Coordination Versatility and Weak Hg···X (X = Cl, O, N) Interactions in Hydrazone-Based Hg(II) Complexes: Structural Evolution from Discrete Units to Extended Architectures

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Materials and physical measurements

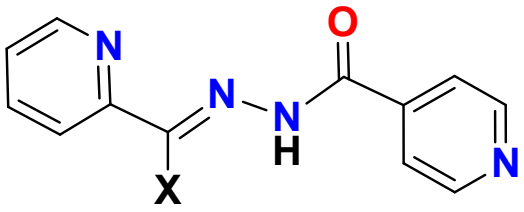
All chemicals were reagent grade and obtained from commercial sources and used without purification. The solvents were purified according to standard procedures. Hydrazone Schiff bases were prepared in a similar manner via a Schiff base condensation between the appropriate aldehyde, ketone, and acid hydrazide based on reported literature [1]**.** Infrared spectra were measured using a Perkin-Elmer FT-IR spectrometer with KBr pellets in the range of 4000–400 cm^{-1}. C, H, and N analyses were carried out with a C.E. Instrument EA-1110 CHNSO microanalyser.

Crystallographic data collection and structure refinement

Diffraction data of the present compounds were collected on a Rigaku XtaLAB (**1-2**) and on a Bruker Smart 1000 CCD (**3**) diffractometer using graphite monochromated Mo-K_α radiation (λ = 0.71073 Å). Experiments were performed at room temperature for **1** and **2**, and at 100 K for **3**. Data reductions were performed with *CrysAlis PRO*, *CrystalClear-SM* [2], and Bruker APEX2, SAINT software package [3]. Empirical absorption corrections were applied by means of programs SADABS [4] and *CrysAlis PRO* [2]. All the structures were solved by direct methods [5] and refined by full matrix least-squares procedures using the SHELXTL program [6] with the contribution of hydrogen atoms placed at calculated positions and constrained to ride to atoms to which they are attached. Drawings were performed with programs Cameron [7] and MERCURY [8]. Details of crystallographic data and refinements are given in **Table 1**.

Computational Details

The DFT calculations based on the experimental X-ray geometries of **1**–**3** were performed using the dispersion-corrected hybrid functional ωB97XD [9] with the help of the Gaussian-09 [10] program package. The Douglas–Kroll–Hess 2^{nd} order scalar relativistic calculations requested relativistic core Hamiltonian were carried out using the DZP-DKH basis sets [11-14] for all atoms. The topological analysis of the electron density distribution with the help of the atoms in molecules (QTAIM) method developed by Bader [15], molecular electrostatic potential (MEP) calculations, and NCI analysis were performed by using the Multiwfn program (version 3.7) [16]. The VMD program (http://www.ks.uiuc.edu/Research/vmd) was used for the visualization of noncovalent interactions. The Cartesian atomic coordinates for model structures used for DFT calculations are presented in the attached **Table S7-S9**.



X = H (HL^1), Ph (HL^2)

Scheme S1: Structure of the ligands.

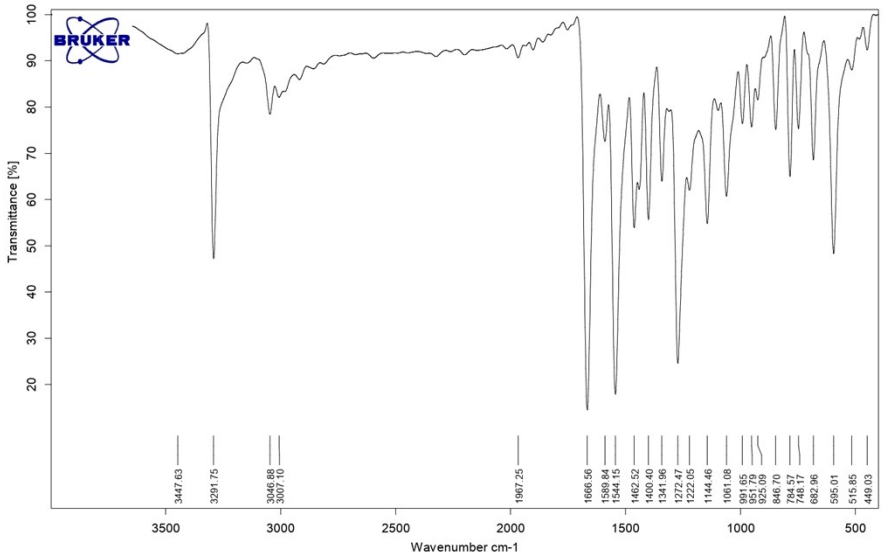


Figure S1. FT-IR spectrum of ligand **HL[1]**.

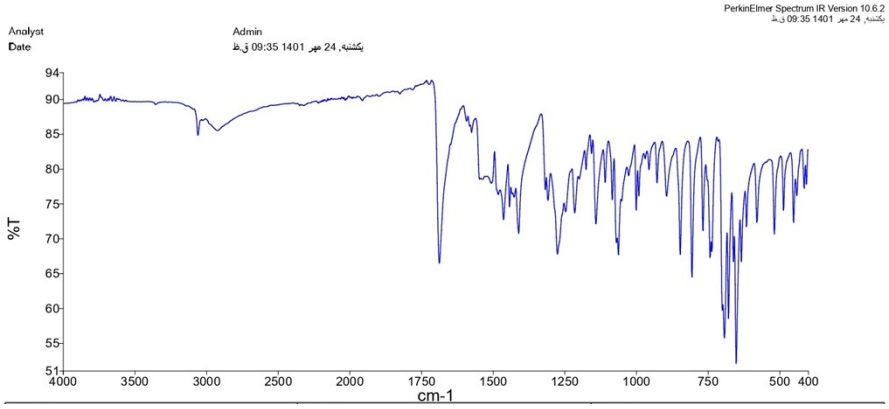


Figure S2. FT-IR spectrum of ligand $\mathbf{HL^2}$.

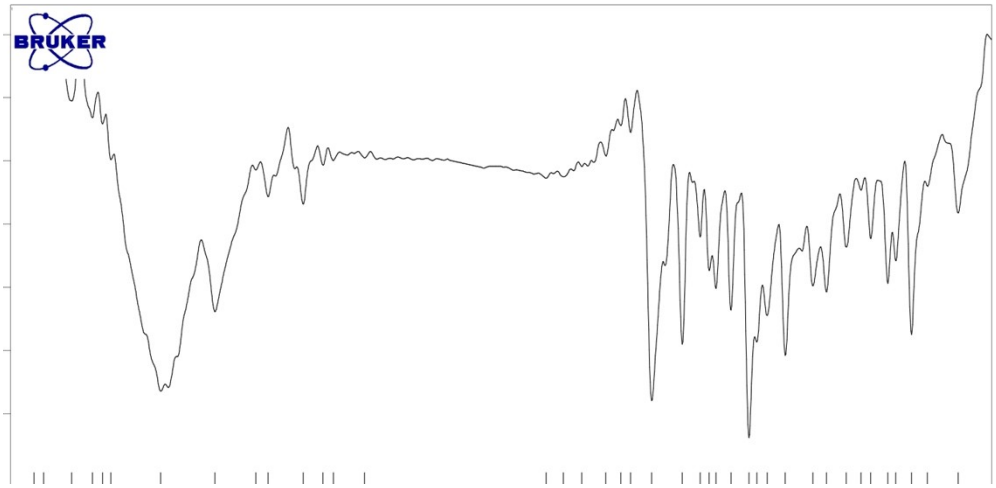


Figure S3. FT-IR spectrum of Hg(II) complex **(1)**.

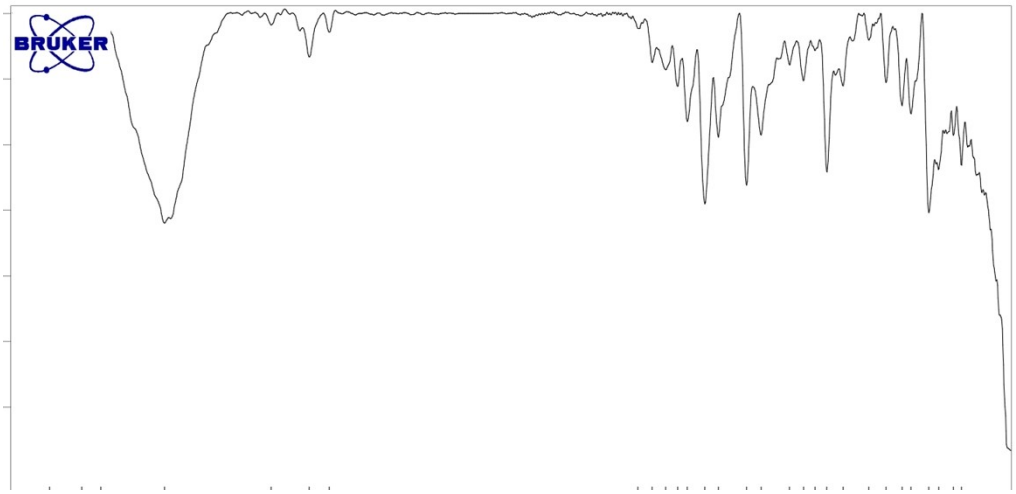


Figure S4. FT-IR spectrum of Hg(II) complex **(2)**.

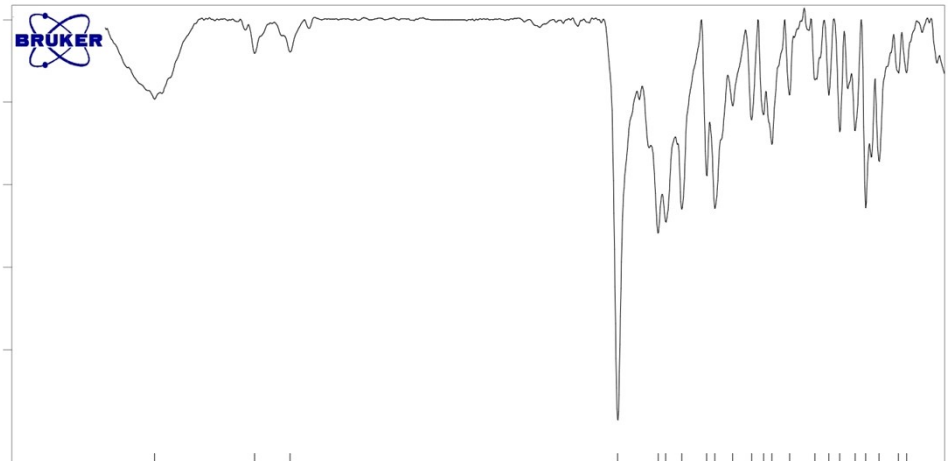


Figure S5. FT-IR spectrum of Hg(II) complex **(3)**.

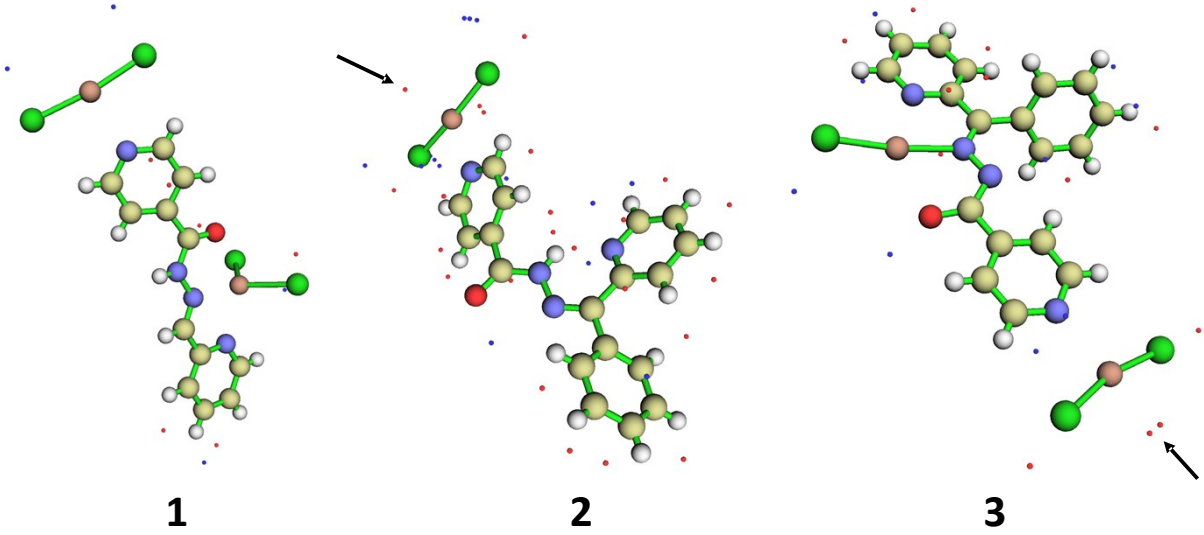


Figure S6. Maxima (red dots) and minima (blue dots) of molecular electrostatic potential (MEP) in model structures **1**–**3** (σ-holes responsible for spodium bonds formation are shown by black arrows).

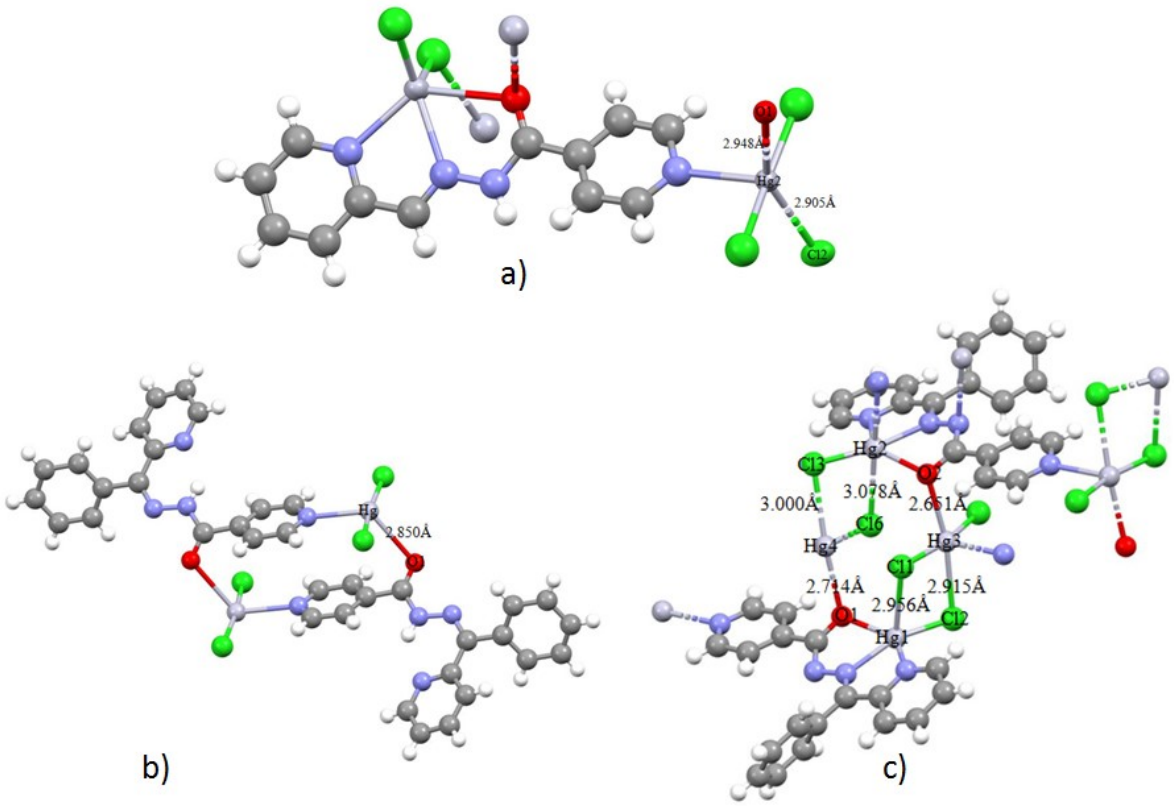


Figure S7. Crystallographic fragments illustrating Hg···O and Hg···Cl contacts in complexes **1**–**3**, with distances labeled in Å (dashed lines).

Additional Hirshfeld Surface Analysis: Shape Index, Curvedness Maps, and Contact Histograms

The curvedness of HS is calculated as the root-mean-square curvature. Flat areas are colored by green and areas of sharp curvature by blue (**Fig. S8**). The shape index is more sensitive to changes in surface curvature (**Fig. S8**). The sign of the shape index shows complementary hollows (with S<1, red color) and bumps (with S>1, blue color). Curvedness and shape index also determine intermolecular interactions. From Fig. SX, it can be seen that dominating interactions Cl···H, H···H, C···H in structures **1**-**3** are caused by bumps of Cl and H on the surface of the molecule. Hollows are located either on the flat surface of the conjugated π-system forming H···π and π···π interactions or Cl and Hg atoms participating in weak coordination bonds, electrostatic interactions and "spodium bonds". The percentage of the interactions also depends on the number of corresponding atoms on the surface. Complex group $\{HgCl_2(HL^1)HgCl_2\}$ of compound **1** has four Cl atoms that results in the abundance of Cl···H interactions (26.7 %, **Fig. 1**). Addition of one phenyl group in ligand HL^2 of compounds **2** and **3** resulted in increasing the part of H···H interactions on the Hirshfeld surface up to 24.4 and 27.9 %, respectively (**Fig. S8**).

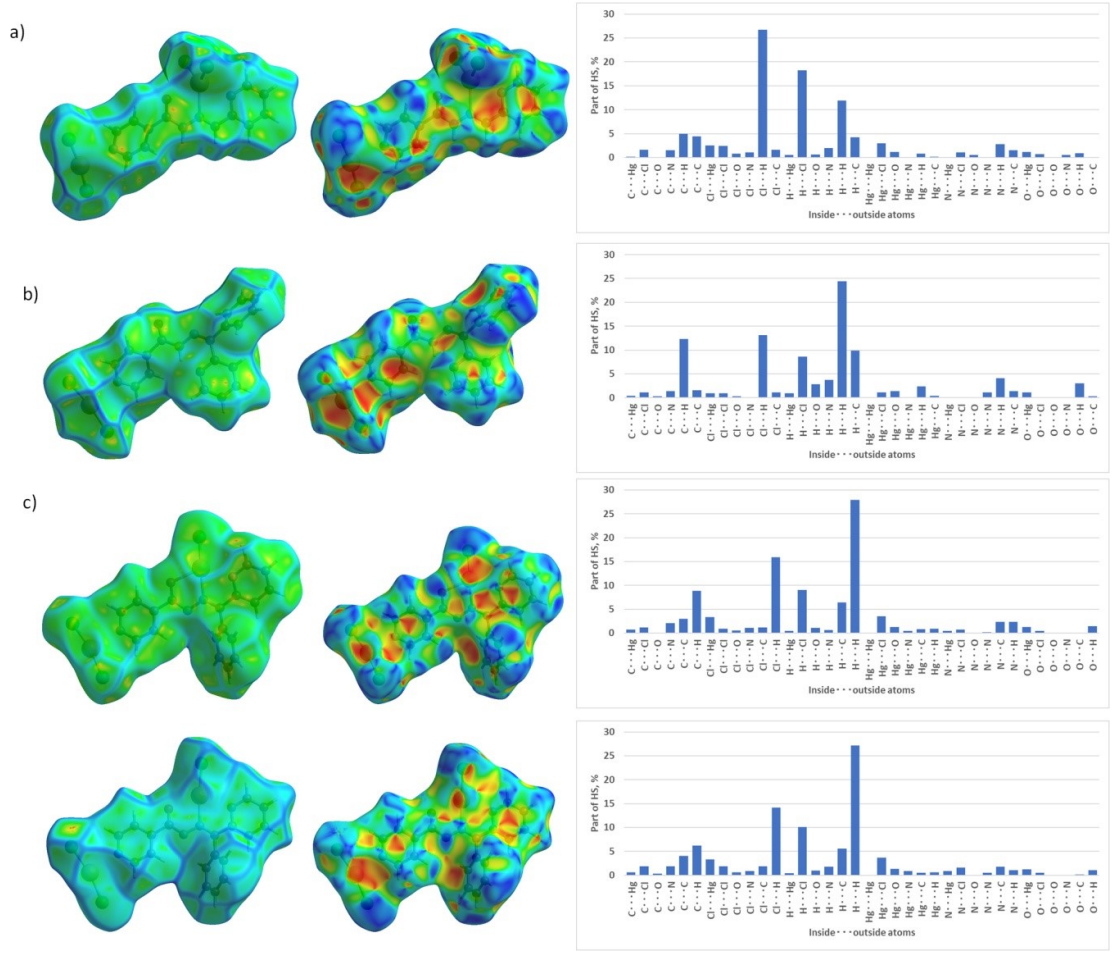


Figure S8. Hirshfeld surfaces (curvedness on the left; shape index in the center) and histograms (on the right) summarizing all types of HS contacts for compounds **1** (a), **2** (b), **3** (c).

Literature-Based List of Hg(II) Complexes with Spodium Bonds

Below is a compiled, representative (but not exhaustive) list of Hg(II) complexes exhibiting spodium bonds (Hg···X, where X = electron-rich atom/anion/π-system), drawn from literature reviews and studies. The list focuses on synthetic complexes (excluding extensive protein examples from PDB surveys, which number in hundreds). Spodium bonds are characterized by Hg···X distances between covalent and van der Waals sums (~2.5-3.5 Å), confirmed via X-ray, DFT/QTAIM, and MEP.

Table S1. A few key examples of reported Hg(II) complexes having spodium bonds**.**

Complex Formula	Ligands/Description	Type of Spodium Bond	Key Features/Analysis	References
$[Hg(HL)(SCN)_2]$	HL = *N′*-(1-(pyridin-2-yl)ethylidene)nicotinohydrazide	Hg···N (from Py and SCN)	Pentacoordinated Hg; SpBs extend to 2D layers; energies –8.04 kcal/mol (–4.02 kcal/mol each spodium bond) to –12.9 kcal/mol (–6.5 kcal/mol each spodium bond)	[17]
$Hg(S_2CNR_2)_2$ (R = Et, iBu, Cy)	Dithiocarbamato (R = ethyl, isobutyl, cyclohexyl)	Intramolecular Hg···S; intermolecular in iBu	Steric-dependent; SpB energies ~2.5 kcal/mol; NBO shows LP(S)→σ*(Hg-S)	[18]
$[Hg_2L(N_3)_4]_n$	L = 1,2-bis(pyridin-2-ylmethylene)hydrazine	Hg···N (from azide/Py)	1D zig-zag polymer extended to 2D via SpBs; pivotal for packing	[19]
$HgCl_2$···L (L = ClR, SR_2, PR_3)	Halide/organics	Hg···Cl/S/P (linear)	SpBs in dimers; MEP supports σ-hole	[20]
HgX_2 dimers (X = Cl, Br, I)	Halides	Hg···X	Purely closed-shell interaction	[21]
$[Hg(L)_2]$ (L = diphenyldithiophosphate derivatives)	Dithiophosphate	Hg···S	Polymeric chains; SpBs + H-bonds; Hirshfeld analysis	[22]
$[Hg(HL)I_2]$)	HL = *o*-nitrobenzaldehyde isonicotinoyl hydrazine ligand	Hg···I (two types)	Supramolecular; SpBs drive aggregation; antibacterial activity	[23]

Table S2. Selected bond distances (Å) and angles (°) for complex **1.**

Hg(1)-N(1)	2.407(6)	Hg(2)-N(4)	2.561(6)
Hg(1)-N(2)	2.345(5)	Hg(2)-Cl(3)	2.3212(19)
Hg(1)-Cl(1)	2.377(2)	Hg(2)-Cl(4)	2.324(2)
Hg(1)-Cl(2)	2.446(2)	Hg(2)-Cl(2)a	2.905(2)
Hg(1)-O(1)	2.635(5)	Hg(2)-O(1)b	2.948(6)
		Hg(2)-Cl(1)b	3.373(2)
N(1)-Hg(1)-N(2)	68.58(19)	Cl(1)-Hg(1)-O(1)	96.07(14)
N(1)-Hg(1)-Cl(1)	113.58(16)	Cl(2)-Hg(1)-O(1)	96.50(13)
N(1)-Hg(1)-Cl(2)	102.79(16)	N(4)-Hg(2)-Cl(3)	91.70(15)
N(1)-Hg(1)-O(1)	133.07(18)	N(4)-Hg(2)-Cl(4)	94.27(15)
N(2)-Hg(1)-Cl(1)	126.26(15)	N(4)-Hg(2)-Cl(2)a	101.25(15)
N(2)-Hg(1)-Cl(2)	117.48(15)	Cl(3)-Hg(2)-Cl(4)	170.09(8)
N(2)-Hg(1)-O(1)	64.55(18)	Cl(3)-Hg(2)-Cl(2)a	96.91(7)
Cl(1)-Hg(1)-Cl(2)	114.07(8)	Cl(4)-Hg(2)-Cl(2)a	89.68(7)
		Hg(1)-Cl(2)-Hg(2)a	114.62(8)

Symmetry codes : a) 2-x, 1-y, 2-z; b) 1-x, 1-y, 2-z.

Table S3. Selected bond distances (Å) and angles (°) for complex **2.**

Hg-N(4)	2.555(6)	Hg-O(1)a	2.850(6)
Hg-Cl(1)	2.294(2)	Hg-Cl(2)b	3.411(3)
Hg-Cl(2)	2.302(2)		
Cl(1)-Hg-Cl(2)	169.65(8)	Cl(2)-Hg-N(4)	96.87(15)
Cl(1)-Hg-N(4)	92.36(15)	N(4)-Hg-O(1)a	119.25(17)
		N(4)-Hg-Cl(2)b	116.73(13)

Symmetry codes: a) 1-x, -y, 1-z; b) x, 1/2-y, -1/2+z.

Table S4. Selected bond distances (Å) and angles (°) for complex **3.**

Hg(1)-N(1)	2.403(3)	Hg(2)-N(5)	2.490(3)
Hg(1)-N(2)	2.232(3)	Hg(2)-N(6)	2.216(3)
Hg(1)-O(1)	2.387(2)	Hg(2)-O(2)	2.498(2)
Hg(1)-Cl(2)	2.3525(9)	Hg(2)-Cl(3)	2.3431(9)
Hg(1)-Cl(1)	2.9556(9)	Hg(2)-N(7)b	2.807(3)
Hg(3)-N(4)a	2.458(3)	Hg(4)-N(8)	2.488(3)
Hg(3)-Cl(1)	2.3930(9)	Hg(4)-Cl(5)	2.3268(9)
Hg(3)-Cl(4)	2.3569(9)	Hg(4)-Cl(6)	2.3609(9)
Hg(3)-Cl(2)	2.9149(9)	Hg(4)-Cl(3)a	2.9997(9)
Hg(3)-O(2)	2.651(3)	Hg(4)-O(1)a	2.714(3)
Hg(3)-Cl(6)c	3.3108(10)	Hg(4)-Cl(1)a	3.3461(10)
N(2)-Hg(1)-Cl(2)	159.43(8)	Cl(4)-Hg(3)-Cl(1)	167.24(3)
N(2)-Hg(1)-O(1)	69.62(9)	Cl(4)-Hg(3)-N(4)a	94.63(8)
Cl(2)-Hg(1)-O(1)	113.18(6)	Cl(1)-Hg(3)-N(4)a	98.09(7)
N(2)-Hg(1)-N(1)	70.86(10)	Cl(4)-Hg(3)-O(2)	89.16(6)
Cl(2)-Hg(1)-N(1)	110.95(8)	Cl(1)-Hg(3)-O(2)	87.23(6)
O(1)-Hg(1)-N(1)	135.62(9)	N(4)a-Hg(3)-O(2)	101.78(9)
N(2)-Hg(1)-Cl(1)	116.57(8)	Cl(4)-Hg(3)-Cl(2)	97.90(3)
Cl(2)-Hg(1)-Cl(1)	83.97(3)	Cl(1)-Hg(3)-Cl(2)	84.18(3)
O(1)-Hg(1)-Cl(1)	91.87(6)	N(4)a-Hg(3)-Cl(2)	85.54(7)
N(1)-Hg(1)-Cl(1)	88.21(8)	O(2)-Hg(3)-Cl(2)	169.44(6)
N(6)-Hg(2)-Cl(3)	170.97(8)	Cl(5)-Hg(4)-Cl(6)	166.72(3)
N(6)-Hg(2)-N(5)	70.12(10)	Cl(5)-Hg(4)-N(8)	92.37(7)
Cl(3)-Hg(2)-N(5)	107.40(7)	Cl(6)-Hg(4)-N(8)	100.87(7)
N(6)-Hg(2)-O(2)	68.21(9)	Hg(3)-Cl(1)-Hg(1)	92.59(3)
Cl(3)-Hg(2)-O(2)	116.47(6)	Hg(1)-Cl(2)-Hg(3)	94.48(3)
N(5)-Hg(2)-O(2)	134.59(9)		

Symmetry codes: a) x+1, y, z; b) 1-x, 2-y, 2-z; c) -1+x, y, z.

Table S5. H-bond parameters (Å /°) for **1-3**.

D-H	A	d(D-H)	d(H…A)	d(D…A)	<DHA	Symmetry code
1						
N3-H3n	Cl2	0.84(8)	2.80(8)	3.410(6)	131(7)	[x,-1+y,z]
N3-H3n	Cl4	0.84(8)	2.70(9)	3.373(7)	139(8)	[2-x,-y,2-z]
C3-H3	Cl3	0.93	2.78	3.503(8)	135	[1+x,y,-1+z]
C4-H4	Cl1	0.93	2.79	3.619(8)	149	[1+x,-1+y,z]
C11-H11	Cl3	0.93	2.80	3.467(7)	130	[-]
2						
N3-H1n	N1	0.86	1.97	2.636(9)	134	-
C4-H4	Cl1	0.93	2.72	3.481(8)	139	[1+x,y,1+z]
3						
C3-H3	Cl4	0.95	2.74	3.555(4)	145	[x,-1+y,z]
C18-H18	O1	0.95	2.48	3.409(5)	167	-x,1-y,1-z]
C21-H21	Cl5	0.95	2.72	3.456(4)	135	-1+x,1+y,z]

Table S6. π···π ring interactions distances (Å) and angles (°) for complexes **1-3**·[a]

1							
Cg(I)	Cg(J)	Symmetry Cg(j)	Cg(I)-Cg(J)	α	β	γ	slippage
Py-N1	Py-N1	2-x, 1-y, 1-z	3.726(5)	0.0(4)	16.6	16.6	1.062
Py-N1	Py-N1	3-x, 1-y, 1-z	4.070(5)	0.0(4)	33.3	33.3	2.234
Py-N4	Py-N4	1-x, 1-y, 2-z	3.912(5)	0.0(4)	28.3	28.3	1.854
2							
Py-N4	Py-N4	1-x, -y, 1-z	3.964(4)	0.0(3)	32.0	32.0	2.100
3							
Py-N1	Py-N4	-x, 1-y, 1-z	4.019(2)	16.64(17)	23.4	33.2	1.597
Py-N1	Py-N5	x, -1+y, z	4.157(2)	21.72(18)	12.2	29.4	
Py-N4	Py-N1	-x, 1-y, 1-z	4.019(2)	16.64(17)	33.2	23.4	2.200
Py-N4	Py-N8	-1+x, y, z	3.6499(19)	2.12(15)	27.5	27.2	1.684
Py-N5	Py-N1	x, 1+y, z	4.157(2)	21.72(18)	29.4	12.2	
Py-N5	Py-N8	1-x, 2-y, 2-z	3.675(2)	9.12(16)	28.5	22.4	1.753
Py-N8	Py-N4	1+x, y, z	3.6500(19)	2.12(15)	27.2	27.5	1.666
Py-N8	Py-N5	1-x, 2-y, 2-z	3.675(2)	9.12(16)	22.4	28.5	1.399

Table S7. Cartesian atomic coordinates for complex **1.**

Hg	5.74243200	2.33342600	19.28336600
Hg	9.52585900	6.61195600	11.01848700
Cl	7.52563600	7.71839400	10.36396400
Cl	11.30258500	8.12018100	11.76097300
Cl	5.98052600	4.42346700	20.26539500
Cl	5.11512900	0.28174000	18.38913800
O	8.69204800	5.92737300	13.42154400
N	10.57794800	5.38747300	9.23278900
N	9.74277000	4.33910200	11.55031800
N	9.30788900	3.86383900	12.75777000
H	9.40212100	3.06008100	12.96712600
N	6.92765700	3.11599100	17.15263600
C	10.95514100	5.85885800	8.02209100
H	10.84645600	6.76709400	7.85471900
C	11.48712300	5.07866800	7.02886400
H	11.73302800	5.44630600	6.21076700
C	11.64570700	3.75021400	7.27717100
H	12.00145700	3.19097400	6.62425400
C	11.27465500	3.24082500	8.49760600
H	11.37618200	2.33402400	8.67721500
C	10.75303000	4.07967700	9.45188300
C	10.33621700	3.56693300	10.73398900
H	10.49958000	2.67969400	10.95985100
C	8.70358500	4.71689800	13.61791700
C	8.10795400	4.10822700	14.83835200
C	7.63727600	2.81725300	14.90164600
H	7.70337400	2.25661800	14.16303900
C	7.94433800	4.91570100	15.95329800
H	8.22874900	5.80088500	15.93580300
C	7.35881000	4.39707100	17.08447300
H	7.25624500	4.94556600	17.82893900
C	7.07044000	2.36195000	16.06690200
H	6.77109500	1.48231300	16.09718600
Cl	7.92087700	1.03254900	20.69741600
O	2.94341400	3.22535700	19.03684500

Table S8. Cartesian atomic coordinates for complex **2.**

Hg	5.594192	2.525689	1.810195
Cl	5.039989	0.740101	0.483677
Cl	6.028961	4.548215	2.821179
O	9.797815	-2.440128	5.536962
N	13.043424	1.229114	5.238749
N	12.248702	-1.416689	6.242052
N	11.286762	-0.705877	5.581898
H	11.429855	0.116083	5.374595
N	7.338075	1.164943	3.099784
C	13.342115	2.509235	4.990374
H	12.859517	2.948178	4.327115
C	14.298508	3.206885	5.639907
H	14.483648	4.089889	5.416696
C	14.984593	2.575051	6.630955
H	15.633442	3.033509	7.115082
C	14.714138	1.245568	6.916913
H	15.188684	0.803284	7.582786
C	13.731482	0.584117	6.202018
C	13.365106	-0.840799	6.491244
C	10.103850	-1.293284	5.250187
C	9.166867	-0.398187	4.473198
C	8.461126	-0.918133	3.441299
H	8.569969	-1.805366	3.185359
C	7.563042	-0.080625	2.772158
H	7.094512	-0.432428	2.049640
C	8.039427	1.675017	4.134134
H	7.898968	2.559074	4.384936
C	8.946170	0.926360	4.822067
H	9.419824	1.304062	5.527729
C	14.324248	-1.684890	7.231467
C	13.885604	-2.507590	8.247026
H	12.979303	-2.533439	8.456821
C	14.780429	-3.305609	8.966005
H	14.469384	-3.841844	9.659486
C	16.124441	-3.299027	8.649818
H	16.718714	-3.818398	9.142025
C	16.584055	-2.535561	7.618735
H	17.485684	-2.555767	7.393196
C	15.691970	-1.711216	6.888317
H	16.007898	-1.189493	6.186111
Hg	7.071046	-2.525689	6.360030
Cl	7.625249	-0.740101	7.686548

Cl	6.636277	-4.548215	5.349047
O	2.867423	2.440128	2.633264
N	-0.378185	-1.229114	2.931477
N	0.416537	1.416689	1.928173
N	1.378476	0.705877	2.588327
H	1.235383	-0.116083	2.795631
N	5.327164	-1.164943	5.070442
C	-0.676877	-2.509235	3.179852
H	-0.194279	-2.948178	3.843111
C	-1.633269	-3.206885	2.530319
H	-1.818410	-4.089889	2.753529
C	-2.319355	-2.575051	1.539270
H	-2.968204	-3.033509	1.055144
C	-2.048900	-1.245568	1.253313
H	-2.523446	-0.803284	0.587439
C	-1.066244	-0.584117	1.968207
C	-0.699868	0.840799	1.678981
C	2.561388	1.293284	2.920039
C	3.498371	0.398187	3.697027
C	4.204112	0.918133	4.728927
H	4.095269	1.805366	4.984867
C	5.102196	0.080625	5.398068
H	5.570727	0.432428	6.120586
C	4.625811	-1.675017	4.036091
H	4.766271	-2.559074	3.785290
C	3.719068	-0.926360	3.348158
H	3.245414	-1.304062	2.642496
C	-1.659010	1.684890	0.938759
C	-1.220366	2.507590	-0.076800
H	-0.314065	2.533439	-0.286595
C	-2.115190	3.305609	-0.795780
H	-1.804146	3.841844	-1.489261
C	-3.459202	3.299027	-0.479592
H	-4.053476	3.818398	-0.971799
C	-3.918817	2.535561	0.551490
H	-4.820446	2.555767	0.777029
C	-3.026732	1.711216	1.281908
H	-3.342660	1.189493	1.984115

Table S9. Cartesian atomic coordinates for complex **3.**

Hg	1.831478	5.900442	8.377050
Hg	2.420678	10.724587	13.197291
Hg	4.140898	8.585872	9.975915
Hg	11.676709	7.906461	11.602816
Cl	3.200396	6.590745	10.903914
Cl	3.361647	7.411981	7.424131
Cl	0.670527	9.469527	14.120334
Cl	4.608933	10.762238	9.201828
Cl	11.243760	5.803419	12.499522
Cl	12.594745	9.814701	10.558852
O	-0.192720	6.940833	9.097899
O	4.439120	9.449199	12.464690
N	2.787488	3.702030	8.546537
N	0.188348	4.395866	8.509723
N	-1.108917	4.832442	8.618749
N	-5.089507	7.711016	9.475385
N	1.544816	13.013176	12.757504
N	4.086027	12.073399	12.632903
N	5.373492	11.587423	12.671133
N	9.381718	8.713718	12.121753
C	4.088705	3.406689	8.515386
H	4.717063	4.116800	8.570990
C	4.561555	2.109720	8.404944
H	5.494104	1.926479	8.399790
C	3.635293	1.089725	8.304413
H	3.926267	0.188378	8.231436
C	2.277321	1.383302	8.308661
H	1.632690	0.690433	8.224257
C	1.876922	2.714931	8.438926
C	0.436762	3.119546	8.474324
C	-1.151774	6.120170	8.923173
C	-2.542232	6.672971	9.077509
C	-3.613359	5.834052	9.377686
H	-3.489469	4.893767	9.442252
C	-4.867099	6.402003	9.580164
H	-5.594759	5.832048	9.800935
C	-4.065730	8.514341	9.168129
H	-4.229945	9.446310	9.076008
C	-2.779335	8.046427	8.976979
H	-2.070360	8.646871	8.779938
C	-0.607772	2.075266	8.433262
C	-0.613697	1.022347	9.359279
H	0.052568	0.980533	10.034747
C	-1.592057	0.042408	9.289898
H	-1.586286	-0.677736	9.910414
C	-2.579367	0.109783	8.319988
H	-3.263900	-0.548887	8.296512
C	-2.574784	1.125966	7.385476

H	-3.240024	1.157554	6.707332
C	-1.588180	2.105387	7.444945
H	-1.582792	2.804210	6.800996
C	0.285690	13.449650	12.782991
H	-0.405546	12.839174	13.012923
C	-0.052808	14.758979	12.487062
H	-0.955924	15.046900	12.541788
C	0.940496	15.638476	12.109010
H	0.730320	16.533896	11.870638
C	2.261552	15.188096	12.086355
H	2.966452	15.772770	11.834178
C	2.531056	13.869842	12.436089
C	3.921775	13.344535	12.467239
C	5.416259	10.267728	12.530956
C	6.808030	9.729868	12.427593
C	7.874807	10.572419	12.162815
H	7.738715	11.508864	12.075877
C	9.141064	10.033315	12.025470
H	9.870514	10.618913	11.858518
C	8.352898	7.895450	12.395027
H	8.518936	6.963974	12.480775
C	7.062792	8.359525	12.553611
H	6.355646	7.754940	12.747352
C	5.064384	14.278405	12.281753
C	5.896501	14.158160	11.170250
H	5.740849	13.476481	10.527107
C	6.960022	15.045331	11.010250
H	7.514590	14.982675	10.241402
C	7.215007	16.017775	11.963169
H	7.950038	16.609999	11.852769
C	6.397484	16.127955	13.076088
H	6.573249	16.791935	13.732851
C	5.319285	15.266001	13.231840
H	4.752316	15.348971	13.989417
Hg	13.893078	10.724587	13.197291
Hg	6.641403	12.105026	15.121253
Hg	-7.331502	8.585872	9.975915
Hg	0.204309	7.906461	11.602816
Cl	12.142927	9.469527	14.120334
Cl	1.122345	9.814701	10.558852
O	11.279680	6.940833	9.097899
N	6.382893	7.711016	9.475385
N	3.688589	11.242191	15.647412

Table S10. Estimated energies of noncovalent interactions in **1**–**3** (E_{int}, kcal/mol).

Contact* (Å)	$E_{int} \approx -V(\mathbf{r})/2$		Contact* (Å)	$E_{int} \approx -V(\mathbf{r})/2$
1			**3**	
Hg–Cl 2.905	8.2		Hg–Cl 3.000	6.3
Hg–O 2.948	4.7		Hg–Cl 3.078	5.0
			Hg–Cl 2.956	7.2
2			Hg–Cl 2.915	7.8
Hg–O 2.850	6.3		Hg–O 2.714	7.8
			Hg–O 2.651	9.1

The estimated energies of noncovalent interactions in **1**–**3** (4.7–9.1 kcal/mol) are typical for such kind of supramolecular contacts in crystals of coordination compounds (e.g., Pt(II) and Pd(II) [24-26], Co(II) [27], Cu(II) [28], Ir(III) [29] complexes, halobismuthates [30-33], haloantimonates [34,35], halotellurates [36-38], molybdates [39,40], etc.

Table S11. The values of descriptors of interactions between complex groups $\{HgCl_2(HL^1)HgCl_2\}$ in the crystal structure of **1.**

Intermolecular distance (length of edge of the underlying net), Å	Solid angle of intermolecular interface, %	Coordinates of a node (molecule center) adjacent to the central node at (0.8081, 0.5064, 0.8811)	Interface area, $Å^2$	Interactions forming the interface (part of all interfaces at %)
4.903	11.748	(1.1919, 0.4936, 1.1189)	70.58	Hg-Cl (21.2%), O-C (1.4 %), O-H (1.6%), O-N (6.4%), C-H (17.9 %), C-C (4.7%), H-H (6.1%), H-N (8.2%), N-Cl (12.3 %), Cl-Cl (5.4%), C-Cl (8.1%), H-Cl (6.7%)
5.981	17.295	(0.1919, 0.4936, 1.1189)	77.04	Hg-Cl (11.8%), Cl-Cl (6.9 %), O-Hg (12.8%), O-Cl (10.3%), C-H (12.6%), C-C (2.2%), C-Hg (1.7 %), C-N (6.1%), C-Cl (9.2 %), H-H (5.4%), H-N (3.1%), H-Hg (2.7%), H-Cl (12.5%), N-Cl (2.8%)
7.588	0.343	(1.8081, 0.5064, 0.8811)	2.23	Cl-Cl (82.7%), Cl-H (17.3%)
7.588	0.343	(-0.1919, 0.5064, 0.8811)	2.23	Cl-Cl (82.7%), Cl-H (17.3 %)
7.931	8.855	(0.8081, 1.5064, 0.8811)	35.29	H-H (15.1%), H-O (11.0%), H-Cl (69.9%), H-Hg (0.3%), Cl-Cl (3.7 %)
7.931	8.855	(0.8081, -0.4936, 0.8811)	35.29	H-H (15.1%), H-O (11.0%), H-Cl (69.9%), H-Hg (0.3%), (0.4 %), Cl-Cl (3.7%)
8.257	7.209	(1.1919, -0.5064, 1.1189)	34.78	C-H (15.1%), C-Cl (0.8%), H-H (18.3%), H-N (7.7%), H-Cl (54.3%), H-Hg (3.8%)
8.806	3.3	(1.8081, -0.4936, 0.8811)	12.37	H-Cl (100.0 %)
8.806	3.3	(-0.1919, 1.5064, 0.8811)	12.37	H-Cl (100.0 %)
11.084	2.926	(0.1919, -0.5064, 1.1189)	14.12	C-Cl (0.3 %), H-Cl (98.8 %), Cl-Cl (0.9 %)
12.625	13.19	(1.1919, 0.4936, 0.1189)	64.37	Hg-H (5.9%), Hg-C (0.2 %), Cl-H (33.5%) (29.2 %), O-H (0.1%), H-H (20.1%), N-H (13.6 %), N-C (11.0%), C-H (3.6%), C-C (12.1%)
14.989	10.903	(1.1919, 1.4936, 0.1189)	44.18	Hg-H (9.9%), Cl-H (65.3%), H-H (24.8%)

15.923	4.989	(2.1919, 0.4936, 0.1189)	30.88	N-H (13.9%), Cl-H (3.8%), C-H (39.9%), H-H (30.0%), C-C (12.4%)
16.466	0.363	(2.1919, -0.5064, 0.1189)	1.81	H-H (100.0%)
17.687	3.191	(1.8081, 0.5064, -0.1189)	12.16	Hg-H (0.1%), Cl-H (99.9%)
17.687	3.191	(-0.1919, 0.5064, 1.8811)	12.16	Hg-H (0.1%), Cl-H (99.9%)

Table S12. The values of descriptors of interactions between complex groups $\{HgCl_2(HL^2)\}$ in the crystal structure of **2.**

Intermolecular distance (length of edge of the underlying net), Å	Solid angle of intermolecular interface, %	Coordinates of a node (molecule center) adjacent to the central node at (0.69958, 0.06220, 0.48020)	Interface area, Å^2	Interactions forming the interface (part of all interfaces at %)
5.864	11.793	(0.3004, -0.0622 0.5198)	58.14	Hg-O (19.6%), Hg-C (6.0%), Hg-H (5.0%), Cl-O (6.5%), Cl-H (16.6%), Cl-C (10.3%), N-C (11.8%), N-H (1.1%), C-H (11.6%), C-C (0.3%), H-H (11.2%)
7.425	3.546	(0.6996, 0.4378, -0.0198)	17.20	Cl-Cl (14.1%), Cl-Hg (26.2%), H-Cl (19.4%), C-H (3.2%), H-H (37.1%)
7.425	3.546	(0.6996, 0.4378, 0.9802)	17.20	Cl-Cl (14.1%), Cl-Hg (26.2%), H-Cl (19.4%), C-H (3.2%), H-H (37.1%)
8.42	17.626	(1.3004 -0.0622 0.5198)	94.65	Hg-H (7.0%), Cl-H (2.5%). N-H (17.8%), C-H (32.8%), C-C (5.2%), H-H (20.4%), C-N (5.1 %). O-C (2.1%), O-H (2.7%), N-N (4.6%)
9.276	2.981	(0.3004, -0.0622, -0.4802)	14.79	Cl-Cl (3.6%), Cl-H (94.8%) Cl-C (1.7%)
10.334	2.138	(0.3004, 0.5622, 0.0198)	10.36	H-Cl (88.8%), H-Hg (11.2%)
10.334	2.138	(0.3004, -0.4378, 0.0198)	10.36	H-Cl (88.8 %), H-Hg (11.2 %)
11.067	3.498	(0.6996, -0.5622, -0.0198)	3.49	Hg-H (0.7%), Cl-H (99.3%)
11.067	3.498	(0.6996, -0.5622, 0.9802)	3.49	Hg-H (0.7 %), Cl-H (99.3 %)
11.308	17.69	(1.3004, -0.0622, 1.5198)	85.15	H-H (31.2%), H-C (45.6%), N-H (14.2%). O-H (6.8%), N-C (0.2%), C-C (2.0%)
12.081	11.228	(1.3004, 0.5622 1.0198)	45.35	Cl-H (16.7%), C-H (9.6 %), H-H (42.3%), H-O (23.4 %), H-N (8.0%)
12.081	11.228	(1.3004, -0.4378 1.0198)	45.35	Cl-H (16.7%), C-H (9.6%), H-H (42.3%), H-O (23.4%), H-N (8.0%)
15.072	3.82	(1.6996, 0.0622 1.4802)	16.80	Hg-H (12.4%). Cl-H (70.6%). Cl-C (8.9%). H-H (8.1%)
15.072	3.82	(-0.3004, 0.0622, -0.5198)	16.80	Hg-H (12.4%), Cl-H (70.6%), Cl-C (8.9%), H-H (8.1%)
15.099	0.725	(-0.3004, 0.4378,	3.49	H-Hg (0.7%), H-Cl (99.3%)

		-0.0198)		
15.099	0.725	(1.6996, 0.4378, 0.9802)	3.49	H-Hg (0.7%), H-Cl (99.3%)

Table S13. The values of descriptors of interactions between complex groups $\{Hg_2Cl_3(L^2)\}$ in the crystal structure of **3.**

Intermolecular distance (length of edge of the underlying net). Å	Solid angle of intermolecular interface. %	Coordinates of a node (molecule center) adjacent to the central nodes at ZA1 (0.87335, 0.54611, 0.63561) and ZA2 (0.65723, 0.90679, 0.87418)	Interface area. Å^2	Interactions forming the interface (part of all interfaces at %)
4.977	22.277	ZA1_ZA1 (1.1267, 0.4539, 0.3644)	117.41	H-N (1.5%), H-C (18.1%), H-H (10.3%), H-Cl (26.3%), H-Hg (3.3%), C-C (3.6 %), C-N (12.8%), C-Cl (4.9 %), C-Hg (5.0%), N-N (1.0 %), N-O (1.1%), O-H (8.9%), Cl-N (0.1%), Hg-N (3.0%)
6.148	11.705	ZA1_ZA2 (0.6572, 0.9068, 0.8742)	60.54	Hg-C (1.4%), Hg-O (19.1%), Hg-H (2.3%), Cl-O (10.5%), Cl-C (6.2 %), Cl-N (6.7%), Cl-H (13.6%), N-H (4.6%), N-C (6.8%), C-C (4.8%), C-H (16.5%), H-H (7.3%), Hg-Cl (0.1%), Cl-Cl (0.1%)
9.067	13.644	ZA1_ZA2 (0.6572, -0.0932, 0.8742)	66.30	Cl-H (24.0%), N-H (5.4 %), C-H (30.3%), H-H (40.4%)
9.302	2.234	ZA1_ZA1 (0.1267, 0.4539, 0.3644)	9.69	Hg-H (26.1%), Cl-H (73.9%)
10.654	1.582	ZA1_ZA2 (1.3428, 0.0932, 0.1258)	7.71	C-Cl (2.6%), H-Cl (97.4%)
11.472	6.985	ZA1_ZA1 (1.8733, 0.5461, 0.6356)	33.38	Hg-Cl (34.0%), Hg-Hg (0.3%), Cl-Cl (3.0%), Cl-H (7.7%), Cl-N (7.9%), Cl-O (2.2%), C-H (1.6%), C-Cl (0.2%), H-H (43.1%)
11.472	6.985	ZA1_ZA1 (-0.1267, 0.5461, 0.6356)	33.38	Hg-Cl (34.0%), Hg-Hg (0.3%), Cl-Cl (3.0%), Cl-H (7.7%), Cl-N (7.9%), Cl-O (2.2%), C-H (1.6%), C-Cl (0.2%), H-H (43.1%)
11.546	1.105	ZA1_ZA2 (0.3428, 1.0932, 1.1258)	6.00	Cl-H (100.0%)
12.497	4.04	ZA1_ZA1 (0.8733, 1.5461, 0.6356)	16.19	Cl-H (28.0%), H-H (71.4%), H-C (0.6%)
12.497	4.04	ZA1_ZA1 (0.8733, -0.4539, 0.6356)	16.19	Cl-H (28.0%), H-H (71.4%), H-C (0.6 %)
13.097	6.794	ZA1_ZA2 (1.6572, -0.0932, 0.8742)	44.02	C-H (29.6%), H-H (36.2%), N-H (17.1%), O-H (0.2%), C-C (12.8%), Hg-H (1.8%) N-C (2.2%)

14.455	7.984	ZA1_ZA1 (1.1267, -0.5461, 0.3644)	38.27	C-C (0.7%), C-H (38.7%), H-H (60.6%)
15.041	4.641	ZA1_ZA1 (2.1267, 0.4539, 0.3644)	20.87	Cl-H (94.0 %), Cl-C (2.7%), H-H (3.3%)
15.358	2.718	ZA1_ZA2 (-0.3428, 0.9068, 0.8742)	13.53	Hg-Cl (71.3%), Cl-Cl (28.7 %)
17.662	1.634	ZA1_ZA1 (1.8733, -0.4539, 0.6356)	7.74	Cl-H (100.0 %)
17.662	1.634	ZA1_ZA1 (-0.1267, 1.5461, 0.6356)	7.74	Cl-H (100.0 %)
5.631	25.009	ZA2_ZA2 (0.3428, 1.0932, 1.1258)	127.33	Hg-N (6.5%), Hg-C (3.1%), Hg-H (2.1%), Cl-H (15.3%), Cl-C (11.4%), Cl-N (0.2%), O-C (1.5%), O-N (0.8%), O-H (8.3%), N-C (9.1%), N-H (3.4%), C-C (7.4%), C-H (13.0%), H-H (16.0%), N-N (2.0 %)
6.148	11.903	ZA2_ZA1 (0.8733, 0.5461, 0.6356)	60.54	Hg-C (1.4%), Hg-O (19.1 %), Hg-H (2.3%), Cl-O (10.5 %), Cl-C (6.2%), Cl-N (6.7%), Cl-H (13.6%), N-H (4.6%), N-C (6.8%), C-C (4.8%), C-H (16.5%), H-H (7.3%), Hg-Cl (0.1 %), Cl-Cl (0.1%)
8.669	1.92	ZA2_ZA2 (1.3428, 1.0932, 1.1258)	12.69	H-Hg (16.4%), H-Cl (83.6 %)
9.067	13.875	ZA2_ZA1 (0.8733, 1.5461, 0.6356)	66.30	Cl-H (24.0%), N-H (5.4%), C-H (30.3 %), H-H (40.4 %)
10.654	1.609	ZA2_ZA1 (1.1267, 0.4539, 0.3644)	7.71	C-Cl (2.6 %), H-Cl (97.4%)
11.472	7.433	ZA2_ZA2 (-0.3428, 0.9068, 0.8742)	37.19	C-H (2.5%), H-H (37.3%), H-Cl (8.1 %), H-Hg (0.1%), Cl-Cl (3.9%), Cl-Hg (31.0%), Cl-O (3.0%), Cl-N (12.5%), Hg-O (0.7 %), Hg-Hg (0.8%)
11.472	7.433	ZA2_ZA2 (1.6572, 0.9068, 0.8742)	37.19	C-H (2.5%), H-H (37.3%), H-Cl (8.1%), H-Hg (0.1 %), Cl-Cl (3.9%), Cl-Hg (31.0%), Cl-O (3.0%), Cl-N (12.5%), Hg-O (0.7%) Hg-Hg (0.8%)
11.546	1.124	ZA2_ZA1 (0.1267, 1.4539, 1.3644	6.00	Cl-H (100.0%)
12.497	4.065	ZA2_ZA2 (0.6572, 1.9068, 0.8742	16.73	C-H (6.3%), H-H (93.7%)
12.497	4.065	ZA2_ZA2 (0.6572, -0.0932, 0.8742	16.73	C-H (6.3%), H-H (93.7 %)
13.097	6.908	ZA2_ZA (1-0.1267, 1.5461, 0.6356)	44.02	C-H (29.6%), H-H (36.2%), N-H (17.1%), O-H (0.2%), C-C (12.8%), Hg-H (1.8 %), N-C (2.2%)

14.003	0.863	ZA2_ZA2 (1.3428, 0.0932, 1.1258)	5.00	Cl-H (9.2%), Cl-Cl (90.8 %)
15.358	2.764	ZA2_ZA1 (1.8733, 0.5461, 0.6356)	13.53	Hg-Cl (71.3%), Cl-Cl (28.7 %)
15.725	1.827	ZA2_ZA2 (0.3428, 2.0932, 1.1258)	16.73	C-H (6.3%), H-H (93.7%)
15.858	4.608	ZA2_ZA2 (-0.6572, 1.0932, 1.1258)	20.19	H-Cl (94.4%), H-H (5.6%)
17.662	2.297	ZA2_ZA2 (-0.3428, 1.9068, 0.8742)	9.68	Cl-H (100.0%)
17.662	2.297	ZA2_ZA2 (1.6572, -0.0932, 0.8742)	9.68	Cl-H (100.0%)

Table S14. Filtering fingerprint by element type for compound **1**, where surface area included (as percentage of the total surface area) for close contacts between atoms inside and outside the surface.

	Outside Atom						
Inside Atom	Hg	Cl	O	N	H	C	Total
C	0.2	1.6	0.1	1.5	**5**	**4.4**	12.8
Cl	2.5	2.4	0.8	1.1	**26.7**	1.6	35.1
H	0.5	**18.2**	0.6	2	**11.9**	**4.2**	37.4
Hg	-	3	1.2	-	0.8	0.2	5.2
N	-	1.1	0.5	-	2.8	1.5	5.9
O	1.2	0.7	-	0.5	0.9	0.1	3.5
Total	4.5	27	3.3	5	48.2	12	

Table S15. Filtering fingerprint by element type for compound **2**, where surface area is included (as a percentage of the total surface area) for close contacts between atoms inside and outside the surface.

	Outside Atom						
Inside Atom	Hg	Cl	O	N	H	C	Total
C	0.4	1.1	0.3	1.4	**12.3**	1.6	17.1
Cl	0.9	0.9	0.3	-	**13.1**	1.1	16.3
H	0.9	**8.6**	2.8	3.7	**24.4**	**9.9**	50.3
Hg	-	1.1	1.4	-	2.4	0.4	5.4
N	-	-	-	1.1	4.1	1.4	6.5
O	1.1	0.1	-	-	3	0.3	4.5
Total	3.3	11.7	4.8	6.2	59.3	14.7	

Table S16. Filtering fingerprint by element type for molecule 1 of compound **3**, where surface area is included (as a percentage of the total surface area) for close contacts between atoms inside and outside the surface.

	Outside Atom						
Inside Atom	Hg	Cl	O	N	C	H	Total
C	0.7	1.2	-	2.1	3	**8.8**	15.8
Cl	3.3	0.9	0.5	1.1	1.2	**15.9**	22.9
H	0.4	**9**	1.1	0.6	**6.4**	**27.9**	45.3
Hg	0	3.5	1.3	0.4	0.8	0.9	6.9
N	0.4	0.7	0.1	0.2	2.3	2.3	6
O	1.3	0.4	-	0.1	-	1.4	3.2
Total	6	15.6	3	4.6	13.6	57.1	

Table S17. Filtering fingerprint by element type for molecule 2 of compound **3**, where surface area is included (as a percentage of the total surface area) for close contacts between atoms inside and outside the surface.

	Outside Atom						
Inside Atom	Hg	Cl	O	N	C	H	Total
C	0.6	1.9	0.3	1.9	4	**6.2**	14.9
Cl	3.3	1.9	0.6	0.9	1.9	**14.2**	22.8
H	0.4	**10.1**	1	1.8	**5.6**	**27.2**	46.1
Hg	0.1	3.7	1.3	0.9	0.5	0.6	7.1
N	0.9	1.6	0.1	0.5	1.8	1.1	5.9
O	1.2	0.5	.	0.1	0.2	1.1	3.2
Total	6.5	19.6	3.3	6.1	14.1	50.5	

Table S18. Coordination types of 35 structures with Schiff base ligand, Hg(II) and pyridine group found in CCDC.

Ref Code	Compound	Coordination Formula	Reference
Compound **3**	tris(chloro)-(2-benzoylpyridine-benzoyl-hydrazone)-di-mercury	$A_2K^{101}M^1_3$	This work
IYANEE	(μ-N'-[1-(pyridin-2-yl)ethylidene]pyridine-4-carbohydrazide)-(μ-chloro)-trichloro-di-mercury(II)	$A_2K^{101}M^1_4$	[41, 42]
YEVQIC	(μ-bromo)-(μ-N'-[1-(pyridin-2-yl)ethylidene]pyridine-3-carbohydrazide)-tribromo-di-mercury	$A_2T^{11}M^1_4$	[43]
Compound **1**	tetrakis(chloro)-(2-pyridinecarbaldehyde-isonicotinoylhydrazone)-di-mercury	$A_2T^{11}M^1_4$	This work
HOSPOW	bis(μ2-N'-(pyridin-2-ylmethylene)nicotinohydrazide)-bis(μ2-iodo)-hexakis(iodo)-tetra-mercury	$A_2T^{11}M^1_4$	[44]
XEHWOY	(μ2-N'-(Pyridin-2-ylmethylene)isonicotinohydrazide)-(μ2-iodo)-tetra-iodo-di-mercury	$A_2T^{11}M^1_4$	[45]
HOSPIQ	(μ2-N'-(pyridin-2-ylmethylene)nicotinohydrazide)-(μ2-iodo)-tris(iodo)-mercury acetonitrile solvate	$A_2T^{11}M^1_4$	[46]
HIMDOZ	(N'-[phenyl(pyridin-2-yl)methylidene]pyridine-4-carbohydrazide)-bis(thiocyanato)-mercury(II)	$AB^{01}M^1_2$	[47]
EMAWUN	{N'-[1-(pyridin-2-yl)ethylidene]pyridine-3-carbohydrazide}-bis(thiocyanato)-mercury	$AB^{01}M^1_2$	[48]
IZUPUQ	dibromo-(N'-(phenyl(pyridin-2-yl)methylene)pyridine-2-carbohydrazide)-mercury(II)	$AB^{01}M^1_2$	[48]
IZUQIF	dibromo-(N'-((pyridin-2-yl)methylene)pyridine-2-carbohydrazide)-mercury(II) methanol solvate	$AB^{01}M^1_2$	[48]
HOSQAJ	(N'-(pyridin-2-ylmethylene)nicotinohydrazide)-dibromo-mercury(II)	$AB^{01}M^1_2$	[44]
IZUQEB	dibromo-(N'-((pyridin-2-yl)methylene)pyridine-2-carbohydrazide)-mercury(II)	$AB^{01}M^1_2$	[48]
IZUQUR	dibromo-(N'-(1-(pyridin-2-yl)ethylidene)pyridine-2-carbohydrazide)-mercury(II)	$AB^{01}M^1_2$	[48]
IZUQOL	dichloro-(N'-(1-(pyridin-2-yl)ethylidene)pyridine-2-carbohydrazide)-mercury	$AB^{01}M^1_2$	[48]
HIDMAL	dichloro-(N'-(bis(pyridin-2-yl)methylidene)acetohydrazide)-mercury(II)	$AB^{01}M^1_2$	[49]
IZUPOK	dichloro-(N'-(phenyl(pyridin-2-yl)methylene)pyridine-2-carbohydrazide)-mercury	$AB^{01}M^1_2$	[48]
COYRAK	dichloro-(N'-(bis(2-pyridinyl)methylene)-2-thiophenecarbohydrazide-N.N')-mercury(II)	$AB^{01}M^1_2$	[50]
HUBMEY	dIIodo-(N'-((pyridin-2-yl)methylene)pyridine-2-carbohydrazide)-mercury(II)	$AB^{01}M^1_2$	[51]
IZUQAX	bis(iodo)-(N'-(phenyl(pyridin-2-yl)methylene)pyridine-2-carbohydrazide)-mercury	$AB^{01}M^1_2$	[48]
YEVQUO	dIIodo-(N'-[1-(pyridin-2-yl)ethylidene]pyridine-3-carbohydrazide)-mercury	$AB^{01}M^1_2$	[43]
YEVREZ	dIIodo-(N'-[phenyl(pyridin-2-yl)methylidene]pyridine-3-carbohydrazide)-mercury methanol solvate	$AB^{01}M^1_2$	[43]
XEHWUE	dIIodo-{N'-[1-(pyridin-2-yl)ethylidene]pyridine-4-carbohydrazide}-mercury(II)	$AB^{01}M^1_2$	[44]
XEHXAL	di-iodo-(N'-((pyridin-2-yl)methylene)isonicotinohydrazide)-mercury	$AB^{01}M^1_2$	[52]
XEHWUE01	bis(iodo)-(N'-(1-(pyridin-2-yl)ethylidene)pyridine-4-carbohydrazide)-mercury(II)	$AB^{01}M^1_2$	[41, 42]
HOSPAI	(N'-(pyridin-2-ylmethylene)nicotinohydrazide)-bis(iodo)-mercury(II) methanol solvate	$AB^{01}M^1_2$	[44]
HOSPEM	(N'-(pyridin-2-ylmethylene)nicotinohydrazide)-bis(iodo)-mercury(II) ethanol solvate	$AB^{01}M^1_2$	[44]
IZUPIE	aqua-bis(iodo)-(N'-(1-(pyridin-2-yl)ethylidene)pyridine-2-carbohydrazide)-mercury	$AB^{01}M^1_3$	[48]
DAXGIV	(μ-N-[pyridin-2-ylmethylidene]pyridine-4-carbohydrazonato)-azido-mercury(II) butan-1-ol solvate	$AK^{101}M^1$	[53]
DAXFUG	(μ-N-[pyridin-2-ylmethylidene]pyridine-4-carbohydrazonato)-azido-mercury(II) hemihydrate	$AK^{101}M^1$	[53]
DAXGAN	(μ-N-[pyridin-2-ylmethylidene]pyridine-4-carbohydrazonato)-azido-mercury(II) methanol solvate	$AK^{101}M^1$	[53]
DAXGER	(μ-N-[pyridin-2-ylmethylidene]pyridine-4-carbohydrazonato)-azido-mercury(II) ethanol solvate	$AK^{101}M^1$	[53]
DAXGOB	(μ-N-[pyridin-2-ylmethylidene]pyridine-4-carbohydrazonato)-azido-mercury(II) propan-1-ol solvate	$AK^{101}M^1$	[53]
YEVQOI	(μ-N-[phenyl(pyridin-2-yl)methylidene]pyridine-3-	$AK^{101}M^1$	[53]

	carbohydrazonato)-bromo-mercury(II)		
HOSPUC	(μ2-N-(pyridin-2-ylmethylene)pyridine-3-carbohydrazonato)-iodo-mercury	$AK^{101}M^{1}$	[54]
YEVRAV	(μ-N-[phenyl(pyridin-2-yl)methylidene]pyridine-3-carbohydrazonato)-iodo-mercury	$AK^{101}M^{1}$	[53]
Compound **2**	dichloro-(2-benzoylpyridine-benzoyl-hydrazone)-mercury	AM^{1}_{3}	This work
HIMDUF	(N-[1-(pyridin-2-yl)ethylidene]pyridin-1-ium-4-carbohydrazonato)-bis(thiocyanato)-mercury(II)	$AT^{001}M^{1}_{2}$	[56]

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