ELECTRONIC SUPPLEMENTARY MATERIALS

Spodium Bonding to Anticrown-Hg_3 Boosts Phosphorescence of Cyclometalated-Pt^{II} Complexes

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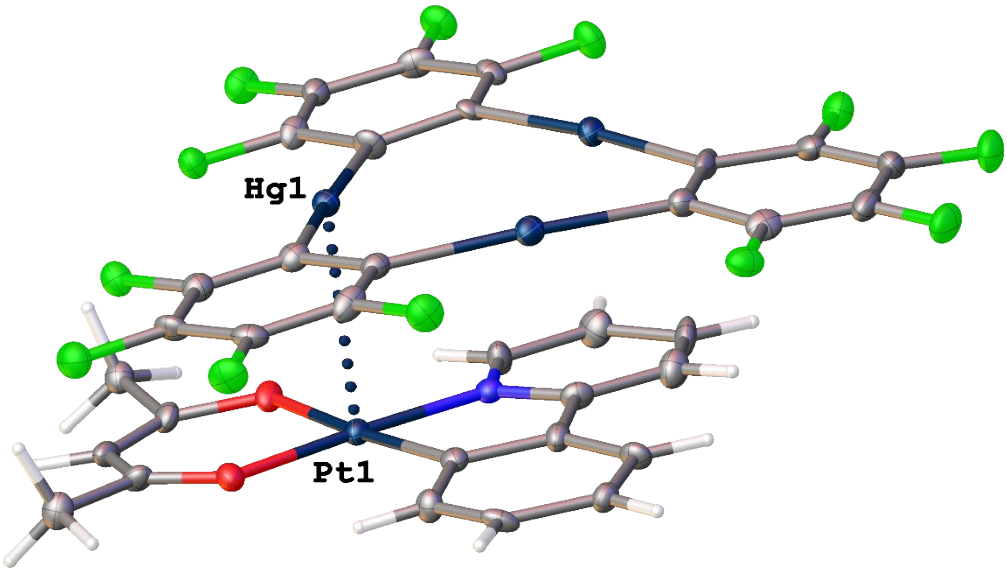


Figure S1. View of the molecular structure of **1**·Hg_3; thermal ellipsoids are shown with the 50% probability.

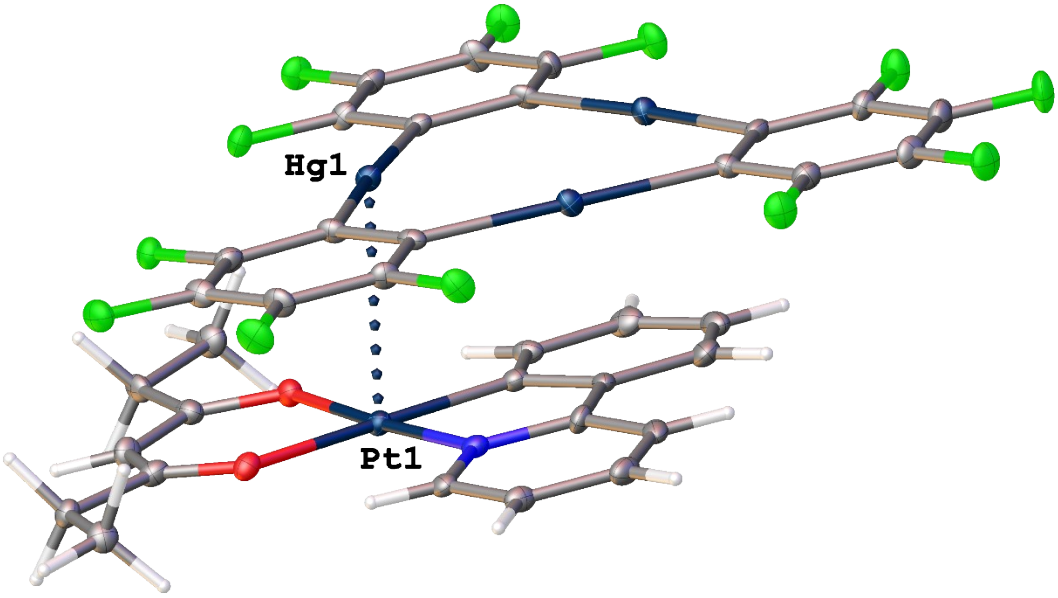


Figure S2. View of the molecular structure of **2**·Hg_3; thermal ellipsoids are shown with the 50% probability.

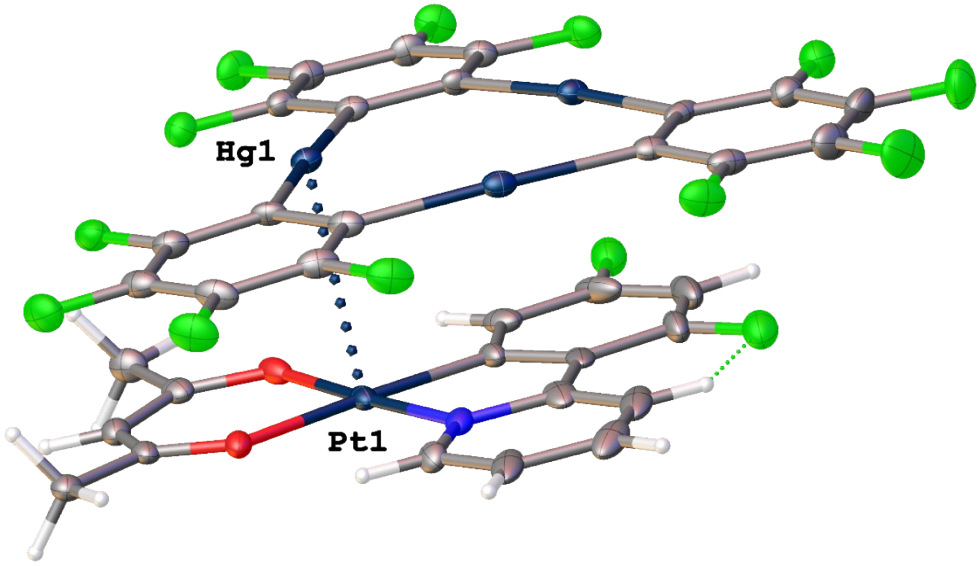


Figure S3. View of the molecular structure of **4**·**Hg$_3$**; thermal ellipsoids are shown with the 50% probability.

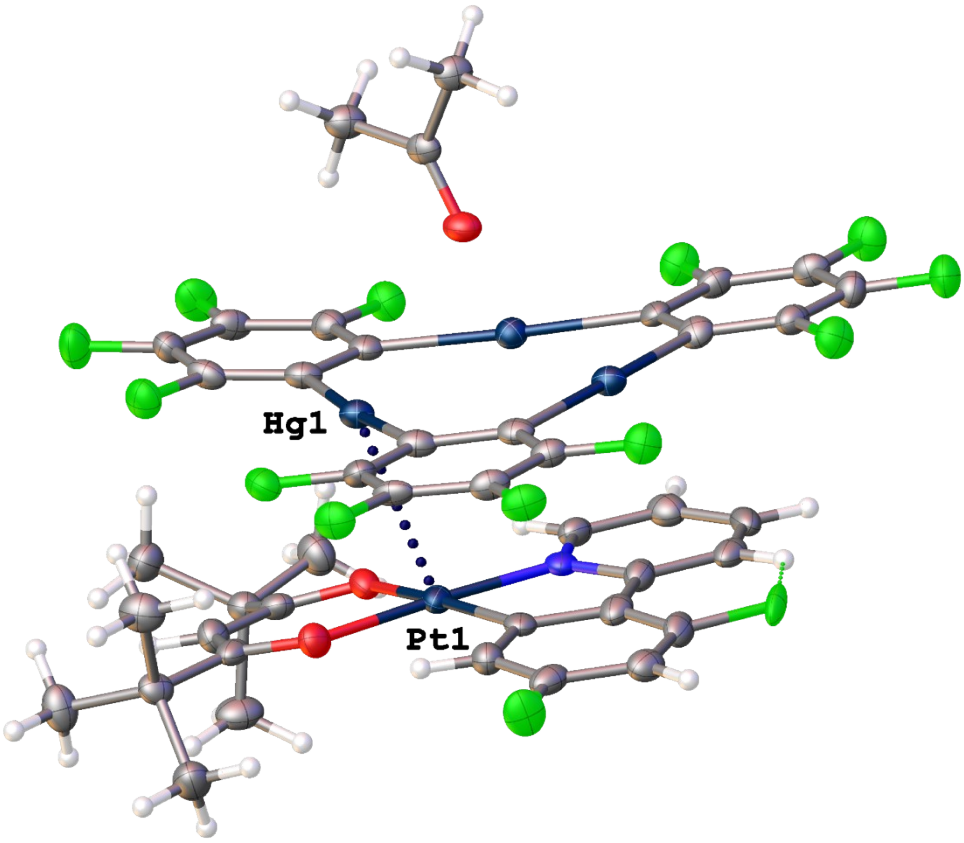


Figure S4. View of the molecular structure of **5**·**Hg$_3$**·Me_2CO; thermal ellipsoids are shown with the 50% probability.

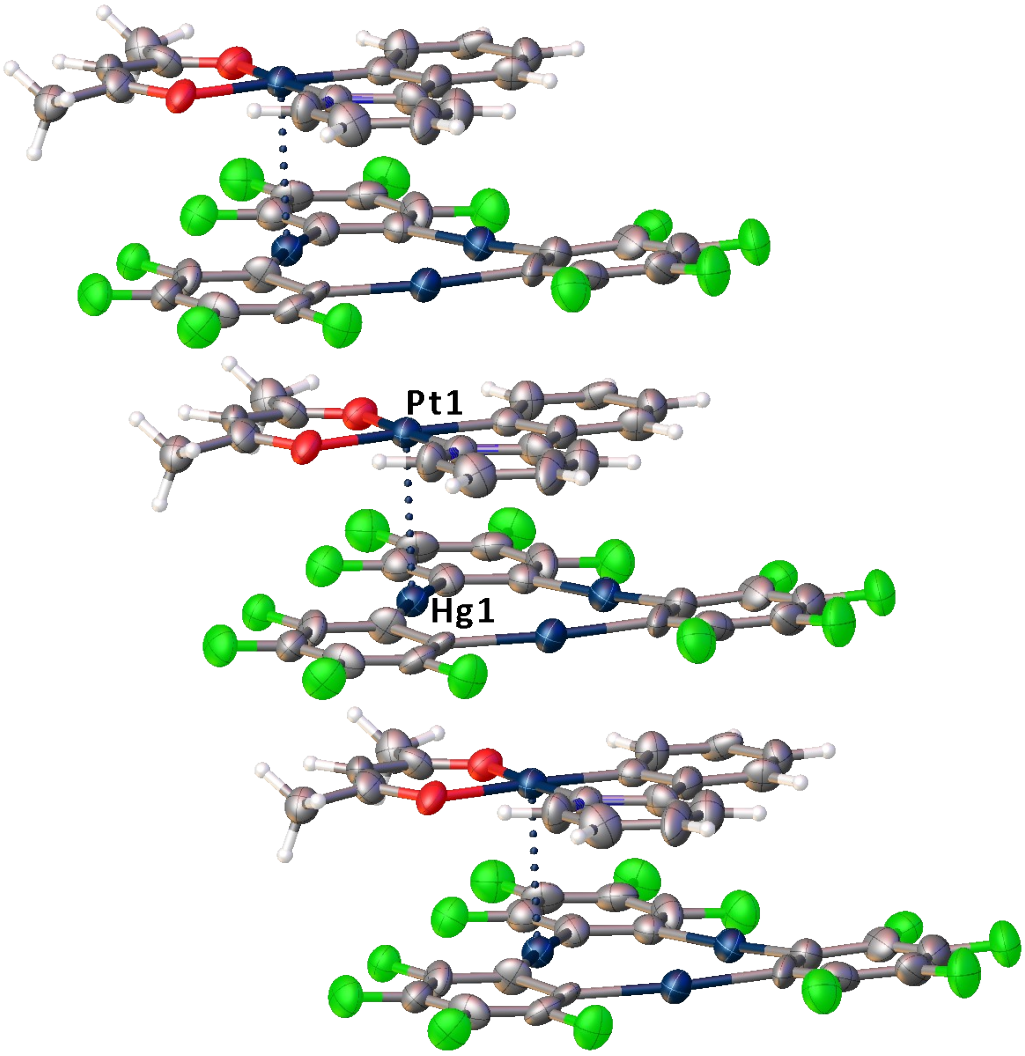


Figure S5. A fragment of crystal packing for **1**·**Hg$_3$**, demonstrating heteropolar stacking between **1** and **Hg$_3$**. Short contacts Hg···Pt are given by dotted lines.

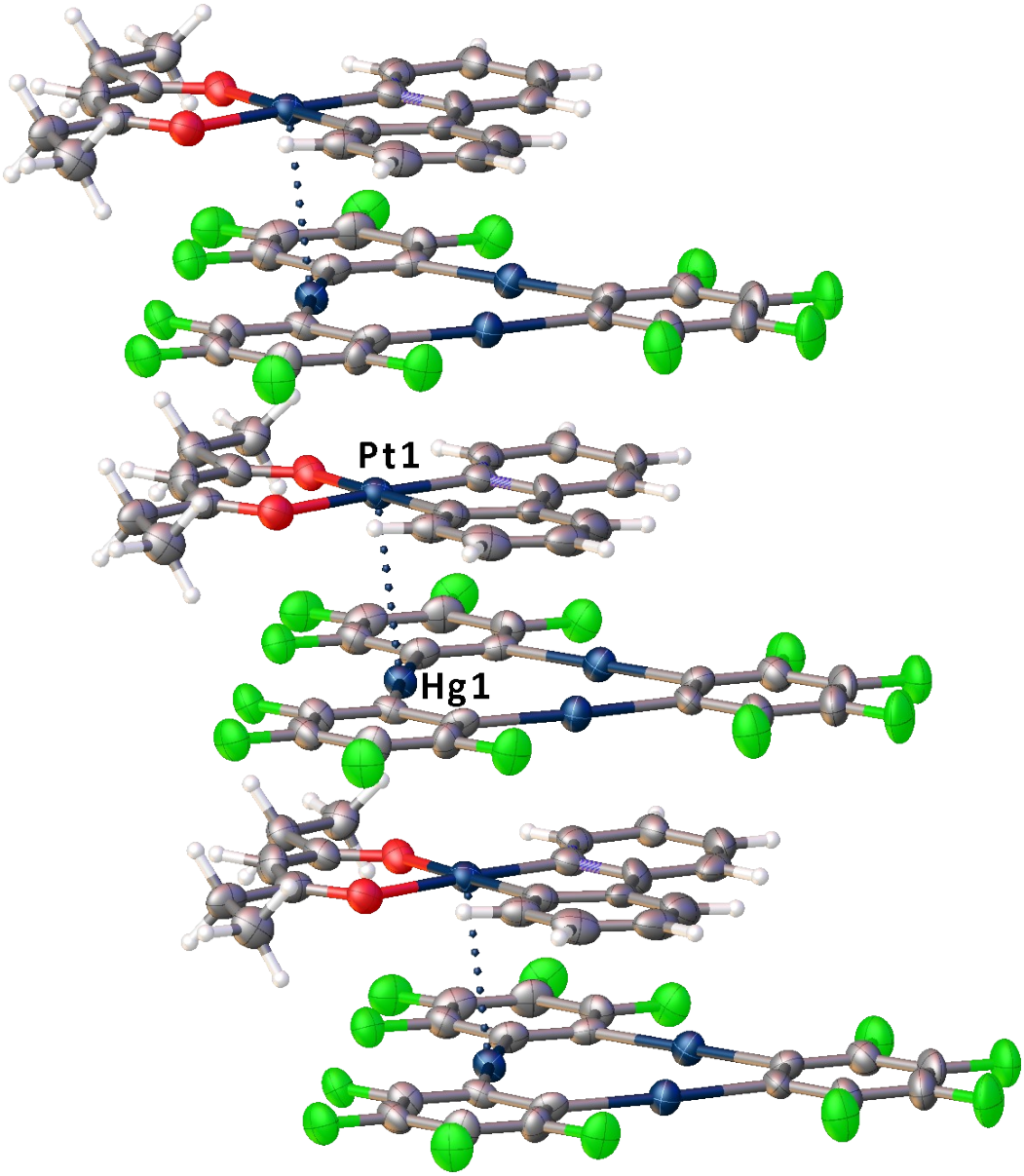


Figure S6. A fragment of crystal packing for **2**·**Hg$_3$** demonstrating heteropolar stacking between **2** and **Hg$_3$**. Short contacts Hg···Pt are given by dotted lines.

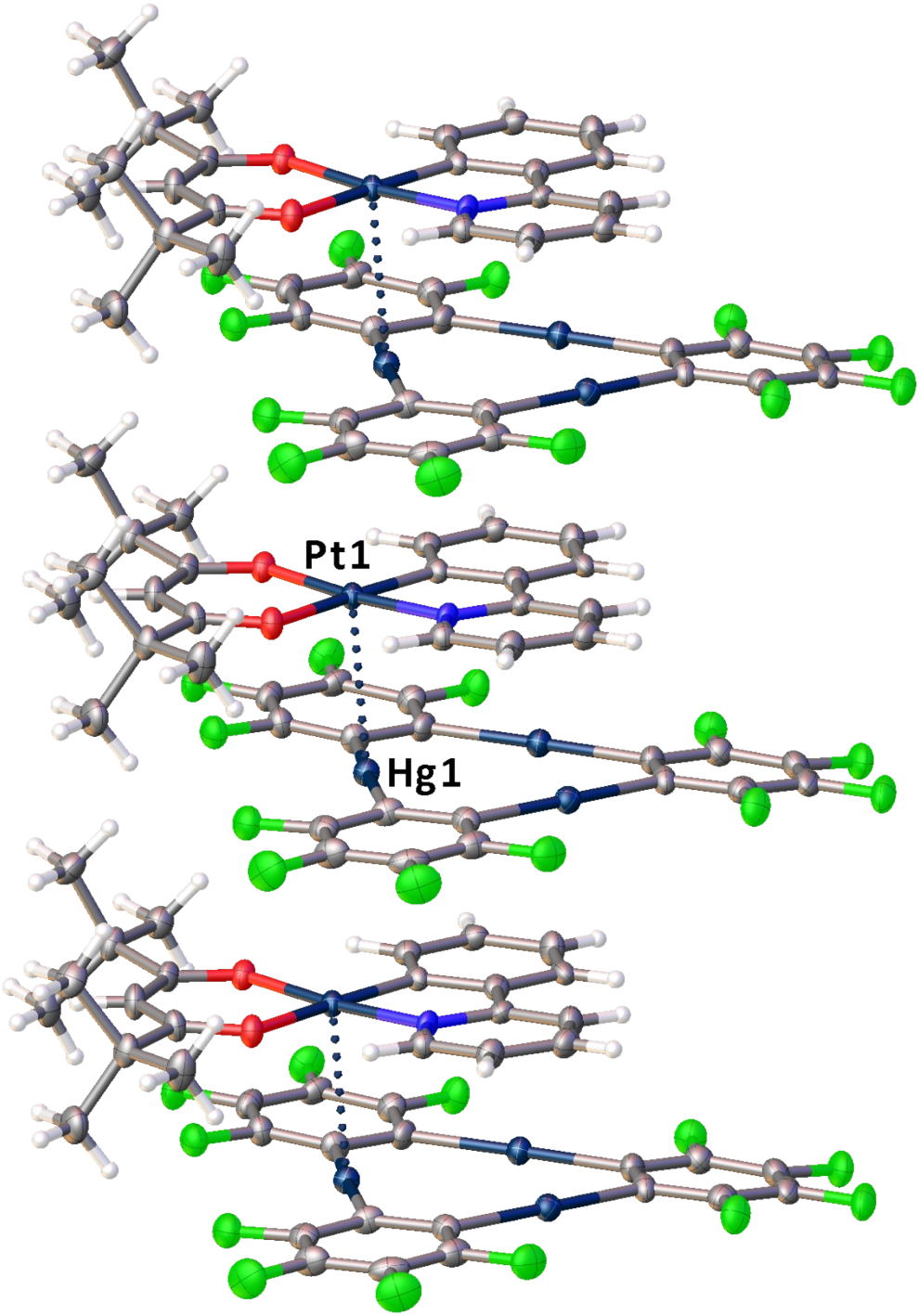


Figure S7. A fragment of crystal packing for **3**·**Hg$_3$** demonstrating heteropolar stacking between **3** and **Hg$_3$**. Short contacts Hg···Pt are given by dotted lines.

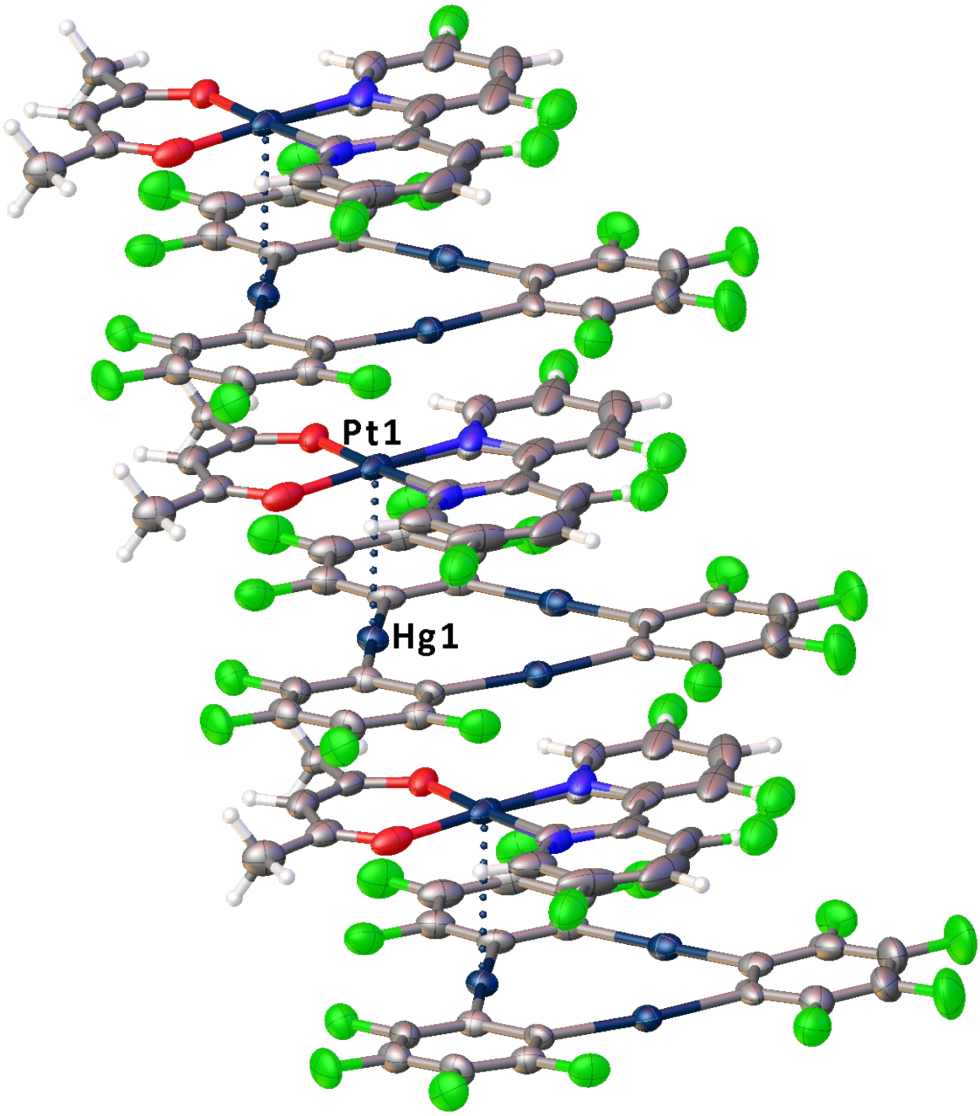


Figure S8. A fragment of crystal packing for **4**·**Hg$_3$**·Me_2CO demonstrating heteropolar stacking between **4** and **Hg$_3$**. Short contacts Hg···Pt are given by dotted lines. Molecules of Me_2CO were omitted for clarity.

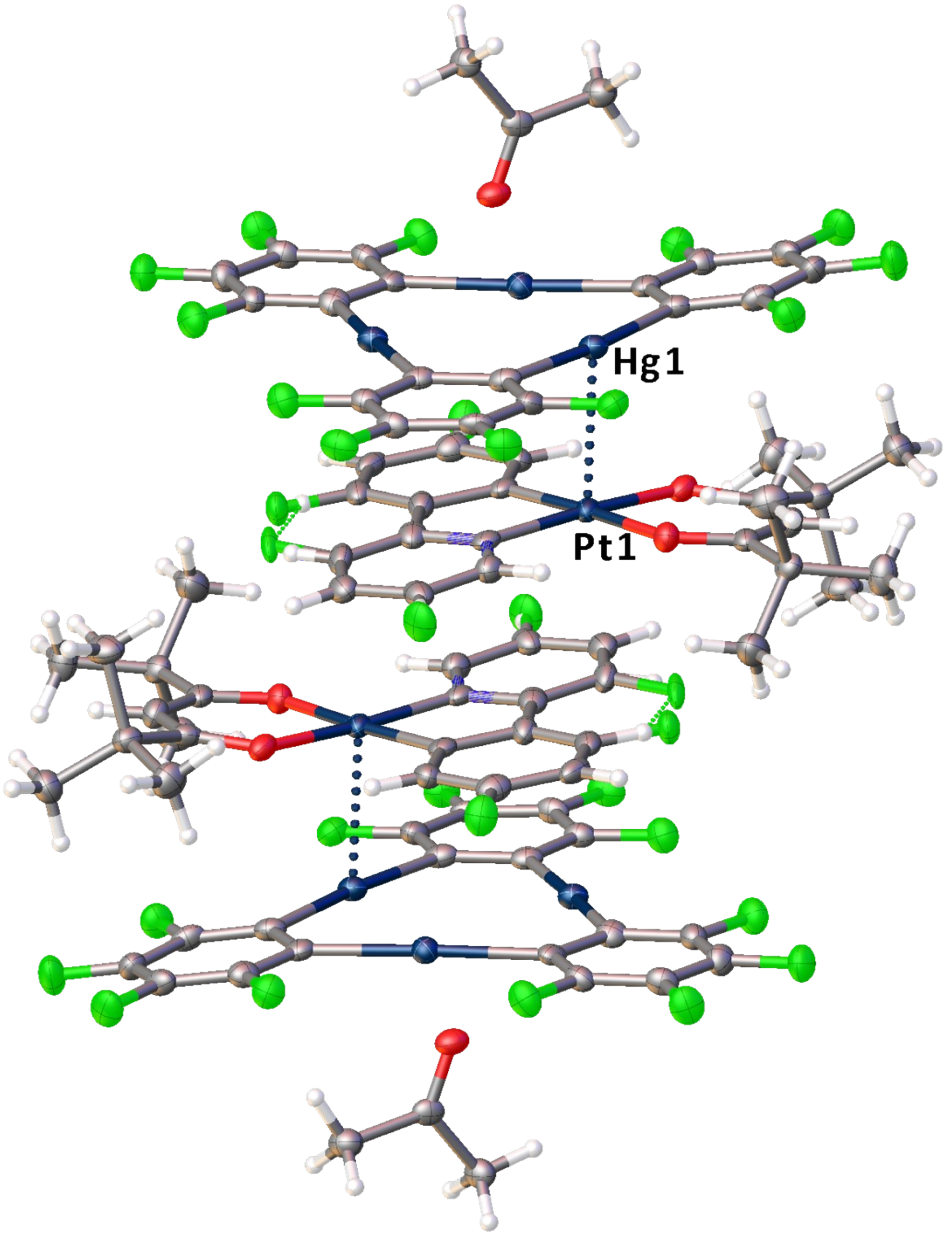


Figure S9. A fragment of crystal packing for **5**·**Hg$_3$**·Me_2CO demonstrating homoplanar stacking between two **5** and heteropolar stacking between **5** and **Hg$_3$**. Short contacts Hg···Pt are given by dotted lines.

Table S1. Crystal data and structure refinement for all compounds studied.

Identification code	**1**·**Hg$_3$**	**2**·**Hg$_3$**	**3**·**Hg$_3$**	**4**·**Hg$_3$**·Me_2CO	**5**·**Hg$_3$**·Me_2CO
Empirical formula	$C_{34}H_{15}F_{12}Hg_3NO_2Pt$	$C_{36}H_{19}F_{12}Hg_3NO_2Pt$	$C_{40}H_{27}F_{12}Hg_3NO_2Pt$	$C_{37}H_{19}F_{14}Hg_3NO_3Pt$	$C_{43}H_{31}F_{14}Hg_3NO_3Pt$
Formula weight	1494.33	1522.38	1578.48	1588.38	1672.55
Temperature, K	100.0(2)	100.0(2)	100.0(2)	100.0(2)	100.0(2)
Crystal size, mm	0.01 × 0.01 × 0.11	0.01 × 0.02 × 0.12	0.01 × 0.02 × 0.21	0.01 × 0.03 × 0.20	0.05 × 0.05 × 0.07
Wavelength, Å	0.74500	0.74500	0.74500	0.74500	0.74500
Crystal system	Triclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	*P*-1	$P2_1/c$	*C*2/c	$P2_1/c$	$P2_1/c$
a, Å	6.8150(6)	24.923(5)	46.347(3)	24.566(5)	10.8111(14)
b, Å	11.8179(12)	6.6890(13)	6.7991(4)	6.6889(13)	14.3859(18)
c, Å	23.580(2)	23.781(5)	25.3750(17)	22.906(4)	27.258(3)
α, deg.	78.260(10)	90	90	90	90
β, deg.	88.380(11)	106.25(3)	101.498(6)	104.207(11)	95.647(11)
γ, deg.	73.801(9)	90	90	90	90
V, Å^3	1784.7(3)	3806.1(14)	7835.7(9)	3648.8(12)	4218.8(9)
Z	2	4	8	4	4
Density (calc.), Mg/m^3	2.781	2.657	2.676	2.891	2.633
μ, mm^{-1}	18.959	17.783	17.239	18.522	16.067
F(000)	1336	2736	5728	2864	3056
Theta range, deg.	1.96 – 27.50	2.92 – 26.00	1.72 – 31.00	1.91 – 31.00	1.68 – 26.00
Index ranges	$-7 \le h \le 8$, $-14 \le k \le 14$, $-29 \le l \le 29$	$-29 \le h \le 29$, $-7 \le k \le 7$, $-27 \le l \le 27$	$-64 \le h \le 63$, $-8 \le k \le 9$, $-35 \le l \le 2335$	$-33 \le h \le 33$, $-9 \le k \le 9$, $-31 \le l \le 30$	$-12 \le h \le 12$, $-16 \le k \le 16$, $-32 \le l \le 31$
Reflections collected	20243	34034	40041	55580	40689
Independent reflections, R_{int}	6769, 0.0525	6426, 0.0611	10454, 0.0307	10031, 0.0520	7143, 0.0233
Reflections observed	5721	5101	9356	9103	6647
R_1 / wR_2 ($I > 2\sigma(I)$)	0.0662 / 0.1578	0.0332 / 0.0809	0.0300 / 0.0785	0.0529 / 0.1277	0.0291 / 0.0633
R_1 / wR_2 (all data)	0.0749 / 0.1628	0.0459 / 0.0869	0.0344 / 0.0806	0.0582 / 0.1308	0.0324 / 0.0648
Goodness-of-fit on F^2	1.052	1.027	1.083	1.090	1.122
Extinction coefficient	0.0021(2)	0.00026(4)	0.000337(12)	0.00192(9)	0.00077(3)
T_{min} / T_{max}	0.212 / 0.824	0.212 / 0.824	0.088 / 0.819	0.101 / 0.818	0.333 / 0.434
$\Delta\rho_{max}$ / $\Delta\rho_{min}$, e·Å^{-3}	3.861 / -3.762	2.603 / -1.288	1.638 / -1.950	2.916 / -3.160	2.500 / -1.829

Powder XRD data for of (1–5)·Hg_3

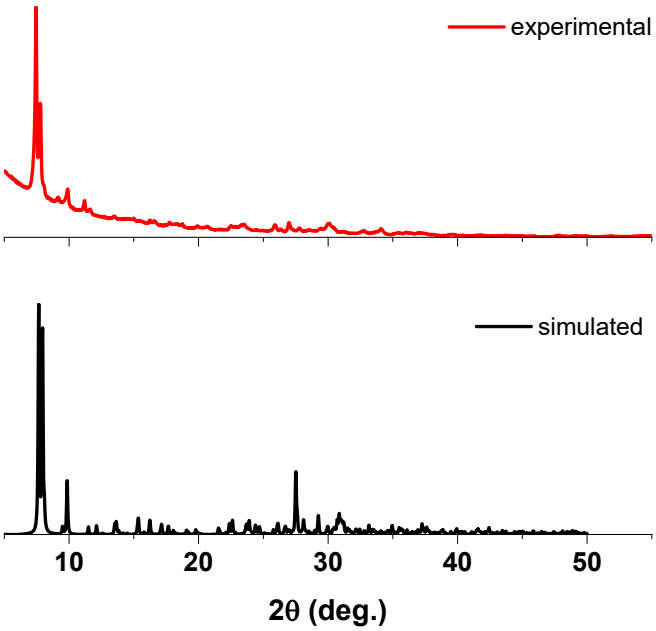


Figure S10. Powder XRD patterns of **1**·Hg_3.

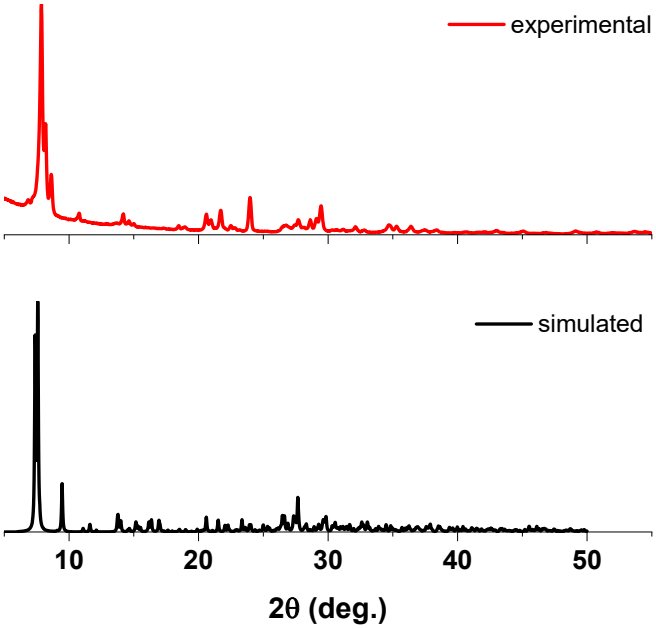


Figure S11. Powder XRD patterns of **2**·Hg_3.

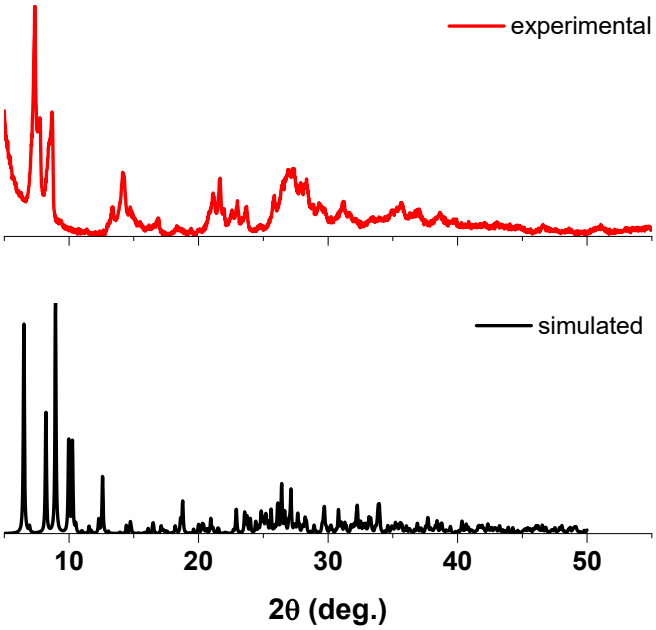


Figure S12. Powder XRD patterns of **3**·Hg_3.

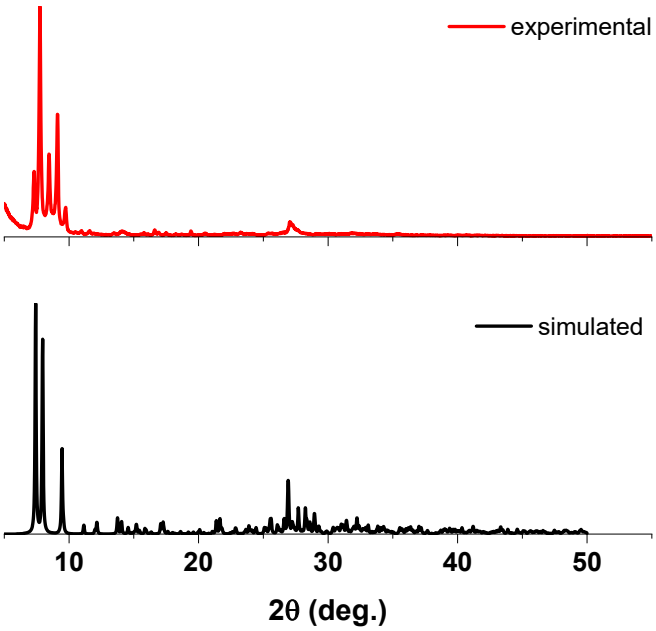


Figure S13. Powder XRD patterns of **4**·Hg_3.

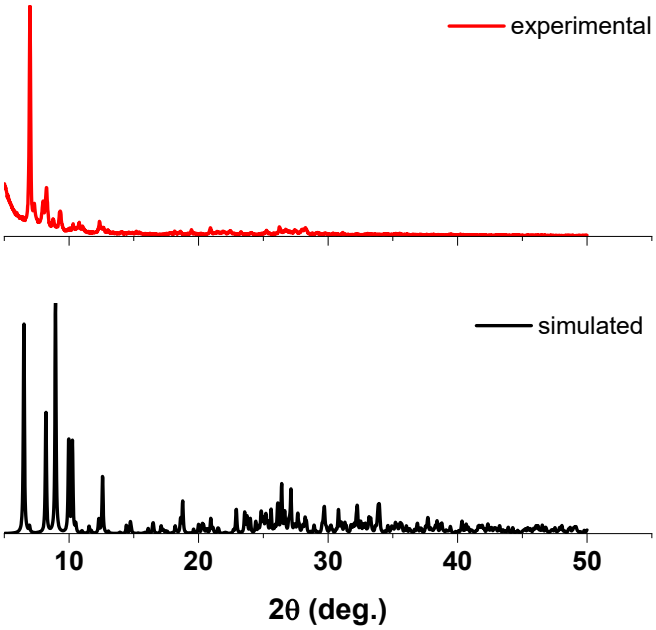


Figure S14. Powder XRD patterns of **5**·Hg_3.

The Cambridge Structural Database (CSD) search for Short Hg···Pt contacts

The search was performed for intermolecular and intramolecular Hg···Pt contacts [3 or more separating bonds], mercury–platinum interatomic separation does not exceed $\sum_{vdW}$ Pt+Hg+0.5 Å, and the category of Hg–Pt bonds (any type). Due to the overlap of ranges of mercury–platinum distances for these two kinds of searches (2.77–3.46 and 2.51–3.16 Å, correspondingly), the results were combined and considered together in **Table S2**. Metal clusters and compounds with bi- or more-center contacts involving Hg and Pt atoms were not included in **Table S2** due to uncertainties in determining bond distances and angles.

Table S2. Covalent (or coordination) Hg–Pt bonds and noncovalent Hg···Pt contacts verified in the CSD search.

Entry	**CSD code and ref. ccdc No**	**Supported/not supported by bridging ligands**	**Hg···Pt distance, Å**	**angle X–Hg···Pt, °**	**Comments, contact/bond between**
1	ACHGPT10	supported	2.5126(9)	172.456(2)	Linkage between $\{O_2Hg^{II}\}$ and $\{N_2C_2Pt^{II}\}$
2	COBTES	unsupported	2.6357(3)	169.5762(14)	Linkage between {Hg} and two $\{P_2CPt\}$
3	COJJAM	unsupported	2.6663(19) 2.629(2)	167.27(5)	Linkage between {Hg} and two $\{P_2CPt\}$
4	DULPAB	unsupported	2.5717(16)	171.92(5)	Linkage between {Hg} and two $\{P_2CPt^0\}$
5	EBUHIT	unsupported	2.6093(4) 2.5914(4)	170.472(12)	Linkage between {Hg} and two $\{O_3C_2Pt\}$
6	EBUHOZ	unsupported	2.5898(3)	170.49(6)	Linkage between {Hg} and two $\{O_3C_2Pt^{II}\}$
7	EBUHUF	unsupported	2.57587(19)	170.25(6)	Linkage between {Hg} and two $\{P_2CPt\}$
8	FEKYAW	supported	2.7909(5), 2.7950(5)	179.576(13)	Linkage between {PHg} and two

					{P_3Pt}
9	FODFEK	unsupported	2.5199(6)	175.01(12)	Linkage between {ClHg} and {N_2C_2Pt}
10	FODFIO	supported	2.5093(7)	176.3(3)	Linkage between {O_2Hg} and {N_2C_2OPt}
11	GEHGSN	semi-supported	2.6177(2)	177.2956(4)	Linkage between {GeHg} and {P_2SnPt}
12	HEZCAT	not applicable	2.5710(7) and 2.9020(5)	177.46(13)	Linkage between {O_2Hg_2} and {P_4Pt_2}, in heterometallic cluster Hg_2Pt_2
13	HEZVOA	semi-supported	2.603(2)	173.92(12)	Linkage between {SiHg} and {P_2HgPt}
14	HUNZAT	unsupported	2.5357(10)	174.85(9)	Linkage between {$ClHg^{I}$} and {$N_2C_2ClPt^{III}$}
15	HUNZEX	unsupported	2.5439(11)	171.94(3)	Linkage between {$BrHg^{I}$} and {$N_2C_2BrPt^{III}$}
16	HUXDUB	unsupported	2.6710(7) 2.5902(7)	176.08(6)	Linkage between {Si_2Hg_2} and {P_2Si_2Pt}
17	HUXFIR	unsupported	2.5965(2)	175.71(3)	Linkage between {$SiHg^{I}$} and {$PSiPt^{I}$}
18	KAXJEY	unsupported	2.530(3)	175.6(7)	Linkage between {CHg^{I}} and {P_3NPt^{0}}
19	KEYGUQ	unsupported	2.5567(9)	174.3(2)	Linkage between {OHg^{I}} and {S_2PCOPt^{III}},
20	LIFYEE	unsupported	2.575(2)	164.66(15)	Linkage between {FeHg} and {PC_2Pt}
21	MICCEG	supported	2.1585(12)*–2.8339(14)	93.6(2)	Linkage between {C_2Hg^{II}} and {$P_2Cl_2Pt^{II}$}
22	MICCOQ	supported	3.1335(6)	157.46(6)	Linkage between {$PCClHg^{II}$} and {$P_2C_2Pt^{II}$}
23	NEBZAV	unsupported	2.7676(14)	113.80(7)–109.45(5)	Linkage between {I_3Hg^{II}} and {PCS_2Pt^{II}}
24	NIDPUO	unsupported	2.603(8)	177.8(8)	Linkage between {$SiHg^{I}$} and {P2SiPt^{I}}

25	OQANOL	unsupported	3.4604(5)	85.5(2)	Linkage between $\{C_2Hg^{II}\}$ and $\{C_4Pt^{II}\}$ in coordination polymer
26	PEDJUF	unsupported	2.5250(2)	172.91(3)	Linkage between $\{IHg^{I}\}$ and $\{P_2IPt^{I}\}$
27	PEJYAE	supported	2.7846(14)	81.9(5)	Linkage between $\{N_2Hg^{II}\}$ and $\{N_4Pt^{II}\}$
28	PEJYEI	supported	2.8349(9)	137.87(6)	between $\{Cl_2N_2Hg^{II}\}$ and $\{N_4Pt^{II}\}$
29	PEJYIM	supported	2.7645(12)	82.7(3)	Linkage between $\{Cl_2N_2Hg^{II}\}$ and $\{N_4Pt^{II}\}$
30	PITFON10	unsupported	2.6153(9)	163.68(5)	Linkage between {Hg} and two $\{P_2CPt\}$
31	PITFUT10	unsupported	2.644(2)	178.22(10)	Linkage between {Hg} and two $\{P_2CPt\}$
32	PITGAA10	unsupported	2.6409(10)	167.25(5)	Linkage between {Hg} and two $\{P_2CPt\}$
33	QIWDUY	unsupported	2.5108(6)	165.93(4)	Linkage between $\{ClHg\}$ and $\{N_2C_2ClPt\}$
34	QUCMAC	unsupported	2.5266(5)	173.51(3)	Linkage between $\{BrHg\}$ and $\{N_2C_2BrPt\}$
35	QUCMIK	unsupported	2.5128(4)	175.1(2)	Linkage between $\{OHg\}$ and $\{N_2C_2OPt\}$
36	QUCMOQ	unsupported	2.6283(3) and 2.5424(3)	150.958(14)	Linkage between {Hg} and $\{N_2C_2Pt\}$ and $\{N_2C_2OPt\}$
37	RETJAB	supported	2.7270(13)	141.7(5)	Linkage between $\{N_2OHg^{II}\}$ and $\{N_4Pt^{II}\}$
38	RUSBIQ	unsupported	2.584(3)	165.5(3)	Linkage between $\{CHg^{I}\}$ and $\{P_2(carboran)Pt^{I}\}$
39	SESDUR	unsupported	2.560(3)	173.5(17)	Linkage between $\{CHg^{I}\}$ and $\{P_2ClPt^{I}\}$
40	SUTTEG	supported	2.7955(14)	135.9(3)	Linkage between $\{N_2O_2Hg^{II}\}$ and $\{N_4Pt^{II}\}$ moieties

41	TEDHEP	unsupported	2.5443(13)	180	Linkage between {Hg} and two $\{N_2C_2OPt^{II}\}$
42	TFMPHG	unsupported	2.5688(4)	174.6238(2)	Linkage between $\{CHg^{I}\}$ and $\{P_2CPt^{I}\}$
43	UMIVUH	supported	2.6130(6)	166.4(3)	Linkage between $\{O_3Hg^{II}\}$ and $\{O_2PCPt^{II}\}$
44	VODMIK	unsupported	2.6050(16)	178.96(12)	Linkage between {MnHg} and $\{P_4Pt\}$
45	VODMOQ	unsupported	2.5511(9)	174.64(8)	Linkage between $\{ClHg^{I}\}$ and $\{P_4Pt^{I}\}$
46	WEDZEK	unsupported	2.559(2)	173.8(6)	Linkage between {CHg} and $\{C_2N_2ClPt\}$
47	XAKHIA	unsupported	2.8078(11)	99.53(6)–111.86(6)	Linkage between $\{Br_3Hg^{II}\}$ and $\{O_2PCPt^{II}\}$
48	XAKHOG	supported	2.6500(9)	159.2(3)	Linkage between $\{O_2CHg^{II}\}$ and $\{O_2PCPt^{II}\}$
49	YIKXIZ	supported	3.154(2) 3.151(2)	91.0(3) 89.4(4)	Linkage between $\{C_2Hg^{II}\}$ and $\{S_4Pt^{II}\}$ moieties
50	YIKXOF	supported	3.021(3)	89.6(3) 87.7(3)	Linkage between $\{C_2Hg^{II}\}$ and $\{S_4Pt^{II}\}$ moieties,
51	YOMVOO	unsupported	2.5458(9) and 2.5483(8)	172.15(2)	Linkage between {Hg} and two$\{C_2N_2ClPt\}$
52	YOMVUU	unsupported	2.6635(7) and 2.5743(7)	142.79(2)	Linkage between {Hg} and $\{C_2N_2ClPt\}$; {PtHg} and $\{C_2N_2Pt\}$
53	UNUJIZ	unsupported	2.5787(7) and 2.5840(6)	174.166(17)	Linkage between {Hg} and $\{O_3NCPt\}$ and $\{O_2NCPt\}$
54	UNUJOF	supported	2.6601(6) and 2.6940(6)	155.63(2)	Linkage between $\{O_2Hg^{I}{}_2\}$ and $\{O_2NCPt^{II}\}$

*This distance was not included into analysis due to the structure two-fold disorder.

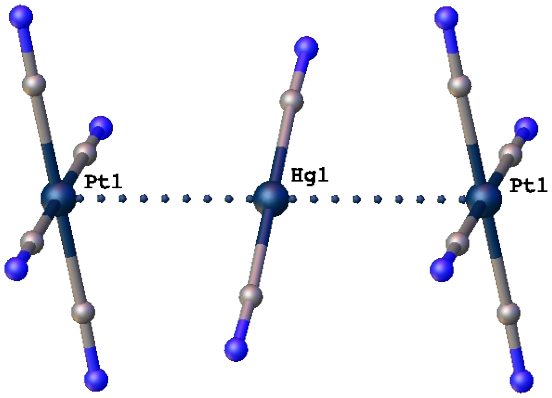


Figure S15. Fragment of Hg···Pt chain, linking the anionic $[Pt(CN)_4]^{2-}$ and neutral $Hg(CN)_2$ complexes, in the structure of the coordination polymer $K_2PtHg(CN)_6 \cdot 2H_2O$.

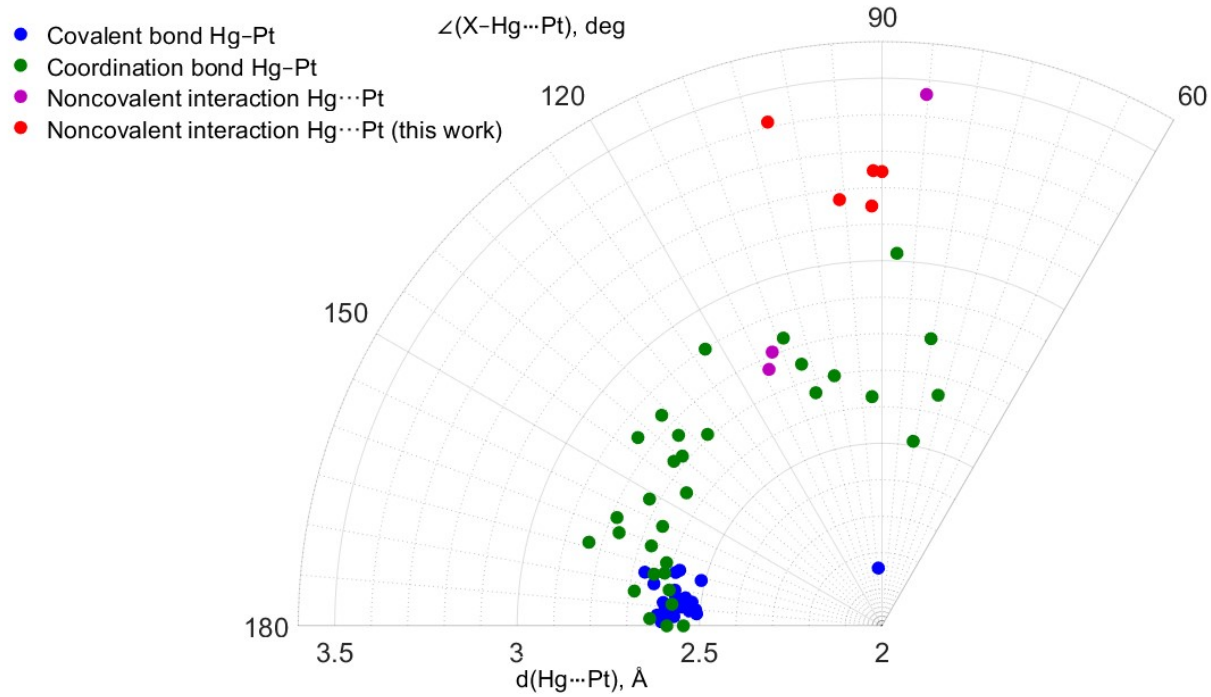


Figure S16. Angular distribution for intermolecular Hg···Pt contacts retrieved from the CCDC (Table S1).

Theoretical considerations

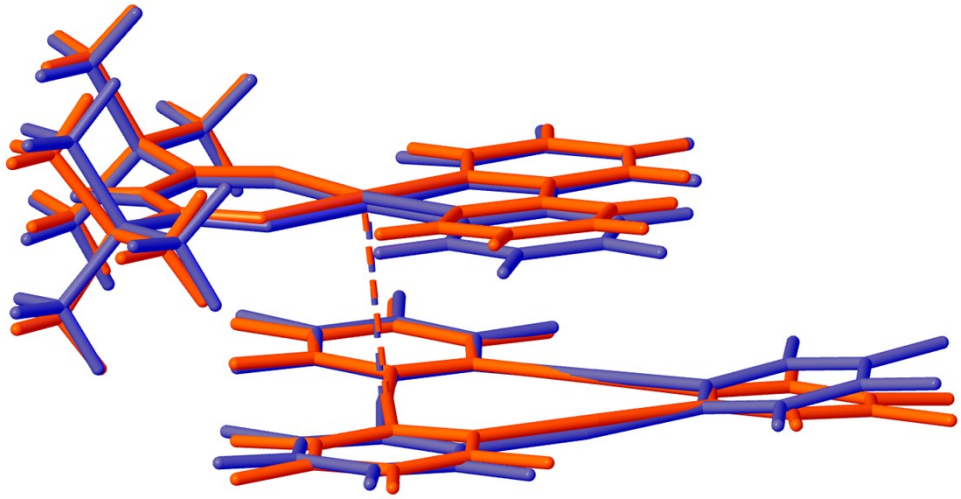


Figure S17. Overlayed images of optimized (blue) and X-Ray (b) geometries of [**3**·**Hg$_3$**] **(**RMSD = 0.2808.

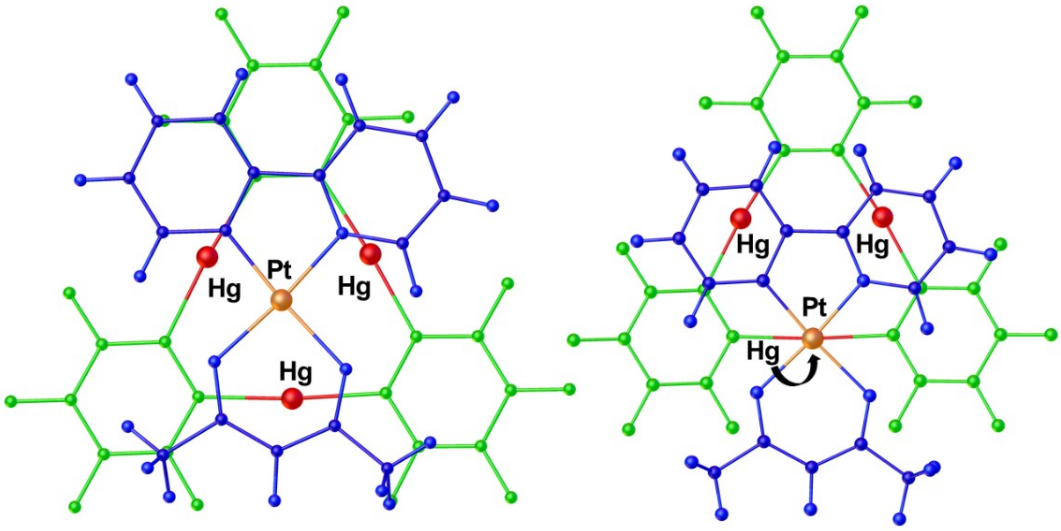


Figure S18. Two possible types of structures of [**1**·**Hg$_3$**]^a (left) and [**1**·**Hg$_3$**]^b (right).

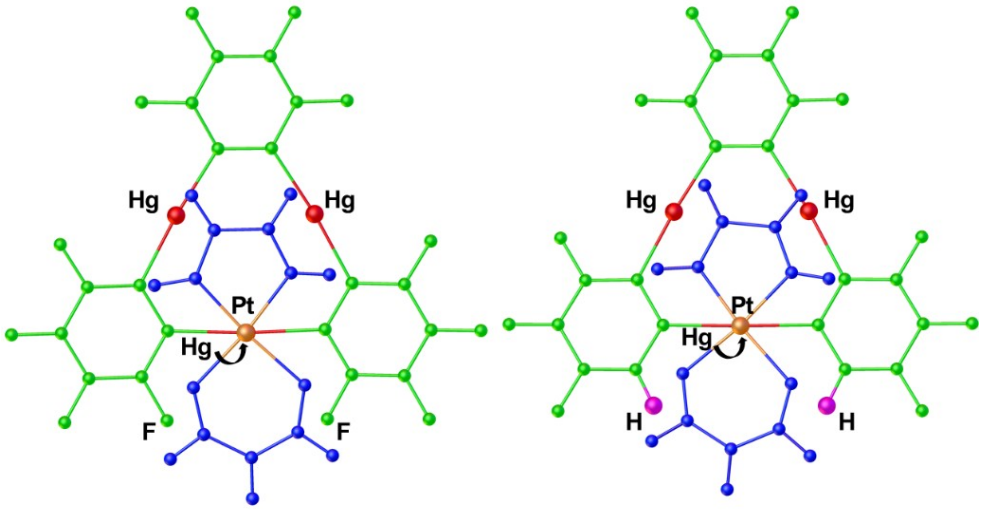


Figure S19. Equilibrium geometries of model complexes **3M1**·**Hg$_3$** (left) and **3M2**·**Hg$_3$** (right).

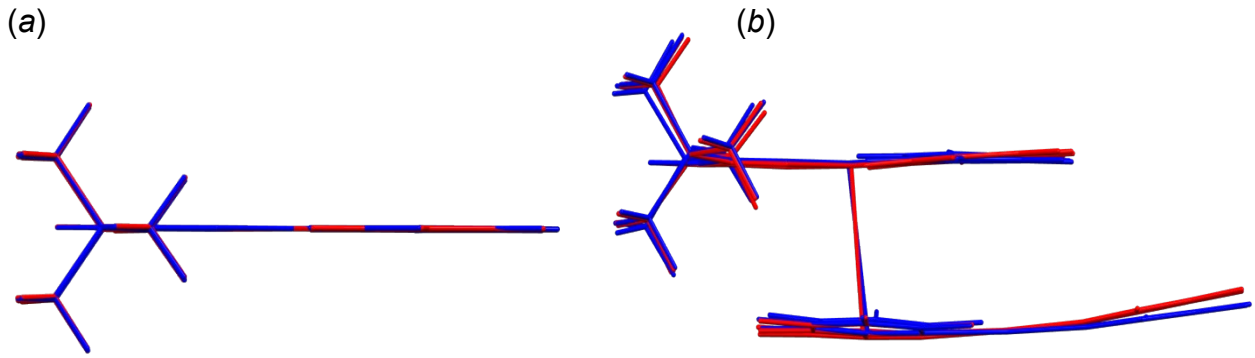


Figure S20. Overlayed images of optimized geometries of **3** (RMSD = 0.0255; *a*) and [**3**·**Hg$_3$**] (RMSD = 0.0828; *b*) in S_0 (red) and T_1 (blue) states.

Table S3. Calculated geometric parameters of **3** and **[3·Hg$_3$]** in ground and excited states.

Entity	d(Pt1···Hg1), Å	d(Pt1–C40), Å	d(Pt1–N1), Å	d(Pt1–O1), Å	d(Pt1–O2), Å	α, °[a]	β, °[b]
3							
S0	-	1.960	1.988	1.999	2.090	0.13	-
^{3}T1	-	1.922	1.976	2.018	2.087	0.08	-
^{3}MC	-	1.995	2.179	2.145	2.109	50.84	-
MECP	-	2.006	2.187	2.133	2.115	95.64	-
[3·Hg$_3$]							
S0	3.111	1.964	1.933	1.996	2.079	0.29	2.97
^{3}T1	3.162	1.923	1.982	2.012	2.073	1.31	1.25
^{3}MC	3.021	1.993	2.170	2.106	2.123	47.24	4.34
MECP	2.954	2.004	2.156	2.100	2.092	92.00	2.90

[a]twist angle between the N1–Pt1–C40 and O1–Pt1–O2 planes (see **Figure S16)**; [b]dihedral angle between the Hg1–Hg2–Hg3 and C1–C7–C13 planes.

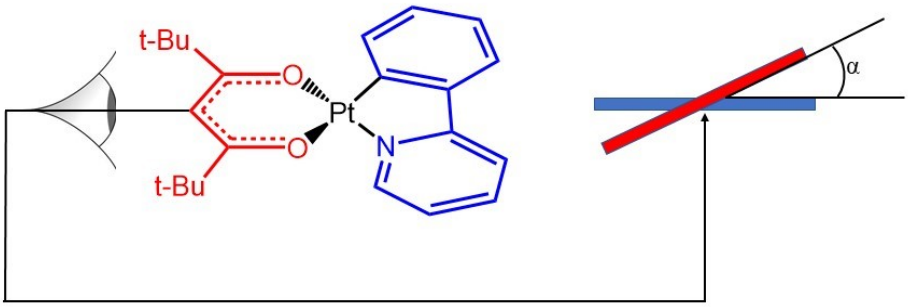


Figure S21. Schematic representation of twist angle.

Table S4. Calculated atomic Hirshfeld spin densities in T_1 optimized structures (in e) of **3** and [**3**·Hg_3].

	Pt, %	**C^N, %**	**O^O, %**	**Hg_3, %**
3	0.36	1.60	0.05	-
[**3**·Hg_3]	0.27	1.61	0.04	0.08

Table S5. The relative energies of ^{3}T1, ^{3}MC states, and the energy barriers in nonradiative decay. The ground state of the open-ring form was treated as the zero point (in kcal/mol).

	3	[**3**·Hg_3]
^{3}T1	59	59
^{3}MC	65	65
MECP	62	59
ΔE_2	3	6

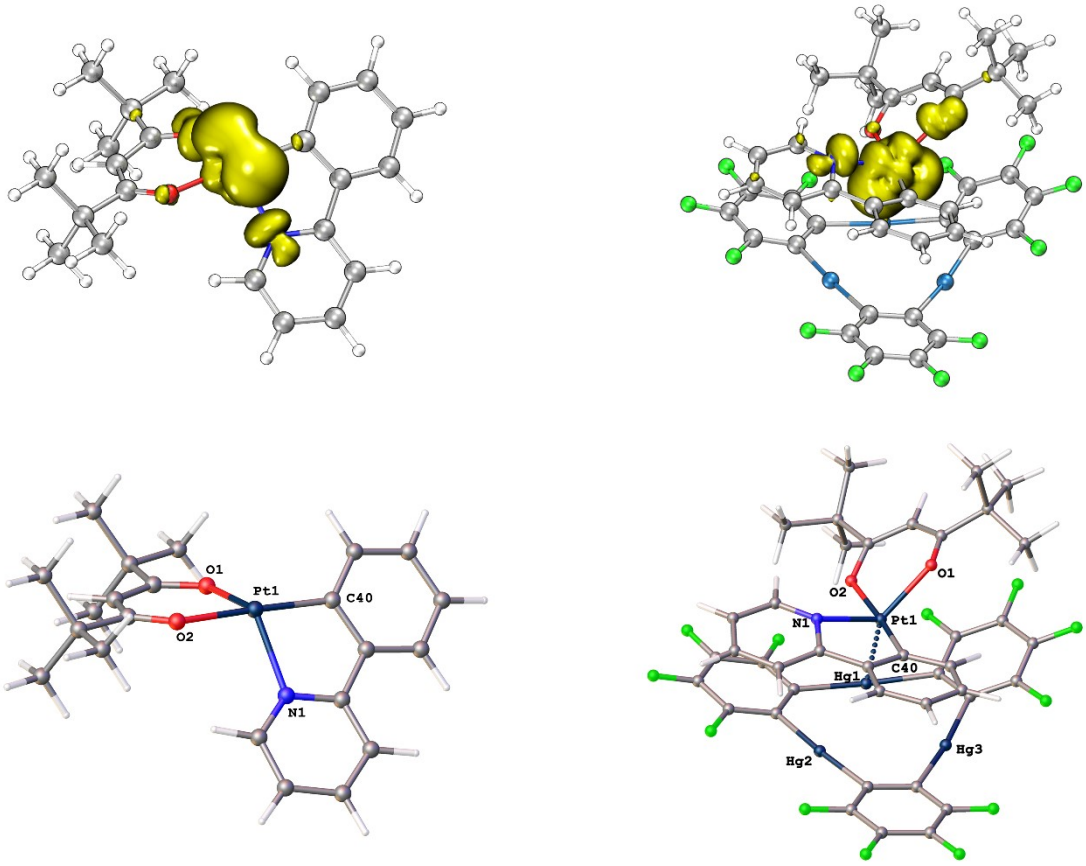


Figure S22. Spin densities computed on ^{3}MC state for **3** and [**3**·**Hg$_3$**] (isovalue = 0.005).

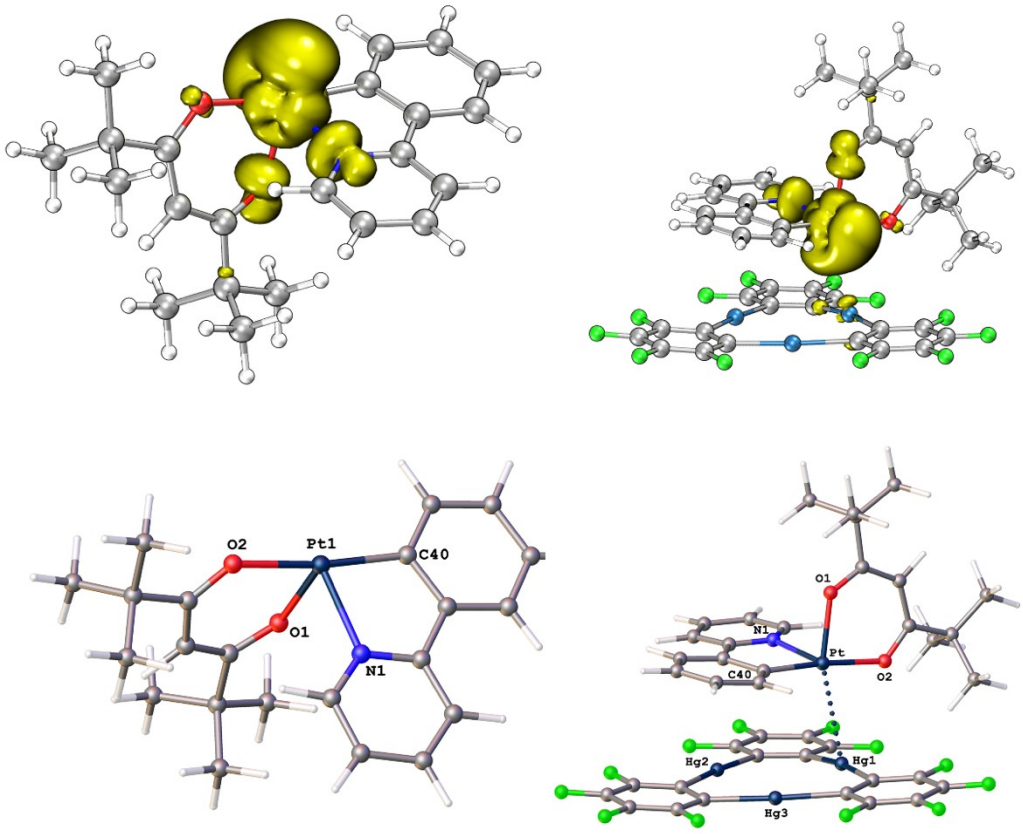


Figure S23. Spin densities computed on MECP (^{3}MC/S$_0$) state for **3** and [**3**·**Hg$_3$**] (isovalue = 0.005).

Table S6. Percentage MO contributions of atoms and ligands to FMOs in **3**.

Pt	Pt, %	C^N, %	O^O, %
HOMO–3	5	88	7
HOMO–2	87	8	5
HOMO–1	33	29	38
HOMO	31	47	21
LUMO	7	91	2
LUMO+1	1	88	10
LUMO+2	4	12	84
LUMO+3	10	86	4
LUMO+4	21	20	59
LUMO+5	28	22	49

Table S7. Percentage MO contributions of atoms and ligands to FMOs in [**3**·**Hg_3**].

Pt-Hg	Pt, %	C^N, %	O^O, %	Hg_3, %
HOMO–3	7	18	4	71
HOMO–2	47	21	6	26
HOMO–1	29	36	25	12
HOMO	23	28	46	3
LUMO	7	78	2	13
LUMO+1	2	30	1	67
LUMO+2	1	63	2	34
LUMO+3	1	9	7	83
LUMO+4	4	11	8	77
LUMO+5	3	7	67	23
LUMO+6	4	13	10	73
LUMO+7	4	46	3	47
LUMO+8	0	4	1	95
LUMO+9	0	4	1	95
LUMO+10	1	8	1	90
LUMO+11	2	25	1	72
LUMO+12	31	38	13	18
LUMO+13	7	65	3	25
LUMO+14	1	13	14	72
LUMO+15	8	14	8	70

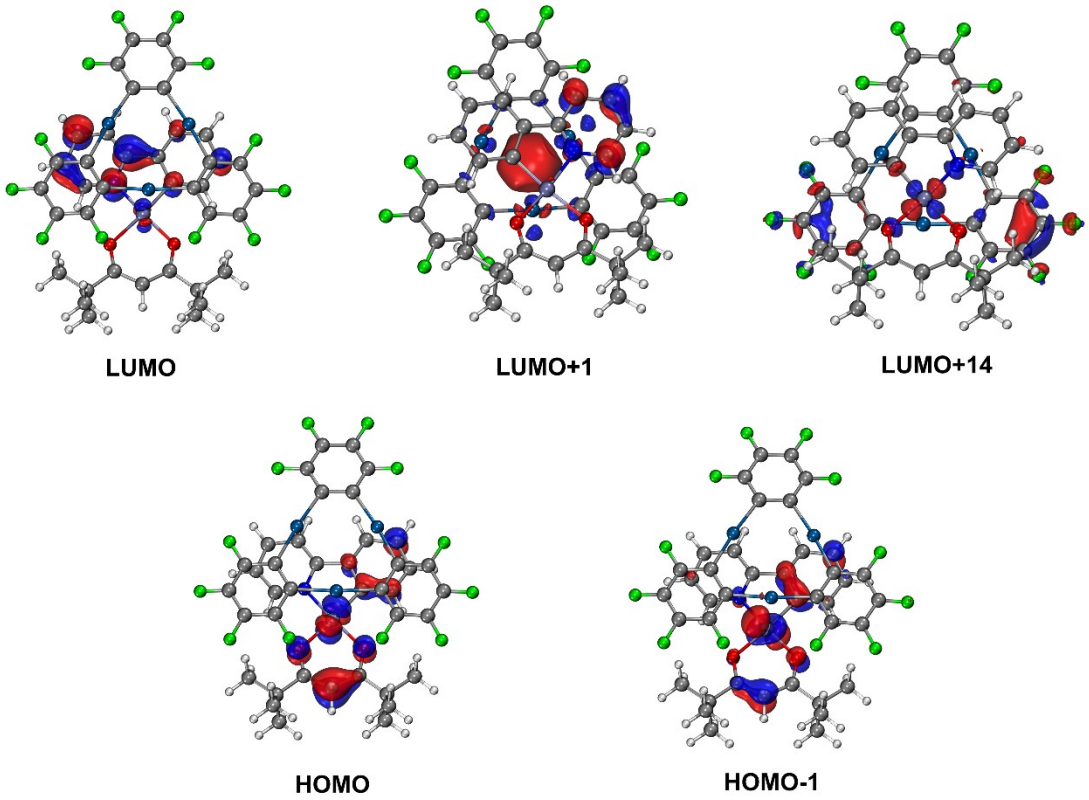


Figure S24. Molecular orbitals for **[3·Hg$_3$]**, calculated at the PBE0-D3BJ/ZORA-def2-TZVP level of theory.

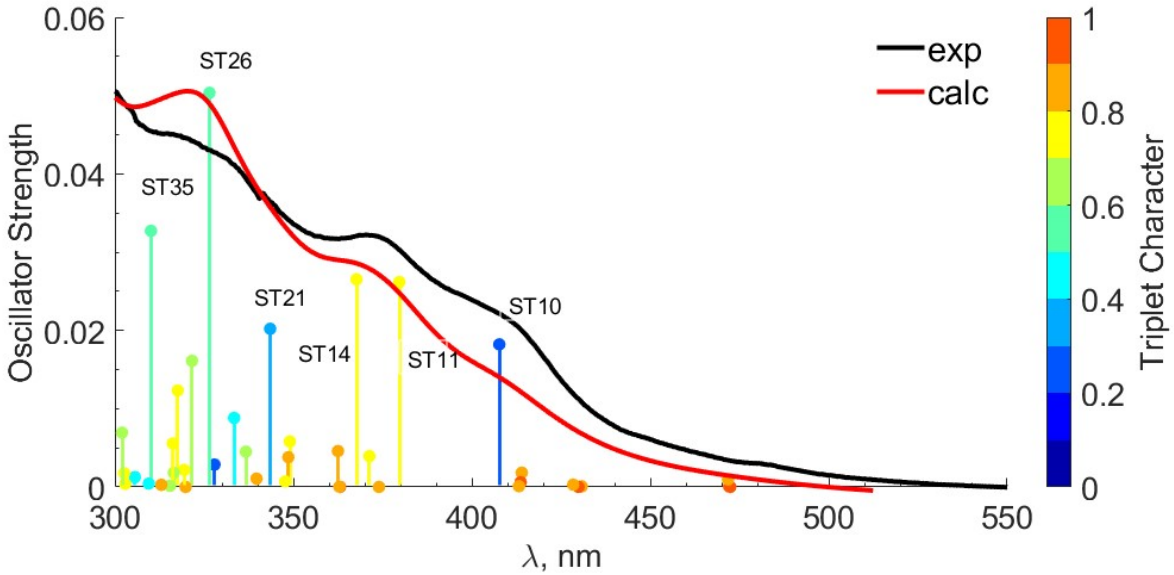


Figure S25. Experimental (black line) and the SOC-TDDFT calculated absorption (red line) spectra for **3**: excitation energies and oscillator strengths are shown by the vertical lines; the spectrum is convoluted with a Lorenzian function having a full width at half-maximum of 0.35 cm^{-1}.

Table S8. Excitation wavelengths (nm), oscillator strengths (f) and contributions of scalar relativistic (SR) states for **3** calculated with SR-TDDFT and SOC-TDDFT.

SR States (TDDFT Singlet-Singlet Excitations)				
State	**Energy(eV)**	**λ(nm)**	**f**	**Transitions**

S1	2.98	403	0.029	H–1 → L (6%); H → L (90%);
S2	3.37	357	0.019	H–2 → L (38%); H–1 → L (53%); H → L (2%); H → L+1 (5%);
S3	3.49	344	0.008	H–2 → L (39%); H–1 → L (7%); H → L (3%); H → L+1 (46%);
S4	3.58	335	0.151	H–2 → L (20%); H–1 → L (29%); H → L (3%); H → L+1 (42%); H → L+2 (2%);
S5	3.67	327	0.001	H–3 → L (2%); H–1 → L+1 (3%); H → L+1 (4%); H → L+2 (88%); H → L+2 (2%);
S6	3.88	309	0.021	H–3 → L (3%); H–2 → L+1 (36%); H–2 → L+2 (14%); H–1 → L+1 (39%); H → L+2 (3%);
S7	3.92	306	0.031	H–3 → L (18%); H–2 → L+1 (29%); H–2 → L+2 (9%); H–1 → L+1 (31%); H–1 → L+2 (7%);
S8	3.97	302	0.006	H–5 → L (11%); H–4 → L (82%); H–2 → L+2 (9%); H–1 → L+1 (31%); H–1 → L+2 (7%);
S9	4.05	297	0.035	H–3 → L (28%); H–2 → L+1 (6%); H–2 → L+2 (2%); H–1 → L+1 (16%); H–1 → L+2 (38%);
S10	4.17	288	0.022	H–3 → L (6%); H–2 → L+1 (24%); H–2 → L+2 (58%); H–1 → L+2 (8%); H–1 → L+2 (38%);
S11	4.30	279	0.156	H–5 → L (11%); H–3 → L (33%); H–2 → L+1 (3%); H–2 → L+2 (11%); H–1 → L+1 (4%); H–1 → L+2 (30%);
S12	4.36	275	0.009	H–5 → L+1 (10%); H–5 → L+2 (5%); H–4 → L+1 (53%); H–4 → L+2 (25%); H–1 → L+1 (4%); H–1 → L+2 (30%);
S13	4.47	268	0.053	H–6 → L (13%); H–6 → L+1 (4%); H–6 → L+2 (3%); H–5 → L (48%); H–4 → L (6%); H–3 → L+1 (7%); H–2 → L+2 (2%); H–1 → L+2 (5%);
S14	4.57	262	0.018	H–6 → L (35%); H–6 → L+1 (15%); H–6 → L+2 (10%); H–5 → L (7%); H–5 → L+2 (3%); H–4 → L (3%); H–4 → L+1 (2%); H–3 → L+1 (4%); H–3 → L+2 (3%); H → L+4 (2%);
S15	4.60	261	0.032	H–6 → L (14%); H–6 → L+1 (13%); H–6 → L+2 (9%); H–5 → L (6%); H–5 → L+1 (4%); H–3 → L+1 (36%); H → L+4 (3%); H–3 → L+1 (4%); H–3 → L+2 (3%); H → L+4 (2%);
SR States (TDDFT Singlet-Triplet Excitations)				
T1	2.46	488	0.000	H–3 → L (5%); H–3 → L+1 (2%); H–1 → L (24%); H → L (54%); H → L+1 (3%); H → L+3 (2%);
T2	2.75	436	0.000	H–5 → L+2 (3%); H–4 → L+2 (2%); H–3 → L+1 (5%); H–1 → L (19%); H–1 → L+1 (9%); H–1 → L+2 (8%); H → L (21%); H → L+1 (17%); H → L+2 (7%);
T3	2.83	424	0.001	H–5 → L+1 (2%); H–4 → L (2%); H–3 → L+2 (4%); H–1 → L (17%); H–1 → L+1 (12%); H–1 → L+2 (10%); H → L (17%); H → L+1 (8%); H → L+2 (12%);
T4	3.20	375	0.000	H–3 → L (39%); H–3 → L+3 (3%); H–3 → L+5 (2%); H → L+1 (13%); H → L+2 (17%); H → L+3 (6%); H → L (17%); H → L+1 (8%); H → L+2 (12%);
T5	3.25	370	0.000	H–3 → L (6%); H–3 → L+1 (5%); H–3 → L+2 (6%); H–2 → L (16%); H–1 → L (22%); H–1 → L+1 (9%); H–1 → L+2 (2%); H → L+1 (19%); H → L+2 (6%);
T6	3.25	369	0.000	H–2 → L (74%); H–1 → L+1 (3%); H → L+1 (9%); H → L+2 (6%); H–1 → L (22%); H–1 → L+1 (9%); H–1 → L+2 (2%); H → L+1 (19%); H → L+2 (6%);
T7	3.47	346	0.002	H–3 → L (2%); H–3 → L+1 (7%); H–1 → L+1 (17%); H–1 → L+2 (21%); H → L+1 (13%); H → L+2 (30%); H–1 → L+2 (2%); H → L+1 (19%); H → L+2 (6%);
T8	3.65	329	0.001	H–8 → L (3%); H–3 → L (28%); H–3 → L+1 (7%); H–3 → L+2 (7%); H–3 → L+3 (3%); H → L+1 (3%); H → L+3 (32%); H → L+1 (19%); H → L+2 (6%);
T9	3.81	315	0.000	H–4 → L (23%); H–4 → L+1 (3%); H–3 → L (7%); H–3 → L+1 (3%); H–3 → L+2 (3%); H–1 → L (8%); H–1 → L+1 (20%); H–1 → L+2 (18%); H → L+2 (6%);

T10	3.83	314	0.018	H–2 → L+1 (59%); H–2 → L+2 (30%); H–3 → L (7%); H–3 → L+1 (3%); H–3 → L+2 (3%); H–1 → L (8%); H–1 → L+1 (20%); H–1 → L+2 (18%); H → L+2 (6%);
T11	3.88	309	0.026	H–5 → L (3%); H–4 → L (40%); H–1 → L+1 (17%); H–1 → L+2 (19%); H → L+1 (3%); H → L+2 (3%); H → L+3 (6%); H–1 → L+2 (18%); H → L+2 (6%);
T12	3.95	304	0.000	H–8 → L+1 (4%); H–8 → L+2 (2%); H–5 → L (10%); H–4 → L (19%); H–3 → L+1 (12%); H–3 → L+2 (7%); H → L+1 (4%); H → L+2 (6%); H → L+3 (15%);
T13	4.09	294	0.004	H–6 → L+1 (4%); H–6 → L+2 (3%); H–5 → L (3%); H–4 → L+1 (33%); H–4 → L+2 (27%); H–1 → L+2 (7%); H → L+2 (3%); H → L+4 (2%); H → L+3 (15%);
T14	4.13	290	0.027	H–6 → L (4%); H–5 → L (5%); H–2 → L+1 (22%); H–2 → L+2 (51%); H → L+4 (4%); H–1 → L+2 (7%); H → L+2 (3%); H → L+4 (2%); H → L+3 (15%);
T15	4.16	288	0.000	H–7 → L+4 (3%); H–2 → L+1 (7%); H–2 → L+2 (4%); H–2 → L+4 (4%); H–2 → L+6 (2%); H → L+4 (32%); H → L+6 (21%); H → L+7 (4%); H → L+3 (15%);
States calculated by SOC-TDDFT				
State	**Energy (eV)**	**λ (nm)**	**f**	**Component Scalar Transitions**
ST1	2.54	472	0.000	T1(95%); T6(1%);
ST2	2.54	472	0.000	T1(95%);
ST3	2.54	472	0.001	T1(94%);
ST4	2.79	431	0.000	S1(3%); T2(64%); T3(19%); T5(2%); T6(7%);
ST5	2.79	430	0.000	T2(65%); T3(17%); T5(3%); T6(10%);
ST6	2.80	428	0.000	S2(7%); S3(2%); T2(71%); T3(15%);
ST7	2.90	414	0.002	S1(4%); T2(26%); T3(66%); T6(1%);
ST8	2.90	414	0.001	T2(27%); T3(68%);
ST9	2.90	413	0.000	S2(1%); T2(21%); T3(73%);
ST10	2.94	408	0.018	S1(68%); T3(4%); T5(6%); T6(16%);
ST11	3.16	380	0.026	S2(13%); S3(3%); S4(4%); T1(1%); T4(7%); T5(18%); T6(48%);
ST12	3.21	374	0.000	T3(4%); T4(24%); T5(38%); T6(26%);
ST13	3.23	371	0.004	S1(1%); S2(13%); S8(2%); T3(2%); T4(33%); T5(28%); T6(14%);
ST14	3.26	368	0.027	S1(1%); S3(10%); S4(4%); T3(2%); T4(37%); T5(37%); T6(1%);
ST15	3.31	363	0.000	T4(66%); T5(18%); T6(12%);
ST16	3.31	363	0.000	T4(57%); T5(23%); T6(15%);
ST17	3.31	363	0.005	S3(1%); T4(46%); T5(31%); T6(16%);
ST18	3.44	349	0.006	S3(3%); S4(3%); T10(3%); T13(2%); T6(4%); T7(71%);
ST19	3.44	349	0.004	S3(1%); S4(2%); T10(5%); T13(2%); T19(2%); T5(2%); T6(3%); T7(72%);
ST20	3.45	348	0.001	S12(4%); S3(1%); S6(6%); S7(2%); T7(80%);
ST21	3.49	344	0.020	S2(7%); S3(28%); S4(22%); S5(2%); T10(25%); T5(1%); T6(3%); T7(4%);
ST22	3.53	340	0.001	S3(1%); S8(1%); T10(1%); T2(3%); T3(5%); T4(5%); T5(28%); T6(30%); T7(11%); T8(4%);
ST23	3.56	337	0.005	S1(12%); S5(5%); T11(1%); T12(2%); T2(3%); T3(4%); T4(4%); T5(25%); T6(30%); T7(3%);
ST24	3.60	333	0.009	S2(37%); S3(8%); S4(1%); T12(3%); T2(2%); T3(3%); T4(3%); T6(16%); T8(9%); T9(3%);
ST25	3.66	328	0.003	S3(5%); S5(64%); T10(5%); T14(5%); T5(2%); T6(2%); T8(3%); T9(2%);
ST26	3.67	327	0.050	S3(9%); S4(22%); S5(3%); T11(4%); T5(9%); T6(3%); T8(32%); T9(4%);
ST27	3.73	322	0.016	S6(9%); S7(7%); S9(7%); T10(47%); T13(6%); T8(6%); T9(6%);
ST28	3.75	320	0.000	S6(1%); T10(2%); T14(2%); T15(1%); T6(2%); T8(73%); T9(8%);

ST29	3.76	319	0.002	S10(4%); S2(3%); S5(1%); S7(1%); S8(1%); S9(2%); T10(7%); T11(2%); T8(59%); T9(10%);
ST30	3.78	318	0.012	S2(1%); S3(1%); S4(4%); T10(9%); T11(14%); T14(5%); T6(2%); T8(28%); T9(20%);
ST31	3.79	317	0.002	S10(4%); S3(1%); S6(12%); T11(16%); T13(2%); T14(4%); T8(12%); T9(37%);
ST32	3.79	316	0.006	S3(4%); S4(3%); S6(1%); S8(1%); T10(9%); T11(3%); T13(5%); T8(30%); T9(25%);
ST33	3.81	315	0.000	S10(3%); S2(1%); S3(2%); S4(2%); S7(7%); S9(1%); T10(2%); T11(19%); T14(7%); T8(15%); T9(27%);
ST34	3.83	313	0.000	S8(2%); T10(31%); T11(7%); T13(22%); T14(5%); T15(2%); T7(3%); T8(1%); T9(13%);
ST35	3.87	310	0.033	S4(4%); S5(1%); S6(4%); S7(11%); S9(3%); T10(21%); T11(2%); T12(4%); T13(23%); T14(5%); T15(2%); T7(2%); T9(2%);
ST36	3.88	310	0.000	S10(5%); S6(21%); S7(16%); T11(6%); T12(2%); T13(24%); T7(3%); T9(6%);
ST37	3.93	306	0.001	S11(4%); S3(2%); S5(2%); S6(3%); S7(7%); S8(2%); S9(18%); T10(5%); T11(11%); T12(8%); T13(2%); T14(17%); T16(4%);
ST38	3.96	303	0.000	S10(2%); S9(1%); T11(37%); T12(15%); T15(3%); T17(3%); T9(21%);
ST39	3.96	303	0.002	S10(3%); S6(2%); S7(2%); S9(2%); T11(39%); T12(8%); T14(4%); T16(1%); T17(2%); T9(21%);
ST40	3.97	302	0.007	S10(2%); S11(3%); S6(1%); S7(4%); S9(3%); T11(23%); T12(18%); T14(17%); T15(1%); T21(1%); T9(13%);
ST41	4.02	299	0.004	S2(3%); S7(3%); S8(1%); S9(1%); T11(12%); T12(32%); T14(5%); T15(9%); T18(2%); T19(2%); T25(2%); T9(7%);
ST42	4.02	298	0.000	S10(1%); T11(9%); T12(37%); T13(2%); T14(5%); T15(7%); T16(3%); T17(1%); T18(1%); T19(2%); T25(3%); T8(1%); T9(7%);
ST43	4.04	297	0.012	S10(2%); S3(1%); S4(4%); S8(5%); T11(14%); T12(30%); T13(1%); T14(1%); T15(9%); T18(4%); T19(2%); T20(2%); T21(6%); T9(4%);
ST44	4.05	296	0.003	S8(22%); S9(1%); T11(3%); T12(6%); T14(2%); T15(12%); T16(10%); T18(14%); T19(3%); T20(5%); T21(5%); T25(2%);
ST45	4.06	296	0.008	S10(1%); S8(11%); T12(19%); T14(4%); T15(25%); T16(7%); T17(3%); T18(9%); T20(5%); T25(2%); T26(1%);
ST46	4.07	295	0.009	S4(3%); S8(14%); T11(6%); T12(18%); T14(1%); T15(22%); T16(5%); T18(4%); T20(4%); T21(2%); T9(5%);
ST47	4.08	294	0.003	S8(1%); T12(19%); T14(1%); T15(38%); T17(2%); T18(3%); T19(2%); T20(11%); T21(10%);
ST48	4.12	292	0.000	S8(13%); S9(2%); T10(2%); T12(5%); T15(12%); T16(10%); T17(7%); T18(14%); T19(3%); T20(8%); T21(9%); T25(3%);
ST49	4.13	290	0.000	S26(3%); T12(7%); T15(21%); T16(18%); T17(5%); T18(21%); T19(2%); T20(5%); T21(7%);
ST50	4.19	286	0.014	S12(1%); S3(4%); S4(4%); S5(3%); S6(3%); S9(9%); T10(35%); T12(1%); T13(7%); T15(7%); T19(7%); T7(3%);
ST51	4.25	282	0.069	S10(4%); S11(20%); S7(10%); S9(14%); T11(4%); T12(4%); T14(18%); T15(4%); T16(1%); T17(1%);
ST52	4.28	280	0.006	S20(6%); S22(5%); S6(2%); T10(2%); T13(17%); T14(4%); T15(7%); T16(25%); T18(8%); T19(3%); T21(1%);
ST53	4.29	280	0.005	S10(3%); S6(2%); S7(1%); T10(10%); T12(3%); T13(26%); T14(3%); T15(3%); T16(11%); T17(5%);

				T18(4%); T19(5%); T21(4%); T7(3%); T9(3%);
ST54	4.30	279	0.008	S10(2%); S11(7%); S6(7%); S8(1%); T10(2%); T12(3%); T13(16%); T14(10%); T15(3%); T16(11%); T17(2%); T18(5%); T19(6%); T7(2%);
ST55	4.31	278	0.001	S16(10%); S22(1%); S7(1%); T11(3%); T12(4%); T13(5%); T14(21%); T16(5%); T17(3%); T18(9%); T20(11%); T21(5%); T25(2%);
ST56	4.32	278	0.013	S12(7%); S16(8%); S9(4%); T10(6%); T13(19%); T14(1%); T16(7%); T17(4%); T18(4%); T19(15%); T20(6%); T25(3%); T7(1%);
ST57	4.35	276	0.001	S10(11%); S13(1%); S20(3%); T11(2%); T13(10%); T14(5%); T15(9%); T16(7%); T17(8%); T18(1%); T19(12%); T20(6%); T21(3%); T9(2%);
ST58	4.37	275	0.001	S10(3%); S11(5%); S5(2%); S7(2%); S8(1%); T11(1%); T12(4%); T13(7%); T14(15%); T15(2%); T16(5%); T17(4%); T18(4%); T19(9%); T20(8%); T21(7%); T9(6%);
ST59	4.39	273	0.001	S10(1%); S16(5%); S9(2%); T13(3%); T14(7%); T15(4%); T16(15%); T17(4%); T18(17%); T19(12%); T20(2%); T21(8%); T9(1%);
ST60	4.40	273	0.010	S10(3%); S11(4%); S20(1%); S22(2%); S6(2%); S8(1%); S9(1%); T11(4%); T14(13%); T15(6%); T16(5%); T17(15%); T18(7%); T19(10%); T21(1%); T25(2%); T9(2%);

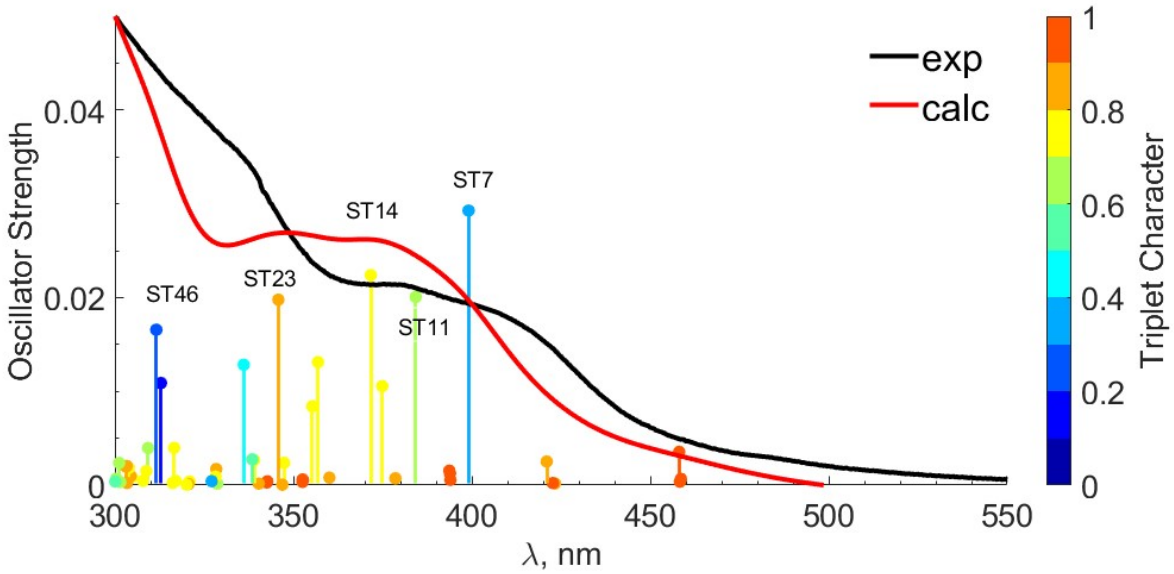


Figure S26. Experimental (black line) and the SOC-TDDFT calculated absorption (red line) spectra for [**3**·**Hg$_3$**]: excitation energies and oscillator strengths are shown by the vertical lines; the spectrum is convoluted with a Lorenzian function having a full width at half-maximum of 0.35 cm^{-1}.

Table S9. Excitation wavelengths (nm), oscillator strengths (f) and contributions of scalar relativistic (SR) states for [**3**·**Hg$_3$**] calculated with SR-TDDFT and SOC-TDDFT.

SR States (TDDFT Singlet-Singlet Excitations)				
State	**Energy(eV)**	**λ(nm)**	**f**	**Transitions**
S1	3.04	395	0.038	H–1 → L (18%); H → L (79%);
S2	3.30	364	0.033	H–2 → L (4%); H–1 → L (74%); H → L (16%);
S3	3.40	353	0.022	H–3 → L (5%); H–2 → L (83%); H–1 → L (2%); H → L

				(3%);
S4	3.64	330	0.003	H–3 → L (3%); H–1 → L+1 (5%); H → L+1 (84%); H → L+2 (3%);
S5	3.76	319	0.025	H–5 → L (2%); H–4 → L (8%); H–3 → L (52%); H–2 → L (6%); H–1 → L+1 (2%); H–1 → L+2 (5%); H → L+1 (10%); H → L+2 (8%);
S6	3.80	315	0.018	H–3 → L (7%); H–1 → L+1 (4%); H → L+2 (82%); H–2 → L (6%); H–1 → L+1 (2%); H–1 → L+2 (5%); H → L+1 (10%); H → L+2 (8%);
S7	3.90	308	0.015	H–4 → L (35%); H–3 → L (22%); H–2 → L+1 (2%); H–1 → L+1 (31%); H–1 → L+1 (2%); H–1 → L+2 (5%); H → L+1 (10%); H → L+2 (8%);
S8	3.95	304	0.002	H–4 → L (42%); H–2 → L+1 (6%); H–1 → L+1 (42%); H–1 → L+1 (31%); H–1 → L+1 (2%); H–1 → L+2 (5%); H → L+1 (10%); H → L+2 (8%);
S9	3.96	303	0.015	H–7 → L (2%); H–5 → L (83%); H–3 → L (4%); H–2 → L+1 (3%); H–1 → L+1 (2%); H–1 → L+2 (5%); H → L+1 (10%); H → L+2 (8%);
S10	4.00	300	0.000	H–11 → L (30%); H–10 → L (40%); H–9 → L (9%); H–8 → L (3%); H–6 → L (4%); H–2 → L+1 (4%); H → L+1 (10%); H → L+2 (8%);
S11	4.03	298	0.002	H–10 → L (9%); H–8 → L (4%); H–6 → L (11%); H–5 → L (7%); H–4 → L (3%); H–2 → L+1 (34%); H–1 → L+2 (18%); H → L+4 (4%);
S12	4.04	297	0.011	H–8 → L (2%); H–4 → L (3%); H–1 → L+2 (3%); H → L+3 (25%); H → L+4 (23%); H → L+5 (32%); H–1 → L+2 (18%); H → L+4 (4%);
S13	4.08	294	0.000	H–11 → L (3%); H–8 → L (3%); H–7 → L (2%); H–2 → L+1 (28%); H–2 → L+2 (4%); H–1 → L+1 (4%); H–1 → L+2 (48%); H → L+4 (4%);
S14	4.10	293	0.021	H–9 → L (2%); H–8 → L (6%); H–6 → L (59%); H–2 → L+1 (11%); H–1 → L+2 (5%); H → L+4 (3%); H–1 → L+2 (48%); H → L+4 (4%);
S15	4.13	291	0.013	H–9 → L (3%); H–8 → L (30%); H–7 → L (26%); H–6 → L (7%); H–3 → L+1 (4%); H–2 → L+2 (2%); H–1 → L+2 (3%); H → L+3 (8%); H → L+5 (5%);
SR States (TDDFT Singlet-Triplet Excitations)				
T1	2.53	475	0.001	H–6 → L (3%); H–2 → L (12%); H–1 → L (37%); H → L (25%);
T2	2.80	428	0.000	H–9 → L (2%); H–2 → L (4%); H–1 → L (5%); H → L (60%); H → L+5 (2%);
T3	2.94	409	0.004	H–1 → L+5 (13%); H → L (3%); H → L+2 (2%); H → L+3 (5%); H → L+4 (5%); H → L+5 (45%); H → L+6 (5%);
T4	3.12	385	0.000	H–2 → L (41%); H–1 → L (31%); H → L+2 (2%); H → L+3 (5%); H → L+4 (5%); H → L+5 (45%); H → L+6 (5%);
T5	3.19	376	0.000	H–11 → L (3%); H–10 → L (3%); H–6 → L (5%); H–4 → L (9%); H–3 → L (22%); H–2 → L (13%); H → L+1 (8%); H → L+2 (7%);
T6	3.28	366	0.003	H–12 → L+8 (4%); H–8 → L+9 (3%); H–7 → L+3 (3%); H–5 → L+3 (6%); H–5 → L+4 (4%); H–4 → L (5%); H–4 → L+4 (7%); H–3 → L+6 (5%); H–3 → L+11 (3%);
T7	3.34	359	0.029	H–3 → L (4%); H–3 → L+2 (2%); H–2 → L (6%); H–2 → L+1 (3%); H–2 → L+2 (4%); H–1 → L (11%); H–1 → L+1 (8%); H–1 → L+2 (8%); H → L+1 (15%); H → L+2 (14%);
T8	3.38	355	0.001	H–12 → L+4 (4%); H–9 → L+3 (2%); H–9 → L+8 (2%); H–8 → L+8 (3%); H–7 → L+3 (4%); H–7 → L+4 (5%); H–7 → L+6 (2%); H–6 → L+9 (3%); H–5 → L+3 (6%); H–4 → L (2%); H–4 → L+9 (4%); H–3 → L+10 (3%); H–3 → L+11 (6%); H–2 → L (3%);
T9	3.38	355	0.001	H–13 → L+3 (3%); H–12 → L+3 (6%); H–9 → L+3 (2%);

				H–9 → L+4 (4%); H–8 → L+3 (3%); H–7 → L+4 (3%); H–7 → L+8 (5%); H–5 → L (2%); H–5 → L+8 (3%); H–5 → L+9 (8%); H–4 → L+6 (2%); H–2 → L (3%); H–3 → L+11 (6%); H–2 → L (3%);
T10	3.55	338	0.002	H–6 → L (3%); H–5 → L (4%); H–4 → L (3%); H–3 → L (14%); H–3 → L+1 (2%); H–2 → L (3%); H–1 → L+4 (3%); H–1 → L+7 (4%); H → L+1 (7%); H → L+4 (7%); H → L+6 (4%); H → L+7 (8%); H–3 → L+11 (6%); H–2 → L (3%);
T11	3.70	324	0.020	H–11 → L (2%); H–8 → L (3%); H–1 → L+1 (3%); H–1 → L+2 (11%); H → L (3%); H → L+1 (35%); H → L+2 (24%); H–1 → L+7 (4%); H → L+1 (7%); H → L+4 (7%); H → L+6 (4%); H → L+7 (8%); H–3 → L+11 (6%); H–2 → L (3%);
T12	3.72	322	0.001	H–11 → L (4%); H–10 → L (4%); H–8 → L (5%); H–7 → L (3%); H–1 → L (6%); H–1 → L+1 (18%); H → L (3%); H → L+1 (16%); H → L+2 (9%); H → L+4 (7%); H → L+6 (4%); H → L+7 (8%); H–3 → L+11 (6%); H–2 → L (3%);
T13	3.82	314	0.011	H–5 → L (40%); H–5 → L+3 (3%); H–3 → L (10%); H–1 → L+1 (14%); H → L+1 (3%); H → L+2 (6%); H → L (3%); H → L+1 (16%); H → L+2 (9%); H → L+4 (7%); H → L+6 (4%); H → L+7 (8%); H–3 → L+11 (6%); H–2 → L (3%);
T14	3.84	313	0.022	H–8 → L (3%); H–6 → L (2%); H–5 → L+3 (4%); H–5 → L+8 (3%); H–4 → L (36%); H–3 → L (23%); H–3 → L+4 (6%); H → L+1 (16%); H → L+2 (9%); H → L+4 (7%); H → L+6 (4%); H → L+7 (8%); H–3 → L+11 (6%); H–2 → L (3%);
T15	3.86	311	0.001	H–9 → L (3%); H–7 → L (3%); H–5 → L (23%); H–1 → L+1 (25%); H–1 → L+4 (3%); H–1 → L+5 (3%); H → L+1 (6%); H → L+2 (9%); H → L+2 (9%); H → L+4 (7%); H → L+6 (4%); H → L+7 (8%); H–3 → L+11 (6%); H–2 → L (3%);
States calculated by SOC-TDDFT				
State	**Energy (eV)**	**λ (nm)**	**f**	**Component Scalar Transitions**
ST1	2.62	459	0.001	T1(95%); T2(1%);
ST2	2.62	458	0.000	T1(96%);
ST3	2.62	458	0.004	T1(96%);
ST4	2.83	423	0.000	S1(1%); T2(83%); T4(8%); T5(2%);
ST5	2.84	423	0.000	T2(81%); T4(11%); T5(4%);
ST6	2.85	421	0.003	S2(3%); S3(6%); T2(86%);
ST7	3.01	399	0.029	S1(63%); T4(23%); T5(5%);
ST8	3.05	394	0.001	T2(2%); T3(94%);
ST9	3.05	394	0.001	T2(2%); T3(95%);
ST10	3.05	394	0.002	T3(97%);
ST11	3.12	384	0.020	S1(1%); S2(13%); S3(8%); T4(59%); T5(9%);
ST12	3.17	379	0.001	T1(1%); T2(4%); T3(2%); T4(52%); T5(26%); T7(6%);
ST13	3.20	375	0.011	S1(9%); S3(5%); T2(4%); T4(39%); T5(32%); T7(4%);
ST14	3.23	372	0.022	S1(1%); S2(16%); S3(2%); T4(11%); T5(57%); T7(5%);
ST15	3.33	360	0.001	T4(15%); T5(56%); T7(19%);
ST16	3.36	357	0.013	S1(7%); S2(3%); S3(1%); T4(8%); T5(39%); T7(32%);
ST17	3.38	355	0.008	S2(10%); S3(4%); T5(22%); T6(4%); T7(51%);
ST18	3.40	353	0.001	T6(98%);
ST19	3.40	353	0.001	T6(98%);
ST20	3.40	353	0.000	T6(95%); T7(3%);
ST21	3.45	347	0.002	S1(3%); S2(4%); S3(6%); T4(13%); T5(7%); T7(19%); T8(28%); T9(14%);
ST22	3.46	347	0.000	T4(9%); T5(4%); T7(45%); T8(24%); T9(10%);
ST23	3.47	346	0.020	S2(5%); S3(4%); T4(7%); T5(3%); T7(15%); T8(45%); T9(17%);

ST24	3.50	343	0.000	T7(1%); T8(43%); T9(52%);
ST25	3.50	343	0.000	T7(2%); T8(47%); T9(50%);
ST26	3.50	343	0.000	T8(36%); T9(62%);
ST27	3.53	340	0.000	T4(4%); T5(2%); T7(20%); T8(26%); T9(38%);
ST28	3.54	339	0.003	S1(8%); S2(1%); S3(1%); T4(6%); T5(4%); T7(19%); T8(25%); T9(21%);
ST29	3.54	339	0.003	S2(31%); T10(2%); T2(4%); T4(2%); T5(5%); T7(12%); T8(13%); T9(23%);
ST30	3.57	336	0.013	S2(1%); S3(42%); T10(8%); T2(2%); T4(5%); T7(18%); T8(5%); T9(4%);
ST31	3.65	329	0.000	S2(1%); S4(18%); T10(66%); T11(3%); T12(1%);
ST32	3.65	328	0.002	T10(85%); T12(3%);
ST33	3.66	328	0.001	S3(4%); S4(4%); T10(74%); T11(5%); T12(3%);
ST34	3.67	327	0.000	S4(48%); T10(22%); T11(9%); T13(1%); T15(2%); T16(2%); T17(2%);
ST35	3.74	321	0.000	S4(2%); T10(5%); T11(63%); T12(8%); T17(6%);
ST36	3.74	321	0.000	T10(7%); T11(64%); T12(7%); T13(2%); T16(3%); T17(5%);
ST37	3.75	320	0.000	S11(3%); S14(1%); S4(6%); S7(2%); S8(2%); T10(6%); T11(55%); T12(13%);
ST38	3.79	317	0.000	S13(4%); S6(1%); S8(2%); T10(2%); T11(8%); T12(66%);
ST39	3.79	317	0.004	S5(1%); S6(5%); T11(6%); T12(62%); T13(3%); T15(4%); T16(5%); T17(2%); T20(1%);
ST40	3.79	316	0.000	S4(3%); S5(1%); T11(13%); T12(60%); T13(2%); T15(2%); T16(3%); T20(3%);
ST41	3.84	313	0.011	S5(22%); S6(50%); T12(4%); T19(2%); T20(4%); T26(3%); T28(2%);
ST42	3.85	312	0.017	S11(2%); S5(44%); S6(15%); S7(2%); S8(1%); T11(3%); T12(2%); T13(3%); T15(7%); T17(5%);
ST43	3.88	309	0.004	S4(2%); S5(2%); S7(3%); S8(3%); T11(4%); T12(4%); T13(26%); T15(26%); T16(3%); T17(5%); T20(3%); T21(1%);
ST44	3.89	309	0.002	T11(3%); T12(7%); T13(29%); T15(27%); T17(3%); T20(4%); T22(1%);
ST45	3.90	308	0.000	S10(2%); S6(1%); S7(3%); S8(3%); T12(7%); T13(28%); T15(24%); T16(5%); T17(8%); T20(3%);
ST46	3.92	306	0.021	S11(2%); S13(1%); S19(1%); S5(12%); S6(5%); S7(9%); S8(4%); T12(4%); T13(10%); T14(11%); T15(10%); T16(6%); T17(9%);
ST47	3.94	305	0.001	S11(2%); S5(1%); S8(2%); T13(46%); T14(3%); T15(21%); T16(5%); T17(5%);
ST48	3.94	304	0.001	T13(42%); T14(22%); T15(15%); T16(4%); T17(6%);
ST49	3.95	304	0.002	S10(4%); S5(2%); T13(31%); T14(18%); T15(27%); T16(3%); T21(2%);
ST50	3.96	303	0.000	T14(88%); T15(4%);
ST51	3.96	303	0.002	T13(12%); T14(68%); T15(9%);
ST52	3.96	303	0.002	S8(1%); T13(6%); T14(71%); T15(8%); T17(3%);
ST53	3.98	302	0.000	S12(1%); S13(4%); T13(4%); T16(29%); T17(1%); T18(3%); T20(4%); T21(12%); T25(3%); T26(3%); T28(8%);
ST54	3.98	301	0.002	S7(2%); T13(6%); T14(1%); T16(28%); T17(5%); T18(4%); T19(1%); T20(4%); T21(8%); T25(4%); T26(2%); T28(8%);
ST55	3.99	300	0.001	S12(3%); S5(1%); S7(7%); T11(1%); T15(2%); T16(8%); T17(17%); T18(4%); T19(3%); T20(7%); T21(5%); T24(3%); T26(3%); T28(6%); T30(3%);
ST56	4.00	300	0.000	S11(2%); S12(6%); S7(6%); S8(1%); S9(3%); T15(1%); T17(21%); T18(5%); T19(2%); T21(16%); T22(1%); T25(1%); T28(5%);
ST57	4.00	300	0.002	S12(4%); S7(3%); S8(1%); T15(8%); T16(9%);

				T17(27%); T18(12%); T19(2%); T20(3%); T21(9%);
ST58	4.01	299	0.004	S10(7%); S11(2%); S13(1%); S8(4%); S9(5%); T15(8%); T16(18%); T17(9%); T18(13%); T19(1%); T21(10%);
ST59	4.02	298	0.009	S10(6%); S11(1%); S12(2%); S13(3%); S14(2%); S15(3%); S19(2%); S7(3%); S8(14%); S9(1%); T15(2%); T16(5%); T17(4%); T18(9%); T19(5%); T21(5%); T26(2%); T28(5%); T30(2%);
ST60	4.03	298	0.001	S10(6%); S11(3%); S12(23%); S13(5%); S7(2%); S8(7%); S9(1%); T17(6%); T20(3%); T22(2%); T25(2%); T26(2%); T28(10%); T30(1%);

Theoretical background of radiative and nonradiative rate constants calculations

To calculate a radiative (k_r)[1] and nonradiative (k_{nr})[2] rate constants we used methodology described earlier using eq. (1) and (4):

$$k_r^{\alpha}(T_1 \rightarrow S_0) = \frac{8\pi^2\eta^3\langle\tilde{\nu}^3\rangle_{fcf}}{3\varepsilon_0\hbar}\left|M_T^{\alpha}\left(Q_0^{T_1}\right)\right|^2 \quad (1)$$

$$M_T^{\alpha}\left(Q_0^{T_1}\right) = \sum_{j\in x,y,z}\left|\sum_m \frac{\langle T_1^{\alpha}|H_{SOC}|S_m\rangle}{E(S_m)-E(T_1)} M_{S_{m,j}}\left(Q_0^{T_1}\right)\right|^2 \quad (2)$$

$$k_r = \frac{k_r^1 + k_r^2 exp(-ZFS_{1,2}/k_BT) + k_r^3 exp(-ZFS_{1,3}/k_BT)}{1 + exp(-ZFS_{1,2}/k_BT) + exp(-ZFS_{1,3}/k_BT)} \quad (3)$$

where η is the refractive index of the solvent, ħ is reduced Planck's constant, and ε_0 is the permittivity of vacuum, $\langle\tilde{\nu}^3\rangle_{fcf}$ is the transition energy of the T_1 excited state (in cm^{-1}), and $M_T^{\alpha}\left(Q_0^{T_1}\right)$ is the transition dipole moment of the $T_1^{\alpha} \rightarrow S_0$ transition, $M_{S_{m,j}}\left(Q_0^{T_1}\right)$ is the j-axis projection of the $S_m \rightarrow S_0$ transition dipole moment

$$k_{nr}(T_1 \rightarrow S_0) = \frac{2\pi}{\hbar} \times \frac{\langle T_1|H_{SOC}|S_0\rangle^2}{\sqrt{2\pi\hbar^2(D_1^2+P^2)}} \times exp\left(-\frac{(E_{0-0} - n_M\hbar\omega_M - \lambda_1 - \mu)^2}{2\pi\hbar^2(D_1^2+P^2)}\right) \times exp(-S_M) \times$$

$$\hbar^2 D_1^2 = \sum_{j\in hf} S_j \left(\frac{\hbar\omega_j^S}{b_j}\right)^2 coth\frac{\hbar\omega_j^T}{2k_BT} \quad (5)$$

$$\hbar^2 P^2 = \frac{1}{2}\sum_{j\in hf}\left[\hbar\omega_j^S \frac{1-b_j^2}{b_j} coth\frac{\hbar\omega_j^T}{2k_BT}\right]^2 \quad (6)$$

$$\lambda_M = \sum_{j\in hf} S_j\hbar\omega_j \quad (7)$$

$$\hbar\omega_M = \frac{\lambda_M}{S_M} \quad (8)$$

$$\lambda_1 = \sum_{j\in hf}\frac{S_j\hbar\omega_j^S}{b_j} \quad (9)$$

$$\mu = \frac{1}{2}\sum_{j\in hf}\hbar\omega_j^S \frac{1-b_j^2}{b_j}\coth\frac{\hbar\omega_j^T}{2k_BT} \quad (10)$$

$$n_M = \frac{\Delta E_{00} - \lambda_1 - \mu}{\hbar\omega_M} \quad (11)$$

$$S_M = \sum_{j\in hf} S_j \quad (12)$$

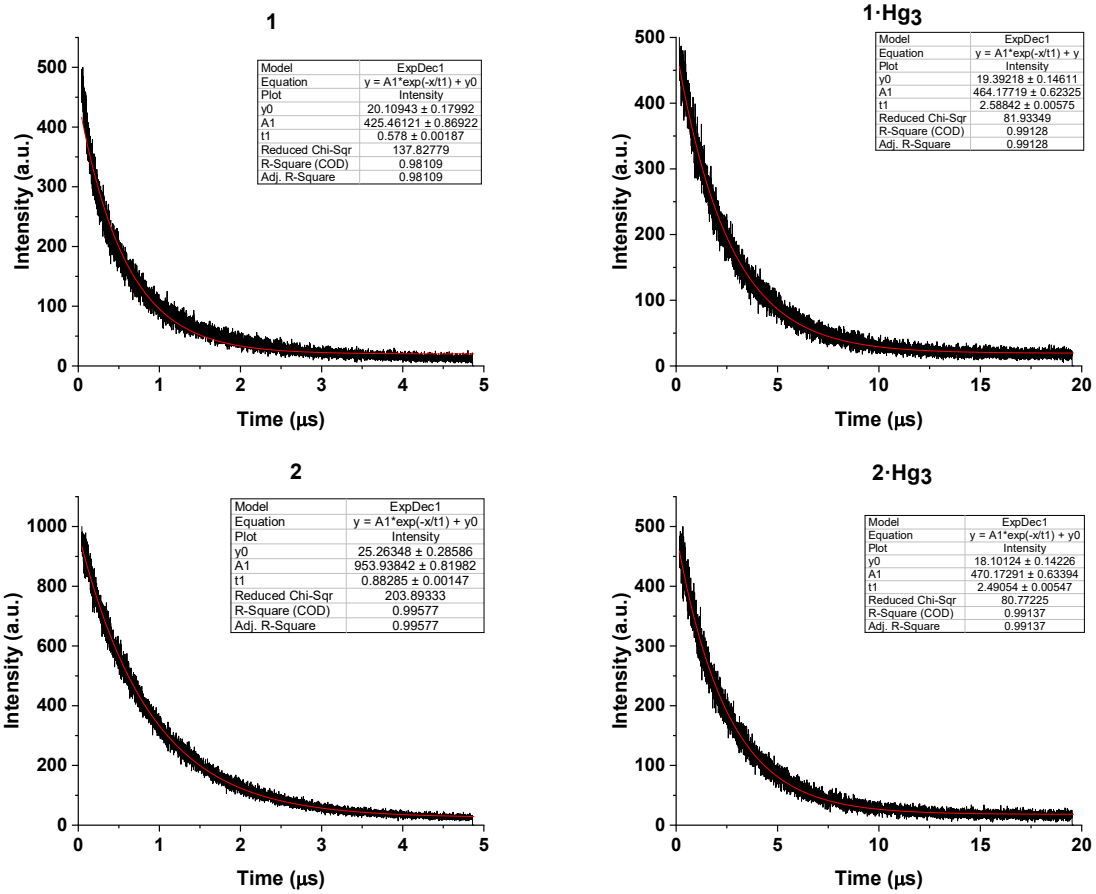
$$S_j = \frac{1}{2}\left(\frac{m_j\omega_j}{\hbar}\right) \quad (13)$$

where S is the Huang–Rhys factor, m_j is the reduced mass of the *j*th normal mode, ΔQ_j represents the equilibrium displacement along the *j*th normal mode coordinate; $\omega_j^{S(T)}$ is the frequency of the *j*th normal mode of the S_0 (T_1) state, $\Delta E_{0\text{-}0}$ is the zeropoint energy difference between the T_1 excited

state and the S_0 ground state. hf and lf designate the high-frequency ligand skeletal modes ($2000>\omega_{hf}>1000$ cm^{-1}) and low-frequency modes $200<\omega_{lf}\leq1000$ cm^{-1}.

Table S8. Values of calculated parameters and k_{nr} at 298K using eq. (4)

	3	**3·Hg$_3$**
$\langle S_0\|H_{SO}\|T_1\rangle$, cm^{-1}	148.7	147.9
S_M	1.22	1.06
S_{lf}	0.60	0.59
$\hbar\omega_M$, cm^{-1}	1416	1396
λ_M, cm^{-1}	1727	1483
λ_{lf}, cm^{-1}	336	312
λ_1, cm^{-1}	364	332
μ, cm^{-1}	946	915
$\hbar^2 D_1^2$, cm^{-2}	2.74×10^5	2.40×10^5
$\hbar^2 P^2$, cm^{-2}	7.40×10^4	7.35×10^4
n_M	13	13
k_{nr}	7.8×10^4	7.1×10^3



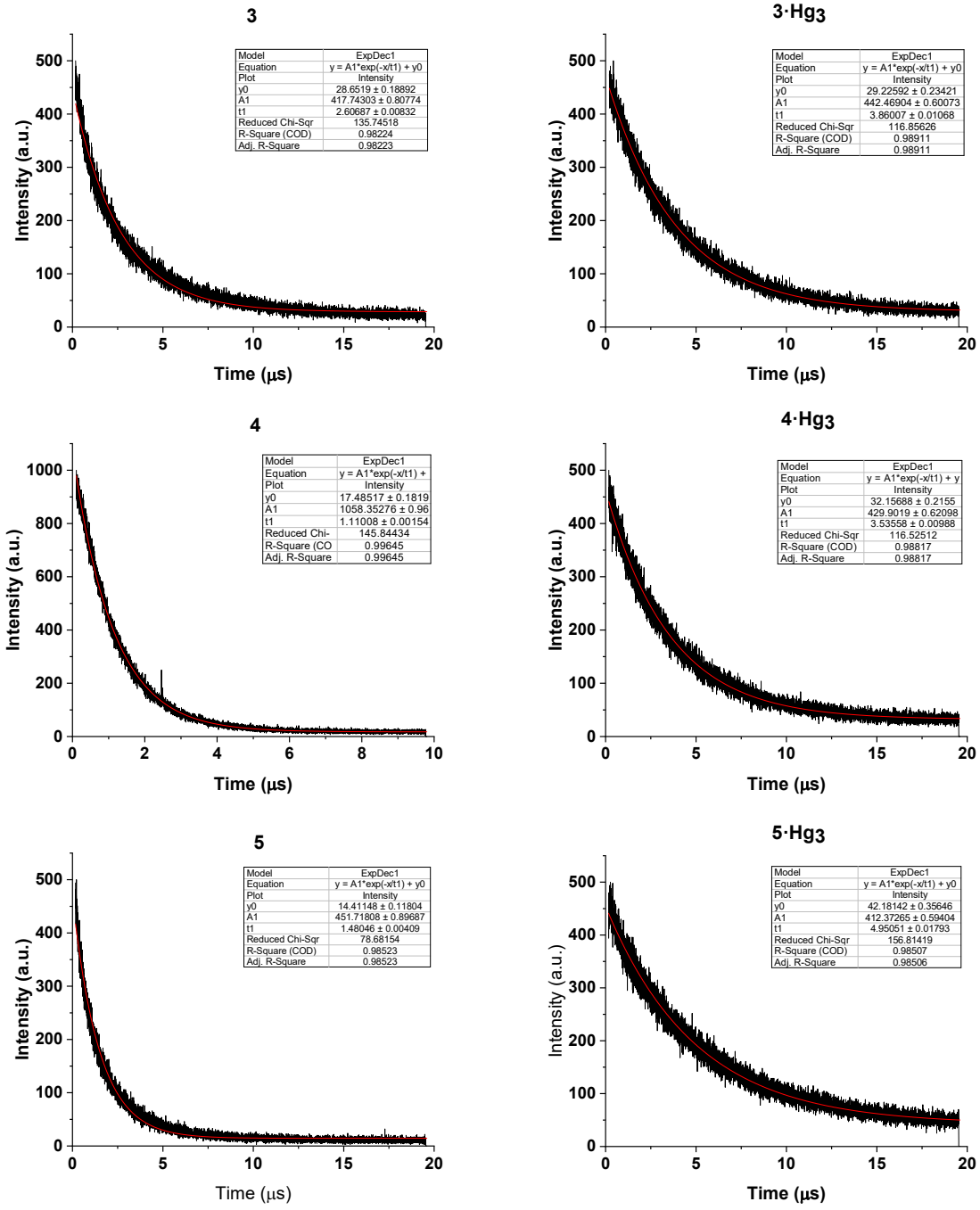
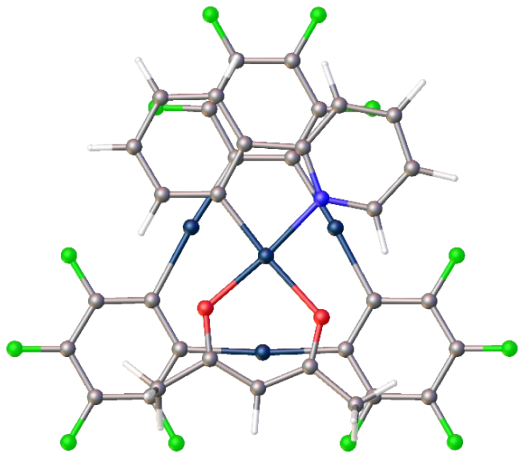


Figure S27. Photoluminescence experimental (black) and fitted (red) decay curves of parent platinum complexes and their adducts in solid state at 298 K.

Cartesian coordinates for the studied molecules

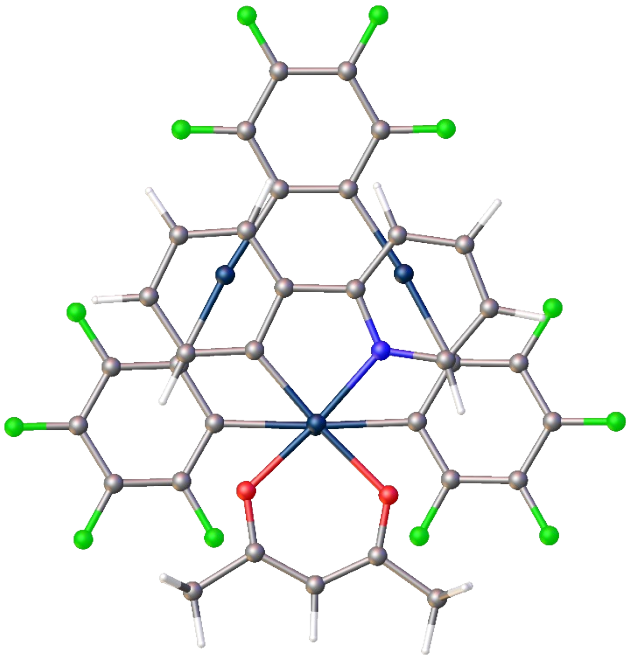
Cartesian coordinate for [**1**·**Hg$_3$**][a] (in Å)



Hg	27.05161993877753	12.00436244608024	10.27745881820301
Hg	28.83894763506038	12.25860732442861	7.16119680678286
Hg	30.58906288397720	11.24455234422889	10.14598105194736
Pt	28.08583150801153	8.86609429899017	8.30953672994455
F	24.06262444408954	12.72187295236358	9.66820759060930
F	22.73755603248919	13.26751631708473	7.39320241561308
F	24.05914201961127	13.39206180745705	5.03910061148354
F	26.72332332152325	12.96344460966769	4.95577535121988
F	30.90295845783867	12.14621264565643	4.81874480103811
F	33.47751435598128	11.35582146902357	4.68409362013034
F	34.81275867390509	10.68707887691831	6.93590675525206
F	33.57355661252510	10.76633832500038	9.32376991688010
F	31.40786619712993	10.30768850828022	13.01533281959152
F	30.05145016961520	10.08086087597728	15.33788312992082
F	27.42806266679850	10.71212521838727	15.44573558110247
F	26.14395686461926	11.56003026827612	13.23505270875149
O	27.68698091160752	8.51860538791919	10.23435086902676
O	26.07997538114116	9.30033396333188	7.93032137805986
N	28.63539491884874	9.11722015025500	6.41143451830161
C	26.11676486527125	12.57529200078416	8.51672251598638
C	24.75071136268212	12.80262208094396	8.52876099350119
C	24.04152690121681	13.08212481945759	7.36303425503679
C	24.72189767485705	13.13802932421552	6.14905769528779
C	26.09810962646187	12.91644975883442	6.13110350320977
C	26.80642332743686	12.64015429116085	7.28979741903741
C	30.86657022283858	11.84022039879770	7.15733699084237
C	31.53568903556690	11.81709342302566	5.94423373315236
C	32.86887865239142	11.42485846845779	5.85356666686760
C	33.55701628874248	11.07967363152445	7.01347490061525
C	32.89379417609327	11.11814053128028	8.23813918651499
C	31.55854042338266	11.47535324652831	8.32884724768266
C	29.48934292824249	11.09406520328931	11.89736772858599
C	30.12019154909039	10.63884578766444	13.04466288307684
C	29.43869154995788	10.51184196859348	14.25465880895483
C	28.08731157725418	10.84457011466207	14.31265081939309
C	27.44800852880732	11.29252773013448	13.15925048110341

C	28.12096223132638	11.42577397295896	11.95544363362743
C	26.56526646417803	8.70496686955368	10.80681248698163
C	25.39183199417522	9.18032942888471	10.20132210660656
H	24.52541663923869	9.29908833035597	10.84755767233116
C	25.18734529484048	9.38778534959987	8.82020202513925
C	27.80181221242668	9.57017314188644	5.46317792990728
H	26.78235387543073	9.76322043492742	5.79266662206314
C	28.22819363735765	9.78868174188024	4.16346535238736
H	27.53143344417613	10.18490211436970	3.42985355717200
C	29.55729937156113	9.50598316387280	3.84134672300591
H	29.92903629665712	9.67578967646935	2.83281711230359
C	30.40917635100581	9.02400701174160	4.82434528819355
H	31.45319847771148	8.82132085461817	4.60042779100673
C	29.93860950573663	8.84469611646720	6.12827300328139
C	30.71664217767257	8.43446102094786	7.28890999038902
C	32.08494459680243	8.14249491362771	7.26711540710620
H	32.64380525116358	8.16676602804440	6.33221086952030
C	32.74652607157164	7.83516047444476	8.45154605125287
H	33.81495272623857	7.62984870801402	8.44118473369766
C	32.03553194226055	7.81045595943327	9.65466258907105
H	32.55439667443070	7.57476716130172	10.58321555981850
C	30.66740093014488	8.08878562036618	9.68177888488089
H	30.11607543814871	8.05168665301841	10.62071530308333
C	29.98550087748785	8.41398224132686	8.50226696706139
C	26.53648012641828	8.33574052759264	12.26091492333812
H	26.17671809147244	7.30324868883379	12.36240521331660
H	27.54796660748773	8.38987547231595	12.67175498112188
H	25.86766355779876	8.98916705688114	12.82838286727473
C	23.79887971851185	9.71036894765728	8.34492896361824
H	23.83490764281304	10.05003661071692	7.30693912163555
H	23.17203980469793	8.81116856022750	8.40210843781468
H	23.33797728520965	10.48095457898129	8.97077552928373

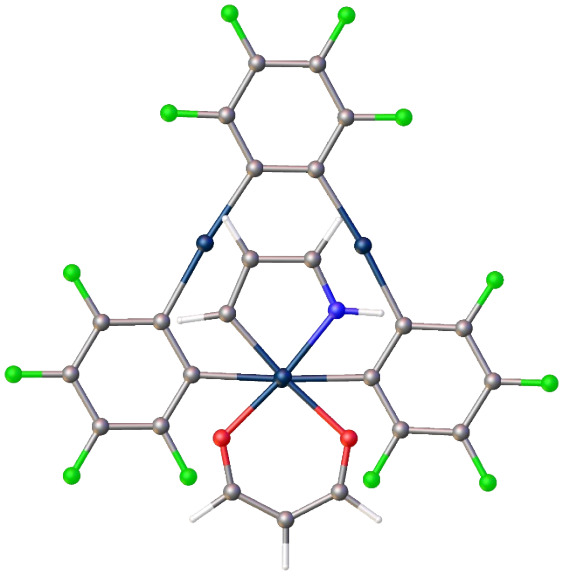
Cartesian coordinate for [**1**·**Hg$_3$**][b] (in Å)



Hg	27.069712000	11.917767000	10.331552000
Hg	28.772044000	12.292089000	7.171645000
Hg	30.620246000	11.267250000	10.142094000
Pt	26.214333000	9.006452000	9.645968000
F	24.071128000	12.556910000	9.814289000
F	22.663042000	13.148767000	7.588063000
F	23.919783000	13.405676000	5.212935000
F	26.596423000	13.085555000	5.052473000
F	30.732399000	12.062427000	4.777569000
F	33.305997000	11.262104000	4.560359000
F	34.686360000	10.525606000	6.757928000
F	33.507429000	10.575674000	9.185618000
F	31.543757000	10.447928000	13.020014000
F	30.197314000	10.054314000	15.328950000
F	27.538681000	10.524362000	15.445822000
F	26.220210000	11.416202000	13.265706000
O	25.745725000	8.664852000	11.556048000
O	24.234693000	9.449821000	9.193725000
N	26.813637000	9.238988000	7.759053000
C	26.090538000	12.528697000	8.606007000
C	24.717464000	12.700453000	8.659180000
C	23.973351000	13.002951000	7.523108000
C	24.620343000	13.138232000	6.296445000
C	26.002459000	12.974285000	6.238344000
C	26.747806000	12.677360000	7.369614000
C	30.777149000	11.770149000	7.115051000
C	31.401904000	11.721460000	5.877585000
C	32.724072000	11.305045000	5.741252000
C	33.437147000	10.923875000	6.877280000
C	32.811178000	10.965388000	8.121603000
C	31.495812000	11.381319000	8.263059000
C	29.581603000	11.159184000	11.927057000
C	30.240327000	10.711656000	13.061557000
C	29.564458000	10.495099000	14.260696000
C	28.194472000	10.742337000	14.321914000
C	27.533722000	11.199328000	13.186215000
C	28.197630000	11.405056000	11.989738000
C	24.575779000	8.718838000	12.058586000
C	23.409339000	9.098583000	11.384328000
H	22.495959000	9.092508000	11.969823000
C	23.274756000	9.398837000	10.018412000
C	25.994437000	9.624526000	6.772813000
H	24.968387000	9.830424000	7.073254000
C	26.440547000	9.766205000	5.467193000
H	25.750804000	10.096600000	4.695248000
C	27.784024000	9.513198000	5.189121000
H	28.173536000	9.634105000	4.180012000
C	28.630509000	9.119034000	6.219004000
H	29.683218000	8.927013000	6.030543000
C	28.128477000	8.977310000	7.517228000
C	28.877520000	8.582537000	8.703571000
C	30.246311000	8.275196000	8.716122000
H	30.838661000	8.335380000	7.804308000
C	30.858041000	7.909792000	9.910883000
H	31.922485000	7.683803000	9.930304000
C	30.098105000	7.838944000	11.086320000
H	30.583687000	7.563351000	12.021936000
C	28.739354000	8.145886000	11.078445000
H	28.164143000	8.120589000	12.002407000
C	28.103752000	8.529587000	9.891826000

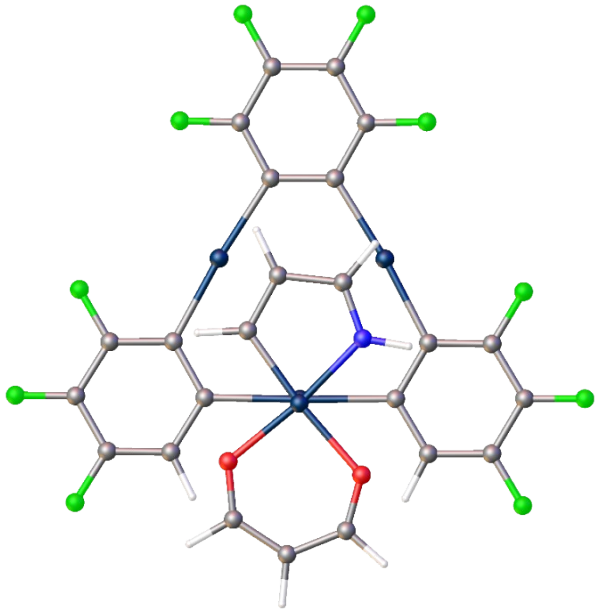
C	21.858707000	9.686547000	9.485845000
H	21.849551000	9.752344000	8.391909000
H	21.155642000	8.897088000	9.774914000
H	21.470217000	10.633851000	9.876741000
C	24.432339000	8.331157000	13.542071000
H	23.379435000	8.222087000	13.825982000
H	24.932137000	7.379540000	13.755931000
H	24.873948000	9.090494000	14.197431000

Cartesian coordinate for ^{3}**M1**·**Hg$_3$** (in Å)



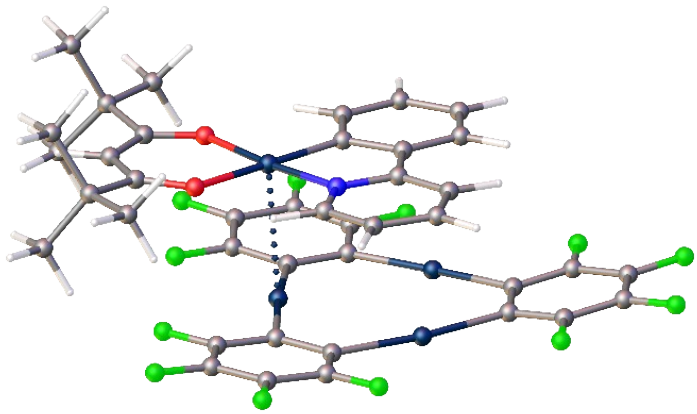
Hg	26.96953289623313	5.09213772572529	10.28251124881927
Hg	28.73457366489796	5.44523858168009	7.15985459821422
Hg	30.50061919677584	4.41748955732479	10.18277442568785
Pt	26.47061694228161	2.16144624869045	9.54989165685373
F	23.97586712904589	5.71585684759858	9.69432477921691
F	22.61535297419034	6.28129417258760	7.43892971550915
F	23.91786899783728	6.53455116190217	5.08913534168445
F	26.59546346456279	6.19880200787280	4.97747972626059
F	30.82951275360745	5.43809732007038	4.85984029620083
F	33.46291101295010	4.85369703355483	4.75846232281368
F	34.77281261967964	4.10132126424803	6.99330866790311
F	33.46382788438243	3.92707050801065	9.34371110982452
F	31.34577968007969	3.53424448356932	13.08210545117330
F	29.94183993224133	3.17502000966012	15.36078228884426
F	27.29218907498490	3.67762731219930	15.41698863555115
F	26.02791860512276	4.56434638191618	13.20507633083332
O	25.93555813470315	1.91734969583013	11.46346335300539
O	24.53547920604439	2.67455943277551	8.99535954964670
N	27.19834779663730	2.32621890466563	7.71631982896695
C	26.02080908338442	5.66709374023188	8.52622142741269
C	24.64737089077687	5.84310430069897	8.55170420997000
C	23.92322113979932	6.13303308087451	7.39841452717117
C	24.59520545823027	6.25989273967061	6.18430999342518
C	25.97740991316233	6.08538033359266	6.14963665503861
C	26.69910837132545	5.78938099690347	7.29729224726939
C	30.75785394496921	4.99650061443758	7.17299173303125
C	31.45463920677049	5.07427442392416	5.97597347903286
C	32.81380708983110	4.77601045278215	5.90055108752229
C	33.49020155382720	4.38753327171084	7.05496261765968
C	32.79379943109549	4.30523258805121	8.25988644142759
C	31.44168217277601	4.60195557368845	8.34182986565278
C	29.41657451971985	4.25877942703294	11.93831610870900
C	30.04432201026458	3.80539342127331	13.08919748341565
C	29.33784667883684	3.60954275141149	14.27434724233515
C	27.96940506018909	3.87169253609340	14.30404825761083
C	27.33872442393062	4.33251622128894	13.15150578790609
C	28.03516038475545	4.53272119999355	11.97113019749540
C	24.76994409493814	2.14817671360302	11.90905270675780
C	23.64037962781688	2.56120968762942	11.20428552327868
H	22.72642932524796	2.71451412514539	11.77220791470589
C	23.59009727481828	2.78557644010953	9.82300191858682
C	28.46159566712150	2.03696148597330	7.57913109013414
C	29.14541107122127	1.66209175403616	8.77894402205376
C	28.32652257238693	1.67085201721523	9.88018754819036
H	26.66397503050633	2.62054923573130	6.90628655200408
H	28.94208130278212	2.09614665171861	6.59960150280649
H	30.20023536482934	1.39254393834864	8.77725127343310
H	28.71029163451681	1.41515155299621	10.87185302877908
H	24.66588995156155	2.00016229707497	12.99203348440376
H	22.62392051634739	3.09756990187580	9.39913710377003

Cartesian coordinate for ^{3}**M2**·**Hg$_3$** (in Å)



Hg	0.923375	0.306411	-1.687391
Hg	-2.204865	1.919097	-1.068926
Hg	-2.095656	-1.380081	-2.573175
H	2.998913	2.524300	-0.809734
F	3.067113	4.870521	0.225119
F	0.691033	6.025952	0.742877
F	-1.596554	4.716158	0.164229
F	-5.218220	2.621664	-0.659721
F	-7.510530	1.324537	-1.254652
F	-7.431904	-1.105350	-2.421231
F	-5.065284	-2.260398	-3.002078
F	-1.309245	-4.154611	-3.758564
F	1.053304	-5.393914	-4.155034
F	3.350595	-4.146108	-3.504841
H	3.132638	-1.789587	-2.518381
C	0.835690	2.249948	-0.936661
C	2.010760	2.947017	-0.631561
C	1.960078	4.215516	-0.068209
C	0.735096	4.823410	0.204964
C	-0.432665	4.129949	-0.101946
C	-0.406711	2.860438	-0.666352
C	-3.923181	0.855213	-1.528964
C	-5.153535	1.425301	-1.237587
C	-6.348701	0.773414	-1.535486
C	-6.308032	-0.481968	-2.138742
C	-5.073664	-1.060348	-2.430991
C	-3.881030	-0.416245	-2.137400
C	-0.242806	-2.242038	-2.891801
C	-0.187476	-3.521258	-3.432926
C	1.020869	-4.178828	-3.645628
C	2.203906	-3.523425	-3.305465
C	2.174237	-2.244798	-2.765735
C	0.957753	-1.588120	-2.545987
Pt	1.176564	-0.668899	1.215678
O	2.494094	-2.027706	0.565590
O	2.690783	0.631734	1.786706
N	-0.279689	0.524498	1.820999
C	3.746642	-1.842198	0.529639
C	4.467823	-0.722847	0.948477
H	5.548355	-0.750717	0.830276
C	3.909385	0.409823	1.556991
C	-1.489217	0.078323	1.645949
C	-1.593589	-1.209715	1.028179
C	-0.369945	-1.757720	0.738343
H	-0.144754	1.450621	2.210738
H	-2.350829	0.676644	1.952904
H	-2.557828	-1.678759	0.839002
H	-0.287785	-2.735978	0.256384
H	4.314995	-2.684238	0.109896
H	4.604404	1.201444	1.877816

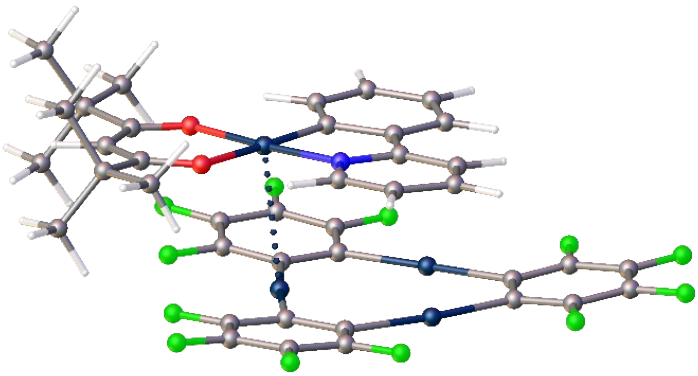
Cartesian coordinate for **S_0 (3·Hg_3)** (in Å)



Hg	27.069712000	11.917767000	10.331552000
Hg	28.772044000	12.292089000	7.171645000
Hg	30.620246000	11.267250000	10.142094000
Pt	26.214333000	9.006452000	9.645968000
F	24.071128000	12.556910000	9.814289000
F	22.663042000	13.148767000	7.588063000
F	23.919783000	13.405676000	5.212935000
F	26.596423000	13.085555000	5.052473000
F	30.732399000	12.062427000	4.777569000
F	33.305997000	11.262104000	4.560359000
F	34.686360000	10.525606000	6.757928000
F	33.507429000	10.575674000	9.185618000
F	31.543757000	10.447928000	13.020014000
F	30.197314000	10.054314000	15.328950000
F	27.538681000	10.524362000	15.445822000
F	26.220210000	11.416202000	13.265706000
O	25.745725000	8.664852000	11.556048000
O	24.234693000	9.449821000	9.193725000
N	26.813637000	9.238988000	7.759053000
C	26.090538000	12.528697000	8.606007000
C	24.717464000	12.700453000	8.659180000
C	23.973351000	13.002951000	7.523108000
C	24.620343000	13.138232000	6.296445000
C	26.002459000	12.974285000	6.238344000
C	26.747806000	12.677360000	7.369614000
C	30.777149000	11.770149000	7.115051000
C	31.401904000	11.721460000	5.877585000
C	32.724072000	11.305045000	5.741252000
C	33.437147000	10.923875000	6.877280000
C	32.811178000	10.965388000	8.121603000
C	31.495812000	11.381319000	8.263059000
C	29.581603000	11.159184000	11.927057000
C	30.240327000	10.711656000	13.061557000
C	29.564458000	10.495099000	14.260696000
C	28.194472000	10.742337000	14.321914000
C	27.533722000	11.199328000	13.186215000
C	28.197630000	11.405056000	11.989738000
C	24.575779000	8.718838000	12.058586000
C	23.409339000	9.098583000	11.384328000
H	22.495959000	9.092508000	11.969823000
C	23.274756000	9.398837000	10.018412000
C	24.469628000	8.258111000	13.518992000
C	23.889587000	9.382359000	14.388020000
H	22.895554000	9.695531000	14.049443000
H	24.547752000	10.255995000	14.380661000
H	23.795933000	9.033414000	15.424191000
C	25.844186000	7.862231000	14.057255000
H	26.299789000	7.073300000	13.449619000
H	25.740252000	7.492550000	15.084397000
H	26.529450000	8.712509000	14.077322000
C	23.547196000	7.028878000	13.567977000
H	23.926484000	6.225019000	12.925225000
H	22.527039000	7.265560000	13.246253000
H	23.496751000	6.646876000	14.595448000
C	21.870641000	9.637146000	9.446165000
C	21.948653000	9.871737000	7.937573000
H	22.421605000	9.026181000	7.426119000
H	22.514193000	10.776772000	7.703842000

H	20.936725000	9.997214000	7.534009000
C	21.011207000	8.391478000	9.711732000
H	21.465112000	7.495726000	9.270273000
H	20.018492000	8.525170000	9.263498000
H	20.872920000	8.205728000	10.782408000
C	21.239121000	10.864268000	10.118633000
H	21.834446000	11.761411000	9.925106000
H	21.152680000	10.738006000	11.203797000
H	20.230722000	11.027466000	9.717535000
C	25.994437000	9.624526000	6.772813000
H	24.968387000	9.830424000	7.073254000
C	26.440547000	9.766205000	5.467193000
H	25.750804000	10.096600000	4.695248000
C	27.784024000	9.513198000	5.189121000
H	28.173536000	9.634105000	4.180012000
C	28.630509000	9.119034000	6.219004000
H	29.683218000	8.927013000	6.030543000
C	28.128477000	8.977310000	7.517228000
C	28.877520000	8.582537000	8.703571000
C	30.246311000	8.275196000	8.716122000
H	30.838661000	8.335380000	7.804308000
C	30.858041000	7.909792000	9.910883000
H	31.922485000	7.683803000	9.930304000
C	30.098105000	7.838944000	11.086320000
H	30.583687000	7.563351000	12.021936000
C	28.739354000	8.145886000	11.078445000
H	28.164143000	8.120589000	12.002407000
C	28.103752000	8.529587000	9.891826000

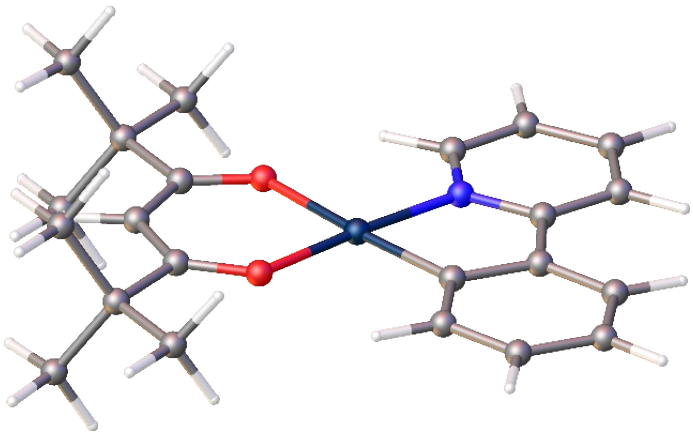
Cartesian coordinate for **T_1 (3·Hg_3)** (in Å)



Hg	27.138294000	11.909366000	10.255866000
Hg	28.760638000	12.347209000	7.059654000
Hg	30.688469000	11.293061000	9.951952000
Pt	26.199836000	8.934705000	9.734928000
F	24.113805000	12.502545000	9.819331000
F	22.650081000	13.110875000	7.632717000
F	23.849441000	13.415294000	5.235094000
F	26.525473000	13.123904000	5.009168000
F	30.702334000	12.306471000	4.626356000
F	33.301699000	11.620817000	4.347805000
F	34.734593000	10.833360000	6.492924000
F	33.582002000	10.724510000	8.933415000
F	31.669776000	10.292093000	12.754097000
F	30.381226000	9.786719000	15.069714000
F	27.732801000	10.290525000	15.289331000
F	26.365225000	11.295419000	13.190567000
O	25.665851000	8.588844000	11.643385000
O	24.240367000	9.383637000	9.229674000
N	26.837380000	9.205993000	7.878207000
C	26.106778000	12.518144000	8.564723000
C	24.732728000	12.669868000	8.651321000
C	23.960664000	12.979136000	7.536307000
C	24.577813000	13.138417000	6.297441000
C	25.959548000	12.989188000	6.205402000
C	26.734271000	12.687422000	7.315635000
C	30.783135000	11.905459000	6.945997000
C	31.394898000	11.939405000	5.701830000
C	32.731434000	11.583332000	5.534237000
C	33.472054000	11.176197000	6.643135000
C	32.859168000	11.133507000	7.893911000
C	31.530678000	11.492586000	8.066654000
C	29.690419000	11.087076000	11.752637000
C	30.371623000	10.569797000	12.843256000
C	29.724958000	10.295590000	14.046543000
C	28.360632000	10.555041000	14.158977000
C	27.674224000	11.073276000	13.065972000
C	28.309593000	11.336940000	11.864518000
C	24.490590000	8.686145000	12.117263000
C	23.348767000	9.079856000	11.404029000
H	22.420885000	9.108140000	11.965233000
C	23.256503000	9.357317000	10.032393000
C	24.342616000	8.288629000	13.591389000
C	23.869112000	9.503774000	14.402447000
H	22.910084000	9.891080000	14.040066000
H	24.606988000	10.310142000	14.355983000
H	23.741133000	9.216200000	15.453673000
C	25.678321000	7.796821000	14.148584000
H	26.057451000	6.941594000	13.578459000
H	25.544015000	7.483606000	15.190852000
H	26.438981000	8.580758000	14.132756000
C	23.313420000	7.152416000	13.698491000
H	23.611073000	6.289665000	13.090098000
H	22.314406000	7.464819000	13.375549000
H	23.239418000	6.822133000	14.742170000
C	21.872405000	9.604309000	9.418819000
C	21.993164000	9.831802000	7.912017000
H	22.492220000	8.991539000	7.417590000
H	22.550888000	10.745159000	7.693380000
H	20.991889000	9.942728000	7.478823000
C	20.997489000	8.365621000	9.667877000

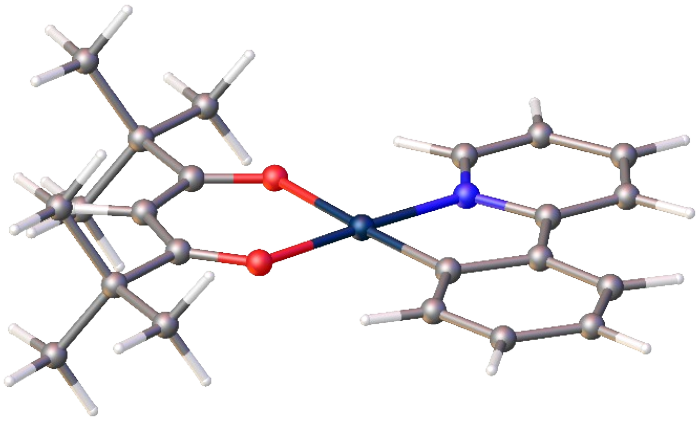
H	21.454639000	7.465550000	9.238735000
H	20.016846000	8.505923000	9.195952000
H	20.833211000	8.183633000	10.735571000
C	21.232111000	10.840374000	10.066646000
H	21.844447000	11.729933000	9.891756000
H	21.102948000	10.718543000	11.148028000
H	20.241646000	11.014201000	9.627384000
C	26.068597000	9.570354000	6.850386000
H	25.018257000	9.733959000	7.086984000
C	26.574040000	9.751740000	5.571803000
H	25.906947000	10.065028000	4.773859000
C	27.967410000	9.567637000	5.343996000
H	28.391404000	9.722664000	4.354427000
C	28.769262000	9.191395000	6.394179000
H	29.837696000	9.046889000	6.252888000
C	28.217937000	8.998627000	7.691746000
C	28.889588000	8.580873000	8.853611000
C	30.278784000	8.282868000	8.969796000
H	30.940455000	8.388182000	8.112450000
C	30.777397000	7.841085000	10.174720000
H	31.839267000	7.610081000	10.254221000
C	29.947018000	7.682811000	11.329892000
H	30.391542000	7.347232000	12.264288000
C	28.601484000	7.990120000	11.254841000
H	27.961569000	7.912344000	12.131664000
C	28.032069000	8.445471000	10.052257000

Cartesian coordinate for **S_0 (3)** (in Å)



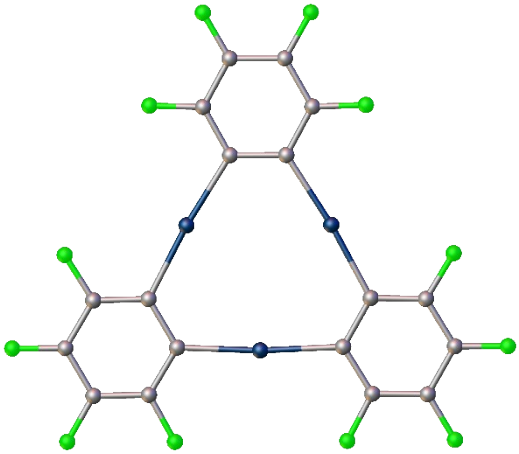
Pt	0.011726000	-0.016947000	-0.165698000
O	-1.979055000	-0.190466000	-0.216169000
O	-0.140275000	2.053811000	-0.404293000
N	1.998310000	0.005917000	-0.095887000
C	-2.815268000	0.757452000	-0.345916000
C	-2.506210000	2.116927000	-0.483814000
H	-3.347955000	2.794654000	-0.584508000
C	-1.224996000	2.694093000	-0.510208000
C	-4.289775000	0.328652000	-0.346911000
C	-5.013119000	1.010440000	0.823466000
H	-5.002855000	2.102454000	0.733594000
H	-4.547243000	0.746204000	1.780531000
H	-6.060841000	0.684777000	0.854248000
C	-4.398351000	-1.187860000	-0.189151000
H	-3.889402000	-1.710736000	-1.005923000
H	-5.454878000	-1.482755000	-0.193212000
H	-3.948630000	-1.523713000	0.751310000
C	-4.936040000	0.744592000	-1.676175000
H	-4.415050000	0.287967000	-2.526400000
H	-4.924088000	1.831072000	-1.817789000
H	-5.982141000	0.413311000	-1.701261000
C	-1.103582000	4.215812000	-0.682027000
C	0.368464000	4.626535000	-0.679870000
H	0.916628000	4.143299000	-1.496131000
H	0.856247000	4.351907000	0.261996000
H	0.449427000	5.713190000	-0.805736000
C	-1.739555000	4.625005000	-2.018241000
H	-1.253558000	4.114063000	-2.858336000
H	-1.629911000	5.706764000	-2.168992000
H	-2.808500000	4.387212000	-2.053931000
C	-1.825056000	4.916327000	0.478029000
H	-1.402171000	4.614951000	1.444130000
H	-2.896225000	4.686604000	0.494154000
H	-1.715808000	6.004482000	0.383686000
C	2.721958000	1.128921000	-0.192652000
H	2.144473000	2.043493000	-0.315108000
C	4.107026000	1.114952000	-0.139022000
H	4.659108000	2.047690000	-0.221226000
C	4.755801000	-0.110862000	0.020807000
H	5.842424000	-0.159702000	0.067333000
C	4.000639000	-1.270727000	0.120444000
H	4.481729000	-2.237195000	0.245676000
C	2.604799000	-1.204015000	0.060517000
C	1.673120000	-2.318664000	0.149007000
C	2.047773000	-3.659196000	0.309664000
H	3.098934000	-3.938520000	0.378412000
C	1.070315000	-4.643905000	0.382046000
H	1.353844000	-5.687523000	0.506745000
C	-0.279738000	-4.284828000	0.293507000
H	-1.045859000	-5.058172000	0.350227000
C	-0.656547000	-2.952756000	0.133770000
H	-1.709431000	-2.684620000	0.065843000
C	0.309059000	-1.941547000	0.058021000

Cartesian coordinate for **T_1 (3)** (in Å)



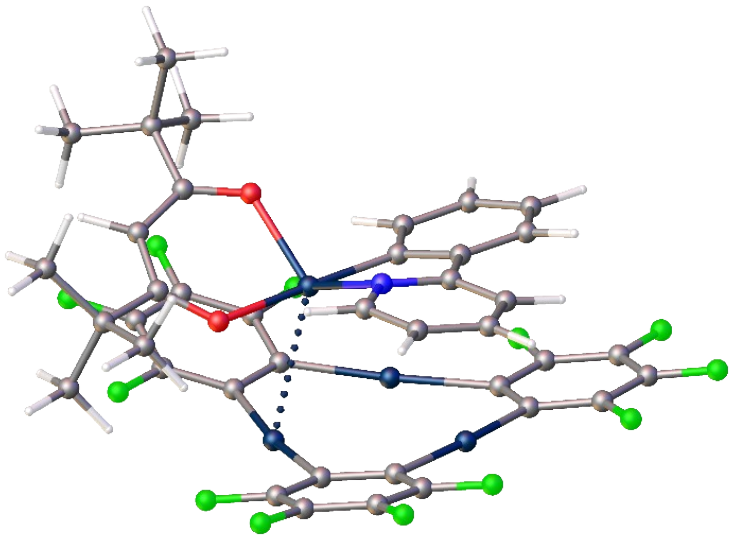
Pt	0.018848000	-0.027673000	-0.164005000
O	-1.990896000	-0.200758000	-0.212988000
O	-0.141957000	2.039714000	-0.403202000
N	1.993186000	0.032557000	-0.101781000
C	-2.823324000	0.746739000	-0.344764000
C	-2.509660000	2.107495000	-0.484647000
H	-3.349195000	2.787411000	-0.586835000
C	-1.229169000	2.680961000	-0.509836000
C	-4.299207000	0.324744000	-0.346943000
C	-5.020667000	1.013454000	0.820661000
H	-5.005404000	2.105140000	0.728428000
H	-4.558350000	0.749249000	1.779455000
H	-6.069865000	0.692788000	0.849965000
C	-4.415297000	-1.190720000	-0.185549000
H	-3.908893000	-1.718313000	-1.000946000
H	-5.473121000	-1.480439000	-0.189955000
H	-3.968951000	-1.526365000	0.756665000
C	-4.940191000	0.741099000	-1.678814000
H	-4.420062000	0.279964000	-2.527114000
H	-4.923077000	1.827108000	-1.822907000
H	-5.987656000	0.414584000	-1.704841000
C	-1.103151000	4.201738000	-0.680318000
C	0.370099000	4.608335000	-0.682344000
H	0.915034000	4.124735000	-1.500424000
H	0.860608000	4.331439000	0.257279000
H	0.452821000	5.694844000	-0.807369000
C	-1.743048000	4.614800000	-2.013615000
H	-1.262751000	4.103089000	-2.856463000
H	-1.628072000	5.696072000	-2.162888000
H	-2.813492000	4.383233000	-2.045479000
C	-1.819215000	4.901350000	0.483956000
H	-1.393028000	4.597862000	1.447902000
H	-2.890957000	4.674438000	0.503684000
H	-1.707199000	5.989193000	0.390670000
C	2.730888000	1.141960000	-0.199764000
H	2.168283000	2.065891000	-0.322930000
C	4.114827000	1.123789000	-0.148534000
H	4.664015000	2.057539000	-0.233611000
C	4.786619000	-0.123041000	0.015252000
H	5.872909000	-0.161955000	0.058642000
C	4.042116000	-1.268373000	0.117085000
H	4.525146000	-2.234890000	0.242989000
C	2.621434000	-1.218544000	0.060765000
C	1.725347000	-2.291538000	0.149376000
C	2.064362000	-3.667006000	0.315222000
H	3.106330000	-3.973422000	0.386216000
C	1.066886000	-4.606083000	0.384891000
H	1.333082000	-5.655373000	0.511541000
C	-0.319387000	-4.251443000	0.296127000
H	-1.076224000	-5.030916000	0.356311000
C	-0.679720000	-2.924350000	0.135216000
H	-1.727223000	-2.637045000	0.065969000
C	0.295258000	-1.916250000	0.057177000

Cartesian coordinate for **Hg_3** (in Å)



Hg	4.44247609856471	2.91426727021404	17.39861939847381
Hg	7.39913335512269	3.11001514712106	15.31629987332506
Hg	4.27717073154918	1.91813488510874	13.92046532054159
F	5.29390178351241	3.87534395491264	20.25520163658952
F	7.62158786048194	4.74536078129470	21.28273373006563
F	9.82312518306212	4.90408885731571	19.72555804719984
F	9.70627423654452	4.19285271254225	17.13585109647597
F	9.50484062171279	3.02616343719421	13.00095777457367
F	9.37605347068481	2.25961161681278	10.42705572938257
F	7.05325571676778	1.34654635678709	9.39263625103142
F	4.84946860183512	1.20349444932940	10.92667189683506
F	1.32088829399984	1.03926419355350	13.37938478742123
F	-0.87339173274703	0.92330327041966	14.92748409371766
F	-0.75056288174247	1.66711491992267	17.52281589679065
F	1.56579368797209	2.53111145792558	18.57647570807645
C	6.26919414651740	3.57012585499521	18.12800970071825
C	6.36558224906317	3.94189532434910	19.45350597629465
C	7.55279136612717	4.39296663568315	20.00759772599866
C	8.68119828883817	4.47426090740178	19.20948747379725
C	8.59400477799582	4.10200633523835	17.87769927666344
C	7.41582700357720	3.65191051234203	17.31734180091778
C	7.22506547348928	2.51842282318144	13.33700334255787
C	8.33605696759774	2.58010863907100	12.52089231853994
C	8.29642259292433	2.19100114684439	11.19171619886956
C	7.10582340286226	1.72371998177768	10.66139113031275
C	5.98481414000781	1.65976352616275	11.47324048351516
C	6.01497207391740	2.04634720078176	12.79760603251202
C	2.62484690505617	1.85259058486335	15.17066243154541
C	1.41884603027019	1.41583849081078	14.66174575847289
C	0.27323991582608	1.34697058364031	15.43808679366777
C	0.33601282984399	1.72825640189548	16.76754231344680
C	1.54267432549481	2.16919690749786	17.28660096720411
C	2.68871248327042	2.24034483300951	16.52125903446525

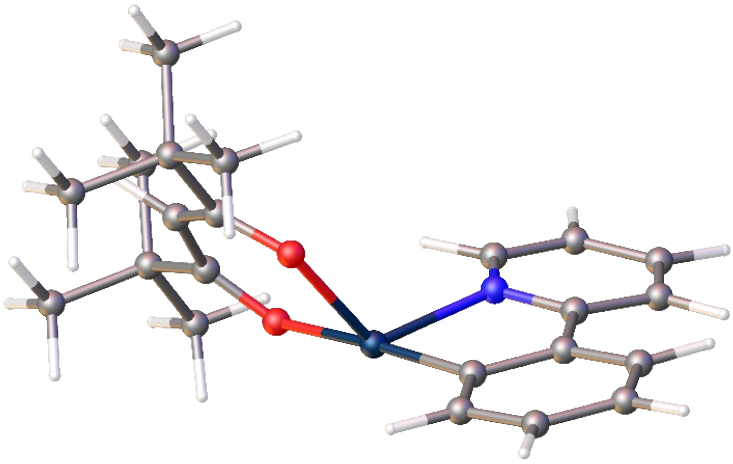
Cartesian coordinate for **MC (3·Hg_3)** (in Å)



Hg	26.486175000	12.110328000	10.018046000
Hg	28.876101000	11.662039000	7.340859000
Hg	29.864577000	11.124716000	10.766553000
Pt	26.591471000	9.115079000	9.638612000
F	23.784506000	12.945685000	8.670407000
F	22.935997000	12.879323000	6.124077000
F	24.676812000	12.367341000	4.117031000
F	27.281051000	11.942716000	4.661202000
F	31.338207000	10.944149000	5.564262000
F	33.862604000	10.168150000	6.150208000
F	34.640697000	9.915886000	8.720476000
F	32.903637000	10.421433000	10.724416000
F	29.835549000	9.959489000	13.665634000
F	27.841193000	9.478113000	15.419329000
F	25.336383000	10.328461000	14.902628000
F	24.802148000	11.659628000	12.615090000
O	26.151119000	7.616045000	11.051067000
O	24.579117000	9.775855000	9.783301000
N	26.513415000	8.663873000	7.517593000
C	25.993664000	12.427611000	8.024426000
C	24.670325000	12.692654000	7.709936000
C	24.209415000	12.677011000	6.395722000
C	25.106943000	12.418557000	5.363162000
C	26.445734000	12.188163000	5.668921000
C	26.903222000	12.175601000	6.977080000
C	30.810226000	11.144769000	7.852362000
C	31.712017000	10.853419000	6.840557000
C	33.012870000	10.444530000	7.119344000
C	33.414900000	10.315290000	8.447663000
C	32.506610000	10.593014000	9.466398000
C	31.212350000	11.008014000	9.194116000
C	28.364991000	11.080833000	12.205394000
C	28.615138000	10.416328000	13.394965000
C	27.600717000	10.159944000	14.315914000
C	26.306640000	10.595139000	14.047305000
C	26.051073000	11.272428000	12.858462000
C	27.051171000	11.512931000	11.928186000
C	25.151464000	7.668595000	11.834224000
C	23.993808000	8.436954000	11.651949000
H	23.195907000	8.268498000	12.361709000
C	23.719819000	9.334854000	10.604699000
C	25.250525000	6.688467000	13.014999000
C	24.291338000	7.031484000	14.155661000
H	23.240196000	6.895630000	13.875360000
H	24.433073000	8.062415000	14.499357000
H	24.486920000	6.363549000	15.003458000
C	26.686394000	6.691662000	13.553649000
H	27.407360000	6.507015000	12.751986000
H	26.794625000	5.904431000	14.309548000
H	26.936968000	7.643632000	14.033056000
C	24.922041000	5.298038000	12.447687000
H	25.622014000	5.032022000	11.647669000
H	23.903580000	5.266938000	12.040991000
H	24.997004000	4.542776000	13.240224000
C	22.293602000	9.870884000	10.409223000
C	22.030218000	10.023069000	8.905583000
H	22.127505000	9.061197000	8.385448000
H	22.719569000	10.739528000	8.453421000
H	21.008781000	10.388888000	8.746198000
C	21.233054000	8.943293000	11.008560000

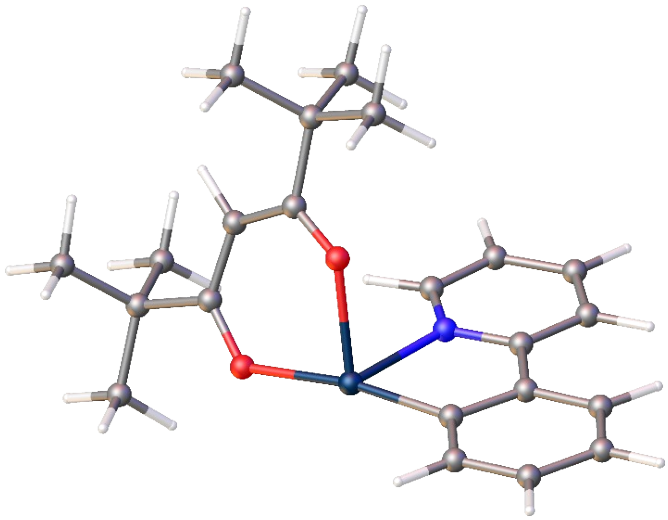
H	21.328130000	7.918162000	10.630246000
H	20.235974000	9.312607000	10.739538000
H	21.278057000	8.911839000	12.103195000
C	22.201384000	11.248165000	11.083442000
H	22.899941000	11.953055000	10.624804000
H	22.425069000	11.184303000	12.153347000
H	21.185869000	11.646826000	10.963815000
C	25.474966000	8.969101000	6.737156000
H	24.522368000	9.112578000	7.245684000
C	25.614182000	9.120806000	5.364176000
H	24.752444000	9.380062000	4.753812000
C	26.881555000	8.956558000	4.803421000
H	27.033919000	9.094999000	3.735231000
C	27.959673000	8.658494000	5.628989000
H	28.962464000	8.568123000	5.218315000
C	27.758932000	8.508349000	7.006062000
C	28.807979000	8.247279000	7.998047000
C	30.084935000	7.776808000	7.661627000
H	30.353481000	7.606310000	6.619766000
C	31.012613000	7.499951000	8.659156000
H	32.004819000	7.138943000	8.395144000
C	30.655729000	7.660504000	10.000941000
H	31.372762000	7.422301000	10.785758000
C	29.391326000	8.142184000	10.341819000
H	29.122353000	8.251112000	11.392646000
C	28.460017000	8.484880000	9.350464000

Cartesian coordinate for ^{3}**MC (3)** (in Å)



Pt	-0.175653000	-0.264334000	-0.385832000
O	-2.113858000	-0.315035000	0.531546000
O	-0.444063000	1.816556000	-0.604214000
N	1.614670000	-0.182801000	0.853722000
C	-2.864257000	0.682680000	0.731571000
C	-2.571843000	2.021527000	0.426800000
H	-3.332530000	2.750861000	0.686261000
C	-1.421307000	2.513951000	-0.212017000
C	-4.229950000	0.357093000	1.366472000
C	-4.344181000	1.088412000	2.711204000
H	-4.305199000	2.177237000	2.593859000
H	-3.534779000	0.792349000	3.389610000
H	-5.298132000	0.835369000	3.191749000
C	-4.350666000	-1.148722000	1.599749000
H	-4.269418000	-1.705089000	0.660142000
H	-5.322530000	-1.373637000	2.056240000
H	-3.559406000	-1.514296000	2.262241000
C	-5.349094000	0.815271000	0.421475000
H	-5.262832000	0.325664000	-0.556198000
H	-5.333767000	1.898632000	0.257946000
H	-6.326287000	0.552334000	0.846802000
C	-1.323465000	4.024649000	-0.485142000
C	0.021678000	4.350819000	-1.133105000
H	0.155233000	3.803097000	-2.071338000
H	0.857043000	4.082205000	-0.476870000
H	0.080247000	5.426060000	-1.342392000
C	-2.455770000	4.431831000	-1.439143000
H	-2.393471000	3.875160000	-2.382070000
H	-2.383053000	5.502224000	-1.671575000
H	-3.444296000	4.247004000	-1.003939000
C	-1.449482000	4.795933000	0.835658000
H	-0.670998000	4.492115000	1.546613000
H	-2.421293000	4.637789000	1.316093000
H	-1.337425000	5.872208000	0.651359000
C	2.219986000	0.939107000	1.242294000
H	1.653526000	1.858935000	1.097216000
C	3.494356000	0.930474000	1.791045000
H	3.962346000	1.860176000	2.105500000
C	4.141123000	-0.300497000	1.926010000
H	5.144303000	-0.352189000	2.346233000
C	3.502698000	-1.460682000	1.508793000
H	4.002565000	-2.422452000	1.587618000
C	2.212950000	-1.389533000	0.964040000
C	1.436016000	-2.523664000	0.454981000
C	1.820218000	-3.856968000	0.660204000
H	2.717560000	-4.093500000	1.231114000
C	1.044756000	-4.892889000	0.155182000
H	1.341469000	-5.927417000	0.319318000
C	-0.122680000	-4.596757000	-0.554828000
H	-0.734774000	-5.406802000	-0.951122000
C	-0.509614000	-3.273528000	-0.758558000
H	-1.425324000	-3.063192000	-1.309929000
C	0.258210000	-2.208379000	-0.269670000

Cartesian coordinate for **MECP (3)** (in Å)



Pt	-0.140703000	-0.252676000	-1.034764000
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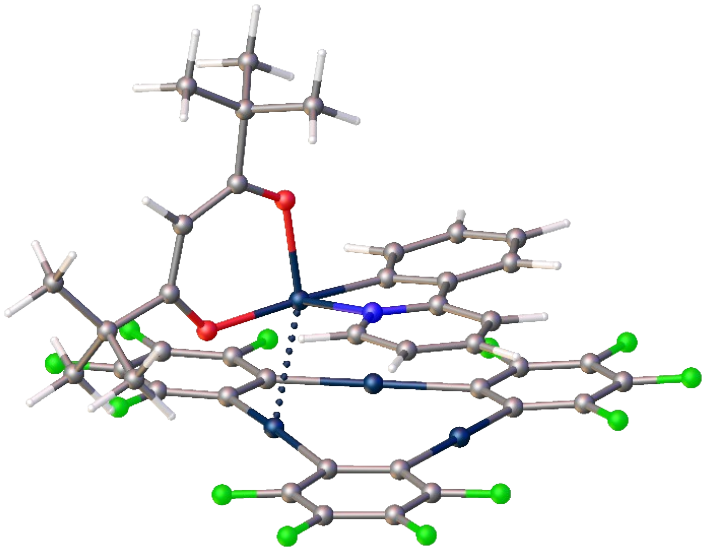
O	-0.584147000	1.788148000	-1.371453000
N	0.816360000	-0.257081000	0.932108000
C	-2.463609000	0.717511000	0.670446000
C	-2.239212000	2.053763000	0.304221000
H	-2.830481000	2.803423000	0.820074000
C	-1.375659000	2.511748000	-0.709357000
C	-3.478831000	0.418280000	1.788098000
C	-2.935873000	1.019950000	3.093121000
H	-2.840965000	2.110256000	3.031915000
H	-1.948309000	0.606268000	3.333690000
H	-3.613172000	0.784006000	3.924191000
C	-3.637830000	-1.092567000	1.957045000
H	-4.004090000	-1.559584000	1.036637000
H	-4.353650000	-1.299476000	2.762120000
H	-2.683633000	-1.568443000	2.204614000
C	-4.839604000	1.037130000	1.446427000
H	-5.219686000	0.649167000	0.493663000
H	-4.793654000	2.129171000	1.370994000
H	-5.567815000	0.786923000	2.228501000
C	-1.363274000	4.012545000	-1.042210000
C	-0.402246000	4.278804000	-2.199925000
H	-0.701130000	3.728648000	-3.098286000
H	0.617239000	3.965875000	-1.952068000
H	-0.392797000	5.350642000	-2.433457000
C	-2.774599000	4.467054000	-1.437557000
H	-3.141091000	3.900881000	-2.302368000
H	-2.761553000	5.530329000	-1.709693000
H	-3.494812000	4.337812000	-0.621958000
C	-0.891532000	4.787252000	0.197268000
H	0.111988000	4.465173000	0.503554000
H	-1.567090000	4.652447000	1.049770000
H	-0.843710000	5.860448000	-0.028198000
C	0.908940000	0.794151000	1.741476000
H	0.437966000	1.713737000	1.393636000
C	1.552254000	0.716901000	2.969462000
H	1.603763000	1.587781000	3.618236000
C	2.118685000	-0.506925000	3.332205000
H	2.638028000	-0.612361000	4.283507000
C	2.019072000	-1.592435000	2.473529000
H	2.461663000	-2.546969000	2.744257000
C	1.343037000	-1.455345000	1.251172000
C	1.148986000	-2.518282000	0.257858000
C	1.593568000	-3.831297000	0.470989000
H	2.103252000	-4.102809000	1.394529000
C	1.379407000	-4.807825000	-0.493468000
H	1.723180000	-5.826920000	-0.324700000
C	0.719036000	-4.470808000	-1.677764000
H	0.550599000	-5.231971000	-2.439394000
C	0.278999000	-3.165842000	-1.894373000
H	-0.225016000	-2.923663000	-2.828621000
C	0.478485000	-2.158884000	-0.939303000

Cartesian coordinate for **MECP (3·Hg_3)** (in Å)



Hg	26.968895000	12.208274000	10.138347000
Hg	29.297073000	11.303450000	7.539731000
Hg	30.501397000	12.015555000	10.860885000
Pt	26.412037000	9.307201000	10.095696000
F	24.166512000	12.614325000	8.709991000
F	23.296115000	12.115665000	6.220125000
F	25.020886000	11.277971000	4.312252000
F	27.628319000	10.964584000	4.887845000
F	31.772329000	10.328096000	5.870794000
F	34.374121000	10.004517000	6.468470000
F	35.295315000	10.626416000	8.930588000
F	33.612459000	11.553026000	10.814060000
F	30.850184000	12.684788000	13.906512000
F	29.106725000	13.308514000	15.860455000
F	26.464802000	13.473593000	15.322751000
F	25.552441000	13.019984000	12.835423000
O	25.852773000	7.392061000	10.752535000
O	24.489585000	9.998689000	10.543898000
N	26.157515000	8.506034000	8.110425000
C	26.376563000	11.995764000	8.140960000
C	25.053877000	12.190238000	7.798660000
C	24.582287000	11.956288000	6.517296000
C	25.464570000	11.532933000	5.539428000
C	26.800403000	11.367572000	5.866161000
C	27.275179000	11.580862000	7.142454000
C	31.304389000	11.136596000	8.041564000
C	32.193534000	10.658284000	7.102654000
C	33.537734000	10.478409000	7.384456000
C	34.009635000	10.794371000	8.646672000
C	33.122790000	11.275712000	9.595760000
C	31.781754000	11.451272000	9.324663000
C	29.110604000	12.519210000	12.316153000
C	29.544697000	12.760536000	13.603723000
C	28.669287000	13.083037000	14.627204000
C	27.315653000	13.167356000	14.350721000
C	26.872071000	12.928428000	13.060235000
C	27.736029000	12.604748000	12.034720000
C	24.670807000	7.069734000	11.087849000
C	23.570236000	7.915604000	11.206031000
H	22.654257000	7.459218000	11.534317000
C	23.526175000	9.294424000	10.960975000
C	24.539107000	5.569517000	11.368841000
C	23.152552000	5.153579000	11.839740000
H	22.386322000	5.357343000	11.088461000
H	22.871308000	5.652156000	12.769922000
H	23.149987000	4.077660000	12.028436000
C	25.567423000	5.199835000	12.440296000
H	26.574094000	5.469184000	12.122244000
H	25.533834000	4.123820000	12.626595000
H	25.354311000	5.713898000	13.380812000
C	24.870790000	4.839488000	10.063748000
H	25.870973000	5.101102000	9.718356000
H	24.154764000	5.095025000	9.278089000
H	24.826734000	3.759599000	10.223932000
C	22.218603000	10.065511000	11.135414000
C	21.673883000	10.320756000	9.724729000
H	21.456535000	9.380060000	9.210994000
H	22.386170000	10.894221000	9.131167000
H	20.744439000	10.892090000	9.786650000
C	21.172862000	9.314885000	11.951053000

H	20.824088000	8.410309000	11.448070000
H	20.303369000	9.960090000	12.094776000
H	21.551450000	9.040204000	12.938115000
C	22.523706000	11.400937000	11.814249000
H	23.245875000	11.977856000	11.239916000
H	22.929776000	11.250199000	12.817199000
H	21.603648000	11.982823000	11.904024000
C	25.011170000	8.504653000	7.441504000
H	24.132252000	8.801967000	8.001513000
C	24.950184000	8.148441000	6.109834000
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C	26.131301000	7.796549000	5.472113000
H	26.127758000	7.531197000	4.421943000
C	27.317774000	7.804495000	6.178018000
H	28.248074000	7.556149000	5.686065000
C	27.317669000	8.165602000	7.522396000
C	28.496007000	8.240710000	8.386658000
C	29.743885000	7.751498000	7.999317000
H	29.884509000	7.314985000	7.017180000
C	30.812079000	7.799513000	8.875837000
H	31.779764000	7.419685000	8.572473000
C	30.634254000	8.331553000	10.145250000
H	31.468882000	8.364399000	10.836736000
C	29.398153000	8.832718000	10.530914000
H	29.275138000	9.235954000	11.530762000
C	28.305246000	8.808314000	9.666151000

References

1. A. Heil and C. M. Marian, *Inorganic Chemistry*, 2019, **58**, 6123-6136.
2. G. S. M. Tong, P. K. Chow, W.-P. To, W.-M. Kwok and C.-M. Che, *Chemistry – A European Journal*, 2014, **20**, 6433-6443.