Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Pd and Pt Metal Atoms as Electron Donor in σ-Hole Bonded Complexes

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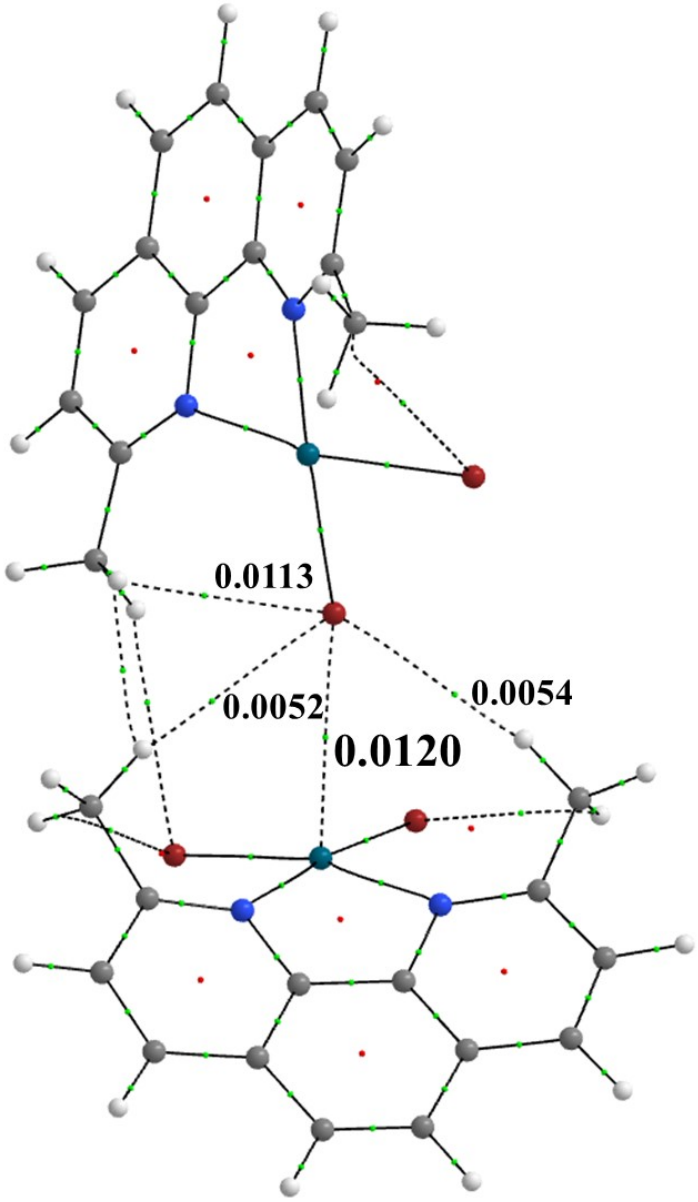


Figure S1. Dimeric form of [Pd(2,9-dimethylphenanthroline)Br_2] extracted from the crystal structure (CSD identifier: **DAPYUQ**). Only hydrogen atoms were optimized using PBE0-D3/def2-TZVP level of theory. Electron density (ρ) [a.u.] values at BCPs are indicated. Green dots show BCPs while red – RCPs. Color coding: carbon, grey; nitrogen, blue; palladium, cyan; hydrogen, white; bromine, brown.

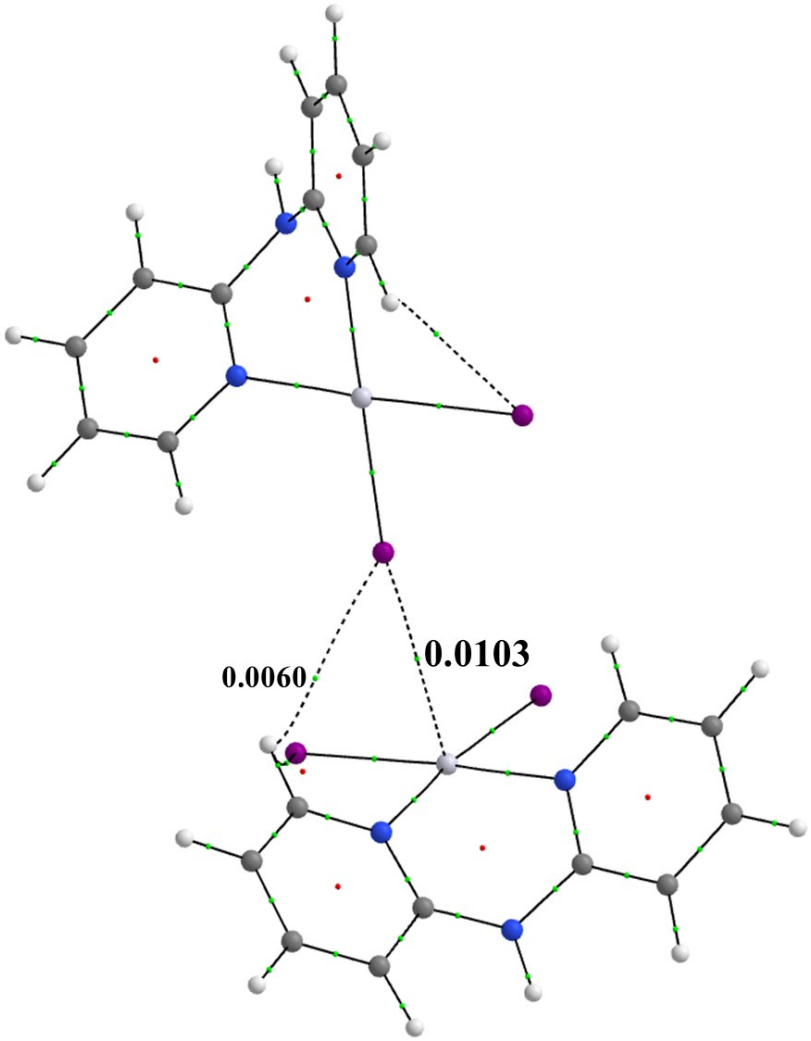


Figure S2. Dimeric form of (Di-2-pyridylamine-$\kappa^2N^2,N^{2'}$)diiodido-platinum(II) extracted from the crystal structure (CSD identifier: **YAVCIJ**). Only hydrogen atoms were optimized using PBE0-D3/def2-TZVP level of theory. Electron density (ρ) [a.u.] values at BCPs are indicated. Green dots show BCPs while red – RCPs. Color coding: carbon, grey; nitrogen, blue; platinum, silver; hydrogen, white; iodine, violet.

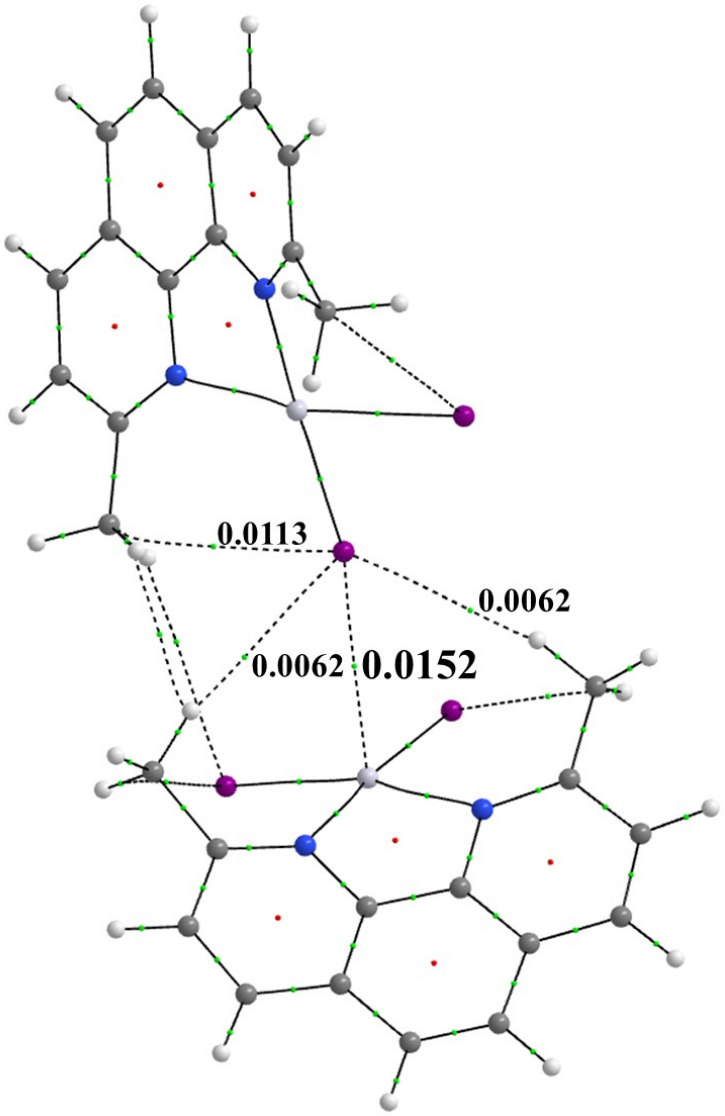


Figure S3. Dimeric form of (2,9-Dimethyl-1,10-phenanthroline)-di-iodo-platinum(II) extracted from the crystal structure (CSD identifier: **ZEWXUU**). Only hydrogen atoms were optimized using PBE0-D3/def2-TZVP level of theory. Electron density (ρ) [a.u.] values at BCPs are indicated. Green dots show BCPs while red – RCPs. Color coding: carbon, grey; nitrogen, blue; platinum, silver; hydrogen, white; iodine, violet.

Table S1. Electron density and its Laplacian at Bond Critical Points (BCPs) and other QTAIM descriptors of dimeric structures extracted from the Cambridge Structural Database (CSD). Only hydrogen atoms were optimized. QTAIM parameters were calculated at the PBE0-D3/def2-TZVP level of theory.

Number	CSD number	Interaction	ρ [a.u.]	∇^2_ρ [a.u.]	V [a.u.]	G [a.u]	H, kcal/mol
1	**DAPYUQ**	**Pd···Br**	0.012	0.034	-0.007	0.008	0.387
2	**YAVCIJ**	**Pt···I**	0.010	0.025	-0.005	0.006	0.336
3	**ZEWXUU**	**Pt···I**	0.015	0.036	-0.009	0.009	0.083

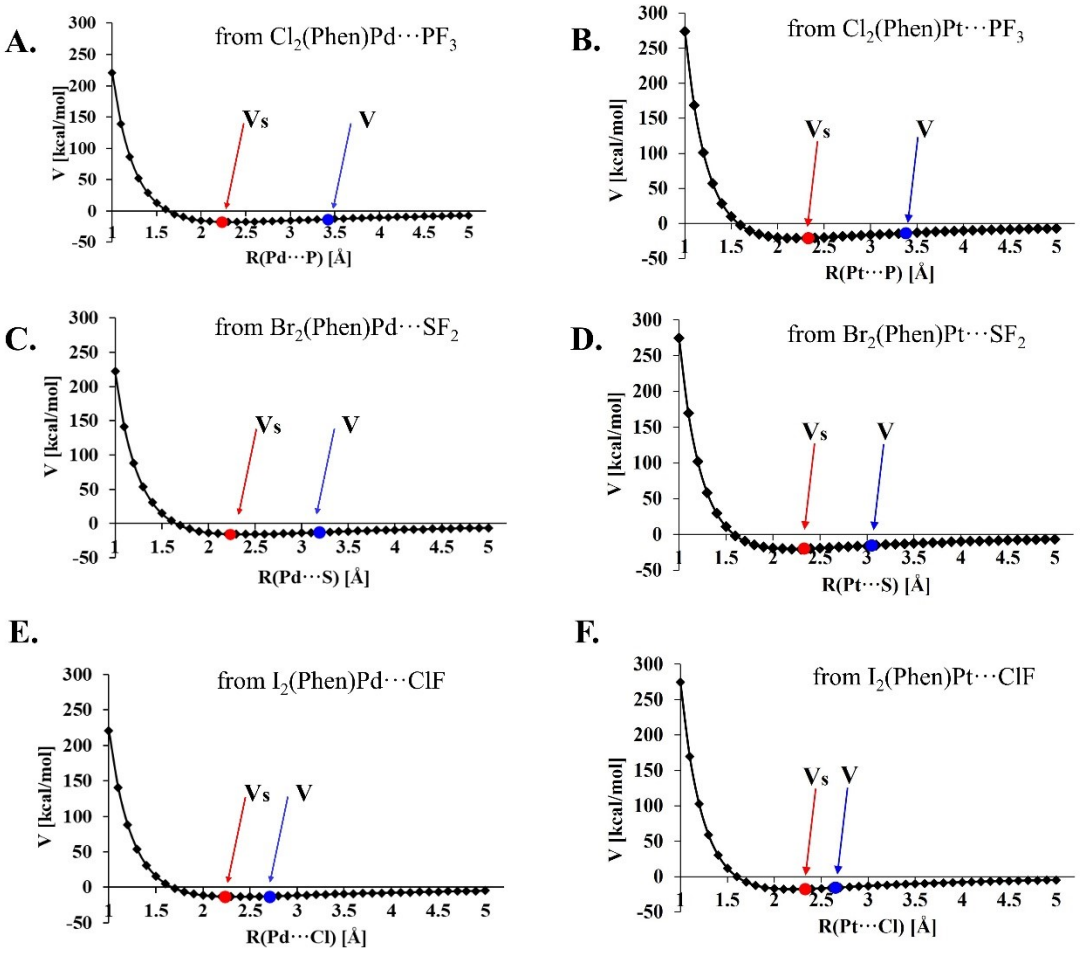


Figure S4. Plots showing the relationship between the value of the electrostatic potential and the distance from the metal atom (M) at the point lying on the axis passing through the M and A atoms. In addition, points corresponding to the values of V_s and V are highlighted (their values are given in Table 2).

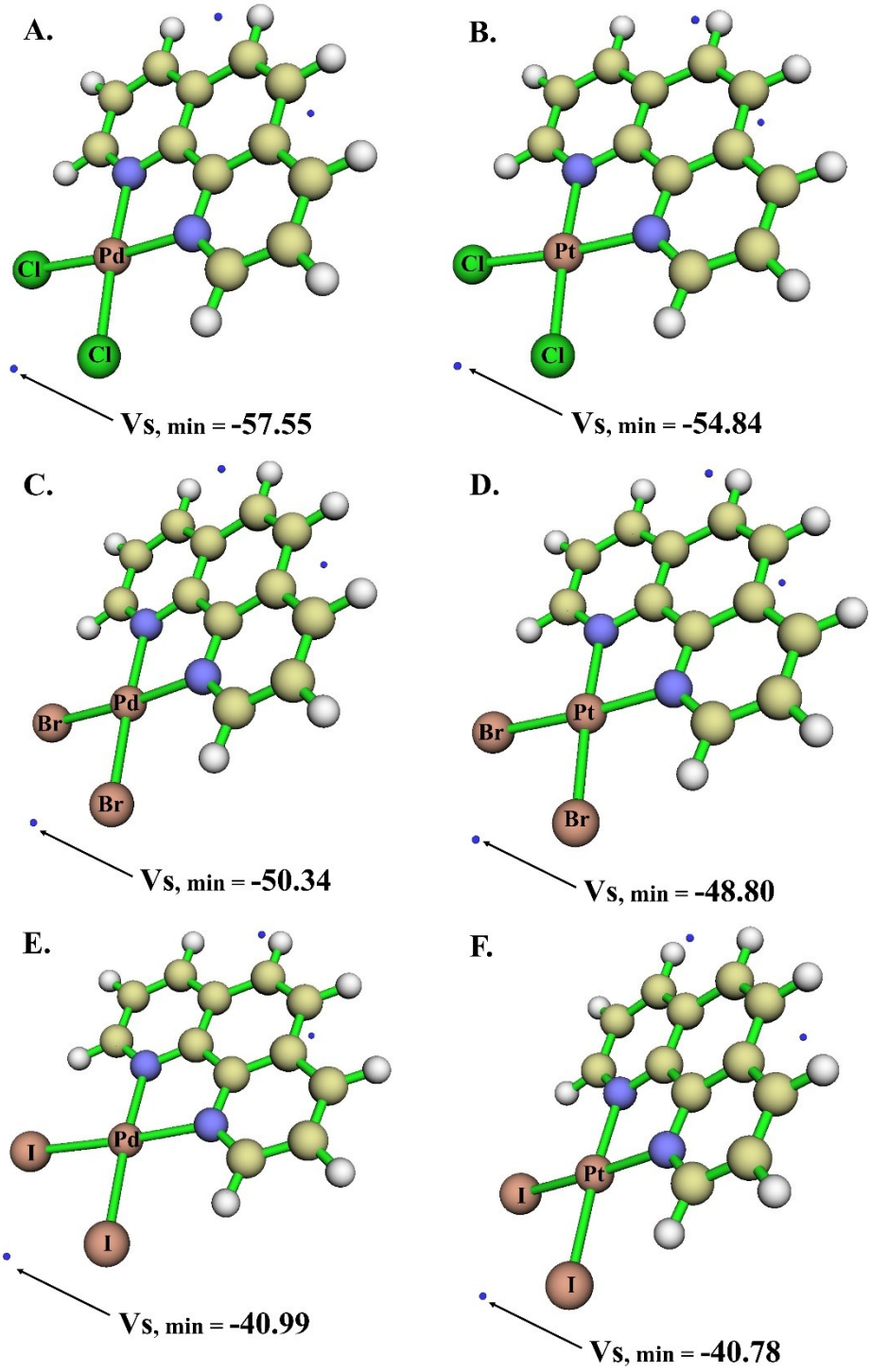
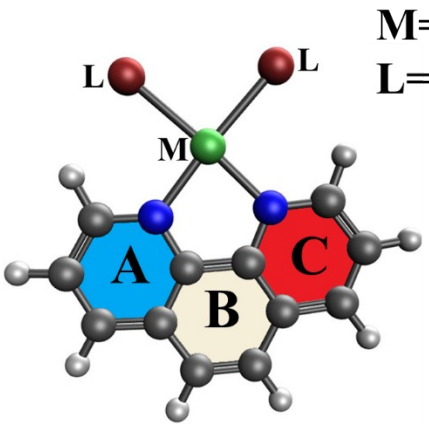


Figure S5. Diagrams representing the positions and values (in kcal/mol) of the minima of electrostatic potential ($V_{s,min}$) near the metal atom for the six selected LBs (in complex geometry). Labeling of compounds corresponds to Figure S4.

Table S2. HOMA index values for rings of the studied Lewis Bases.



Complex	*HOMA index*			Complex	*HOMA index*		
	RING A	**RING B**	**RING C**		**RING A**	**RING B**	**RING C**
Cl_2(Phen)Pd	0.954	0.750	0.954	Cl_2(Phen)Pt	0.960	0.766	0.960
Br_2(Phen)Pd	0.952	0.746	0.952	Br_2(Phen)Pt	0.958	0.764	0.958
I_2(Phen)Pd	0.949	0.734	0.949	I_2(Phen)Pt	0.956	0.758	0.956

Table S3. HOMA index values for rings of the studied complexes. The rings designation is shown above Table S2.

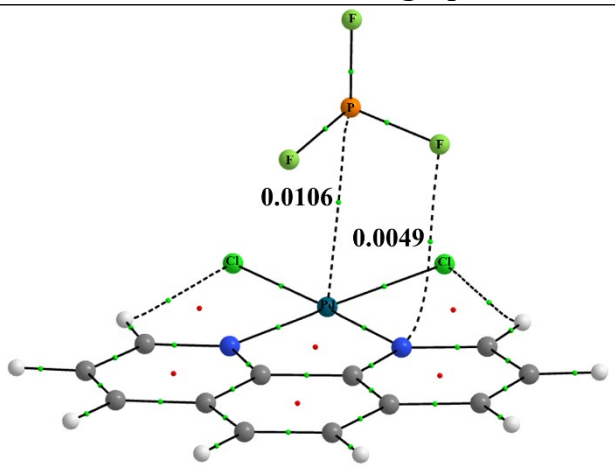
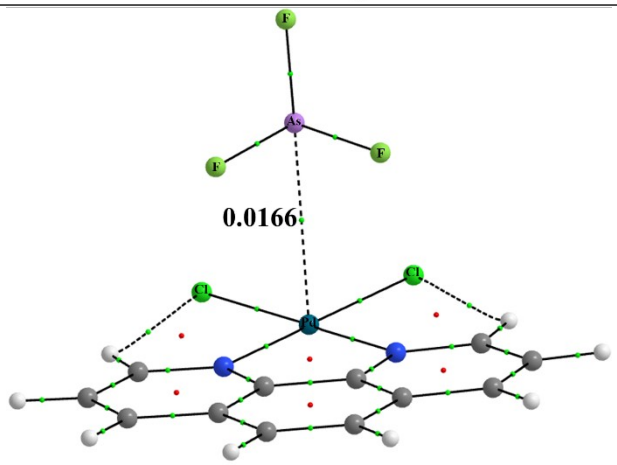
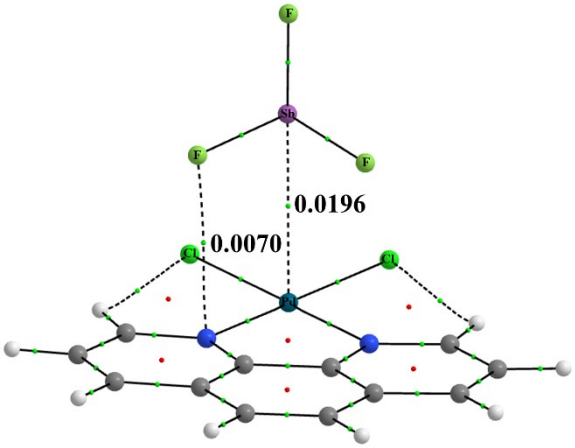
Complex	*HOMA index*			Complex	*HOMA index*		
	RING A	**RING B**	**RING C**		**RING A**	**RING B**	**RING C**
Cl_2(Phen)Pd···PF_3	0.955	0.753	0.955	Cl_2(Phen)Pt···PF_3	0.960	0.768	0.960
Cl_2(Phen)Pd···AsF_3	0.954	0.756	0.954	Cl_2(Phen)Pt···AsF_3	0.960	0.769	0.960
Cl_2(Phen)Pd···SbF_3	0.955	0.759	0.954	Cl_2(Phen)Pt···SbF_3	0.959	0.772	0.960
Cl_2(Phen)Pd···SF_2	0.955	0.753	0.956	Cl_2(Phen)Pt···SF_2	0.960	0.767	0.960
Cl_2(Phen)Pd···SeF_2	0.955	0.755	0.956	Cl_2(Phen)Pt···SeF_2	0.960	0.768	0.961
Cl_2(Phen)Pd···TeF_2	0.956	0.758	0.956	Cl_2(Phen)Pt···TeF_2	0.961	0.770	0.961
Cl_2(Phen)Pd···ClF	0.954	0.753	0.954	Cl_2(Phen)Pt···ClF	0.959	0.766	0.959
Cl_2(Phen)Pd···BrF	0.954	0.754	0.954	Cl_2(Phen)Pt···BrF	0.959	0.766	0.959
Cl_2(Phen)Pd···IF	0.954	0.755	0.954	Cl_2(Phen)Pt···IF	0.959	0.767	0.959
Br_2(Phen)Pd···PF_3	0.953	0.749	0.953	Br_2(Phen)Pt···PF_3	0.959	0.766	0.959
Br_2(Phen)Pd···AsF_3	0.953	0.752	0.953	Br_2(Phen)Pt···AsF_3	0.958	0.768	0.958
Br_2(Phen)Pd···SbF_3	0.953	0.756	0.953	Br_2(Phen)Pt···SbF_3	0.958	0.770	0.958
Br_2(Phen)Pd···SF_2	0.954	0.749	0.953	Br_2(Phen)Pt···SF_2	0.959	0.765	0.959
Br_2(Phen)Pd···SeF_2	0.954	0.751	0.953	Br_2(Phen)Pt···SeF_2	0.959	0.766	0.959
Br_2(Phen)Pd···TeF_2	0.955	0.753	0.954	Br_2(Phen)Pt···TeF_2	0.959	0.768	0.960
Br_2(Phen)Pd···ClF	0.952	0.748	0.952	Br_2(Phen)Pt···ClF	0.957	0.763	0.957
Br_2(Phen)Pd···BrF	0.952	0.749	0.952	Br_2(Phen)Pt···BrF	0.957	0.764	0.957
Br_2(Phen)Pd···IF_3	0.952	0.750	0.952	Br_2(Phen)Pt···IF	0.957	0.765	0.957
I_2(Phen)Pd···PF_3	0.950	0.738	0.950	I_2(Phen)Pt···PF_3	0.956	0.760	0.956
I_2(Phen)Pd···AsF_3	0.950	0.742	0.950	I_2(Phen)Pt···AsF_3	0.956	0.763	0.956
I_2(Phen)Pd···SbF_3	0.951	0.746	0.951	I_2(Phen)Pt···SbF_3	0.956	0.765	0.956
I_2(Phen)Pd···SF_2	0.951	0.738	0.950	I_2(Phen)Pt···SF_2	0.957	0.759	0.956
I_2(Phen)Pd···SeF_2	0.952	0.740	0.951	I_2(Phen)Pt···SeF_2	0.957	0.760	0.956
I_2(Phen)Pd···TeF_2	0.953	0.742	0.952	I_2(Phen)Pt···TeF_2	0.958	0.761	0.957
I_2(Phen)Pd···ClF	0.949	0.736	0.950	I_2(Phen)Pt···ClF	0.955	0.756	0.955
I_2(Phen)Pd···BrF	0.950	0.737	0.950	I_2(Phen)Pt···BrF	0.955	0.757	0.955
I_2(Phen)Pd···IF	0.950	0.738	0.950	I_2(Phen)Pt···IF	0.955	0.759	0.955

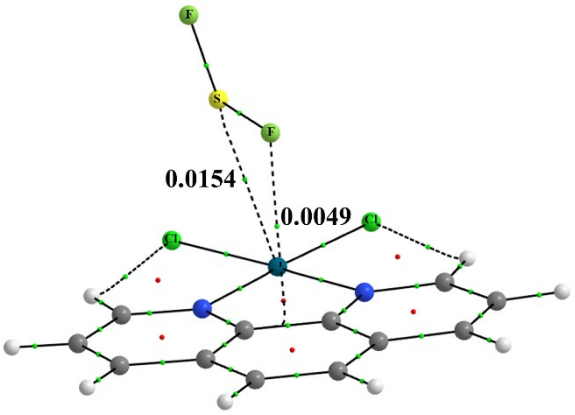
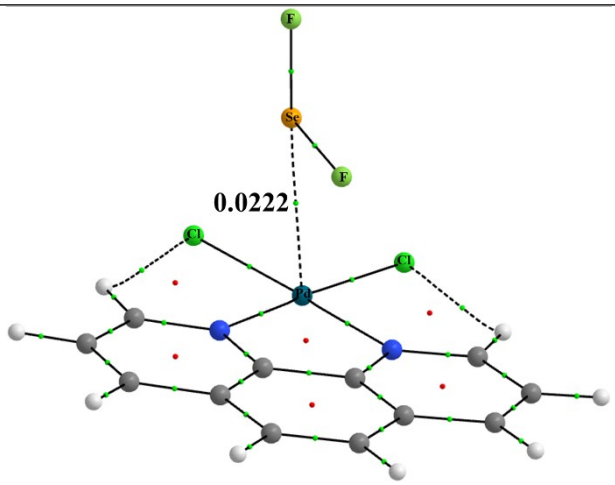
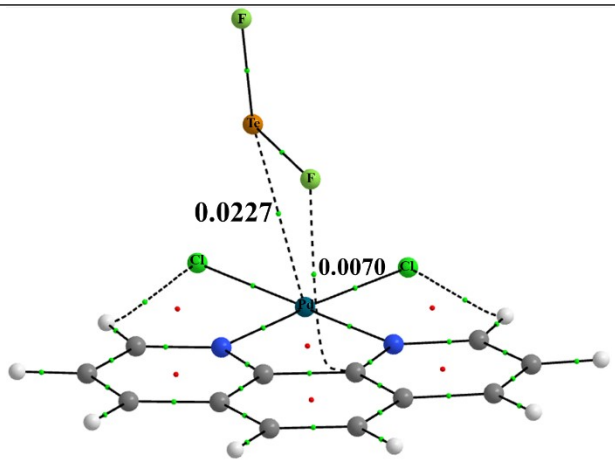
Table S4. Bond Critical Points (BCPs) and other descriptors derived from Quantum Theory of Atoms In Molecules (QTAIM) for the studied complexes. QTAIM parameters were calculated at the PBE0-D3/def2-TZVP level of theory.

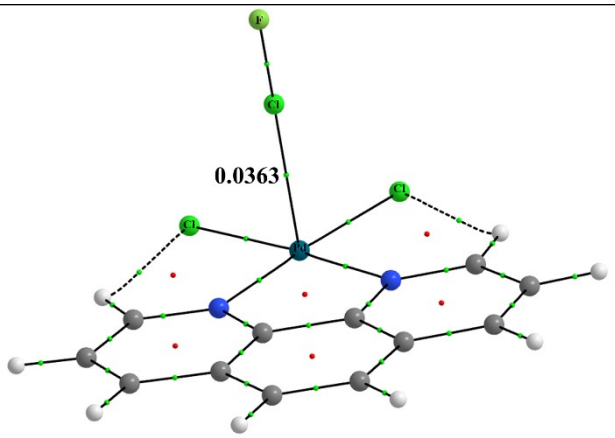
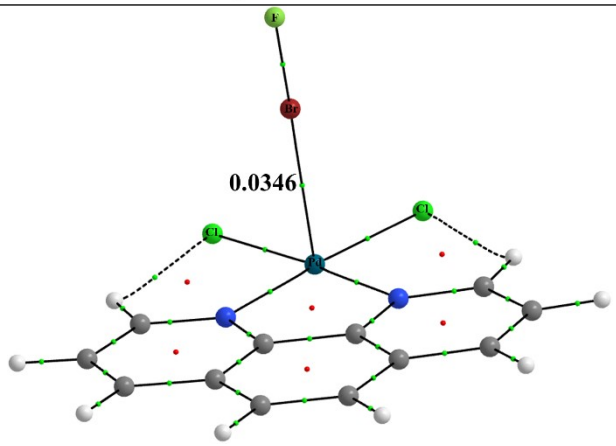
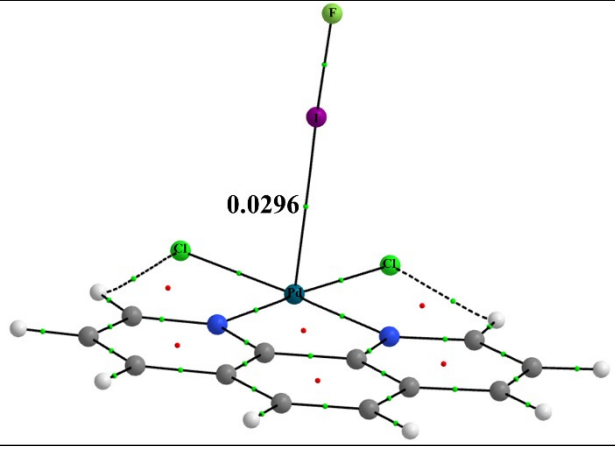
Complex	Interaction	Electron density (ρ) [a.u.]	Laplacian (∇^2_ρ) [a.u.]	V [a.u.]	G [a.u.]	H [kcal/mol]
Cl_2(Phen)Pd···PF_3	Pd···P	0.011	0.024	-0.005	0.006	0.247
Cl_2(Phen)Pd···AsF_3	Pd···As	0.017	0.034	-0.009	0.009	-0.261
Cl_2(Phen)Pd···SbF_3	Pd···Sb	0.020	0.034	-0.011	0.010	-0.879
Cl_2(Phen)Pd···SF_2	Pd···S	0.015	0.039	-0.009	0.010	0.164
Cl_2(Phen)Pd···SeF_2	Pd···Se	0.022	0.046	-0.014	0.013	-0.769
Cl_2(Phen)Pd···TeF_2	Pd···Te	0.023	0.042	-0.014	0.012	-1.199
Cl_2(Phen)Pd···ClF	Pd···Cl	0.036	0.084	-0.029	0.025	-2.393
Cl_2(Phen)Pd···BrF	Pd···Br	0.035	0.070	-0.025	0.021	-2.528
Cl_2(Phen)Pd···IF	Pd···I	0.030	0.055	-0.020	0.017	-2.084
Br_2(Phen)Pd···PF_3	Pd···P	0.010	0.023	-0.005	0.005	0.263
Br_2(Phen)Pd···AsF_3	Pd···As	0.016	0.032	-0.009	0.008	-0.162
Br_2(Phen)Pd···SbF_3	Pd···Sb	0.019	0.033	-0.010	0.009	-0.718
Br_2(Phen)Pd···SF_2	Pd···S	0.015	0.038	-0.009	0.009	0.223
Br_2(Phen)Pd···SeF_2	Pd···Se	0.021	0.045	-0.013	0.012	-0.665
Br_2(Phen)Pd···TeF_2	Pd···Te	0.022	0.041	-0.014	0.012	-1.128
Br_2(Phen)Pd···ClF	Pd···Cl	0.036	0.084	-0.028	0.025	-2.348
Br_2(Phen)Pd···BrF	Pd···Br	0.034	0.069	-0.025	0.021	-2.472
Br_2(Phen)Pd···IF	Pd···I	0.029	0.055	-0.020	0.017	-2.022
I_2(Phen)Pd···PF_3	Pd···P	0.010	0.022	-0.005	0.005	0.260
I_2(Phen)Pd···AsF_3	Pd···As	0.014	0.030	-0.008	0.008	-0.051
I_2(Phen)Pd···SbF_3	Pd···Sb	0.017	0.031	-0.010	0.009	-0.574
I_2(Phen)Pd···SF_2	Pd···S	0.015	0.037	-0.009	0.009	0.206
I_2(Phen)Pd···SeF_2	Pd···Se	0.021	0.044	-0.013	0.012	-0.663
I_2(Phen)Pd···TeF_2	Pd···Te	0.022	0.041	-0.014	0.012	-1.166
I_2(Phen)Pd···ClF	Pd···Cl	0.037	0.085	-0.029	0.025	-2.542

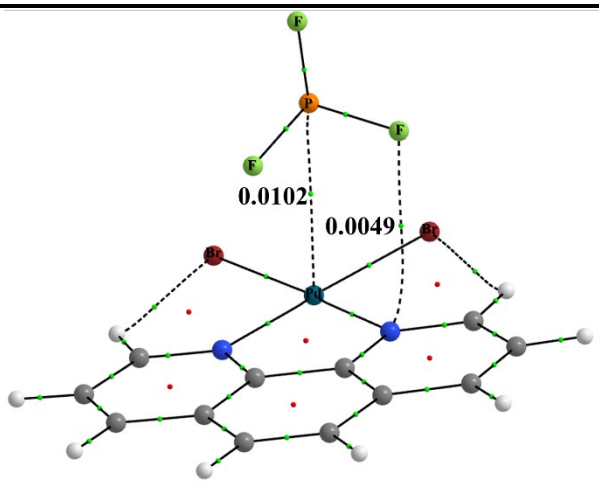
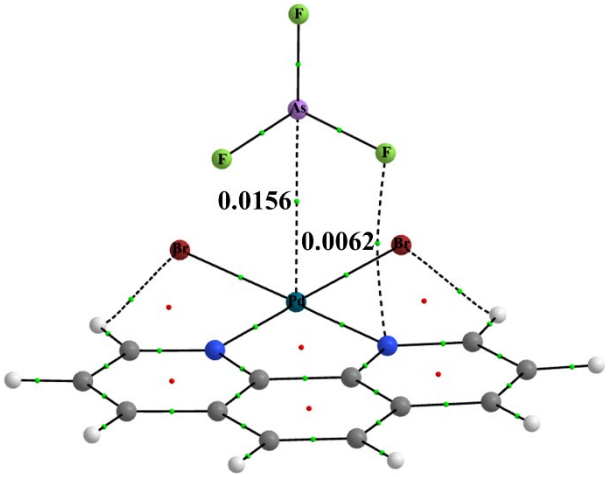
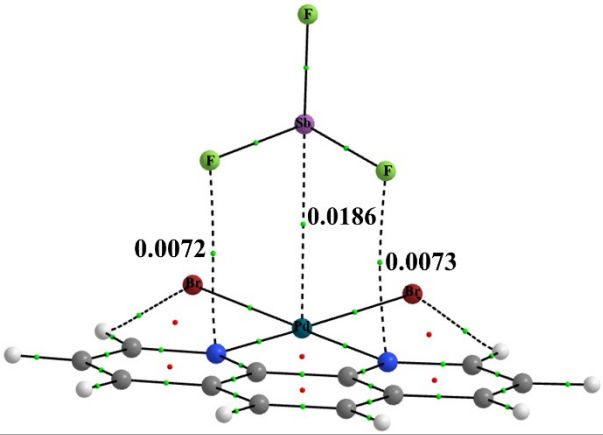
I_2(Phen)Pd···BrF	Pd···Br	0.035	0.069	-0.026	0.022	-2.611
I_2(Phen)Pd···IF	Pd···I	0.029	0.054	-0.020	0.017	-2.119
Cl_2(Phen)Pt···PF_3	Pt···P	0.014	0.028	-0.007	0.007	-0.063
Cl_2(Phen)Pt···AsF_3	Pt···As	0.023	0.038	-0.013	0.011	-1.113
Cl_2(Phen)Pt···SbF_3	Pt···Sb	0.027	0.038	-0.016	0.013	-2.004
Cl_2(Phen)Pt···SF_2	Pt···S	0.025	0.053	-0.016	0.014	-0.763
Cl_2(Phen)Pt···SeF2	Pt···Se	0.033	0.056	-0.021	0.018	-2.251
Cl_2(Phen)Pt···TeF_2	Pt···Te	0.034	0.049	-0.022	0.017	-3.074
Cl_2(Phen)Pt···ClF	Pt···Cl	0.050	0.099	-0.039	0.032	-4.622
Cl_2(Phen)Pt···BrF	Pt···Br	0.046	0.078	-0.033	0.026	-4.237
Cl_2(Phen)Pt···IF	Pt···I	0.039	0.061	-0.027	0.021	-3.585
Br_2(Phen)Pt···PF_3	Pt···P	0.013	0.027	-0.007	0.007	-0.009
Br_2(Phen)Pt···AsF_3	Pt···As	0.022	0.036	-0.012	0.011	-0.953
Br_2(Phen)Pt···SbF_3	Pt···Sb	0.025	0.037	-0.015	0.012	-1.776
Br_2(Phen)Pt···SF_2	Pt···S	0.023	0.051	-0.015	0.014	-0.620
Br_2(Phen)Pt···SeF_2	Pt···Se	0.032	0.055	-0.020	0.017	-2.084
Br_2(Phen)Pt···TeF_2	Pt···Te	0.033	0.048	-0.021	0.017	-2.906
Br_2(Phen)Pt···ClF	Pt···Cl	0.050	0.099	-0.039	0.032	-4.541
Br_2(Phen)Pt···BrF	Pt···Br	0.045	0.078	-0.033	0.026	-4.164
Br_2(Phen)Pt···IF	Pt···I	0.038	0.060	-0.026	0.021	-3.498
I_2(Phen)Pt···PF_3	Pt···P	0.012	0.026	-0.006	0.006	0.056
I_2(Phen)Pt···AsF_3	Pt···As	0.020	0.035	-0.011	0.010	-0.760
I_2(Phen)Pt···SbF_3	Pt···Sb	0.024	0.035	-0.014	0.011	-1.551
I_2(Phen)Pt···SF_2	Pt···S	0.022	0.049	-0.014	0.013	-0.510
I_2(Phen)Pt···SeF_2	Pt···Se	0.031	0.054	-0.020	0.017	-1.995
I_2(Phen)Pt···TeF_2	Pt···Te	0.032	0.048	-0.021	0.016	-2.821
I_2(Phen)Pt···ClF	Pt···Cl	0.050	0.099	-0.039	0.032	-4.651
I_2(Phen)Pt···BrF	Pt···Br	0.045	0.077	-0.033	0.026	-4.176
I_2(Phen)Pt···IF	Pt···I	0.038	0.060	-0.026	0.020	-3.465

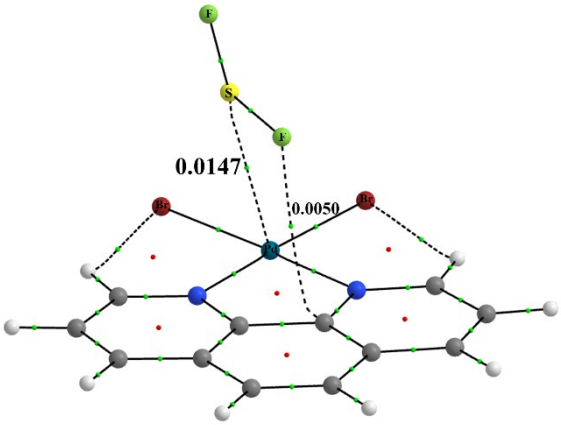
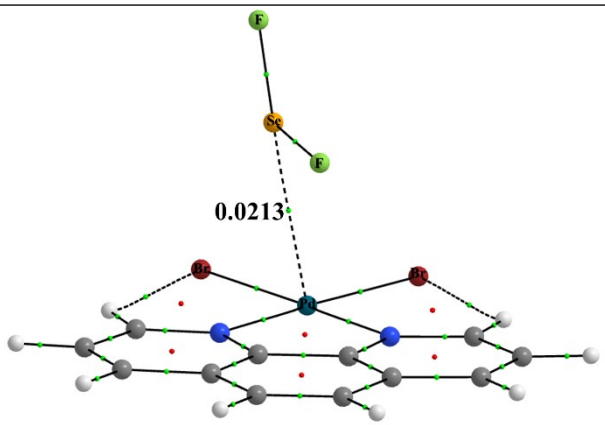
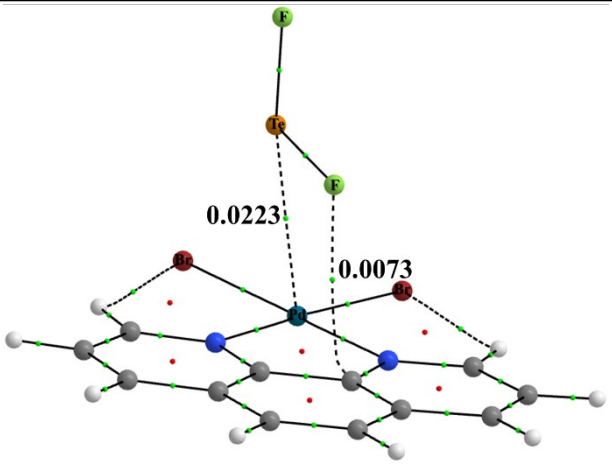
Table S5. QTAIM molecular graphs presenting the Bond Critical Points (BCPs) (green dots) in the studied complexes. Solid and dashed lines identified bond paths. Electron density (ρ) value is given in a.u.

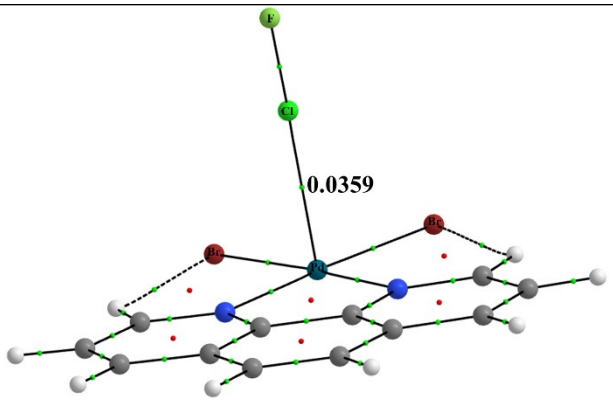
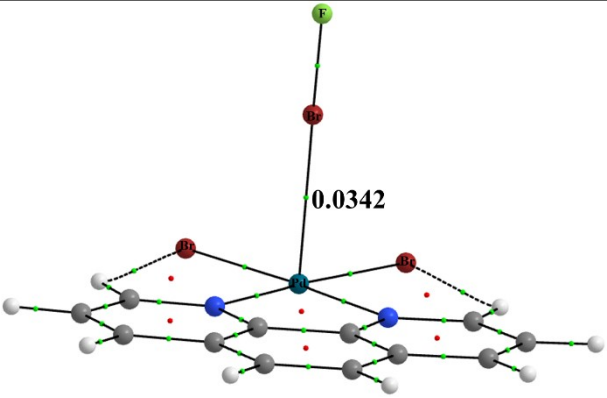
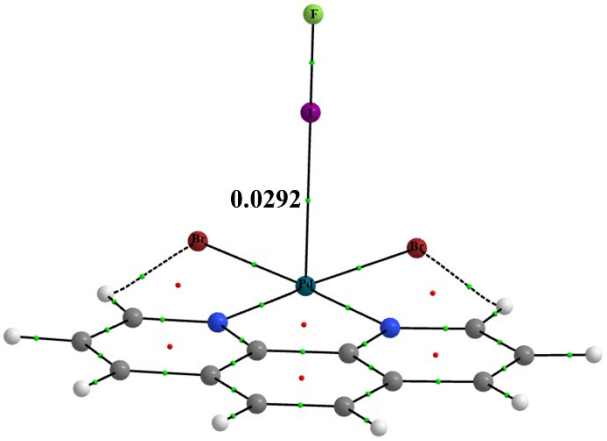
Complex	QTAIM molecular graph
$Cl_2(Phen)Pd\cdots PF_3$	
$Cl_2(Phen)Pd\cdots AsF_3$	
$Cl_2(Phen)Pd\cdots SbF_3$	

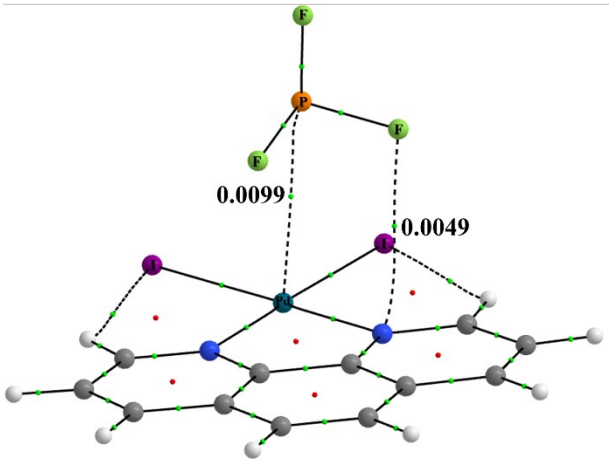
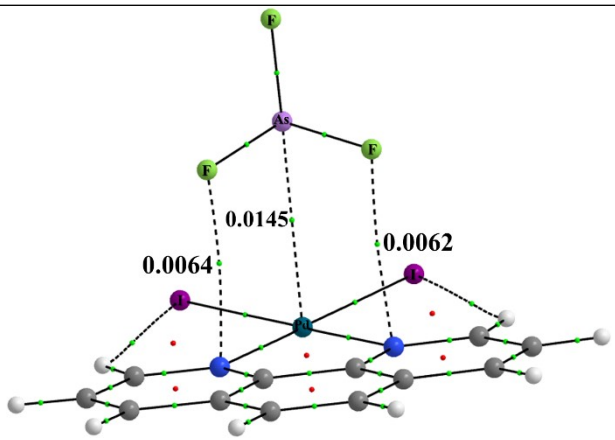
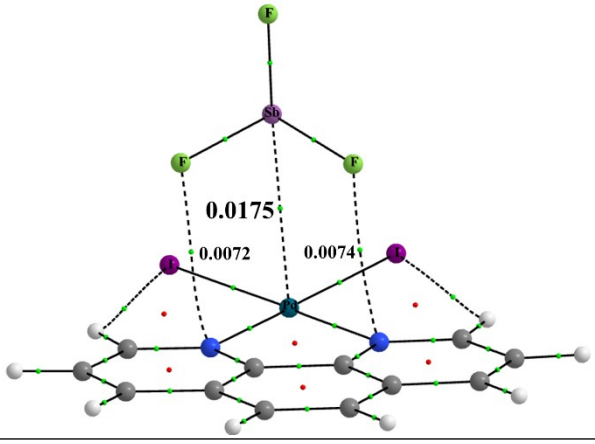
$Cl_2(Phen)Pd\cdots SF_2$	
$Cl_2(Phen)Pd\cdots SeF_2$	
$Cl_2(Phen)Pd\cdots TeF_2$	

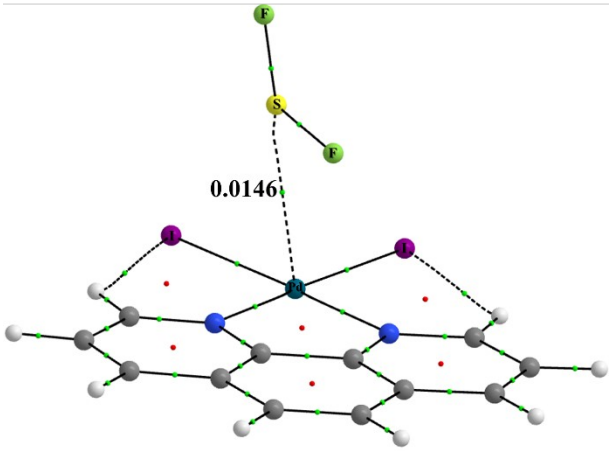
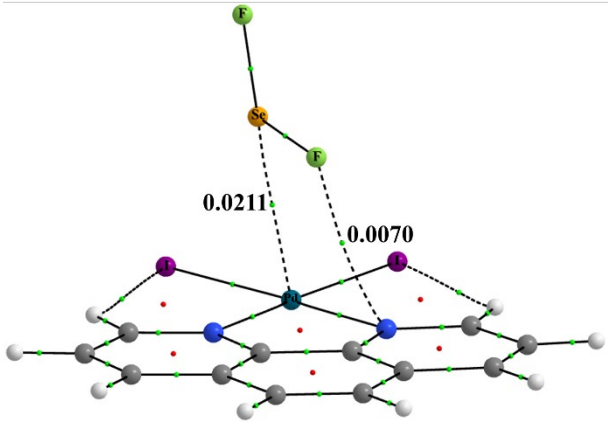
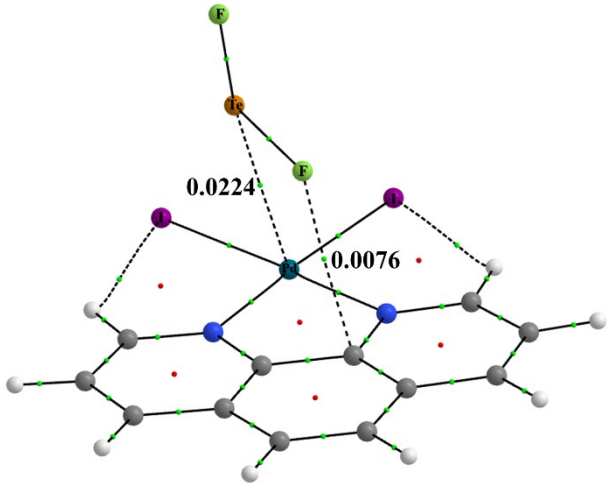
Cl_2(Phen)Pd···ClF	
Cl_2(Phen)Pd···BrF	
Cl_2(Phen)Pd···IF	

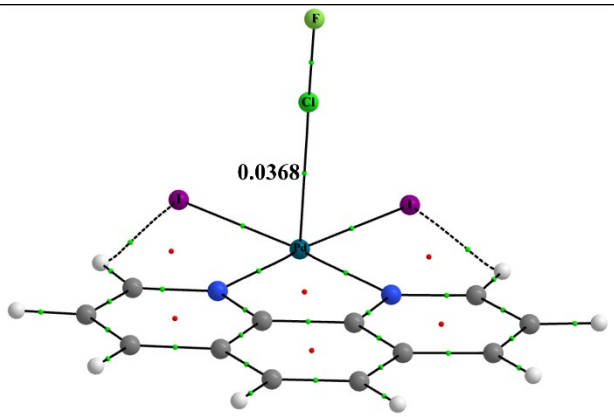
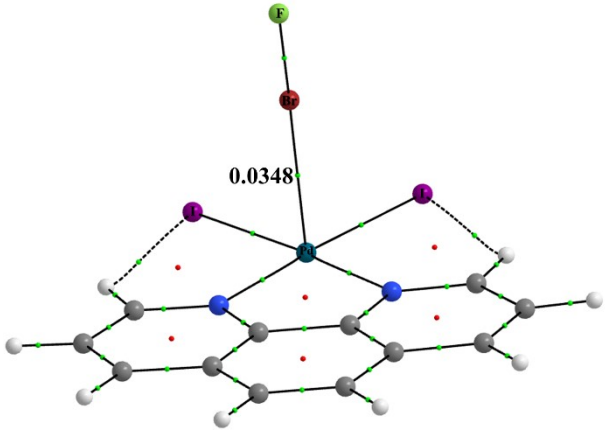
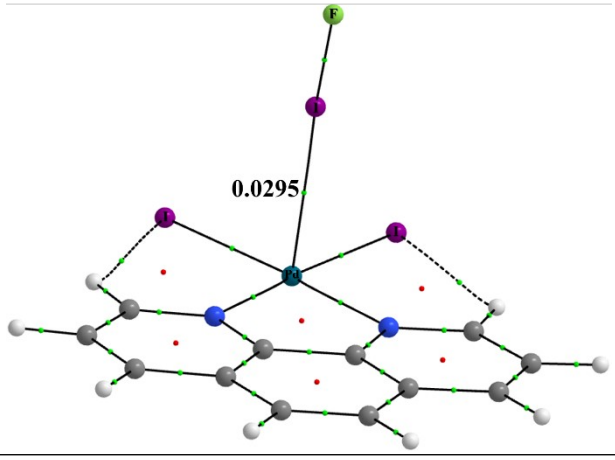
$Br_2(Phen)Pd\cdots PF_3$	
$Br_2(Phen)Pd\cdots AsF_3$	
$Br_2(Phen)Pd\cdots SbF_3$	

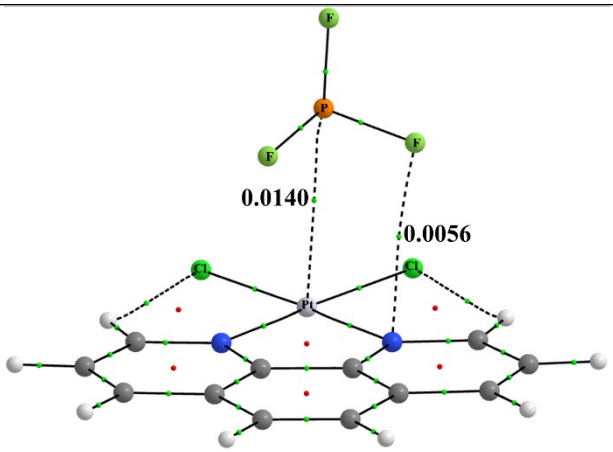
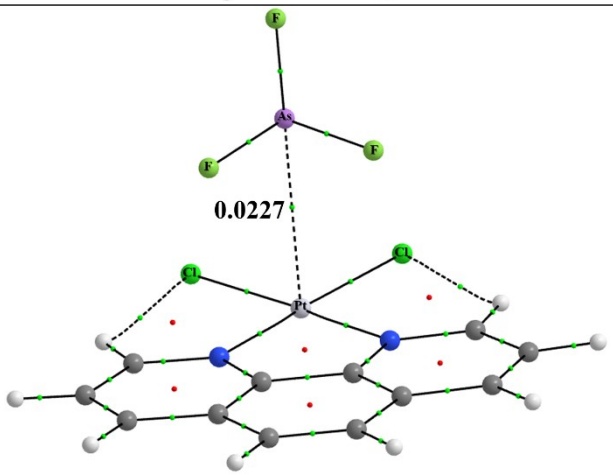
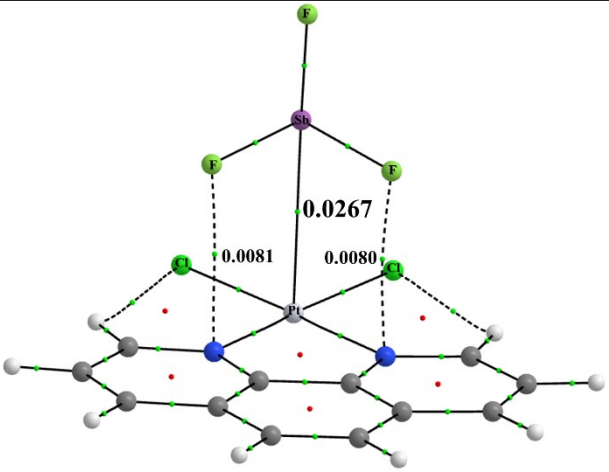
$Br_2(Phen)Pd\cdots SF_2$	
$Br_2(Phen)Pd\cdots SeF_2$	
$Br_2(Phen)Pd\cdots TeF_2$	

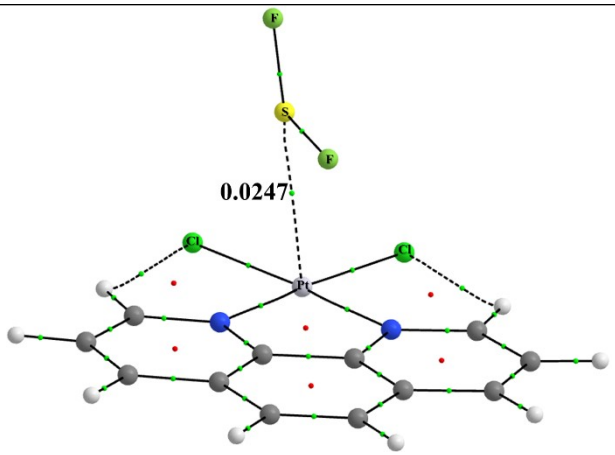
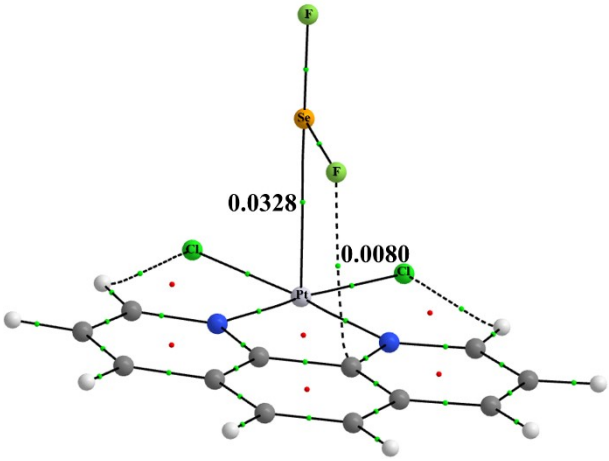
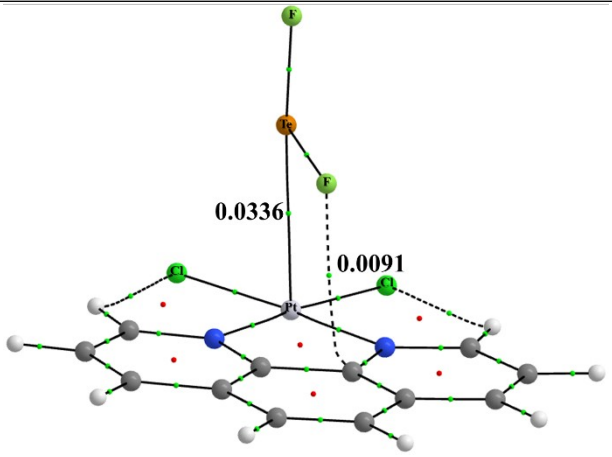
Br_2(Phen)Pd···ClF	
Br_2(Phen)Pd···BrF	
Br_2(Phen)Pd···IF	

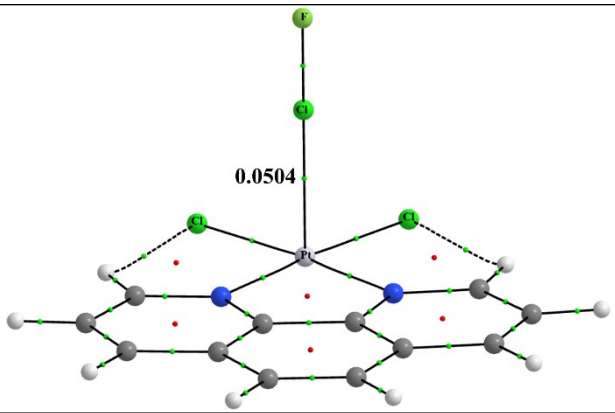
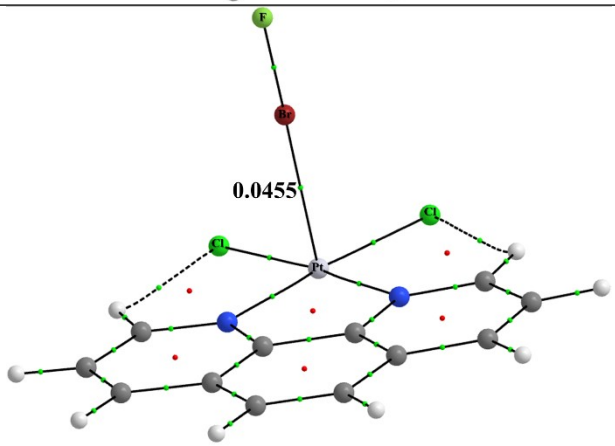
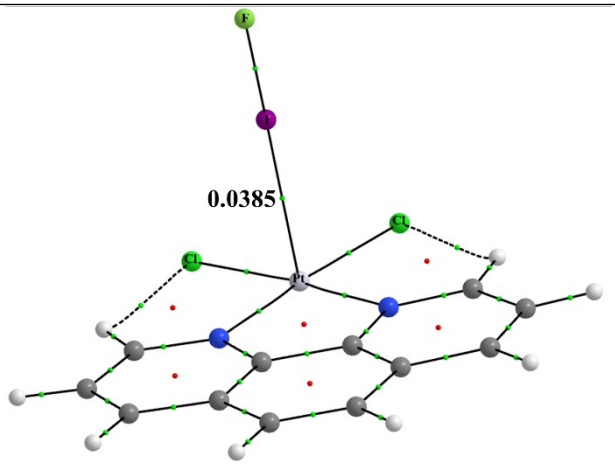
$I_2(Phen)Pd\cdots PF_3$	
$I_2(Phen)Pd\cdots AsF_3$	
$I_2(Phen)Pd\cdots SbF_3$	

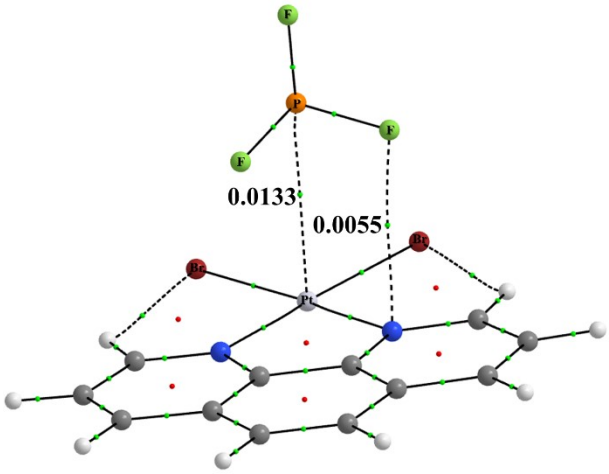
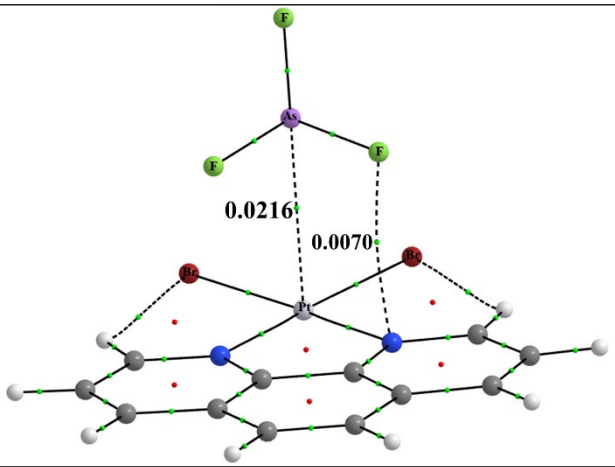
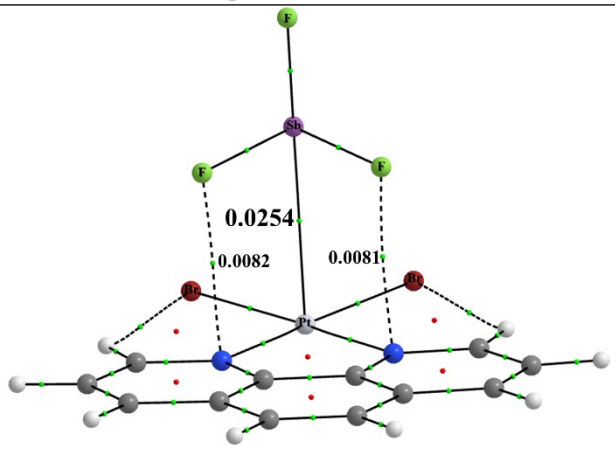
$I_2(Phen)Pd\cdots SF_2$	
$I_2(Phen)Pd\cdots SeF_2$	
$I_2(Phen)Pd\cdots TeF_2$	

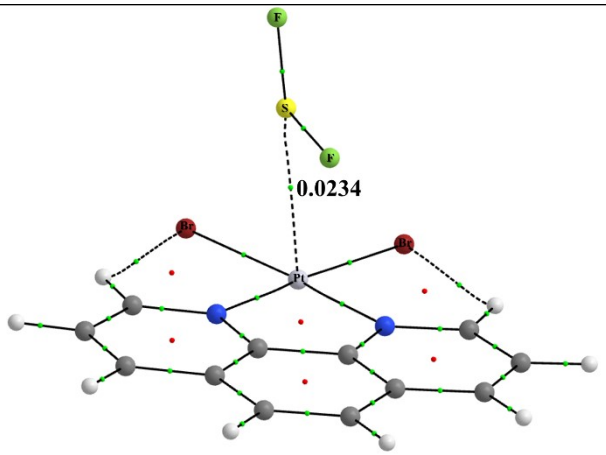
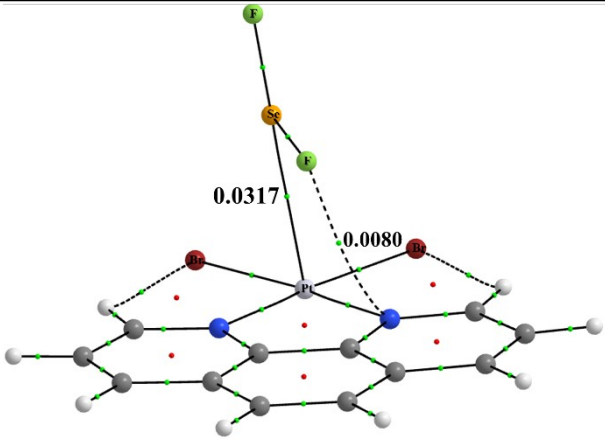
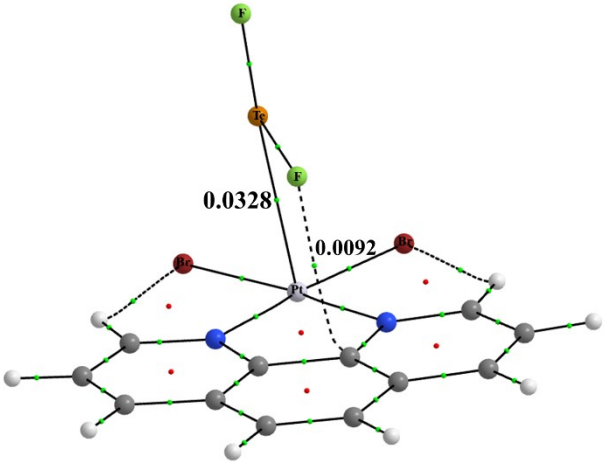
I_2(Phen)Pd···ClF	
I_2(Phen)Pd···BrF	
I_2(Phen)Pd···IF	

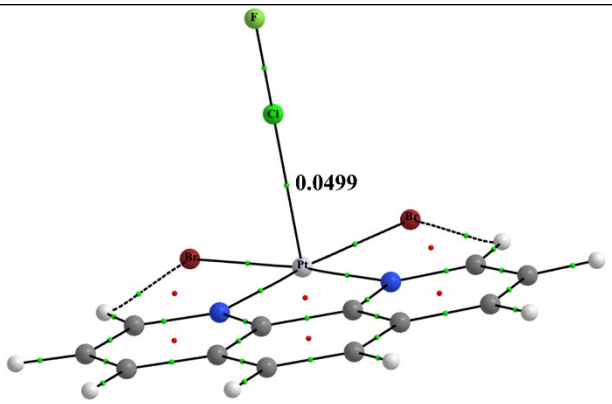
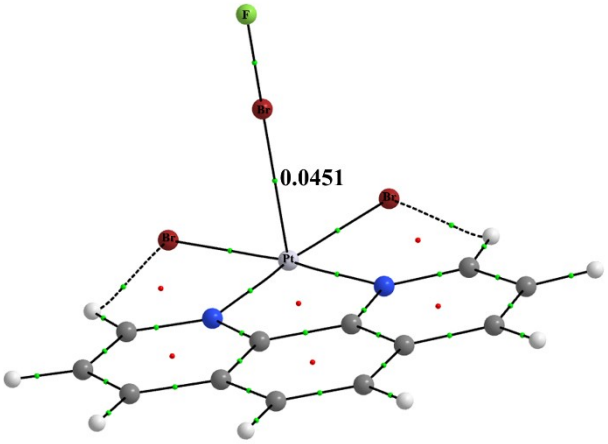
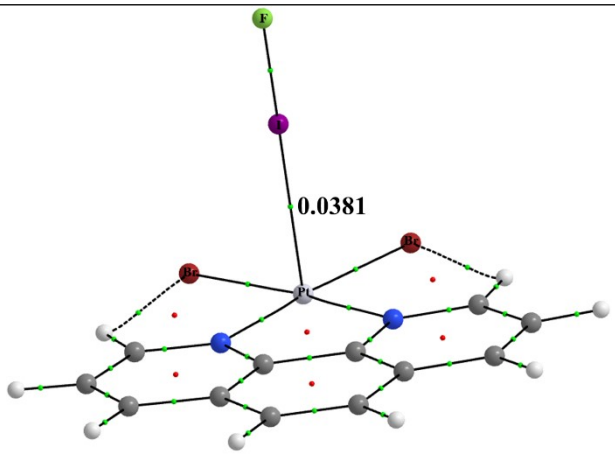
$Cl_2(Phen)Pt\cdots PF_3$	
$Cl_2(Phen)Pt\cdots AsF_3$	
$Cl_2(Phen)Pt\cdots SbF_3$	

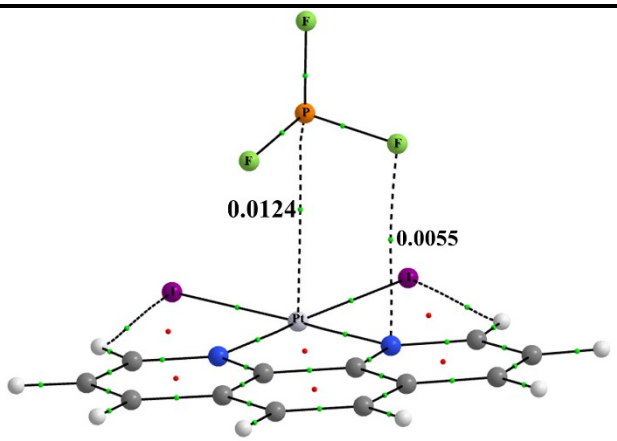
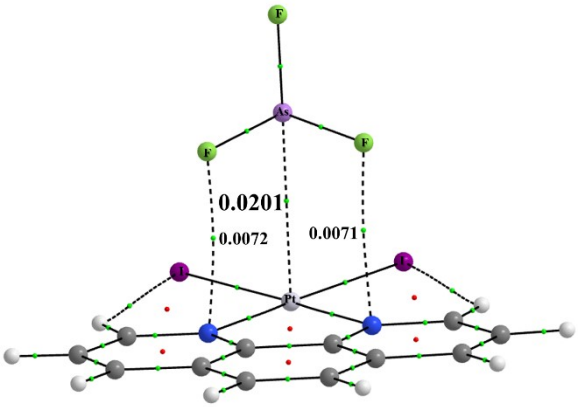
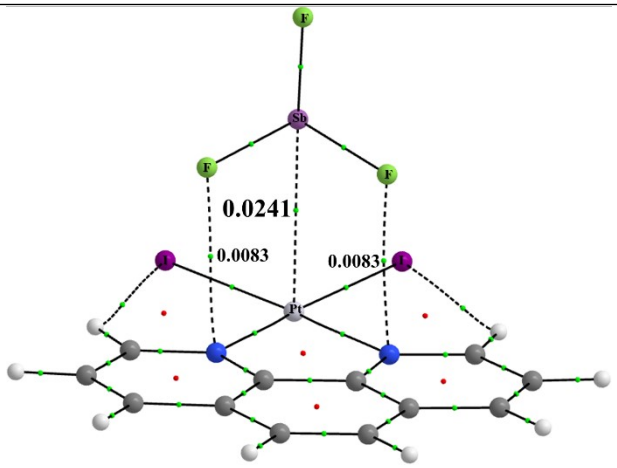
$Cl_2(Phen)Pt\cdots SF_2$	
$Cl_2(Phen)Pt\cdots SeF_2$	
$Cl_2(Phen)Pt\cdots TeF_2$	

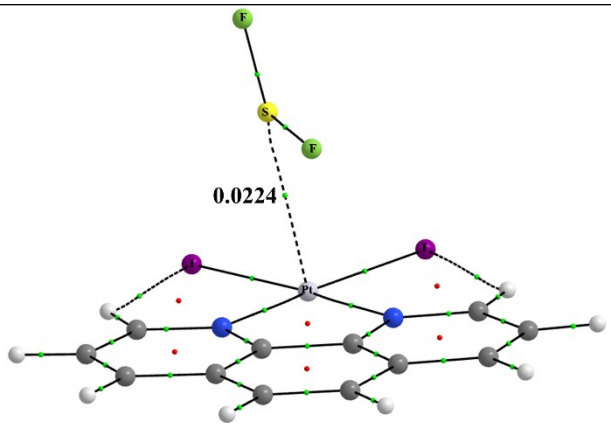
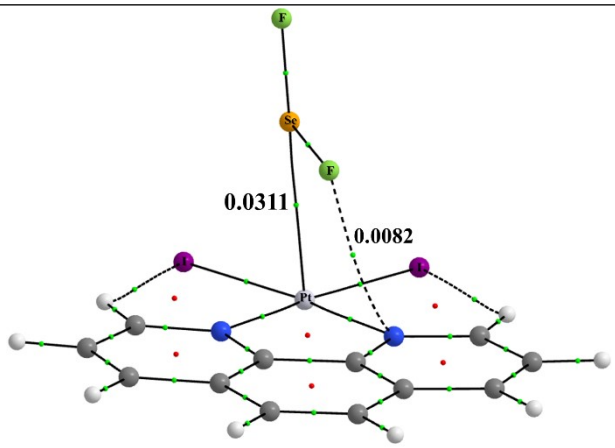
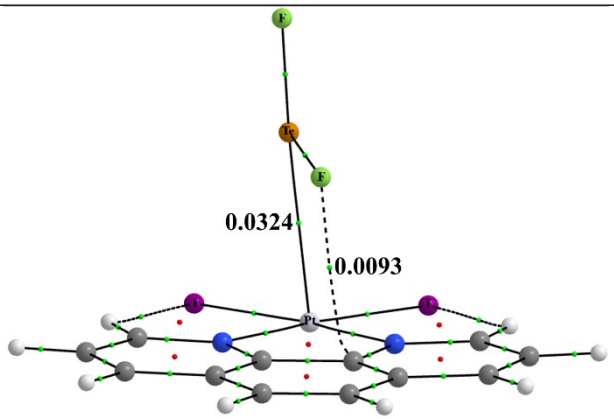
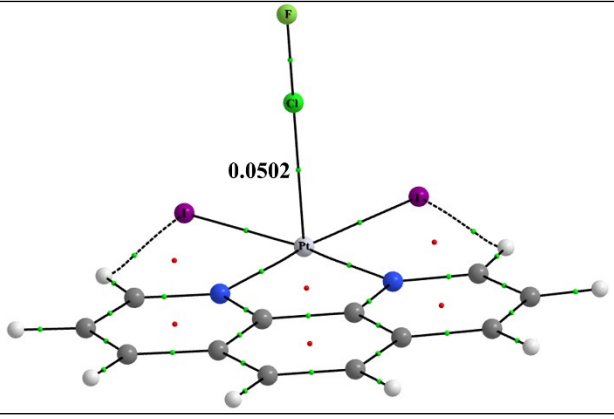
Cl_2(Phen)Pt···ClF	
Cl_2(Phen)Pt···BrF	
Cl_2(Phen)Pt···IF	

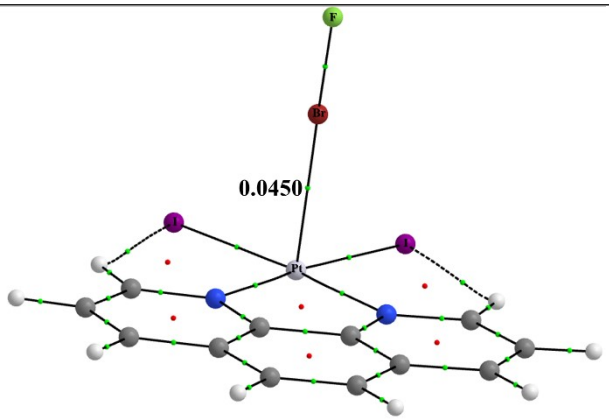
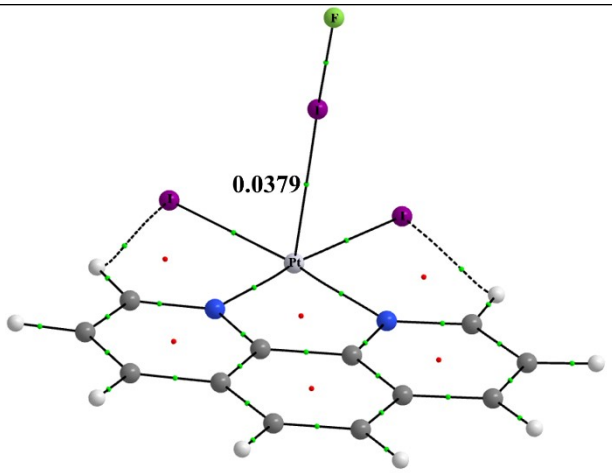
$Br_2(Phen)Pt\cdots PF_3$	
$Br_2(Phen)Pt\cdots AsF_3$	
$Br_2(Phen)Pt\cdots SbF_3$	

$Br_2(Phen)Pt\cdots SF_2$	
$Br_2(Phen)Pt\cdots SeF_2$	
$Br_2(Phen)Pt\cdots TeF_2$	

Br_2(Phen)Pt···ClF	
Br_2(Phen)Pt···BrF	
Br_2(Phen)Pt···IF	

$I_2(Phen)Pt\cdots PF_3$	
$I_2(Phen)Pt\cdots AsF_3$	
$I_2(Phen)Pt\cdots SbF_3$	

$I_2(Phen)Pt\cdots SF_2$	
$I_2(Phen)Pt\cdots SeF_2$	
$I_2(Phen)Pt\cdots TeF_2$	
$I_2(Phen)Pt\cdots ClF$	

I_2(Phen)Pt···BrF	
I_2(Phen)Pt···IF	

1. **2.** **3.**

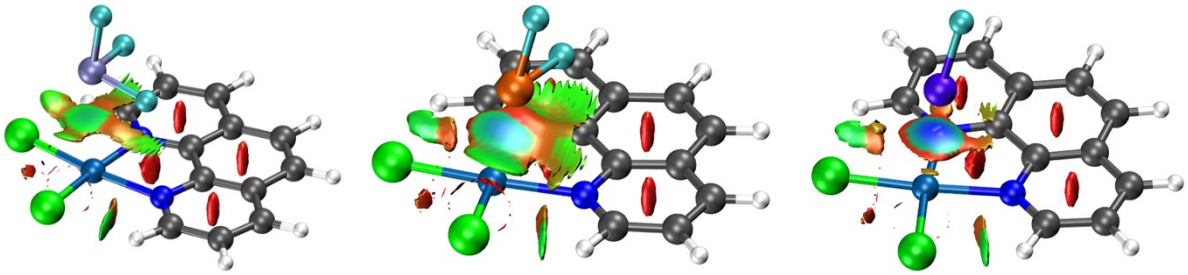


Figure S6. NCI isosurfaces at the RDG 0.5 a.u. isovalue for the dichloro(1,10-phenanthroline)palladium (II) with Lewis acid (**1.** AsF_3, **2.** TeF_2 and **3.** IF) complexes containing the discussed non-covalent interactions.

1. **2.** **3.**

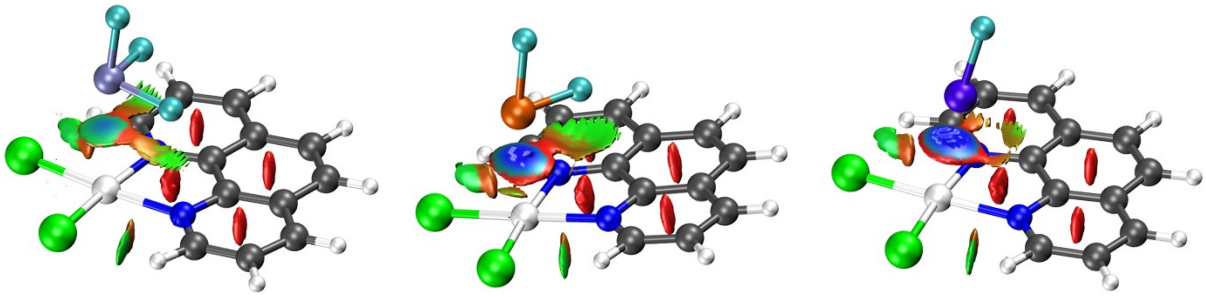


Figure S7. NCI isosurfaces at the RDG 0.5 a.u. isovalue for the dichloro(1,10-phenanthroline) platinum (II) with Lewis acid (**1.** AsF_3, **2.** TeF_2 and **3.** IF) complexes containing the discussed non-covalent interactions.

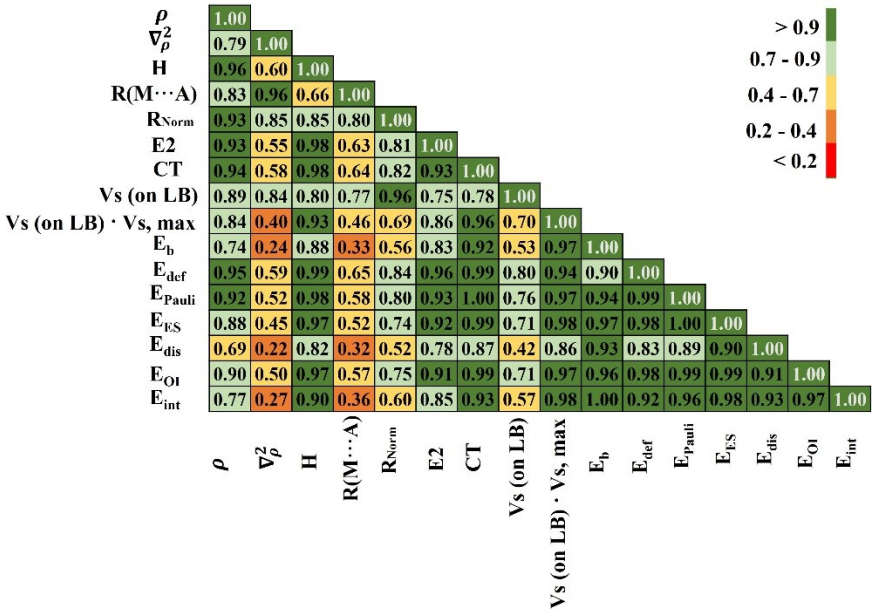


Figure S8. Correlation coefficients of selected features obtained for all complexes containing a chalcogen bond. The absolute values of the correlation matrix are presented on a five-point scale: high values are green and low values are red.

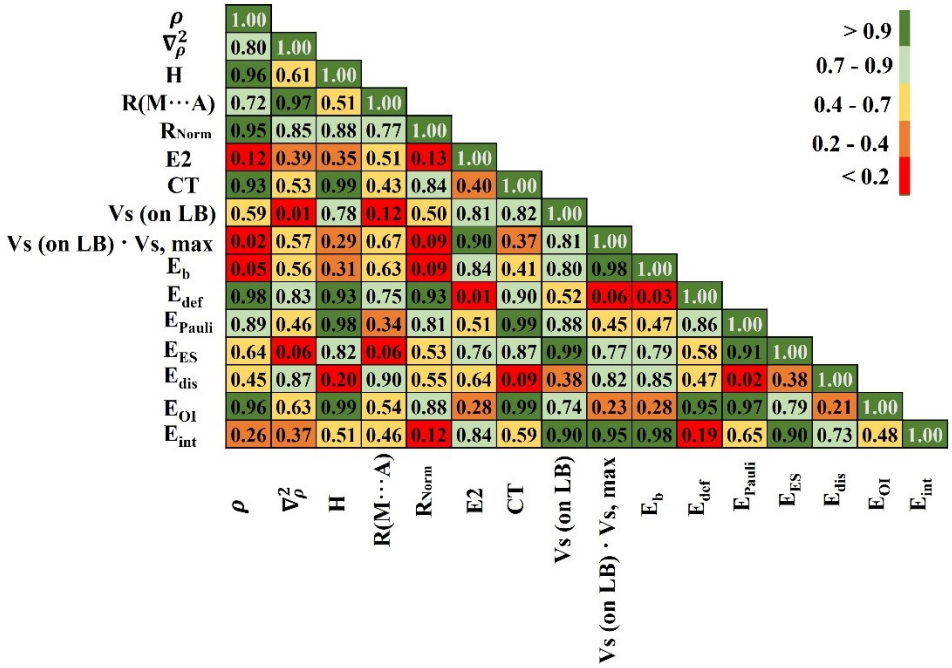


Figure S9. Correlation coefficients of selected features obtained for all complexes containing a halogen bond. The absolute values of the correlation matrix are presented on a five-point scale: high values are green and low values are red.

Table S6. XYZ coordinates of the optimized geometries for the studied complexes.

$Cl_2(Phen)Pd\cdots PF_3$	N 0.79086500 2.39455100 5.94653800 N -0.60822900 3.76369300 4.15498600 C -1.26889300 4.43335300 3.23063300 C -0.29735900 3.06196000 6.39421800 C 1.52118500 1.70576200 6.80185300 C -0.69043000 3.05560200 7.73981800 C 1.19862300 1.64333700 8.16158600 H 1.83070000 1.06523200 8.82312400 C -2.41443200 5.17596000 3.53714700 H -2.92097400 5.70858500 2.74265100 C 0.09922900 2.31424000 8.63370800 H -0.16539500 2.28220400 9.68490100 C -1.04698400 3.79568400 5.43412900 C -2.18352400 4.51550200 5.82868000 H -2.15027100 3.78781500 9.16100300 C -2.56622700 4.49405000 7.20387300 H -3.44514800 5.05345500 7.50382900 C -2.87326700 5.22073200 4.82922600 H -3.75736500 5.79293800 5.08813600 H 2.38580100 1.20558700 6.37873600 H -0.85906000 4.36990100 2.22799100 Cl 1.28587000 3.13289500 1.73718800 Cl 3.01911900 1.45818900 3.94566700 P 3.14581400 5.18892000 5.03453700 F 3.90497500 6.46666200 5.57286400 F 1.68308800 5.70394000 5.36695300 F 3.32693100 4.31209100 6.33439700 C -1.85122700 3.79515300 8.11891900 Pd 1.10626100 2.66904800 3.94463200
$Cl_2(Phen)Pd\cdots AsF_3$	N 0.77977300 2.32976200 6.01509700 N -0.54937400 3.76923800 4.22437300 C -1.16709300 4.48179100 3.30347600 C -0.30917600 3.00310000 6.45103600 C 1.48247300 1.61576000 6.87171400 C -0.73457200 2.97242300 7.78622300 C 1.12627300 1.52721400 8.22160800 H 1.73611600 0.92806500 8.88521000 C -2.30590400 5.23822300 3.60007100 H -2.77694500 5.80669100 2.80871500 C 0.02375600 2.20085100 8.68166800 H -0.26599100 2.14985900 9.72543000 C -1.02130800 3.77373500 5.49182200 C -2.15294200 4.50601500 5.87634200 H -2.21615000 3.69587000 9.18900300 C -2.57123800 4.45653700 7.24023000 H -3.44644600 5.02562600 7.53258200 C -2.80013300 5.25387900 4.87934400 H -3.67826200 5.83823600 5.13116600 H 2.35308900 1.11622900 6.46126600 H -0.72734300 4.44800700 2.31275000 Cl 1.46861500 3.26655000 1.87227800 Cl 3.09813600 1.49058700 4.06984600 As 3.11088300 5.15779700 4.66511800

	F 3.98657200 6.56524400 5.16705400 F 1.58498500 5.97706300 4.62371600 F 2.89468900 4.57096100 6.27977100 C -1.89193500 3.72226600 8.15483100 Pd 1.16912700 2.67946200 4.04018400
$Cl_2(Phen)Pd\cdots SbF_3$	Pd 1.17807200 2.64046700 4.06511800 N 0.75831700 2.27483700 6.02960100 N -0.52672800 3.75105600 4.23653300 C -1.11475900 4.48916500 3.31700000 C -0.31595700 2.97308800 6.46157200 C 1.44070900 1.54335900 6.88713100 C -0.74654700 2.95113800 7.79496200 C 1.07648200 1.45997600 8.23511200 H 1.66941000 0.84563900 8.90005100 C -2.23239600 5.27700100 3.61125900 H -2.67943600 5.86607300 2.82121900 C -0.01083200 2.15967000 8.69172300 H -0.30492700 2.11514900 9.73454600 C -1.00352100 3.76397000 5.50186400 C -2.11426800 4.52799200 5.88410100 H -2.21198300 3.71239400 9.19444800 C -2.53900200 4.48681500 7.24615700 H -3.39789000 5.08092800 7.53698100 C -2.73320300 5.29983500 4.88745000 H -3.59357500 5.91045300 5.13815100 H 2.30318100 1.02623400 6.48238300 H -0.66881600 4.45483700 2.32975500 Cl 1.52968300 3.25078700 1.90727700 Cl 3.11372200 1.45815600 4.11496900 Sb 3.12214100 5.14592500 4.54703400 F 3.95843900 6.73711500 5.19049600 F 1.45153700 6.04009200 4.33480700 F 2.67605300 4.59353600 6.31895200 C -1.88422900 3.73134200 8.16127800
$Cl_2(Phen)Pd\cdots SF_2$	N 0.91089200 2.32354200 6.01968800 N -0.39567400 3.87389300 4.30725700 C -1.00216300 4.64226300 3.42338300 C -0.14145300 3.02330100 6.50128100 C 1.59879500 1.54937500 6.83601500 C -0.54251600 2.96213200 7.84304700 C 1.26607800 1.42887400 8.18972700 H 1.86200700 0.78100500 8.81945000 C -2.10383500 5.43190100 3.76931900 H -2.56782800 6.04535000 3.00790700 C 0.20098800 2.13000500 8.69563300 H -0.07147400 2.05243200 9.74245100 C -0.84187700 3.85360300 5.58367500 C -1.93633900 4.61523400 6.01613200 H -1.96916700 3.69099000 9.29936400 C -2.33027700 4.53376100 7.38592500 H -3.17769100 5.12433900 7.71528900 C -2.57259000 5.42174700 5.05865700 H -3.42283400 6.02962300 5.34785700 H 2.43328600 1.02232000 6.38545300 H -0.58503400 4.61995900 2.42222000 Cl 1.45559000 3.23516600 1.84824300

	Cl 3.03725500 1.30962300 3.95066000 F 3.28819400 6.93547600 4.65674000 F 2.01132800 5.33954000 5.91264100 C -1.66289900 3.74232600 8.26064700 Pd 1.24131600 2.67779800 4.03232400 S 2.61350700 5.49653400 4.42876500
$Cl_2(Phen)Pd\cdots SeF_2$	N 0.90827900 2.33865600 6.01140500 N -0.41607200 3.87721900 4.29953600 C -1.02775500 4.64237800 3.41673900 C -0.14813400 3.03091400 6.49366400 C 1.60953900 1.57727600 6.82759700 C -0.54165800 2.97264300 7.83730900 C 1.28507800 1.46069600 8.18359000 H 1.89216300 0.82412700 8.81407100 C -2.13377100 5.42461400 3.76486800 H -2.60265100 6.03601800 3.00490200 C 0.21499800 2.15305000 8.69045200 H -0.05056900 2.07946900 9.73930900 C -0.85791000 3.85369700 5.57709800 C -1.95523800 4.60936100 6.01188200 H -1.96631500 3.69628500 9.29801000 C -2.34322900 4.52908700 7.38336500 H -3.19277500 5.11540200 7.71467500 C -2.59870800 5.41136600 5.05549500 H -3.45101200 6.01520300 5.34702000 H 2.44870500 1.05807400 6.37719700 H -0.61189500 4.62583700 2.41519600 Cl 1.45881800 3.26571100 1.84225700 Cl 3.04298200 1.35098800 3.93871100 F 3.45611800 6.88954600 4.75312100 F 1.94116400 5.24368300 5.98717900 C -1.66605300 3.74556900 8.25748600 Se 2.66487500 5.36398000 4.39242300 Pd 1.23660700 2.70126400 4.02519300
$Cl_2(Phen)Pd\cdots TeF_2$	N 0.89147900 2.30863800 6.01552400 N -0.42083700 3.85791900 4.30362800 C -1.02591600 4.62853700 3.42067400 C -0.15578500 3.01378800 6.49849000 C 1.58985000 1.54533000 6.83215300 C -0.54469300 2.96467000 7.84356200 C 1.27017400 1.43847900 8.18995000 H 1.87483100 0.80031200 8.82107800 C -2.12650500 5.41837300 3.76834200 H -2.59047300 6.03334200 3.00835300 C 0.20831300 2.14269100 8.69748900 H -0.05319200 2.07704900 9.74787600 C -0.86064800 3.83961800 5.58176600 C -1.95026100 4.60570600 6.01677400 H -1.95674100 3.70750700 9.30672400 C -2.33445100 4.53434200 7.38965000 H -3.17743900 5.12973500 7.72140500 C -2.58905400 5.41066400 5.05964900 H -3.43524500 6.02272600 5.35175200 H 2.42292500 1.01661800 6.38200600 H -0.61054600 4.61235400 2.41935000 Cl 1.50657600 3.29087600 1.86598400

	Cl 3.01942900 1.30656000 3.94468200 F 3.52129800 7.07749400 4.79525000 F 1.87254600 5.23224100 5.95427100 C -1.66055400 3.74919100 8.26474100 Te 2.68001100 5.44872500 4.22402000 Pd 1.23049100 2.67862800 4.03460600
Cl_2(Phen)Pd···ClF	N 0.43899500 1.63808000 5.82734200 N -0.87753800 3.04590300 3.99395100 C -1.48548300 3.74248900 3.05498100 C -0.69599100 2.25833400 6.22064700 C 1.13394300 0.94060200 6.70318500 C -1.17931900 2.18756000 7.53461200 C 0.72254900 0.81683200 8.03491100 H 1.32698300 0.23392300 8.71766800 C -2.66822700 4.44466800 3.31208000 H -3.13066400 5.00336700 2.50878100 C -0.42807900 1.43557800 8.45281300 H -0.76224600 1.35523400 9.48136400 C -1.39986000 3.01125800 5.24035100 C -2.57958700 3.68588900 5.58425600 C -2.38483000 2.87883800 7.86116600 H -2.75364400 2.82082400 8.87895100 C -3.05537800 3.59646000 6.92715500 H -3.96803300 4.12048900 7.18740600 C -3.21621000 4.41901000 4.56926000 H -4.13013800 4.95938100 4.79010800 H 2.03919700 0.48043300 6.32140300 H -1.00427400 3.73553900 2.08266900 Cl 1.16696000 2.49497500 1.67678400 Cl 2.77464900 0.77735100 3.91506600 F 2.53264100 5.71229600 5.51977100 Pd 0.88350600 2.00300300 3.85846500 Cl 1.97850000 4.28776700 4.82577500
Cl_2(Phen)Pd···BrF	N 0.41932300 1.60975100 5.81938800 N -0.89722300 3.01857300 3.98587300 C -1.50310400 3.71776200 3.04756300 C -0.71048400 2.23809500 6.21470300 C 1.11618500 0.91471100 6.69557400 C -1.18668000 2.17780800 7.53166200 C 0.71139700 0.80085000 8.03011700 H 1.31714700 0.21986800 8.71329700 C -2.67937400 4.42949100 3.30760700 H -3.14045700 4.99015700 2.50494500 C -0.43394400 1.42776000 8.45026900 H -0.76239100 1.35602200 9.48127900 C -1.41418900 2.99113300 5.23466800 C -2.58685400 3.67617500 5.58164200 C -2.38587300 2.87851100 7.86120100 H -2.74919000 2.82849700 8.88135700 C -3.05646700 3.59615200 6.92726200 H -3.96374100 4.12824800 7.18983900 C -3.22201200 4.41139000 4.56720100 H -4.13029900 4.96011800 4.79062100 H 2.01809300 0.44911600 6.31278700 H -1.02558500 3.70639000 2.07360700 Cl 1.14446600 2.45798000 1.66739400

	Cl 2.74822400 0.74099100 3.90093000 Br 2.06118700 4.32629400 4.80006400 F 2.65570400 5.86099900 5.55821200 Pd 0.85946900 1.96717600 3.84726400
Cl_2(Phen)Pd···IF	N 0.39818000 1.58429800 5.81490700 N -0.91994700 2.99264000 3.98236900 C -1.52601100 3.69309100 3.04489100 C -0.72763200 2.21857900 6.21295100 C 1.09631800 0.89026500 6.69114900 C -1.19738400 2.16620800 7.53251300 C 0.69754600 0.78389900 8.02798400 H 1.30448600 0.20377500 8.71081700 C -2.69696900 4.41218800 3.30797800 H -3.15795000 4.97366700 2.50584400 C -0.44312500 1.41738000 8.45086900 H -0.76653600 1.35193300 9.48387100 C -1.43213200 2.97131200 5.23351600 C -2.59915800 3.66426900 5.58354200 C -2.39158900 2.87389900 7.86499000 H -2.75016600 2.82980000 8.88707900 C -3.06296000 3.59141900 6.93153000 H -3.96609700 4.12931900 7.19647600 C -3.23431000 4.40057200 4.56988000 H -4.13820000 4.95549600 4.79574000 H 1.99514400 0.41996900 6.30716200 H -1.05267200 3.67784500 2.06907000 Cl 1.12187400 2.43091000 1.66267200 Cl 2.72691800 0.71814000 3.89316800 F 2.84389600 6.08589200 5.57714700 I 2.22022200 4.42747800 4.75644300 Pd 0.83160200 1.93350400 3.84000800

Table S6 (Continuation). XYZ coordinates of the optimized geometries for the studied complexes.

$Br_2(Phen)Pd\cdots PF_3$	N 0.79372800 2.37891300 5.94678000 N -0.60668500 3.75933400 4.14886000 C -1.27262700 4.43219500 3.23045800 C -0.29048300 3.05560700 6.39090100 C 1.51536800 1.68775400 6.80774700 C -0.68384000 3.05517700 7.73761100 C 1.19256400 1.63087200 8.16733600 H 1.82015700 1.04940500 8.83022100 C -2.41351900 5.17961700 3.54113900 H -2.92153600 5.71336900 2.74832300 C 0.09844300 2.31155300 8.63561600 H -0.16872200 2.28582000 9.68635800 C -1.03857700 3.79259300 5.43052000 C -2.17113700 4.51825600 5.82970700 H -2.13484000 3.79656200 9.16225500 C -2.55176900 4.50220400 7.20501200 H -3.42720600 5.06715700 7.50475200 C -2.86429500 5.22650400 4.83519400 H -3.74441100 5.80197700 5.10042600 H 2.37768200 1.17693000 6.39214400 H -0.87271800 4.37068100 2.22349900 P 3.13376500 5.21214500 5.04340700 F 3.86379200 6.50241300 5.59132800 F 1.65705300 5.71259900 5.33025200 F 3.28812200 4.34766800 6.35502700 C -1.83892700 3.80132300 8.11926800 Pd 1.11911500 2.65072800 3.92806200 Br 1.34155700 3.13473600 1.58842400 Br 3.14400500 1.36167900 3.89800200
$Br_2(Phen)Pd\cdots AsF_3$	Pd 1.17323100 2.65394700 4.01800700 N 0.77832800 2.31310000 6.01142200 N -0.55550000 3.75890900 4.21373500 C -1.18284900 4.46867900 3.29704100 C -0.30121800 3.00241700 6.44614700 C 1.47113900 1.59474300 6.87267000 C -0.72091500 2.98519100 7.78452300 C 1.11996600 1.51829100 8.22428400 H 1.72421700 0.91416600 8.88850900 C -2.31336900 5.23468100 3.59935700 H -2.78963100 5.79936400 2.80840100 C 0.02953000 2.21052800 8.68338800 H -0.25797400 2.17172800 9.72831700 C -1.01354400 3.77393900 5.48632600 C -2.13684600 4.51764600 5.87721800 H -2.18292400 3.73164600 9.19490700 C -2.54570900 4.48307900 7.24389000 H -3.41336200 5.06289000 7.53767200 C -2.79123100 5.26341000 4.88382500 H -3.66211300 5.85527400 5.14326000 H 2.33446700 1.07830900 6.46732800 H -0.75909900 4.42830100 2.29944000 Br 1.50994200 3.25314600 1.71574000 Br 3.21634300 1.38906600 4.01925900

	As 3.06985700 5.19246400 4.72001900 F 3.90232100 6.61246800 5.25704000 F 1.52573000 5.97438700 4.66126800 F 2.83794200 4.57648900 6.32096300 C -1.86705300 3.74878300 8.15796700
$Br_2(Phen)Pd\cdots SbF_3$	Pd 1.18238900 2.61393300 4.04149500 N 0.75764400 2.25751200 6.02450600 N -0.53178800 3.73977200 4.22410500 C -1.13122100 4.47304400 3.30780600 C -0.30553600 2.97341200 6.45571800 C 1.42832600 1.52002700 6.88639300 C -0.72971600 2.96559700 7.79241900 C 1.06963600 1.44932700 8.23619400 H 1.65563600 0.82864100 8.90141200 C -2.23975500 5.27083300 3.60769700 H -2.69329300 5.85437500 2.81723300 C -0.00327400 2.16987300 8.69239700 H -0.29452800 2.13811200 9.73649700 C -0.99308500 3.76511500 5.49525500 C -2.09464100 4.54116500 5.88372400 H -2.17316500 3.75203500 9.19991900 C -2.50843800 4.51645000 7.24899900 H -3.35875500 5.12204700 7.54130200 C -2.72191900 5.30929600 4.88994100 H -3.57439400 5.92783400 5.14813800 H 2.28157100 0.98405700 6.48619400 H -0.70300600 4.42957300 2.31291700 Br 1.56521900 3.22767300 1.74611400 Br 3.23161100 1.35398100 4.06620500 Sb 3.07566100 5.18718200 4.61464700 F 3.86872300 6.78341500 5.29662200 F 1.39361800 6.05112800 4.37733400 F 2.60069700 4.60066900 6.36697300 C -1.85454100 3.76096300 8.16376600
$Br_2(Phen)Pd\cdots SF_2$	Pd 1.25629400 2.67262500 4.02296600 N 0.90909100 2.32153400 6.02654500 N -0.39759300 3.87545400 4.30031400 C -1.00862000 4.64329100 3.41889200 C -0.14535700 3.02492900 6.49904200 C 1.58773100 1.54941800 6.85272500 C -0.55371100 2.96784000 7.83993400 C 1.24785700 1.43283200 8.20466700 H 1.83925900 0.78534100 8.83905800 C -2.11074100 5.43239400 3.76321900 H -2.57533400 6.04403600 3.00069300 C 0.18172900 2.13776200 8.70098400 H -0.09862600 2.06544200 9.74610900 C -0.84315300 3.85469400 5.57728500 C -1.93933400 4.61663300 6.00855100 H -1.98263700 3.69849800 9.29226300 C -2.33808200 4.53892300 7.37663200 H -3.18623300 5.13100800 7.70135400 C -2.57781600 5.42244000 5.05241300 H -3.42840000 6.02899200 5.34345100 H 2.42539700 1.01672400 6.41435200 H -0.59655100 4.62403500 2.41532200

	Br 1.51295600 3.24057000 1.70410300 Br 3.17159400 1.23682700 3.91882100 F 3.27436900 6.95690900 4.74271900 F 2.02122800 5.31179700 5.96036600 C -1.67414700 3.74881700 8.25415500 S 2.62441000 5.51234500 4.48281500
$Br_2(Phen)Pd\cdots SeF_2$	Pd 1.24013300 2.69344800 4.01052100 N 0.90710700 2.33746300 6.01587500 N -0.42535100 3.87954100 4.29655800 C -1.04533800 4.64430800 3.41900100 C -0.14854700 3.03412300 6.49424100 C 1.60247200 1.57745700 6.83856000 C -0.54292700 2.98014300 7.83896300 C 1.27748700 1.46509200 8.19442800 H 1.88262200 0.82836700 8.82665500 C -2.14933500 5.42704800 3.77083100 H -2.62215400 6.03682800 3.01197100 C 0.20927800 2.16205400 8.69695800 H -0.05917400 2.09380900 9.74545600 C -0.85993800 3.85653600 5.57689100 C -1.95643400 4.61320700 6.01570200 H -1.96249300 3.70641300 9.30247800 C -2.34256600 4.53701300 7.38742400 H -3.19099000 5.12524400 7.71821300 C -2.60627900 5.41464300 5.06363100 H -3.45712100 6.01773000 5.36098200 H 2.44203300 1.05169300 6.39608900 H -0.63975800 4.62955600 2.41297400 Br 1.48646300 3.25936100 1.68825300 Br 3.16110300 1.26963200 3.89119800 F 3.43811200 6.90585700 4.79531700 F 1.95515500 5.21668800 6.01271600 C -1.66497500 3.75449400 8.26110700 Se 2.66699700 5.37436600 4.41675700
$Br_2(Phen)Pd\cdots TeF_2$	Pd 1.23096400 2.67169900 4.01507400 N 0.89242800 2.31212400 6.01706200 N -0.43221700 3.86126500 4.29772000 C -1.04738000 4.62970500 3.41967100 C -0.15522200 3.01967400 6.49633200 C 1.58789800 1.55337300 6.84056200 C -0.54327200 2.97591300 7.84293400 C 1.26969900 1.45209600 8.19876900 H 1.87489500 0.81646500 8.83196700 C -2.14718500 5.41812100 3.77115200 H -2.61682200 6.03011000 3.01220400 C 0.20842300 2.15879800 8.70210900 H -0.05444600 2.09950800 9.75254700 C -0.86412900 3.84302900 5.57878000 C -1.95386100 4.60868000 6.01796700 H -1.95042200 3.71997000 9.30936300 C -2.33490100 4.54181500 7.39147800 H -3.17766100 5.13770000 7.72291600 C -2.60095200 5.41126100 5.06499800 H -3.44657100 6.02131500 5.36296600 H 2.42187900 1.01927200 6.39809500 H -0.64211500 4.61520800 2.41390000

	Br 1.52051500 3.27423700 1.70355800 Br 3.13132000 1.22117400 3.89015800 F 3.51358400 7.07563100 4.86801700 F 1.88084000 5.19775500 5.99904800 C -1.65811300 3.75993500 8.26621300 Te 2.68840800 5.44628500 4.27418800
Br_2(Phen)Pd···ClF	Pd 0.89338600 2.00148000 3.84815400 N 0.43639600 1.63435900 5.83350600 N -0.88675900 3.04819300 3.99343700 C -1.50287400 3.74542500 3.06013600 C -0.69772400 2.25883900 6.22323100 C 1.12487700 0.93695800 6.71464900 C -1.18235900 2.19120700 7.53812400 C 0.71274500 0.81639400 8.04611900 H 1.31500700 0.23270900 8.73016300 C -2.68414400 4.44787400 3.32159400 H -3.15001100 5.00619800 2.51999100 C -0.43596300 1.43969900 8.46019200 H -0.77334300 1.36368500 9.48804500 C -1.40276800 3.01246700 5.24265300 C -2.58207300 3.68783600 5.59128800 C -2.38585600 2.88368300 7.86731000 H -2.75227100 2.82605500 8.88598500 C -3.05666400 3.60106500 6.93424300 H -3.96845100 4.12669300 7.19431800 C -3.22485200 4.42168300 4.58113500 H -4.13764600 4.96132200 4.80847300 H 2.03023100 0.47043600 6.34022800 H -1.03114600 3.74173900 2.08292200 Br 1.22107000 2.51141400 1.53482900 Br 2.90665800 0.71128900 3.87906900 F 2.51039100 5.71635200 5.53782600 Cl 1.98256700 4.29103000 4.82330300
Br_2(Phen)Pd···BrF	Pd 0.86940100 1.96505200 3.83708400 N 0.41718100 1.60606600 5.82570600 N -0.90636700 3.02007300 3.98528100 C -1.52104200 3.71915700 3.05242600 C -0.71152700 2.23904400 6.21758900 C 1.10725400 0.91076200 6.70724500 C -1.18879200 2.18226100 7.53556300 C 0.70179200 0.80025100 8.04149500 H 1.30502100 0.21795500 8.72582900 C -2.69570900 4.43126200 3.31679900 H -3.16073200 4.99072600 2.51553600 C -0.44119600 1.43234800 8.45798200 H -0.77264600 1.36520300 9.48835800 C -1.41658500 2.99245700 5.23713200 C -2.58866300 3.67849800 5.58881900 C -2.38561700 2.88470400 7.86777600 H -2.74624000 2.83567300 8.88894000 C -3.05654300 3.60191300 6.93470400 H -3.96265600 4.13601700 7.19723700 C -3.23046200 4.41368400 4.57900000 H -4.13741700 4.96197900 4.80888900 H 2.00898700 0.43847900 6.33167500 H -1.05342800 3.71025900 2.07341300

	Br 1.19741700 2.47184600 1.52508300 Br 2.87972100 0.67371100 3.86537400 Br 2.06594100 4.33156100 4.79549100 F 2.62623500 5.86907600 5.57590000
Br_2(Phen)Pd···IF	N 0.40095200 1.57675500 5.81477200 N -0.92267200 2.99095800 3.97474100 C -1.53724300 3.69088300 3.04225400 C -0.72278200 2.21741200 6.20915900 C 1.09150500 0.88204100 6.69662500 C -1.19331900 2.17012100 7.52987900 C 0.69228700 0.78047800 8.03334600 H 1.29607300 0.19868500 8.71759100 C -2.70597900 4.41149000 3.30927400 H -3.17071300 4.97136000 2.50815000 C -0.44497300 1.42109900 8.45241700 H -0.77124700 1.36143300 9.48488700 C -1.42790000 2.97071600 5.22898400 C -2.59354700 3.66611800 5.58344900 C -2.38414200 2.88129800 7.86485500 H -2.73969900 2.83939200 8.88809500 C -3.05531100 3.59837800 6.93186800 H -3.95660100 4.13952900 7.19649600 C -3.23498600 4.40208000 4.57395900 H -4.13701600 4.95748500 4.80607000 H 1.98941400 0.40363600 6.31999400 H -1.07405800 3.67694400 2.06133300 F 2.80756200 6.08817600 5.60951600 I 2.23014400 4.43048500 4.75168300 Br 1.18079600 2.44059400 1.51395600 Br 2.86259100 0.64396200 3.85222700 Pd 0.84711000 1.92647700 3.82312200

Table S6 (Continuation). XYZ coordinates of the optimized geometries for the studied complexes.

I_2(Phen)Pd···PF_3	N 0.79858300 2.35923700 5.94864800 N -0.60540900 3.75579900 4.14001800 C -1.27924000 4.43221100 3.23046800 C -0.28016800 3.04834200 6.38657800 C 1.50856300 1.66693100 6.81796300 C -0.67409500 3.05693700 7.73489200 C 1.18632100 1.61829200 8.17753300 H 1.80814000 1.03378800 8.84326800 C -2.41441700 5.18541800 3.54625800 H -2.92554000 5.72039000 2.75620000 C 0.09860500 2.31180700 8.63935400 H -0.17219200 2.29562000 9.68939600 C -1.02704900 3.78975000 5.42493200 C -2.15460700 4.52267100 5.83089200 H -2.11328700 3.81066400 9.16406600 C -2.53224100 4.51425400 7.20643400 H -3.40321700 5.08627700 7.50582300 C -2.85331600 5.23455400 4.84336100 H -3.72823500 5.81372900 5.11773900 H 2.36805800 1.14185000 6.41356800 H -0.89358000 4.37382800 2.21743600 P 3.09910900 5.24374400 5.05772800 F 3.80258100 6.54188200 5.62095200 F 1.61165100 5.72473600 5.31491900 F 3.23923500 4.37867500 6.37031000 C -1.82178200 3.81156500 8.11981000 Pd 1.14298000 2.62436000 3.89885200 I 1.42953600 3.12615200 1.39142300 I 3.30468700 1.22963500 3.81454200
I_2(Phen)Pd···AsF_3	Pd 1.19327900 2.61959000 3.97591800 N 0.78404900 2.29009000 6.00137900 N -0.55816100 3.74534500 4.19241500 C -1.19862600 4.45231200 3.28289800 C -0.28412900 2.99883100 6.43259800 C 1.46341700 1.56781000 6.86973900 C -0.69774100 2.99829200 7.77473000 C 1.11844900 1.50600000 8.22316000 H 1.71531400 0.89644500 8.88918900 C -2.31901700 5.22938500 3.59221800 H -2.80273900 5.78988600 2.80273900 C 0.04233100 2.22076700 8.67908200 H -0.24351000 2.19743300 9.72496000 C -0.99764000 3.77178500 5.47121000 C -2.11113400 4.52863700 5.87083900 H -2.13601200 3.77154600 9.19408300 C -2.50843200 4.51193100 7.24059900 H -3.36715100 5.10418900 7.53586900 C -2.77558100 5.27230500 4.88315800 H -3.63765900 5.87237600 5.15307600 H 2.31815200 1.03029600 6.47271400 H -0.79610900 4.40539300 2.27644300 As 3.02354700 5.23709700 4.78949000 F 3.80522900 6.67002500 5.36478700

	F 1.46010600 5.97492600 4.71115000 F 2.77955100 4.58602900 6.37339000 C -1.83032300 3.77791100 8.15395400 I 1.58433400 3.22409500 1.50218000 I 3.38097100 1.25903700 3.92940400
I_2(Phen)Pd···SbF_3	Pd 1.21343000 2.57220200 4.01378700 N 0.76808300 2.22527700 6.02736500 N -0.51490800 3.73047900 4.21638600 C -1.11994300 4.46839300 3.30761800 C -0.28346700 2.96104900 6.45321400 C 1.41643200 1.47563800 6.89563300 C -0.70966100 2.96277800 7.79101700 C 1.05562400 1.41227900 8.24476700 H 1.62718300 0.77959200 8.91136000 C -2.21641300 5.27961100 3.61293300 H -2.67070500 5.86531600 2.82446300 C -0.00240600 2.15619600 8.69590900 H -0.29840900 2.13417000 9.73896400 C -0.96381100 3.76200500 5.49187400 C -2.05458300 4.55266400 5.88708400 H -2.13454500 3.77167700 9.20375500 C -2.46457800 4.53888400 7.25300800 H -3.30511300 5.15797700 7.54539400 C -2.68369700 5.32655200 4.89948300 H -3.52627700 5.95470900 5.16690200 H 2.26007200 0.91716400 6.50483100 H -0.70833500 4.42151300 2.30552900 Sb 2.99828000 5.26241100 4.64775700 F 3.74877800 6.86541400 5.35924700 F 1.33490900 6.11937300 4.29585400 F 2.41770500 4.69187200 6.37243800 C -1.81985000 3.77549900 8.16635100 I 1.64130800 3.16569300 1.53889100 I 3.40094300 1.20551200 3.99826800
I_2(Phen)Pd···SF_2	Pd 1.27293600 2.66672700 3.98511500 N 0.91382300 2.32399600 6.02264700 N -0.41233300 3.87800700 4.28434500 C -1.03788800 4.64312700 3.41115000 C -0.14149100 3.02986900 6.48889500 C 1.58778700 1.55788200 6.85771000 C -0.54958300 2.97917000 7.83192000 C 1.24937000 1.44681500 8.21001200 H 1.84085400 0.80249200 8.84763300 C -2.13924600 5.43007400 3.76095400 H -2.61233100 6.03819300 3.00074800 C 0.18361900 2.15504200 8.69996700 H -0.09937900 2.09069700 9.74494100 C -0.84570200 3.85661800 5.56534300 C -1.94262300 4.61685200 6.00351600 H -1.97243700 3.71016500 9.28909500 C -2.33700600 4.54453600 7.37251200 H -3.18512600 5.13677000 7.69710600 C -2.59347700 5.41975300 5.05385700 H -3.44349700 6.02275000 5.35394300 H 2.42809400 1.01943100 6.43080600 H -0.64162000 4.62787700 2.40078600

	F 3.28697700 6.93937300 4.82126500 F 2.07290200 5.24571100 6.01140900 C -1.66896300 3.75877400 8.24940400 S 2.66126000 5.48838500 4.53538900 I 1.56516300 3.22419000 1.48794700 I 3.34890300 1.15998100 3.83034600
I_2(Phen)Pd···SeF_2	Pd 1.26308100 2.68411100 3.97857400 N 0.91499900 2.33537500 6.01735800 N -0.42986500 3.88351100 4.28610600 C -1.05970500 4.64968900 3.41720200 C -0.14181200 3.03507700 6.48827000 C 1.60184300 1.57800300 6.84909900 C -0.54000100 2.98470400 7.83379100 C 1.27420000 1.46826800 8.20404700 H 1.87639900 0.83193100 8.83955300 C -2.16192600 5.43203500 3.77343200 H -2.63939100 6.04164200 3.01726500 C 0.20596800 2.16903300 8.69889500 H -0.06847300 2.10644400 9.74623200 C -0.85564900 3.85785700 5.56918400 C -1.95241700 4.61405100 6.01371000 H -1.95647700 3.71005300 9.29983600 C -2.33837600 4.54044100 7.38500200 H -3.18654100 5.12969100 7.71470800 C -2.60995600 5.41664700 5.06850000 H -3.45962400 6.01733800 5.37407800 H 2.44405600 1.04565400 6.41885600 H -0.66695700 4.64029500 2.40562300 F 3.41989700 6.91643100 4.83499600 F 1.96695900 5.18717500 6.03340400 C -1.66083700 3.75862000 8.25792700 Se 2.67650100 5.37379100 4.44079800 I 1.54076500 3.23176200 1.47534100 I 3.33340200 1.17285200 3.80703600
I_2(Phen)Pd···TeF_2	Pd 1.25105600 2.66307100 3.97899600 N 0.90235500 2.31439500 6.01616300 N -0.43674600 3.86830200 4.28537000 C -1.06283800 4.63731700 3.41597000 C -0.14776800 3.02296600 6.48809200 C 1.59197700 1.56131600 6.84922500 C -0.53894600 2.98281200 7.83563400 C 1.27238000 1.46330800 8.20682300 H 1.87693000 0.83056700 8.84361300 C -2.16255700 5.42285900 3.77172000 H -2.63781600 6.03403500 3.01553500 C 0.20916300 2.17101600 8.70231600 H -0.05902200 2.11758000 9.75175500 C -0.86059200 3.84556400 5.56894200 C -1.95207700 4.60871300 6.01373900 H -1.94457800 3.72307200 9.30451300 C -2.33295500 4.54347000 7.38678500 H -3.17676700 5.13851700 7.71711900 C -2.60798400 5.41157300 5.06771000 H -3.45371900 6.01750000 5.37379400 H 2.42937300 1.02200100 6.41883600 H -0.66937000 4.62920100 2.40497900

	F 3.50351100 7.07355100 4.92821300 F 1.89759500 5.16386100 6.04267300 C -1.65438200 3.76392600 8.26077900 Te 2.70299600 5.43483700 4.32180700 I 3.29031300 1.10963500 3.79826000 I 1.56207900 3.23726500 1.48337600
I_2(Phen)Pd···ClF	Pd 0.92579200 1.99923500 3.82300600 N 0.44046600 1.62733800 5.83763200 N -0.89132400 3.05063000 3.98556100 C -1.51792800 3.74835400 3.06004600 C -0.69266300 2.25722600 6.22013900 C 1.11894800 0.93071500 6.72665500 C -1.18096100 2.19399300 7.53580800 C 0.70464600 0.81371100 8.05727000 H 1.30268300 0.22909000 8.74431400 C -2.69809800 4.45018600 3.32562700 H -3.16898700 5.00777100 2.52636300 C -0.44233600 1.44319900 8.46409700 H -0.78546900 1.37320200 9.49051500 C -1.39910500 3.01231900 5.23768400 C -2.57862400 3.68799800 5.59218000 C -2.38224500 2.88797000 7.86733000 H -2.74639700 2.83112800 8.88689200 C -3.05272200 3.60474000 6.93490600 H -3.96362200 4.13238600 7.19412300 C -3.22955500 4.42235700 4.58820100 H -4.14127800 4.96032900 4.82384200 H 2.02532600 0.45609900 6.36403000 H -1.05829000 3.75037500 2.07667000 F 2.48952700 5.71094200 5.55053400 Cl 1.99681600 4.28168900 4.80759200 I 1.32296500 2.52421800 1.34248500 I 3.09484200 0.62756000 3.80880400
I_2(Phen)Pd···BrF	Pd 0.90240400 1.96095200 3.81191700 N 0.42158200 1.59867600 5.83020600 N -0.90966600 3.02201700 3.97715300 C -1.53432800 3.72186800 3.05196300 C -0.70613200 2.23744200 6.21445100 C 1.10084000 0.90396700 6.72011300 C -1.18772200 2.18513400 7.53295500 C 0.69268800 0.79723900 8.05334100 H 1.29128800 0.21390400 8.74094200 C -2.70740300 4.43427500 3.32003600 H -3.17671700 4.99339400 2.52095600 C -0.44856500 1.43582100 8.46204000 H -0.78637700 1.37470500 9.49076500 C -1.41198600 2.99238500 5.23183400 C -2.58415000 3.67919000 5.58887700 C -2.38234000 2.88925300 7.86694800 H -2.74128200 2.84080200 8.88876100 C -3.05225700 3.60615100 6.93424000 H -3.95754300 4.14238400 7.19538900 C -3.23335400 4.41535100 4.58506300 H -4.13905600 4.96238500 4.82294500 H 2.00343600 0.42301600 6.35672400 H -1.07869300 3.71798800 2.06684500

	Br 2.08001500 4.32558800 4.78156000 F 2.60001500 5.86747800 5.59167600 I 3.06715800 0.58620700 3.79606600 I 1.29724100 2.48005200 1.33183900
I_2(Phen)Pd···IF	Pd 0.88535500 1.94352000 3.80890600 N 0.40777400 1.58488800 5.82858400 N -0.92414300 3.00843700 3.97628200 C -1.54959700 3.70857200 3.05163400 C -0.71728900 2.22776800 6.21462700 C 1.08768600 0.89086900 6.71874100 C -1.19404300 2.18155500 7.53506200 C 0.68392500 0.78978400 8.05362000 H 1.28338700 0.20715800 8.74104700 C -2.71946600 4.42529500 3.32159100 H -3.18910500 4.98438100 2.52270100 C -0.45373700 1.43346700 8.46422700 H -0.78773300 1.37748700 9.49447000 C -1.42359400 2.98240500 5.23248800 C -2.59186200 3.67465300 5.59158600 C -2.38494200 2.89083400 7.87120300 H -2.74009500 2.84710500 8.89453500 C -3.05565300 3.60720400 6.93868500 H -3.95789100 4.14775600 7.20140800 C -3.24145500 4.41116800 4.58828500 H -4.14414900 4.96235500 4.82792400 H 1.98825500 0.40678000 6.35484600 H -1.09674000 3.70272200 2.06538700 F 2.75086600 6.10935000 5.67512300 I 2.23324800 4.45312700 4.76925100 I 1.28707600 2.47609800 1.33365500 I 3.05632800 0.58002100 3.79643400

Table S6 (Continuation). XYZ coordinates of the optimized geometries for the studied complexes.

$Cl_2(Phen)Pt\cdots PF_3$	N 0.79502100 2.36828000 5.95386300 N -0.56108100 3.75351100 4.17425800 C -1.20611800 4.43805700 3.24350100 C -0.28755600 3.04707700 6.40955500 C 1.51424100 1.66238300 6.81129400 C -0.68356100 3.03798400 7.75271200 C 1.18427400 1.59914800 8.16708000 H 1.80721400 1.00808600 8.82585900 C -2.34059100 5.19576400 3.54437900 H -2.82994900 5.73766600 2.74539800 C 0.09257600 2.28129800 8.64438400 H -0.17357300 2.24530500 9.69479800 C -1.01808900 3.79307200 5.45090000 C -2.14546600 4.52943600 5.83528500 H -2.14248700 3.78736000 9.16570500 C -2.53555900 4.50678800 7.20876500 H -3.40774900 5.07776000 7.50638300 C -2.81434400 5.24769400 4.83199800 H -3.69145300 5.83410900 5.08161900 H 2.37207000 1.15129500 6.38945400 H -0.79040300 4.37098100 2.24445000 Cl 1.31746400 3.07729100 1.74856000 Cl 3.00636000 1.36796100 3.95540500 P 3.00024600 5.25248000 4.98498200 F 3.78400500 6.52424600 5.50859800 F 1.54812900 5.82538000 5.26542600 F 3.12497500 4.41334900 6.31783300 C -1.83636100 3.79368500 8.12572600 Pt 1.11744100 2.63959700 3.97375500
$Cl_2(Phen)Pt\cdots AsF_3$	N 0.79407400 2.33803500 5.99894400 N -0.52440800 3.76692800 4.22114200 C -1.14366400 4.47721000 3.29401900 C -0.29225600 3.01437700 6.44651300 C 1.49752900 1.61650400 6.85454300 C -0.71014600 2.98482700 7.78242400 C 1.14508900 1.53117400 8.20366900 H 1.75563700 0.92791000 8.86284800 C -2.27741100 5.23798600 3.58995200 H -2.74605800 5.80286900 2.79464300 C 0.04860000 2.20982600 8.67350400 H -0.23400000 2.15877900 9.71898400 C -1.00182000 3.78310400 5.48984300 C -2.12901700 4.52156400 5.86967100 H -2.18580700 3.71962300 9.18538500 C -2.54238300 4.47655200 7.23557100 H -3.41421300 5.04989300 7.52947700 C -2.77331900 5.26626500 4.86937700 H -3.64849300 5.85675500 5.11614400 H 2.36224400 1.11127400 6.44049900 H -0.70732100 4.43454300 2.30290300 Cl 1.44324200 3.18884900 1.83248700 Cl 3.07459700 1.41772000 4.03190000 As 2.98287100 5.14889000 4.73445700

	F 3.86673700 6.55860900 5.23118900 F 1.46411700 5.98549400 4.70903200 F 2.79069100 4.57184400 6.35736000 C -1.86363100 3.74151000 8.15053500 Pt 1.16819300 2.66812800 4.03490600
$Cl_2(Phen)Pt\cdots SbF_3$	Pt 1.17306100 2.64024600 4.04821500 N 0.77431800 2.29845500 6.00747600 N -0.51131800 3.75625400 4.22607600 C -1.10782300 4.48514100 3.29975100 C -0.30066400 2.99431100 6.45064400 C 1.46290400 1.56538700 6.86403000 C -0.72209300 2.97305700 7.78527100 C 1.10510100 1.48555200 8.21209500 H 1.70355200 0.87239600 8.87310300 C -2.22600300 5.26933700 3.59343300 H -2.67662000 5.84972800 2.79903700 C 0.02031200 2.18444000 8.67820100 H -0.26501900 2.14019900 9.72324600 C -0.99165800 3.77832500 5.49302700 C -2.10283200 4.54093600 5.87112300 H -2.18436400 3.73805000 9.18582600 C -2.52077500 4.50340000 7.23566300 H -3.37993800 5.09618700 7.52812900 C -2.72593800 5.30336300 4.87062400 H -3.58734100 5.91403700 5.11669700 H 2.32128300 1.04634300 6.45469400 H -0.66642200 4.44242300 2.31137700 Cl 1.48303000 3.17336500 1.85024200 Cl 3.07408200 1.37676500 4.05541300 Sb 3.03064200 5.10931000 4.65531500 F 3.87730000 6.69856600 5.30299200 F 1.36601700 6.02657800 4.47942200 F 2.63714100 4.55178800 6.43929600 C -1.86025600 3.75309000 8.15151000
$Cl_2(Phen)Pt\cdots SF_2$	N 0.92112700 2.37029200 5.99967000 N -0.40307600 3.88684200 4.30087500 C -1.01744600 4.65244900 3.41424200 C -0.14408800 3.04916900 6.49261400 C 1.63009900 1.60904200 6.81645900 C -0.53582900 2.98085600 7.83499400 C 1.30385900 1.48503000 8.16940100 H 1.91689100 0.84971000 8.79544100 C -2.12631800 5.42821600 3.76122500 H -2.59375600 6.03698700 2.99818200 C 0.22734700 2.16399200 8.68394000 H -0.03638800 2.08044700 9.73228200 C -0.85631700 3.86596900 5.57851700 C -1.95850100 4.61533100 6.00758000 H -1.97184200 3.69008200 9.29162000 C -2.34818100 4.52666000 7.37849700 H -3.20284000 5.10534800 7.71003600 C -2.60141400 5.41449600 5.04926600 H -3.45882600 6.01371400 5.33445000 H 2.47196100 1.09739600 6.36385300 H -0.60083300 4.63379500 2.41362400 Cl 1.40136500 3.20797100 1.80853400

	Cl 3.02784700 1.33038100 3.91252300 F 3.39119600 6.74267300 4.79204600 F 1.95329100 5.26801600 5.99857400 C -1.66788600 3.74472700 8.25245900 Pt 1.22642800 2.71226200 4.02511000 S 2.64771300 5.33026000 4.54373700
Cl_2(Phen)Pt···SeF_2	N 0.92347900 2.38587800 5.99270200 N -0.41904900 3.89183300 4.29341700 C -1.03381000 4.65939900 3.40973300 C -0.14856800 3.05320000 6.48415600 C 1.64861500 1.64159400 6.80953400 C -0.53400900 2.98672200 7.82797400 C 1.32963000 1.52026800 8.16454200 H 1.95556300 0.89961100 8.79238700 C -2.14596500 5.42926400 3.75973200 H -2.61478600 6.04096200 2.99999400 C 0.24444700 2.18546200 8.67806900 H -0.01344800 2.10504600 9.72811400 C -0.86978200 3.86336100 5.57103900 C -1.97461800 4.60640800 6.00301700 H -1.97179100 3.68539800 9.28786800 C -2.36127700 4.51519200 7.37451800 H -3.21901500 5.08824200 7.70772100 C -2.62078400 5.40646700 5.04749000 H -3.47993900 6.00178200 5.33561200 H 2.49708700 1.14097600 6.35731000 H -0.61693300 4.64786200 2.40925700 Cl 1.36820200 3.19020600 1.78734000 Cl 3.01108100 1.33217400 3.88735200 F 3.56899100 6.70113400 4.93142300 F 1.80462800 5.24918900 6.03038200 C -1.67214500 3.74018300 8.24751400 Se 2.72160100 5.20125400 4.52957500 Pt 1.21817900 2.72304900 4.01197800
Cl_2(Phen)Pt···TeF_2	N 0.91415500 2.37057600 5.98660200 N -0.43254800 3.87319000 4.28534900 C -1.04331700 4.64428600 3.40217000 C -0.15404500 3.04267700 6.47826600 C 1.64660500 1.63532000 6.80448000 C -0.53024600 2.98818700 7.82488000 C 1.33718500 1.52625600 8.16266200 H 1.96871400 0.91316600 8.79224100 C -2.15017100 5.42079900 3.75407500 H -2.61698700 6.03505000 2.99525200 C 0.25464200 2.19511900 8.67665300 H 0.00463000 2.12521400 9.72935200 C -0.87764400 3.84978600 5.56452600 C -1.97578200 4.60090900 5.99878200 H -1.95610200 3.70151400 9.28923000 C -2.35529300 4.51926200 7.37273700 H -3.20824700 5.09843200 7.70750900 C -2.62053200 5.40232700 5.04341000 H -3.47442200 6.00418000 5.33360100 H 2.49292800 1.13169200 6.35194200 H -0.62916000 4.63067500 2.40079700 Cl 1.34303900 3.14433400 1.77103000

	Cl 2.97473600 1.28196100 3.86859100 F 3.63430700 6.85384500 5.07569600 F 1.72304700 5.23303700 6.07145700 C -1.66354500 3.74757100 8.24647900 Te 2.78925900 5.22735100 4.47124300 Pt 1.20037500 2.69539900 4.00073900
Cl_2(Phen)Pt···ClF	N 0.43987500 1.64723400 5.82139000 N -0.86749300 3.04793800 3.99989400 C -1.47050100 3.75114600 3.05793600 C -0.69856800 2.26244800 6.22269100 C 1.14197300 0.95161600 6.69809900 C -1.17864300 2.18702500 7.53593200 C 0.73052900 0.82574400 8.02781000 H 1.34025000 0.24576400 8.70828100 C -2.65253100 4.45159200 3.31371900 H -3.10846700 5.01381400 2.50922600 C -0.42303400 1.43699800 8.45128900 H -0.75339200 1.35255800 9.48051600 C -1.40014500 3.01427500 5.24515300 C -2.57968100 3.68872800 5.58369400 C -2.38619700 2.87636600 7.86025800 H -2.75655200 2.81713600 8.87733000 C -3.05648500 3.59490000 6.92623300 H -3.96970300 4.11761100 7.18683700 C -3.21017400 4.42441800 4.56750600 H -4.12439600 4.96601200 4.78302100 H 2.04869700 0.49648800 6.31588700 H -0.98527200 3.74745700 2.08844000 Cl 1.15993400 2.47013400 1.66242100 Cl 2.76606300 0.75013000 3.89987100 F 2.49373600 5.69252800 5.53779800 Pt 0.87802800 2.01005600 3.86746900 Cl 1.90056900 4.24596700 4.85222100
Cl_2(Phen)Pt···BrF	N 0.42238200 1.62212800 5.81424800 N -0.88710100 3.02130800 3.99254500 C -1.48900400 3.72622000 3.05114000 C -0.71205400 2.24343100 6.21761600 C 1.12765000 0.93035600 6.69146000 C -1.18514500 2.17760800 7.53379100 C 0.72286000 0.81379800 8.02399700 H 1.33487900 0.23687500 8.70496500 C -2.66573700 4.43437600 3.30975800 H -3.12111700 4.99776600 2.50580100 C -0.42677200 1.43085600 8.44958900 H -0.75145700 1.35424400 9.48122000 C -1.41465500 2.99418900 5.24016600 C -2.58841400 3.67698800 5.58160200 C -2.38782200 2.87407200 7.86082100 H -2.75296000 2.82202100 8.88014600 C -3.05924400 3.59149000 6.92675600 H -3.96819000 4.12046500 7.18955300 C -3.21845000 4.41366600 4.56579900 H -4.12809600 4.96197800 4.78362500 H 2.03160300 0.47106400 6.30788600 H -1.00738100 3.71814100 2.07996000 Cl 1.12537600 2.41842900 1.64761800

	Cl 2.73157400 0.70136900 3.88216200 Br 1.98287000 4.30220700 4.83578600 F 2.63568600 5.85319100 5.56317000 Pt 0.85204700 1.97178300 3.85514700
Cl_2(Phen)Pt···IF	N 0.40430400 1.60014800 5.81050700 N -0.90603600 2.99901400 3.98950700 C -1.50698800 3.70612900 3.04892000 C -0.72761800 2.22523900 6.21568300 C 1.11069700 0.90928300 6.68779500 C -1.19613900 2.16514100 7.53368800 C 0.71000600 0.79792300 8.02191500 H 1.32291600 0.22171100 8.70265700 C -2.67929800 4.42055700 3.30990400 H -3.13368600 4.98567800 2.50662400 C -0.43655600 1.41939700 8.44933900 H -0.75772000 1.34727400 9.48238200 C -1.43055400 2.97600500 5.23867700 C -2.59976100 3.66526000 5.58242100 C -2.39514400 2.86683500 7.86282600 H -2.75699100 2.81897200 8.88351500 C -3.06669300 3.58473000 6.92919600 H -3.97240300 4.11833200 7.19374600 C -3.22871700 4.40403100 4.56744100 H -4.13468500 4.95762000 4.78717800 H 2.01243800 0.44658700 6.30327100 H -1.02815500 3.69519600 2.07645900 Cl 1.09508600 2.37709900 1.63821800 Cl 2.70198900 0.66286900 3.87118100 F 2.82890700 6.07790900 5.57894700 Pt 0.82684600 1.93880100 3.84748100 I 2.11730400 4.41000500 4.81508900

Table S6 (Continuation). XYZ coordinates of the optimized geometries for the studied complexes.

$Br_2(Phen)Pt\cdots PF_3$	N 0.79141200 2.36246500 5.95856600 N -0.56836700 3.75305800 4.17365600 C -1.21943900 4.43839400 3.24777900 C -0.28933000 3.04624000 6.41113000 C 1.50471200 1.65674600 6.82101800 C -0.68615000 3.04107800 7.75510500 C 1.17434900 1.59720900 8.17669000 H 1.79506700 1.00496800 8.83652000 C -2.35201600 5.19740300 3.55170200 H -2.84361100 5.73866000 2.75364800 C 0.08532400 2.28453100 8.65049100 H -0.18325200 2.25315400 9.70046200 C -1.01998700 3.79291100 5.45218300 C -2.14604900 4.53126000 5.84020600 H -2.13978800 3.79421800 9.17072500 C -2.53486600 4.51226800 7.21356500 H -3.40561500 5.08569900 7.51063300 C -2.81942800 5.25015900 4.84078800 H -3.69478700 5.83705300 5.09548700 H 2.36243600 1.13933700 6.40598900 H -0.81169800 4.37397400 2.24498000 Br 1.35504600 3.09041700 1.60608700 Br 3.12756000 1.28779400 3.92555500 P 3.00842800 5.26472100 5.00173600 F 3.77239500 6.54215800 5.53982300 F 1.54676400 5.82993200 5.24350400 F 3.10366700 4.43051200 6.34017100 C -1.83604400 3.79926600 8.13005400 Pt 1.12293900 2.63144600 3.96368900
$Br_2(Phen)Pt\cdots AsF_3$	N 0.79139300 2.32911100 5.99958700 N -0.53049100 3.76319300 4.21678800 C -1.15670700 4.47295700 3.29399700 C -0.29001400 3.01452200 6.44538500 C 1.48770900 1.60592600 6.85957900 C -0.70592700 2.99238900 7.78305100 C 1.13733500 1.52745200 8.20945900 H 1.74471000 0.92153200 8.86915100 C -2.28606000 5.23837600 3.59383700 H -2.75771700 5.80145200 2.79901100 C 0.04727700 2.21621900 8.67737000 H -0.23558600 2.17246400 9.72313400 C -0.99958000 3.78389200 5.48855800 C -2.12272900 4.52797000 5.87287800 H -2.17081700 3.73819900 9.19063700 C -2.53163700 4.49084300 7.23980600 H -3.39965400 5.06977000 7.53400500 C -2.77223100 5.27229100 4.87606100 H -3.64362500 5.86598400 5.12854600 H 2.34920900 1.09036700 6.45097100 H -0.73092000 4.42907200 2.29810200 Br 1.47626700 3.19074300 1.68436000 Br 3.19058900 1.32554700 3.99706500 As 2.96741600 5.17093500 4.76447100

	F 3.82448600 6.58785500 5.28515800 F 1.43653300 5.98395300 4.72776900 F 2.76186200 4.57451200 6.37832800 C -1.85331300 3.75580100 8.15427500 Pt 1.17189600 2.65371200 4.02058400
$Br_2(Phen)Pt\cdots SbF_3$	Pt 1.17860400 2.62352900 4.03503800 N 0.77314100 2.28798000 6.00908300 N -0.51430700 3.75148200 4.22236400 C -1.11770900 4.47938400 3.29970900 C -0.29581100 2.99426900 6.45050200 C 1.45250500 1.55113800 6.86980300 C -0.71551100 2.98064300 7.78674200 C 1.09626600 1.47815700 8.21843500 H 1.68983500 0.86061600 8.87979400 C -2.23064400 5.26922900 3.59697500 H -2.68419400 5.84741100 2.80262000 C 0.01954700 2.18923100 8.68276900 H -0.26618100 2.15239800 9.72801100 C -0.98590200 3.77940600 5.49254400 C -2.09218500 4.54875800 5.87475200 H -2.16577300 3.75871800 9.19173200 C -2.50535600 4.52004100 7.24042500 H -3.35979600 5.11950900 7.53307100 C -2.72015700 5.31051500 4.87721900 H -3.57706900 5.92532800 5.12868100 H 2.30631700 1.02013000 6.46572300 H -0.68727300 4.43412300 2.30641600 Br 1.51469200 3.16562300 1.70085800 Br 3.18930100 1.27783200 4.02319500 Sb 3.00684100 5.13772500 4.68809100 F 3.82074100 6.73463400 5.35709200 F 1.33375200 6.03206100 4.48360300 F 2.58232900 4.56816500 6.46076600 C -1.84632600 3.76899500 8.15591900
$Br_2(Phen)Pt\cdots SF_2$	N 0.91839300 2.36718400 6.00530900 N -0.40946100 3.88836200 4.30086700 C -1.02863400 4.65586400 3.41921600 C -0.14622900 3.04959800 6.49463300 C 1.62241700 1.60773000 6.82797200 C -0.53945500 2.98483200 7.83779900 C 1.29527200 1.48726400 8.18080600 H 1.90695900 0.85217200 8.80841100 C -2.13575400 5.43254500 3.76879800 H -2.60447500 6.04152700 3.00669200 C 0.21976000 2.16943600 8.69120300 H -0.04696100 2.09030000 9.73915700 C -0.85836300 3.86690500 5.58004300 C -1.95984700 4.61742600 6.01217100 H -1.97219700 3.69553100 9.29612800 C -2.34950500 4.53132000 7.38274300 H -3.20340500 5.11165800 7.71332200 C -2.60625500 5.41791200 5.05776400 H -3.46241300 6.01675000 5.34756700 H 2.46523600 1.09077300 6.38256300 H -0.61911800 4.64069200 2.41530800 Br 1.42542900 3.20985800 1.66174100

	Br 3.14045400 1.24169700 3.87723700 F 3.36891100 6.76921900 4.81217500 F 1.96931700 5.25278000 6.01482300 C -1.66977800 3.74966500 8.25650100 Pt 1.23016800 2.70375300 4.01499200 S 2.64511700 5.34936000 4.55380900
Br_2(Phen)Pt···SeF_2	N 0.92188500 2.38310600 6.00071900 N -0.42216000 3.89508200 4.29570700 C -1.03956200 4.66645800 3.41712500 C -0.15045500 3.05313800 6.48784500 C 1.64122500 1.64006700 6.82377100 C -0.53936500 2.98859000 7.83179400 C 1.31940400 1.52075900 8.17804500 H 1.94334300 0.89990200 8.80770200 C -2.15028600 5.43704900 3.76893400 H -2.61874000 6.05045300 3.01032600 C 0.23410800 2.18810800 8.68661700 H -0.02830200 2.11077000 9.73579600 C -0.87044400 3.86469600 5.57412500 C -1.97514100 4.60858200 6.00833800 H -1.97635600 3.68677400 9.29193600 C -2.36392500 4.51810300 7.37879500 H -3.22145700 5.09232200 7.71049300 C -2.62296400 5.41139600 5.05673500 H -3.48126800 6.00607700 5.34875300 H 2.49153000 1.13499100 6.37939600 H -0.62780400 4.65975600 2.41421300 Br 1.39269400 3.18935700 1.64182100 Br 3.12288600 1.23963900 3.85514400 F 3.53162000 6.73723300 4.92591800 F 1.83093600 5.22578300 6.04953500 C -1.67662400 3.74233000 8.25165200 Se 2.70610800 5.22591900 4.52368500 Pt 1.22469500 2.71567200 4.00483100
Br_2(Phen)Pt···TeF_2	N 0.91492000 2.37175400 5.99477200 N -0.43538300 3.87795600 4.28738000 C -1.04890000 4.65295800 3.40944800 C -0.15558400 3.04385900 6.48159200 C 1.64391600 1.64077300 6.81957300 C -0.53556700 2.99059500 7.82820500 C 1.33166300 1.53356200 8.17700000 H 1.96309900 0.92280300 8.80896400 C -2.15610300 5.42783000 3.76271000 H -2.62275100 6.04377800 3.00513700 C 0.24651900 2.20109400 8.68532500 H -0.00820600 2.13381000 9.73708300 C -0.87917500 3.85089500 5.56696400 C -1.97891500 4.60053100 6.00294900 H -1.96345700 3.69948900 9.29196000 C -2.36147400 4.51815700 7.37553400 H -3.21583500 5.09637700 7.70833500 C -2.62585600 5.40427400 5.05150400 H -3.48035400 6.00360000 5.34518600 H 2.49349600 1.13480300 6.37528900 H -0.63859000 4.64580000 2.40617900 Br 1.35988600 3.13751600 1.62344900

	Br 3.08132000 1.18403500 3.83456600 F 3.61870000 6.87212800 5.08448800 F 1.72842100 5.22386400 6.08039600 C -1.67026400 3.74722100 8.24946700 Te 2.78333900 5.24317500 4.47326500 Pt 1.20671900 2.68947700 3.99303000
Br_2(Phen)Pt···ClF	N 0.43851900 1.64736700 5.82838400 N -0.87467500 3.05080300 4.00112700 C -1.48452400 3.75430600 3.06380700 C -0.70018600 2.26435200 6.22615800 C 1.13581700 0.95332900 6.71015100 C -1.18212900 2.19091400 7.53991600 C 0.72323400 0.82963700 8.03947400 H 1.33192500 0.24997800 8.72116900 C -2.66632000 4.45364500 3.32243800 H -3.12485700 5.01512100 2.51887900 C -0.43002500 1.44257100 8.45907500 H -0.76364700 1.36125900 9.48752400 C -1.40295600 3.01563800 5.24819900 C -2.58328400 3.68918900 5.58998800 C -2.38919600 2.87937800 7.86574900 H -2.75804600 2.81988000 8.88334600 C -3.06003800 3.59682700 6.93212400 H -3.97339800 4.11968800 7.19190100 C -3.21908700 4.42495200 4.57758100 H -4.13324900 4.96473600 4.79795200 H 2.04373100 0.49422300 6.33474500 H -1.00644100 3.75418100 2.09043700 Br 1.19866900 2.48228500 1.52058600 Br 2.89025400 0.67559100 3.87400100 F 2.47849000 5.69783600 5.54728700 Pt 0.88643800 2.00885600 3.85970900 Cl 1.90340400 4.24954500 4.84921400
Br_2(Phen)Pt···BrF	N 0.42030200 1.62120700 5.82072700 N -0.89369000 3.02514700 3.99381600 C -1.50153900 3.73167300 3.05751100 C -0.71423000 2.24451700 6.22056200 C 1.12029000 0.93035400 6.70281000 C -1.18962000 2.18006600 7.53706300 C 0.71401300 0.81537600 8.03479300 H 1.32466100 0.23824800 8.71684300 C -2.67766500 4.43930300 3.31909500 H -3.13488400 5.00306800 2.51642500 C -0.43527500 1.43423800 8.45648800 H -0.76359800 1.36028600 9.48718500 C -1.41732400 2.99579000 5.24299800 C -2.59159200 3.67811300 5.58782000 C -2.39162200 2.87594300 7.86569400 H -2.75564500 2.82304600 8.88536900 C -3.06293100 3.59328400 6.93232200 H -3.97186700 4.12264100 7.19436500 C -3.22606200 4.41621800 4.57623800 H -4.13539800 4.96307600 4.79907300 H 2.02541500 0.46704200 6.32605400 H -1.02656800 3.72782000 2.08271400 Br 1.16570700 2.43269900 1.50630300

	Br 2.85516200 0.62600500 3.85651200 Br 1.98774400 4.30572200 4.83326800 F 2.61882700 5.85849400 5.57714600 Pt 0.86071900 1.97064100 3.84713400
Br_2(Phen)Pt···IF	N 0.40777100 1.59669800 5.81130800 N -0.90667600 2.99990600 3.98472200 C -1.51314700 3.70880700 3.04906600 C -0.72422100 2.22404700 6.21278100 C 1.10896800 0.90729900 6.69387300 C -1.19492800 2.16608000 7.53119300 C 0.70686100 0.79828100 8.02751800 H 1.31845400 0.22227500 8.70964800 C -2.68456700 4.42323300 3.31277100 H -3.14048100 4.98879200 2.51063900 C -0.43932700 1.42173900 8.45081600 H -0.76402800 1.35282700 9.48299600 C -1.42745100 2.97512800 5.23542100 C -2.59689900 3.66449100 5.58229600 C -2.39313900 2.86751200 7.86161900 H -2.75391900 2.81927000 8.88266300 C -3.06440600 3.58514500 6.92841100 H -3.96999200 4.11941300 7.19202300 C -3.22987100 4.40475400 4.57131500 H -4.13534000 4.95729100 4.79581800 H 2.01189400 0.44047500 6.31639300 H -1.04076800 3.70174300 2.07311200 F 2.81386600 6.08097200 5.59188700 Pt 0.84042500 1.93346200 3.83349700 I 2.12892300 4.41099600 4.80717300 Br 1.13857900 2.38516900 1.49035800 Br 2.82966300 0.58218000 3.83938400

Table S6 (Continuation). XYZ coordinates of the optimized geometries for the studied complexes.

I_2(Phen)Pt···PF_3	N 0.79980800 2.33682300 5.95193700 N -0.56547000 3.74452300 4.16293700 C -1.22598400 4.43360500 3.24728900 C -0.27330300 3.03310200 6.40278000 C 1.50219500 1.62660000 6.81891100 C -0.66746200 3.03489500 7.74922200 C 1.17538100 1.57265900 8.17535600 H 1.79091700 0.97448800 8.83476600 C -2.35163100 5.19902700 3.55929300 H -2.84758500 5.74175500 2.76489100 C 0.09561800 2.27376900 8.64737000 H -0.17365800 2.25007900 9.69740800 C -1.00408900 3.78530900 5.44566400 C -2.12363200 4.53133900 5.84348000 H -2.10476200 3.80028700 9.17386900 C -2.50582900 4.51908400 7.21805700 H -3.37062500 5.10019000 7.51759900 C -2.80417600 5.25452800 4.85252800 H -3.67331400 5.84583200 5.11828600 H 2.35530600 1.09484800 6.41144200 H -0.83417600 4.37242900 2.23753100 P 2.99596800 5.30303400 5.00132400 F 3.72677000 6.59129700 5.55844800 F 1.52246800 5.86591600 5.15213700 F 3.01943400 4.49108000 6.35680300 C -1.80795400 3.80242200 8.13118700 Pt 1.14702400 2.60651800 3.93050800 I 1.42821200 3.09972100 1.40844600 I 3.29422600 1.16793800 3.85389400
I_2(Phen)Pt···AsF_3	Pt 1.19135000 2.62985400 3.98688000 N 0.79685500 2.31246400 5.99217300 N -0.53200800 3.75411900 4.20015700 C -1.16952500 4.46194100 3.28418900 C -0.27672700 3.01185300 6.43440600 C 1.48178600 1.58695300 6.85873800 C -0.68930900 3.00186800 7.77486300 C 1.13524800 1.51895800 8.20977500 H 1.73717500 0.90901300 8.87082500 C -2.29202600 5.23458500 3.58944600 H -2.76943000 5.79433400 2.79564100 C 0.05540300 2.22411000 8.67429900 H -0.22749400 2.19214000 9.72051900 C -0.98712500 3.78205100 5.47659400 C -2.10385500 4.53491900 5.86804300 H -2.13689500 3.76597200 9.18947300 C -2.50494300 4.51082300 7.23686600 H -3.36678300 5.09859600 7.53169500 C -2.76194300 5.27795500 4.87646100 H -3.62723800 5.87678100 5.13781300 H 2.33799600 1.05526400 6.45871600 H -0.76096500 4.41541200 2.28080400 As 2.94105700 5.20537400 4.81211400 F 3.75595100 6.63300300 5.36816500

	F 1.39221100 5.98108000 4.76136800 F 2.72202000 4.57765900 6.41139600 C -1.82696400 3.77621900 8.15072100 I 1.53796200 3.18133100 1.48078200 I 3.35298000 1.20513500 3.93044900
$I_2(Phen)Pt\cdots SbF_3$	Pt 1.20404100 2.59865500 4.00864600 N 0.78221100 2.26984600 6.00836500 N -0.50611000 3.74614200 4.21280400 C -1.11658300 4.47642700 3.29716400 C -0.28024400 2.98827800 6.44502300 C 1.44690800 1.52769700 6.87544200 C -0.70120500 2.98210600 7.78249700 C 1.08987500 1.46052500 8.22377700 H 1.67536100 0.83658500 8.88642400 C -2.22278600 5.27327200 3.59873000 H -2.67853500 5.85174100 2.80579700 C 0.02202200 2.18620100 8.68347800 H -0.26731000 2.15738600 9.72801800 C -0.96767900 3.77752200 5.48635300 C -2.06820100 4.55495700 5.87433000 H -2.13889000 3.77340100 9.19199800 C -2.47822400 4.53437300 7.24041600 H -3.32706100 5.14187800 7.53280500 C -2.70062600 5.31943600 4.88226700 H -3.55180400 5.93898600 5.14159800 H 2.29588200 0.98130300 6.48070700 H -0.69979200 4.43153500 2.29766700 Sb 2.97032600 5.18142500 4.72315800 F 3.74565100 6.78760500 5.41452100 F 1.29906500 6.05793700 4.44969700 F 2.47980000 4.61625100 6.47955100 C -1.82329200 3.78011400 8.15497500 I 1.57420000 3.13786400 1.49912600 I 3.34904600 1.14244900 3.96474700
$I_2(Phen)Pt\cdots SF_2$	Pt 1.26171600 2.69638600 3.99481200 N 0.92494300 2.36454300 6.01058800 N -0.40345500 3.89158700 4.28974100 C -1.02544100 4.66253700 3.41364700 C -0.14471700 3.04741300 6.48742000 C 1.61751300 1.60830600 6.84516200 C -0.54976200 2.98385800 7.82880200 C 1.27964900 1.48812900 8.19499900 H 1.88631100 0.85382800 8.82833600 C -2.13371200 5.43784900 3.76106100 H -2.60083700 6.04825100 2.99904300 C 0.19967800 2.17089900 8.69250500 H -0.07903300 2.09514600 9.73762700 C -0.85349000 3.86531800 5.56820400 C -1.95855400 4.61409200 5.99947100 H -1.98998200 3.68963100 9.28114200 C -2.35732600 4.52772300 7.36671200 H -3.21375500 5.10766200 7.69140900 C -2.60562400 5.41743700 5.04847100 H -3.46311200 6.01311600 5.34098900 H 2.46702800 1.08763400 6.41600900 H -0.62070200 4.65546200 2.40727100

	F 3.36428700 6.79201800 4.86928400 F 1.98712200 5.23288500 6.04507300 C -1.68260700 3.74611500 8.24308800 S 2.66587200 5.36392000 4.58909200 I 1.49535800 3.20387700 1.46737200 I 3.32161800 1.14763700 3.83143200
$I_2(Phen)Pt\cdots SeF_2$	Pt 1.24702500 2.70610400 3.98107100 N 0.93029200 2.38099200 6.00479700 N -0.42035200 3.90088500 4.28994400 C -1.04141500 4.67922400 3.42069000 C -0.14564100 3.05056900 6.48386100 C 1.64343600 1.64331400 6.83728700 C -0.54111100 2.98638300 7.82757700 C 1.31674400 1.52420100 8.19003500 H 1.93961100 0.90586900 8.82330500 C -2.15165400 5.44852500 3.77520900 H -2.61977000 6.06606400 3.01968800 C 0.22732800 2.18961400 8.68978200 H -0.04300600 2.11496400 9.73718400 C -0.86560900 3.86365200 5.56892700 C -1.97212200 4.60561000 6.00705700 H -1.98115200 3.67703900 9.28731000 C -2.36570000 4.51264300 7.37529700 H -3.22482800 5.08581000 7.70469600 C -2.62270300 5.41379600 5.06247600 H -3.48118900 6.00511400 5.36087600 H 2.49918400 1.13556200 6.40549800 H -0.63671700 4.68290200 2.41449000 F 3.51129400 6.76050100 4.92745500 F 1.84962200 5.20685400 6.05488500 C -1.68009600 3.73619300 8.24760000 Se 2.70762500 5.23766800 4.52043100 I 1.43098600 3.16828300 1.43887400 I 3.27998300 1.12414100 3.79252200
$I_2(Phen)Pt\cdots TeF_2$	Pt 1.22808900 2.68075400 3.96827000 N 0.92522900 2.37281200 5.99880300 N -0.43153200 3.88821200 4.28269500 C -1.04695800 4.67271500 3.41522600 C -0.15053700 3.04188100 6.47740400 C 1.64966800 1.64901500 6.83317200 C -0.53815100 2.98675500 7.82342700 C 1.33191400 1.54034600 8.18882900 H 1.96352500 0.93357800 8.82453400 C -2.15477300 5.44471400 3.77127100 H -2.61979900 6.06694200 3.01777900 C 0.24016300 2.20222100 8.68791600 H -0.02327200 2.13593900 9.73763000 C -0.87423200 3.85094200 5.56205100 C -1.97715900 4.59662600 6.00191800 H -1.97248000 3.68293000 9.28605300 C -2.36645200 4.50833300 7.37157800 H -3.22386900 5.08339500 7.70201600 C -2.62570300 5.40775100 5.05842800 H -3.48147500 6.00216600 5.35846000 H 2.50614100 1.14274800 6.40162600 H -0.64159000 4.67881800 2.40954600

	F 3.61316100 6.88250200 5.09192400 F 1.73643400 5.21325700 6.07933300 C -1.67669300 3.73647300 8.24456400 Te 2.79070000 5.24839100 4.47313800 I 3.22464000 1.05285000 3.76730400 I 1.38661900 3.10916400 1.41784300
I_2(Phen)Pt···ClF	Pt 0.91445400 2.00663000 3.83685600 N 0.44377100 1.64207900 5.83090100 N -0.87718500 3.05362900 3.99394900 C -1.49645300 3.75837000 3.06440200 C -0.69468000 2.26275200 6.22235800 C 1.13207900 0.94909800 6.71984000 C -1.18048500 2.19193400 7.53660900 C 0.71743700 0.82774500 8.04833300 H 1.32320300 0.24754300 8.73224700 C -2.67751900 4.45675900 3.32685500 H -3.13979100 5.01826900 2.52539500 C -0.43499400 1.44464700 8.46143100 H -0.77426400 1.36789000 9.48842600 C -1.39858100 3.01511000 5.24342900 C -2.57978000 3.68787200 5.59053300 C -2.38632800 2.88009100 7.86469900 H -2.75346500 2.81991100 8.88288600 C -3.05700700 3.59718000 6.93191100 H -3.97021200 4.12086300 7.19061300 C -3.22281900 4.42498600 4.58421400 H -4.13648000 4.96251300 4.81225300 H 2.04147700 0.48307200 6.35544800 H -1.02922100 3.76450000 2.08529500 F 2.46544200 5.69850400 5.55647500 Cl 1.91731500 4.24628300 4.83569900 I 1.27732900 2.49992600 1.33000700 I 3.06916400 0.58659900 3.82124200
I_2(Phen)Pt···BrF	Pt 0.88857200 1.96615400 3.82408200 N 0.42561600 1.61529400 5.82331000 N -0.89556100 3.02684100 3.98616600 C -1.51239300 3.73475300 3.05739200 C -0.70853800 2.24268400 6.21656100 C 1.11637400 0.92569100 6.71299500 C -1.18787400 2.18158100 7.53358500 C 0.70786900 0.81367800 8.04412900 H 1.31528700 0.23605100 8.72872000 C -2.68735800 4.44220600 3.32253100 H -3.14799200 5.00606500 2.52181000 C -0.44041900 1.43700300 8.45902400 H -0.77444300 1.36809600 9.48828400 C -1.41243700 2.99487000 5.23771000 C -2.58723400 3.67717500 5.58756700 C -2.38841000 2.87771500 7.86411700 H -2.75082700 2.82464100 8.88436600 C -3.05917000 3.59467400 6.93129600 H -3.96772300 4.12535100 7.19203500 C -3.22840100 4.41674600 4.58184100 H -4.13690900 4.96199600 4.81209200 H 2.02283700 0.45504800 6.34749700 H -1.04820900 3.73649600 2.07691700

	Br 2.00155300 4.30482200 4.82156600 F 2.59827200 5.86234700 5.59122200 I 3.03329200 0.53363300 3.80390300 I 1.24332500 2.44600800 1.31488700
I_2(Phen)Pt···IF	Pt 0.87526800 1.95212500 3.82337500 N 0.41594500 1.60848500 5.82504100 N -0.90498300 3.01955100 3.98820800 C -1.51979000 3.73076900 3.06039200 C -0.71967900 2.23391400 6.21803800 C 1.10823200 0.92133700 6.71569300 C -1.19833400 2.17354600 7.53524200 C 0.70016800 0.80989500 8.04689100 H 1.30909700 0.23444100 8.73195000 C -2.69384200 4.43944000 3.32573700 H -3.15238500 5.00600900 2.52574600 C -0.44932000 1.43131200 8.46134800 H -0.78282000 1.36311400 9.49080500 C -1.42343000 2.98599200 5.23932300 C -2.59735600 3.66953800 5.58928200 C -2.39923000 2.86909700 7.86554000 H -2.76165200 2.81609200 8.88577800 C -3.06980500 3.58631200 6.93274700 H -3.97815900 4.11727200 7.19355000 C -3.23642700 4.41205500 4.58435100 H -4.14414900 4.95848400 4.81481300 H 2.01590000 0.45244000 6.35115500 H -1.05451000 3.73461200 2.08052400 F 2.77408400 6.11056100 5.64830100 I 2.13808100 4.43757600 4.82303200 I 1.22555000 2.42551600 1.31325500 I 3.01595200 0.51527700 3.80218700