Supplementary information for

Syntheses, structure and properties of a new series of organic-inorganic Hg-based halides: adjusting halogens resulted in huge performance mutations

Contents

Table S1. Selected bond lengths (Å) for $[N(CH_3)_4]HgCl_{0.63}Br_{2.37}$

bond	lengths (Å)	bond	lengths (Å)
Hg1-Br6	2.485(5)	Hg2-Cl5A	2.23(2)
Hg1-Br41	3.009(9)	Hg2-Cl4A	2.28(2)
Hg1-Br2	2.500(5)	N2-C1	1.45(2)
Hg1-Br1	2.507(8)	N2-C2	1.48(2)
Hg1-Cl1A	2.23(2)	N2-C5	1.48(2)
Hg1-Cl4A1	2.88(5)	N2-C6	1.48(2)
Hg2-Br3	2.475(5)	C3-N1	1.47(7)
Hg2-Br4	2.533(8)	C4-N1	1.63(6)
Hg2-Br2	2.983(5)	N1-C7	1.54(6)
Hg2-Br5	2.531(10)	N1-C8	1.5000(14)

[1]1+X,+Y,+Z; [2]-1+X,+Y,+Z

Table S2. Selected bond lengths (Å) for $[N(CH_3)_4]HgBrI_2$

bond	lengths (Å)	bond	lengths (Å)
Hg2-Br2	2.651(4)	N1-C1	1.480(14)
Hg2-I2	2.845(3)	N1-C3[2]	1.481(14)
Hg2-I2[1]	2.845(3)	N1-C3	1.481(14)
Hg2-I3	2.666(5)	N1-C2	1.486(14)
Hg1-I1	2.682(4)	N2-C5	1.474(14)
Hg1-I2[2]	2.858(3)	N2-C4[1]	1.489(12)
Hg1-I2	2.858(3)	N2-C4	1.489(12)
Hg1-Br1	2.625(4)	N2-C6	1.481(13)

[1]2-X,+Y,+Z; [2]1-X,+Y,+Z

Table S3. Selected bond lengths (Å) for $[N(CH_3)_4]HgCl_{0.45}I_{2.55}$

bond	lengths (Å)	bond	lengths (Å)
Hg1-I2	2.690(6)	Hg2-I42	2.863(4)
Hg1-I4	2.881(4)	Hg2-Cl2	2.40(3)
Hg1-I4[1]	2.881(4)	N1-C3	1.482(14)
Hg1-I5	2.666(11)	N1-C4	1.479(14)
Hg1-Cl1	2.40(3)	N1-C5	1.479(14)
Hg2-I1	2.733(12)	N2-C1	1.479(14)
Hg2-I3	2.658(6)	N2-C2	1.480(14)
Hg2-I4	2.863(4)	N2-C6	1.49(3)

[1]2-X,+Y,+Z; [2]1-X,+Y,+Z

Table S4. Selected bond angles (°) for $[N(CH_3)_4]HgCl_{0.63}Br_{2.37}$

bond	angles (°)	bond	angles (°)
Br6-Hg1-Br4[1]	95.3(2)	Cl5A-Hg2-Br2	96.1(16)
Br6-Hg1-Br2	118.8(2)	Cl5A-Hg2-Cl4A	105.9(18)
Br6-Hg1-Br1	121.5(4)	Cl4A-Hg2-Br3	129.8(14)
Br6-Hg1-Cl4A1	86.9(7)	Cl4A-Hg2-Br2	97.7(13)
Br2-Hg1-Br41	89.34(19)	Hg2-Br4-Hg1[2]	92.8(3)
Br2-Hg1-Br1	118.7(4)	Hg1-Br2-Hg2	95.35(17)

Br2-Hg1-Cl4A1	87.2(7)	C1-N2-C2	110.9(19)
Br1-Hg1-Br4[1]	94.9(4)	C1-N2-C5	110.7(19)
Br1-Hg1-Cl4A1	105.4(12)	C1-N2-C6	108.9(19)
Cl1A-Hg1-Br6	119.8(15)	C2-N2-C6	108.7(19)
Cl1A-Hg1-Br2	121.2(15)	C5-N2-C2	108.2(19)
Cl1A-Hg1-Cl4A1	100(2)	C5-N2-C6	109.4(19)
Br3-Hg2-Br4	120.5(3)	C3-N1-C4	112(4)
Br3-Hg2-Br2	93.63(17)	C3-N1-C7	119(4)
Br3-Hg2-Br5	122.6(4)	C3-N1-C8	106(4)
Br4-Hg2-Br2	91.0(2)	C7-N1-C4	123(4)
Br5-Hg2-Br4	116.5(5)	C8-N1-C4	84(3)
Br5-Hg2-Br2	91.8(5)	C8-N1-C7	105(3)
Cl5A-Hg2-Br3	121.3(11)	Hg2-Cl4A-Hg1[2]	102.0(15)

[1]1+X,+Y,+Z; [2]-1+X,+Y,+Z

Table S5. Selected bond angles (°) for $[N(CH_3)_4]HgBrI_2$

bond	angles (°)	bond	angles (°)
Br2-Hg2-I2[1]	111.32(9)	C1-N1-C3[2]	111(3)
Br2-Hg2-I2	111.32(9)	C1-N1-C3	111(3)
Br2-Hg2-I3	126.62(15)	C1-N1-C2	122(5)
I2-Hg2-I2[1]	96.36(13)	C32-N1-C3	103(5)
I3-Hg2-I2	103.40(11)	C3-N1-C2	104(3)
I3-Hg2-I2[1]	103.40(11)	C32-N1-C2	104(3)
I1-Hg1-I2[2]	109.31(10)	C5-N2-C4	99(2)
I1-Hg1-I2	109.31(10)	C5-N2-C4[1]	99(2)
I2-Hg1-I22	92.55(12)	C5-N2-C6	115.5(15)
Br1-Hg1-I1	123.47(14)	C4-N2-C4[1]	113(2)
Br1-Hg1-I2[2]	108.91(10)	C6-N2-C4	114.3(11)
Br1-Hg1-I2	108.91(10)	C6-N2-C4[1]	114.3(11)
Hg2-I2-Hg1	100.23(9)	C1-N1-C32	111(3)

[1]2-X,+Y,+Z; [2]1-X,+Y,+Z

Table S6. Selected bond angles (°) for $[N(CH_3)_4]HgCl_{0.45}I_{2.55}$

bond	angles (°)	bond	angles (°)
I2-Hg1-I4[1]	109.75(14)	I3-Hg2-I4	112.03(13)
I2-Hg1-I4	109.75(14)	I3-Hg2-I4[2]	112.03(13)
I4-Hg1-I4[1]	91.47(19)	I4-Hg2-I4[2]	96.21(19)
I5-Hg1-I2	122.7(5)	Cl2-Hg2-I3	122(2)
I5-Hg1-I4	109.4(3)	Cl2-Hg2-I4	105.6(15)
I5-Hg1-I4[1]	109.4(3)	Hg2-I4-Hg1	99.45(15)
Cl1-Hg1-I2	128(3)	C4-N1-C3	108(2)
Cl1-Hg1-I4[1]	105.9(18)	C5-N1-C3	108(2)
Cl1-Hg1-I4	105.9(18)	C5-N1-C4	109(2)

I1-Hg2-I4[2]	102.2(2)	C1-N2-C2	115.4(16)
I1-Hg2-I4	102.2(2)	C1-N2-C6	93(6)
I3-Hg2-I1	127.4(3)	C2-N2-C6	115(2)

[1]2-X,+Y,+Z; [2]1-X,+Y,+Z

Table S7. Intermolecular C-H···X Interactions in $[N(CH_3)_4]HgCl_{0.63}Br_{2.37}$ (Å, °)

C - H···X	d (H···X)	d (C···X)	∠(C - H···X)
[C1 - H1B···Br6]	3.016	3.659	125.798
[C3- H3A···Br6]	2.676	3.755	136.18
[C7 - H7C···Br4]	2.851	3.603	125.968

Table S8. Infrared Vibrations (cm^{-1}) for $[N(CH_3)_4]HgCl_{0.45}I_{2.55}$

Wavenumber (cm^{-1})	Assignments
3030	ν(C-H)
1475	δ(C-H)
1281	ω (CH_2)
946	ν(C-N)

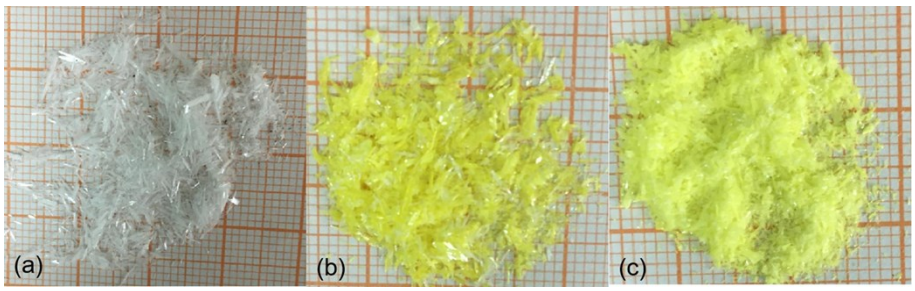

Figure S1. Photographs of polycrystalline powders of $[N(CH_3)_4]HgCl_{0.63}Br_{2.37}$ (a) 、$[N(CH_3)_4]HgBrI_2$ (b) and $[N(CH_3)_4]HgCl_{0.45}I_{2.55}$ (c)

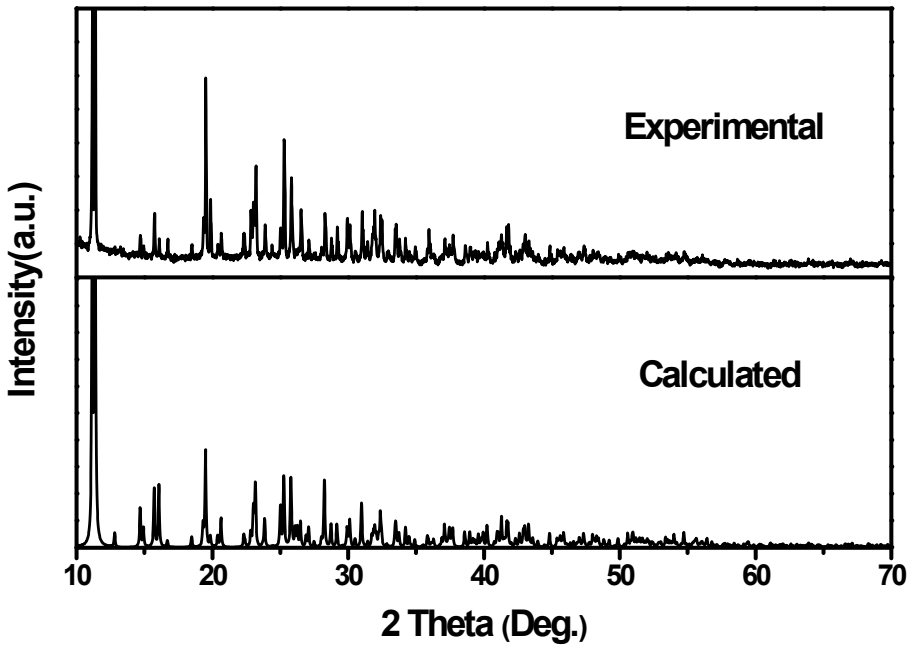

Figure S2. Simulated and measured powder X-ray diffraction patterns of $[N(CH_3)_4]HgCl_{0.63}Br_{2.37}$

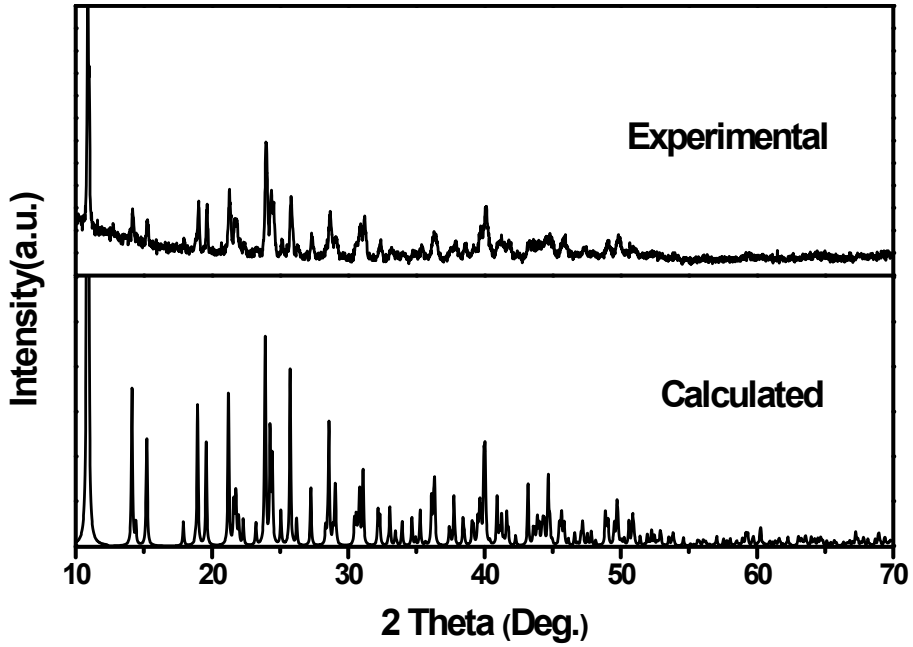

Figure S3. Simulated and measured powder X-ray diffraction patterns of $[N(CH_3)_4]HgBrI_2$

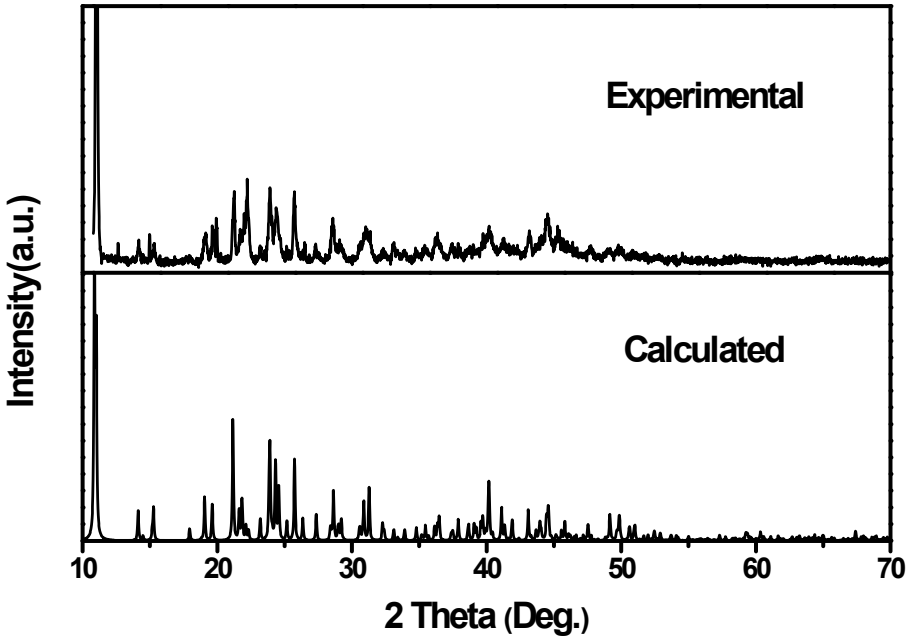

Figure S4. Simulated and measured powder X-ray diffraction patterns of $[N(CH_3)_4]HgCl_{0.45}I_{2.55}$

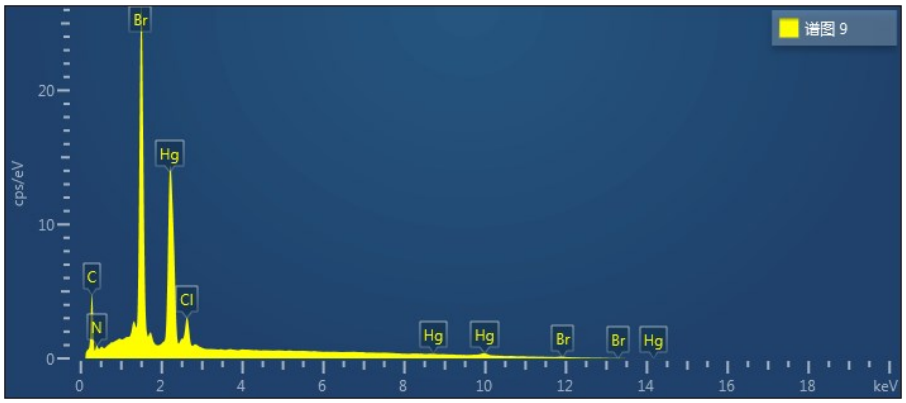

Figure S5. EDS patterns of $[N(CH_3)_4]HgCl_{0.63}Br_{2.37}$

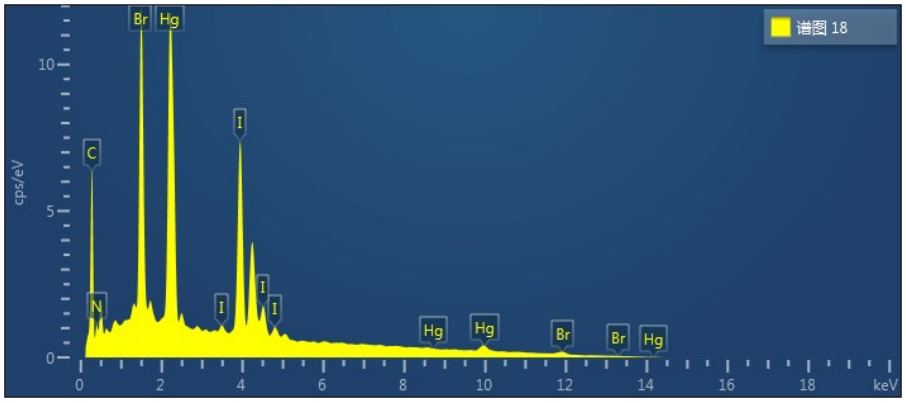

Figure S6. EDS patterns of $[N(CH_3)_4]HgBrI_2$

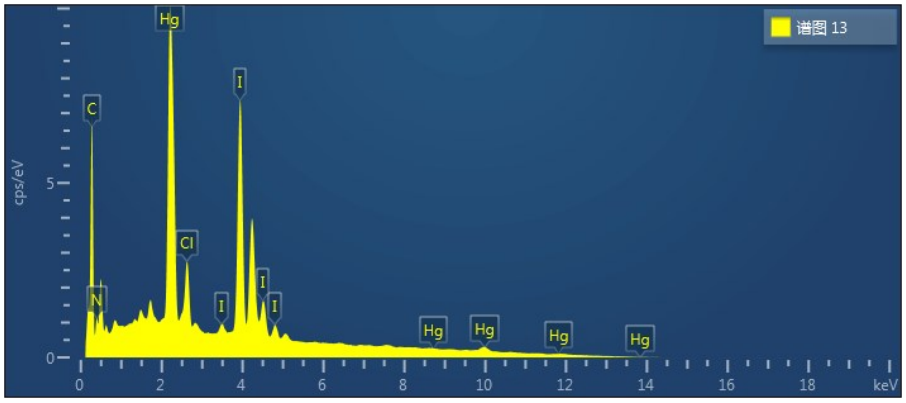

Figure S7. EDS patterns of $[N(CH_3)_4]HgCl_{0.45}I_{2.55}$

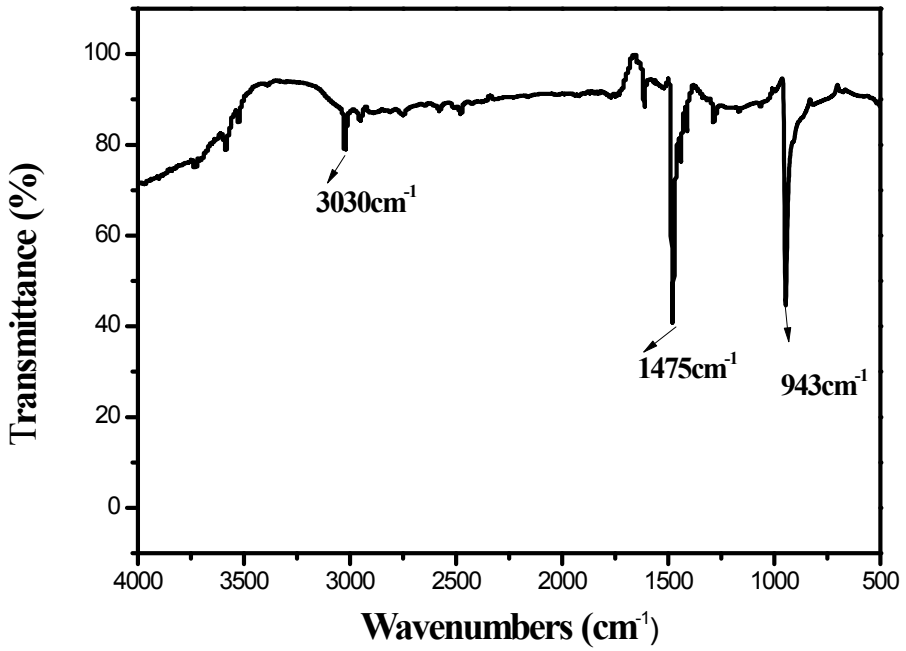

Figure S8. The infrared spectrum of $[N(CH_3)_4]HgCl_{0.63}Br_{2.37}$

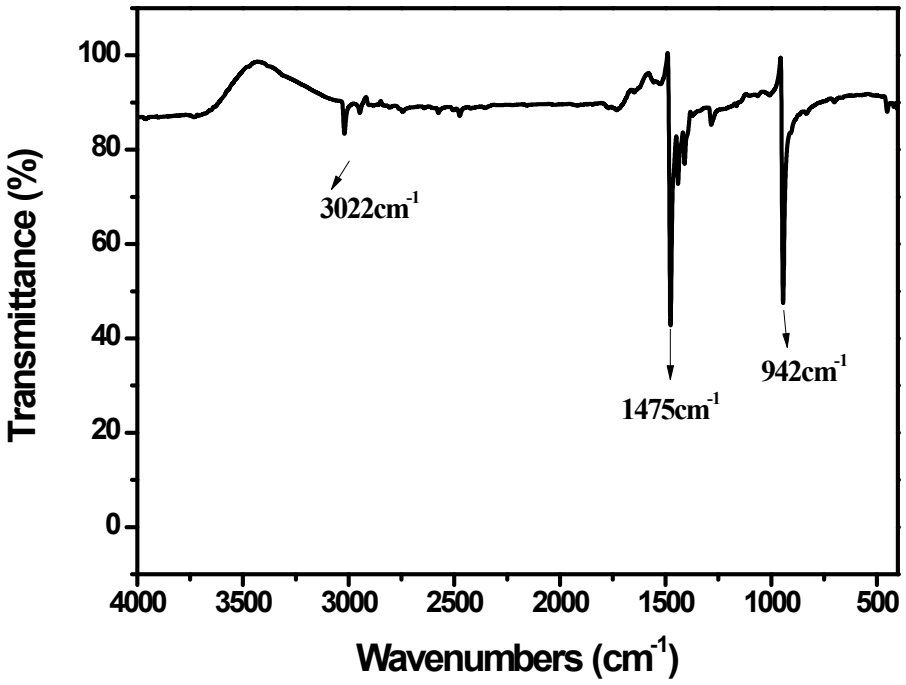

Figure S9. The infrared spectrum of $[N(CH_3)_4]HgBrI_2$

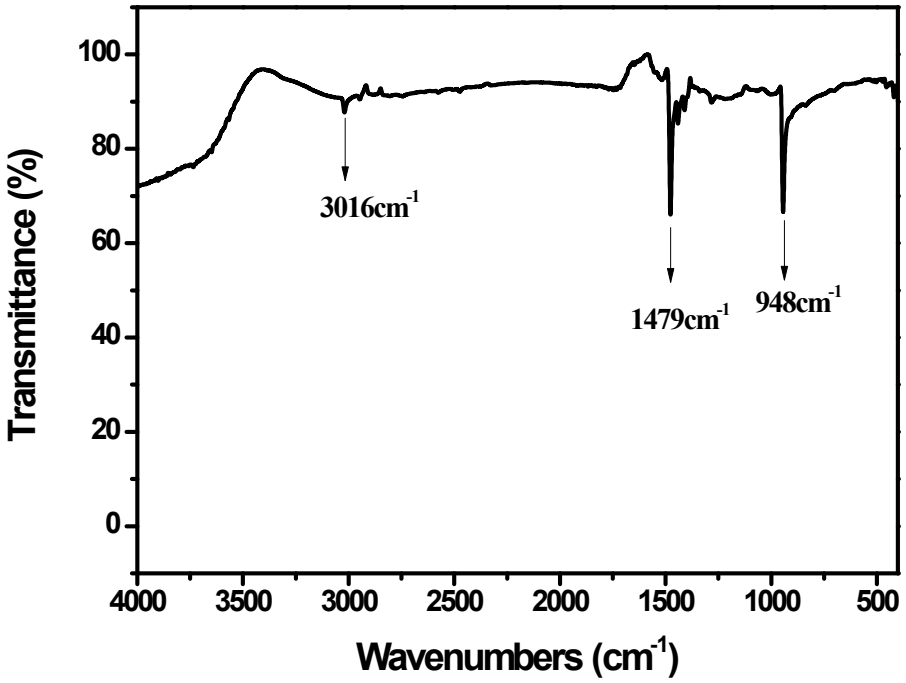

Figure S10. The infrared spectrum of $[N(CH_3)_4]HgCl_{0.45}I_{2.55}$

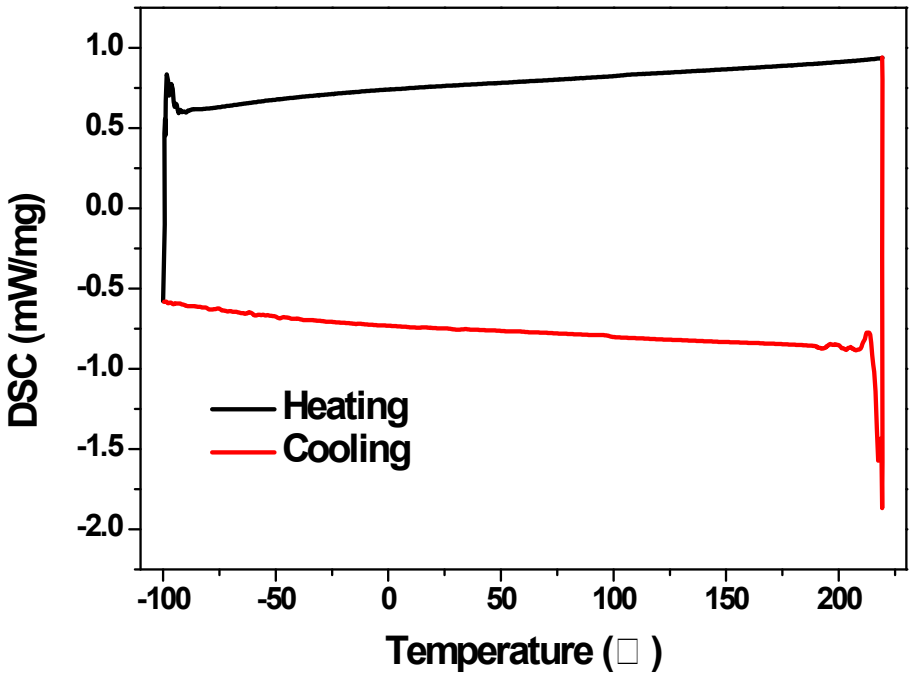

Figure S11. The DSC curves of $[N(CH_3)_4]HgCl_{0.63}Br_{2.37}$

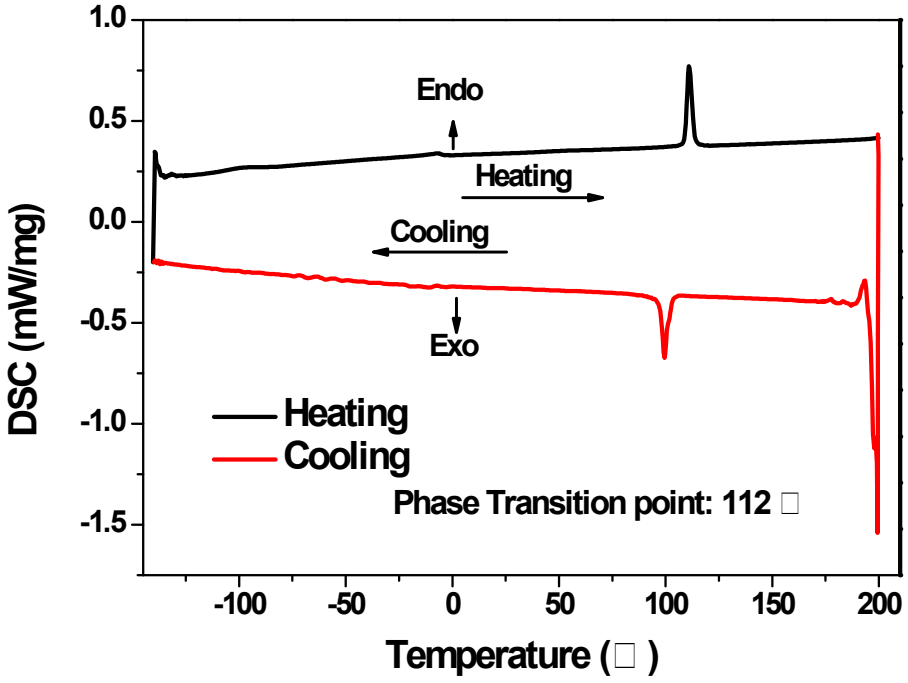

Figure S12. The DSC curves of $[N(CH_3)_4]HgBrI_2$

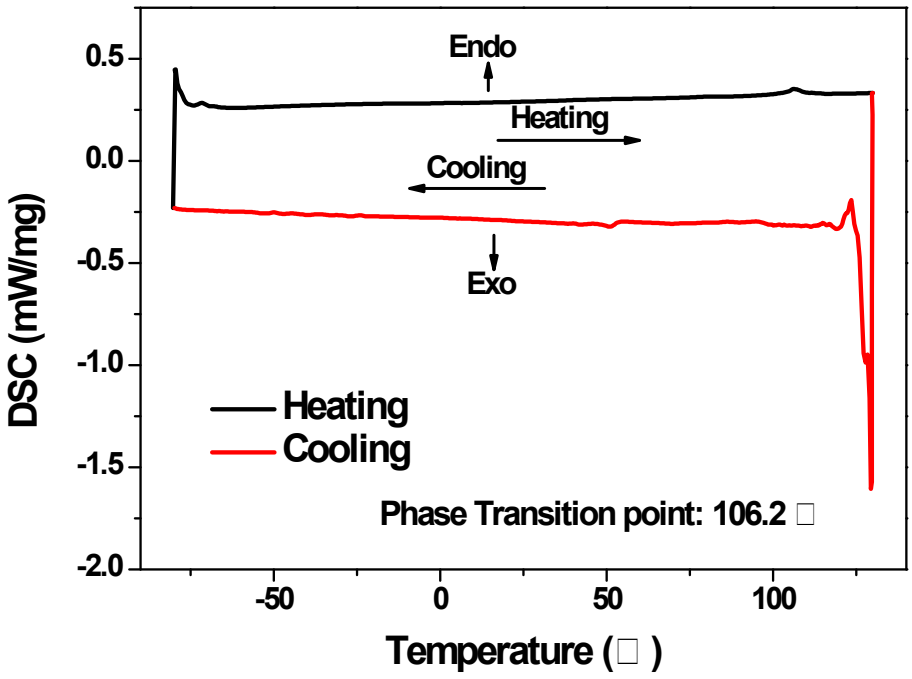

Figure S13. The DSC curves of $[N(CH_3)_4]HgCl_{0.45}I_{2.55}$

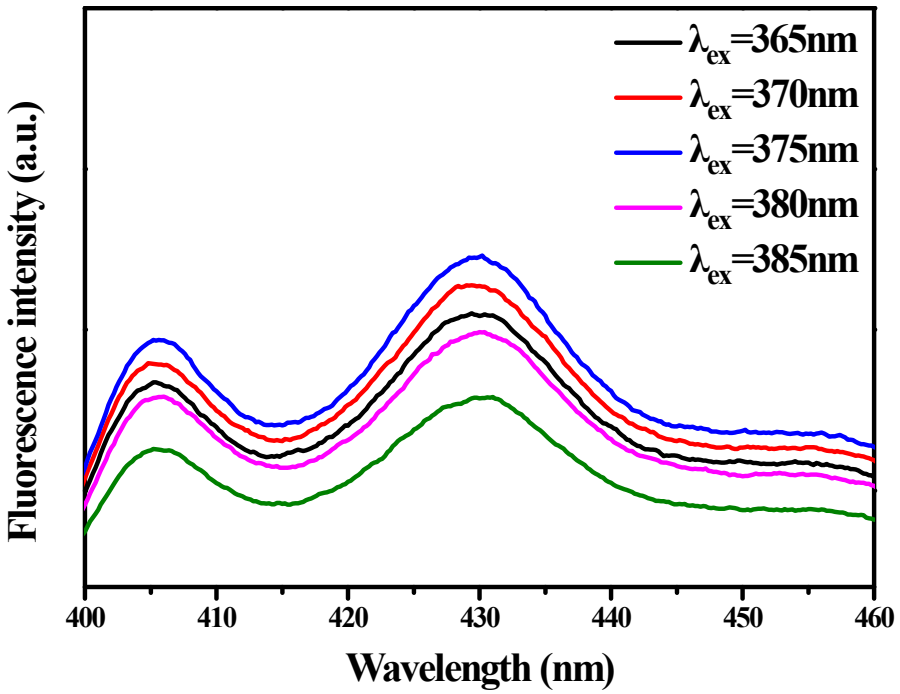

Figure S14. Emission spectra of $[N(CH_3)_4]HgCl_{0.63}Br_{2.37}$ under different excitation wavelengths.

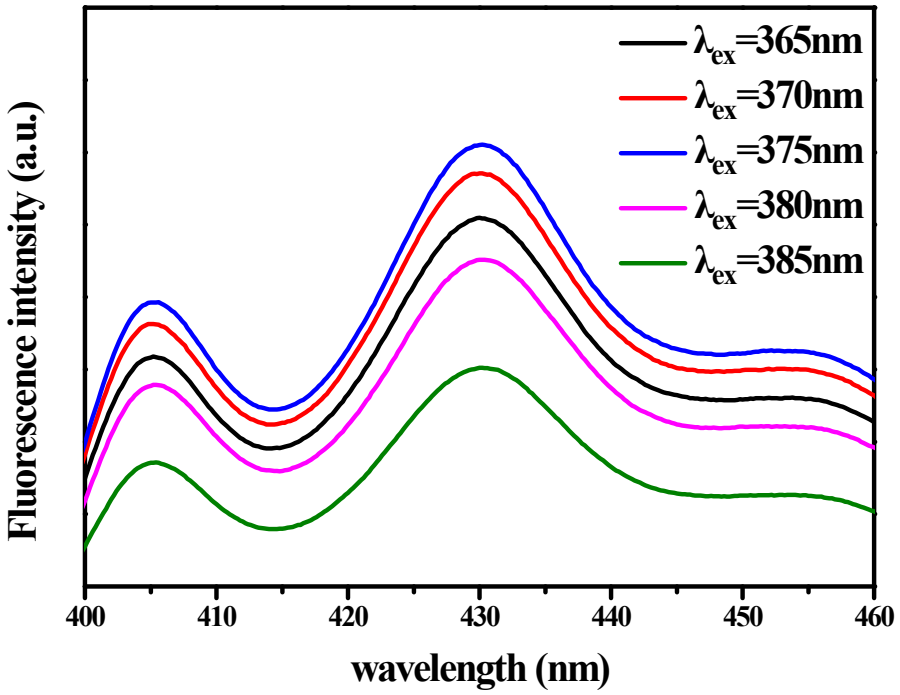

Figure S15. Emission spectra of $[N(CH_3)_4]HgBrI_2$ under different excitation wavelengths.

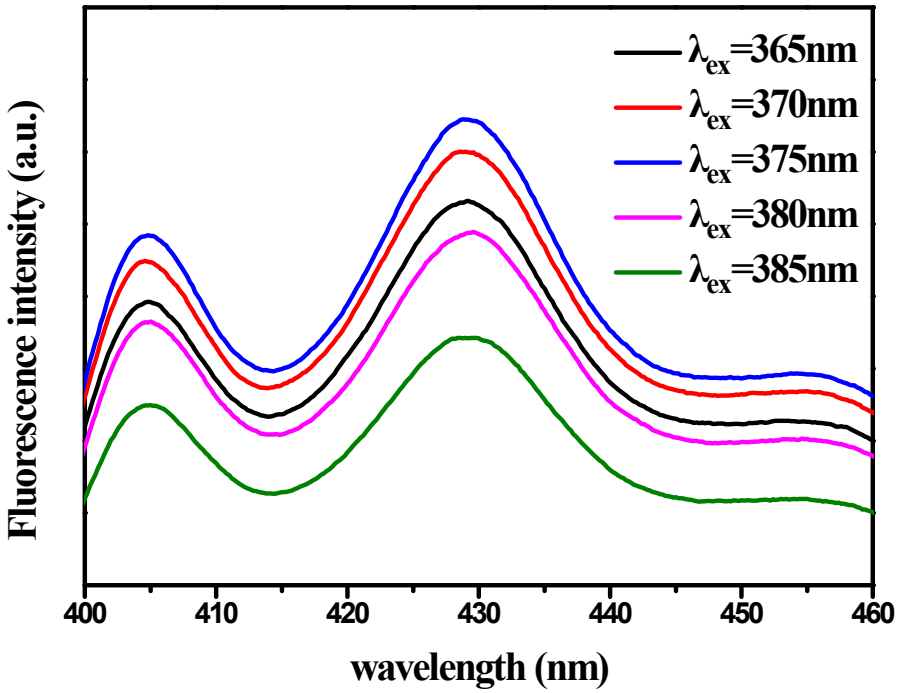

Figure S16. Emission spectra of $[N(CH_3)_4]HgCl_{0.45}I_{2.55}$ under different excitation wavelengths.

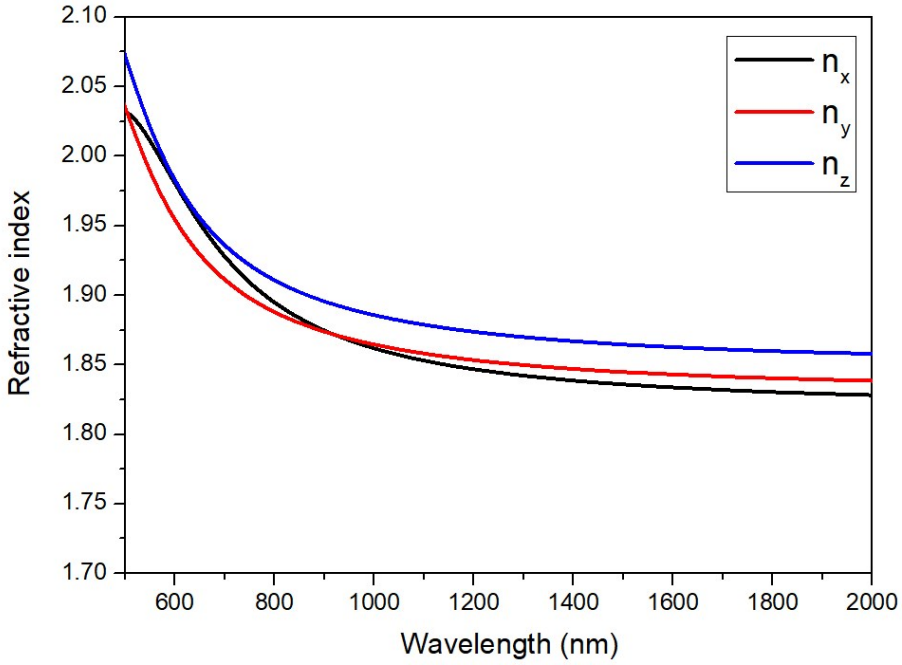

Figure S17. The simulated refractive index of $[N(CH_3)_4]HgBrI_2$