Electronic Supplementary Material (ESI) for RSC Advances.

Table S1

Complete crystal data and structure refinement for mercury iodide and thiocyanate complex.

Compound	$HgLI_2$	$HgL(SCN)_2$
Empirical formula	$C_{22}H_{23}HgI_2N_5O_4$	$C_{24}H_{23}HgN_7O_4S_2$
Formula weight	875.84	738.20
Temperature (K)	173(2)	173(2)
Wavelength (Å)	0.71073	0.71073
Crystal system	Triclinic	Monoclinic
Space group	$P\bar{1}$	$P2_1/n$
Unit cell dimensions	a = 7.1329(3) Å b = 7.3046(3) Å c = 14.7198(7) Å α = 97.922(2)° β = 97.425(2)° γ = 117.0955(18)°	a = 8.4523(8) Å b = 11.6846(12) Å c = 27.114(3) Å α = 90° β = 91.952(4)° γ = 90°
Volume ($Å^3$)	660.03(5)	2676.3(5)
Z	1	4
Calculated density (Mg/m^3)	2.203	1.832
Absorption coefficient(mm^{-1})	8.205	5.952
F(000)	408	1440
Crystal size (mm)	0.096 x 0.062 x 0.034	0.260 x 0.114 x 0.076
Theta range for data collection (°)	2.863 to 27.632	1.743 to 26.181
Index ranges	$-6 \le h \le 9$ $-9 \le k \le 9$ $-19 \le l \le 19$	$-10 \le h \le 7$ $-14 \le k \le 13$ $-32 \le l \le 33$
Reflections collected	7494	29879
Independent reflections	4034	5364
R_{int}	0.0278	0.0651
Completeness to theta (%)	94.4	100
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents
Max. and min. transmission	0.7456 and 0.5998	0.7453 and 0.5799
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data/restraints/parameters	4034/3/302	5364/327/351
Goodness-of-fit on F^2	1.004	1.166
Final R indices [$I>2\sigma(I)$]	$R_1 = 0.0326$, $wR_2 = 0.0767$	$R_1 = 0.0822$, $wR_2 = 0.2136$
R indices (all data)	$R_1 = 0.0359$, $wR_2 = 0.0778$	$R_1 = 0.0916$, $wR_2 = 0.2204$
Largest diff. peak and hole($e.Å^{-3}$)	1.744 and -1.024	4.827 and -4.178

Table S2

Bond lengths (Å) and bond angles (˚) optimized of mercury chloride, bromide and azide complexes by using LANL2DZ basis set.

	$HgLCl_2$	$HgLBr_2$	$HgL(N_3)_2$	
Bond length (Å)	*B3LYP*	*B3LYP*	*Bond length (Å)*	*B3LYP*
Hg–N2	2.57049	2.62221	Hg1–N2	2.62468
Hg–N3	2.57709	2.56954	Hg1–N3	2.52692
Hg–N4	2.57048	2.62221	Hg1–N4	2.57720
Hg–I1	2.61379	2.75913	Hg1–S1	2.32198
Hg–I2	2.62447	2.76001	Hg1–S2	2.30152
Bond angle (°)			*Bond angle (°)*	
N2–Hg–N3	69.97588	69.62670	N2–Hg1–N3	71.14563
N2–Hg–N4	130.90818	132.70187	N2–Hg1–N4	131.84860
N2–Hg–I1	99.50708	98.59538	N2–Hg1–S1	94.25254
N2–Hg–I2	100.68438	100.66516	N2–Hg1–S2	107.87220
N3–Hg–N4	69.97579	69.62672	N3–Hg1–N4	70.03299
N3–Hg–I1	78.94284	82.08764	N3–Hg1–S1	72.31888
N3–Hg–I2	150.99300	147.26229	N3–Hg1–S2	151.87792
N4–Hg–I1	99.50809	98.59512	N4–Hg1–S1	99.99616
N4–Hg–I2	100.68496	100.66519	N4–Hg1–S2	93.85728
I1–Hg–I2	130.06416	130.65008	S1–Hg1–S2	134.74335
			Hg1–S1–C1S	132.00542
			Hg1–S2–C2S	93.85728
			S1–C1S–N1S	176.92143
			S2–C2S–N2S	176.73458