Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Varying Coordination Modes of Amide Ligand in Group 12 Hg(II) and Cd(II) Complexes: Synthesis, Crystal Structure and Nonlinear Optical Properties

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Table-S1 Selected bond lengths (Å) and bond angles(°) of 1

Bond distance	**(Å)**
Hg(1)-N(10)	2.120(4)
Hg(1)-N(2)	2.118(4)
Hg(1)-N(9)	2.494(4)
Hg(1)-N(3)	2.522(4)
Hg(1)-N(1)	2.694(4)
Hg(1)-Hg(2)	3.3481(2)
Hg(2)-N(7)	2.121(3)
Hg(2)-N(4)	2.128(3)
Hg(2)-N(8)	2.475(4)
Hg(2)-N(5)	2.495(4)
Hg(2)-N(1)	2.644(3)
Hg(2)-N(6)	2.698(4)
Bond angle	**(°)**
N(2)-Hg(1)-N(10)	168.19(13)
N(2)-Hg(1)-N(9)	111.43(14)
N(10)-Hg(1)-N(9)	74.16(13)
N(2)-Hg(1)-N(3)	73.14(13)
N(10)-Hg(1)-N(3)	112.83(13)
N(9)-Hg(1)-N(3)	124.90(12)

N(2)-Hg(1)-N(1)	69.77(12)
N(10)-Hg(1)-N(1)	102.64(13)
N(9)-Hg(1)-N(1)	75.88(11)
N(3)-Hg(1)-N(1)	142.37(11)
N(2)-Hg(1)-Hg(2)	81.14(9)
N(10)-Hg(1)-Hg(2)	87.04(9)
N(9)-Hg(1)-Hg(2)	117.31(8)
N(3)-Hg(1)-Hg(2)	117.60(9)
N(1)-Hg(1)-Hg(2)	50.49(7)
N(7)-Hg(2)-N(4)	172.40(14)
N(7)-Hg(2)-N(8)	73.80(13)
N(4)-Hg(2)-N(8)	113.80(13)
N(7)-Hg(2)-N(5)	102.64(13)
N(4)-Hg(2)-N(5)	73.66(13)
N(8)-Hg(2)-N(5)	121.68(12)
N(7)-Hg(2)-N(1)	112.88(12)
N(4)-Hg(2)-N(1)	70.25(12)
N(8)-Hg(2)-N(1)	76.42(12)
N(5)-Hg(2)-N(1)	143.82(11)
N(7)-Hg(2)-N(6)	69.79(12)
N(4)-Hg(2)-N(6)	102.85(12)
N(8)-Hg(2)-N(6)	140.84(11)
N(5)-Hg(2)-N(6)	80.70(12)

N(1)-Hg(2)-N(6)	104.89(11)
N(7)-Hg(2)-Hg(1)	89.69(9)
N(4)-Hg(2)-Hg(1)	87.15(9)
N(8)-Hg(2)-Hg(1)	113.71(9)
N(5)-Hg(2)-Hg(1)	124.55(9)
N(1)-Hg(2)-Hg(1)	51.83(8)
N(6)-Hg(2)-Hg(1)	53.19(7)

Table-S2 Selected bond lengths (Å) and bond angles(°) of 2

Bond distance	**(Å)**
Cd(1)-O(4)	2.380(4)
Cd(1)-N(5)	2.387(4)
Cd(1)-N(10)	2.396(4)
Cd(1)-O(2)	2.410(4)
Cd(1)-Cl(2)	2.5185(12)
Cd(1)-Cl(1)	2.5271(12)
Cd(2)-O(1)	2.331(4)
Cd(2)-N(4)	2.341(4)
Cd(2)-Cl(3)	2.5969(14)
Bond angle	**(°)**
O(4)-Cd(1)-N(5)	71.41(14)
O(4)-Cd(1)-N(10)	88.81(13)
N(5)-Cd(1)-N(10)	155.50(13)
O(4)-Cd(1)-O(2)	79.72(15)
N(5)-Cd(1)-O(2)	90.75(14)
N(10)-Cd(1)-O(2)	71.09(14)
O(4)-Cd(1)-Cl(2)	94.63(13)
N(5)-Cd(1)-Cl(2)	96.54(11)
N(10)-Cd(1)-Cl(2)	99.41(10)
O(2)-Cd(1)-Cl(2)	168.89(10)
O(4)-Cd(1)-Cl(1)	164.21(12)
N(5)-Cd(1)-Cl(1)	96.08(10)
N(10)-Cd(1)-Cl(1)	100.46(10)
O(2)-Cd(1)-Cl(1)	91.14(10)
Cl(2)-Cd(1)-Cl(1)	96.39(5)
O(1)#1-Cd(2)-O(1)	180.0(2)
O(1)#1-Cd(2)-N(4)	85.97(14)

O(1)-Cd(2)-N(4)	94.03(14)
N(4)-Cd(2)-N(4)#1	180.0(1)
O(1)#1-Cd(2)-Cl(3)	92.96(11)
O(1)-Cd(2)-Cl(3)	87.04(11)
N(4)-Cd(2)-Cl(3)	89.76(11)

Table-S3: Hydrogen Bonding in 1 and 2 [Å and (°)].

	D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
			1		
1	C(28)-H(28)…O(4)#(7)	0.950(1)	2.476(1)	3.251(1)	138.74(3)
2	C(34) -H(34)…O(2)#(8)	0.950(1)	2.541(1)	3.417(1)	153.29(4)
Equivalent positions (7)-x,-y+2,-z+1 (8) -x,-y+2,-z+2					
			2		
1	C(10)-H(10)…Cl(1)#(2)	0.950(1)	2.884(1)	3.797(1)	161.58(1)
2	C(17) -H(17)…Cl(2)#(2)	0.950(1)	2.672(1)	3.570(1)	157.97(1)
Equivalent Position (2) x-1/2,+y,-z+1/2					

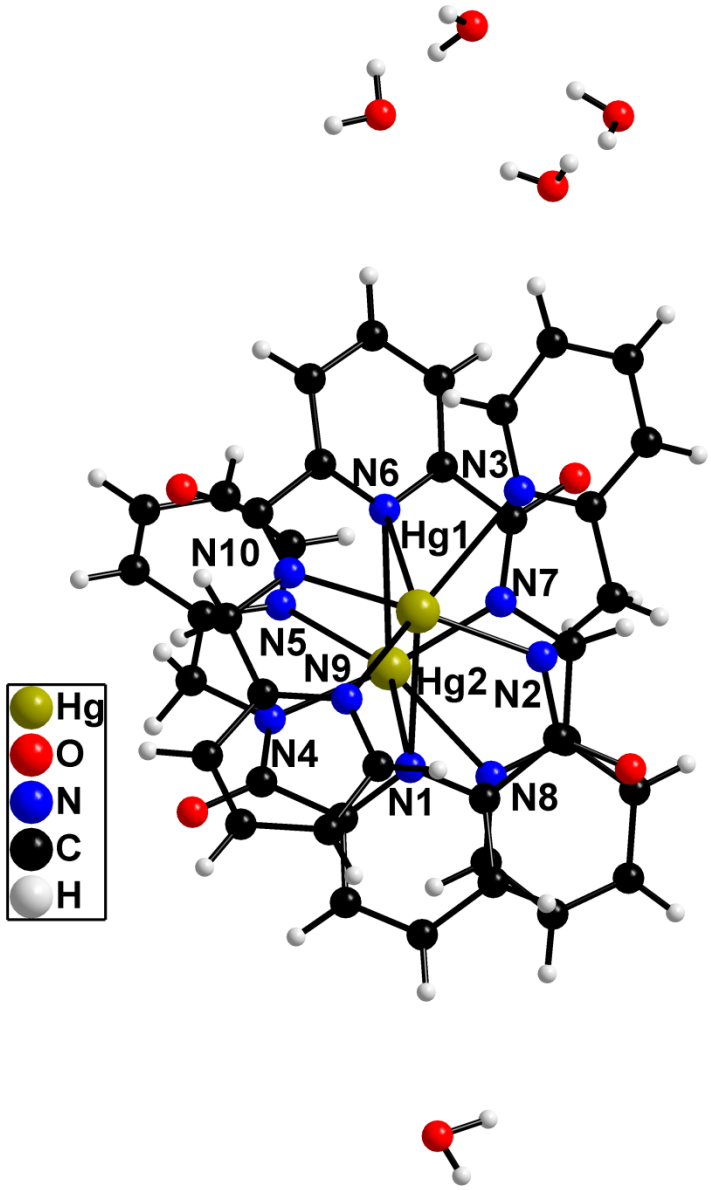


Fig. S1. Crystal structure of complex **1**showing five lattice water molecules.

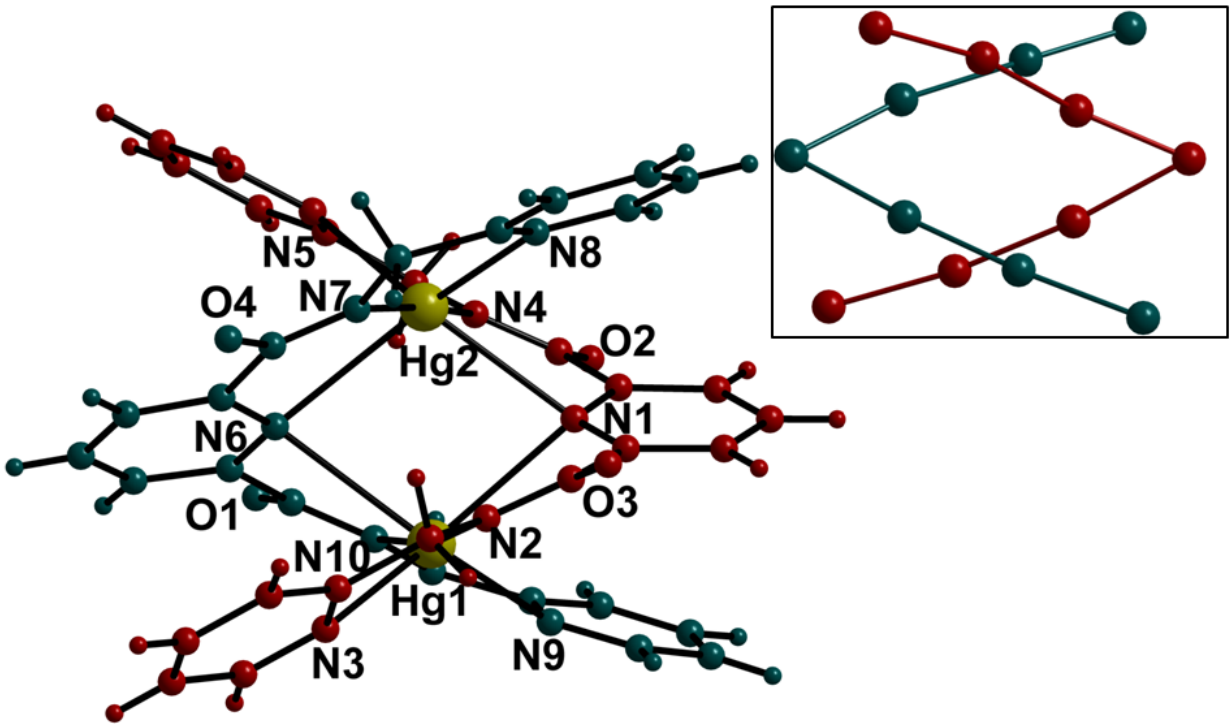


Fig. S2. Doubly helical wrapped crystal structure of **1.**

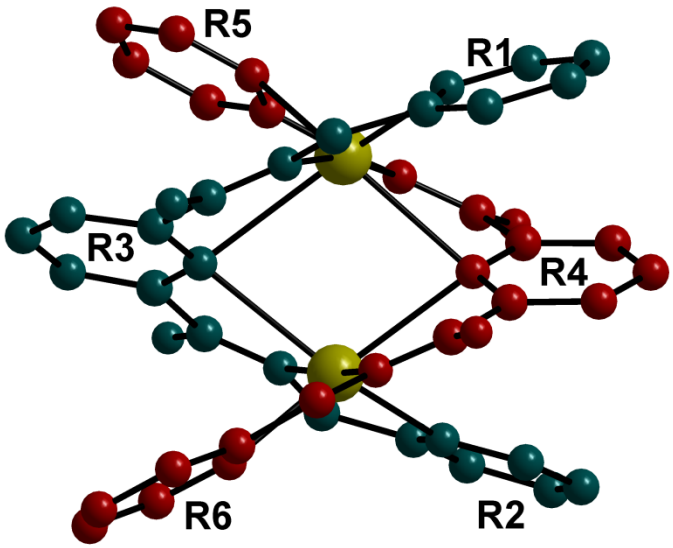


Fig. S3. Complex**1** showing dihedral angle between terminal and central pyridine rings.

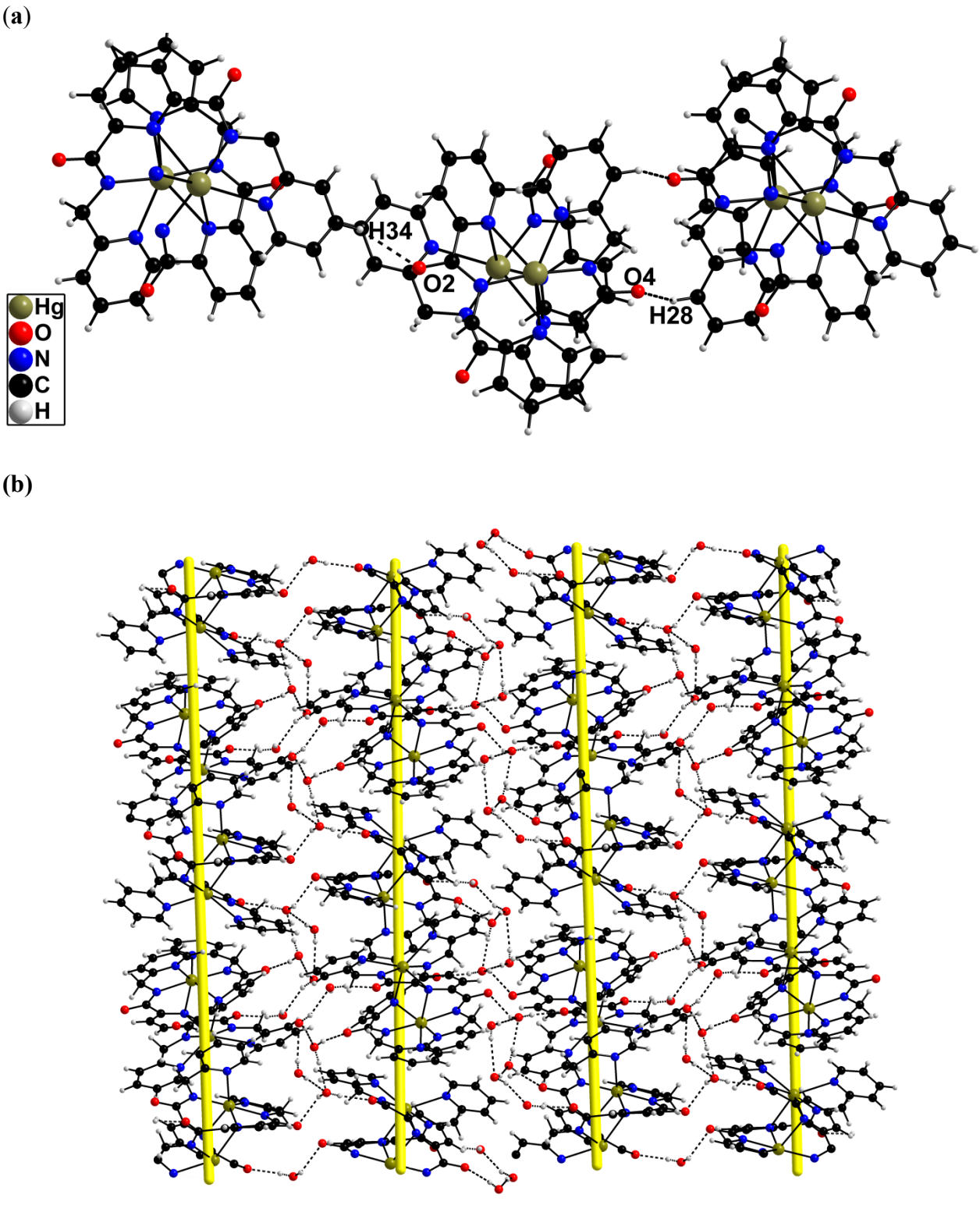
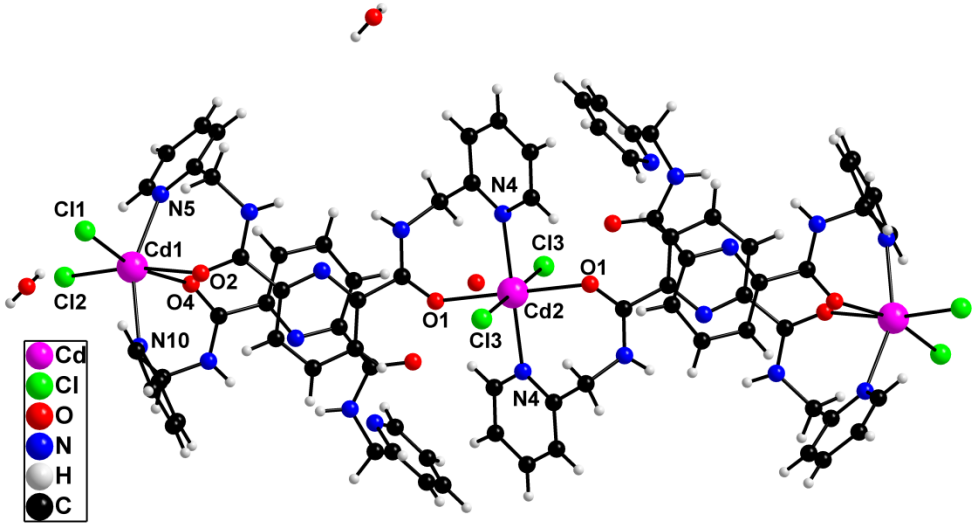


Fig. S4. (a) Showing hydrogen bonded 1D chain of complex **1** (b) Packing of complex **1** represents water tetramer between two helical layers.

(a)



(b)

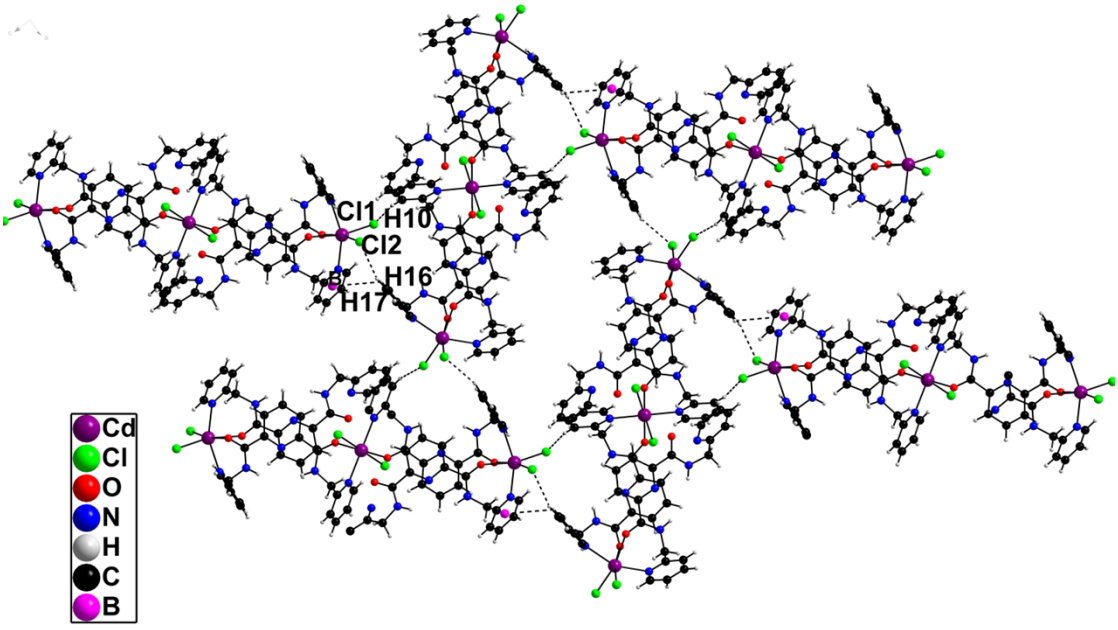


Fig. S5. (a) Crystal structure of complex **2.** (b) Packing diagram of the H-bonded 2D layer in **2** along *b* axis.

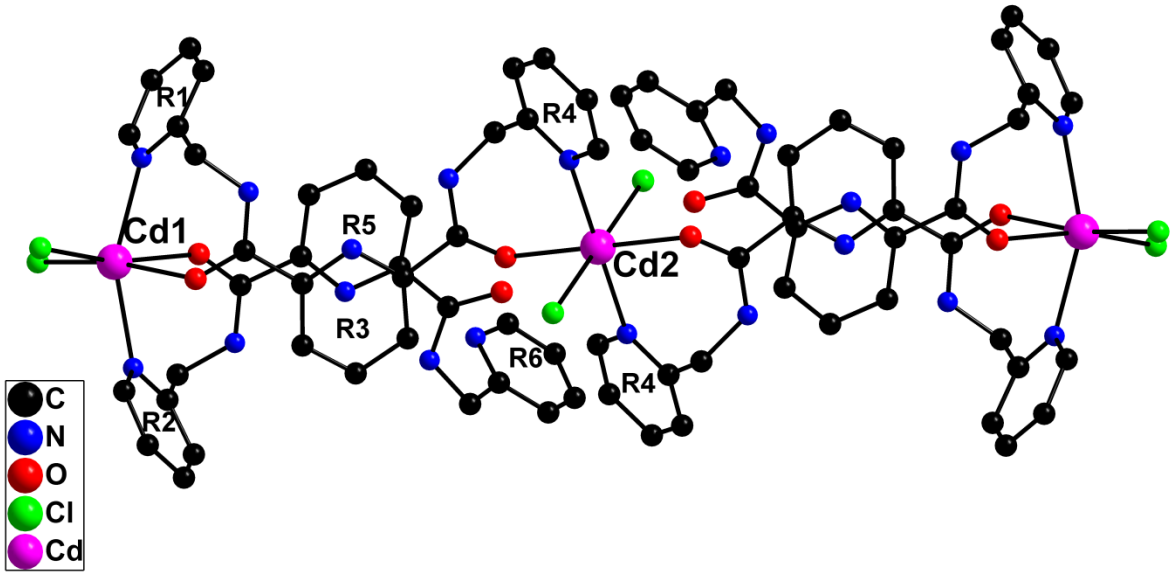


Fig. S6. Crystal structure of **2** shows dihedral angle between terminal and central pyridine rings. Dihedral angle between rings R1, R2 and R4, R4 are 78.84° and 0°. Other dihedral angles between rings R1, R3 and R5, R6 are found to be 84.14° and 65.48°.

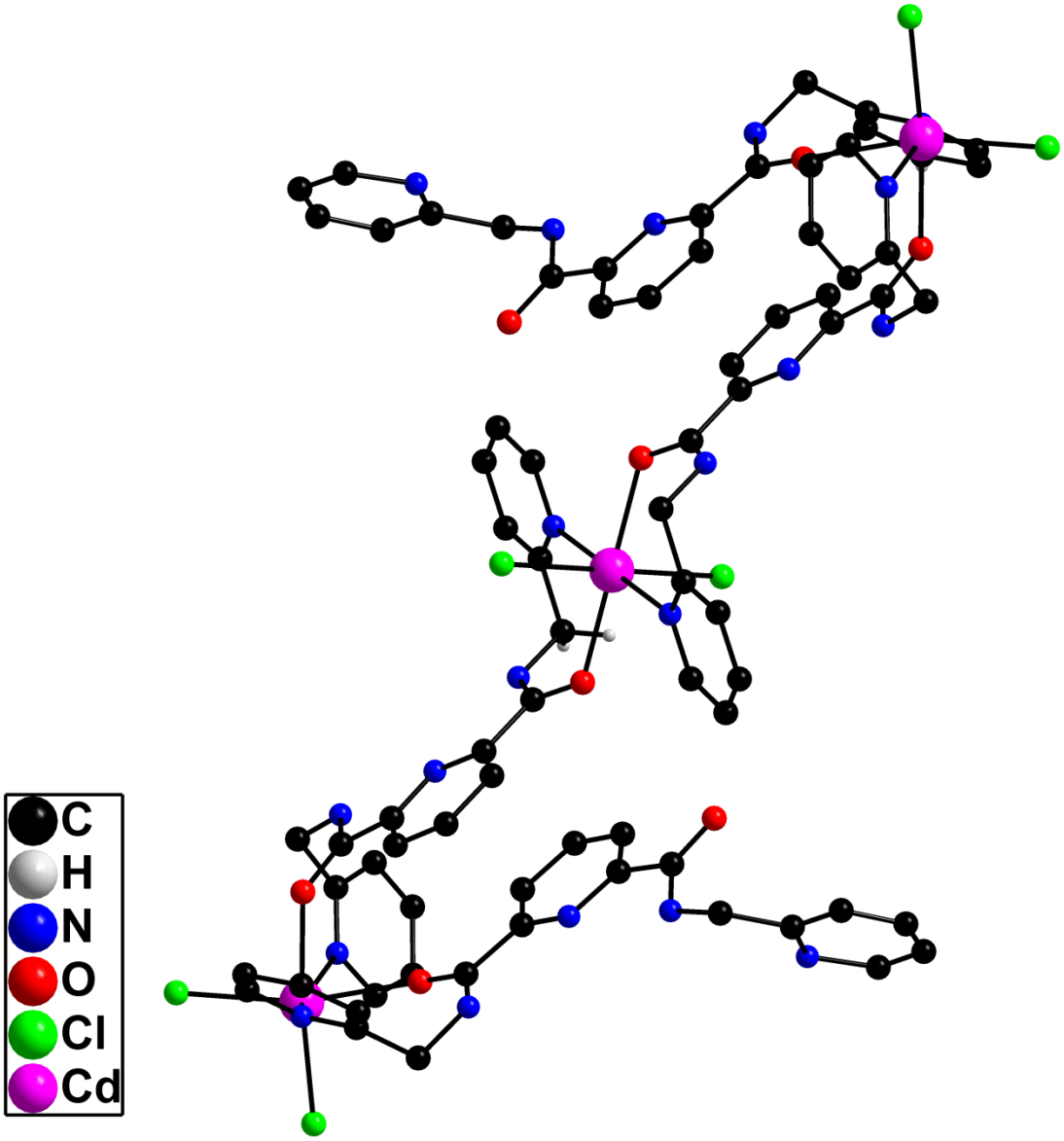


Fig. S7. Z shaped structure of **2**(Hydrogen atoms removed for clarity).

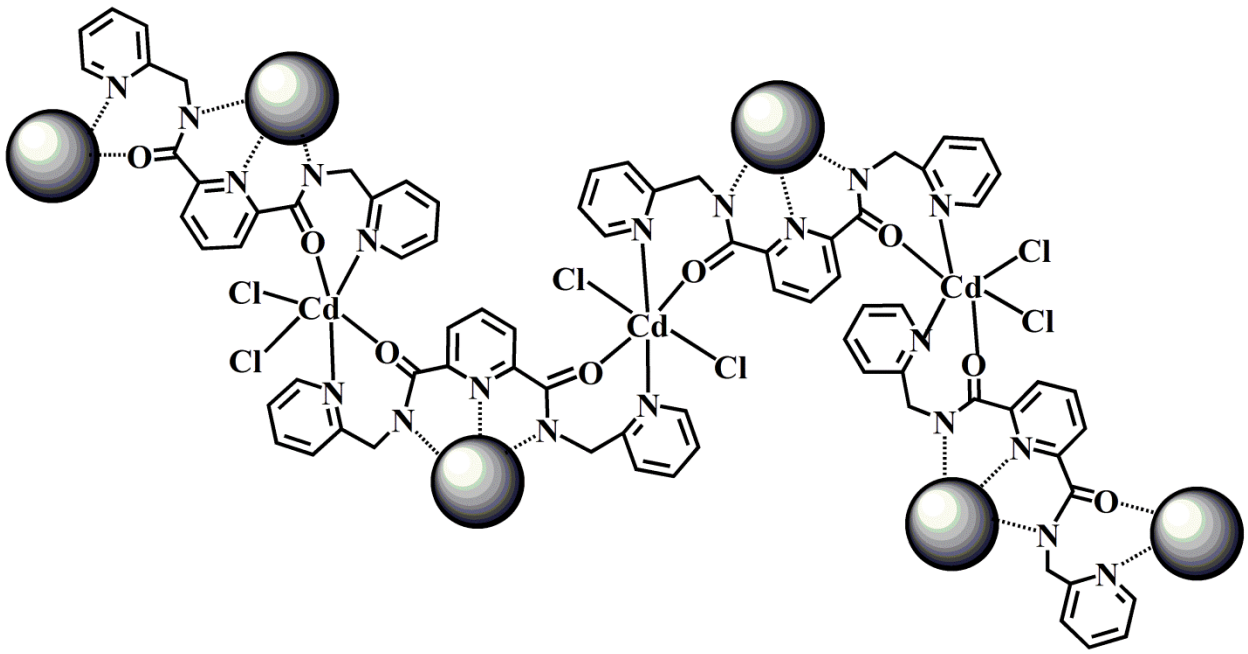


Chart B. Showing six vacant coordination sites for further growth.

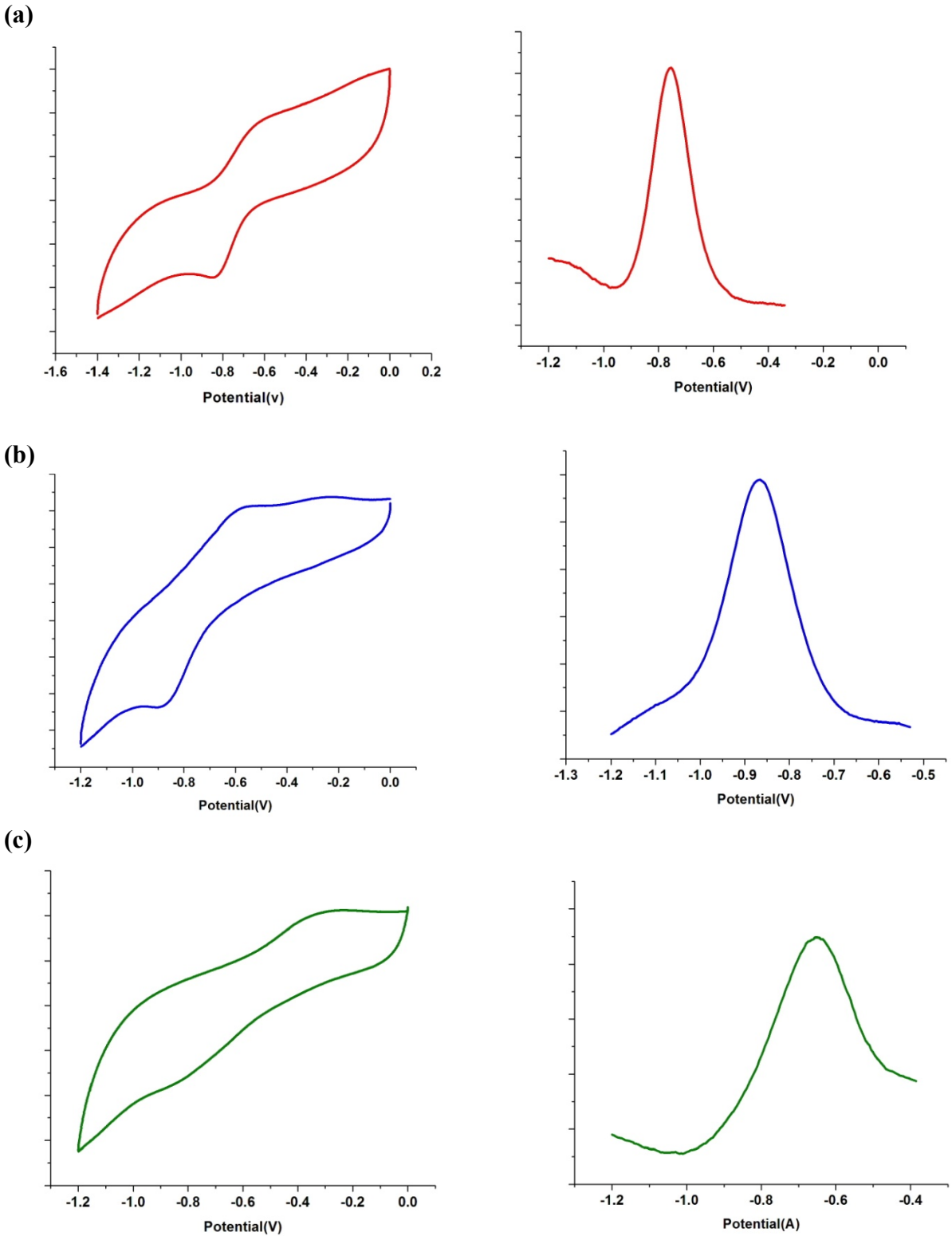


Fig. S8. Cyclic voltammograms and Differential potentialvoltammograms of **H_2L** (a) Complexes **1**(b) **2**(c) at 0.001M concentration in 0.1M TBAPF6 in DMSO recorded at a scan rate of 100 mV s^{-1}.

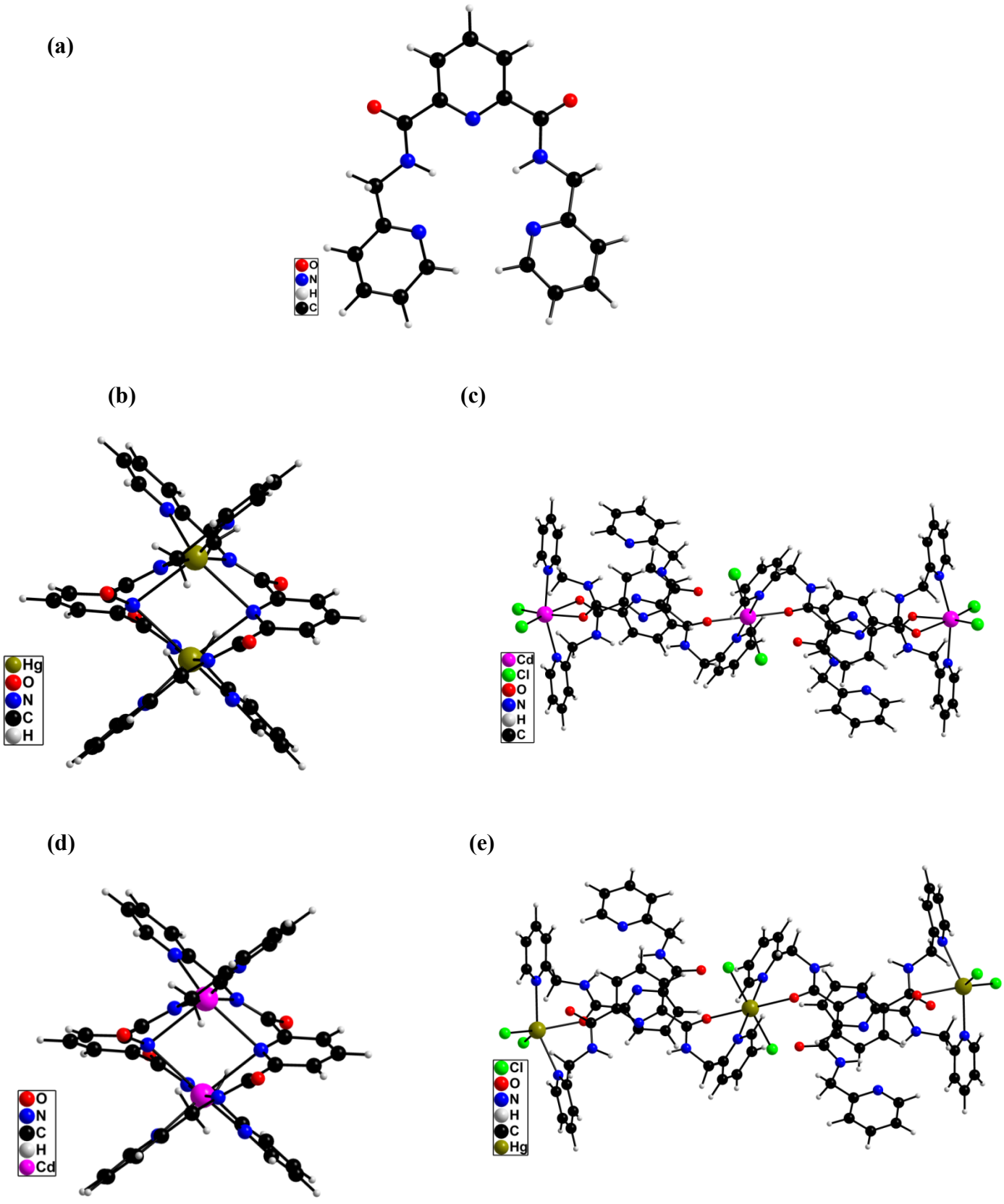


Fig. S9. Optimized structures of H_2L (a),**1** (b),**2** (c), Cd analogue of **1** (d) and Hg analogue of **2** (e)

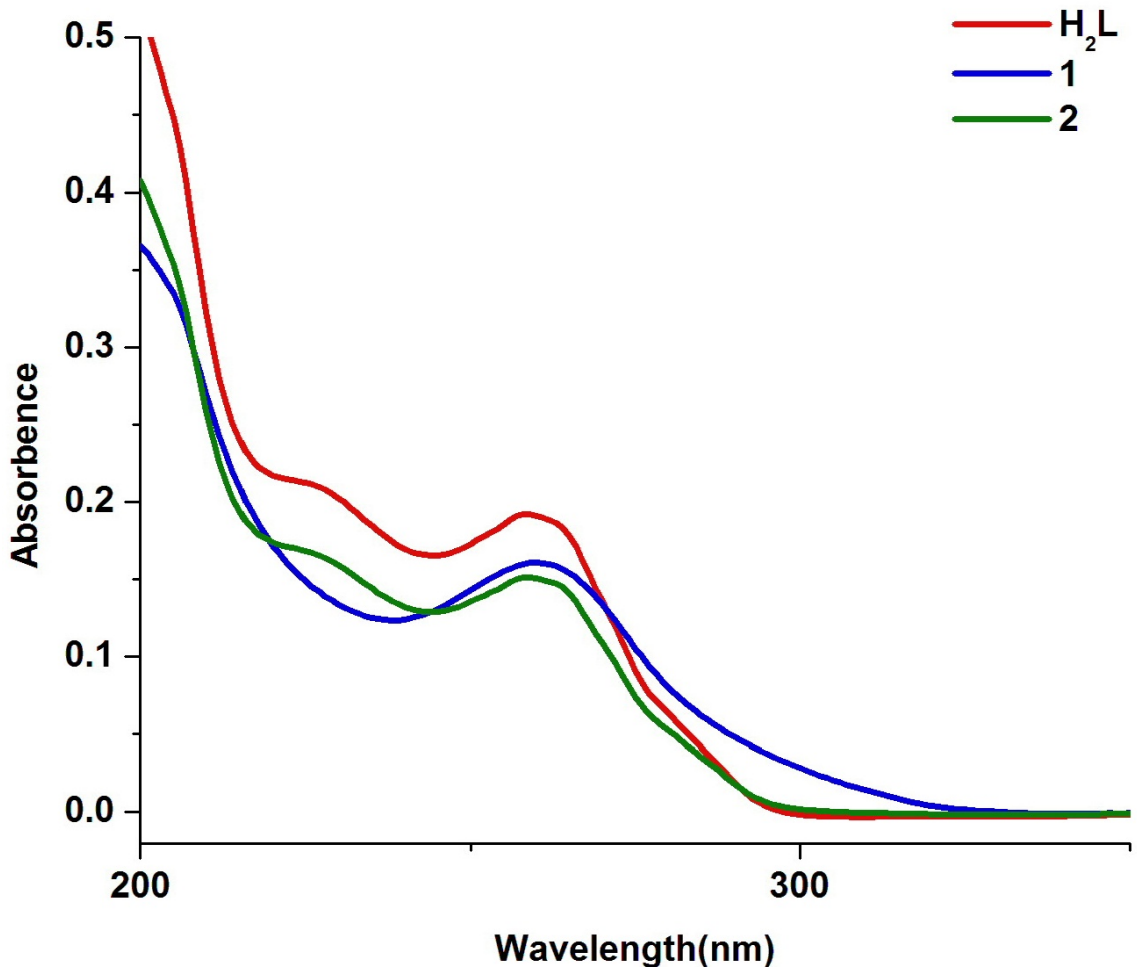


Fig. S10. Uv-Vis spectra of **H_2L,** complexes **1** and **2.**

Table-S4: Cartesian coordinates (Å) for calculated geometry of **H_2L**

O	-2.740400	-3.494600	0.769100
O	-2.742700	3.492900	-0.768900
N	-2.215600	-0.000700	0.000000
N	-0.794900	-2.344200	0.284500
H	-0.350100	-1.471200	0.004200
N	-0.796500	2.343900	-0.284300
H	-0.351000	1.471200	-0.003900
N	1.737000	-1.978100	-0.473600
N	1.735500	1.979300	0.474000
C	-2.909600	-1.144600	0.225000
C	-4.317700	-1.187900	0.242500
H	-4.803100	-2.137300	0.439400
C	-5.031300	-0.001600	-0.000300
H	-6.117700	-0.002000	-0.000400
C	-4.318500	1.185100	-0.242900
H	-4.804500	2.134200	-0.439800
C	-2.910400	1.142800	-0.225200
C	-2.140800	-2.423100	0.455300
C	-2.142400	2.421800	-0.455200
C	0.051600	-3.519800	0.434300
H	0.078300	-3.843500	1.486800
H	-0.383700	-4.361200	-0.123700
C	1.463400	-3.237900	-0.053400
C	2.441100	-4.256300	-0.061300

H	2.187800	-5.255700	0.282900
C	3.732600	-3.956200	-0.522900
H	4.501700	-4.723900	-0.542300
C	4.015300	-2.647000	-0.964900
H	4.999400	-2.375400	-1.334500
C	2.985900	-1.691900	-0.920000
H	3.149400	-0.670000	-1.251700
C	0.049200	3.520000	-0.433700
H	0.075500	3.844200	-1.486100
H	-0.386500	4.361000	0.124700
C	1.461200	3.238800	0.053600
C	2.438500	4.257700	0.061000
H	2.184800	5.256900	-0.283300
C	3.730300	3.958300	0.522400
H	4.499000	4.726300	0.541500
C	4.013700	2.649300	0.964700
H	4.998000	2.378200	1.334100
C	2.984700	1.693700	0.920200
H	3.148700	0.671900	1.252000

Table S5-Cartesian coordinates (Å) for calculated geometry of **1**

Hg	-1.792900	-0.000300	-0.000300
Hg	1.791900	0.000300	0.000000
O	-0.707100	3.466600	2.566100
O	0.708600	3.482600	-2.546800

O	-0.705200	-3.467300	-2.565600
O	0.708900	-3.482800	2.545600
N	0.001000	0.006400	-2.142000
N	-1.580400	-2.052100	-0.912700
N	-3.262600	-1.604900	1.298600
N	1.582500	2.057700	-0.901600
N	3.260100	1.596700	1.310400
N	0.000900	-0.006700	2.141800
N	1.583100	-2.057300	0.901100
N	3.262000	-1.595300	-1.309500
N	-3.262500	1.604100	-1.299400
N	-1.580900	2.051500	0.912400
C	0.418200	1.111400	-2.822500
C	0.390400	1.162500	-4.229500
H	0.681000	2.085000	-4.719100
C	-0.000800	0.014800	-4.942100
H	-0.001500	0.018100	-6.029200
C	-0.391100	-1.137100	-4.235900
H	-0.682300	-2.056600	-4.730700
C	-0.417000	-1.094400	-2.828600
C	-0.914700	-2.306100	-2.060900
C	-2.052600	-3.221800	-0.168900
H	-1.204900	-3.753100	0.299000
H	-2.507900	-3.951100	-0.857500
C	-3.047600	-2.895200	0.935800

C	-3.718700	-3.948500	1.598800
H	-3.523400	-4.974400	1.299400
C	-4.614800	-3.657500	2.635800
H	-5.133900	-4.459400	3.154200
C	-4.832100	-2.311200	2.999400
H	-5.516300	-2.041100	3.797400
C	-4.132000	-1.317400	2.304200
H	-4.255000	-0.265700	2.547600
C	0.917000	2.318500	-2.048300
C	2.056100	3.223000	-0.151800
H	1.208800	3.754600	0.316400
H	2.514800	3.954000	-0.836200
C	3.047900	2.889100	0.953700
C	3.719000	3.938000	1.623700
H	3.526100	4.965700	1.329200
C	4.612200	3.640200	2.661400
H	5.131300	4.438500	3.185200
C	4.826300	2.291700	3.018600
H	5.508200	2.016500	3.816900
C	4.126400	1.302600	2.316600
H	4.247000	0.249400	2.554900
C	-0.417900	1.093700	2.828500
C	-0.392400	1.136000	4.235800
H	-0.684200	2.055300	4.730800
C	-0.002000	-0.016000	4.941900

H	-0.003000	-0.019500	6.028900
C	0.389800	-1.163300	4.229000
H	0.680500	-2.085900	4.718400
C	0.418000	-1.111800	2.822000
C	0.917300	-2.318500	2.047600
C	2.057200	-3.222200	0.151100
H	1.210200	-3.753000	-0.318700
H	2.514700	-3.954000	0.835500
C	3.050500	-2.887800	-0.952800
C	3.723600	-3.936200	-1.621600
H	3.531200	-4.964000	-1.327200
C	4.618000	-3.637800	-2.658100
H	5.138600	-4.435700	-3.180900
C	4.831400	-2.289100	-3.015300
H	5.514200	-2.013500	-3.812600
C	4.129600	-1.300500	-2.314500
H	4.249600	-0.247300	-2.552800
C	-4.131500	1.316500	-2.305300
H	-4.254200	0.264800	-2.548900
C	-4.831500	2.310200	-3.000700
H	-5.515400	2.040100	-3.799000
C	-4.614700	3.656500	-2.636900
H	-5.133700	4.458300	-3.155400
C	-3.718900	3.947600	-1.599500
H	-3.524000	4.973500	-1.300000

C	-3.048000	2.894300	-0.936300
C	-2.053400	3.221100	0.168800
H	-1.205800	3.752900	-0.298700
H	-2.509300	3.950000	0.857400
C	-0.915800	2.305400	2.061000

Table S6-Cartesian coordinates (Å) for calculated geometry of **2**

Cd	6.750700	5.298000	-7.157000
Cd	0.000000	0.000000	0.000000
Cl	7.782500	3.788900	-8.955500
Cl	7.034400	7.839800	-7.533200
Cl	-2.251200	1.278200	-0.292600
O	1.132200	1.457400	-1.446600
O	6.193700	3.133000	-5.998300
N	3.376900	1.826100	-4.185200
N	0.786500	0.849600	-3.651000
H	1.238900	0.712300	-4.548900
N	4.118300	2.447800	-6.766700
H	3.216100	2.089800	-6.468100
N	-0.619700	-1.370200	-1.954800
N	4.482700	5.262900	-8.167100
C	3.021600	1.495000	-2.918400
C	3.946600	1.376600	-1.861700
H	3.597100	1.045800	-0.888700
C	5.297000	1.661400	-2.128800

H	6.041900	1.566600	-1.344600
C	5.666500	2.076600	-3.419700
H	6.684400	2.345900	-3.678600
C	4.677200	2.138500	-4.420200
C	1.568600	1.263600	-2.623600
C	5.057800	2.611700	-5.798600
C	-0.653900	0.552600	-3.498000
H	-1.162100	0.845200	-4.422900
H	-1.052300	1.158300	-2.674300
C	-0.928700	-0.915900	-3.202600
C	-1.495200	-1.766800	-4.169800
H	-1.736800	-1.377700	-5.155100
C	-1.758200	-3.110000	-3.840200
H	-2.209700	-3.778600	-4.568300
C	-1.435300	-3.576100	-2.553900
H	-1.650200	-4.596800	-2.251800
C	-0.856000	-2.671100	-1.646100
H	-0.583400	-2.975900	-0.641400
C	4.355900	2.800100	-8.180600
H	3.903600	2.022900	-8.806400
H	5.439000	2.802900	-8.360800
C	3.783400	4.158500	-8.557100
C	2.583800	4.270300	-9.286300
H	2.060100	3.372100	-9.601600
C	2.087700	5.546300	-9.612300

H	1.167900	5.651600	-10.181700
C	2.808700	6.678600	-9.197700
H	2.472300	7.683200	-9.433000
C	4.004200	6.496400	-8.479400
H	4.621800	7.333700	-8.164600
O	2.899800	6.312000	1.480300
O	5.428700	5.814200	-5.177200
N	4.570600	6.349900	-1.721900
N	4.949800	7.180000	0.850100
H	5.613800	7.362700	0.099000
N	6.678300	6.676700	-3.418700
H	6.636500	6.891300	-2.425600
N	7.275300	8.461100	0.928800
N	8.580400	5.051800	-5.543700
C	3.542900	6.189000	-0.851500
C	2.289300	5.685500	-1.248900
H	1.506200	5.581300	-0.506700
C	2.096700	5.341800	-2.597800
H	1.138400	4.957000	-2.933500
C	3.161100	5.500100	-3.502100
H	3.075500	5.253200	-4.554100
C	4.383900	6.002900	-3.019000
C	3.770500	6.564400	0.593000
C	5.549600	6.161700	-3.964400
C	5.325700	7.629500	2.182400

H	5.409000	6.771900	2.867500
H	4.538000	8.273600	2.598900
C	6.647100	8.383100	2.130000
C	7.184100	8.973700	3.292900
H	6.653700	8.893300	4.238100
C	8.402500	9.666000	3.205600
H	8.835000	10.131700	4.086900
C	9.053000	9.751700	1.957800
H	9.993600	10.281700	1.845500
C	8.451600	9.133800	0.849200
H	8.914400	9.177800	-0.133100
C	7.888000	7.006500	-4.201800
H	8.428400	7.782100	-3.649200
H	7.585600	7.425500	-5.170800
C	8.811100	5.817300	-4.440000
C	9.880900	5.532700	-3.567500
H	10.050500	6.165000	-2.700400
C	10.724000	4.439400	-3.837900
H	11.557500	4.210000	-3.178900
C	10.477300	3.658400	-4.980800
H	11.108300	2.813400	-5.237500
C	9.394500	3.996500	-5.810500
H	9.164900	3.442700	-6.717200
Cd	-6.750700	-5.298000	7.157000
Cl	-7.782500	-3.788900	8.955500

Cl	-7.034400	-7.839800	7.533200
Cl	2.251200	-1.278200	0.292600
O	-1.132200	-1.457400	1.446600
O	-6.193700	-3.133000	5.998300
N	-3.376900	-1.826100	4.185200
N	-0.786500	-0.849600	3.651000
H	-1.238900	-0.712300	4.548900
N	-4.118300	-2.447800	6.766700
H	-3.216100	-2.089800	6.468100
N	0.619700	1.370200	1.954800
N	-4.482700	-5.262900	8.167100
C	-3.021600	-1.495000	2.918400
C	-3.946600	-1.376600	1.861700
H	-3.597100	-1.045800	0.888700
C	-5.297000	-1.661400	2.128800
H	-6.041900	-1.566600	1.344600
C	-5.666500	-2.076600	3.419700
H	-6.684400	-2.345900	3.678600
C	-4.677200	-2.138500	4.420200
C	-1.568600	-1.263600	2.623600
C	-5.057800	-2.611700	5.798600
C	0.653900	-0.552600	3.498000
H	1.162100	-0.845200	4.422900
H	1.052300	-1.158300	2.674300
C	0.928700	0.915900	3.202600

C	1.495200	1.766800	4.169800
H	1.736800	1.377700	5.155100
C	1.758200	3.110000	3.840200
H	2.209700	3.778600	4.568300
C	1.435300	3.576100	2.553900
H	1.650200	4.596800	2.251800
C	0.856000	2.671100	1.646100
H	0.583400	2.975900	0.641400
C	-4.355900	-2.800100	8.180600
H	-3.903600	-2.022900	8.806400
H	-5.439000	-2.802900	8.360800
C	-3.783400	-4.158500	8.557100
C	-2.583800	-4.270300	9.286300
H	-2.060100	-3.372100	9.601600
C	-2.087700	-5.546300	9.612300
H	-1.167900	-5.651600	10.181700
C	-2.808700	-6.678600	9.197700
H	-2.472300	-7.683200	9.433000
C	-4.004200	-6.496400	8.479400
H	-4.621800	-7.333700	8.164600
O	-2.899800	-6.312000	-1.480300
O	-5.428700	-5.814200	5.177200
N	-4.570600	-6.349900	1.721900
N	-4.949800	-7.180000	-0.850100
H	-5.613800	-7.362700	-0.099000

N	-6.678300	-6.676700	3.418700
H	-6.636500	-6.891300	2.425600
N	-7.275300	-8.461100	-0.928800
N	-8.580400	-5.051800	5.543700
C	-3.542900	-6.189000	0.851500
C	-2.289300	-5.685500	1.248900
H	-1.506200	-5.581300	0.506700
C	-2.096700	-5.341800	2.597800
H	-1.138400	-4.957000	2.933500
C	-3.161100	-5.500100	3.502100
H	-3.075500	-5.253200	4.554100
C	-4.383900	-6.002900	3.019000
C	-3.770500	-6.564400	-0.593000
C	-5.549600	-6.161700	3.964400
C	-5.325700	-7.629500	-2.182400
H	-5.409000	-6.771900	-2.867500
H	-4.538000	-8.273600	-2.598900
C	-6.647100	-8.383100	-2.130000
C	-7.184100	-8.973700	-3.292900
H	-6.653700	-8.893300	-4.238100
C	-8.402500	-9.666000	-3.205600
H	-8.835000	-10.131700	-4.086900
C	-9.053000	-9.751700	-1.957800
H	-9.993600	-10.281700	-1.845500
C	-8.451600	-9.133800	-0.849200

H	-8.914400	-9.177800	0.133100
C	-7.888000	-7.006500	4.201800
H	-8.428400	-7.782100	3.649200
H	-7.585600	-7.425500	5.170800
C	-8.811100	-5.817300	4.440000
C	-9.880900	-5.532700	3.567500
H	-10.050500	-6.165000	2.700400
C	-10.724000	-4.439400	3.837900
H	-11.557500	-4.210000	3.178900
C	-10.477300	-3.658400	4.980800
H	-11.108300	-2.813400	5.237500
C	-9.394500	-3.996500	5.810500
H	-9.164900	-3.442700	6.717200

Table S7-Cartesian coordinates (Å) for calculated geometry of Cd analogue of **1**

O	-0.672200	-2.498200	3.458800
O	0.690100	2.422400	3.516600
O	-0.672900	2.496900	-3.459200
O	0.684900	-2.421600	-3.518100
N	0.006900	2.053300	0.024200
N	-1.565100	0.863100	-2.018800
N	-3.135500	-1.344700	-1.439000
N	1.577500	0.818800	2.039500
N	3.124100	-1.390600	1.406900
N	0.005300	-2.053700	-0.024800

N	1.575500	-0.819800	-2.041000
N	3.124400	1.388200	-1.408700
N	-3.131100	1.347800	1.442000
N	-1.564600	-0.863500	2.019700
C	0.403000	2.730400	1.143300
C	0.370800	4.136100	1.204700
H	0.643800	4.616600	2.137500
C	0.003600	4.858800	0.055700
H	0.002400	5.945900	0.067900
C	-0.362100	4.161300	-1.109200
H	-0.636100	4.662000	-2.031000
C	-0.390900	2.754400	-1.079300
C	-0.889700	1.996200	-2.297500
C	-2.064400	0.100800	-3.164400
H	-1.230400	-0.340000	-3.738300
H	-2.590800	0.759300	-3.874400
C	-2.991000	-1.035100	-2.755900
C	-3.673800	-1.777300	-3.746000
H	-3.532600	-1.521100	-4.792100
C	-4.509600	-2.836400	-3.368300
H	-5.037100	-3.415300	-4.121800
C	-4.653800	-3.144400	-1.998500
H	-5.289000	-3.957700	-1.662500
C	-3.945300	-2.374200	-1.068900
H	-4.010700	-2.573000	-0.002800

C	0.904000	1.946200	2.344000
C	2.078200	0.031200	3.167000
H	1.244600	-0.411100	3.740100
H	2.617400	0.671300	3.884300
C	2.989500	-1.106700	2.730500
C	3.668100	-1.877100	3.701700
H	3.534900	-1.641000	4.753600
C	4.489300	-2.938200	3.298200
H	5.013400	-3.538700	4.037000
C	4.623000	-3.219800	1.921600
H	5.246500	-4.033600	1.565900
C	3.919500	-2.422000	1.011700
H	3.977500	-2.599400	-0.058700
C	-0.392100	-2.755000	1.078700
C	-0.364400	-4.161900	1.107900
H	-0.637900	-4.662800	2.029600
C	-0.000300	-4.859200	-0.057700
H	-0.002300	-5.946300	-0.070400
C	0.366500	-4.136300	-1.206700
H	0.638100	-4.616500	-2.140000
C	0.399900	-2.730600	-1.144700
C	0.900500	-1.946300	-2.345400
C	2.076000	-0.032000	-3.168500
H	1.242200	0.411600	-3.740400
H	2.613700	-0.672200	-3.886800

C	2.988900	1.104700	-2.732300
C	3.668000	1.874400	-3.703600
H	3.534200	1.638700	-4.755400
C	4.490400	2.934500	-3.300200
H	5.015000	3.534600	-4.039100
C	4.625000	3.215800	-1.923600
H	5.249500	4.029000	-1.568000
C	3.921000	2.418600	-1.013500
H	3.979700	2.595800	0.056800
C	-3.938500	2.379600	1.072900
H	-4.004500	2.578900	0.006900
C	-4.644000	3.151400	2.003400
H	-5.277400	3.966500	1.668300
C	-4.499300	2.842700	3.373000
H	-5.024400	3.422800	4.127200
C	-3.665900	1.781200	3.749500
H	-3.524300	1.524400	4.795500
C	-2.986100	1.037500	2.758600
C	-2.062300	-0.101200	3.165900
H	-1.227400	0.336900	3.740600
H	-2.590500	-0.759100	3.875100
C	-0.889600	-1.997000	2.297400
Cd	1.748400	-0.000900	-0.000700
Cd	-1.749900	0.000300	0.000700

Table S8-Cartesian coordinates (Å) for calculated geometry of Hg analogue of **2**

Cl	7.859700	3.952800	-9.111900
Cl	6.687000	8.043200	-7.384700
Cl	-2.317600	1.204500	-0.293600
O	1.148900	1.628500	-1.548100
O	6.335500	2.926700	-6.098700
N	3.453600	1.805900	-4.249300
N	0.853800	0.849800	-3.711200
H	1.330300	0.643100	-4.583000
N	4.199900	2.380600	-6.825000
H	3.282200	2.089300	-6.501600
N	-0.605700	-1.389200	-2.101100
N	4.362600	5.193700	-8.215000
C	3.075600	1.530400	-2.975800
C	3.985600	1.443000	-1.903500
H	3.620400	1.165100	-0.920500
C	5.344600	1.689000	-2.165200
H	6.077600	1.614300	-1.367600
C	5.738600	2.039500	-3.468000
H	6.764700	2.276200	-3.726300
C	4.762700	2.083100	-4.481800
C	1.612700	1.337200	-2.694400
C	5.168200	2.496500	-5.873700
C	-0.592100	0.577000	-3.586500
H	-1.086600	0.904200	-4.508000

H	-0.984400	1.170700	-2.752700
C	-0.902500	-0.892900	-3.334400
C	-1.492300	-1.703300	-4.322900
H	-1.724800	-1.283500	-5.297900
C	-1.789700	-3.047500	-4.026600
H	-2.258100	-3.685000	-4.771700
C	-1.481900	-3.555300	-2.752100
H	-1.724700	-4.576500	-2.473100
C	-0.879800	-2.687900	-1.821600
H	-0.622200	-3.022900	-0.821900
C	4.416600	2.727400	-8.240700
H	4.015000	1.920400	-8.864800
H	5.497100	2.792800	-8.416700
C	3.754900	4.043600	-8.622700
C	2.557600	4.075200	-9.364100
H	2.104800	3.144700	-9.695200
C	1.970100	5.315100	-9.678200
H	1.050300	5.358500	-10.255600
C	2.597500	6.493700	-9.240300
H	2.185800	7.472800	-9.463600
C	3.797800	6.392100	-8.513500
H	4.345200	7.269200	-8.177300
O	2.924700	6.277700	1.634800
O	5.369200	5.640100	-5.045800
N	4.540900	6.263200	-1.596100

N	4.951200	7.156500	0.947700
H	5.600600	7.326100	0.181100
N	6.603000	6.617600	-3.331300
H	6.556100	6.868100	-2.347000
N	7.276200	8.443000	0.962800
N	8.577600	5.098600	-5.543900
C	3.531900	6.101300	-0.704200
C	2.285700	5.555700	-1.066400
H	1.517300	5.452400	-0.309200
C	2.080300	5.168500	-2.401400
H	1.127600	4.747600	-2.707400
C	3.125600	5.327400	-3.327300
H	3.030100	5.046200	-4.369800
C	4.342800	5.874500	-2.879600
C	3.776100	6.519000	0.725700
C	5.489300	6.038700	-3.849200
C	5.344100	7.640900	2.262500
H	5.432300	6.801800	2.969300
H	4.563800	8.299000	2.671300
C	6.667000	8.388600	2.175000
C	7.224300	8.998500	3.318400
H	6.708900	8.936600	4.273200
C	8.443300	9.684900	3.199400
H	8.891100	10.164800	4.065300
C	9.074200	9.746000	1.940200

H	10.014500	10.270700	1.803500
C	8.453200	9.110400	0.852600
H	8.900400	9.135400	-0.137500
C	7.794800	6.966500	-4.130500
H	8.331600	7.747700	-3.581700
H	7.473400	7.389300	-5.090100
C	8.731500	5.789500	-4.381600
C	9.734200	5.435100	-3.455700
H	9.845600	6.005800	-2.537800
C	10.584400	4.350600	-3.737800
H	11.366300	4.067400	-3.037700
C	10.413700	3.646500	-4.943700
H	11.051700	2.808800	-5.206700
C	9.395200	4.050700	-5.823400
H	9.216800	3.551700	-6.772000
Cl	-7.859700	-3.952800	9.111900
Cl	-6.687000	-8.043200	7.384700
Cl	2.317600	-1.204500	0.293600
O	-1.148900	-1.628500	1.548100
O	-6.335500	-2.926700	6.098700
N	-3.453600	-1.805900	4.249300
N	-0.853800	-0.849800	3.711200
H	-1.330300	-0.643100	4.583000
N	-4.199900	-2.380600	6.825000
H	-3.282200	-2.089300	6.501600

N	0.605700	1.389200	2.101100
N	-4.362600	-5.193700	8.215000
C	-3.075600	-1.530400	2.975800
C	-3.985600	-1.443000	1.903500
H	-3.620400	-1.165100	0.920500
C	-5.344600	-1.689000	2.165200
H	-6.077600	-1.614300	1.367600
C	-5.738600	-2.039500	3.468000
H	-6.764700	-2.276200	3.726300
C	-4.762700	-2.083100	4.481800
C	-1.612700	-1.337200	2.694400
C	-5.168200	-2.496500	5.873700
C	0.592100	-0.577000	3.586500
H	1.086600	-0.904200	4.508000
H	0.984400	-1.170700	2.752700
C	0.902500	0.892900	3.334400
C	1.492300	1.703300	4.322900
H	1.724800	1.283500	5.297900
C	1.789700	3.047500	4.026600
H	2.258100	3.685000	4.771700
C	1.481900	3.555300	2.752100
H	1.724700	4.576500	2.473100
C	0.879800	2.687900	1.821600
H	0.622200	3.022900	0.821900
C	-4.416600	-2.727400	8.240700

H	-4.015000	-1.920400	8.864800
H	-5.497100	-2.792800	8.416700
C	-3.754900	-4.043600	8.622700
C	-2.557600	-4.075200	9.364100
H	-2.104800	-3.144700	9.695200
C	-1.970100	-5.315100	9.678200
H	-1.050300	-5.358500	10.255600
C	-2.597500	-6.493700	9.240300
H	-2.185800	-7.472800	9.463600
C	-3.797800	-6.392100	8.513500
H	-4.345200	-7.269200	8.177300
O	-2.924700	-6.277700	-1.634800
O	-5.369200	-5.640100	5.045800
N	-4.540900	-6.263200	1.596100
N	-4.951200	-7.156500	-0.947700
H	-5.600600	-7.326100	-0.181100
N	-6.603000	-6.617600	3.331300
H	-6.556100	-6.868100	2.347000
N	-7.276200	-8.443000	-0.962800
N	-8.577600	-5.098600	5.543900
C	-3.531900	-6.101300	0.704200
C	-2.285700	-5.555700	1.066400
H	-1.517300	-5.452400	0.309200
C	-2.080300	-5.168500	2.401400
H	-1.127600	-4.747600	2.707400

C	-3.125600	-5.327400	3.327300
H	-3.030100	-5.046200	4.369800
C	-4.342800	-5.874500	2.879600
C	-3.776100	-6.519000	-0.725700
C	-5.489300	-6.038700	3.849200
C	-5.344100	-7.640900	-2.262500
H	-5.432300	-6.801800	-2.969300
H	-4.563800	-8.299000	-2.671300
C	-6.667000	-8.388600	-2.175000
C	-7.224300	-8.998500	-3.318400
H	-6.708900	-8.936600	-4.273200
C	-8.443300	-9.684900	-3.199400
H	-8.891100	-10.164800	-4.065300
C	-9.074200	-9.746000	-1.940200
H	-10.014500	-10.270700	-1.803500
C	-8.453200	-9.110400	-0.852600
H	-8.900400	-9.135400	0.137500
C	-7.794800	-6.966500	4.130500
H	-8.331600	-7.747700	3.581700
H	-7.473400	-7.389300	5.090100
C	-8.731500	-5.789500	4.381600
C	-9.734200	-5.435100	3.455700
H	-9.845600	-6.005800	2.537800
C	-10.584400	-4.350600	3.737800
H	-11.366300	-4.067400	3.037700

C	-10.413700	-3.646500	4.943700
H	-11.051700	-2.808800	5.206700
C	-9.395200	-4.050700	5.823400
H	-9.216800	-3.551700	6.772000
Hg	6.740400	5.409700	-7.258800
Hg	0.000000	0.000000	0.000000
Hg	-6.740400	-5.409700	7.258800