Electronic Supporting Information

Pure Heterometallic Spodium Bonding

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S1. Crystal data and structure refinement

Table S1. Crystal data and structure refinement for $Ph^F_2Hg{\cdot}Pd(acac)_2$ and $Ph^F_2Hg{\cdot}Pt(acac)_2$

Identification code	$Ph^F_2Hg{\cdot}Pd(acac)_2$	$Ph^F_2Hg{\cdot}Pt(acac)_2$
Empirical formula	$C_{22}H_{14}F_{10}HgO_4Pd$	$C_{22}H_{14}F_{10}HgO_4Pt$
Formula weight	839.32	928.01
Temperature, K	100(2)	100(2)
Crystal size, mm	0.12 × 0.04 × 0.02	0.06 × 0.04 × 0.03
Wavelength, Å	1.54184	1.54184
Crystal system	monoclinic	monoclinic
Space group	I2/m	I2/m
a, Å	11.8573(9)	11.8245(3)
b, Å	6.2066(5)	6.2102(2)
c, Å	15.9257(12)	15.9199(4)
α, deg.	90	90
β, deg.	99.161(7)	99.276(2)
γ, deg.	90	90
V, Å^3	1157.08(16)	1153.75(6)
Z	2	2
Density (calc.), g/cm^3	2.409	2.671
μ, mm^{-1}	19.045	23.988
F(000)	788.0	824.0
2Θ range for data collection, deg.	8.67 to 144.78	8.68 to 159.698
Index ranges	-14 ≤ h ≤ 14, -6 ≤ k ≤ 7, -19 ≤ l ≤ 19	-14 ≤ h ≤ 15, -7 ≤ k ≤ 7, -19 ≤ l ≤ 20
Reflections collected	3301	6349
Independent reflections	1210 [R_{int} = 0.0620, R_{sigma} = 0.0449]	1336 [R_{int} = 0.0545, R_{sigma} = 0.0325]
R_1 / wR_2 ($I > 2\sigma(I)$)	0.0405/0.1134	0.0348/0.0964
R_1 / wR_2 (all data)	0.0408/0.1137	0.0358/0.0981
Goodness-of-fit on F^2	1.189	1.174
Largest diff. peak/hole, e Å^{-3}	0.24/-0.21	2.00/-1.54

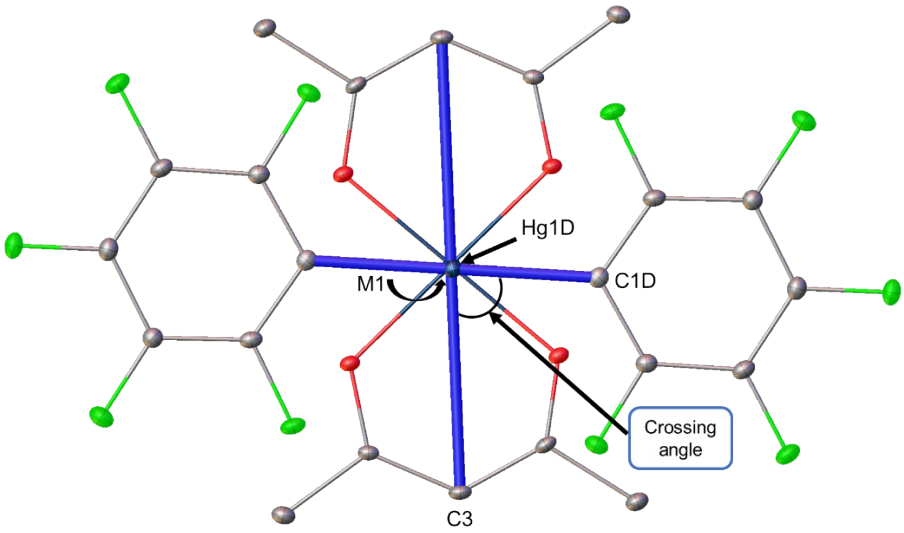


Figure S1. Schematic representation of the crossing angle.

S2. The Cambridge Structural Database (CSD) search for short $Ph^{F}Hg\cdots M$ contacts

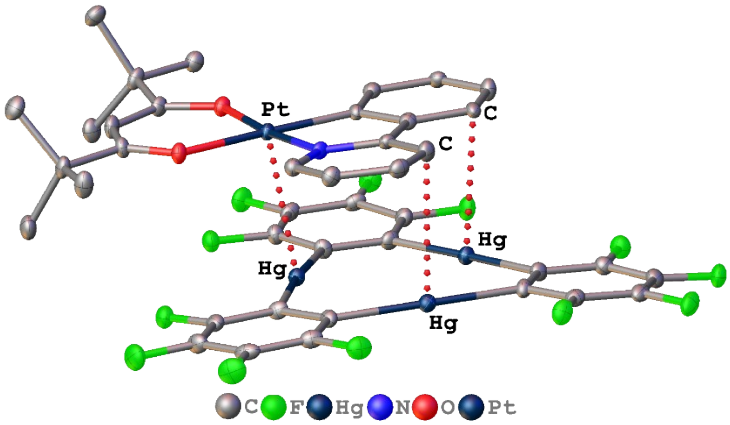


Figure S2. A view of the molecular structure of the cocrystal from ref. 24. The identified SpB contacts are shown by doted lines; H-atoms were omitted for clarity.

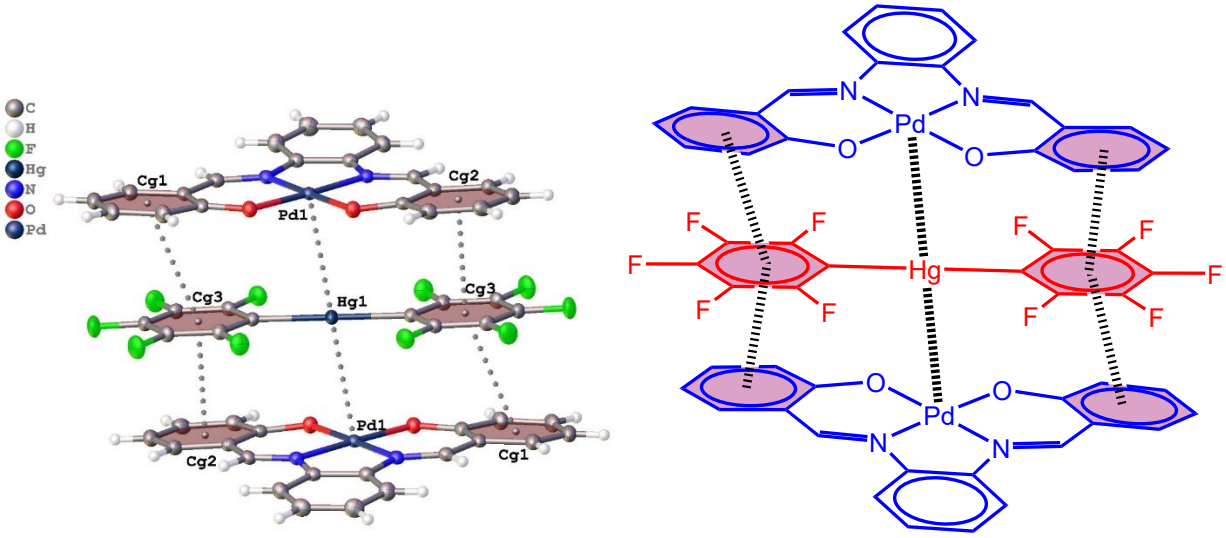
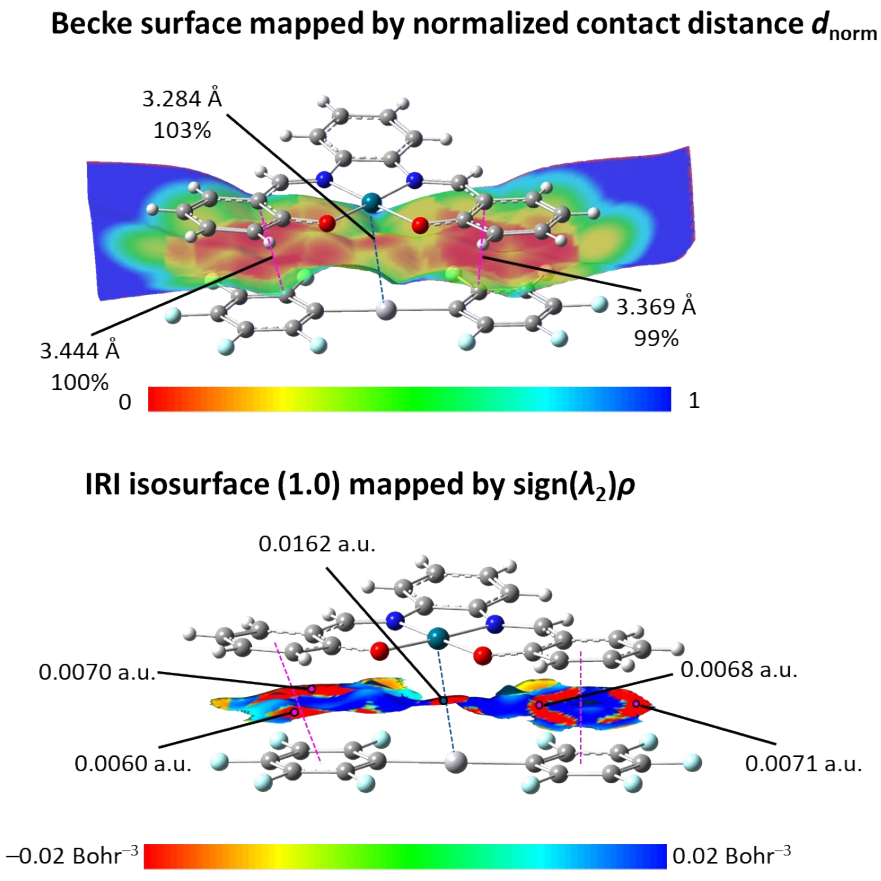


Figure S3. A fragment of the crystal structure of COJBIN (left) and its graphical representation (right) showing structure-determining NCIs (dotted lines).

Table S2. Parameters of short contacts in COJBIN.

Contact	d, Å	R[a], %
Hg1···Pd1	3.2841(2)	103
Cg1···Cg3	3.5675(11)	
Cg2···Cg3	3.4095(11)	

[a]Normalization of the experimentally observed Ch···($ChB_{acceptor}$) distances to the corresponding Bondi $\sum_{vdW}$[1]



	Geometric criteria	Electron density criteria
Pd···Hg	no	yes
π···π	borderline	yes

Figure S4. Theoretical analysis of COJBIN. Top: Becke surface mapped by normalized contact distance $d_{norm} = \frac{d_1 - r^{vdW}_1}{r^{vdW}_1} + \frac{d_2 - r^{vdW}_2}{r^{vdW}_2}$, where d_1 (d_2) is the distance from a point on the surface to the nearest nucleus inside (outside) the surface, r^{vdW}_1 and r^{vdW}_2 denote van der Waals radius of atoms 1 and 2. Interatomic distances for contacts with low d_{norm} values and their percentage of the sum of van der Waals radii are given in black. Middle: IRI isosurface (1.0) mapped by sign(λ_2)ρ, electron density critical points of (3; –1) type and ρ values. Bottom: table summarizing the results of the two-criterion test for non-covalent interactions (see Computational Details section).

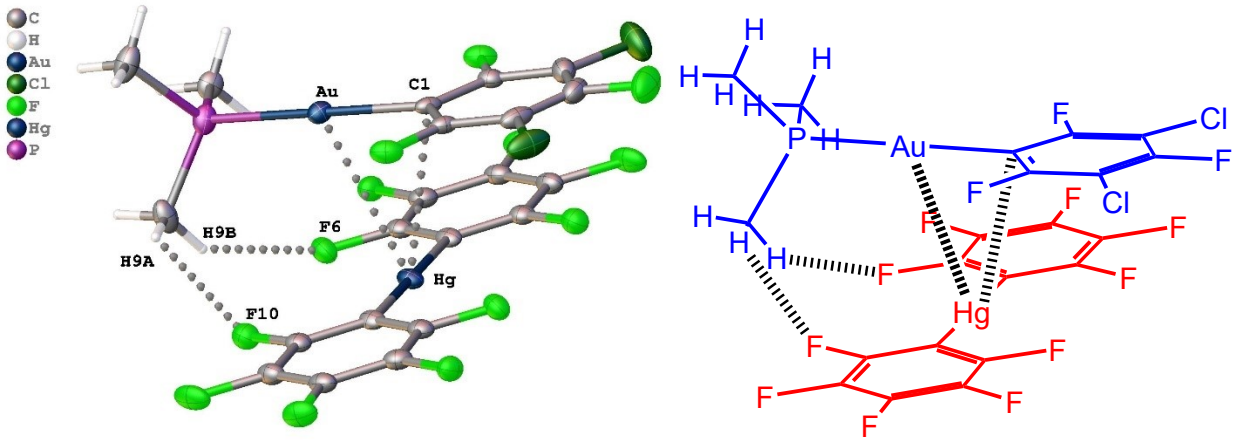
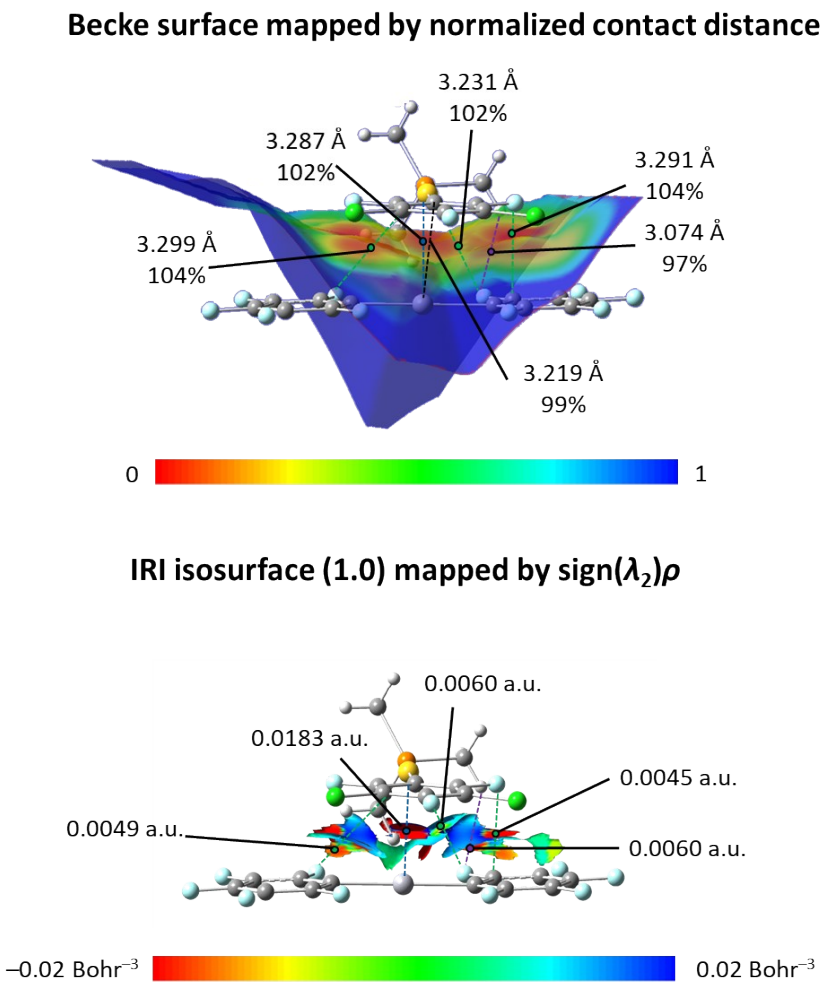


Figure S5. A fragment of the crystal structure of KEWWIU (left) and its graphical representation (right) showing structure-determining NCIs (dotted lines).

Table S3. Parameters of short contacts in KEWWIU.

Contact	d, Å	R[a], %
Hg···Au	3.2865(3)	102
Hg···C1	3.219(6)	99
H9B···F6	2.522(4)	94
H9A···F10	2.578(5)	97

[a]Normalization of the experimentally observed Ch···($ChB_{acceptor}$) distances to the corresponding Bondi $\sum_{vdW}$[1]



	Geometric criteria	Electron density criteria
Au···Hg	no	yes
Hg···C	yes	no
LP(F)···π	no	borderline
CH···F	in part	yes

Figure S6. Theoretical analysis of KEWWIU. Top: Becke surface mapped by normalized contact distance $d_{norm} = \frac{d_1 - r^{vdW}_1}{r^{vdW}_1} + \frac{d_2 - r^{vdW}_2}{r^{vdW}_2}$, where d_1 (d_2) is the distance from a point on the surface to the nearest nucleus inside (outside) the surface, r^{vdW}_1 and r^{vdW}_2 denote van der Waals radius of atoms 1 and 2. Interatomic distances for contacts with low d_{norm} values and their percentage of the sum of van der Waals radii are given in black. Middle: IRI isosurface (1.0) mapped by sign(λ_2)ρ, electron density critical points of (3; –1) type and ρ values. Bottom: table summarizing the results of the two-criterion test for non-covalent interactions (see Computational Details section).

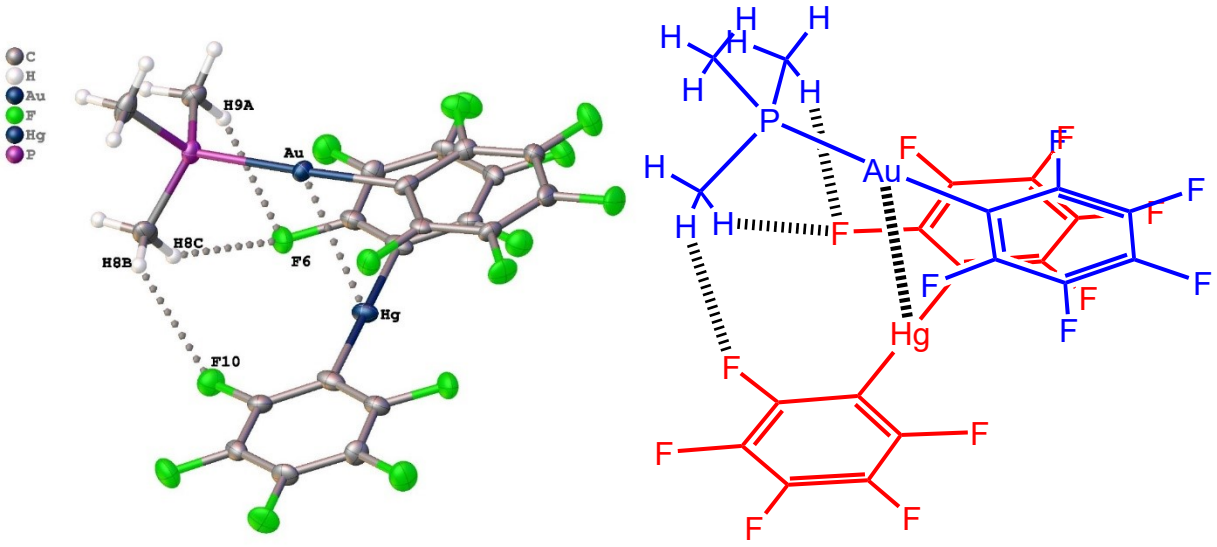
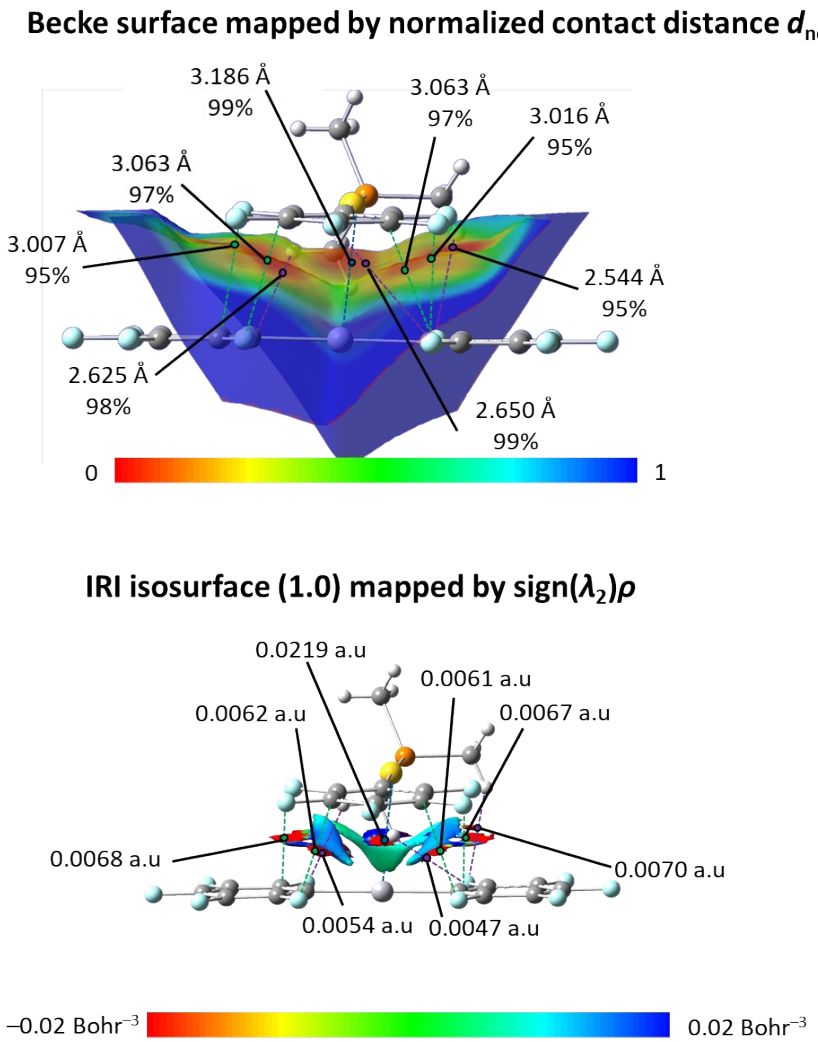


Figure S7. A fragment of the crystal structure of ITEBUF (left) and its graphical representation (right) showing structure-determining NCIs (dotted lines).

Table S4. Parameters of short contacts in ITEBUF.

Contact	d, Å	R[a], %
Hg···Au	3.1860(3)	99
H8C···F6	2.650(3)	99
H9A···F6	2.625(4)	98
H8B···F10	2.544(3)	95

[a]Normalization of the experimentally observed Ch···($ChB_{acceptor}$) distances to the corresponding Bondi $\sum_{vdW}$[1]



	Geometric criteria	Electron density criteria
Au···Hg	yes	yes
LP(F)···π	yes	yes
CH···F	yes	in part

Figure S8. Theoretical analysis of ITEBUF. Top: Becke surface mapped by normalized contact distance $d_{norm} = \frac{d_1 - r^{vdW}_1}{r^{vdW}_1} + \frac{d_2 - r^{vdW}_2}{r^{vdW}_2}$, where d_1 (d_2) is the distance from a point on the surface to the nearest nucleus inside (outside) the surface, r^{vdW}_1 and r^{vdW}_2 denote van der Waals radius of atoms 1 and 2. Interatomic distances for contacts with low d_{norm} values and their percentage of the sum of van der Waals radii are given in black. Middle: IRI isosurface (1.0) mapped by sign(λ_2)ρ, electron density critical points of (3; –1) type and ρ values. Bottom: table summarizing the results of the two-criterion test for non-covalent interactions (see Computational Details section).

S3. Theoretical considerations

To confirm that short Hg···Pt/Pd contacts in the $M(acac)_2(Ph^F{}_2Hg)$ cocrystals are structure-determining, we optimized the geometry of $[M(acac)_2(Ph^F{}_2Hg)]_3$ fragments (at the same level of theory) in vacuum and also checked whether the structures belong to the minimum PES, or not (**Figure S9**).

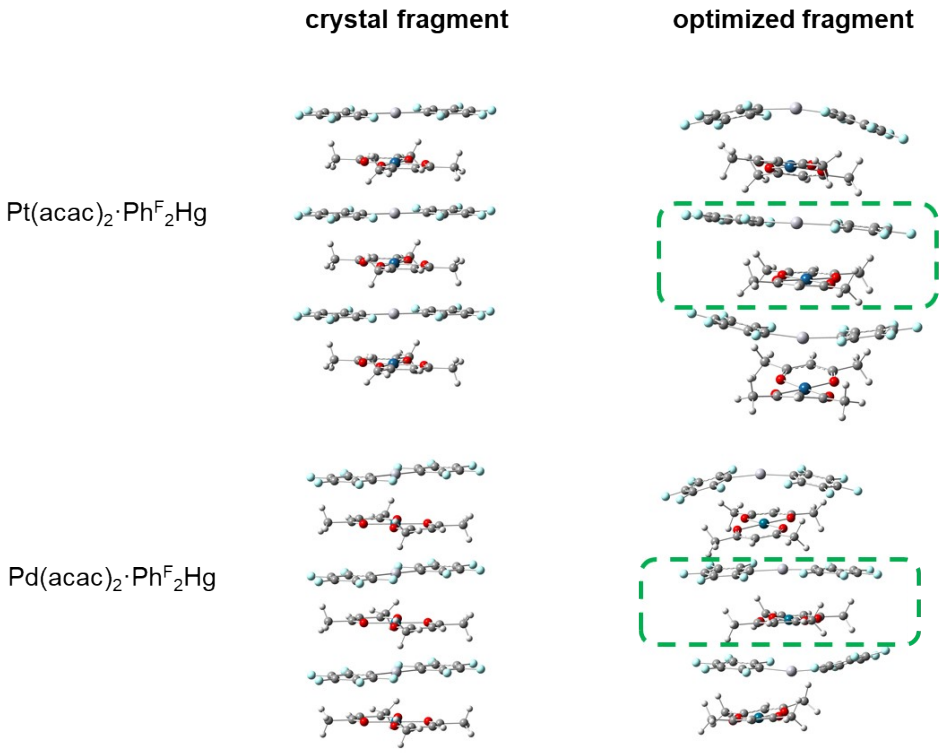


Figure S9. Left row: fragments of $[M(acac)_2(Ph^F{}_2Hg)]_3$ (M = Pt, Pd) from the experimental crystal structures; right row: optimized geometries of $[M(acac)_2(Ph^F{}_2Hg)]_3$. The green dashed line indicates the least deformed $Ph^F{}_2Hg{\cdot}M(acac)_2$ structure in the absence of crystal field, which was used for further theoretical analysis.

Notably, all three Hg···Pt/Pd contacts are preserved despite significant distortion of the terminal fragments during the gas phase optimization.

Table S5. Electron density properties in (3; –1) critical point between Hg and M are given on the right panel: the electron density with sign of second eigenvalue λ_2 sign(λ_2)ρ, Laplacian of electron density $\nabla^2\rho$, local electronic kinetic energy density G, local electronic potential energy density V.

	sign(λ_2)ρ, Bohr^{-3}	**$\nabla^2\rho$, Bohr^{-5}**	***G*, Hartree·Bohr^{-3}**	***V*, Hartree·Bohr^{-3}**
$Ph^F_2Hg{\cdot}Pt(acac)_2$	–0.0198	0.0524	0.0136	–0.0140
$Ph^F_2Hg{\cdot}Pd(acac)_2$	–0.0184	0.0507	0.0129	–0.0131

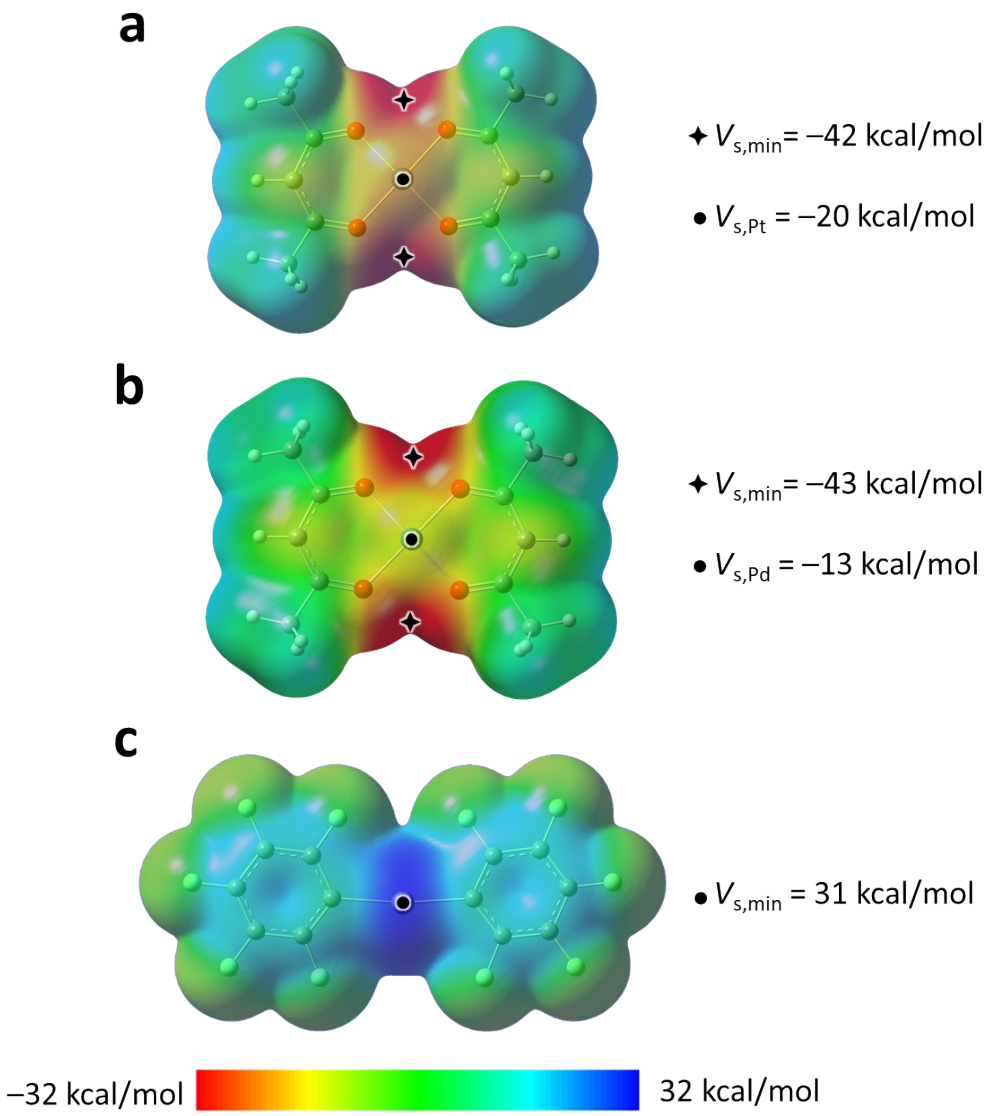


Figure S10. Distribution of MEP on electron density isosurface (0.001 a.u.) for (a) $Pt(acac)_2$, (b) $Pd(acac)_2$, and (c) $Ph^F{}_2Hg$. The values of the potential on the surface above any one of the metal atoms are shown.

In the structures of $Ph^F_2Hg{\cdot}Pt(acac)_2$ and $Ph^F_2Hg{\cdot}Pd(acac)_2$, hydrogens of the methyl group are disordered in two equilibrium positions (1 and 2) with an occupancy of 0.5. Hydrogen bonds were found in one of these two configurations (position 2). To estimate the contribution of these interactions to the total energy, the corresponding theoretical calculations were carried out. Considering the disorder of hydrogens of the CH_3 groups of the $Ph^F_2Hg{\cdot}Pt(acac)_2$ and $Ph^F_2Hg{\cdot}Pd(acac)_2$ complexes, we performed a two criteria test for the structures $Ph^F_2Hg{\cdot}Pt(acac)_2$ and $Ph^F_2Hg{\cdot}Pd(acac)_2$. Our analysis revealed that short contacts (hydrogen bonds CH···F) are easily cleaved by the thermal motion (**Figures S11** and **S12, Table S6**). It is clear from the latter that these interactions are quite weak, their energy value do not exceed 0.1 kcal and, consequently, they are far from being structure-determining.

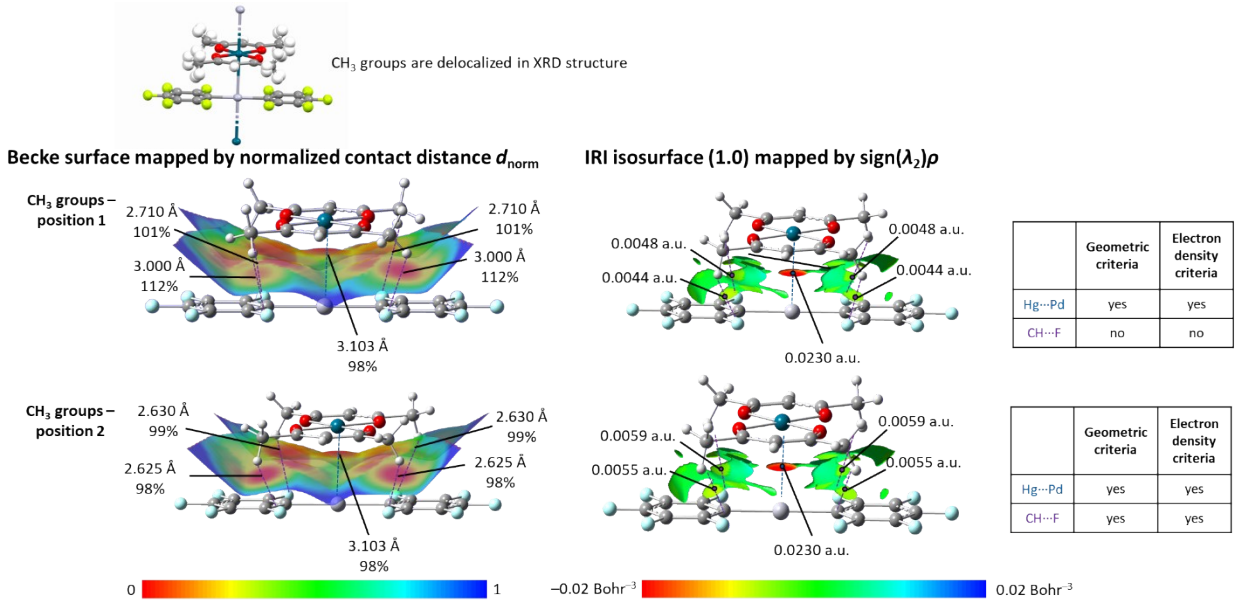


Figure S11. Theoretical analysis of $Ph^F_2Hg{\cdot}Pd(acac)_2$ with two types of the CH_3 group localization. Left: Becke surface mapped by normalized contact distance $d_{norm} = \frac{d_1 - r^{vdW}_1}{r^{vdW}_1} + \frac{d_2 - r^{vdW}_2}{r^{vdW}_2}$, where d_1 (d_2) is the distance from a point on the surface to the nearest nucleus inside (outside) the surface, r^{vdW}_1 and r^{vdW}_2 denote van der Waals radius of atoms 1 and 2. Interatomic distances for contacts with low d_{norm} values and their percentage of the sum of van der Waals radii are given in black. Middle: IRI isosurface (1.0) mapped by sign(λ_2)ρ, electron density critical points of (3; –1) type and ρ values. Right: table summarizing the results of the two-criterion test for non-covalent interactions (see Computational Details section).

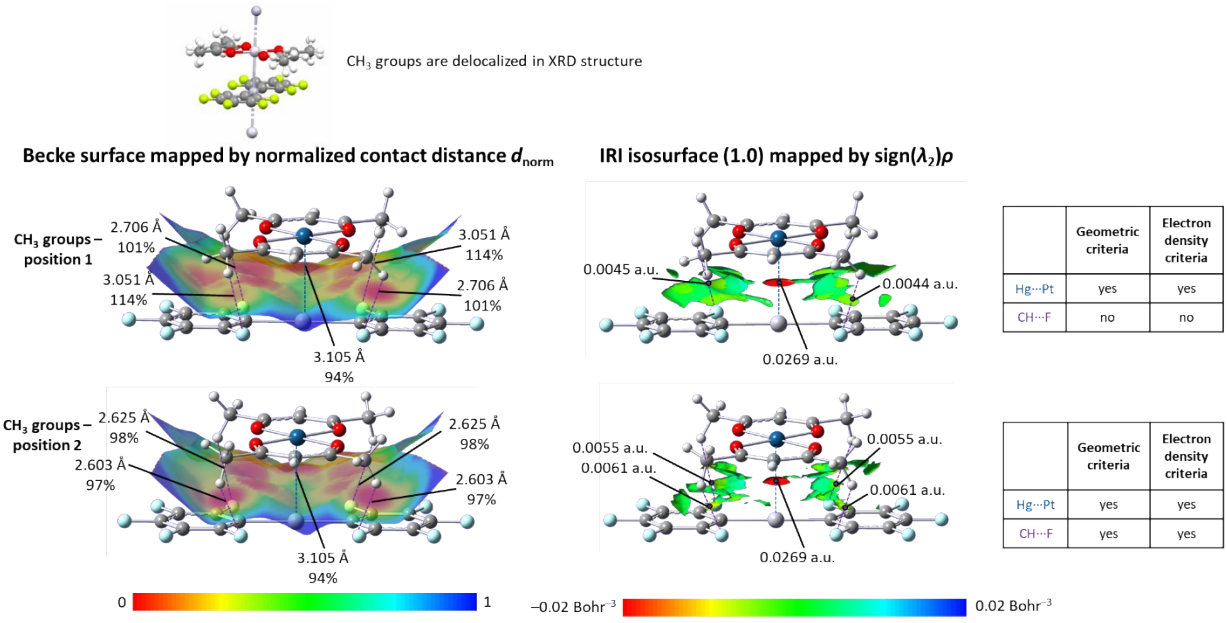


Figure S12. Theoretical analysis of $Ph^F_2Hg{\cdot}Pt(acac)_2$ with two types of the CH_3 group localization. Left: Becke surface mapped by normalized contact distance $d_{norm} = \frac{d_1 - r^{vdW}_1}{r^{vdW}_1} + \frac{d_2 - r^{vdW}_2}{r^{vdW}_2}$, where d_1 (d_2) is the distance from a point on the surface to the nearest nucleus inside (outside) the surface, r^{vdW}_1 and r^{vdW}_2 denote van der Waals radius of atoms 1 and 2. Interatomic distances for contacts with low d_{norm} values and their percentage of the sum of van der Waals radii are given in black. Middle: IRI isosurface (1.0) mapped by sign(λ_2)ρ, electron density critical points of (3; –1) type and ρ values. Right: table summarizing the results of the two-criterion test for non-covalent interactions (see Computational Details section).

Table S6. Decomposition of the interaction energy (SAPT0) between Ph^F_2Hg and $M(acac)_2$ and fragments in the cocrystals.

	E_{ES}, kcal/mol	E_{EX}, kcal/mol	E_{IND}, kcal/mol	E_{DISP}, kcal/mol	E_{TOT}, kcal/mol
$Ph^F_2Hg{\cdot}Pt(acac)_2$ CH_3 – position 1	–15.4	23.7	–5.5	–20.2	–17.2
$Ph^F_2Hg{\cdot}Pt(acac)_2$ CH_3 – position 2	–14.7	23.2	–5.4	–20.1	–17.1
$Ph^F_2Hg{\cdot}Pd(acac)_2$ CH_3 – position 1	–9.7	18.6	–3.8	–17.8	–12.6
$Ph^F_2Hg{\cdot}Pd(acac)_2$ CH_3 – position 2	–10.1	19.2	–3.8	–17.9	–12.6

A partially dispersive nature of the Hg···Pt/Pd contacts is also shown through visualization of the van der Waals potential:[2] the dispersion contribution prevails over the exchange-repulsive contribution in the region above the metal atom.

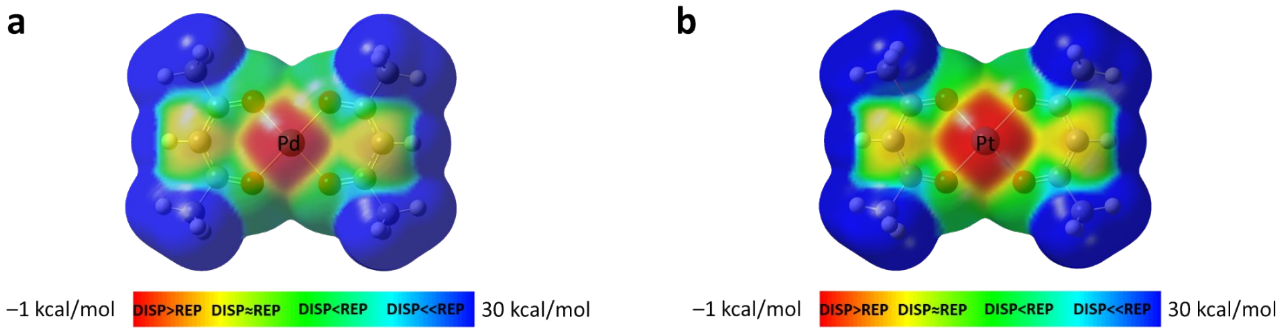
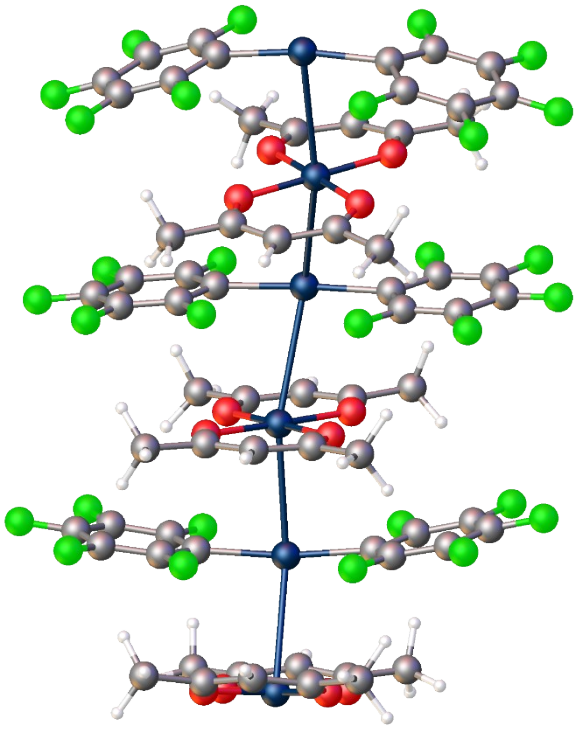


Figure S13. Van der Waals potential distribution on the ED isosurface (ρ = 0.001 e/Bohr^3) for (a) $Pd(acac)_2$ and (b) $Pt(acac)_2$.

S4. Cartesian coordinates for the studied $[M(acac)_2(Ph^F{}_2Hg)]_3$ (M = Pt, Pd) systems



$Pt(acac)_2(Ph^F{}_2Hg)]_3$

Hg	1.36955200	0.19200600	-1.16034200
F	1.03379900	1.95074600	1.39245200
F	1.02917800	2.71395600	-3.27941700
F	0.56843700	4.57313000	1.82754000
O	-2.05625100	1.84983700	-1.63388800
F	0.25366900	6.27310400	-0.29312300
O	-1.64030800	-1.03924100	-1.88063600
F	0.47207600	5.32175900	-2.84788000
C	0.65732400	4.50482600	-1.80905200
C	0.68862100	4.11816800	0.57523500
C	0.52558600	4.99086700	-0.50447400
C	-2.07212700	1.74802400	-2.90984600
C	1.09592300	2.26240000	-0.95539900
C	-1.68741000	-0.73004000	-3.12390700
C	0.95067900	2.77232100	0.32999400
C	-1.89519900	0.55947900	-3.64433000
H	-1.92037400	0.64942300	-4.72927100
C	-2.26989900	3.05526700	-3.63223800
C	0.94019400	3.15282500	-2.00659000
C	-1.45681200	-1.89362800	-4.05143500
H	-1.35274700	3.65750200	-3.54510100
H	-2.49061900	2.90975500	-4.69732100

H	-3.08692800	3.62018300	-3.16451600
H	-2.07628800	-2.74655000	-3.74297100
H	-1.67582900	-1.64276700	-5.09713400
H	-0.40080600	-2.19706700	-3.97227600
F	1.91895600	-2.17073200	-3.41134500
F	1.39466100	-1.76225600	1.27692500
F	2.34268000	-4.82157500	-3.12834700
O	-1.51598400	-1.25968400	0.87112000
F	2.23777800	-5.97139600	-0.64836100
O	-1.88167000	1.62866100	1.12304200
F	1.73134700	-4.42648600	1.55087900
C	1.77470200	-3.87189400	0.33390700
C	2.06702000	-4.07888300	-2.05454200
C	2.03255200	-4.66700500	-0.78651500
C	-1.45717800	-1.15752400	2.14764000
C	1.60697400	-1.89098400	-1.07983200
C	-1.75417100	1.32613100	2.36232100
C	1.85191300	-2.70535800	-2.17456000
C	-1.56014900	0.03556500	2.88282500
H	-1.48116100	-0.04793700	3.96559400
C	-1.25591800	-2.47117300	2.85462200
H	-2.07829300	-3.15190800	2.59356000
H	-1.21462400	-2.35612500	3.94520400
H	-0.32075800	-2.92939300	2.50150500
C	1.58342400	-2.50225000	0.16909400

C	-1.82554300	2.51563600	3.28007700
H	-1.05410900	3.23974700	2.97862100
H	-1.68379000	2.24354200	4.33365500
H	-2.80275000	3.00576600	3.15973200
Hg	-4.91983800	-0.16272400	-0.49210400
Pt	-7.76315800	-0.60870900	1.08122900
F	-4.80128100	1.61737000	2.12383500
F	-5.17581400	2.36892900	-2.53502300
F	-4.77369200	4.27755200	2.55760800
O	-8.23639700	0.93180000	-0.13061300
F	-4.87992500	6.00948300	0.44013800
O	-7.87105300	-1.95003200	-0.42171600
F	-5.05448600	5.03351300	-2.11177700
C	-5.04353800	4.19738100	-1.07066300
C	-4.89103200	3.81012200	1.30855400
C	-4.93679700	4.69872200	0.23048600
C	-8.22475900	0.85712900	-1.40448700
C	-5.05641900	1.91279600	-0.21391300
C	-7.90306600	-1.62372600	-1.65603000
C	-4.93111800	2.43866100	1.06560300
C	-8.01071600	-0.31282400	-2.16109000
H	-8.00895400	-0.20189000	-3.24620300
C	-8.44525500	2.16401300	-2.12514900
C	-5.10177200	2.81727900	-1.26359700
C	-7.77626700	-2.77391200	-2.62363900

H	-8.52805100	-2.70724600	-3.42416400
H	-7.88090000	-3.72539700	-2.08731500
H	-7.54301200	2.41897500	-2.70186500
H	-9.28389200	2.08301800	-2.83384700
H	-8.64864100	2.96018600	-1.39830100
H	-6.78136000	-2.73487200	-3.09475200
F	-4.45864600	-2.22841500	-2.98794900
F	-4.32604600	-2.31104400	1.74341600
F	-3.54676100	-4.77038800	-3.05315100
O	-7.22611400	-2.13340800	2.26747200
F	-3.09460600	-6.12498100	-0.71936400
O	-7.58124800	0.74120800	2.55262900
F	-3.51810400	-4.88117800	1.68343000
C	-3.76543100	-4.23717000	0.53677400
C	-3.78956000	-4.18406200	-1.87796900
C	-3.54007400	-4.87348000	-0.68717400
C	-6.74902500	-1.98747100	3.44531900
C	-4.48018100	-2.21117500	-0.61898600
C	-7.05079500	0.49023000	3.68928500
C	-4.25544100	-2.87064000	-1.81798900
C	-6.63204100	-0.77291800	4.14603900
H	-6.19546700	-0.81785300	5.14305600
C	-6.28050800	-3.27663400	4.06939800
H	-7.09131600	-4.01958600	4.01804300
H	-5.95915000	-3.15180500	5.11153000

H	-5.44186700	-3.66669200	3.47182400
C	-4.20859700	-2.91600400	0.54667000
C	-6.88230000	1.71054800	4.55696600
H	-7.84764700	2.23354100	4.63863500
H	-6.50617300	1.47031900	5.55981200
H	-6.18077400	2.39678500	4.05732800
Pt	-1.77669800	0.29665600	-0.37428200
Hg	7.49048400	0.32801800	0.73134200
Pt	4.39940200	-0.12971600	0.14046900
F	6.63511400	2.44866700	2.97209500
F	7.30333500	2.41784400	-1.71246500
F	5.59621700	4.94044200	2.80774100
O	4.44378200	1.31973000	-1.26192700
F	5.39500100	6.17533800	0.38089100
O	4.85439500	-1.57889300	-1.18773100
F	6.25669900	4.90943600	-1.87453400
C	6.38921400	4.31679600	-0.68489100
C	6.05021600	4.33454300	1.70842500
C	5.93215900	4.96386500	0.46626700
C	4.61023900	1.10197000	-2.51561200
C	7.05597000	2.38255900	0.64277800
C	4.98749600	-1.38379400	-2.44626700
C	6.60242500	3.05513100	1.77234600
C	4.86364500	-0.14675800	-3.10657600
H	4.98926800	-0.15830900	-4.18819700

C	4.47107900	2.32933700	-3.37463900
C	6.93575100	3.03755900	-0.57838000
C	5.26447900	-2.62992200	-3.24495100
H	5.02297400	3.16466900	-2.92504100
H	4.82710700	2.16211700	-4.39920100
H	3.40640700	2.61018900	-3.41267500
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H	5.67168000	-2.39912300	-4.23773800
H	5.96454900	-3.27695300	-2.70242600
F	7.95304900	-1.88251800	-1.55693500
F	7.12537900	-1.80179900	3.10154600
F	7.62990200	-4.57015800	-1.56433600
O	4.31782200	-1.57528200	1.53139700
F	7.06303800	-5.88107400	0.75888900
O	3.95001100	1.32331900	1.45678100
F	6.81769400	-4.48864800	3.09322900
C	7.13422600	-3.85084400	1.96372400
C	7.55132800	-3.89170200	-0.41683300
C	7.24361100	-4.56579700	0.76801700
C	3.97445300	-1.37740900	2.75142500
C	7.61473100	-1.76940700	0.78424300
C	3.68042000	1.11622000	2.69341400
C	7.72452500	-2.50767500	-0.38947200
C	3.67368500	-0.13471500	3.33398400
H	3.41004100	-0.14195900	4.39039300

C	3.90401900	-2.63807400	3.56824700
C	7.31189400	-2.46736000	1.94872500
C	3.35829200	2.36625300	3.46771300
H	4.89527700	-3.11366600	3.58931900
H	3.56984000	-2.45408100	4.59703700
H	3.21302200	-3.33689500	3.07377900
H	2.54343800	2.90410400	2.96319400
H	3.06776600	2.15040500	4.50366100
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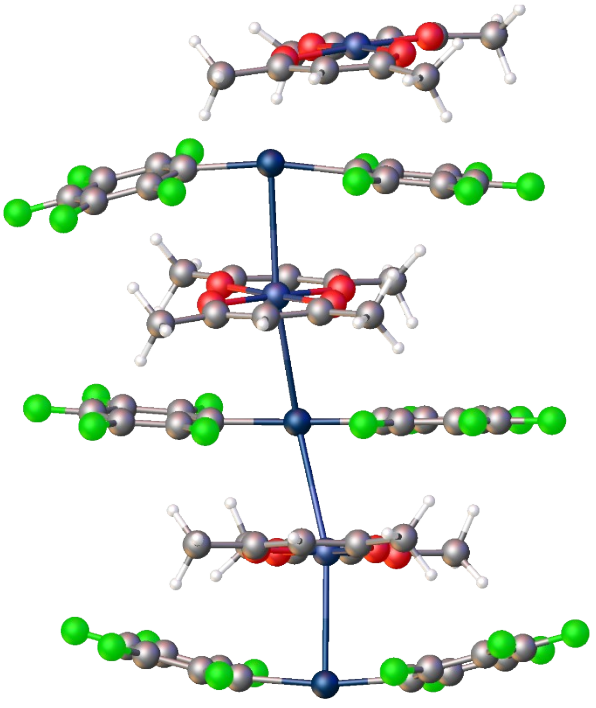
$[Pd(acac)_2(Ph^F{}_2Hg)]_3$



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O	2.06637400	2.26891500	-1.43240200
F	-1.40542500	-4.64859700	-2.97519700
O	1.89896700	-0.62793500	-1.67894400
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F	-1.37486600	-1.95834200	-3.18018300
F	-1.09221200	-4.29746900	1.73784700
C	2.22503700	3.49213800	-3.42586300
H	1.31566100	4.08237800	-3.23987200
H	2.34859000	3.36680600	-4.50898500
H	3.07598900	4.06019300	-3.02649600
C	-1.21326700	-1.70069600	-0.83116000

C	2.11719500	2.17128300	-2.70508100
C	1.91365400	-1.51059000	-3.84681800
H	0.91798500	-1.97294800	-3.76721000
H	2.65879900	-2.25506600	-3.53378300
H	2.09454500	-1.23126400	-4.89268400
C	-1.15834400	-2.33560300	0.40431900
C	-1.15703700	-3.72266200	0.53114900
C	-1.29990600	-3.90370500	-1.87251300
C	-1.28702300	-2.51141300	-1.95351700
C	2.06846200	0.97567700	-3.44596400
H	2.11730000	1.06531400	-4.52993400
C	-1.23897800	-4.51562700	-0.61672800
C	1.96870300	-0.32370600	-2.91782400
F	-0.97042300	2.89944700	-3.01593800
O	1.75014800	-0.86362200	1.06502800
F	-1.01511700	4.87766200	2.06648600
O	1.80423500	2.03553700	1.32122700
F	-0.71577300	6.56515200	-0.06837000
F	-1.21272500	2.21806100	1.66160600
F	-0.67681500	5.55622100	-2.60862100
C	1.62262300	-2.10483100	3.04603900
H	0.78497400	-2.69815500	2.65290000
H	1.51109200	-1.99516500	4.13235600
H	2.55197600	-2.65408700	2.83511300
C	-1.14668300	2.48457900	-0.69162600

C	1.66562200	-0.77372700	2.33646300
C	1.51747200	2.91157000	3.46995600
C	-1.00315000	3.36756000	-1.75161300
C	-0.85615800	4.74247600	-1.56650900
C	-1.01254200	4.39530000	0.81995000
C	-1.13365000	3.02687300	0.58788600
C	1.61070700	0.42011700	3.07775400
H	1.51088500	0.32692700	4.15798000
C	-0.85583800	5.26014600	-0.26706500
C	1.65788200	1.72390100	2.55247000
H	2.38447500	3.57539900	3.34653400
H	0.62345400	3.47938400	3.17203800
H	1.42863300	2.62009600	4.52422300
Hg	-7.41959400	-0.30781300	0.41273400
Pd	-4.26071000	-0.37993200	0.10580100
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O	-4.35389100	1.05956300	-1.29608100
F	-6.85756400	-5.18017500	-1.87010700
O	-4.46328800	-1.85152100	-1.25408200
F	-6.29743300	-6.42749500	0.48999600
F	-7.47995900	-2.54572700	-1.89248300
F	-6.35759200	-5.02505400	2.82957400
C	-4.32980400	2.08457800	-3.40274600
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H	-3.30839400	2.49210600	-3.33508800
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C	-4.58595600	-2.93079000	-3.33452400
H	-5.27762800	-3.64356300	-2.86877000
H	-3.58773500	-3.39526900	-3.35670200
H	-4.89924200	-2.73684300	-4.36840800
C	-7.00228000	-3.06767900	1.64970900
C	-6.67172400	-4.42251500	1.68046200
C	-6.92961700	-4.50201500	-0.72241900
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C	-4.48051300	-0.42009000	-3.17155200
H	-4.52051100	-0.43620700	-4.25951600
C	-6.62409900	-5.14085600	0.48256500
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F	-6.27336200	4.47908900	2.63468600
O	-4.07543200	1.09751200	1.44768300
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F	-6.99787400	1.87339000	2.71318900
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C	-3.71153800	-2.84382000	3.55035500
C	-7.22826600	1.78392900	0.35833700
C	-3.88833500	-1.59057800	2.73282700

C	-3.78695900	2.18909200	3.50025800
C	-7.09970900	2.46283700	-0.84902100
C	-6.71365200	3.80202200	-0.91013600
C	-6.56203600	3.83363700	1.50288500
C	-6.95035400	2.49403400	1.52166800
C	-3.78559600	-0.32932400	3.34520700
H	-3.60754900	-0.31575000	4.41925100
C	-6.43108800	4.48739000	0.27458400
C	-3.89043700	0.91517700	2.69992900
H	-2.86866700	-3.41474500	3.13184600
H	-3.52111400	-2.63238600	4.61015200
H	-4.61138000	-3.46894000	3.45924700
H	-2.99082200	2.81639100	3.07540900
H	-4.73091100	2.74588400	3.41399300
H	-3.57805300	1.99984900	4.56087600
Hg	5.08525700	0.69590400	0.12475600
Pd	7.87935800	-1.53271600	0.45097700
F	4.76545600	-1.73371400	2.23641000
O	7.77118700	-0.19183100	-1.04971200
F	4.47161100	-3.84108400	-2.77987800
O	7.99140000	-3.08731400	-0.81157300
F	4.36043600	-5.47036600	-0.60090700
F	4.75692800	-1.16342400	-2.46056200
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C	7.43198900	0.67052400	-3.19725000

H	6.40525300	1.02938100	-3.01905500
H	7.53966400	0.41630300	-4.25963300
H	8.11014800	1.49643300	-2.93634800
C	4.80669300	-1.37712300	-0.10256500
C	7.69113000	-0.50401700	-2.28795500
C	7.84750200	-4.31989800	-2.79786200
C	4.69750500	-2.23095200	0.98717000
C	4.54445800	-3.60773600	0.84813000
C	4.54376000	-3.31679000	-1.54935600
C	4.70009800	-1.94472200	-1.36505900
C	7.77283200	-1.80083900	-2.81970300
H	7.68044100	-1.89949500	-3.90054600
C	4.47760600	-4.15698200	-0.43529700
C	7.89537800	-2.99339900	-2.07689200
H	8.49395100	-5.04518700	-2.28468300
H	6.81217800	-4.69707900	-2.75183700
H	8.13475800	-4.23382600	-3.85448100
F	5.21474800	3.01953300	-2.07876200
O	7.80136800	-2.87487000	1.93628400
F	4.02211700	5.32763100	2.71361300
O	7.67435300	0.01967900	1.71343500
F	4.02023300	6.82084400	0.42519900
F	4.61906000	2.69495500	2.60865900
F	4.62059200	5.65312100	-1.96816800
C	7.37799600	-3.78831400	4.04202100

H	6.39907200	-4.21431800	3.76544400
H	7.37671400	-3.54188200	5.11176900
H	8.13853200	-4.55454500	3.83050400
C	5.00244100	2.78982800	0.27141000
C	7.60926100	-2.58578400	3.16077000
C	7.47075500	1.23019400	3.70675300
H	6.51433400	1.70427900	3.43768100
H	8.27218600	1.90073500	3.36055300
H	7.52339400	1.12246700	4.79791700
C	4.98119200	3.57653000	-0.87434600
C	4.66422100	4.93480900	-0.84382400
C	4.35619400	4.76912400	1.54811600
C	4.67907600	3.41466000	1.46915900
C	7.55831000	-1.28967400	3.71325000
H	7.43466100	-1.21429100	4.79285600
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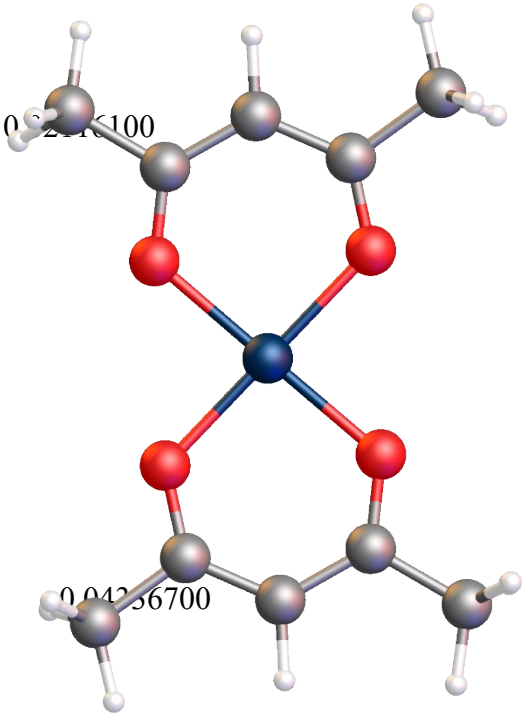

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C	-2.65310900	-1.25272000	-
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C	-2.64465300	1.26379100	
0.02144000			
C	-3.27836600	0.00870200	
0.01561700			
H	-4.36696200	0.01177100	
C	-3.48883500	-2.50620000	-0.00612100
C	-3.46150200	2.52485400	0.12093500
H	-3.40668400	-2.98304900	0.98247100
H	-4.54792400	-2.29920100	-0.20555700
H	-3.10928700	-3.21611300	-0.75271100
H	-3.11482900	3.25493000	-0.62282900
H	-4.53365000	2.33925900	-0.02203300
H	-3.30640800	2.96132400	1.12039900
O	1.38391000	1.45904600	-0.03063100
O	1.38049300	-1.46304400	0.00265900
C	2.64913200	1.25418200	-0.00528000
C	2.64510900	-1.25593900	0.04068900
C	3.27831800	-0.00170100	0.03274100
H	4.36684700	-0.00359800	0.05921900
C	3.47021200	2.51581200	-0.01618600
H	3.22596900	3.09831600	-0.91556800

H	4.54843300	2.31216800	0.00050800
H	3.20177200	3.12648800	0.85799800
C	3.45787000	-2.52000500	0.10273200
H	3.13612000	-3.10286900	0.97855700
H	4.53583300	-2.32468500	0.16598600
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Pt	0.00409900	-0.00289800	-0.02468900

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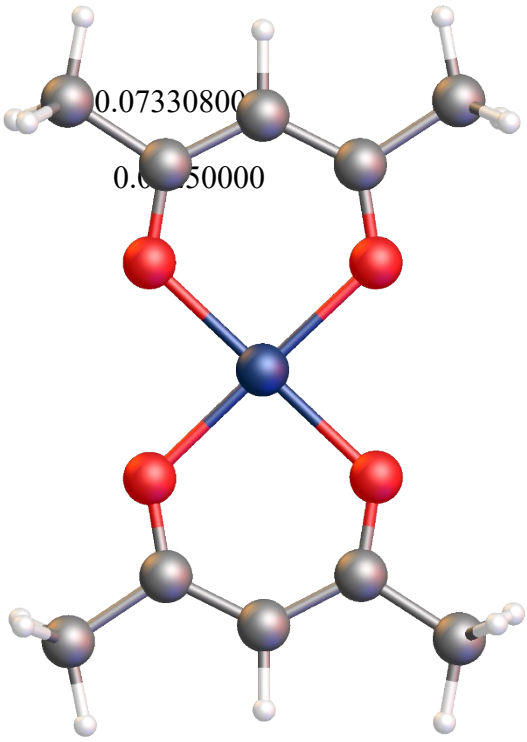

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O	1.39232000	-1.45552700	-
O	1.37536500	1.45498500	
C	3.49011500	-2.50161400	-
H	3.29108300	-3.08370900	
H	4.56444200	-2.28425800	-
H	3.20323800	-3.12317600	-0.91512600
C	2.65218700	-1.24726700	-0.03883700
C	3.45445800	2.52482400	0.13108500
H	3.26413400	3.00239200	1.10431400
H	3.13253900	3.22047200	-0.65626400
H	4.53078500	2.33454100	0.03163000
C	3.28174500	0.00986600	0.02465600
H	4.37011000	0.01504300	0.05373900

C	2.63767500	1.25962900	0.04800400
O	-1.38229500	1.45123100	-0.02627100
O	-1.38285400	-1.45968100	-0.00968200
C	-3.46704000	2.51557100	-0.07406000
H	-3.18757900	3.16142400	0.77034700
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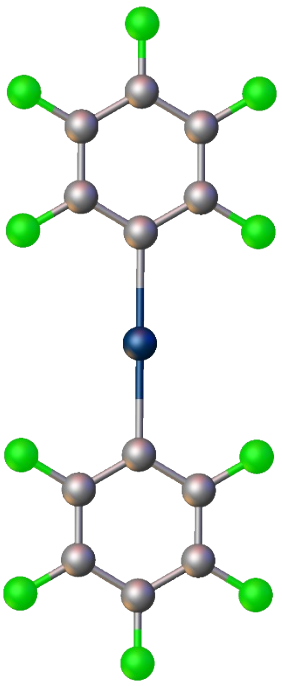
H	-3.23826300	3.05856900	-1.00286800
C	-2.64400800	1.25160300	-0.02728300
C	-3.46298400	-2.51463200	0.15415400
C	-3.28154800	-0.00129400	0.01249300
H	-4.37015100	-0.00136600	0.03439900
C	-2.64370300	-1.25441600	0.04151500
H	-3.22095600	-3.18583700	-0.68161100
H	-3.18199400	-3.03207800	1.08352400
H	-4.54211400	-2.31522800	0.16086900

$Ph^{F}_{2}Hg$

Hg	-0.00033802	0.08631892	0.02893056
F	-2.24009100	2.42343526	-0.41536636
F	-4.98335611	-2.25980639	0.49158014
F	-6.36311252	0.07838344	0.04510225
F	-2.23196713	-2.25637450	0.48458944
F	-4.99147997	2.42000366	-0.40837414
C	-2.21032917	0.08356214	0.03454469
C	-2.91309527	1.27449689	-0.19286723



C	-4.31448966	1.27274896	-0.18930620
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C	-2.90895745	-1.10912063	0.26551720
C	-5.01311794	0.08006637	0.04166723
F	2.23941502	-2.25079132	0.47325926
F	4.98268007	2.43244336	-0.43372346
F	6.36243656	0.09426117	0.01279419
F	2.23129106	2.42900935	-0.42674384
F	4.99080404	-2.24735637	0.46628451
C	2.20965315	0.08907694	0.02332291
C	2.91241928	-1.10185493	0.25074984
C	4.31381369	-1.10010509	0.24719879
C	4.30967582	1.28350734	-0.21121212
C	2.90828142	1.28175824	-0.20765720
C	5.01244195	0.09257561	0.01621556

COJBEJ

Hg	1.25591000	-2.30461800	-0.19116600
C	-0.58938000	-3.24247000	-0.14243000
C	-1.30157100	-3.51028000	-1.29929600
C	-2.56772800	-4.07892500	-1.29437400
C	-3.15033200	-4.35221200	-0.06699400
C	-2.47087000	-4.05992400	1.10329800
C	-1.21352900	-3.55682800	1.04331900
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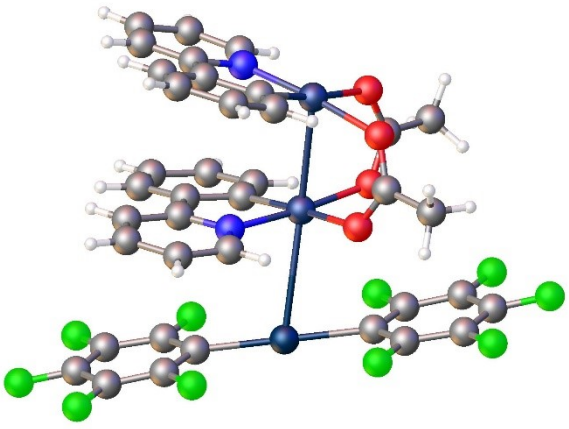

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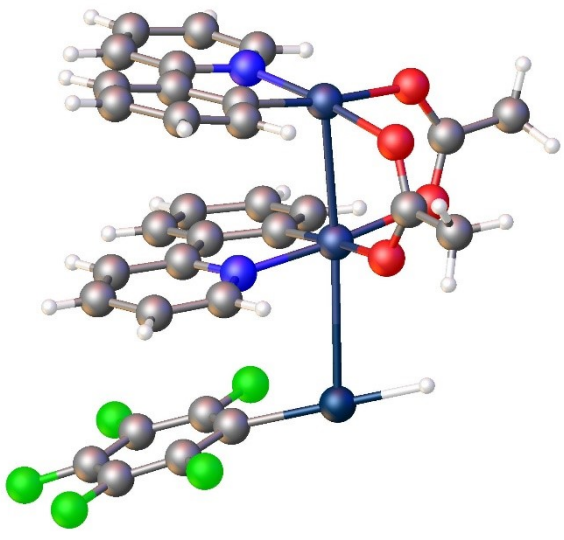
F	-4.40927200	-4.84318300	-0.03492900
F	-3.07754700	-4.35022600	2.27962400
F	-0.58488100	-3.30478600	2.20299800
Pd	-0.76050700	0.02441700	0.20728900
Pd	-2.56845600	2.21221300	0.12241700
O	-2.12850700	-0.76094000	1.55371500
O	-3.32670900	1.12538500	1.78842500
O	-1.99717200	-0.54299900	-1.40128100
O	-3.62596000	0.99834800	-1.18303200
C	3.10120000	-1.36676600	-0.23990200
C	3.81339100	-1.09895600	0.91696400
C	5.07954900	-0.53031100	0.91204200
C	5.66215200	-0.25702400	-0.31533800
C	4.98269000	-0.54931200	-1.48563000
C	3.72534900	-1.05240800	-1.42565200
C	0.44702800	0.28468700	2.95637000
H	-0.24287200	-0.28828900	3.26653400
C	1.38087200	0.79772100	3.86311900
H	1.33252000	0.56890800	4.78321000
C	2.38082600	1.64688000	3.40258800
H	3.01237300	2.00843200	4.01307900
C	2.45868100	1.96382600	2.07105600
H	3.14431900	2.54427200	1.76144100
C	1.52972000	1.43707200	1.16863100

C	1.54233500	1.61834100	-0.28440400
C	2.44533100	2.41693800	-0.97821800
H	3.08015400	2.94445400	-0.50892400
C	2.40841700	2.42956700	-2.34772300
H	3.02777000	2.96403400	-2.83061800
C	1.47414800	1.67188100	-3.03353800
H	1.45926000	1.66930800	-3.98342700
C	0.56852600	0.92407900	-2.32352800
H	-0.08269800	0.41380500	-2.79074800
C	0.51515400	0.60441300	1.61941300
C	-1.23277400	3.33425100	2.55386000
H	-1.72057500	2.68398100	3.04477500
C	-0.36129300	4.16811500	3.21925400
H	-0.25998000	4.09548200	4.16093100
C	0.36231500	5.10755300	2.51964200
H	0.95252200	5.69683200	2.97520500
C	0.22123000	5.18724400	1.12649700
H	0.73945400	5.80510000	0.62207600
C	-0.67971300	4.35810000	0.50201000
C	-1.00041600	4.35392000	-0.94690600
C	-0.47555800	5.25323900	-1.86106200
H	0.16746300	5.89581600	-1.58516600
C	-0.89369500	5.21261400	-3.17397000
H	-0.54448400	5.83083500	-3.80672200
C	-1.82394100	4.26626000	-3.56337100

H	-2.11856700	4.24079400	-4.46671500
C	-2.32584600	3.36798500	-2.66893200
H	-2.95218200	2.71290700	-2.95640100
C	-1.92243900	3.40314100	-1.31836300
C	-3.03077000	-0.06602500	2.09208900
C	-3.79295600	-0.71468800	3.20521000
H	-4.56603000	-0.15932800	3.43749600
H	-4.09931700	-1.59867900	2.91834500
H	-3.21080300	-0.80779000	3.98848700
C	-3.13014200	-0.04592500	-1.69838500
C	-3.93745600	-0.73969300	-2.74697400
H	-4.33162300	-0.07674500	-3.34910300
H	-3.35778700	-1.34161700	-3.26053800
H	-4.65043400	-1.25939500	-2.31988800
F	3.27916200	-1.38839200	2.12110800
F	5.73673300	-0.28861600	2.04668900
F	6.92109300	0.23394700	-0.34740300
F	5.58936700	-0.25901000	-2.66195600
F	3.09670200	-1.30445000	-2.58533000
N	0.59649300	0.90147200	-0.94196200
N	-1.41294900	3.42454800	1.19818700

COJBEJ with PhF replaced by H atom

Hg	1.25591000	-2.30461800	-0.19116600
Pd	-0.76050700	0.02441700	0.20728900



Pd	-2.56845600	2.21221300	0.12241700
O	-2.12850700	-0.76094000	1.55371500
O	-3.32670900	1.12538500	1.78842500
O	-1.99717200	-0.54299900	-1.40128100
O	-3.62596000	0.99834800	-1.18303200
C	3.10120000	-1.36676600	-0.23990200
C	3.81339100	-1.09895600	0.91696400
C	5.07954900	-0.53031100	0.91204200
C	5.66215200	-0.25702400	-0.31533800
C	4.98269000	-0.54931200	-1.48563000
C	3.72534900	-1.05240800	-1.42565200
C	0.44702800	0.28468700	2.95637000
H	-0.24287200	-0.28828900	3.26653400
C	1.38087200	0.79772100	3.86311900
H	1.33252000	0.56890800	4.78321000
C	2.38082600	1.64688000	3.40258800
H	3.01237300	2.00843200	4.01307900
C	2.45868100	1.96382600	2.07105600
H	3.14431900	2.54427200	1.76144100
C	1.52972000	1.43707200	1.16863100
C	1.54233500	1.61834100	-0.28440400
C	2.44533100	2.41693800	-0.97821800
H	3.08015400	2.94445400	-0.50892400
C	2.40841700	2.42956700	-2.34772300
H	3.02777000	2.96403400	-2.83061800

C	1.47414800	1.67188100	-3.03353800
H	1.45926000	1.66930800	-3.98342700
C	0.56852600	0.92407900	-2.32352800
H	-0.08269800	0.41380500	-2.79074800
C	0.51515400	0.60441300	1.61941300
C	-1.23277400	3.33425100	2.55386000
H	-1.72057500	2.68398100	3.04477500
C	-0.36129300	4.16811500	3.21925400
H	-0.25998000	4.09548200	4.16093100
C	0.36231500	5.10755300	2.51964200
H	0.95252200	5.69683200	2.97520500
C	0.22123000	5.18724400	1.12649700
H	0.73945400	5.80510000	0.62207600
C	-0.67971300	4.35810000	0.50201000
C	-1.00041600	4.35392000	-0.94690600
C	-0.47555800	5.25323900	-1.86106200
H	0.16746300	5.89581600	-1.58516600
C	-0.89369500	5.21261400	-3.17397000
H	-0.54448400	5.83083500	-3.80672200
C	-1.82394100	4.26626000	-3.56337100
H	-2.11856700	4.24079400	-4.46671500
C	-2.32584600	3.36798500	-2.66893200
H	-2.95218200	2.71290700	-2.95640100
C	-1.92243900	3.40314100	-1.31836300
C	-3.03077000	-0.06602500	2.09208900

C	-3.79295600	-0.71468800	3.20521000
H	-4.56603000	-0.15932800	3.43749600
H	-4.09931700	-1.59867900	2.91834500
H	-3.21080300	-0.80779000	3.98848700
C	-3.13014200	-0.04592500	-1.69838500
C	-3.93745600	-0.73969300	-2.74697400
H	-4.33162300	-0.07674500	-3.34910300
H	-3.35778700	-1.34161700	-3.26053800
H	-4.65043400	-1.25939500	-2.31988800
F	3.27916200	-1.38839200	2.12110800
F	5.73673300	-0.28861600	2.04668900
F	6.92109300	0.23394700	-0.34740300
F	5.58936700	-0.25901000	-2.66195600
F	3.09670200	-1.30445000	-2.58533000
N	0.59649300	0.90147200	-0.94196200
N	-1.41294900	3.42454800	1.19818700
H	-0.29481673	-3.09276087	-0.15020972

S5. References

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2. T. Lu and Q. Chen, van der Waals potential: an important complement to molecular electrostatic potential in studying intermolecular interactions, *Journal of Molecular Modeling*, 2020, **26**, 315.