **3** and **4** (blue node: $\{Hg_2Se_6\}$ group; pink node: $\{SbSe_3\}$ group).

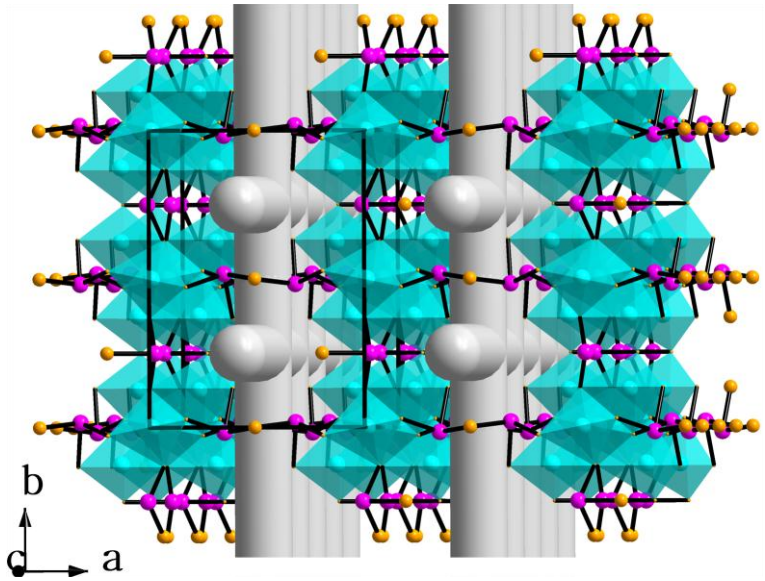


**Fig. S2** The intersecting 2D channels in compound **5** running along the *b* and *c* axes.

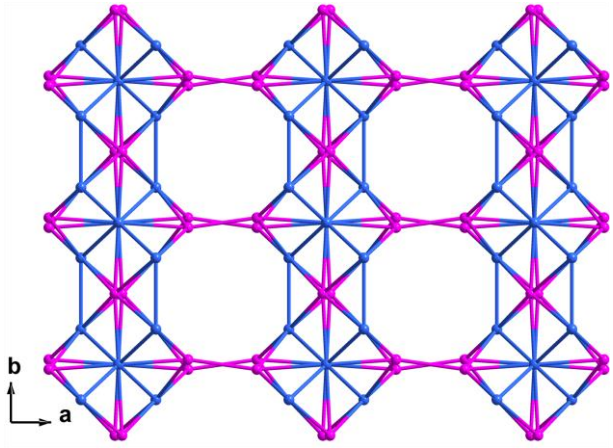


**Fig. S3** The framework topology of compound **5** (blue node: $\{HgSe_4\}$ group; pink node: $\{SbSe_3\}$ group).

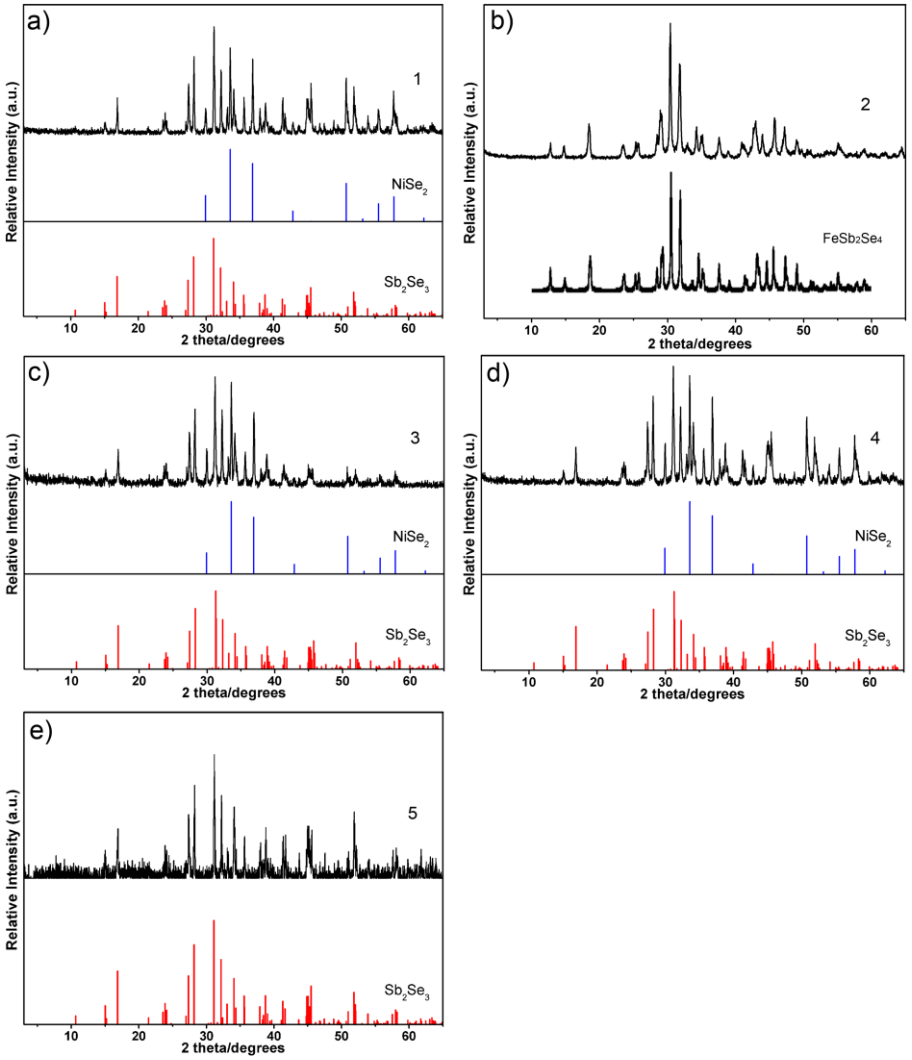


**Fig. S4** The PXRD patterns of the TG residues for compounds **1**-**5**.

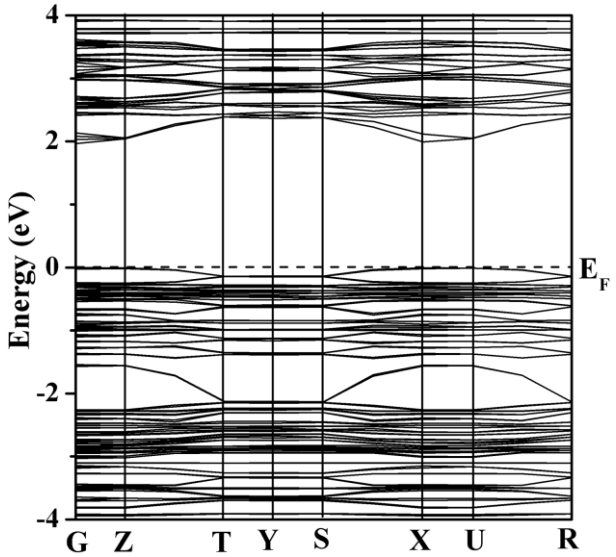


**Fig. S5** The band structure of **2**. Fermi level is set at 0 eV (dashed line).