Electronic Supplementary Information

Metal-involving C···d_z^2-Pt^{II} Tetrel Bonding as a Principal Component of Stacking Interaction between Arenes and the Platinum(II) Square-plane

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1. Crystal data and structure refinement

Table S1. Crystal data and structure refinement for **1**·$(OFA)_2$, **1**·C_6F_6, and **2**·C_6F_6.

Identification code	**1**·$(OFA)_2$	**1**·C_6F_6	**2**·C_6F_6
Empirical formula	$C_{58}H_{28}F_8N_4O_2Pt_2S_4$	$C_{50}H_{28}F_6N_4Pt_2S_4$	$C_{42}H_{24}F_6N_4Pt_2S_4$
Formula weight	1483.26	1317.18	1217.07
Temperature/K	100(2)	100.0(5)	100.00(10)
Crystal system	triclinic	monoclinic	monoclinic
Space group	P-1	C2/c	P2/n
a/Å	10.7456(2)	10.02350(10)	10.0312(2)
b/Å	14.0684(2)	29.0365(4)	11.5989(2)
c/Å	16.9039(3)	15.6254(2)	16.5342(3)
α/°	87.4668(13)	90	90
β/°	83.8451(15)	105.9290(10)	98.669(2)
γ/°	70.6288(18)	90	90
Volume/Å^3	2396.78(8)	4373.11(10)	1901.79(6)
Z	2	4	2
ρ_{calc}g/cm^3	2.055	2.001	2.125
μ/mm^{-1}	13.117	14.166	16.211
F(000)	1424.0	2520.0	1156.0
Crystal size/mm^3	0.17 × 0.14 × 0.11	0.07 × 0.06 × 0.03	0.15 × 0.12 × 0.1
Radiation	CuKα (λ = 1.54184)	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	5.258 to 133.202	6.088 to 141.402	7.622 to 139.996
Index ranges	-12 ≤ h ≤ 12, -16 ≤ k ≤ 11, -20 ≤ l ≤ 19	-12 ≤ h ≤ 11, -35 ≤ k ≤ 33, -18 ≤ l ≤ 19	-12 ≤ h ≤ 12, -9 ≤ k ≤ 14, -20 ≤ l ≤ 20
Reflections collected	16859	14582	15928
Independent reflections	16859 [R_{int} =n/a, R_{sigma} = 0.0209]	4181 [R_{int} = 0.0384, R_{sigma} = 0.0307]	3607 [R_{int} = 0.0394, R_{sigma} = 0.0333]
Data/restraints/parameters	16859/0/704	4181/180/342	3607/0/252
Goodness-of-fit on F^2	1.015	1.034	1.035
Final R indexes [I>=2σ (I)]	R_1 = 0.0540, wR_2 = 0.1545	R_1 = 0.0275, wR_2 = 0.0719	R_1 = 0.0298, wR_2 = 0.0750
Final R indexes [all data]	R_1 = 0.0626, wR_2 = 0.1651	R_1 = 0.0288, wR_2 = 0.0729	R_1 = 0.0314, wR_2 = 0.0762
Largest diff. peak/hole / e Å^{-3}	2.86/-1.51	2.09/-0.81	2.54/-1.24
CCDC Nos	2245750	2245749	2245751

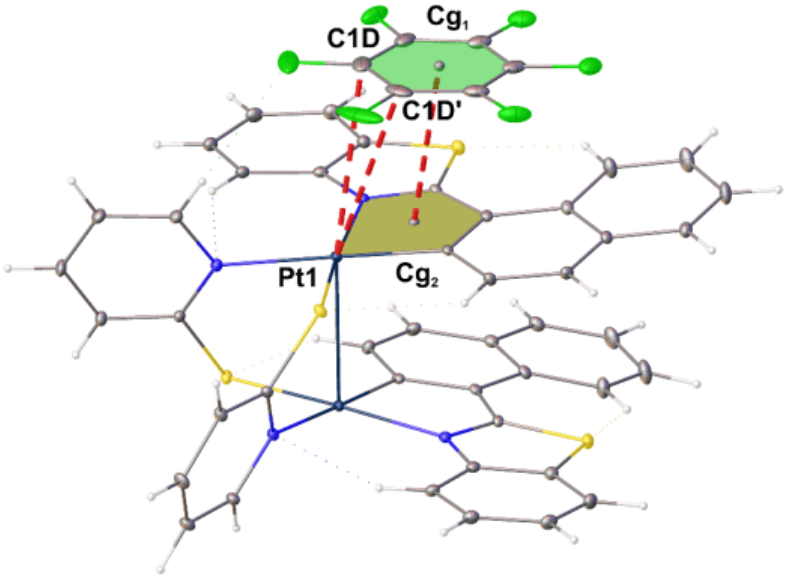


Figure S1. A fragment of the crystal structure of **1**·C_6F_6. Short contacts are given by dotted lines and thermal ellipsoids are shown at the 50% probability level

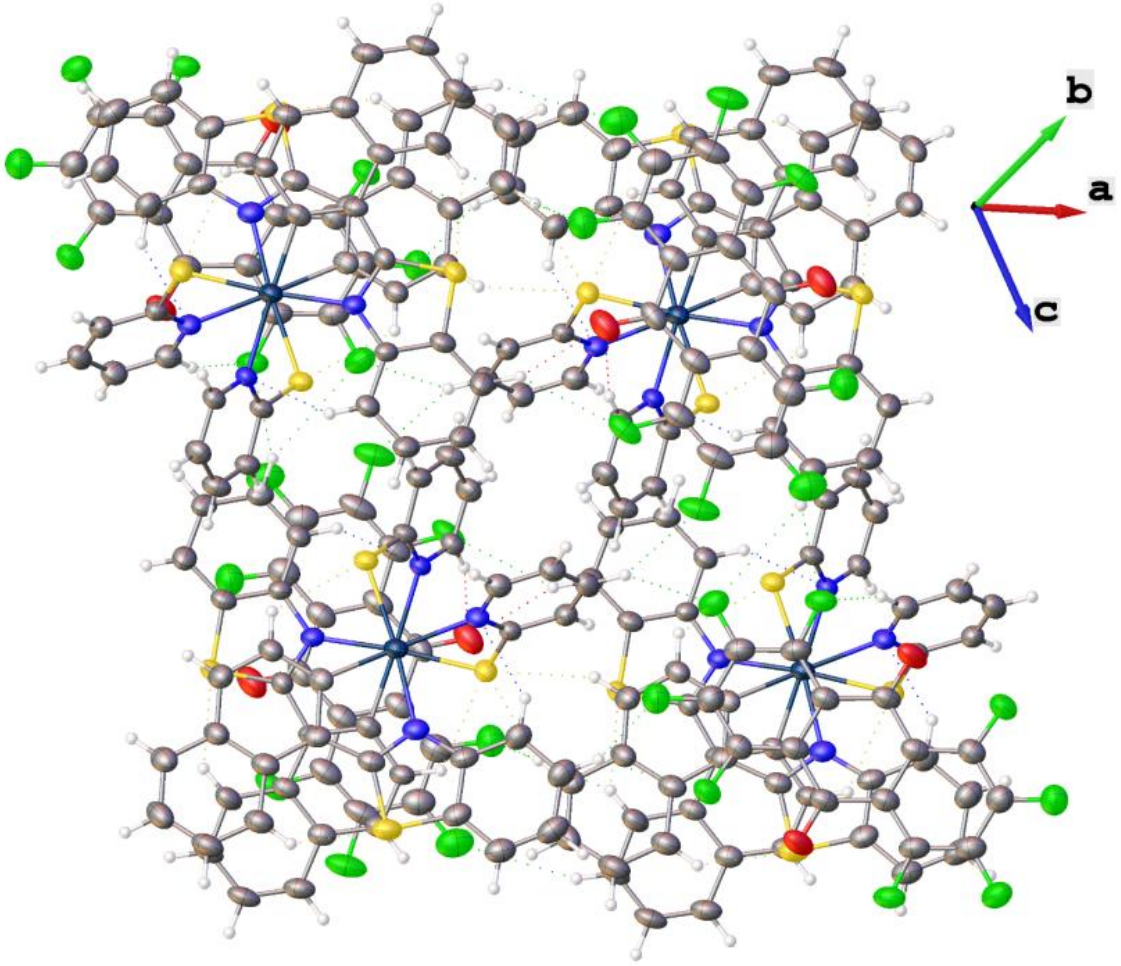


Figure S2. A fragment of the crystal packing of **1**·$(OFA)_2$.

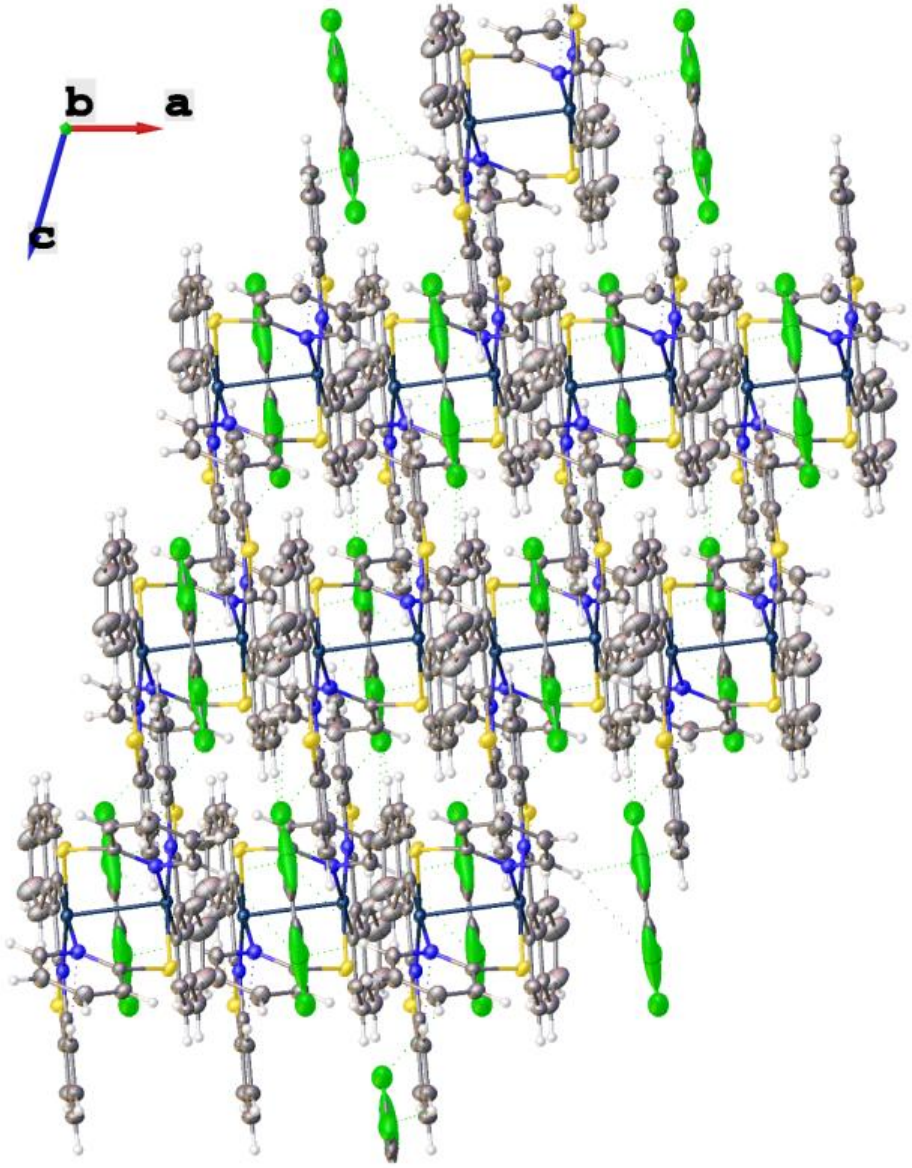


Figure S3. A fragment of the crystal packing of **1**·C_6F_6.

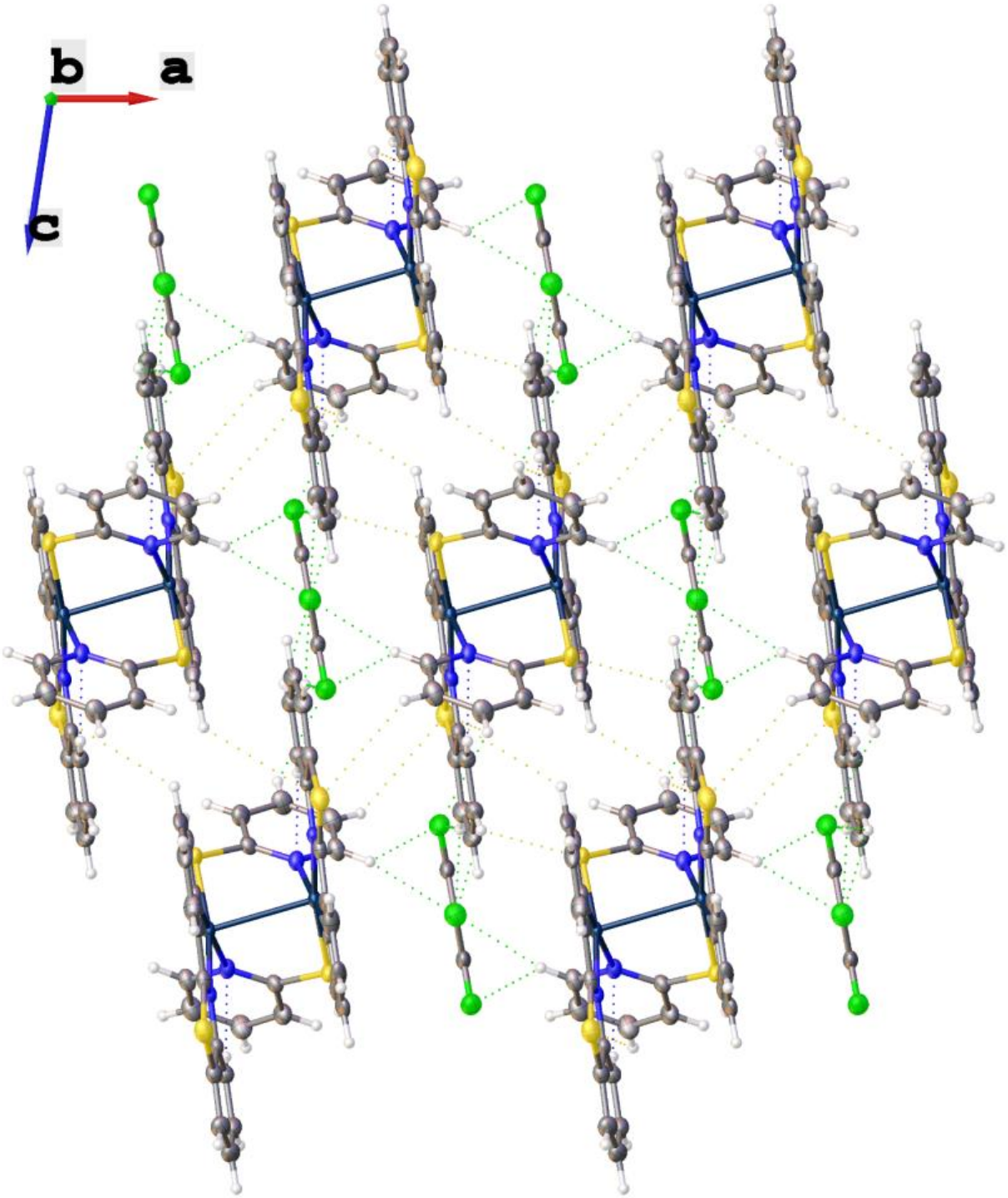


Figure S4. A fragment of the crystal packing of **2**·C_6F_6.

2. CSD search for π-hole···M contacts

We analyzed the Cambridge Structural Database[1] (CSD version 5.43 updates March, 2022; search and processing was carried out in the program ConQuest version 2022.2.0) (**Table S2**) to demonstrate the occurrence of short contacts between a π-hole and a metal ion. The search was

carried out based on the following three geometrical parameters: (i) Cg···M distances were set in the range from 3.0 to 4.5 Å (where Cg is centroid of an aromatic ring; M is a transition metal in a square-planar environment), (ii) the angle between the normal of the aromatic ring varied from 0 to 45°; (iii) only structures with halogen substituents at an aromatic ring were considered. Notably, C(isocyanide)···M contacts can also be considered as π-hole···M interaction and we found several examples of relevant contacts in CSD (**Table S2**, group 3). We did consider not include these results because of the difference of C(isocyanide)···M contacts from contacts involving aromatic ring π-hole; the latter are closer to structures obtained in this work.

According to these criteria, we revealed 60 structures with π-hole···M short contacts; they were divided into two groups. The first group consists of 33 structures (blue dots, **Figure S5** and **Table S2**, group 1) of cocrystals formed on cocrystallization of perfluoro(het)arenes (including substituted fluorinated derivatives) with mononuclear platinum(II), palladium(II), nickel(II), copper(II), and gold(I) complexes. In this group, typical π-hole···M separations are of 3.2–4.2 Å with the angles in the range 0–35°.

The second group (27 structures, black dots, **Figure S2**) includes contacts in the crystal structures of metal complexes and metalloporphyrins bearing perfluoroaromatic ligands.[2] These contacts are most likely induced by crystal packing effects as follows from more diffuse character of the scatter in bond lengths and angles (3.3–4.6 Å and 6–44°). All identified contacts include only mononuclear Pt^{II}, Pd^{II}, Ni^{II}, and Au^{III} complexes, while binuclear (or higher) complexes functioning as acceptors of π-hole···[M–M] interactions were not found.

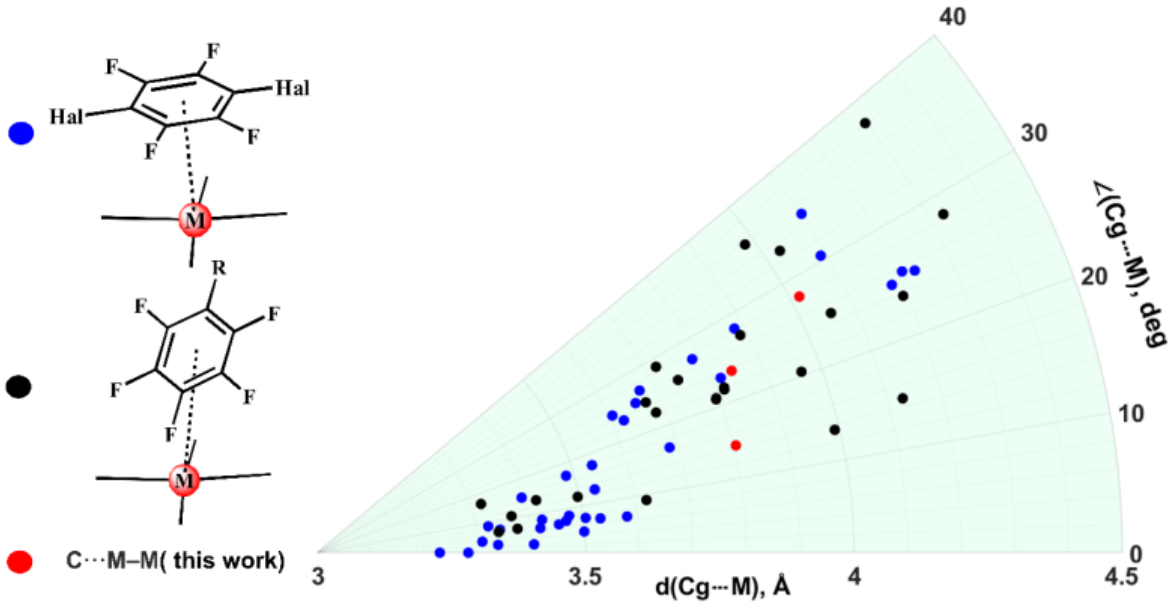
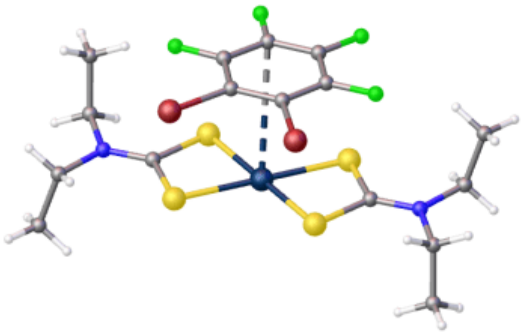
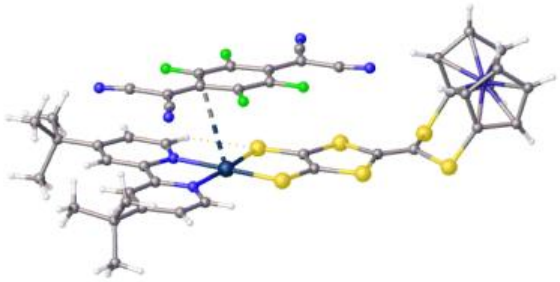
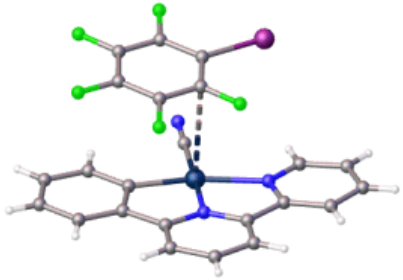
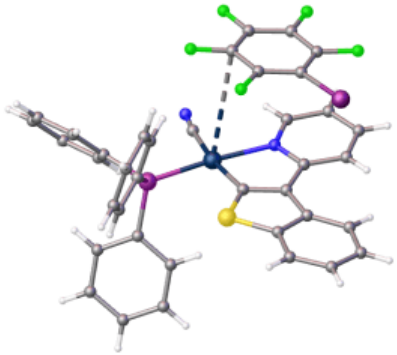
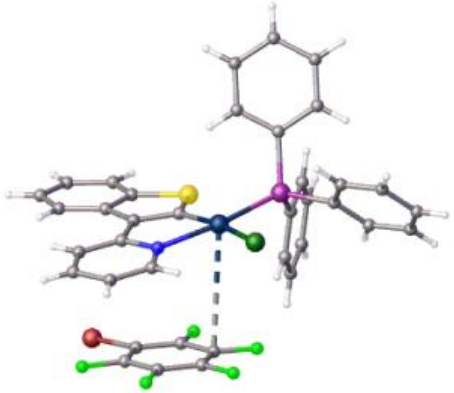


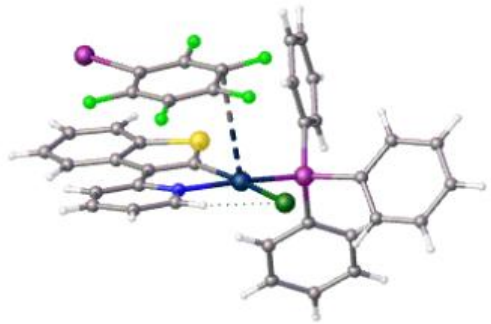
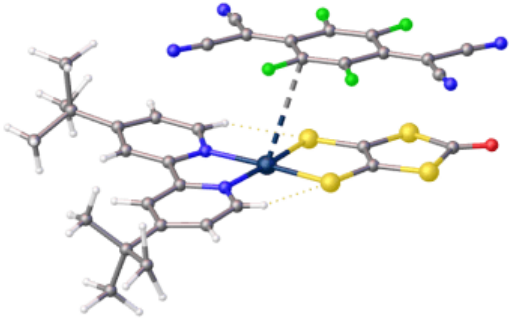
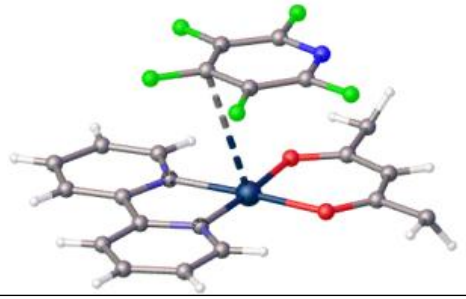
Figure S5. Angular distribution for intermolecular π-hole···M contacts retrieved from the CSD. The distances were set as the range between 3.0 and 4.5 Å, while the angularity was set in the 0–

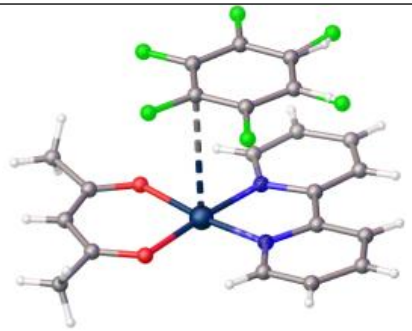
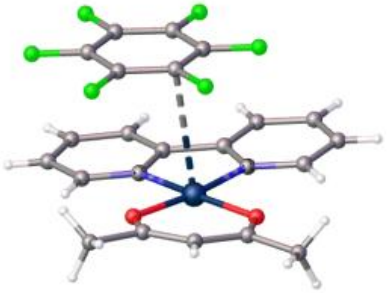
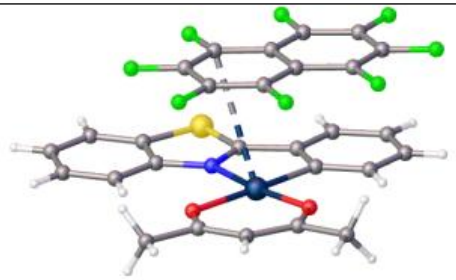
40° range. *R* factor ≤6%.

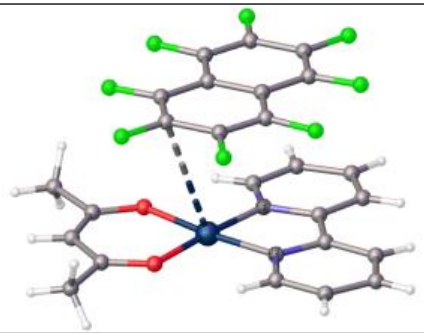
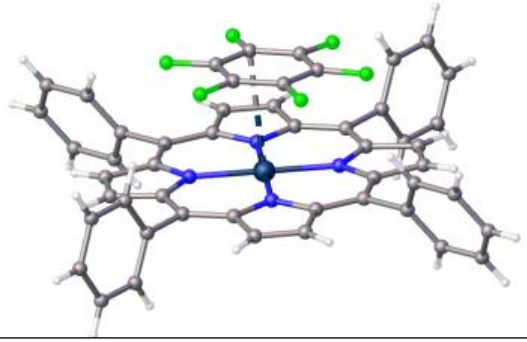
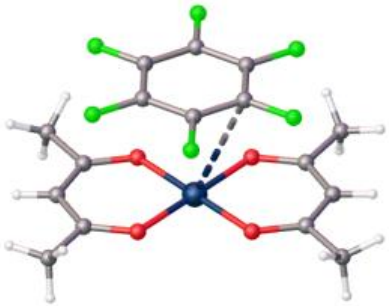
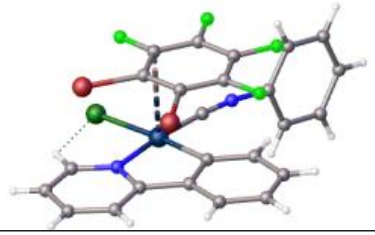
Table S2. Results of CSD search for π-hole···M contacts.

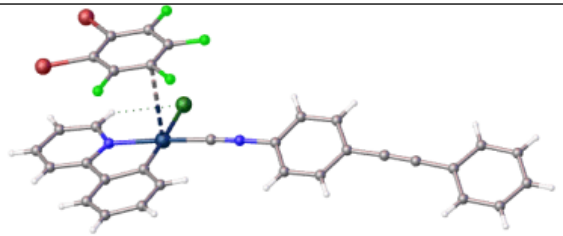
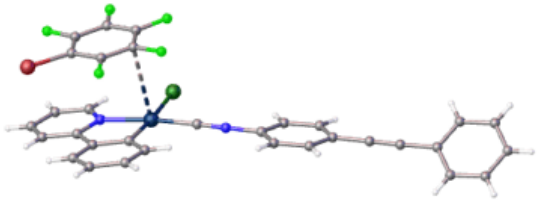
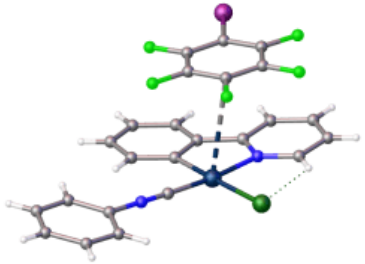
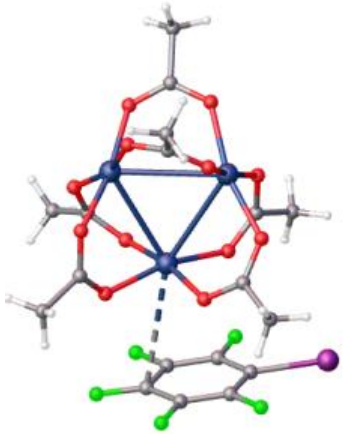
	Refcode	d(C···M), Å	d(Cg···M), Å	Θ(Cg···M),°	d(C···M)/ ΣAvdW	Type of interaction	Ref
Group 1 (X–C···M), X= Hal							
M = Pt							
	FEBLAD	3.584(5)	3.4677(16)	7.30	0.883	Classified as π-hole···Pt^{II} interaction	[3]
	GEMWUS	3.543(11)	3.418	6.29	0.873	Classified by as π-π stacking	[4]
	JUXBIQ	3.3418(16)	3.622	23.347	0.823	Classified as π-hole···Pt^{II} interactions	[5]

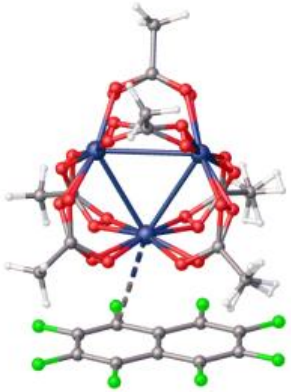
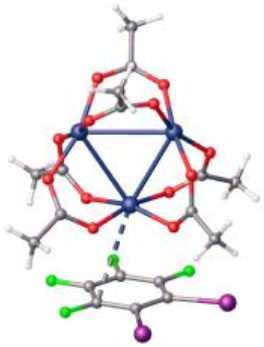
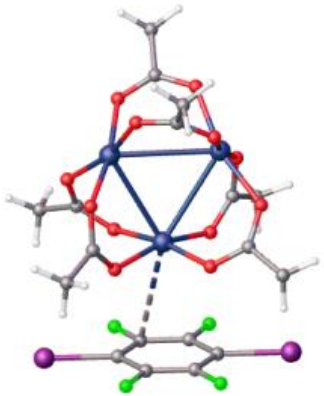
	MIRHIH	3.8456(14)	4.209	25.674	0.947	Classified as π-π stacking	[6]
	MIRHUT	3.6930(15)	4.089	30.529	0.910	Classified as π-π stacking	[6]
	NUQTEA	3.863(3)	4.231	25.273	0.951	Classified as π-π stacking	[7]

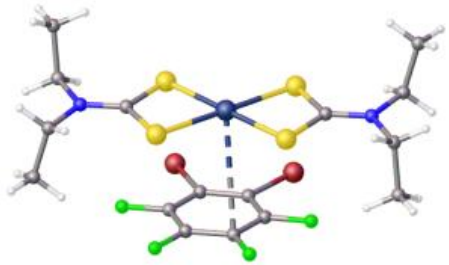
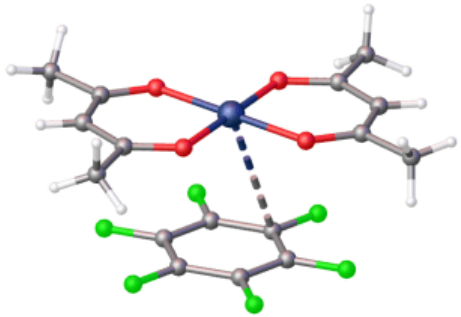
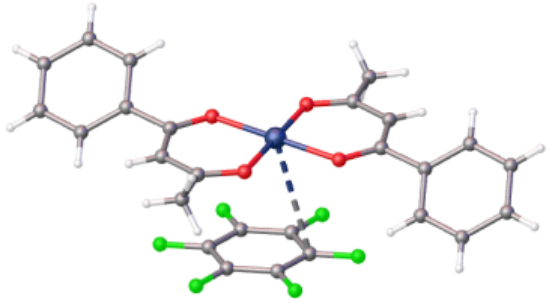
	NUQTIE	3.8332(16)	4.181	24.98	0.944	Classified as π-π stacking	[7]
	OJIXEK	3.528(8)	4.101	34.97	0.869	Classified as π-interactions	[8]
	PUNNIY	3.405(3)	3.322	8.78	0.839	Classified as π-hole···Pt^{II} interaction	[9]

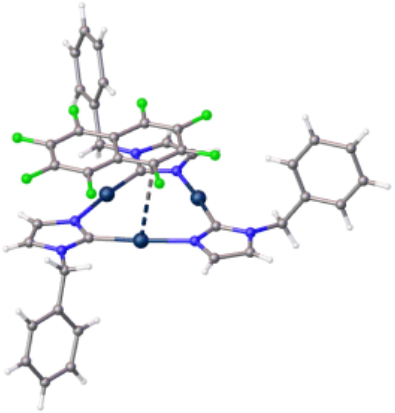
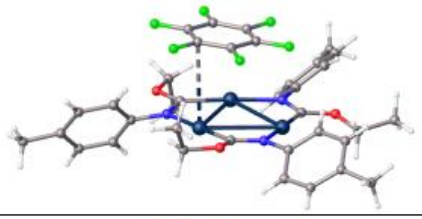
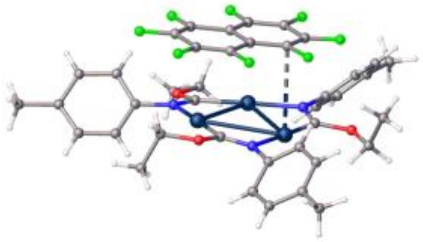
	PUNNUK	3.347(5)	3.655	25.171	0.824	Classified as π-hole···Pt^{II} interaction	[9]
	PUNPAS	3.316(4)	3.606	24.915	0.817	Classified as π-hole···Pt^{II} interaction	[9]
	PUNPEW	3.576(9)	3.343(5)	7.18	0.881	Classified as π-hole···Pt^{II} interaction	[9]

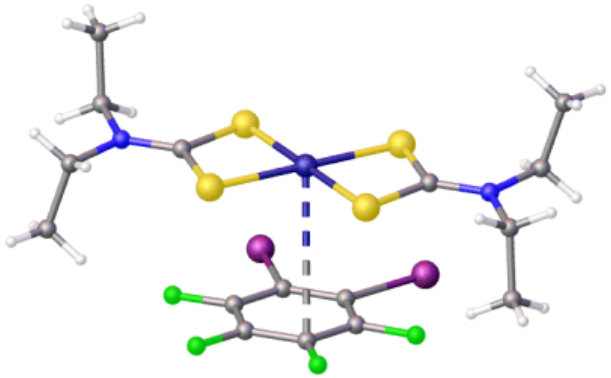
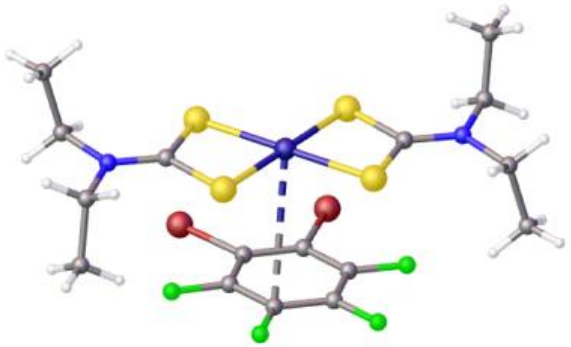
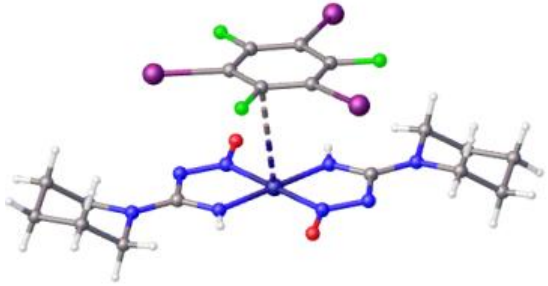
	PUNPIA	3.563(4)	3.3371(14)	2.50	0.878	Classified as π-hole···Pt^{II} interaction	[9]
	RIRKOV	3.329(5)	3.394	15.075	0.820	Classified as π-hole···Pt^{II} interaction	[10]
	RIRMEN	3.557(2)	3.28125(15)	0	0.876	Classified as π-hole···Pt^{II} interaction	[10]
	ULUZIN	3.555(5)	3.882	28.246	0.876	Classified as π-hole···Pt^{II} interaction	[11]

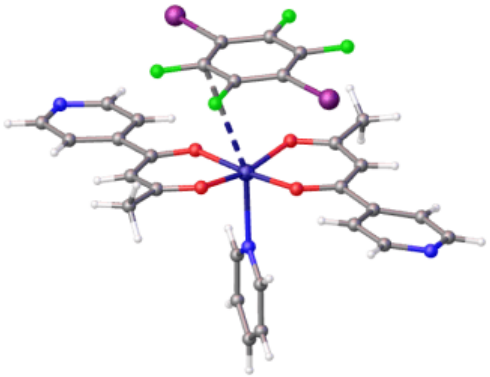
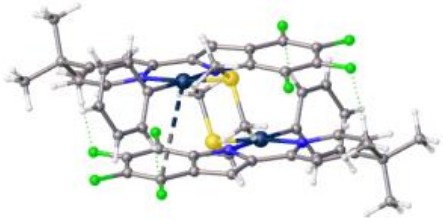
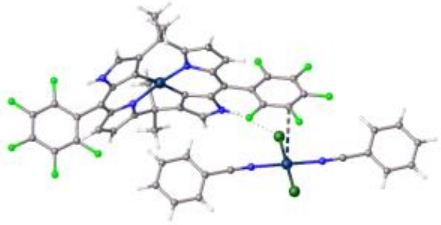
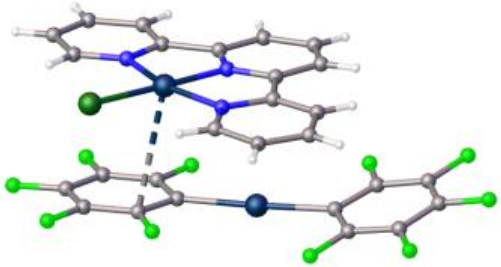
	ULUZOT	3.394(7)	3.537	17.671	0.836	Classified as π-hole···Pt^{II} interaction	[11]
	ULUZUZ	3.489(5)	3.53	12.847	0.859	Classified as π-hole···Pt^{II} interaction	[11]
	UMACAP	3.456(5)	3.786	27.289	0.851	Classified as π-hole···Pt^{II} interaction	[11]
M = Pd							
	CANZEA	3.56(1)	3.474	8.35	0.908	Classified as π-hole···Pd^{II} interaction	[12]

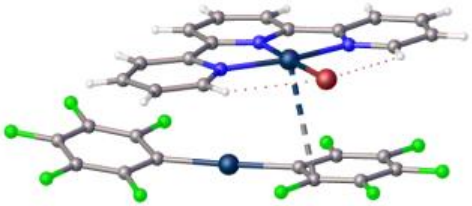
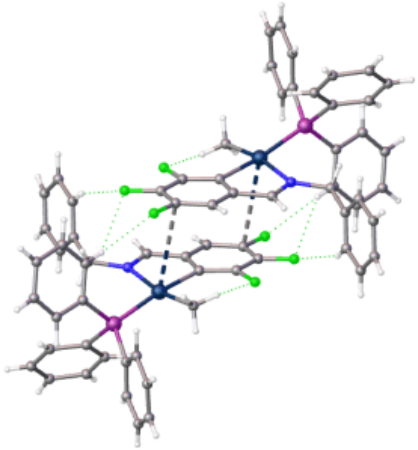
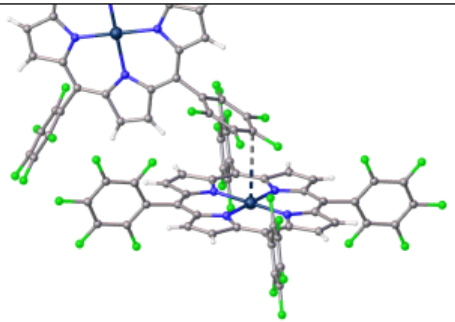
	CANZOK	3.577(3)	3.485	17.17	0.913	Classified as π-hole···Pd^{II} interaction	[12]
	CAPBAA	3.507(3)	3.308	3.83	0.895	Classified as π-hole···Pd^{II} interaction	[12]
	CAPBEE	3.641(4)	3.404	2.21	0.929	Classified as π-hole···Pd^{II} interaction	[12]

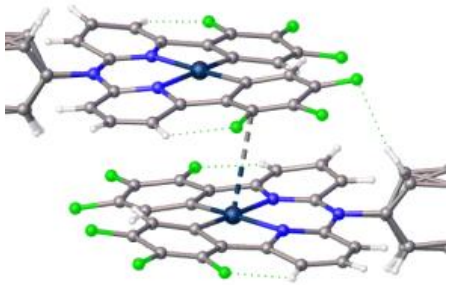
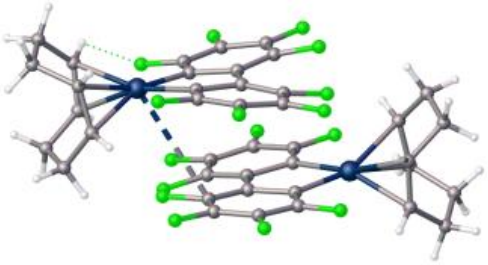
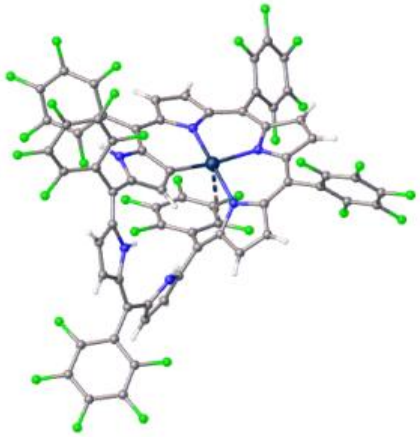
	FEBKUW	3.581(4)	3.4527(13)	6.66	0.914	Classified as π-hole···Pd^{II} interaction	[3]
	RIRMAJ	3.5119(8)	3.228(15)	0	0.896	Classified as π-hole···Pd^{II} interaction	[10]
	RIRMIR	3.423(2)	3.32670(7)	8.349	0.873	Classified as π-hole···Pd^{II} interaction	[10]
M = Au							

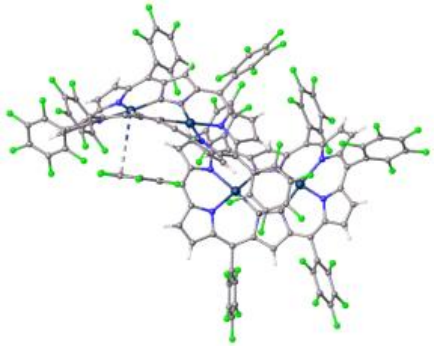
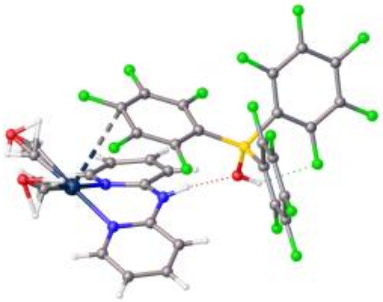
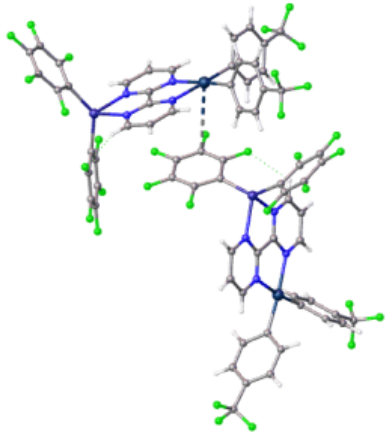
	EKUJAW	3.364(9)	3.672	26.71	0.822	Classified as π-acid–base interactions	[13]
	VOQCAF	3.545(8)	3.685	16.62	0.867	Classified as π-acid–base interactions	[14]
	XASNOV	3.516(12)	3.819(5)	23.42	0.860	Classified as π-interactions	[15]
M = Ni							

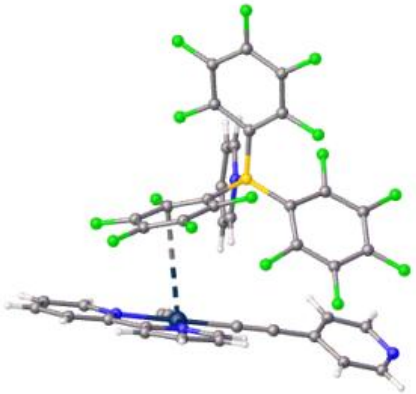
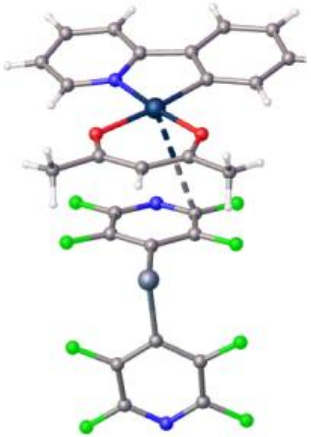
	FEBKIK	3.668(3)	3.4988(10)	4.52	0.880	Classified as π-hole···Ni^{II} interaction	[3]
	FEBKOQ	3.576(3)	3.4532(10)	6.67	0.858	Classified as π-hole···Ni^{II} interaction	[3]
	LAGHUA	3.591(4)	3.504	7.382	0.861	This contact was not mentioned in the original article	[16]
M = Cu							

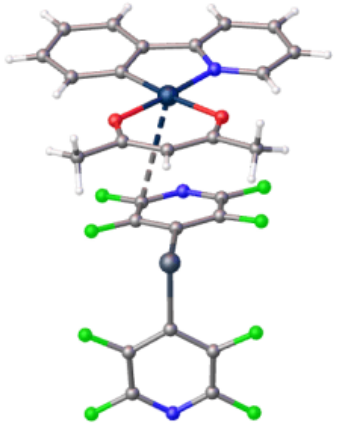
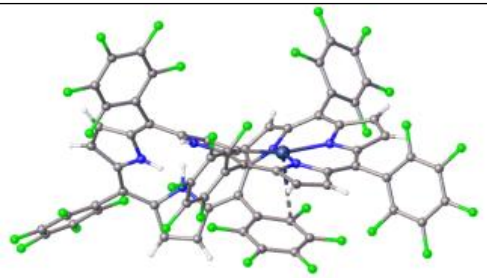
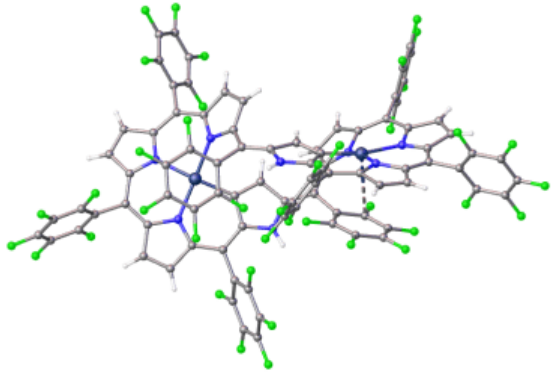
	PEHVEH	3.632(3)	3.5312(11)	6.91	0.875	Classified as π-hole···Cu interaction	[17]
Group 2 (F–C···M)							
M = Pt							
	ACUZUW	3.930(2)	4.1917(9)	23.66	0.968	This contact was not mentioned in the original article	[18]
	ADELED	3.493(9)	3.886	27.207	0.860	This contact was not mentioned in the original article	[19]
	AVEWAA	3.399(3)	3.368	10.65	0.837	Classified as π-stacking and Coulomb forces	[20]

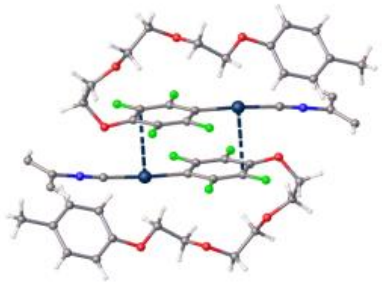
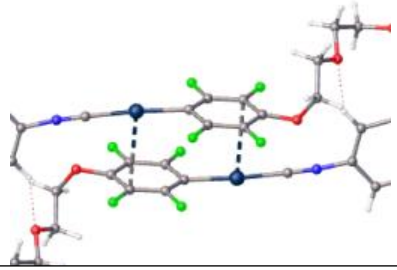
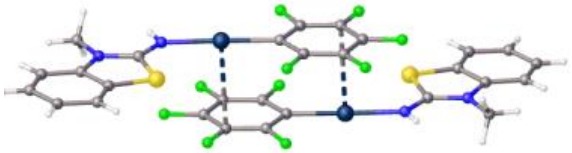
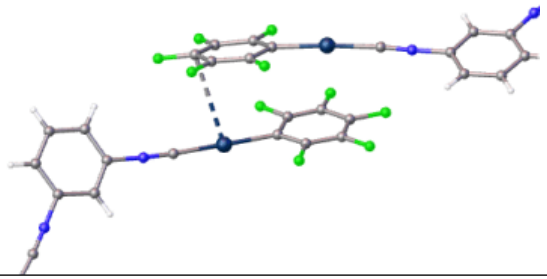
	AVEWEE	3.435(4)	3.419	13.492	0.846	Classified as π-stacking and Coulomb forces	[20]
	BACXEJ	3.746(6)	4.056(2)	25.0	0.923	These contacts were not mentioned in the original article	[21]
	BARVEW	3.56(1)	4.357	44.284	0.877	This contact was not mentioned in the original article	[2]

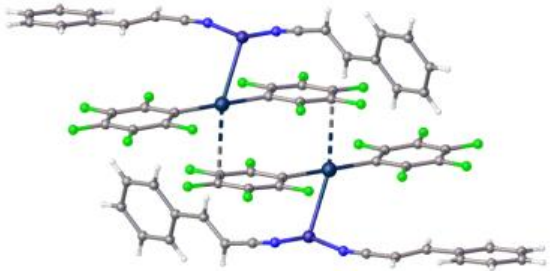
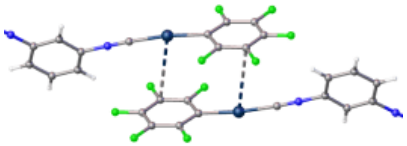
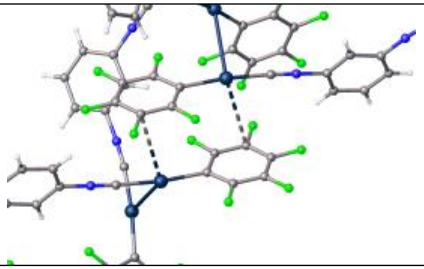
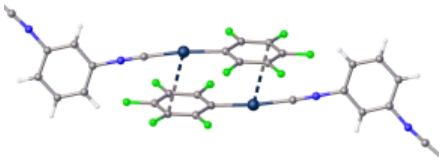
	CIZPAF	3.44(4)	3.982(14)	35.76	0.847	Classified as Pt-π interactions	[22]
	DIFHIM	3.792(2)	4.577	43.69	0.934	This contact was not mentioned in the original article	[23]
	KISYER	3.274(7)	4.128	14.764	0.806	This contact was not mentioned in the original article	[24]

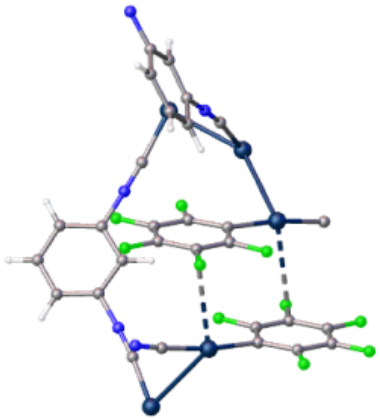
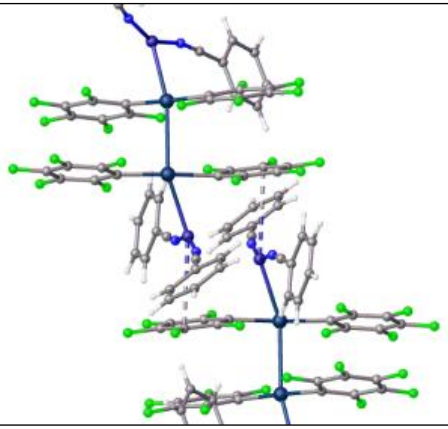
	LURFAI	3.963(11)	4.238(4)	20.49	0.976	This contact was not mentioned in the original article	[25]
	SAXVAP	3.542(4)	4.029	33.115	0.872	This contact was not mentioned in the original article	[26]
	ULAYAJ	3.665(13)	4.297	38.079	0.903	This contact was not mentioned in the original article	[27]

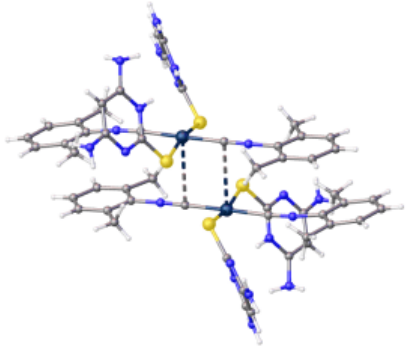
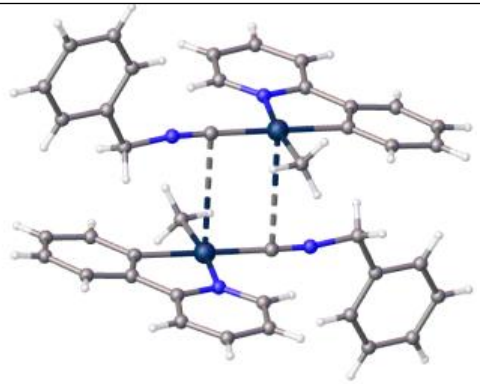
	UWIBIN	3.905(3)	4.326	28.387	0.962	Classified as Pt-Pt and/or π-π interactions	[11]
	VALVUD	3.512(5)	3.3755(17)	6.81(12)	0.865	This contact was not mentioned in the original article	[28]

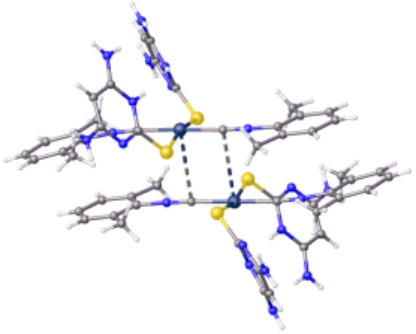
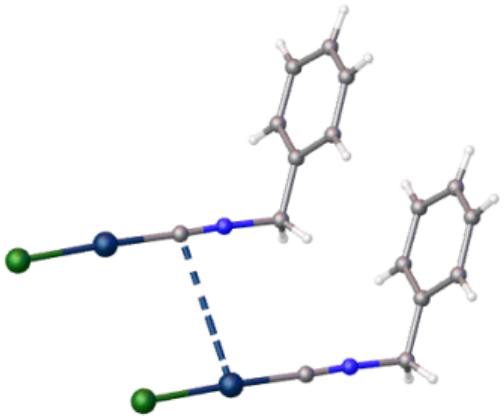
	VALWAK	3.551(7)	3.340(2)	6.54	0.875	This contact was not mentioned in the original article	[28]
M = Pd							
	KAHLUC	3.289(5)	3.991	13.351	0.839	This contact was not mentioned in the original article	[29]
	KISXOA	3.389(5)	3.318(2)	16.58	0.865	This contact was not mentioned in the original article	[24]

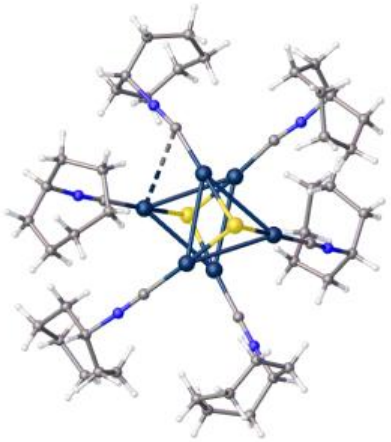
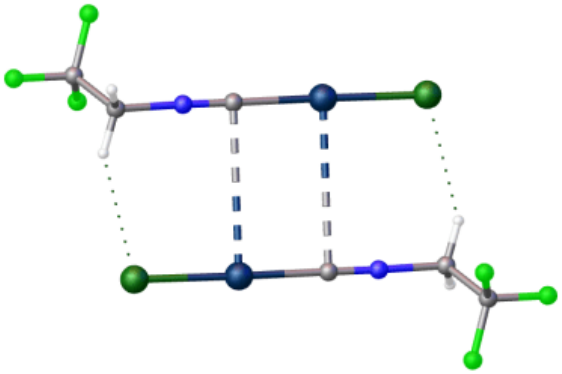
	DEFRUE01	3.403(6)	3.745	25.58	0.832	Classified as π-hole···Au intercations	[30]
	DEFSEP	3.404(13)	3.683	22.47	0.832	Classified as π-hole···Au intercations	[30]
	OLIKUQ	3.346(6)	3.673(2)	24.59	0.818	This contact was not mentioned in the original article	[31]
	TEDSID	3.501(11)	3.496(4)	12.11	0.856	Classified by the authors as Au–π interactions, π-π stacking	[32]

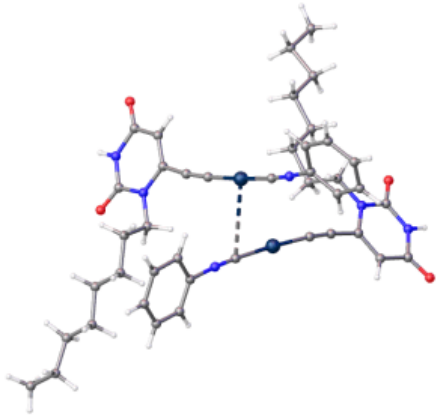
	TUDCEB	3.329(4)	3.7196(17)	28.75	0.814	These contacts were not mentioned in the original article	[33]
	WUHJUH	3.603(5)	3.818	22.1	0.881	These contacts were not mentioned in the original article	[34]
	WUHKAO	3.606(5)	3.796	21.03	0.882	These contacts were not mentioned in the original article	[34]
	WUHKES	3.609(12)	3.817	21.84	0.882	These contacts were not mentioned in the original article	[34]

	WUHKUI	3.578(10)	3.797	21.16	0.875	These contacts were not mentioned in the original article	[34]
M = Cu							
	TUDCAX	3.688(9)	3.621(4)	9.09	0.889	These contacts were not mentioned in the original article	[33]
Group 3 (N–C···M)							
M = Pt							

	BOJKIX	3.537(9)	-	88.0	0.871	Classified as π-hole···Pt^{II} interactions	[35]
	KEJGUE	3.573(14)	-	85.5	0.880	These contacts were not mentioned in the original article; no π-π interactions observed; classified by the authors as C-H-π or C-H-Pt interactions	[36]
M = Pd							

	BOJJIW	3.527(3)	-	90.23[e]	0.900	Classified as π-hole···Pd^{II} interactions	[35]
M = Au							
	BESYOQ	3.729(17)	-	100.1	0.912	This contact was not mentioned in the original article	[37]

	CAVMUI01	3.489(19)	-	71.1	0.853	This contact was not mentioned in the original article	[38]
	HUDMEY	3.644(15)	-	92.1	0.891	These contacts were not mentioned in the original article	[39]

	XORGES	3.556(10)	-	89.2	0.869	Classified as π-π interactions	[40]

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3. Computational details

3.1. Geometry

The optimization of [**1**·OFA·**1**] led to a negligible geometry distortion: the distance $Q_{Pt(\mathbf{A})}$ was reduced, while the $Q_{Pt(\mathbf{C})}$ separations increased by 0.1 Å (for $Q_{Pt(\mathbf{A})}$) and 0.5 Å (for $Q_{Pt(\mathbf{C})}$) (**Figure S5**). A similar trend was also verified for the distances, which reflect the π-π stacking between cyclometalated ligands and perfluoroarenes. Indeed, the distance between the centroids of the naphthyl fragment in complex **A** and the perfluoroarene decreases (by 0.2 Å), while the separation between- the benzothiazole fragment in complex **C** and the perfluoroarene increases (by 0.2 Å) (**Table S3**). Notably, when the optimization was performed for [**1**·OFA], OFA undergoes the greatest distortion of the molecular plane: two planes involving the terminal aromatic rings intersect along the central C−C direction with the torsion angle 17.6° (**Figure S7**).

The geometry parameters of the [**1**·OFA·**1**] most closely matched the geometry of the X-ray structure. The optimized geometry for [**1**·C_6F_6·**1**] exhibits a shift of the perfluoroarene toward the naphthyl fragment, as follows from an increased Q_{Pt} distance (by 0.1 Å) and π-π stacking (by 0.3 Å) between the naphthyl fragments and the C_6F_6 fragment. Considering the optimized geometries of the bimolecular and trimolecular models, it can be concluded that, in general, the geometries are similar (**Figure S6**). However, a comparison of the geometry of the bimolecular and trimolecular models with X-ray diffraction analysis shows that the geometry in the binuclear model agrees best with the experimental geometry. Finally, in the optimized structure of **2**·C_6F_6, we did not observe significant changes in the geometric position of the perfluoroarene in both the bimolecular and trimolecular models. Thus, the optimized structures of the trinuclear for (**1**–**2**)·Ar^F are in a good agreement with the geometry obtained from the XRD experiments.

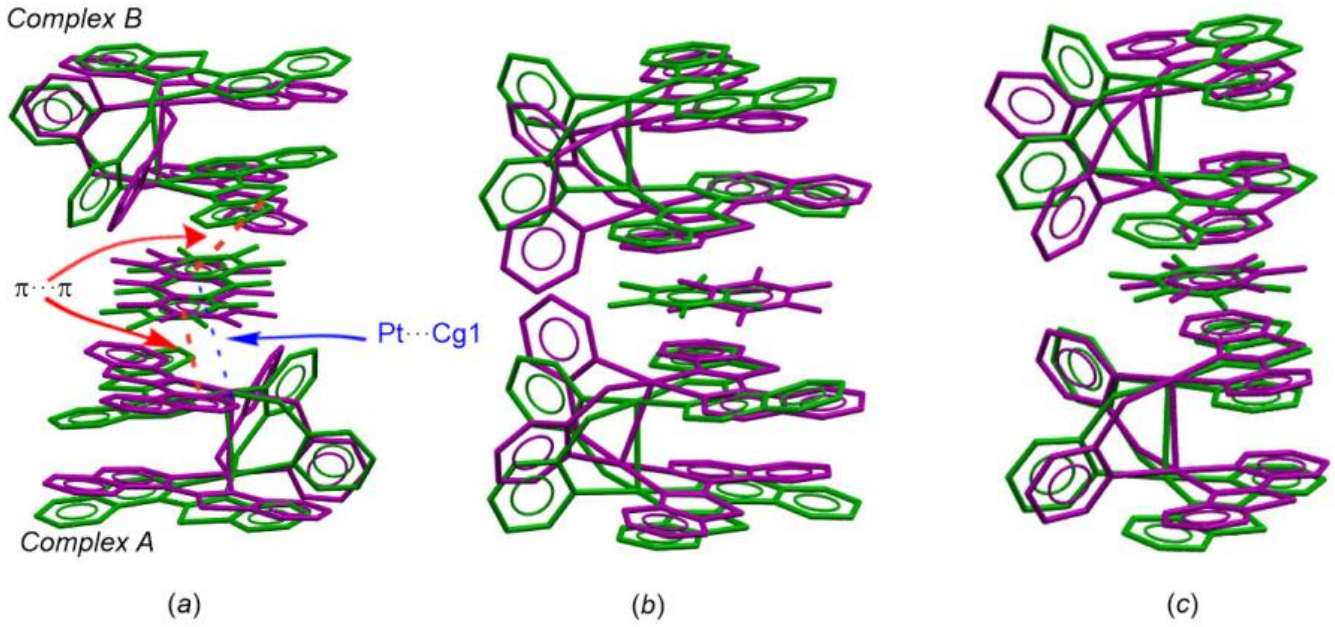


Figure S6. Overlayed images of [**1**·OFA·**1**] (a), [**1**·C_6F_6·**1**] (b), [**2**·C_6F_6·**2**] (c) in X-ray (green) and optimized (purple) geometries (hydrogen atoms were omitted for the sake of simplicity).

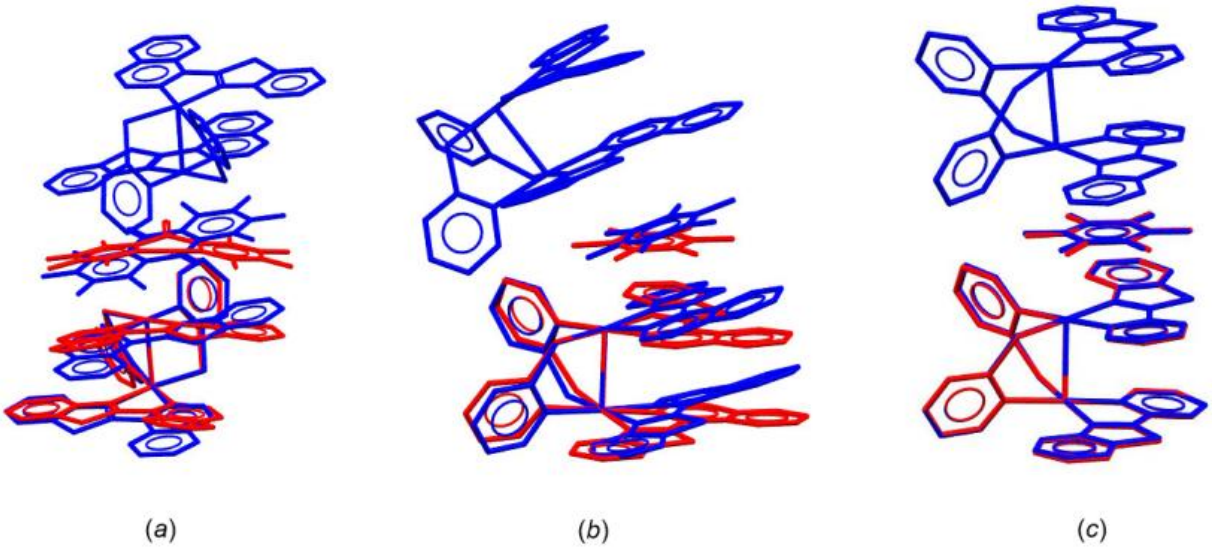


Figure S7. Overlayed images of [**1**·OFA·**1**] (a), [**1**·C_6F_6·**1**] (b), and [**2**·C_6F_6·**2**] (c) in trimolecular (blue) and bimolecular (red) optimized geometries (hydrogen atoms were omitted for the sake of simplicity).

Figure S8. X-ray (a) and optimized structures (b) of OFA.

Table S3. Intermolecular distances of optimized and X-ray structures for the trimolecular and bimolecular models [(**1**/**2**)·Ar^F]

	Pt(A, B)···Cg1, Å	M···C, Å	Q_{Pt}, Å	π-π, Å
[**1**·OFA·**1**] (X-ray)	3.805	3.755	3.653	3.548* 3.548**
[**1**·OFA·**1**]	3.817 3.852	3.474 3.487	3.507 3.520	3.309* 3.720**
[**1**·OFA]	4.163	3.727	3.501	3.327* 3.323**
[**1**·C_6F_6·**1**] (X-ray)	3.996 3.996	3.642 3.642	3.412	3.695* 3.695*
[**1**·C_6F_6·**1**]	4.301 4.289	3.541 3.548	3.296 3.206	3.387* 3.374*
[**1**·C_6F_6].	3.747	3.354	3.231	3.501*
[**2**·C_6F_6·**2**] (X-ray)	3.843 3.843	3.351	3.6122	3.458** 3.457**
[**2**·C_6F_6·**2**]	3.682 3.682	3.357 3.364	3.305 3.294	3.520** 3.516**
[**2**·C_6F_6]	3.668	3.346	3.264	3.553**

* – the distance between the centroids of the naphthyl fragment of the C^N ligand and Ar^F

** – the distance between the centroids of the benzothiazole fragment of the C^N ligand and Ar^F

3.2. QTAIM

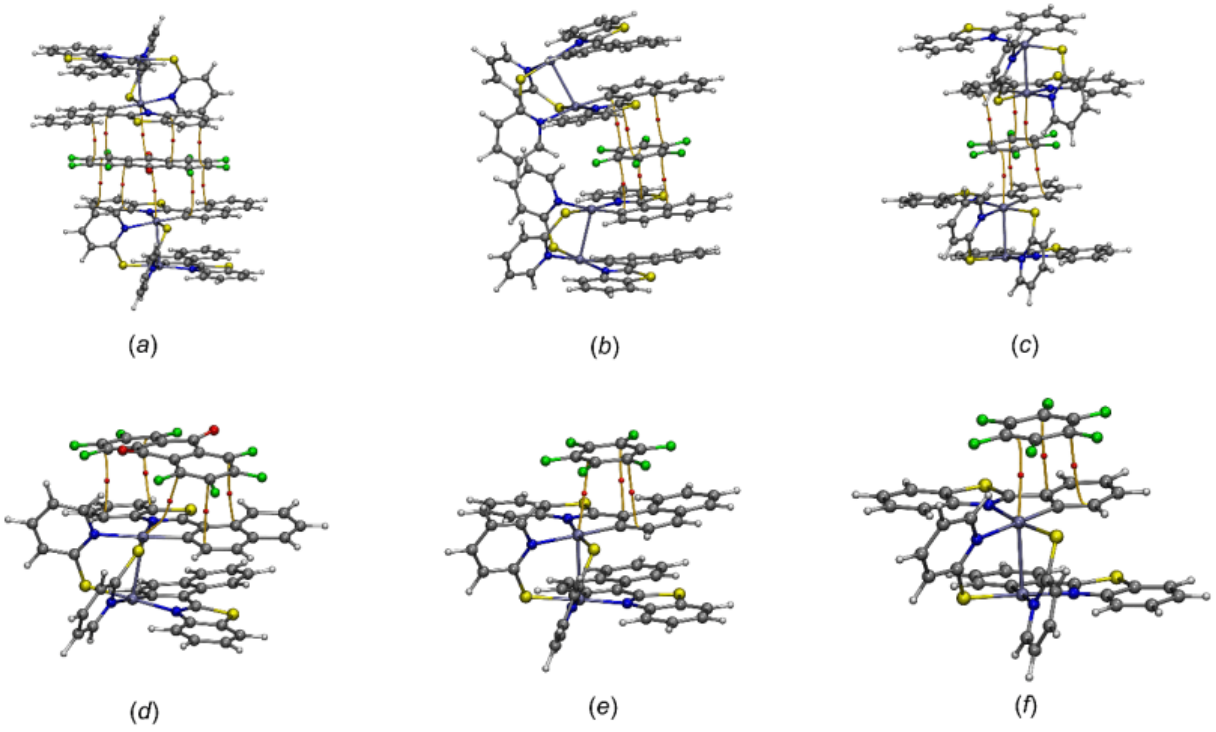


Figure S9. QTAIM distribution of bond critical points (red) and bond paths for (a) [**1**·OFA·**1**]; (b) [**1**·C_6F_6·**1**]; (c) [**2**·C_6F_6·**2**]; (d) [**1**·OFA]; (e) [**1**·C_6F_6]; (f) [**2**·C_6F_6].

Table S4. Electron density (ρ_b), its Laplacian ($\nabla^2\rho_b$), potential and kinetic energy densities (V_b and G_b), second eigenvalue of the Hessian matrix (λ_2), elliptical bond index (ε), electron localization function at BCPs (in a.u.) calculated at the PBE0-D3BJ/ZORA-def2-TZVP level of theory.

Contact	Clusters	ρ_b	$\nabla^2\rho_b$	V_b	G_b	H	ε	λ_2	ELF
C···Pt	[**1**·OFA·**1**]	0.0084	0.0211	–0.0040	0.0047	0.0006	2.18	–0.0014	0.04
C···Pt	[**1**·OFA]	0.0076	0.0210	–0.0036	0.0045	0.0008	8.1	–0.0003	0.03
C···Pt	[**1**· C_6F_6]	0.0122	0.0305	–0.0066	0.0071	0.0005	1.30	–0.0032	0.06
C···Pt	[**2**·C_6F_6·**2**]	0.0128	0.0317	–0.0069	0.0074	0.0005	1.34	–0.0035	0.067
C···Pt	[**2**·C_6F_6]	0.0128	0.0318	–0.0069	0.0074	0.0005	1.47	–0.0033	0.07
C···C^{naph}	[**1**·OTA·**1**]	0.0082	0.0245	–0.0040	0.0051	0.0011	1.06	–0.0019	0.03
C···C^{naph}	[**1**·OTA·**1**]	0.0073	0.0232	–0.0035	0.0047	0.0011	5.99	–0.0006	0.03
C···C^{naph}	[**1**·OTA]	0.0081	0.0254	–0.0041	0.0052	0.0011	3.15	–0.0012	0.03
C···C^{naph}	[**1**·OTA]	0.0084	0.0267	–0.0043	0.0055	0.0012	0.66	–0.0021	0.03
C···C^{naph}	[**1**·C_6F_6·**1**]	0.0098	0.0309	–0.0053	0.0065	0.0012	0.11	–0.0029	0.04
C···C^{naph}	[**1**·C_6F_6·**1**]	0.0083	0.0263	–0.0043	0.0055	0.0011	0.80	–0.0017	0.03
C···C^{naph}	[**1**·C_6F_6·**1**]	0.0090	0.0290	–0.0047	0.0060	0.0013	2.17	–0.0015	0.03
C···C^{naph}	[**1**·C_6F_6]	0.0082	0.0256	–0.0042	0.0053	0.0011	0.84	–0.0018	0.03
C···C^{naph}	[**1**·C_6F_6]	0.0090	0.0281	–0.0047	0.0059	0.0012	1.49	–0.0020	0.04
C···C^{ph}	[**2**·C_6F_6·**2**]	0.0082	0.0245	–0.0040	0.0050	0.0011	0.37	–0.0024	0.03
C···C^{ph}	[**2**·C_6F_6·**2**]	0.0091	0.0282	–0.0047	0.0059	0.0012	0.99	–0.0024	0.036
C···C^{ph}	[**2**·C_6F_6]	0.0081	0.0246	–0.0040	0.0050	0.0011	0.19	–0.0025	0.033
C···C^{ph}	[**2**·C_6F_6]	0.0089	0.0280	–0.0046	0.0058	0.0012	0.76	–0.0025	0.034
C···C^{bt}	[**1**·OTA·**1**]	0.0081	0.0253	–0.0041	0.0052	0.0011	9.30	–0.0004	0.02
C···C^{bt}	[**1**·OTA·**1**]	0.0093	0.0297	–0.0050	0.0062	0.0012	2.56	–0.0014	0.03
C···C^{bt}	[**1**·OTA]	0.0090	0.0273	–0.0046	0.0057	0.0011	3.12	–0.0013	0.04
C···C^{bt}	[**1**·OTA]	0.0083	0.0259	–0.0041	0.0053	0.0012	9.71	–0.0005	0.03

3.3 ETS–NOCV–CDF

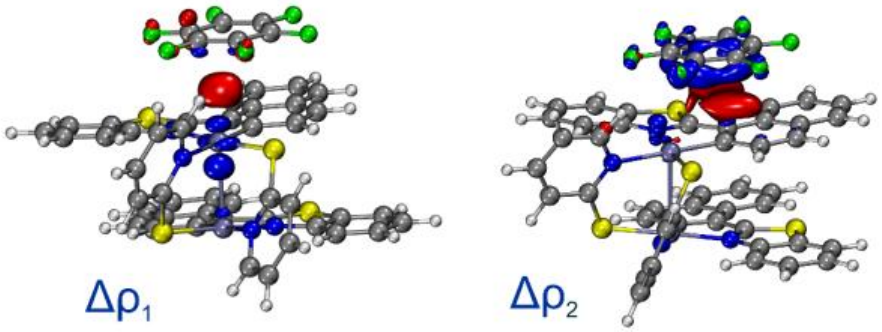


Figure S10 ETS–NOCV deformation densities for [**1**·C_6F_6] (isovalues 0.0005 a.u., electrons transfer occurs from the decreased electron density regions (blue) to the increased electron density regions (red)).

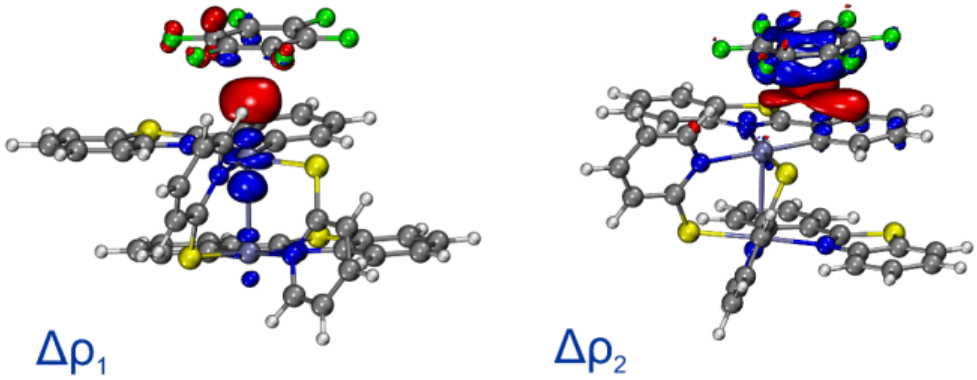


Figure S11 ETS–NOCV deformation densities for [**2**·C_6F_6·**2**] (isovalues 0.0005 a.u., electrons transfer occurs from the decreased electron density regions (blue) to the increased electron density regions (red), the second molecule of the Pt complex in trimolecular clusters was omitted for clarity).

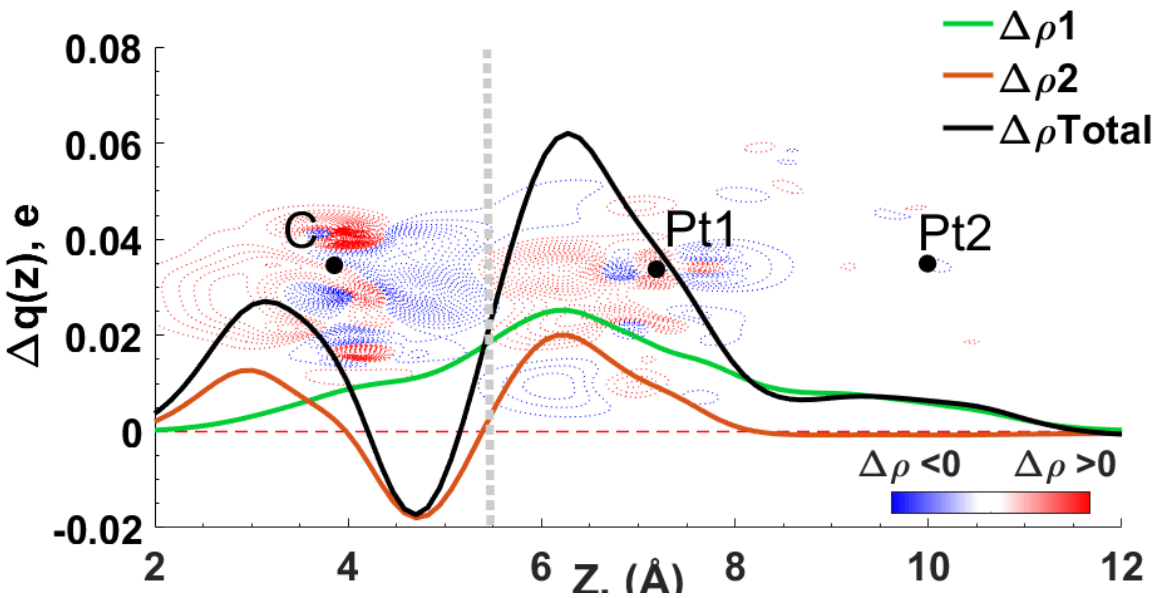


Figure S12. EDD contour plot (red – charge concentration, blue – charge depletion, range – 0.01 to 0.01 a.u., step 0.0005 a.u.) and CDF functions for the C···Pt interaction in [**1**·C_6F_6] (black dots indicate positions of the atomic nuclei, grey vertical lines identify the boundaries between the C, Pt2 and Pt1 atoms, which are placed along the *z* axis).

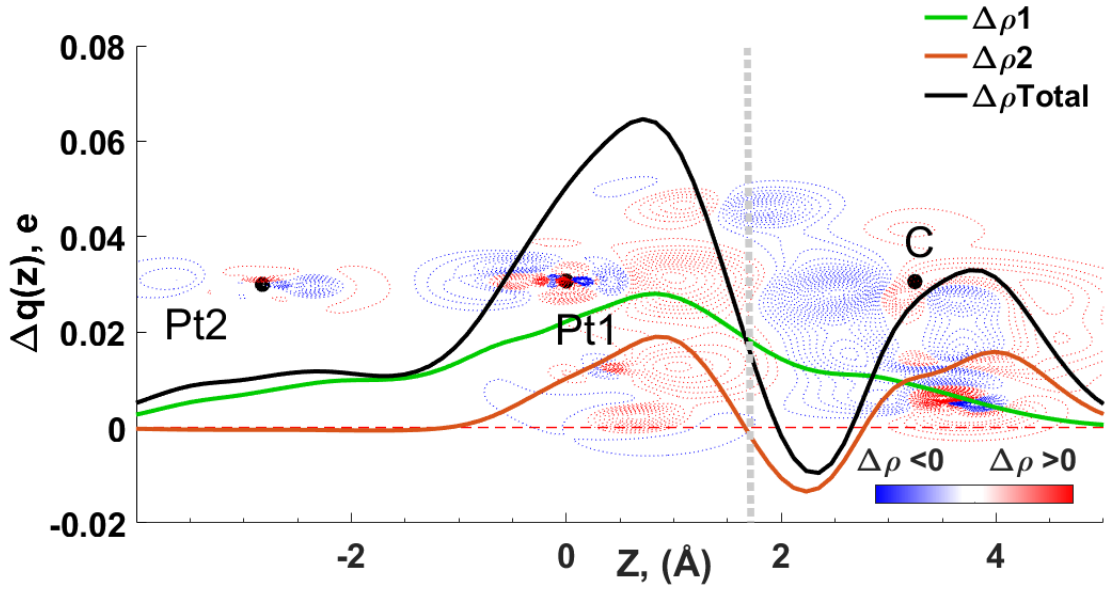
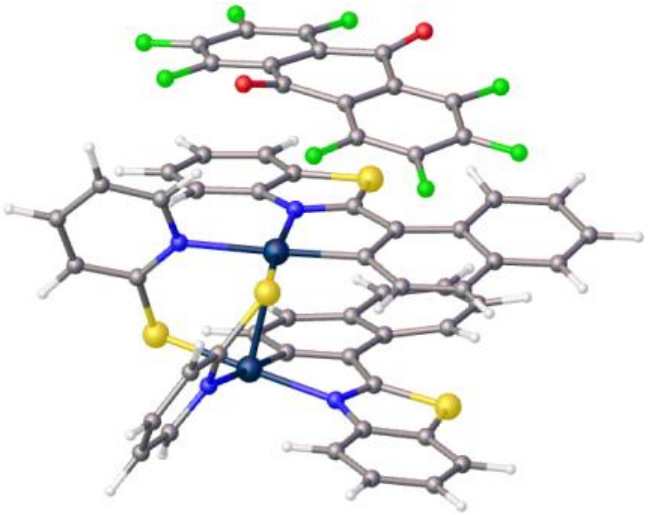


Figure S13. EDD contour plot (red – charge concentration, blue – charge depletion, range – 0.01 to 0.01 a.u., step 0.0005 a.u.) and CDF functions for the C···Pt interaction in [**2**·C_6F_6·**2**] (black dots indicate positions of the atomic nuclei, grey vertical lines identify the boundaries between the C, Pt2 and Pt1 atoms, which are placed along the *z* axis).

4. Cartesian coordinates for the studied molecules

Optimized geometries

Cartesian coordinates for [**1**·OFA] (in Å)



Pt	-0.094091000	-2.812509000	7.307402000
Pt	-0.107045000	-2.997332000	10.148798000
S	0.005481000	-5.101961000	7.264754000
S	2.043004000	-2.214308000	10.165001000
S	-1.954629000	1.264629000	6.973936000
S	-4.584068000	-2.870447000	10.085239000
N	-0.392701000	-0.775295000	7.144832000
N	0.784886000	-4.920201000	9.868014000
N	2.045366000	-2.925517000	7.531670000
N	-2.098674000	-3.510484000	10.210675000
C	-0.913722000	-1.209027000	10.390965000
C	-2.629018000	-1.501984000	6.774885000
C	2.680193000	-3.303898000	6.405559000
H	2.046434000	-3.481783000	5.540411000
C	-1.662614000	-0.445345000	6.918087000
C	-2.901012000	-2.453065000	10.136993000
C	-2.308528000	-1.141327000	10.196580000
C	0.410030000	0.318053000	7.399318000
C	1.777910000	0.326772000	7.692560000
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H	1.316728000	-7.491395000	7.773661000
C	-2.048170000	-2.770539000	6.988950000
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H	3.460959000	1.544271000	8.201813000
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C	1.410309000	-5.409489000	10.956510000
H	1.417743000	-4.747701000	11.820321000
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H	-1.162583000	-6.135565000	10.358331000
C	-2.775811000	-4.710624000	10.212488000
C	1.989537000	-6.661834000	10.999688000
H	2.467740000	-7.010329000	11.911147000
C	-2.914846000	-3.896643000	7.002244000
H	-2.495058000	-4.883575000	7.183696000
C	4.165453000	-2.840370000	8.634698000
H	4.712754000	-2.672555000	9.559320000

C	-2.256574000	1.304981000	10.351185000
C	-2.998402000	0.111770000	10.084422000
C	-0.878005000	1.205331000	10.674846000
H	-0.327849000	2.121743000	10.889717000
C	0.332752000	2.761374000	7.625980000
H	-0.228273000	3.692784000	7.585282000
C	4.812903000	-3.183086000	7.463073000
H	5.898304000	-3.273035000	7.444419000
C	-3.092226000	-7.090660000	10.240707000
H	-2.673930000	-8.094592000	10.284086000
C	1.941052000	-7.445613000	9.838484000
H	2.386011000	-8.439572000	9.819597000
C	-2.883903000	2.566812000	10.226525000
H	-2.298029000	3.459927000	10.443957000
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F	-2.884374000	-5.012596000	4.025604000
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F	1.652147000	3.745991000	4.884188000
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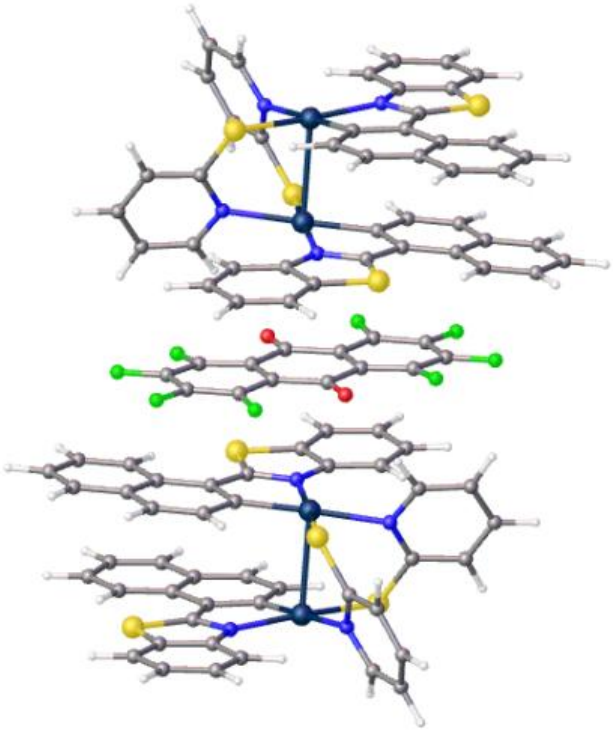
Cartesian coordinates for [**1**·OFA·**1**] (in Å)



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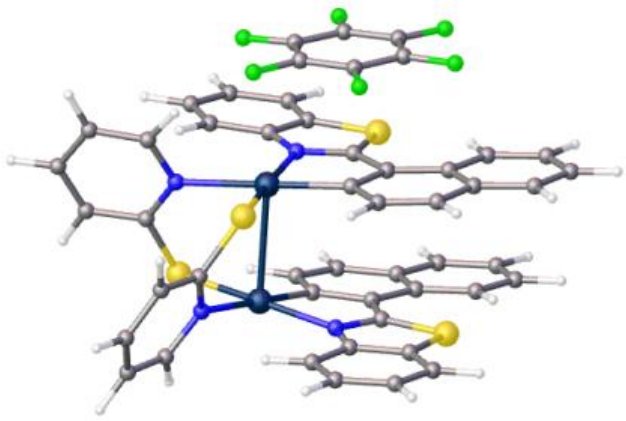
Cartesian coordinates for [**1**·C_6F_6] (in Å)



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H	-0.410025000	1.804561000	11.722205000
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C	2.257356000	-2.609023000	10.098121000
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C	2.643346000	-3.993699000	10.120452000
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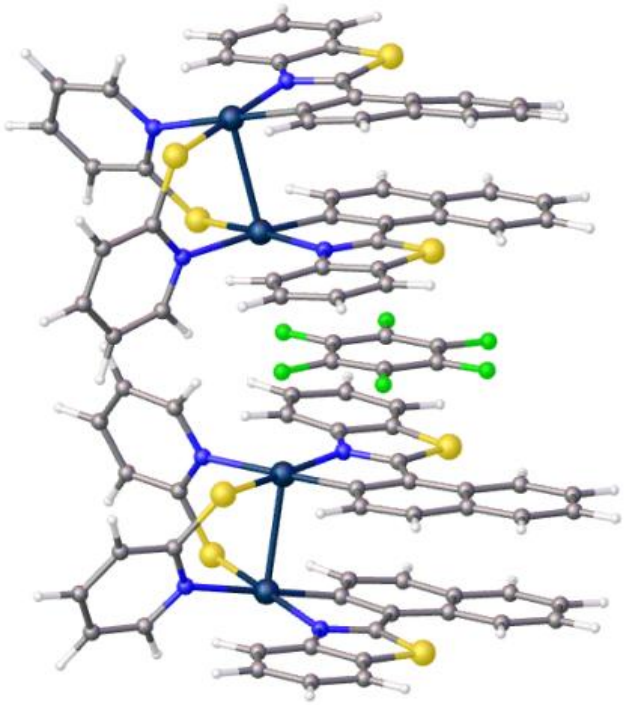
Cartesian coordinates for [**1**·C_6F_6·**1**] (in Å)



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N	3.446226000	0.194361000	-2.871340000
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C	2.964435000	3.954927000	-1.435432000
H	2.345591000	3.417833000	-0.720187000
C	0.871651000	-0.088675000	-3.062063000
C	4.815398000	0.297524000	-2.757116000
C	1.607680000	-1.287740000	-3.166474000
C	3.026544000	-1.050545000	-3.081494000
C	0.965978000	-2.566791000	-3.304122000
C	3.656950000	5.094443000	-1.076278000
H	3.579724000	5.472601000	-0.059480000
C	-0.463699000	-2.598103000	-3.307256000
C	5.571126000	1.445112000	-2.490974000
H	5.075554000	2.393360000	-2.325554000
C	4.490421000	5.176869000	-3.324176000
H	5.066848000	5.642866000	-4.120928000
C	-1.146632000	-3.829164000	-3.438675000
H	-2.237174000	-3.817320000	-3.433243000
C	5.479100000	-0.935881000	-2.916223000
C	3.759171000	4.007147000	-3.629237000
C	-1.184348000	-1.379954000	-3.199793000
H	-2.274706000	-1.418416000	-3.205018000
C	6.952789000	1.340197000	-2.428411000
H	7.541681000	2.233507000	-2.224480000
C	7.602561000	0.110963000	-2.618960000
H	8.689212000	0.057381000	-2.567164000
C	-0.544709000	-0.172367000	-3.099243000
H	-1.131256000	0.743009000	-3.043109000
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H	7.358059000	-2.006744000	-2.993857000
C	-0.459078000	-5.014632000	-3.568282000
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C	4.449666000	5.712439000	-2.051598000
H	5.012580000	6.616970000	-1.820921000
C	1.637669000	-3.806172000	-3.439692000
H	2.721357000	-3.853558000	-3.463311000
C	0.948394000	-4.993314000	-3.571874000
H	1.506575000	-5.922398000	-3.684290000
Pt	2.003621000	2.156831000	-5.659013000
S	0.075121000	2.948771000	-2.763151000
S	-0.625070000	-1.345921000	-6.633502000
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N	0.966138000	3.971750000	-5.121543000
C	1.066203000	4.966790000	-6.023465000
H	1.703169000	4.747818000	-6.879124000
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C	-0.961370000	1.177060000	-6.213591000
C	2.142259000	-0.644322000	-6.412448000
C	0.742273000	-0.302807000	-6.400605000
C	2.698497000	-1.953243000	-6.622685000
C	0.407433000	6.174010000	-5.897406000
H	0.514601000	6.936755000	-6.664981000
C	4.123029000	-2.077120000	-6.644538000
C	-1.647613000	2.389350000	-6.066868000
H	-1.095877000	3.312507000	-5.939126000
C	-0.454438000	5.372911000	-3.807789000
H	-1.030768000	5.495961000	-2.892870000
C	4.722608000	-3.343992000	-6.834502000
H	5.811705000	-3.402450000	-6.848810000
C	-1.702131000	-0.003035000	-6.431662000
C	0.246106000	4.158671000	-3.993588000
C	4.921972000	-0.924518000	-6.425094000
H	6.007507000	-1.036455000	-6.431521000
C	-3.034519000	2.386377000	-6.100864000
H	-3.568123000	3.328417000	-5.981371000
C	-3.759023000	1.199268000	-6.287752000
H	-4.847728000	1.224702000	-6.306646000
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H	5.007624000	1.149033000	-5.948388000
C	-3.096006000	-0.009141000	-6.463712000
H	-3.645658000	-0.935956000	-6.622242000
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H	-0.925071000	7.305922000	-4.611013000
C	1.946452000	-3.144990000	-6.768231000
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H	1.936637000	-5.263659000	-7.027556000
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F	4.047470000	-0.986618000	-0.015250000
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C	2.016885000	-2.156538000	-0.146477000
C	2.730644000	-0.971257000	-0.013526000
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F	-0.048470000	-3.261979000	-0.221654000
F	-1.365048000	-0.899003000	-0.027245000
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C	0.626225000	-2.135541000	-0.132550000
C	-0.048705000	-0.925501000	-0.032400000
C	0.667176000	0.260395000	0.052588000
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S	-1.087040000	3.462728000	5.634691000
S	-1.339846000	-2.224469000	3.045215000
N	-0.595179000	0.235437000	3.029474000
N	-0.324836000	3.482116000	3.015462000
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H	0.260661000	3.496428000	1.039763000

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H	-2.355632000	2.395375000	2.943053000
C	-1.750401000	5.257707000	3.744489000
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C	4.209277000	-3.571173000	2.803910000
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C	-4.173067000	1.237661000	3.001209000
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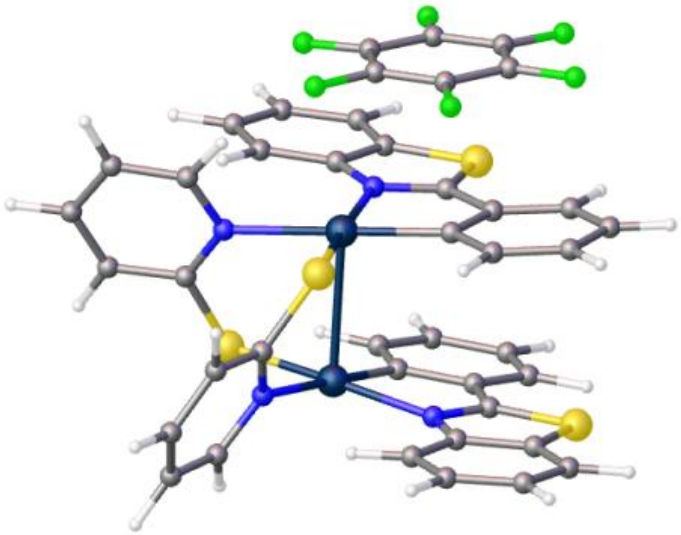
C	3.411784000	0.046321000	3.163511000
H	3.946989000	0.987518000	3.273676000
C	-3.949915000	-1.175380000	3.051734000
H	-4.384971000	-2.173578000	3.073056000
C	3.588318000	-4.790047000	2.655596000
H	4.174380000	-5.702916000	2.556250000
C	-1.776903000	5.789562000	2.470959000
H	-2.350910000	6.693606000	2.267370000
C	1.428326000	-3.694494000	2.754430000
H	0.349563000	-3.796644000	2.698495000
C	2.181712000	-4.842607000	2.629253000
H	1.675909000	-5.798007000	2.492114000
Pt	0.774333000	2.154912000	5.917341000
S	2.659074000	3.122944000	3.050259000
S	3.269974000	-1.526954000	6.439139000
N	2.335110000	0.860173000	6.277581000
N	1.866742000	3.959041000	5.514327000
C	1.827474000	4.872163000	6.503847000
H	1.206245000	4.599252000	7.355617000
C	-0.235176000	0.484422000	6.262463000
C	3.700521000	1.018129000	6.357055000
C	0.534492000	-0.697045000	6.282183000
C	1.946993000	-0.411857000	6.303990000
C	-0.074486000	-1.997170000	6.270272000
C	2.524971000	6.062977000	6.465597000
H	2.466225000	6.756952000	7.300669000
C	-1.495610000	-2.067738000	6.418809000
C	4.426503000	2.215711000	6.363112000
H	3.905551000	3.165603000	6.322430000
C	3.295775000	5.426429000	4.285675000

H	3.851265000	5.611825000	3.368343000
C	-2.146051000	-3.323551000	6.398483000
H	-3.229651000	-3.346686000	6.521253000
C	4.395685000	-0.205969000	6.444149000
C	2.561174000	4.221366000	4.386925000
C	-2.242629000	-0.863894000	6.506474000
H	-3.325889000	-0.932608000	6.618711000
C	5.811585000	2.160370000	6.426326000
H	6.378825000	3.090282000	6.425607000
C	6.492161000	0.934681000	6.489994000
H	7.580247000	0.919853000	6.536113000
C	-1.642525000	0.363561000	6.388892000
H	-2.255623000	1.262902000	6.379134000
C	5.786983000	-0.263152000	6.505053000
H	6.303629000	-1.220386000	6.560230000
C	-1.440194000	-4.486924000	6.187812000
H	-1.952856000	-5.447867000	6.158063000
C	3.289763000	6.335832000	5.322394000
H	3.858441000	7.262227000	5.241669000
C	0.613974000	-3.210543000	6.024324000
H	1.677779000	-3.208945000	5.802447000
C	-0.049668000	-4.419307000	5.976146000
H	0.513557000	-5.326490000	5.758858000

Cartesian coordinates for [**2**·C_6F_6] (in Å)



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N	4.280792000	-1.762140000	-9.527964000
C	-0.451276000	-2.977950000	-9.617178000
C	0.163498000	-1.700312000	-9.676013000
C	0.492794000	-4.050680000	-9.459266000
C	1.815344000	-6.076492000	-9.133925000
C	4.825884000	-1.249483000	-8.408273000
H	4.117477000	-0.838888000	-7.693916000
C	2.554482000	-4.873360000	-9.107904000
C	3.931195000	-4.921656000	-8.863436000
H	4.502473000	-4.003740000	-8.802632000
C	2.425049000	-7.318537000	-8.961613000
H	1.840814000	-8.236222000	-8.990894000
C	6.184280000	-1.259196000	-8.156737000
H	6.567472000	-0.844875000	-7.228042000
C	5.081275000	-2.255747000	-10.499122000
C	6.478925000	-2.296877000	-10.298287000
H	7.099751000	-2.701430000	-11.094230000
C	4.537585000	-6.156917000	-8.688589000
H	5.609109000	-6.199221000	-8.502356000
C	-0.700319000	-0.599579000	-9.790320000
H	-0.283809000	0.404044000	-9.860561000
C	-2.083412000	-0.766682000	-9.813153000
H	-2.723084000	0.112605000	-9.885411000
C	3.797459000	-7.347892000	-8.745344000
H	4.299103000	-8.304137000	-8.608570000
C	7.028303000	-1.812607000	-9.127939000
H	8.106380000	-1.844090000	-8.975506000
C	-2.662926000	-2.039254000	-9.743565000
H	-3.744940000	-2.153872000	-9.759654000
C	-1.841185000	-3.152501000	-9.654533000
H	-2.270325000	-4.152943000	-9.596245000
Pt	2.477844000	-1.889994000	-12.412589000
S	2.334724000	0.533870000	-9.810894000
S	-1.913760000	-1.538752000	-13.263620000
N	0.613061000	-1.144268000	-12.937807000
N	3.536892000	-0.043038000	-12.180881000
C	0.124956000	-3.471077000	-12.937487000
C	1.510888000	-3.607095000	-12.662437000
C	-0.294973000	-2.100307000	-13.036225000
C	-1.337981000	0.101035000	-13.225642000
C	4.388894000	0.243829000	-13.182915000
H	4.470768000	-0.522900000	-13.950847000
C	0.064037000	0.118561000	-13.053859000
C	0.731553000	1.348388000	-13.037035000
H	1.809655000	1.378454000	-12.942541000

C	-2.082292000	1.274350000	-13.340430000
H	-3.162922000	1.239487000	-13.464512000
C	5.102993000	1.424145000	-13.257127000
H	5.766596000	1.607820000	-14.097873000
C	3.401198000	0.820731000	-11.149658000
C	4.103731000	2.046516000	-11.167621000
H	3.976625000	2.722804000	-10.325526000
C	-0.008031000	2.516789000	-13.152465000
H	0.509067000	3.474318000	-13.132727000
C	1.994500000	-4.920221000	-12.548433000
H	3.044341000	-5.086727000	-12.312443000
C	1.152030000	-6.017805000	-12.714852000
H	1.565169000	-7.022335000	-12.622679000
C	-1.403438000	2.486188000	-13.294059000
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C	4.940938000	2.353581000	-12.221424000
H	5.482462000	3.298588000	-12.232620000
C	-0.212556000	-5.853911000	-12.982984000
H	-0.860068000	-6.720809000	-13.100760000
C	-0.730067000	-4.571505000	-13.088080000
H	-1.791269000	-4.418700000	-13.288104000
F	0.712792000	-4.502177000	-6.376810000
F	2.768880000	-2.746188000	-6.354999000
C	0.471329000	-3.207652000	-6.410701000
C	1.527105000	-2.306079000	-6.394405000
F	2.282388000	-0.088908000	-6.496875000
F	-1.837328000	-3.600321000	-6.523683000
F	-2.323973000	-0.938842000	-6.669828000
F	-0.258907000	0.809628000	-6.710698000
C	-0.838061000	-2.743878000	-6.493967000
C	1.276589000	-0.941866000	-6.474506000
C	-1.088455000	-1.378710000	-6.574295000
C	-0.028263000	-0.477445000	-6.576864000

Cartesian coordinates for [**2**·C_6F_6·**2**] (in Å)

Pt	5.232705000	4.093024000	4.326219000
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S	5.525096000	0.055493000	6.264188000
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F	2.422202000	3.934373000	6.374899000
N	5.323569000	2.567487000	5.730790000
N	5.540893000	5.765635000	5.619215000
C	5.026501000	1.273944000	3.760526000
C	4.920617000	2.539805000	3.128320000
C	5.290495000	1.369952000	5.170743000
C	2.167238000	1.882198000	5.270466000
C	5.657693000	1.186056000	7.576943000
C	4.440969000	6.497577000	5.881078000
H	3.539148000	6.186407000	5.361284000
C	5.509799000	2.506420000	7.097321000
C	5.535891000	3.569502000	8.006418000

H	5.384238000	4.583650000	7.659039000
C	5.870056000	0.912332000	8.927448000
H	5.988787000	-0.111307000	9.277439000
C	4.430376000	7.554605000	6.770389000
H	3.506933000	8.096623000	6.955825000
C	6.720157000	6.099256000	6.189980000
C	6.772476000	7.170586000	7.109741000
H	7.733059000	7.415745000	7.556744000
C	5.742880000	3.297270000	9.350857000
H	5.767084000	4.122596000	10.060006000
C	2.158263000	3.270080000	5.267559000
C	4.612776000	2.527548000	1.759071000
H	4.538565000	3.469243000	1.217370000
C	4.391833000	1.331701000	1.078863000
H	4.132436000	1.362809000	0.020971000
C	5.917699000	1.983297000	9.811564000
H	6.081586000	1.797916000	10.871563000
C	5.631471000	7.887463000	7.409479000
H	5.674176000	8.711707000	8.120384000
C	4.492632000	0.096990000	1.730588000
H	4.312114000	-0.829140000	1.188510000
C	4.823342000	0.067668000	3.077070000
H	4.900578000	-0.882311000	3.606278000
F	1.885153000	5.280743000	4.091093000
F	1.888630000	-0.133775000	4.105779000
F	1.319241000	1.217896000	1.825336000
F	1.352925000	3.921283000	1.814530000
C	1.887511000	1.183742000	4.102429000
C	1.886140000	3.957203000	4.094960000
C	1.607003000	1.875446000	2.930514000
C	1.614977000	3.263101000	2.926040000
Pt	8.021214000	4.236659000	3.859920000
S	4.971983000	5.621018000	2.647258000
S	7.905301000	0.916486000	0.846559000
N	8.014214000	3.182208000	2.071629000
N	7.590100000	6.195500000	3.108663000
C	8.431070000	1.395925000	3.583466000
C	8.459900000	2.428742000	4.557020000
C	8.138629000	1.879807000	2.262442000
C	7.622382000	2.361945000	-0.076196000
C	8.644547000	7.032199000	3.090698000
H	9.561369000	6.625048000	3.512669000
C	7.736235000	3.498011000	0.755659000
C	7.583780000	4.770568000	0.194003000
H	7.706981000	5.652796000	0.809492000
C	7.322664000	2.468555000	-1.433570000
H	7.231329000	1.580501000	-2.055978000
C	8.591725000	8.308778000	2.565370000
H	9.479473000	8.935543000	2.565187000
C	6.389206000	6.621442000	2.656217000
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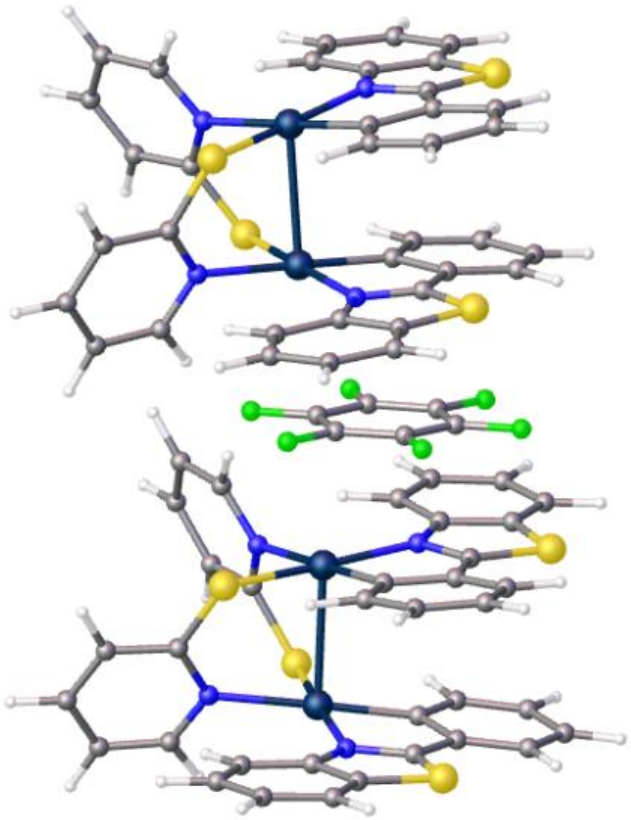
H	5.294097000	8.234751000	1.746991000



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C	8.987791000	0.696638000	6.189446000
H	9.203651000	0.426978000	7.223379000
C	7.146282000	3.740197000	-1.966025000
H	6.907684000	3.852146000	-3.022105000
C	7.367800000	8.752935000	2.047650000
H	7.273505000	9.751776000	1.623547000
C	8.951096000	-0.301900000	5.208417000
H	9.137567000	-1.341439000	5.471739000
C	8.663860000	0.050015000	3.898064000
H	8.621989000	-0.711292000	3.118148000
Pt	-1.465545000	4.072038000	3.837660000
S	-4.429690000	5.214716000	2.260502000
S	-1.754548000	0.031149000	1.906182000
N	-1.558570000	2.544180000	2.436623000
N	-1.772299000	5.743525000	2.542472000
C	-1.256222000	1.253856000	4.408089000
C	-1.153144000	2.520988000	5.038440000
C	-1.521268000	1.347389000	2.997895000
C	-1.893530000	1.160085000	0.592643000
C	-0.669376000	6.468553000	2.274339000
H	0.236613000	6.139894000	2.775564000
C	-1.749254000	2.481389000	1.070789000
C	-1.785028000	3.543889000	0.161345000
H	-1.638909000	4.559088000	0.507992000
C	-2.109553000	0.884513000	-0.756884000
H	-2.225268000	-0.139860000	-1.105709000
C	-0.660459000	7.535223000	1.396566000
H	0.265377000	8.071161000	1.205611000
C	-2.954557000	6.089701000	1.985550000
C	-3.008837000	7.171614000	1.078494000
H	-3.972150000	7.427973000	0.643833000
C	-1.995939000	3.269815000	-1.182152000
H	-2.027841000	4.094631000	-1.891583000
C	-0.846267000	2.511311000	6.407864000
H	-0.774040000	3.454023000	6.948076000
C	-0.623576000	1.316906000	7.090152000
H	-0.365048000	1.350253000	8.148185000
C	-2.165487000	1.954698000	-1.641486000
H	-2.332562000	1.767887000	-2.700738000
C	-1.866225000	7.884772000	0.775626000
H	-1.910858000	8.717796000	0.075148000
C	-0.721327000	0.081053000	6.440246000
H	-0.539338000	-0.843918000	6.983807000
C	-1.051026000	0.049077000	5.093523000
H	-1.126052000	-0.901869000	4.565719000
Pt	-4.252846000	4.223372000	4.313166000
S	-1.198289000	5.602953000	5.513529000
S	-4.133468000	0.898319000	7.321163000

N	-4.242238000	3.165847000	6.099541000
N	-3.818074000	6.180387000	5.065863000
C	-4.663807000	1.382306000	4.585860000
C	-4.693598000	2.416714000	3.614012000
C	-4.368795000	1.863913000	5.907143000
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H	-5.791130000	6.611967000	4.672790000
C	-3.960536000	3.479456000	7.415220000
C	-3.803682000	4.750998000	7.977927000
H	-3.926363000	5.634187000	7.363716000
C	-3.543314000	2.446443000	9.602048000
H	-3.452015000	1.557434000	10.223095000
C	-4.814514000	8.294542000	5.614990000
H	-5.701602000	8.922218000	5.620323000
C	-2.614258000	6.604940000	5.511617000
C	-2.491402000	7.900725000	6.062654000
H	-1.512266000	8.217153000	6.414563000
C	-3.501593000	4.855962000	9.328244000
H	-3.371132000	5.843870000	9.766068000
C	-4.974329000	2.021355000	2.296458000
H	-4.984687000	2.767826000	1.503922000
C	-5.222317000	0.687158000	1.979149000
H	-5.438585000	0.419098000	0.944887000
C	-3.362726000	3.717063000	10.135560000
H	-3.120974000	3.827205000	11.191112000
C	-3.587156000	8.737439000	6.125727000
H	-3.489426000	9.736171000	6.549313000
C	-5.185023000	-0.312911000	2.958602000
H	-5.371553000	-1.352045000	2.693732000
C	-4.897044000	0.036924000	4.269346000
H	-4.854587000	-0.725644000	5.048000000