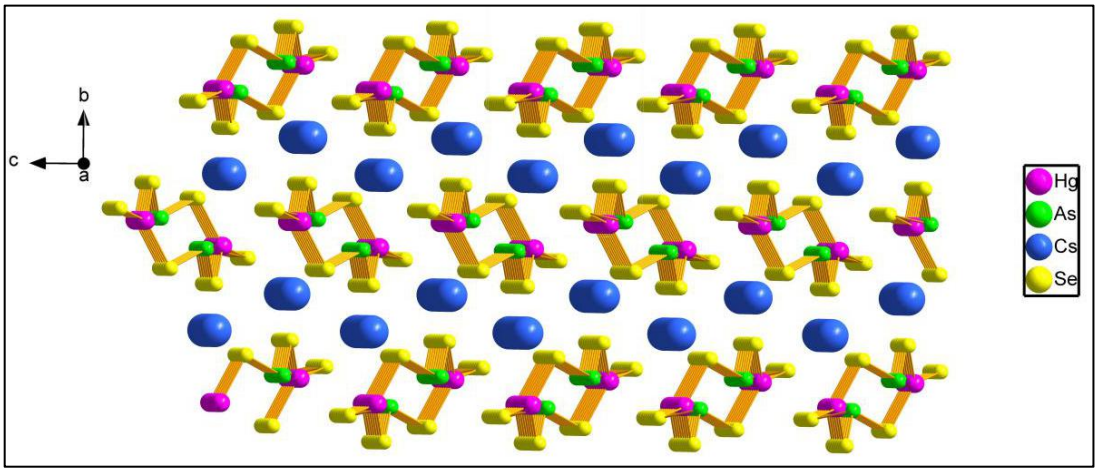
Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Content:



FigS1.one-dimensional chains structure of compound 1

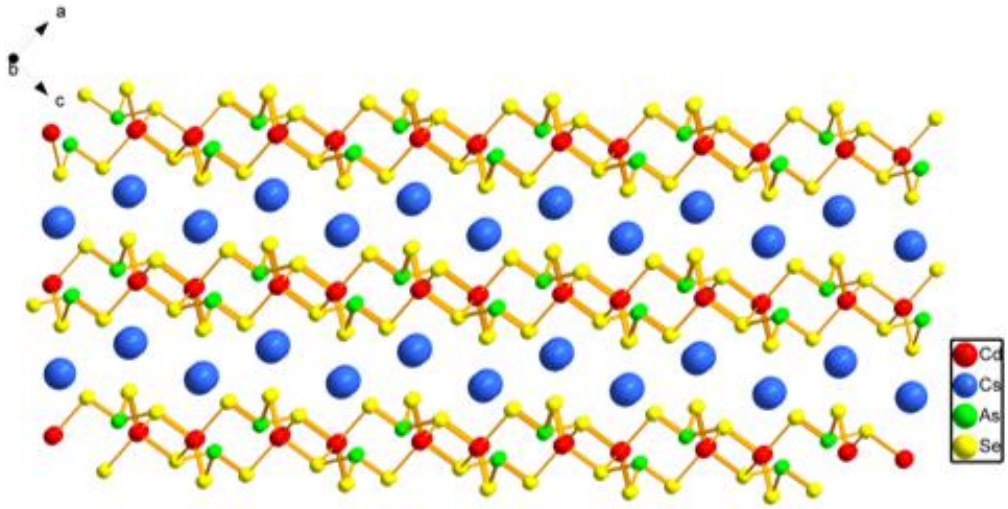


Fig S2. 2-D layer structure of compound $CsCdAsSe_3$(2) .

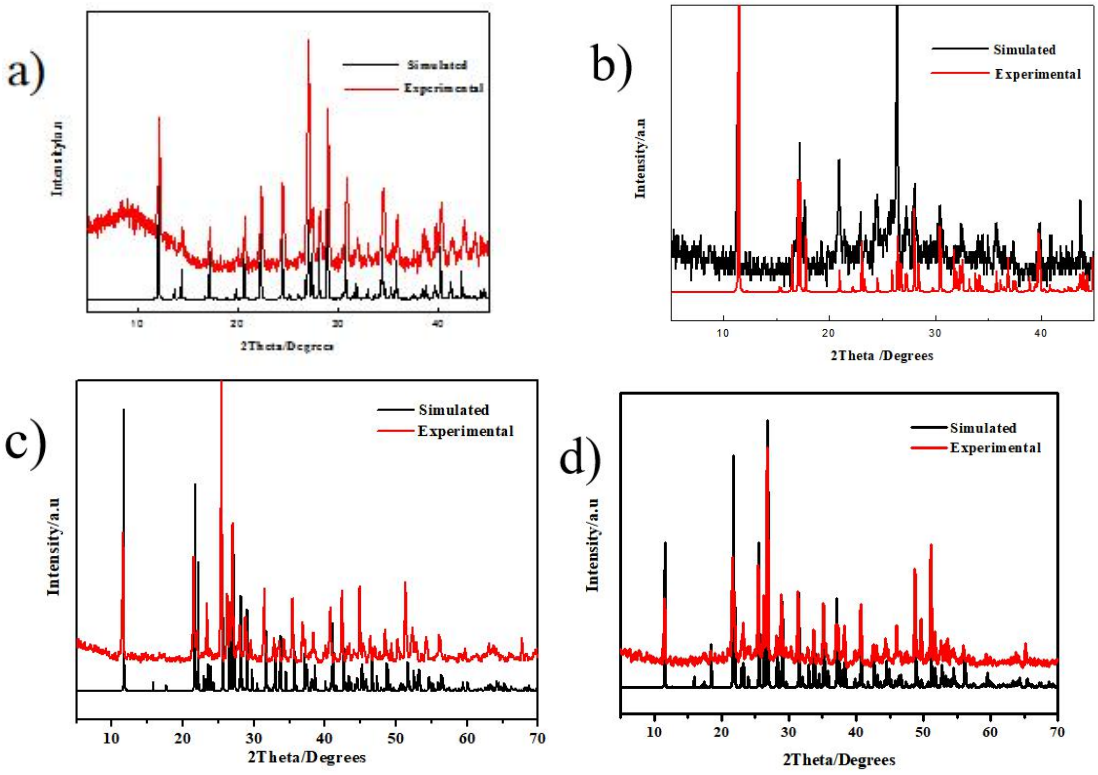


Figure S3. Powder X-ray Diffraction (PXRD) 1 -4（a-d）.

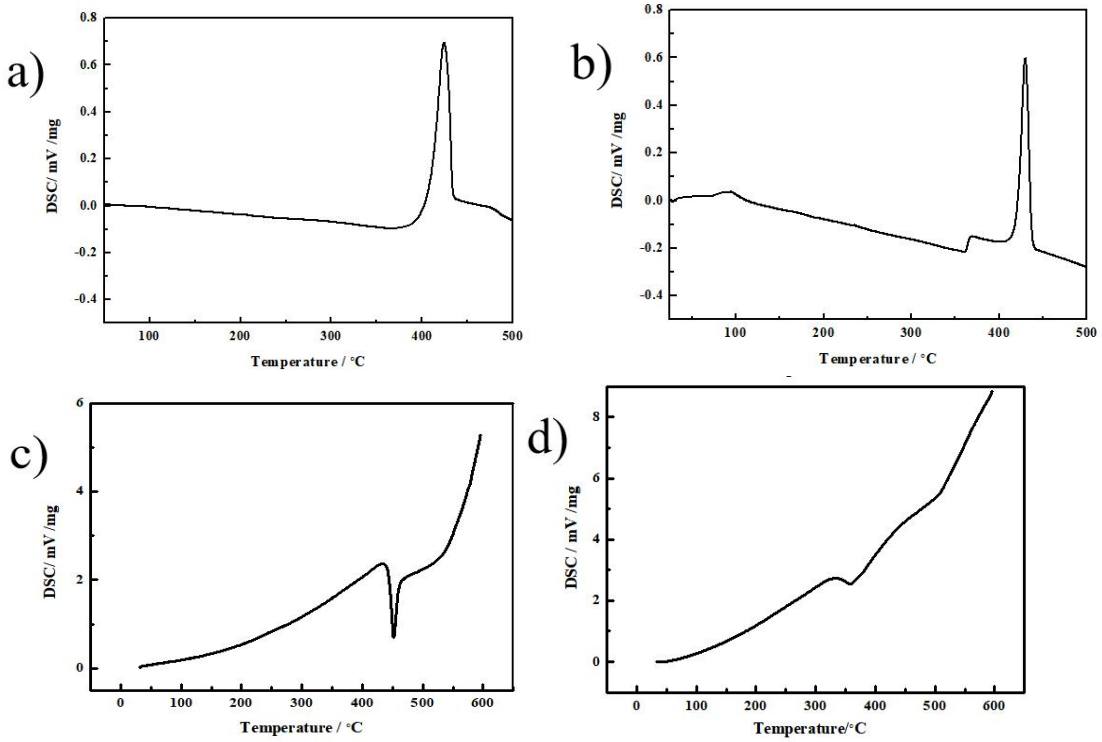


Figure S4. Thermogravimetric And Differeential Scanning Calorimeter Analyses (TG-DSC).1 -4（a-d）

Table S1. Summary of Crystal Data for Compounds 1−4.

	1	2	3	4
Empirical formula	$CsHgAsSe_3$	$CsCdAsSe_3$	$Cs_2Cd_2As_2S_6$	$Cs_2Hg_2As_2S_6$
Formula wt	645.3	557.11	832.82	1009.20
Cryst syst	monoclinic	monoclinic	monoclinic	monoclinic
Space group	P2(1)/n	P2(1)/n	P2(1)/n	P2(1)/n
a /Å	6.957(5)	10.428(6)	10.233(3)	10.090(2)
b /Å	14.9717(11)	6.869(5)	6.631(2)	6.6510(16)
c /Å	7.415(6)	10.794(7)	10.447(3)	10.428(3)
α /deg	90	90	90	90
β /deg	96.926(13)	93.676(10)	95.300(5)	94.686(4)
γ /deg	90	90	90	90
V/Å^3	763.9(10)	771.6(8)	705.9(4)	697.5(3)

Z	4	4	2	2
D_c/(Mg·m^{-3})	5.611	4.796	3.918	4.806
μ/mm^{-1}	43.322	25.771	13.587	32.688
F(000)	1080	952	736	864
GOF	1.025	1.085	1.090	1.180
R1,[a] *wR2[I*>2σ(I)]	0.0357,0.0846	0.0758, 0.1663	0.0311,0.0886	0.066,0.1710
R1, wR2(all data)	0.0463, 0.0879	0.0854,0.1695	0.0386,0.0916	0.0719,0.1725

$aR1 = \Sigma // Fo| - |Fc // /\Sigma|Fo|$, $wR_2 = \Sigma[(w(Fo^2 - Fc^2)^2)/\Sigma[w(Fo^2)^2)]^{1/2}$.

Table S2. Selected bond lengths(Å) and angles(°) for compound $CsHgAsSe_3$(1)

Hg(1)-Se(1)	2.571(2)	As(1)-Se(3)	2.372(2)
Hg(1)-Se(3)	2.581(19)	As(1)-Se(2)#2	2.386(2)
Hg(1)-Se(2)	2.592(2)	As(1)-Se(1)#3	2.404(2)
Se(1)-Hg(1)-Se(3)	120.24(6)	Se(1)-Hg(1)-Se(2)	121.95(5)
Se(3)-Hg(1)-Se(2)	117.41(6)	Se(3)-As(1)-Se(2)#2	101.20(7)
Se(3)-As(1)-Se(1)#3	97.94(7)	Se(2)#2-As(1)-Se(1)#3	102.77(8)
As(1)#11-Se(1)-Hg(1)	91.87(7)	As(1)#2-Se(2)-Hg(1)	93.31(7)
As(1)-Se(3)-Hg(1)	90.48(8)		

Symmetry transformations used to generate equivalent atoms: #2 -*x*+1,-*y*,-*z*; #3 *x*-1,*y*,*z*; #11 *x*+1,*y*,*z*

Table S3. Selected bond lengths(Å) and angles(°) for compound $CsCdAsSe_3$(2)

Cd(1)-Se(1)	2.541(3)	As(1)-Se(2)#8	2.357(4)
Cd(1)-Se(2)	2.616(3)	As(1)-Se(3)	2.406(4)

Cd(1)-S(2)^{ii}	2.6696(15)	Se(3)-Cd(1)#2	2.719(4)
Cd(1)-Se(3)	2.621(4)	Se(2)-As(1)#9	2.357(4)
As(1)-Se(1)#7	2.351(4)	As(1)#7-Se(1)-Cd(1)	95.55(12)
Se(1)-Cd(1)-Se(2)	118.18(11)	Se(1)-Cd(1)-Se(3)	122.96(12)
Se(2)-Cd(1)-Se(3)	103.27(11)	Se(3)-Cd(1)-Se(3)#1	109.52(9)
Se(2)-Cd(1)-Se(3)#1	106.98(11)	Se(1)#7-As(1)-Se(2)#8	102.00(14)
Se(1)#7-As(1)-Se(3)	100.51(14)	Se(2)#8-As(1)-Se(3)	98.58(14)
As(1)-Se(3)-Cd(1)	97.14(12)	As(1)-Se(3)-Cd(1)#2	102.33(12)
Cd(1)-Se(3)-Cd(1)#2	115.22(11)	As(1)#9-Se(2)-Cd(1)	88.34(12)

Symmetry transformations used to generate equivalent atoms: #1 -*x*+1/2,*y*+1/2,-*z*+3/2; *#2* -*x*+1/2,*y*-1/2,-*z*+3/2; #7 -*x*,-*y*,-*z*+1; #8 *x*,*y*-1,*z* ; #9 *x*,*y*+1,*z*

Table S4 Selected bond lengths (Å) and angles (°) for compound $Cs_2Cd_2As_2S_6$ (**3**)

Cd(1)-S(1)	2.501(2)	S(2)-Cd(1)-S(3)	103.01(7)
Cd(1)-S(2)	2.519(2)	S(1)-Cd(1)-S(3)#1	96.97(7)
Cd(1)-S(3)	2.521(2)	S(2)-Cd(1)-S(3)#1	105.16(7)
Cd(1)-S(3)#1	2.616(2)	S(3)-Cd(1)-S(3)#1	111.04(5)
As(1)-S(1)	2.215(2)	S(1)-As(1)-S(2)#9	103.12(9)
As(1)-S(2)#9	2.218(2)	S(1)-As(1)-S(3)#4	100.25(9)
As(1)-S(3)#4	2.278(2)	S(2)#9-As(1)-S(3)#4	98.94(9)
S(3)-As(1)#4	2.278(2)	As(1)-S(1)-Cd(1)	96.86(8)
S(2)-As(1)#9	2.218(2)	As(1)#4-S(3)-Cd(1)	97.89(8)
S(3)-Cd(1)#12	2.616(2)	As(1)#4-S(3)-Cd(1)#12	100.80(8)
S(1)-Cd(1)-S(2)	118.21(7)	Cd(1)-S(3)-Cd(1)#12	114.33(8)

S(1)-Cd(1)-S(3)	121.36(8)	As(1)#9-S(2)-Cd(1)	90.32(8)

Symmetry transformations used to generate equivalent atoms: #1 -*x*+1/2,*y*+1/2,-*z*+3/2; #2 -*x*,-*y*,-*z*+2; #3 *x*+1/2,-*y*-1/2,*z*-1/2; #4 -*x*+1,-*y*,-*z*+2; #5 *x*,*y*-1,*z*; #6 -*x*+1/2,*y*-1/2,-*z*+5/2; #7 *x*-1/2,-*y*-1/2,*z*+1/2; #8 *x*-1/2,-*y*+1/2,*z*+1/2; #9 -*x*+1,-*y*+1,-*z*+2; #10 -*x*+1/2,*y*+1/2,-*z*+5/2; #11 *x*+1/2,-*y*+1/2,*z*-1/2; #12 -*x*+1/2,*y*-1/2,-*z*+3/2; #13 *x*,*y*+1,*z*

Table S5 Selected bond lengths (Å) and angles (°) for compound $Cs_2Hg_2As_2S_6$ (**4**)

Hg(1)-S(2)	2.482(7)	S(3)-Hg(1)-S(1)	104.1(2)
Hg(1)-S(3)	2.485(6)	S(2)-Hg(1)-S(3)#1	91.4(2)
Hg(1)-S(1)	2.529(6)	S(3)-Hg(1)-S(3)#1	109.17(13)
Hg(1)-S(3)#1	2.749(6)	S(1)-Hg(1)-S(3)#1	102.1(2)
As(1)-S(1)#7	2.212(7)	S(1)#7-As(1)-S(2)#4	102.7(3)
As(1)-S(2)#4	2.236(7)	S(1)#7-As(1)-S(3)	98.6(3)
As(1)-S(3)	2.278(7)	S(2)#4-As(1)-S(3)	100.6(3)
S(1)-As(1)#9	2.212(7)	As(1)#9-S(1)-Hg(1)	91.8(2)
S(2)-As(1)#4	2.236(7)	As(1)#4-S(2)-Hg(1)	96.1(3)
S(3)-Hg(1)#5	2.749(6)	As(1)-S(3)-Hg(1)	96.6(2)
S(2)-Hg(1)-S(3)	128.5(2)	As(1)-S(3)-Hg(1)#5	101.0(2)
S(2)-Hg(1)-S(1)	117.4(2)	Hg(1)-S(3)-Hg(1)#5	115.8(2)

Symmetry transformations used to generate equivalent atoms: #1 -*x*+1/2,*y*+1/2,-*z*+1/2; #2 -*x*-1/2,*y*-1/2,-*z*+1/2; #3 *x*-1/2,-*y*+1/2,*z*+1/2; #4 -*x*,-*y*,-*z*; #5 -*x*+1/2,*y*-1/2,-*z*+1/2; #6 *x*-1/2,-*y*-1/2,*z*+1/2; #7 *x*,*y*-1,*z*; #8 *x*+1/2,-*y*-1/2,*z*-1/2; #9 *x*,*y*+1,*z*; #10 *x*+1/2,-*y*+1/2,*z*-1/2; #11 -*x*-1/2,*y*+1/2,-*z*+1/2