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Supplementary information for

Pyridine imines as ligands in luminescent iridium complexes

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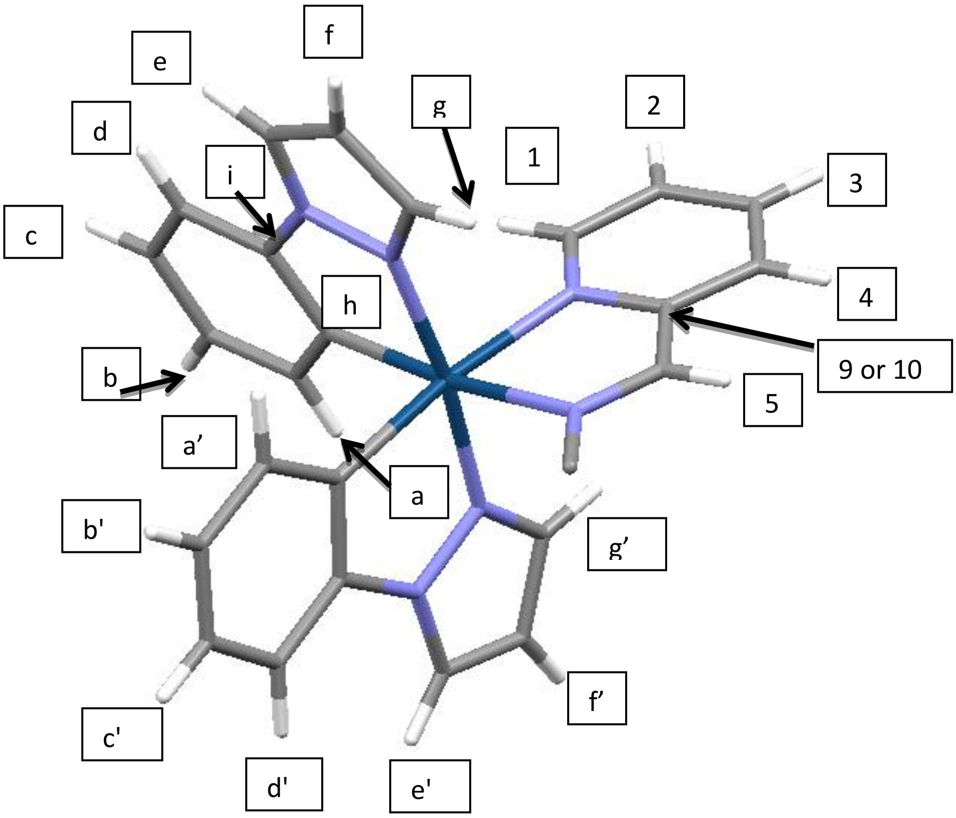
Contents



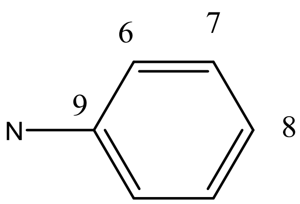
NMR labelling

Ppz the protons (and attached carbons) are labelled a-g, with quaternary carbons being h and i).

The non-prime labels refer to the phenyl (and associated pyrazole) which is trans to imine

The prime labels refer to the phenyl (and associated pyrazole) which is trans to pyridine

The pyridine is numbered 1-4 with the quanternary carbon being C9 for the isopropyl complex but C10 for the aryl complexes. The imine is C and H5 and substituent is numbered as shown below.



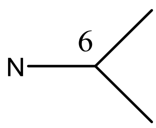


Figure S1a,b c Significant parts of 2-D NMR spectra of 4b

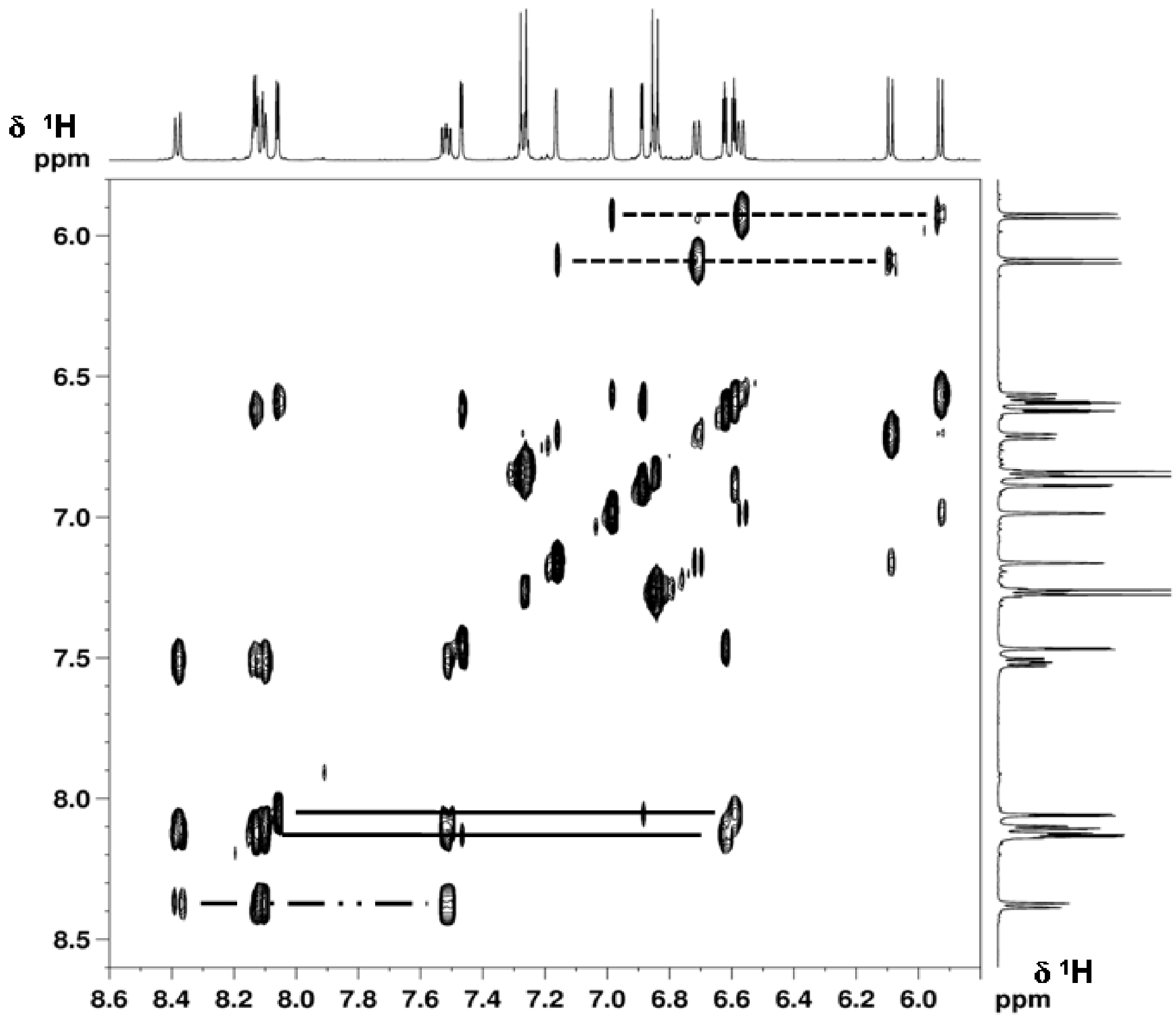


Fig. S.1a: Aromatic part of the TOCSY spectrum of 4b showing identification of two cyclometallated phenyls (----), two pyrazoles (——) and one pyridine ring (··—··).

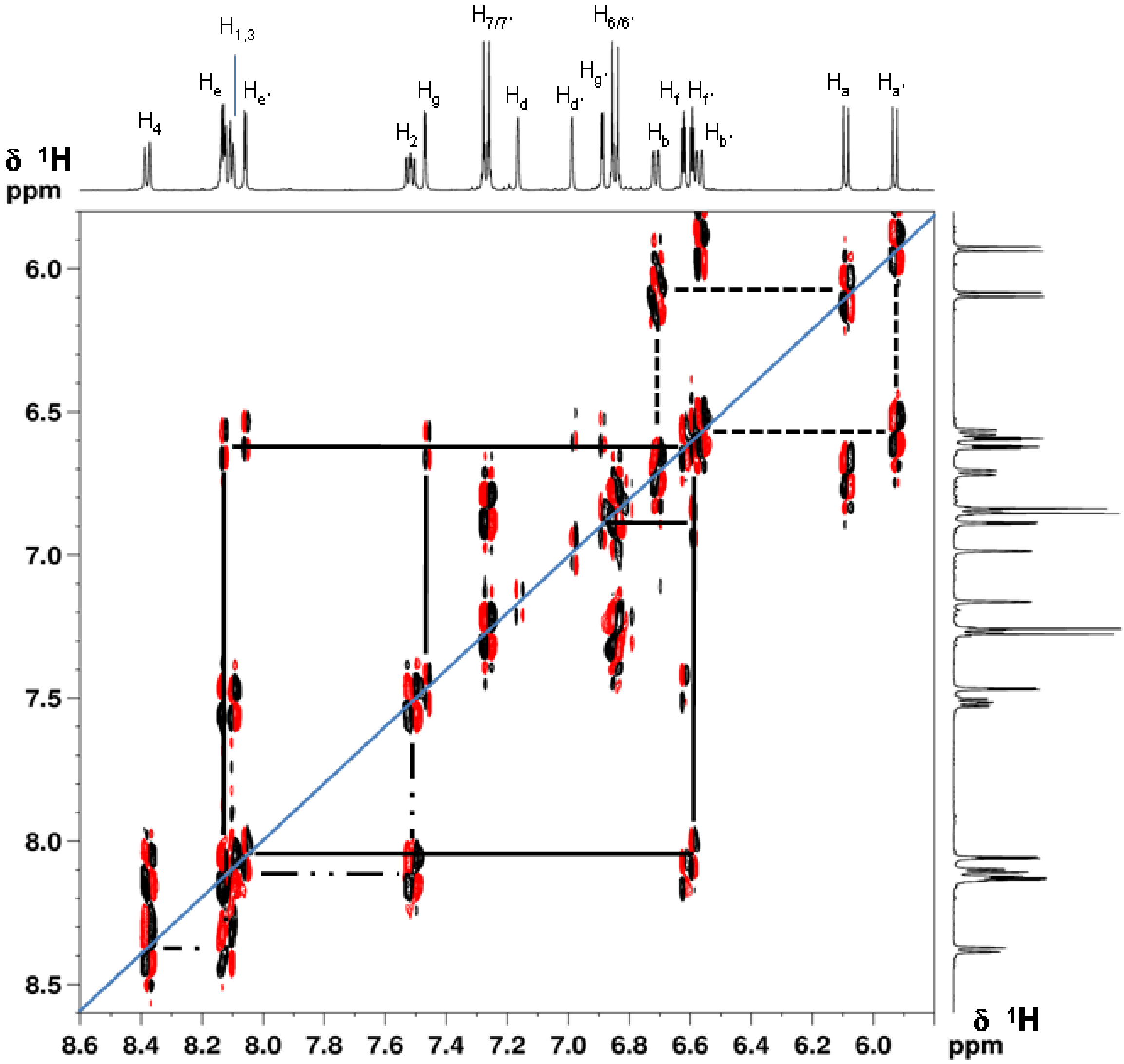


Fig. S1b: COSY spectrum of 4b showing one bond correlations.

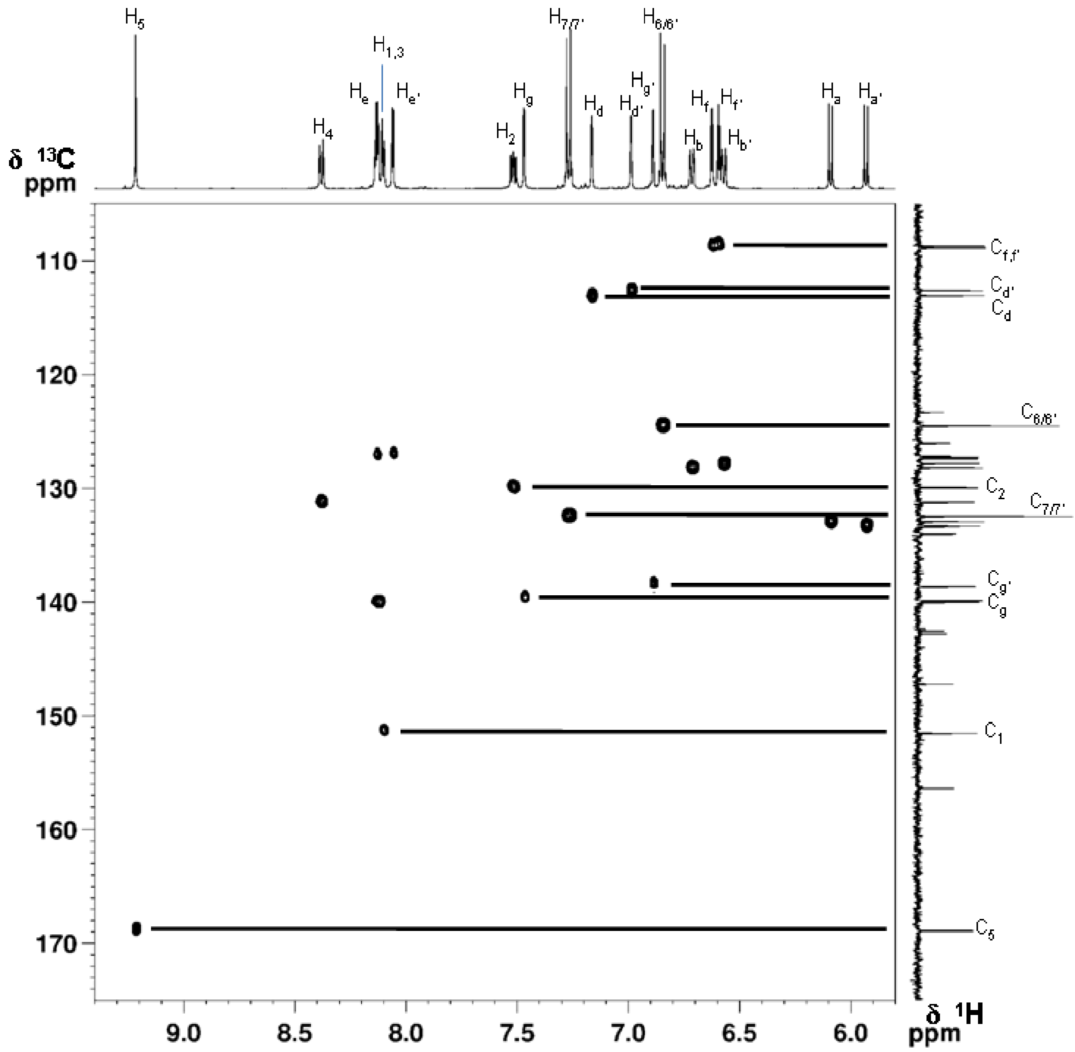


Fig. S1c: HMQC spectrum of 4b showing some direct C-H couplings.

Figure. S2: X-ray structures of 4b and 4c

Table S1 X-ray data for compounds 4b and 4c

Compound reference	**4b**	**4c**
Chemical formula	$C_{32}H_{27}BrIrN_6PF_6$ 0.5(CH_2Cl_2) 0.5(C_2H_5OH) 0.5 (C_6H_{14})	$C_{34}H_{31}IrN_6(PF_6)$
Formula Mass	1021.26	940.73
Temperature/K	150(2)	150(2)
Crystal system	Triclinic	Monoclinic
Space group	*P*-1	*P*2(1)/n
a/Å	10.898(2)	8.7123(17)
b/Å	12.910(3)	20.055(4)
c/Å	27.523(6)	18.908(4)
α/°	90.069(4)	90
β/°	98.453(4)	92.520(4)
γ/°	97.286(4)	90
U/$Å^3$	3798.7(15)	3300.5(11)
No. of formula units per unit cell, *Z*	4	4
Density (calc.) Mg/m^3	1.786	1.893
Abs. coefficient/ mm^{-1}	4.746	5.375
F(000)	2004	1832
Crystal size mm	0.30 x 0.18 x 0.16	0.20 x 0.10 x 0.05
Theta range °	1.59 to 26.00	2.03 to 26.00
Index ranges	-13<=h<=13, -15<=k<=15, -33<=l<=33	-10<=h<=10, -24<=k<=24, -23<=l<=23
No. of reflections measured	29649	25460
No. of independent reflections	14714 [R(int) = 0.0630]	6479 [R(int) = 0.1233]
Data / restraints / parameters	14714 / 0 / 887	6479 / 0 / 446
Goodness-of-fit, F^2	0.902	0.790
Final R indices [I>2sigma(I)]	0.0541, wR2 = 0.1140	0.0497, wR2 = 0.0687
R indices (all data)	0.0849, wR2 = 0.1208	0.0969, wR2 = 0.0793
Largest diff. peak and hole e.$Å^{-3}$	2.483 and -1.467	1.435 and -1.076

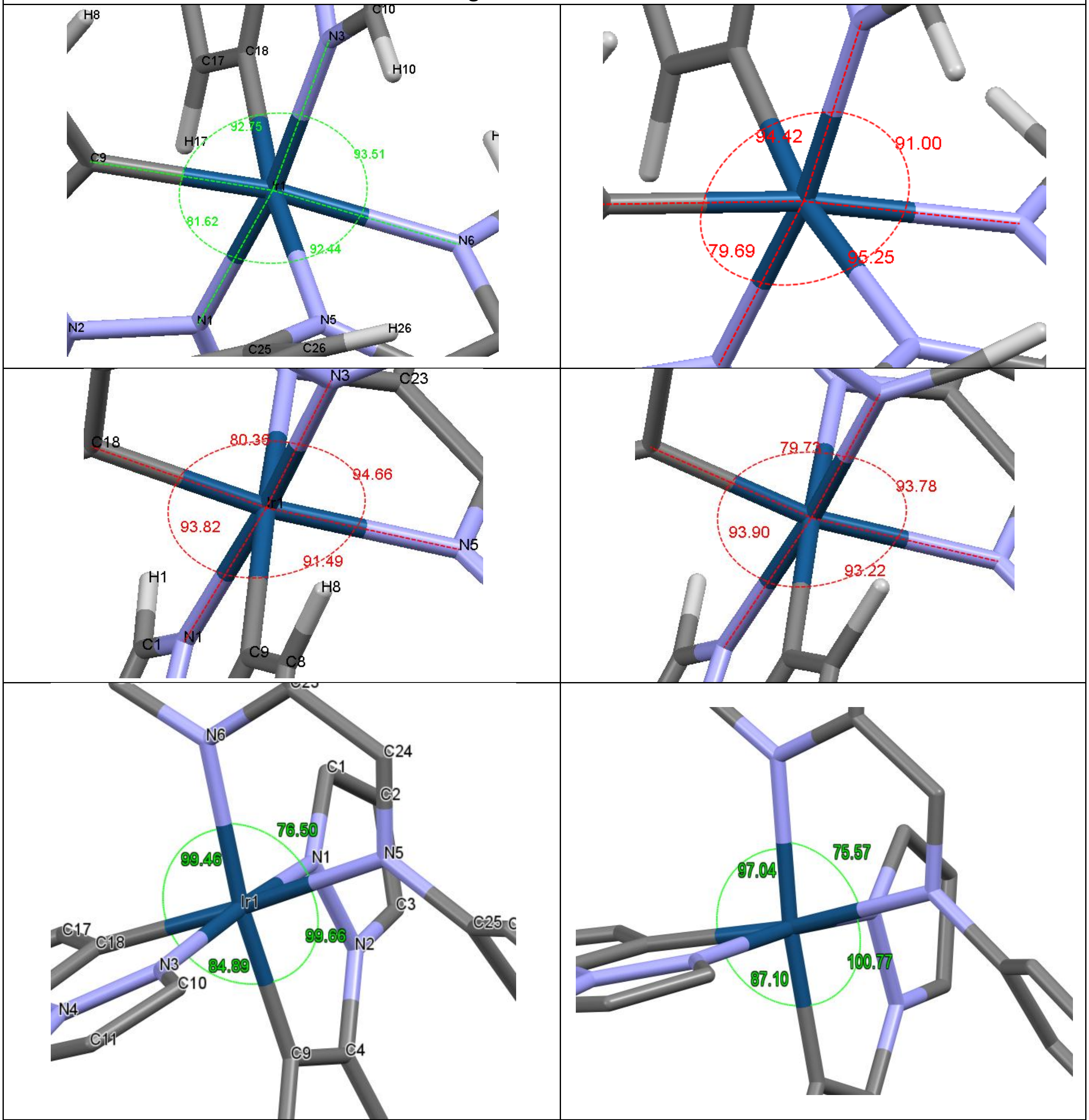
Table S2 Comparison of computed and calculated bond lengths and the most significant effects of including PF_6 and solvent (DCM) in calculated geometry for 4a.

Table :

4a Bond	**4a** cation Calc (Å)	**4a** (PF_6) Calc (Å)	**4a** Exp. (Å)	Difference Calc-Exp 4a	Difference Calc-Exp 4a(PF_6)
Ir1 N1	2.051		2.003	0.048	
Ir1 N3	2.052		2.021	0.031	
Ir1 N5	2.239	2.217	2.157	0.082	0.060
Ir1 N6	2.195	2.189	2.135	0.060	0.055
Ir1 C9	2.028		2.026	0.002	
Ir1 C18	2.021		2.023	-0.002	
Br1 C28	1.914		1.892	0.022	

Figure. S3a: Experimental and calculated bond angles for 4a

Bond angles around the Ir atom



a | b

Bond angles around the Ir atom in the three pseudo octahedral planes. a): X-ray results. b): DFT computed data

The majority of the bond angles excluding hydrogen atoms (72%) are within 1.0 deg compared to the experimental ones; among these 46% fall in the range 0-0.5 deg. Only four show values in the range [2,2.5]. The largest discrepancy (2.85 deg) is found for θ(N1-Ir1-N6) whose values are 92.75 and 94.42 for X-ray and DFT data respectively.

Figure. S3b: Plot showing distribution of differences between calculated and experimental bond angles for 4a

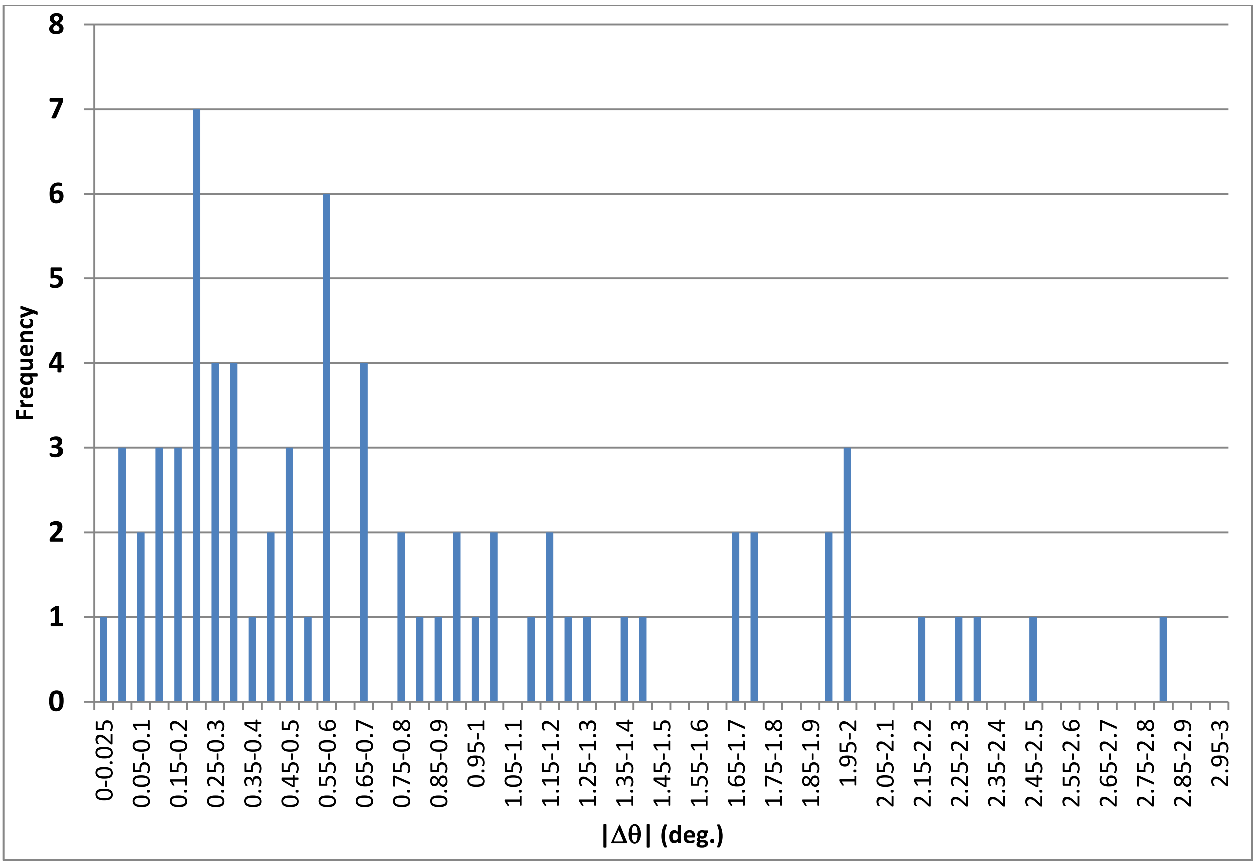
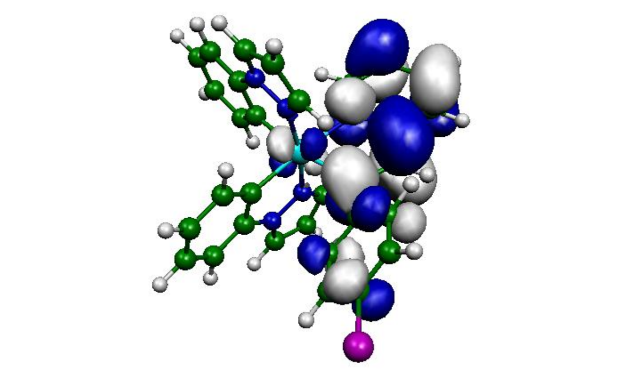
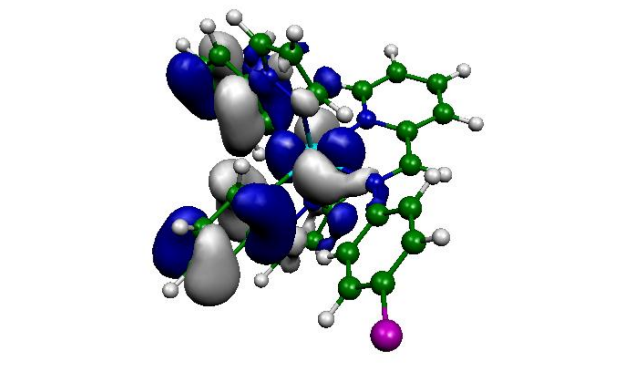
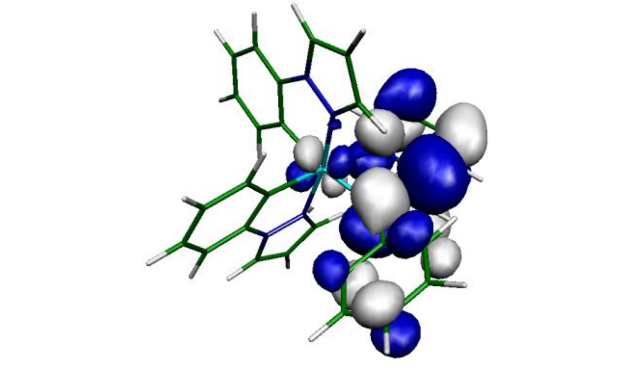
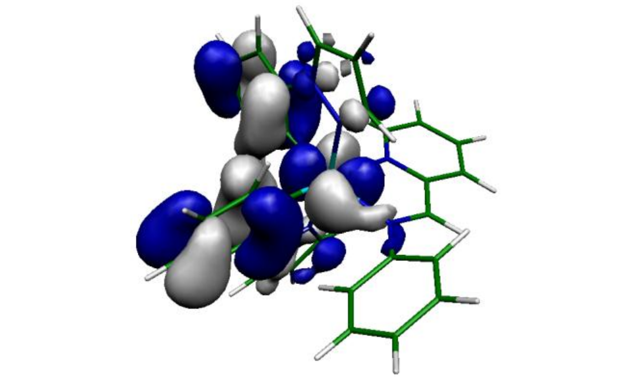
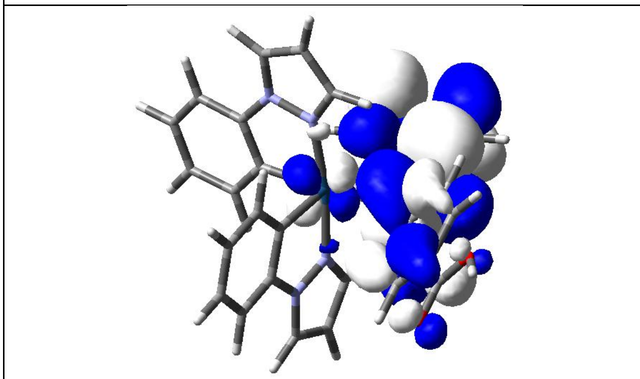
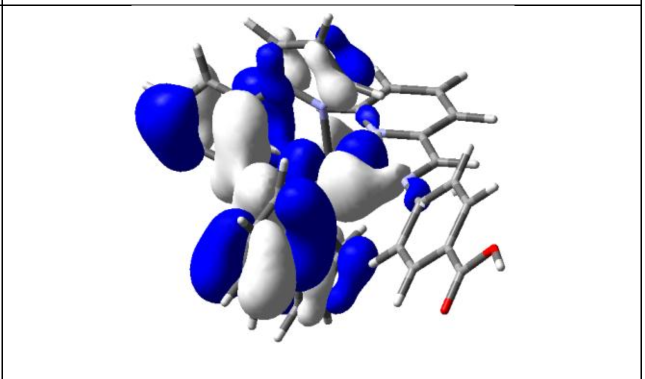
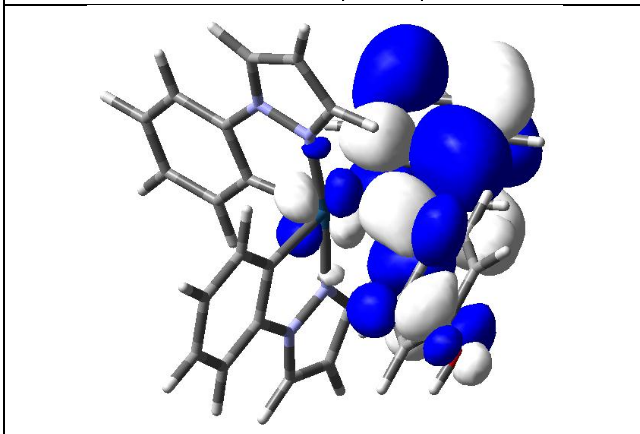
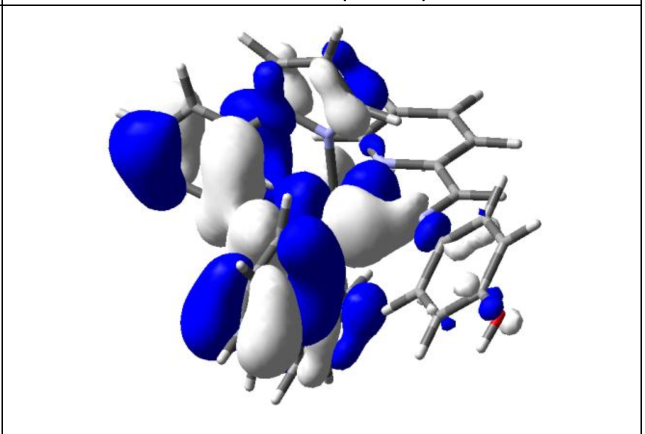


Figure S4: HOMO LUMO diagram of 4a,5a,6a, 7a,8a (p-Br,p-H,p-COOH, p-OH,iPr)cations at D95(d)/SDD/M06/ACN level of theory

	
LUMO 4a	HOMO 4a
	
LUMO 5a	HOMO 5a
	
LUMO 6a (COOH)	HOMO 6a (COOH)
	
LUMO 7a (OH)	HOMO 7a (OH)

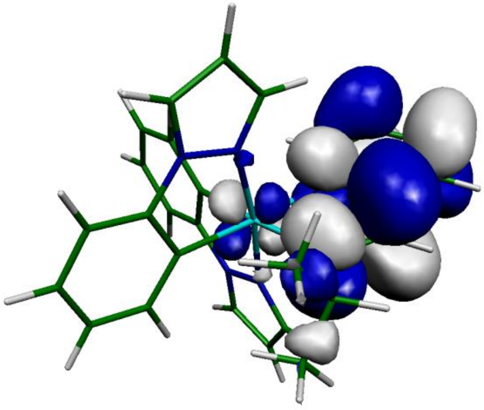
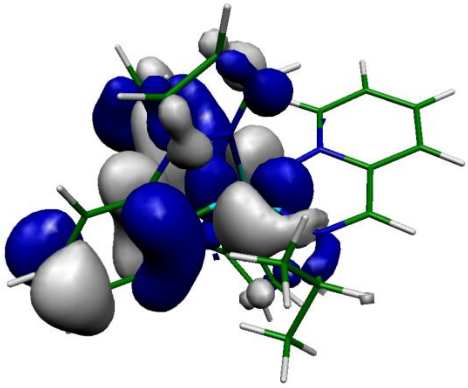
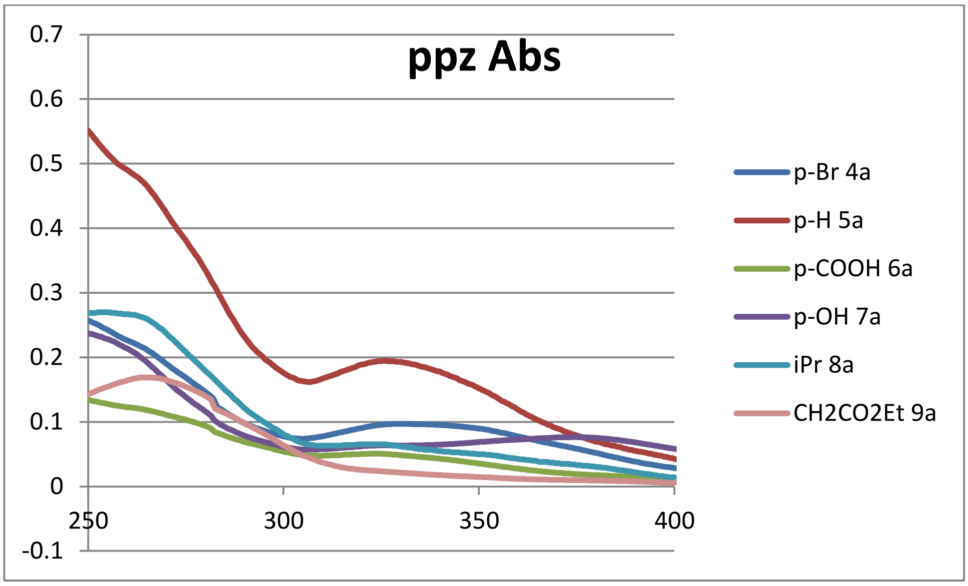
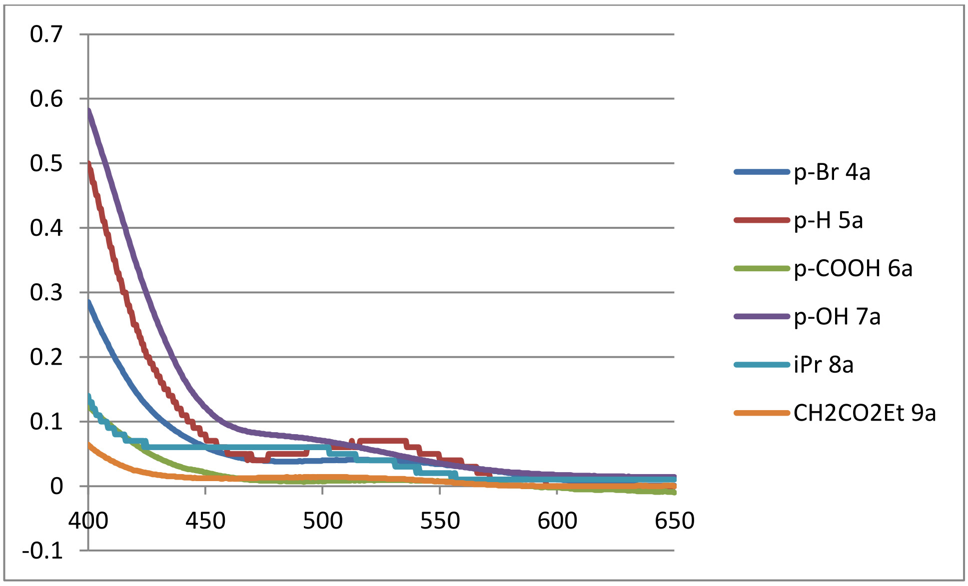
	
LUMO 8a (iPr)	HOMO 8a (iPr)

Figure S5a: Absorption spectra for 4a-4c and 5a-8a

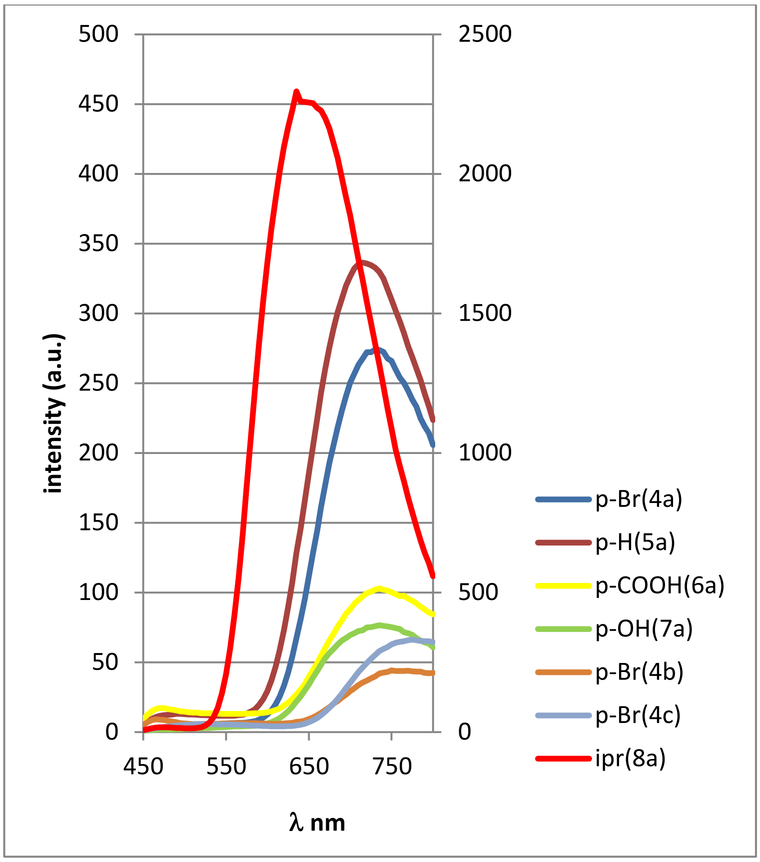


250 -400 nm 0.01 M solutions



400-460 nm intensity x 10

Figure S5b: Emission spectra for 4a-4c and 5a-8a



Emission spectra of approximately 10^{-5}M solutions of complexes in degassed CH_2Cl_2

Intensity for complex **8a** is on the right hand axis

Figure S5c: Excitation spectra for 4a-4c and 5a-8a

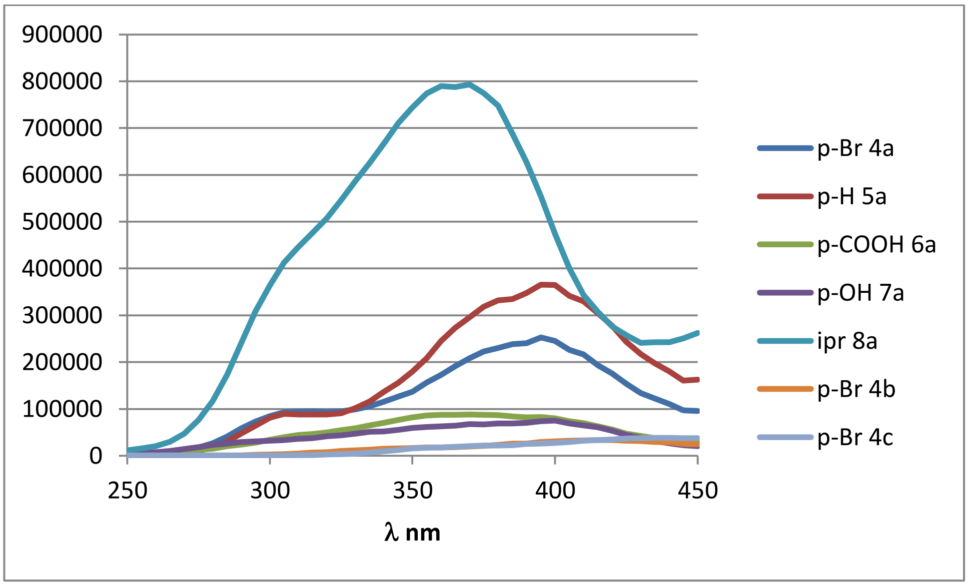
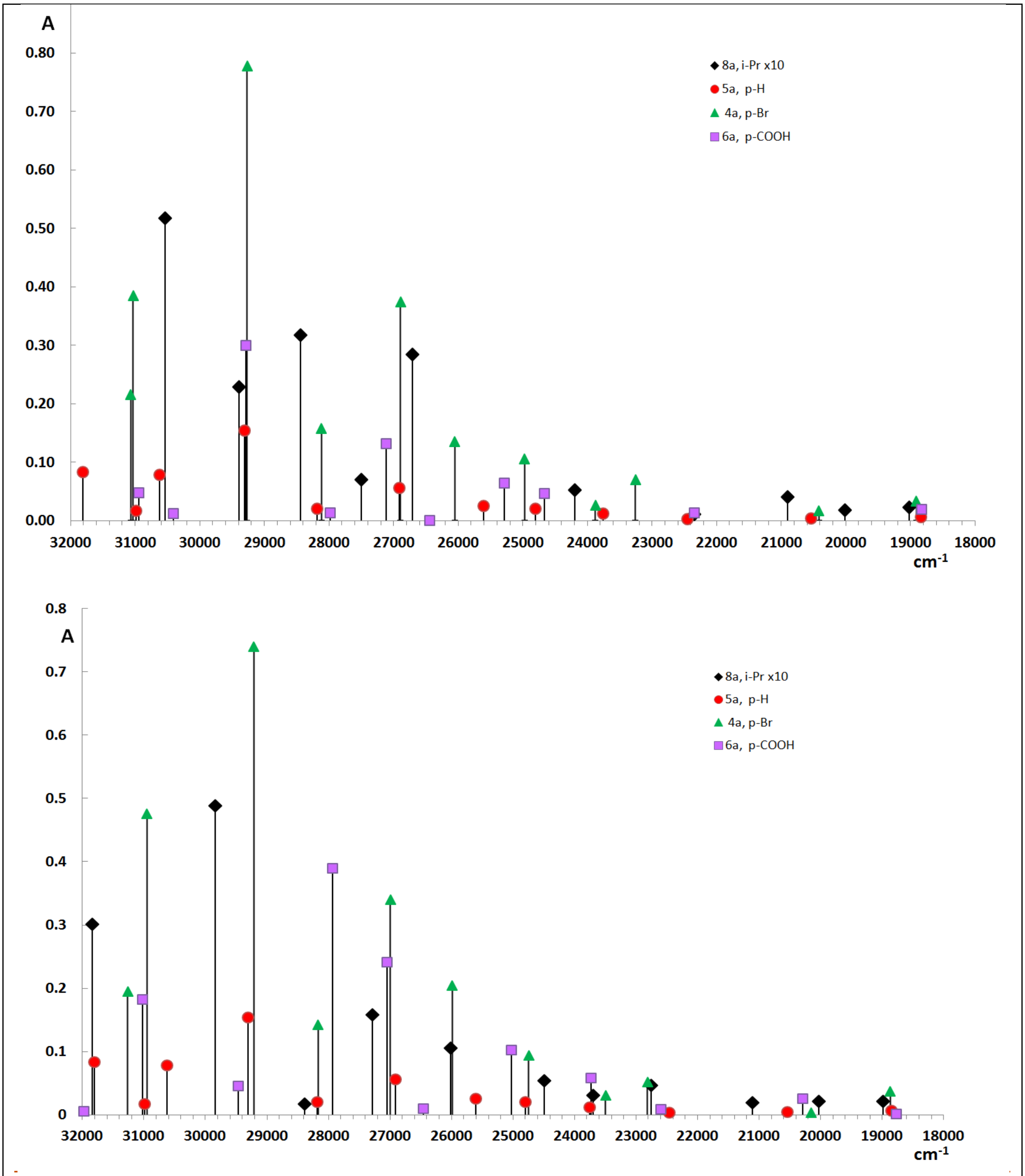


Table S3: Parameters for each Gaussian function $\epsilon(\tilde{\nu}_i) \times \left(e^{-\left((\ln 2) \times (\tilde{\nu}_i - \tilde{\nu})^2/(\Delta_i)^2\right)}\right)$, for absorption spectra of 8a, 5a, 4a, 6a.

λ (nm), $\tilde{\nu}$ and Δ (cm^{-1})

8a, i-Pr				5a, p-H				4a, p-Br				6a, p-COOH			
λ	$\tilde{\nu}_i$	$\epsilon(\tilde{\nu}_i)$	Δ_i	λ	$\tilde{\nu}_i$	$\epsilon(\tilde{\nu}_i)$	Δ_i	λ	$\tilde{\nu}_i$	$\epsilon(\tilde{\nu}_i)$	Δ_i	λ	$\tilde{\nu}_i$	$\epsilon(\tilde{\nu}_i)$	Δ_i
235	42533	4.13489	2248	230	43493	0.56240	2651	231	43342	2.55527	2501	229	43700	1.38000	2280
253	39532	0.73894	877	236	42456	0.00934	582	237	42127	0.02168	590	234	42720	0.00000	120
262	38130	1.82694	1212	246	40731	0.23186	1326	246	40650	0.97883	1405	245	40782	0.78192	1537
276	36260	1.58093	1327	255	39229	0.24410	1182	258	38730	1.54838	1431	259	38633	0.88816	1433
287	34897	0.45203	847	264	37888	0.17070	1037	266	37620	0.44012	842	266	37596	0.27544	819
297	33701	0.61233	879	275	36415	0.30386	1605	275	36342	1.10446	1096	276	36281	0.71225	1035
311	32112	0.46575	987	287	34866	0.07341	1493	289	34649	0.74797	1140	288	34673	0.44497	1165
327	30539	0.51724	980	299	33419	0.09491	1190	297	33714	0.01694	447	297	33621	0.02957	568
340	29391	0.22911	666	306	32692	0.02967	963	301	33251	0.34756	861	311	32134	0.44462	1976
352	28446	0.31776	721	314	31809	0.08321	794	311	32185	0.31561	794	310	32233	0.00241	509
364	27502	0.06966	593	323	30987	0.01679	578	322	31067	0.21565	860	323	30945	0.04827	740
374	26710	0.28398	1252	327	30624	0.07842	946	322	31031	0.38466	1268	329	30407	0.01201	679
413	24190	0.05276	1964	341	29303	0.15388	1485	342	29268	0.77723	1393	342	29281	0.29927	1407
448	22345	0.01124	660	355	28179	0.01991	832	356	28116	0.15783	823	357	27986	0.01298	694
478	20906	0.04022	1029	372	26910	0.05652	1022	372	26892	0.37422	1108	369	27112	0.13208	1329
500	20016	0.01801	477	391	25608	0.02575	903	384	26056	0.13502	1287	378	26439	0.00000	1671
526	19014	0.02323	634	403	24800	0.02076	1024	400	24972	0.10523	964	396	25284	0.06378	1275
				421	23756	0.01185	1185	419	23875	0.02661	944	405	24671	0.04710	1818
				445	22455	0.00328	888	430	23256	0.06972	1741	448	22344	0.01389	1505
				487	20536	0.00408	1028	490	20418	0.01682	1023	531	18825	0.01882	1854
				531	18843	0.00613	989	529	18908	0.03318	1178				
								574	17419	0.01221	905				

Figure S6: Gaussian function parameters used for the decomposition of the spectra of (▲)4a p-Br, (●)5a p-H, (■) 6a p-COOH (♦)8a i-Pr and their wavenumbers $\tilde{\nu}_i$ (cm^{-1})



Comparison of the coefficient $\epsilon(\tilde{\nu}_i)$ of the Gaussian functions simulating (i) the $A(\nu)$ spectrum

$$A(\nu) = \sum_i \epsilon(\tilde{\nu}_i) \times \left(e^{-((\ln 2) \times (\tilde{\nu}_i - \tilde{\nu})^2/(\Delta_i)^2)}\right)$$

used for the decomposition in case of (▲)4a p-Br, (●)5a p-H, (■) 6a p-COOH and (♦)8a i-Pr (10x) and their wavenumbers $\tilde{\nu}_i$(cm^{-1}) in the range 32000 to 18000 cm^{-1}. Δ_i is half of the Gaussian width at half height. In case of **8a** the plotted $\epsilon(\tilde{\nu}_i)'s$ are 10 times the actual value.

Figure S7:Optimized geometries of the ion-couples with different position of PF_6^- anion for 4a, 5a and 8a

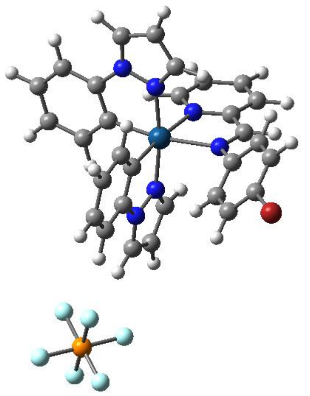
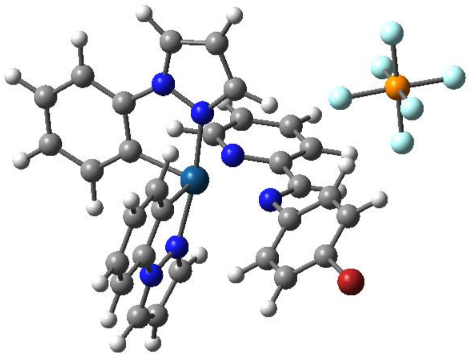
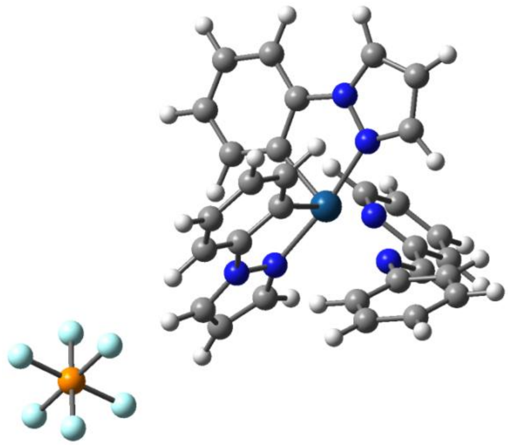
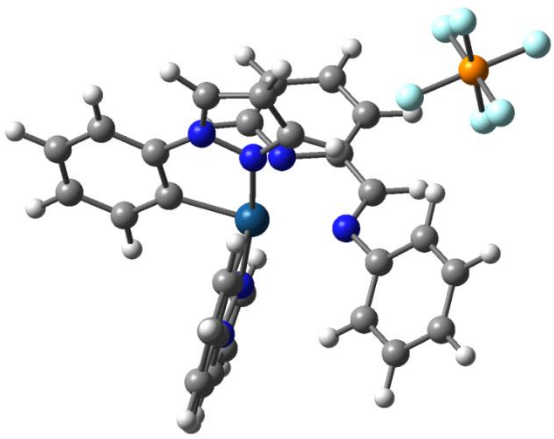
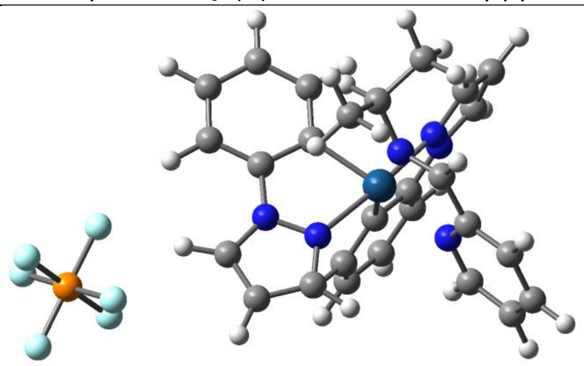
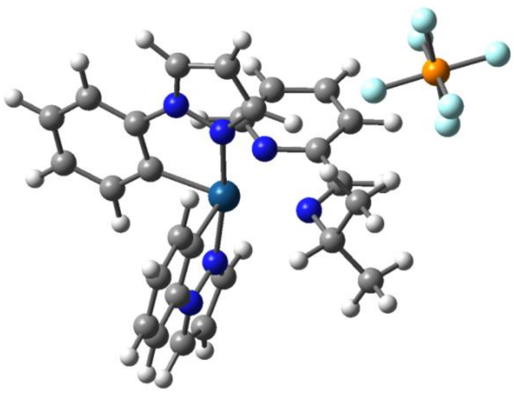
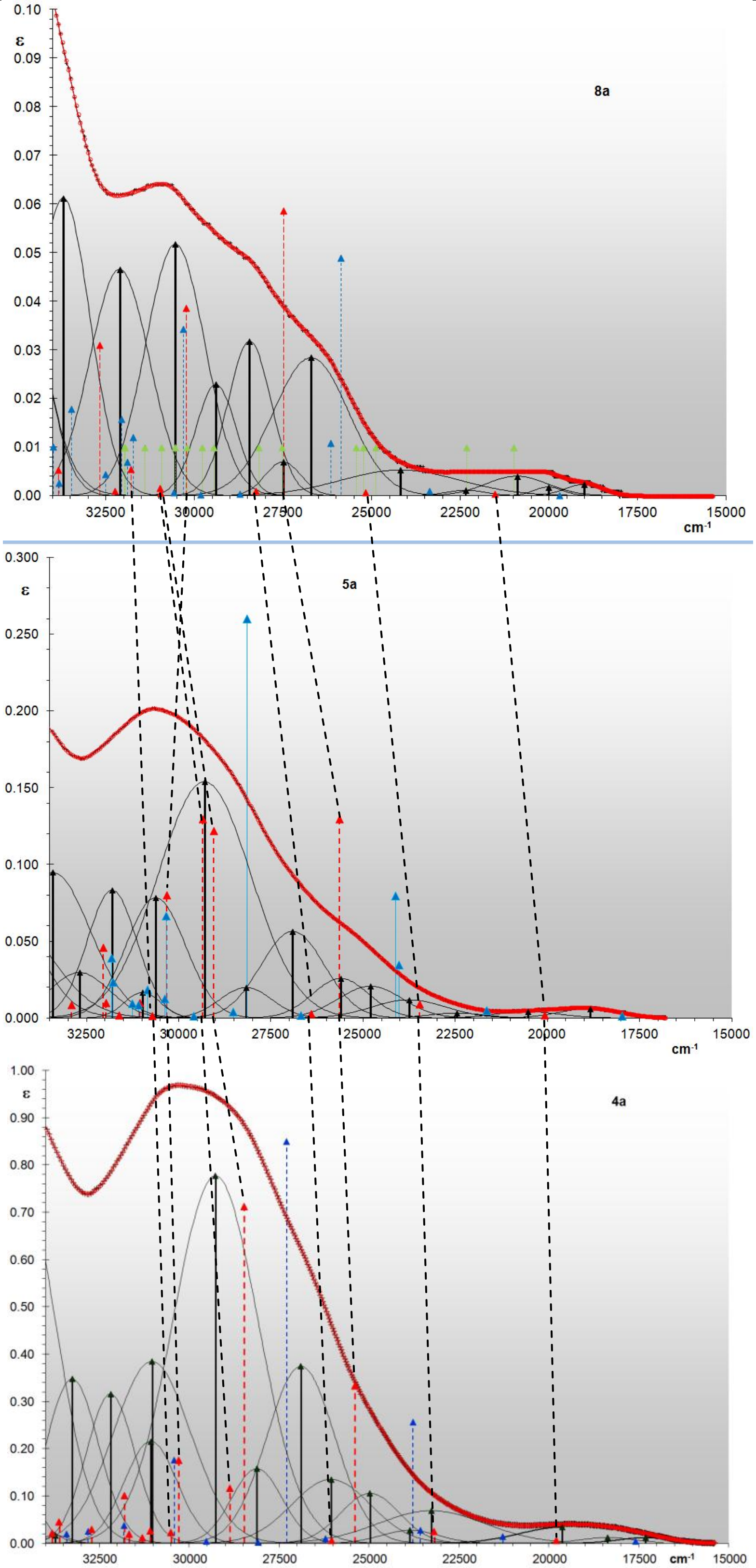
 **A -2542.81487333hartree**	 **B -2542.90479931 hartree**
ion-couples 4a-PF_6^- (**A**) close to the Phenylpyrazole side (**B**) close to the Phenylimine side	
 **A -2530.14636480hartree**	 **B-2530.15542774hartree**
ion-couples 5a-PF_6^- (**A**) close to the Phenylpyrazole side (**B**) close to the Phenylimine side	
 **A -2417.11628454hartree**	 **B-2417.12249972hartree**
Ion-couples 8a-PF_6^- (**A**) close to the Phenylpyrazole side (**B**) close to the imine side	

Figure S8:Low energy part of the absorption spectra for 4a,5a and 8a.

Low energy part of the absorption spectra of **8a,5a** and **4a**. (o) Experimental data and (**+**) fitted data; (▲) Position of fitting Gaussian functions; TD-DFT computed intensities and wavenumbers for **4a** and (▲) PF_6^- on the phenylpyrazole side (**4a**-PF6PZ) and (▲)PF_6^- on the Phenylimine side (**4a**-PF6PI). Black dotted lines connect transitions that are very close in MO's involved in excitations and related only to PF6PI.



Where necessary spectra were adjusted to set the lowest absorption at zero to remove negative absorption

Assignment of bands in the region 270-650 nm:

In the case of **4a** the contribution to this band by the **4a**-PF6PI ion pair is the most relevant and is due mainly to four transitions at around 30290 (330 nm; f = 0.0700), 28468 (351 nm; f = 0.2848) and 25387 cm^{-1} (393 nm; f = 0.1329) and a less intense one at 28865 cm^{-1} (346 nm; f = 0.0465) and some further ones of very low intensity. The "free" ion and **4a**-PF6PZ contribute with similar transitions but at longer wavelength (See Table S4 below). The major contribution to the longest wavelength transition in this region (394, 390, 364 nm for **4a, 5a, 8a** respectively) is given by the (HOMO-3)→LUMO excitation. In the case of the aromatic pyridineimines **4a** and **5a** there is a further contribution, though small, from the (HOMO-2)→LUMO excitation (See Table 4 and Tables S4-S6 in SI)

Table S4 : Computed electronic transitions at D95(d))/SDD/M06/DCM level of theory for 4a- PF6PI; 5a- PF6PI and 8a- PF6PI

	4a		**5a**		**8a**	
	λ (*f*)	Excitation MOs (contribution %)	λ (*f*)	Excitation MOs (contribution %)	λ (*f*)	Excitation MOs (contribution %)
1	505 (0.0022)	HOMO → LUMO (0.98)	498 (0.0018)	HOMO → LUMO (0.98)	464(0.0009)	HOMO → LUMO (0.97)
2	431 (0.0098)	HOMO -3 → LUMO (0.08) HOMO -2 → LUMO (0.88)	426 (0.0091)	HOMO -3 → LUMO (0.08) HOMO -2 → LUMO (0.90)	397 (0.0014)	HOMO -2 →LUMO (0.95)
3	394 (0.1329)	HOMO -3 → LUMO (0.85) HOMO -2 → LUMO (0.07)	390 (0.1297)	HOMO -3 → LUMO (0.87) HOMO -2 → LUMO (0.07)	363 (0.1174)	HOMO -3 → LUMO (0.93)
4	384 (0.0020)	HOMO -1 → LUMO (0.96)	379 (0.0027)	HOMO -1 → LUMO (0.97)	353 (0.0019)	HOMO -1 → LUMO (0.96)
5	351 (0.2848)	HOMO -5 → LUMO (0.71) HOMO -4 → LUMO (0.20)	344 (0.1222)	HOMO -6 → LUMO (0.30) HOMO -5 → LUMO (0.12) HOMO -4 → LUMO (0.54)	330 (0.0772)	HOMO → LUMO +2 (0.92)
6	346 (0.0465)	HOMO -5 → LUMO (0.19) HOMO -4 → LUMO (0.78)	341(0.1297)	HOMO -6 → LUMO (0.41) HOMO -5 → LUMO (0.12) HOMO -4 → LUMO (0.44)	323 (0.0011)	HOMO -4 → LUMO (0.66) HOMO → LUMO +1 (0.23) HOMO → LUMO +3 (0.08))
7	330 (0.0700)	HOMO → LUMO +1 (0.13) HOMO → LUMO +2 (0.73)	330 (0.0802)	HOMO → LUMO +1 (0.06) HOMO → LUMO +2 (0.85)	322 (0.0031)	HOMO -4 → LUMO (0.31) HOMO → LUMO +1 (0.41) HOMO → LUMO +3 (0.24)

f = oscillator strength

For the aryl pyridineimines (**4a** and **5a**) the computed most intense transitions in this wave-number range are definitely multideterminantal involving (HOMO-4,-5)→LUMO excitations and some contribution from (HOMO-6)→LUMO for **5a**. As can be seen (HOMO -4 and -5) have a non-negligible contribution from the *d*-orbitals of Ir and significant contributions from the ppz orbitals; (HOMO-5 for **4a**) (and HOMO-6 for **5a**) have a large contribution from the N-aryl of the imine. On the other hand, the LUMO has only a very small metal contribution with the major contribution from the π system of the pyridineimine (see Fig S4). Then these absorptions can be described as spin allowed metal+ligand to ligand charge transfer (^{1}ML,L'CT) [dπ (Ir)+ πC^N]→ π* (X^Y) transitions. This pattern occurs for **4a**, **5a** and even **8a**, though with some minor differences concerning the imine substituent, suggesting that this behaviour is common to this class of compounds.

Table S5: TD-DFT results for Structure 4a p-Br /D95(d)/SDD/M06/DCM level of theory

4a-PF_6^-Pyridineimine side

06075_Ir_2PhPzol_PyImminoPh_pBr_PF6_SDD_D95d_M06_DCM_TD15.out
HOMO is orbital 169 and LUMO is orbital 170

>>>> Singlet states <<<<

eV	nm	cm-1	f
2.4540;	505.23;	19793.0;	0.0022
2.8747;	431.30;	23185.7;	0.0098
3.1477;	393.89;	25387.8;	0.1329
3.2287;	384.01;	26041.0;	0.0020
3.5297;	351.26;	28468.9;	0.2848
3.5788;	346.44;	28865.0;	0.0465
3.7555;	330.14;	30290.2;	0.0700
3.7818;	327.84;	30502.7;	0.0087
3.8534;	321.76;	31079.1;	0.0102
3.8803;	319.52;	31296.9;	0.0043
3.9264;	315.77;	31668.6;	0.0076
3.9431;	314.44;	31802.6;	0.0399
4.0548;	305.77;	32704.3;	0.0115
4.1671;	297.53;	33610.1;	0.0176
4.1916;	295.79;	33807.8;	0.0086

Excited State: 2
2.4540 eV 505.23 nm 19793.cm-1 f=0.0022
169 →170 97.94 % 0→0

Excited State: 5
2.8747 eV 431.30 nm 23186.cm-1 f=0.0098
166 →170 7.84 % -3→0
167 →170 88.23 % -2→0

Excited State: 9
3.1477 eV 393.89 nm 25388.cm-1 f=0.1329
164 →170 3.78 % -5→0
166 →170 85.40 % -3→0
167 →170 7.43 % -2→0

Excited State: 11
3.2287 eV 384.01 nm 26041.cm-1 f=0.0020
166 →170 2.10 % -3→0
168 →170 96.28 % -1→0

Excited State: 13
3.5297 eV 351.26 nm 28469.cm-1 f=0.2848
164 →170 70.62 % -5→0
165 →170 19.74 % -4→0
166 →170 2.35 % -3→0

Excited State: 15
3.5788 eV 346.44 nm 28865.cm-1 f=0.0465
164 →170 18.81 % -5→0
165 →170 78.19 % -4→0

Excited State: 19
3.7555 eV 330.14 nm 30290.cm-1 f=0.0700
163 →170 5.94 % -6→0
169 →171 12.94 % 0→1
169 →172 73.41 % 0→2

Excited State: 22
3.7818 eV 327.84 nm 30503.cm-1 f=0.0087
163 →170 86.24 % -6→0
164 →170 2.91 % -5→0
169 →172 8.04 % 0→2

Excited State: 23
3.8534 eV 321.76 nm 31079.cm-1 f=0.0102
163 →170 3.10 % -6→0
169 →171 67.44 % 0→1
169 →172 8.53 % 0→2
169 →173 17.29 % 0→3

Excited State: 25
3.8803 eV 319.52 nm 31297.cm-1 f=0.0043
169 →171 16.89 % 0→1
169 →173 75.02 % 0→3

Excited State: 26
3.9264 eV 315.77 nm 31669.cm-1 f=0.0076
162 →170 91.35 % -7→0
164 →174 2.42 % -5→4

Excited State: 27
3.9431 eV 314.44 nm 31803.cm-1 f=0.0399
166 →172 3.88 % -3→2
167 →171 20.57 % -2→1
167 →172 59.64 % -2→2

Excited State: 28
4.0548 eV 305.77 nm 32704.cm-1 f=0.0115
161 →170 7.93 % -8→0
167 →171 56.78 % -2→1
167 →172 22.00 % -2→2

Excited State: 29
4.1671 eV 297.53 nm 33610.cm-1 f=0.0176
166 →171 24.11 % -3→1
166 →172 26.66 % -3→2
167 →173 7.94 % -2→3
168 →171 2.87 % -1→1
168 →172 17.38 % -1→2

Excited State: 30
4.1916 eV 295.79 nm 33808.cm-1 f=0.0086
166 →172 10.79 % -3→2
166 →173 8.58 % -3→3
167 →173 57.77 % -2→3
168 →173 8.48 % -1→3

>>>> Triplet states <<<<

eV	nm	cm-1	f
2.3699;	523.15;	19115.0;	0.0000
2.4684;	502.28;	19909.2;	0.0000
2.8366;	437.09;	22878.6;	0.0000
3.0723;	403.55;	24780.1;	0.0000
3.1131;	398.27;	25108.6;	0.0000
3.1438;	394.38;	25356.3;	0.0000
3.2229;	384.70;	25994.3;	0.0000
3.4086;	363.74;	27492.2;	0.0000
3.5688;	347.42;	28783.6;	0.0000
3.6456;	340.09;	29404.0;	0.0000
3.7069;	334.46;	29898.9;	0.0000
3.7255;	332.80;	30048.1;	0.0000
3.7586;	329.87;	30315.0;	0.0000
3.7707;	328.81;	30412.7;	0.0000
3.8590;	321.29;	31124.5;	0.0000

Excited State: 1
2.3699 eV 523.15 nm 19115.cm-1 f=0.0000
161 →170 3.95 % -8→0
164 →170 5.15 % -5→0
166 →170 9.09 % -3→0
167 →170 32.16 % -2→0
169 →170 41.96 % 0→0

Excited State: 3
2.4684 eV 502.28 nm 19909.cm-1 f=0.0000
161 →170 3.65 % -8→0
164 →170 2.58 % -5→0
166 →170 4.85 % -3→0
167 →170 28.72 % -2→0
169 →170 55.32 % 0→0

Excited State: 4
2.8366 eV 437.09 nm 22879.cm-1 f=0.0000
166 →170 74.65 % -3→0
167 →170 15.73 % -2→0
168 →170 3.44 % -1→0

Excited State: 6
3.0723 eV 403.55 nm 24780.cm-1 f=0.0000
162 →174 3.42 % -7→4
164 →170 61.44 % -5→0
164 →175 3.36 % -5→5
166 →170 3.32 % -3→0
167 →170 12.75 % -2→0

Excited State: 7
3.1131 eV 398.27 nm 25109.cm-1 f=0.0000
163 →179 2.98 % -6→9
165 →172 11.63 % -4→2
168 →172 9.47 % -1→2
168 →173 11.80 % -1→3
169 →172 36.88 % 0→2
169 →178 3.19 % 0→8

Excited State: 8
3.1438 eV 394.38 nm 25356.cm-1 f=0.0000
163 →178 4.19 % -6→8
165 →173 10.49 % -4→3
168 →170 2.15 % -1→0
168 →172 16.72 % -1→2
168 →173 10.84 % -1→3
169 →173 28.03 % 0→3
169 →179 4.81 % 0→9

Excited State: 10
3.2229 eV 384.70 nm 25994.cm-1 f=0.0000
166 →170 2.56 % -3→0
168 →170 91.30 % -1→0

Excited State: 12
3.4086 eV 363.74 nm 27492.cm-1 f=0.0000
153 →170 2.85 % -16→0
156 →170 3.26 % -13→0
159 →170 4.30 % -10→0
161 →170 41.80 % -8→0
161 →171 2.33 % -8→1
162 →174 6.45 % -7→4
164 →175 8.49 % -5→5
167 →170 5.15 % -2→0
167 →175 2.99 % -2→5

Excited State: 14
3.5688 eV 347.42 nm 28784.cm-1 f=0.0000
165 →170 95.10 % -4→0

Excited State: 16
3.6456 eV 340.09 nm 29404.cm-1 f=0.0000
163 →172 2.10 % -6→2
163 →179 5.20 % -6→9
164 →172 3.00 % -5→2
165 →172 7.52 % -4→2
165 →178 2.11 % -4→8
167 →172 5.09 % -2→2
169 →171 2.41 % 0→1
169 →172 28.37 % 0→2
169 →173 5.92 % 0→3
169 →174 2.06 % 0→4
169 →178 3.14 % 0→8
169 →179 3.14 % 0→9

Excited State: 17
3.7069 eV 334.46 nm 29899.cm-1 f=0.0000
163 →173 3.91 % -6→3
163 →178 6.86 % -6→8
163 →179 2.39 % -6→9
165 →173 4.61 % -4→3
165 →178 2.10 % -4→8
166 →172 3.01 % -3→2
166 →173 4.50 % -3→3
167 →173 3.30 % -2→3

169 →171 8.55 % 0→1
169 →172 8.47 % 0→2
169 →173 25.54 % 0→3
169 →178 4.35 % 0→8
169 →179 2.42 % 0→9

Excited State: 18
3.7255 eV 332.80 nm 30048.cm-1 f=0.0000
163 →172 2.29 % -6→2
164 →172 3.97 % -5→2
165 →172 3.05 % -4→2
166 →173 6.75 % -3→3
167 →171 3.27 % -2→1
167 →172 47.48 % -2→2
167 →173 2.80 % -2→3
169 →172 5.64 % 0→2

Excited State: 20
3.7586 eV 329.87 nm 30315.cm-1 f=0.0000
162 →170 3.66 % -7→0
163 →170 84.51 % -6→0
169 →171 2.58 % 0→1

Excited State: 21
3.7707 eV 328.81 nm 30413.cm-1 f=0.0000
160 →173 3.47 % -9→3
166 →172 14.48 % -3→2
166 →173 20.65 % -3→3
167 →173 22.85 % -2→3
168 →173 2.28 % -1→3
169 →171 4.48 % 0→1
169 →173 5.99 % 0→3

Excited State: 24
3.8590 eV 321.29 nm 31125.cm-1 f=0.0000
161 →171 2.57 % -8→1
162 →174 7.26 % -7→4
164 →170 6.23 % -5→0
166 →171 5.81 % -3→1
169 →171 41.12 % 0→1
169 →173 6.50 % 0→3

4a-PF_6^- Phenylpyrazole side.

06075_Ir_2PhPzol_PF6_PyImminoPh_pBr_SDD_D95d_M06_DCM_TD46.out
HOMO is orbital 169 and LUMO is orbital 170

>>>> Singlet states <<<<

eV	nm	cm-1	f
2.1800;	568.50;	17590.1;	0.0017
2.6380;	469.92;	21280.2;	0.0057
2.9230;	424.17;	23575.5;	0.0110
2.9470;	420.58;	23776.7;	0.1026
3.2490;	381.54;	26209.6;	0.0039
3.3830;	366.41;	27291.8;	0.3398
3.4820;	356.05;	28085.9;	0.0010
3.6600;	338.75;	29520.3;	0.0019
3.7710;	328.78;	30415.5;	0.0703
3.9440;	314.35;	31811.7;	0.0150
4.0680;	304.75;	32813.8;	0.0102
4.1410;	299.34;	33406.8;	0.0079
4.2500;	291.69;	34283.0;	0.0254
4.2880;	289.08;	34592.5;	0.0267
4.3040;	288.06;	34715.0;	0.0272
4.3320;	286.17;	34944.3;	0.0085
4.3610;	284.29;	35175.3;	0.0234
4.3770;	283.24;	35305.7;	0.1146
4.4110;	281.05;	35580.9;	0.0344
4.4200;	280.46;	35655.7;	0.0152
4.4450;	278.87;	35859.0;	0.0068
4.4690;	277.42;	36046.4;	0.0340
4.5100;	274.90;	36376.9;	0.0441
4.5420;	272.97;	36634.1;	0.0277
4.6130;	268.73;	37212.1;	0.0298
4.6380;	267.28;	37413.9;	0.1338
4.6550;	266.30;	37551.6;	0.0266
4.6660;	265.66;	37642.1;	0.0320
4.7020;	263.68;	37924.8;	0.0185
4.7470;	261.16;	38290.7;	0.0468
4.7580;	260.56;	38378.9;	0.0127
4.7690;	259.97;	38466.0;	0.0759
4.8010;	258.20;	38729.7;	0.0971
4.8130;	257.58;	38822.9;	0.0848
4.8630;	254.91;	39229.5;	0.0215
4.8740;	254.35;	39315.9;	0.0108
4.8810;	253.98;	39373.2;	0.0085
4.9030;	252.83;	39552.3;	0.0241
4.9360;	251.16;	39815.3;	0.0267
4.9380;	251.07;	39829.5;	0.0172
4.9490;	250.48;	39923.3;	0.0758
5.0170;	247.10;	40469.4;	0.0136
5.0560;	245.20;	40783.0;	0.0233
5.0920;	243.48;	41071.1;	0.0046
5.1020;	242.98;	41155.7;	0.0024
5.1200;	242.11;	41303.5;	0.0168

1 1 Excited State: Singlet
2.1800 eV 568.50 nm
17590.cm-1 f=0.0017
169 →170 97.75 % 0 → 0

2 2 Excited State: Singlet
2.6380 eV 469.92 nm
21280.cm-1 f=0.0057
166 →170 7.47 % -3 → 0
167 →170 90.34 % -2 → 0

3 3 Excited State: Singlet
2.9230 eV 424.17 nm
23575.cm-1 f=0.0110
168 →170 97.48 % -1 → 0

4 4 Excited State: Singlet
2.9470 eV 420.58 nm
23777.cm-1 f=0.1026
166 →170 88.14 % -3 → 0
167 →170 7.20 % -2 → 0

5 5 Excited State: Singlet
3.2490 eV 381.54 nm
26210.cm-1 f=0.0039
165 →170 97.41 % -4 → 0

6 6 Excited State: Singlet
3.3830 eV 366.41 nm
27292.cm-1 f=0.3398
163 →170 82.95 % -6 → 0
164 →170 10.62 % -5 → 0

7 7 Excited State: Singlet
3.4820 eV 356.05 nm
28086.cm-1 f=0.0010
163 →170 10.87 % -6 → 0
164 →170 87.10 % -5 → 0

8 8 Excited State: Singlet
3.6600 eV 338.75 nm
29520.cm-1 f=0.0019
169 →171 95.99 % 0 → 1

9 9 Excited State: Singlet
3.7710 eV 328.78 nm
30415.cm-1 f=0.0703
169 →172 89.56 % 0 → 2

10 10 Excited State: Singlet
3.9440 eV 314.35 nm
31812.cm-1 f=0.0150
169 →173 88.34 % 0 → 3

11 11 Excited State: Singlet
4.0680 eV 304.75 nm
32814.cm-1 f=0.0102
162 →170 91.34 % -7 → 0

12 12 Excited State: Singlet
4.1410 eV 299.34 nm
33407.cm-1 f=0.0079
160 →170 2.40 % -9 → 0
161 →170 5.87 % -8 → 0
162 →170 2.03 % -7 → 0
167 →171 83.13 % -2 → 1

13 13 Excited State: Singlet
4.2500 eV 291.69 nm
34283.cm-1 f=0.0254
159 →170 3.06 % -10 → 0
160 →170 23.31 % -9 → 0
161 →170 24.43 % -8 → 0
166 →171 29.44 % -3 → 1
167 →171 8.87 % -2 → 1

14 14 Excited State: Singlet
4.2880 eV 289.08 nm
34593.cm-1 f=0.0267
159 →170 3.53 % -10 → 0
160 →170 3.54 % -9 → 0
166 →171 5.51 % -3 → 1
166 →172 2.16 % -3 → 2
167 →172 69.58 % -2 → 2
167 →178 2.12 % -2 → 8
168 →172 2.28 % -1 → 2

15 15 Excited State: Singlet
4.3040 eV 288.06 nm
34715.cm-1 f=0.0272
159 →170 18.87 % -10 → 0
160 →170 21.58 % -9 → 0
166 →171 21.88 % -3 → 1
167 →172 11.12 % -2 → 2
168 →171 17.00 % -1 → 1

16 16 Excited State: Singlet
4.3320 eV 286.17 nm
34944.cm-1 f=0.0085
159 →170 2.12 % -10 → 0
160 →170 4.56 % -9 → 0
166 →171 10.36 % -3 → 1
168 →171 66.48 % -1 → 1
169 →174 2.38 % 0 → 4
169 →175 7.34 % 0 → 5

17 17 Excited State: Singlet
4.3610 eV 284.29 nm
35175.cm-1 f=0.0234
167 →172 2.12 % -2 → 2
168 →171 8.41 % -1 → 1
169 →174 31.65 % 0 → 4
169 →175 29.93 % 0 → 5
169 →178 6.08 % 0 → 8
169 →179 3.20 % 0 → 9

18 18 Excited State: Singlet
4.3770 eV 283.24 nm
35306.cm-1 f=0.1146
156 →170 6.93 % -13 → 0
159 →170 3.08 % -10 → 0
160 →170 7.07 % -9 → 0
161 →170 40.62 % -8 → 0
166 →171 14.47 % -3 → 1
166 →172 5.23 % -3 → 2
167 →172 3.41 % -2 → 2
167 →173 4.21 % -2 → 3
168 →172 6.63 % -1 → 2

19 19 Excited State: Singlet
4.4110 eV 281.05 nm
35581.cm-1 f=0.0344
161 →170 8.87 % -8 → 0
166 →171 6.49 % -3 → 1
166 →172 6.14 % -3 → 2
167 →173 5.87 % -2 → 3
168 →172 47.40 % -1 → 2
169 →174 3.39 % 0 → 4
169 →175 4.01 % 0 → 5

20 20 Excited State: Singlet
4.4200 eV 280.46 nm
35656.cm-1 f=0.0152
165 →172 2.19 % -4 → 2
166 →172 8.52 % -3 → 2
167 →173 12.88 % -2 → 3
168 →172 7.34 % -1 → 2
168 →173 5.38 % -1 → 3
169 →174 35.66 % 0 → 4
169 →175 7.74 % 0 → 5
169 →181 3.19 % 0 →11

21 21 Excited State: Singlet
4.4450 eV 278.87 nm
35859.cm-1 f=0.0068
167 →172 2.07 % -2 → 2
167 →173 32.79 % -2 → 3
167 →179 3.86 % -2 → 9
167 →181 7.18 % -2 →11
168 →173 3.37 % -1 → 3
169 →173 2.14 % 0 → 3
169 →174 10.17 % 0 → 4
169 →175 15.97 % 0 → 5
169 →179 3.75 % 0 → 9

22 22 Excited State: Singlet
4.4690 eV 277.42 nm
36046.cm-1 f=0.0340
155 →170 2.07 % -14 → 0
156 →170 20.97 % -13 → 0
159 →170 33.92 % -10 → 0
160 →170 22.04 % -9 → 0
161 →170 5.90 % -8 → 0
166 →171 2.02 % -3 → 1

23 23 Excited State: Singlet
4.5100 eV 274.90 nm
36377.cm-1 f=0.0441
164 →172 2.16 % -5 → 2
166 →172 46.51 % -3 → 2
166 →181 2.00 % -3 →11
167 →181 2.31 % -2 →11
168 →172 19.63 % -1 → 2
169 →174 3.80 % 0 → 4
169 →175 5.12 % 0 → 5
169 →178 3.20 % 0 → 8

24 24 Excited State: Singlet
4.5420 eV 272.97 nm
36634.cm-1 f=0.0277
166 →172 2.79 % -3 → 2
166 →173 52.10 % -3 → 3
166 →179 4.06 % -3 → 9
166 →181 4.76 % -3 →11
167 →173 7.39 % -2 → 3
168 →173 16.97 % -1 → 3

25 25 Excited State: Singlet
4.6130 eV 268.73 nm
37212.cm-1 f=0.0298
156 →170 3.74 % -13 → 0
164 →172 3.75 % -5 → 2
165 →172 3.39 % -4 → 2
166 →172 5.40 % -3 → 2
169 →174 5.61 % 0 → 4
169 →178 45.72 % 0 → 8
169 →181 8.43 % 0 →11
169 →186 2.00 % 0 →16

26 26 Excited State: Singlet
4.6380 eV 267.28 nm
37414.cm-1 f=0.1338
156 →170 11.49 % -13 → 0
159 →170 5.43 % -10 → 0
165 →171 3.68 % -4 → 1
166 →172 4.01 % -3 → 2
166 →173 10.89 % -3 → 3
167 →181 2.00 % -2 →11
168 →173 39.27 % -1 → 3
169 →181 2.04 % 0 →11

27 27 Excited State: Singlet
4.6550 eV 266.30 nm
37552.cm-1 f=0.0266
156 →170 13.89 % -13 → 0
159 →170 7.34 % -10 → 0
165 →171 34.32 % -4 → 1
166 →173 2.42 % -3 → 3
167 →181 3.30 % -2 →11
168 →173 8.89 % -1 → 3
169 →175 3.97 % 0 → 5
169 →179 2.24 % 0 → 9
169 →181 3.46 % 0 →11

28 28 Excited State: Singlet
4.6660 eV 265.66 nm
37642.cm-1 f=0.0320
156 →170 17.23 % -13 → 0
159 →170 7.41 % -10 → 0
161 →170 2.19 % -8 → 0
164 →171 4.77 % -5 → 1
165 →171 49.32 % -4 → 1
167 →181 2.21 % -2 →11

29 29 Excited State: Singlet
4.7020 eV 263.68 nm
37925.cm-1 f=0.0185
156 →170 2.44 % -13 → 0
165 →172 2.81 % -4 → 2
165 →173 3.37 % -4 → 3
166 →173 2.18 % -3 → 3
168 →173 2.71 % -1 → 3
169 →175 14.39 % 0 → 5
169 →176 11.93 % 0 → 6
169 →178 2.77 % 0 → 8
169 →179 17.00 % 0 → 9
169 →181 20.61 % 0 →11

30 30 Excited State: Singlet
4.7470 eV 261.16 nm
38291.cm-1 f=0.0468
157 →170 2.53 % -12 → 0
164 →172 5.18 % -5 → 2
165 →172 12.28 % -4 → 2
166 →181 2.12 % -3 →11
167 →173 5.92 % -2 → 3
167 →175 3.42 % -2 → 5
167 →181 6.82 % -2 →11
169 →176 35.52 % 0 → 6
169 →181 6.41 % 0 →11

31 31 Excited State: Singlet
4.7580 eV 260.56 nm
38379.cm-1 f=0.0127
157 →170 8.40 % -12 → 0
164 →173 2.56 % -5 → 3
165 →172 4.53 % -4 → 2
165 →173 7.49 % -4 → 3
167 →173 5.61 % -2 → 3
167 →175 6.34 % -2 → 5
167 →181 7.47 % -2 →11
168 →173 3.63 % -1 → 3
169 →176 28.43 % 0 → 6
169 →179 3.79 % 0 → 9

32 32 Excited State: Singlet
4.7690 eV 259.97 nm
38466.cm-1 f=0.0759
157 →170 61.24 % -12 → 0
158 →170 10.30 % -11 → 0
167 →173 3.50 % -2 → 3
167 →181 4.68 % -2 →11
168 →173 2.02 % -1 → 3

33 33 Excited State: Singlet

4.8010 eV 258.20 nm
38730.cm-1 f=0.0971
164 →172 16.62 % -5 → 2
165 →172 19.29 % -4 → 2
165 →173 11.39 % -4 → 3
166 →172 3.56 % -3 → 2
167 →173 4.41 % -2 → 3
167 →175 5.31 % -2 → 5
167 →181 4.42 % -2 →11
168 →178 3.26 % -1 → 8
169 →176 4.90 % 0 → 6
169 →178 2.46 % 0 → 8
169 →179 3.06 % 0 → 9

34 34 Excited State: Singlet
4.8130 eV 257.58 nm
38823.cm-1 f=0.0848
164 →172 3.82 % -5 → 2
165 →172 30.16 % -4 → 2
165 →173 7.12 % -4 → 3
167 →173 3.12 % -2 → 3
169 →176 12.54 % 0 → 6
169 →178 6.03 % 0 → 8
169 →181 8.69 % 0 →11

35 35 Excited State: Singlet
4.8630 eV 254.91 nm
39230.cm-1 f=0.0215
153 →170 4.53 % -16 → 0
155 →170 24.35 % -14 → 0
157 →170 5.39 % -12 → 0
158 →170 16.80 % -11 → 0
163 →171 12.15 % -6 → 1
164 →171 23.85 % -5 → 1

36 36 Excited State: Singlet
4.8740 eV 254.35 nm
39316.cm-1 f=0.0108
157 →170 2.33 % -12 → 0
158 →170 10.42 % -11 → 0
163 →171 16.92 % -6 → 1
164 →171 55.37 % -5 → 1
165 →171 5.14 % -4 → 1

37 37 Excited State: Singlet
4.8810 eV 253.98 nm
39373.cm-1 f=0.0085
155 →170 6.45 % -14 → 0
156 →170 5.76 % -13 → 0
157 →170 4.81 % -12 → 0
158 →170 54.11 % -11 → 0
163 →171 18.53 % -6 → 1

38 38 Excited State: Singlet
4.9030 eV 252.83 nm
39552.cm-1 f=0.0241
166 →173 10.02 % -3 → 3
166 →175 4.14 % -3 → 5
166 →179 4.47 % -3 → 9
166 →181 21.64 % -3 →11
167 →174 20.73 % -2 → 4
167 →175 6.91 % -2 → 5
167 →178 6.01 % -2 → 8

39 39 Excited State: Singlet
4.9360 eV 251.16 nm
39815.cm-1 f=0.0267
163 →172 3.04 % -6 → 2
164 →172 27.18 % -5 → 2
164 →173 2.84 % -5 → 3
165 →172 11.53 % -4 → 2
165 →173 22.47 % -4 → 3
167 →174 3.80 % -2 → 4
168 →172 2.80 % -1 → 2
168 →179 2.36 % -1 → 9
169 →186 2.45 % 0 →16
169 →189 2.33 % 0 →19

40 40 Excited State: Singlet
4.9380 eV 251.07 nm
39830.cm-1 f=0.0172
162 →175 3.48 % -7 → 5
163 →172 2.16 % -6 → 2
163 →174 6.96 % -6 → 4
165 →173 2.15 % -4 → 3
166 →173 4.15 % -3 → 3
166 →174 2.61 % -3 → 4
166 →175 3.10 % -3 → 5
166 →179 2.26 % -3 → 9
166 →181 7.08 % -3 →11
167 →174 36.91 % -2 → 4
168 →174 11.32 % -1 → 4

41 41 Excited State: Singlet
4.9490 eV 250.48 nm
39923.cm-1 f=0.0758
155 →170 43.70 % -14 → 0
163 →171 36.30 % -6 → 1
164 →171 6.14 % -5 → 1

42 42 Excited State: Singlet
5.0170 eV 247.10 nm
40469.cm-1 f=0.0136
155 →170 2.23 % -14 → 0
165 →174 2.24 % -4 → 4
166 →174 4.34 % -3 → 4
166 →175 6.68 % -3 → 5
167 →174 11.26 % -2 → 4
167 →175 3.57 % -2 → 5
167 →178 2.57 % -2 → 8
168 →174 45.30 % -1 → 4

43 43 Excited State: Singlet
5.0560 eV 245.20 nm
40783.cm-1 f=0.0233
163 →174 6.37 % -6 → 4
165 →173 5.62 % -4 → 3
166 →174 10.99 % -3 → 4
166 →175 7.80 % -3 → 5
167 →175 5.56 % -2 → 5
167 →178 3.68 % -2 → 8
167 →181 3.53 % -2 →11
168 →174 12.09 % -1 → 4
168 →175 14.76 % -1 → 5

44 44 Excited State: Singlet
5.0920 eV 243.48 nm
41071.cm-1 f=0.0046
163 →174 2.69 % -6 → 4
166 →175 6.32 % -3 → 5
166 →178 2.33 % -3 → 8
167 →174 12.12 % -2 → 4
167 →175 11.15 % -2 → 5
168 →174 5.57 % -1 → 4
168 →175 25.91 % -1 → 5
169 →177 10.08 % 0 → 7

45 45 Excited State: Singlet
5.1020 eV 242.98 nm
41156.cm-1 f=0.0024
163 →177 5.67 % -6 → 7
167 →174 2.04 % -2 → 4
167 →175 3.04 % -2 → 5
168 →175 3.01 % -1 → 5
169 →177 71.53 % 0 → 7

46 46 Excited State: Singlet
5.1200 eV 242.11 nm
41304.cm-1 f=0.0168
154 →170 4.12 % -15 → 0
163 →172 5.30 % -6 → 2
163 →173 3.06 % -6 → 3
163 →174 4.66 % -6 → 4
166 →174 16.15 % -3 → 4
167 →174 4.13 % -2 → 4
167 →175 14.96 % -2 → 5
167 →181 3.97 % -2 →11
168 →174 6.12 % -1 → 4
168 →175 20.71 % -1 → 5
169 →177 2.00 % 0 → 7

4a-Cation in DCM solution

06075_Ir_2PhPzol_PyImminoPh_pBr_SDD_D95Vd_M06_DCM_TD15.out
HOMO is orbital 134 and LUMO is orbital 135

>>>> Singlet states <<<<

eV	nm	cm-1	f
2.2342;	554.93;	18020.3;	0.0019
2.6889;	461.10;	21687.3;	0.0056
2.9865;	415.15;	24087.7;	0.0427
2.9960;	413.83;	24164.5;	0.0774
3.3176;	373.72;	26758.0;	0.0187
3.3841;	366.37;	27294.8;	0.3547
3.5264;	351.59;	28442.2;	0.0021
3.7118;	334.02;	29938.3;	0.0132
3.7806;	327.95;	30492.5;	0.0724
3.7964;	326.58;	30620.4;	0.0028
3.8714;	320.26;	31224.6;	0.0081
3.9043;	317.56;	31490.1;	0.0098
3.9188;	316.38;	31607.6;	0.0222
3.9717;	312.17;	32033.8;	0.0355
4.0597;	305.40;	32743.9;	0.0409

1 2 Excited State: Singlet
2.2342 eV 554.93 nm 18020.cm-1 f=0.0019
134 → 135 0.69972 97.92 % 0 → 0

2 5 Excited State: Singlet
2.6889 eV 461.10 nm 21687.cm-1 f=0.0056
131 → 135 -0.12641 3.20 % -3 → 0
132 → 135 0.68775 94.60 % -2 → 0

3 8 Excited State: Singlet
2.9865 eV 415.15 nm 24088.cm-1 f=0.0427
131 → 135 -0.28900 16.70 % -3 → 0
133 → 135 0.63351 80.27 % -1 → 0

4 9 Excited State: Singlet
2.9960 eV 413.83 nm 24165.cm-1 f=0.0774
129 → 135 -0.10303 2.12 % -5 → 0
131 → 135 0.61261 75.06 % -3 → 0
133 → 135 0.30730 18.89 % -1 → 0

5 13 Excited State: Singlet
3.3176 eV 373.72 nm 26758.cm-1 f=0.0187
130 → 135 0.68662 94.29 % -4 → 0

6 15 Excited State: Singlet
3.3841 eV 366.37 nm 27295.cm-1 f=0.3547
128 → 135 0.43881 38.51 % -6 → 0
129 → 135 0.50388 50.78 % -5 → 0
130 → 135 0.13930 3.88 % -4 → 0
131 → 135 0.11774 2.77 % -3 → 0

7 17 Excited State: Singlet
3.5264 eV 351.59 nm 28442.cm-1 f=0.0021
128 → 135 0.52755 55.66 % -6 → 0
129 → 135 -0.46116 42.53 % -5 → 0

8 20 Excited State: Singlet
3.7118 eV 334.02 nm 29938.cm-1 f=0.0132
134 → 136 0.65628 86.14 % 0 → 1
134 → 137 -0.21254 9.03 % 0 → 2

9 23 Excited State: Singlet
3.7806 eV 327.95 nm 30492.cm-1 f=0.0724
134 → 136 0.22229 9.88 % 0 → 1
134 → 137 0.64174 82.37 % 0 → 2

10 25 Excited State: Singlet
3.7964 eV 326.58 nm 30620.cm-1 f=0.0028
134 → 138 0.67491 91.10 % 0 → 3

11 26 Excited State: Singlet
3.8714 eV 320.26 nm 31225.cm-1 f=0.0081
127 → 135 0.68353 93.44 % -7 → 0

12 27 Excited State: Singlet
3.9043 eV 317.56 nm 31490.cm-1 f=0.0098
125 → 135 -0.15017 4.51 % -9 → 0
126 → 135 0.21184 8.98 % -8 → 0
132 → 136 0.61444 75.51 % -2 → 1
132 → 137 -0.11541 2.66 % -2 → 2

13 28 Excited State: Singlet
3.9188 eV 316.38 nm 31608.cm-1 f=0.0222
124 → 135 0.16578 5.50 % -10 → 0
125 → 135 -0.18020 6.49 % -9 → 0
126 → 135 0.25284 12.79 % -8 → 0
131 → 136 -0.23699 11.23 % -3 → 1
132 → 137 0.46816 43.83 % -2 → 2
133 → 138 -0.12408 3.08 % -1 → 3

14 29 Excited State: Singlet
3.9717 eV 312.17 nm 32034.cm-1 f=0.0355
124 → 135 -0.18946 7.18 % -10 → 0
125 → 135 0.19495 7.60 % -9 → 0
126 → 135 -0.17851 6.37 % -8 → 0
131 → 136 0.28289 16.01 % -3 → 1
132 → 136 0.26777 14.34 % -2 → 1
132 → 137 0.41664 34.72 % -2 → 2

15 30 Excited State: Singlet
4.0597 eV 305.40 nm 32744.cm-1 f=0.0409
123 → 135 0.13733 3.77 % -11 → 0
124 → 135 0.35949 25.85 % -10 → 0
125 → 135 -0.20998 8.82 % -9 → 0
131 → 136 0.38205 29.19 % -3 → 1
131 → 137 -0.13639 3.72 % -3 → 2
132 → 138 -0.15696 4.93 % -2 → 3
133 → 136 -0.20874 8.71 % -1 → 1
133 → 137 0.16813 5.65 % -1 → 2

>>>> Triplet states <<<<

eV	nm	cm-1	f
2.1814;	568.37;	17594.2;	0.0000
2.3230;	533.72;	18736.4;	0.0000
2.6541;	467.15;	21406.4;	0.0000
2.8963;	428.08;	23360.1;	0.0000
2.9827;	415.68;	24057.0;	0.0000
3.1042;	399.40;	25037.6;	0.0000
3.1415;	394.67;	25337.6;	0.0000
3.3123;	374.32;	26715.1;	0.0000
3.3738;	367.49;	27211.6;	0.0000
3.5136;	352.87;	28339.0;	0.0000
3.6649;	338.30;	29559.6;	0.0000

3.6834; 336.60; 29708.9; 0.0000
3.7413; 331.40; 30175.0; 0.0000
3.7460; 330.98; 30213.3; 0.0000
3.7808; 327.93; 30494.3; 0.0000

1 1 Excited State: Triplet
2.1814 eV 568.37 nm 17594.cm-1 f=0.0000
131 → 135 -0.13908 3.87 % -3 → 0
132 → 135 -0.17534 6.15 % -2 → 0
134 → 135 0.64439 83.05 % 0 → 0

2 3 Excited State: Triplet
2.3230 eV 533.72 nm 18736.cm-1 f=0.0000
126 → 135 0.16866 5.69 % -8 → 0
128 → 135 0.12760 3.26 % -6 → 0
129 → 135 0.15498 4.80 % -5 → 0
131 → 135 0.28417 16.15 % -3 → 0
132 → 135 0.48770 47.57 % -2 → 0
134 → 135 0.26633 14.19 % 0 → 0

3 4 Excited State: Triplet
2.6541 eV 467.15 nm 21406.cm-1 f=0.0000
131 → 135 0.58016 67.32 % -3 → 0
132 → 135 -0.36458 26.58 % -2 → 0

4 6 Excited State: Triplet
2.8963 eV 428.08 nm 23360.cm-1 f=0.0000
127 → 139 0.10474 2.19 % -7 → 4
128 → 135 0.36314 26.37 % -6 → 0
129 → 135 0.43797 38.36 % -5 → 0
131 → 135 -0.17963 6.45 % -3 → 0
132 → 135 -0.24940 12.44 % -2 → 0

5 7 Excited State: Triplet
2.9827 eV 415.68 nm 24057.cm-1 f=0.0000
133 → 135 0.68843 94.79 % -1 → 0

6 10 Excited State: Triplet
3.1042 eV 399.40 nm 25038.cm-1 f=0.0000
130 → 137 -0.21234 9.02 % -4 → 2
133 → 137 -0.17820 6.35 % -1 → 2
133 → 138 -0.28333 16.06 % -1 → 3
134 → 137 0.40880 33.42 % 0 → 2
134 → 138 0.16816 5.66 % 0 → 3
134 → 143 -0.11919 2.84 % 0 → 8

7 11 Excited State: Triplet
3.1415 eV 394.67 nm 25338.cm-1 f=0.0000
128 → 143 0.11358 2.58 % -6 → 8
130 → 138 -0.22222 9.88 % -4 → 3
133 → 137 -0.33339 22.23 % -1 → 2
133 → 138 0.18184 6.61 % -1 → 3
134 → 137 -0.16304 5.32 % 0 → 2
134 → 138 0.34391 23.65 % 0 → 3
134 → 144 -0.14685 4.31 % 0 → 9

8 12 Excited State: Triplet
3.3123 eV 374.32 nm 26715.cm-1 f=0.0000
126 → 135 0.14530 4.22 % -8 → 0
130 → 135 0.66542 88.56 % -4 → 0

9 14 Excited State: Triplet
3.3738 eV 367.49 nm 27212.cm-1 f=0.0000
117 → 135 0.11934 2.85 % -17 → 0
121 → 135 -0.15882 5.04 % -13 → 0
122 → 135 0.11322 2.56 % -12 → 0
124 → 135 -0.22626 10.24 % -10 → 0
125 → 135 -0.11852 2.81 % -9 → 0
126 → 135 0.35796 25.63 % -8 → 0
127 → 139 -0.16500 5.45 % -7 → 4
128 → 135 -0.10767 2.32 % -6 → 0
128 → 140 0.13418 3.60 % -6 → 5
129 → 140 0.16609 5.52 % -5 → 5
130 → 135 -0.20569 8.46 % -4 → 0
132 → 135 -0.11299 2.55 % -2 → 0

10 16 Excited State: Triplet
3.5136 eV 352.87 nm 28339.cm-1 f=0.0000
128 → 135 0.52096 54.28 % -6 → 0
129 → 135 -0.44934 40.38 % -5 → 0

11 18 Excited State: Triplet
3.6649 eV 338.30 nm 29560.cm-1 f=0.0000
129 → 137 -0.11993 2.88 % -5 → 2
130 → 137 -0.15203 4.62 % -4 → 2
130 → 138 -0.14290 4.08 % -4 → 3
130 → 144 -0.10674 2.28 % -4 → 9
132 → 137 0.13208 3.49 % -2 → 2
132 → 138 0.11086 2.46 % -2 → 3
134 → 136 0.30660 18.80 % 0 → 1
134 → 137 -0.22013 9.69 % 0 → 2
134 → 138 -0.29899 17.88 % 0 → 3
134 → 144 -0.11031 2.43 % 0 → 9

12 19 Excited State: Triplet
3.6834 eV 336.60 nm 29709.cm-1 f=0.0000
128 → 144 -0.11897 2.83 % -6 → 9
129 → 138 0.11259 2.54 % -5 → 3
130 → 137 0.14381 4.14 % -4 → 2
130 → 143 0.11106 2.47 % -4 → 8
132 → 137 -0.11461 2.63 % -2 → 2
134 → 136 0.38327 29.38 % 0 → 1
134 → 137 0.35543 25.27 % 0 → 2
134 → 138 -0.13963 3.90 % 0 → 3
134 → 143 0.15954 5.09 % 0 → 8

13 21 Excited State: Triplet
3.7413 eV 331.40 nm 30175.cm-1 f=0.0000
128 → 143 -0.10197 2.08 % -6 → 8
131 → 137 -0.20846 8.69 % -3 → 2
132 → 138 -0.24135 11.65 % -2 → 3
134 → 136 0.43533 37.90 % 0 → 1
134 → 138 0.23778 11.31 % 0 → 3

14 22 Excited State: Triplet
3.7460 eV 330.98 nm 30213.cm-1 f=0.0000
128 → 137 -0.10356 2.14 % -6 → 2
128 → 138 -0.14309 4.09 % -6 → 3
130 → 137 0.11759 2.77 % -4 → 2
131 → 138 0.25297 12.80 % -3 → 3
132 → 137 0.46962 44.11 % -2 → 2
132 → 138 0.11470 2.63 % -2 → 3
134 → 137 0.18022 6.50 % 0 → 2

15 24 Excited State: Triplet
3.7808 eV 327.93 nm 30494.cm-1 f=0.0000
128 → 137 -0.15450 4.77 % -6 → 2
130 → 138 0.10872 2.36 % -4 → 3
131 → 137 0.28128 15.82 % -3 → 2
131 → 138 -0.15988 5.11 % -3 → 3
132 → 138 0.35111 24.66 % -2 → 3
134 → 136 0.17483 6.11 % 0 → 1
134 → 138 0.27014 14.60 % 0 → 3

Table S6: TD-DFT results for Structure 5a p-H /D95(d)/SDD/M06/DCM level of theory .

5a-PF_6^- Phenylpyrazoleside.

07058_Ir_2PhPzol_PF6_PyImminoPh_SDD_D95d_M06_DCM_TD15.out
HOMO is orbital 166 and LUMO is orbital 167

>>>> Singlet states <<<<

eV	nm	cm-1	f
2.2290;	556.20;	17979.1;	0.0013
2.6830;	462.00;	21645.0;	0.0053
2.9790;	416.16;	24029.2;	0.0346
2.9900;	414.60;	24119.6;	0.0798
3.3090;	374.62;	26693.7;	0.0019
3.4900;	355.25;	28149.2;	0.2602
3.5380;	350.40;	28538.8;	0.0041
3.6690;	337.86;	29598.1;	0.0015
3.7620;	329.55;	30344.4;	0.0669
3.7660;	329.21;	30375.7;	0.0127
3.8260;	324.03;	30861.3;	0.0184
3.8560;	321.49;	31105.2;	0.0085
3.8770;	319.77;	31272.5;	0.0098
3.9410;	314.60;	31786.4;	0.0236
3.9450;	314.23;	31823.8;	0.0394

1 2 Excited State: Singlet
2.2290 eV 556.20 nm 17979.cm-1 f=0.0013
166 →167 97.70 % 0→0

2 4 Excited State: Singlet
2.6830 eV 462.00 nm 21645.cm-1 f=0.0053
163 →167 6.92 % -3→0
164 →167 90.94 % -2→0

3 7 Excited State: Singlet
2.9790 eV 416.16 nm 24029.cm-1 f=0.0346
163 →167 13.74 % -3→0
165 →167 84.90 % -1→0

4 9 Excited State: Singlet
2.9900 eV 414.60 nm 24120.cm-1 f=0.0798
163 →167 77.14 % -3→0
164 →167 6.96 % -2→0
165 →167 13.63 % -1→0

5 13 Excited State: Singlet
3.3090 eV 374.62 nm 26694.cm-1 f=0.0019
162 →167 97.66 % -4→0

6 15 Excited State: Singlet
3.4900 eV 355.25 nm 28149.cm-1 f=0.2602
160 →167 89.46 % -6→0
161 →167 5.74 % -5→0

7 17 Excited State: Singlet
3.5380 eV 350.40 nm 28539.cm-1 f=0.0041
160 →167 5.51 % -6→0
161 →167 91.34 % -5→0

8 22 Excited State: Singlet
3.6690 eV 337.86 nm 29598.cm-1 f=0.0015
166 →168 95.64 % 0→1

9 24 Excited State: Singlet
3.7620 eV 329.55 nm 30344.cm-1 f=0.0669
166 →169 89.56 % 0→2

10 25 Excited State: Singlet
3.7660 eV 329.21 nm 30376.cm-1 f=0.0127
159 →167 96.77 % -7→0

11 26 Excited State: Singlet
3.8260 eV 324.03 nm 30861.cm-1 f=0.0184
166 →170 89.26 % 0→3

12 27 Excited State: Singlet
3.8560 eV 321.49 nm 31105.cm-1 f=0.0085
158 →167 5.28 % -8→0
164 →168 86.69 % -2→1

13 28 Excited State: Singlet
3.8770 eV 319.77 nm 31272.cm-1 f=0.0098
155 →167 2.67 % -11→0
157 →167 12.35 % -9→0
158 →167 20.86 % -8→0
163 →168 46.33 % -3→1
164 →168 6.38 % -2→1
164 →169 4.94 % -2→2
165 →168 2.13 % -1→1

14 29 Excited State: Singlet
3.9410 eV 314.60 nm 31786.cm-1 f=0.0236
158 →167 4.70 % -8→0
164 →169 80.10 % -2→2
164 →174 2.17 % -2→7

15 30 Excited State: Singlet
3.9450 eV 314.23 nm 31824.cm-1 f=0.0394
156 →167 16.71 % -10→0
157 →167 26.83 % -9→0
158 →167 3.86 % -8→0
163 →168 13.25 % -3→1
165 →168 30.28 % -1→1

>>>> Triplet states <<<<

eV	nm	cm-1	f
2.1840;	567.62;	17617.4;	0.0000
2.3310;	531.89;	18800.9;	0.0000
2.6850;	461.71;	21658.6;	0.0000
2.9160;	425.11;	23523.3;	0.0000
2.9820;	415.76;	24052.3;	0.0000
3.1140;	398.13;	25117.4;	0.0000
3.1420;	394.59;	25342.8;	0.0000
3.3010;	375.58;	26625.5;	0.0000
3.4040;	364.18;	27458.9;	0.0000
3.5080;	353.35;	28300.6;	0.0000
3.5720;	347.03;	28816.0;	0.0000
3.5880;	345.51;	28942.7;	0.0000
3.6220;	342.22;	29221.0;	0.0000
3.6400;	340.56;	29363.4;	0.0000
3.7460;	330.93;	30217.9;	0.0000

1 1 Excited State: Triplet
2.1840 eV 567.62 nm 17617.cm-1 f=0.0000
160 →167 2.79 % -6→0
164 →167 5.41 % -2→0
166 →167 85.38 % 0→0

2 3 Excited State: Triplet
2.3310 eV 531.89 nm 18801.cm-1 f=0.0000
158 →167 4.35 % -8→0
160 →167 11.53 % -6→0
163 →167 6.13 % -3→0
164 →167 56.41 % -2→0
166 →167 11.52 % 0→0

3 5 Excited State: Triplet
2.6850 eV 461.71 nm 21659.cm-1 f=0.0000
163 →167 81.79 % -3→0
164 →167 12.62 % -2→0

4 6 Excited State: Triplet

2.9160 eV 425.11 nm 23523.cm-1 f=0.0000
155 →167 2.38 % -11→0
160 →167 50.74 % -6→0
160 →172 2.26 % -6→5
163 →167 5.90 % -3→0
164 →167 19.82 % -2→0
165 →167 7.84 % -1→0

5 8 Excited State: Triplet
2.9820 eV 415.76 nm 24052.cm-1 f=0.0000
160 →167 9.51 % -6→0
165 →167 86.38 % -1→0

6 10 Excited State: Triplet
3.1140 eV 398.13 nm 25117.cm-1 f=0.0000
161 →175 2.23 % -5→8
162 →169 6.31 % -4→2
162 →170 3.47 % -4→3
165 →169 2.58 % -1→2
165 →170 19.75 % -1→3
166 →169 21.75 % 0→2
166 →170 18.18 % 0→3
166 →174 3.30 % 0→7

7 11 Excited State: Triplet
3.1420 eV 394.59 nm 25343.cm-1 f=0.0000
161 →169 4.42 % -5→2
161 →174 4.79 % -5→7
162 →169 6.56 % -4→2
162 →170 5.69 % -4→3
165 →169 23.39 % -1→2
165 →170 3.50 % -1→3
166 →169 10.34 % 0→2
166 →170 17.73 % 0→3
166 →175 4.25 % 0→8

8 12 Excited State: Triplet
3.3010 eV 375.58 nm 26625.cm-1 f=0.0000
158 →167 2.49 % -8→0
162 →167 92.16 % -4→0

9 14 Excited State: Triplet
3.4040 eV 364.18 nm 27459.cm-1 f=0.0000
153 →167 10.46 % -13→0
155 →167 15.75 % -11→0
156 →167 15.88 % -10→0
158 →167 20.92 % -8→0
160 →167 3.26 % -6→0
160 →172 6.80 % -6→5
162 →167 5.06 % -4→0

10 16 Excited State: Triplet
3.5080 eV 353.35 nm 28301.cm-1 f=0.0000
159 →167 15.55 % -7→0
161 →167 79.34 % -5→0

11 18 Excited State: Triplet
3.5720 eV 347.03 nm 28816.cm-1 f=0.0000
150 →167 5.28 % -16→0
151 →167 2.76 % -15→0
156 →167 3.15 % -10→0
157 →167 2.84 % -9→0
158 →167 8.50 % -8→0
159 →167 2.95 % -7→0
159 →171 5.97 % -7→4
159 →173 6.10 % -7→6
160 →172 3.79 % -6→5
163 →168 5.39 % -3→1
164 →170 2.49 % -2→3
166 →168 3.47 % 0→1
166 →169 4.85 % 0→2
166 →170 2.43 % 0→3

12 19 Excited State: Triplet
3.5880 eV 345.51 nm 28943.cm-1 f=0.0000
152 →170 3.97 % -14→3
161 →175 2.79 % -5→8
162 →175 2.12 % -4→8
163 →169 7.83 % -3→2
164 →168 2.17 % -2→1
164 →169 4.05 % -2→2
164 →170 9.58 % -2→3
166 →168 6.01 % 0→1
166 →169 5.34 % 0→2
166 →170 4.89 % 0→3

13 20 Excited State: Triplet
3.6220 eV 342.22 nm 29221.cm-1 f=0.0000
159 →167 67.58 % -7→0
159 →172 3.04 % -7→5
159 →173 2.28 % -7→6
160 →167 2.50 % -6→0
161 →167 12.51 % -5→0
166 →168 4.39 % 0→1

14 21 Excited State: Triplet
3.6400 eV 340.56 nm 29363.cm-1 f=0.0000
161 →167 2.44 % -5→0
161 →169 3.65 % -5→2
161 →174 3.97 % -5→7
166 →168 56.86 % 0→1
166 →169 15.99 % 0→2
166 →174 2.46 % 0→7

15 23 Excited State: Triplet
3.7460 eV 330.93 nm 30218.cm-1 f=0.0000
161 →174 2.19 % -5→7
162 →175 2.13 % -4→8
163 →169 30.09 % -3→2
164 →169 11.64 % -2→2
164 →170 5.38 % -2→3
166 →168 4.84 % 0→1
166 →170 12.79 % 0→3
166 →175 3.33 % 0→8

5a-PF6⁻Pyridineimine side

07058_Ir_2PhPzol_PyImminoPh_PF6_SDD_D95d_M06_DCM_TD15.out

HOMO is orbital 166 and LUMO is orbital 167

>>>> Singlet states <<<<

eV	nm	cm-1	f
2.4900;	497.91;	20084.0;	0.0018
2.9090;	426.09;	23469.2;	0.0091
3.1790;	390.01;	25640.4;	0.1297
3.2740;	378.69;	26406.8;	0.0027
3.6020;	344.21;	29052.0;	0.1222
3.6390;	340.62;	29358.2;	0.1297
3.7600;	329.68;	30332.4;	0.0802
3.8090;	325.47;	30724.8;	0.0017
3.8510;	321.95;	31060.7;	0.0102
3.9200;	316.27;	31618.6;	0.0021
3.9650;	312.64;	31985.7;	0.0101
3.9740;	311.93;	32058.5;	0.0460
4.0800;	303.87;	32908.8;	0.0087
4.2120;	294.33;	33975.5;	0.0232
4.2610;	290.95;	34370.2;	0.0052

1 2 Excited State: Singlet
2.4900 eV 497.91 nm 20084.cm-1 f=0.0018
166 →167 97.93 % 0→0

2 5 Excited State: Singlet
2.9090 eV 426.09 nm 23469.cm-1 f=0.0091
163 →167 7.59 % -3→0
164 →167 90.00 % -2→0

3 9 Excited State: Singlet
3.1790 eV 390.01 nm 25640.cm-1 f=0.1297
163 →167 87.44 % -3→0
164 →167 7.43 % -2→0

4 11 Excited State: Singlet
3.2740 eV 378.69 nm 26407.cm-1 f=0.0027
163 →167 2.00 % -3→0
165 →167 97.09 % -1→0

5 13 Excited State: Singlet
3.6020 eV 344.21 nm 29052.cm-1 f=0.1222
160 →167 29.89 % -6→0
161 →167 12.08 % -5→0
162 →167 54.11 % -4→0

6 15 Excited State: Singlet
3.6390 eV 340.62 nm 29358.cm-1 f=0.1297
160 →167 41.45 % -6→0
161 →167 11.71 % -5→0
162 →167 43.73 % -4→0

7 20 Excited State: Singlet
3.7600 eV 329.68 nm 30332.cm-1 f=0.0802
166 →168 5.82 % 0→1
166 →169 85.40 % 0→2

8 22 Excited State: Singlet
3.8090 eV 325.47 nm 30725.cm-1 f=0.0017
159 →167 3.21 % -7→0
160 →167 20.08 % -6→0
161 →167 65.68 % -5→0
166 →168 6.14 % 0→1

9 24 Excited State: Singlet
3.8510 eV 321.95 nm 31061.cm-1 f=0.0102
160 →167 2.95 % -6→0
161 →167 4.96 % -5→0
166 →168 59.85 % 0→1
166 →169 3.44 % 0→2
166 →170 24.40 % 0→3

10 25 Excited State: Singlet
3.9200 eV 316.27 nm 31619.cm-1 f=0.0021
166 →168 25.77 % 0→1
166 →170 67.14 % 0→3

11 26 Excited State: Singlet
3.9650 eV 312.64 nm 31986.cm-1 f=0.0101
159 →167 92.45 % -7→0
161 →167 3.08 % -5→0

12 27 Excited State: Singlet
3.9740 eV 311.93 nm 32058.cm-1 f=0.0460
163 →169 3.70 % -3→2
164 →168 10.98 % -2→1
164 →169 70.55 % -2→2
165 →170 2.20 % -1→3
166 →169 2.04 % 0→2

13 28 Excited State: Singlet
4.0800 eV 303.87 nm 32909.cm-1 f=0.0087
158 →167 7.32 % -8→0
164 →168 69.53 % -2→1
164 →169 12.61 % -2→2
164 →170 2.43 % -2→3

14 29 Excited State: Singlet
4.2120 eV 294.33 nm 33975.cm-1 f=0.0232
163 →168 19.30 % -3→1
163 →169 22.11 % -3→2
164 →170 20.41 % -2→3
165 →169 17.65 % -1→2

15 30 Excited State: Singlet
4.2610 eV 290.95 nm 34370.cm-1 f=0.0052
163 →168 3.13 % -3→1
163 →169 18.38 % -3→2
163 →170 9.47 % -3→3
164 →168 2.52 % -2→1
164 →170 51.97 % -2→3
165 →170 4.76 % -1→3

>>>> Triplet states <<<<

eV	nm	cm-1	f
2.3850;	519.75;	19240.0;	0.0000
2.4980;	496.22;	20152.4;	0.0000
2.8740;	431.26;	23187.9;	0.0000
3.1150;	398.00;	25125.6;	0.0000
3.1180;	397.54;	25154.7;	0.0000
3.1450;	394.15;	25371.1;	0.0000
3.2680;	379.39;	26358.1;	0.0000
3.4520;	359.14;	27844.3;	0.0000
3.6160;	342.88;	29164.7;	0.0000
3.6420;	340.38;	29378.9;	0.0000
3.6730;	337.55;	29625.2;	0.0000
3.6990;	335.12;	29840.1;	0.0000
3.7180;	333.40;	29994.0;	0.0000
3.7650;	329.29;	30368.4;	0.0000
3.8320;	323.52;	30910.0;	0.0000

1 1 Excited State: Triplet
2.3850 eV 519.75 nm 19240.cm-1 f=0.0000
158 →167 3.19 % -8→0
160 →167 8.06 % -6→0
161 →167 3.11 % -5→0
163 →167 8.95 % -3→0
164 →167 40.90 % -2→0
166 →167 26.97 % 0→0

2 3 Excited State: Triplet
2.4980 eV 496.22 nm 20152.cm-1 f=0.0000
158 →167 2.20 % -8→0
163 →167 2.32 % -3→0
164 →167 19.13 % -2→0
166 →167 70.25 % 0→0

3 4 Excited State: Triplet
2.8740 eV 431.26 nm 23188.cm-1 f=0.0000
163 →167 76.69 % -3→0
164 →167 14.23 % -2→0
165 →167 2.69 % -1→0

4 6 Excited State: Triplet
3.1150 eV 398.00 nm 25126.cm-1 f=0.0000
161 →175 2.08 % -5→8
162 →169 11.80 % -4→2
165 →169 6.13 % -1→2
165 →170 14.53 % -1→3
166 →169 37.36 % 0→2
166 →174 2.08 % 0→7

5 7 Excited State: Triplet
3.1180 eV 397.54 nm 25155.cm-1 f=0.0000
160 →167 41.80 % -6→0
161 →167 15.22 % -5→0
163 →167 4.29 % -3→0
164 →167 17.48 % -2→0

6 8 Excited State: Triplet
3.1450 eV 394.15 nm 25371.cm-1 f=0.0000
161 →174 2.51 % -5→7
162 →170 10.93 % -4→3
165 →169 20.55 % -1→2
165 →170 7.76 % -1→3
166 →170 28.09 % 0→3
166 →174 2.45 % 0→7
166 →175 3.80 % 0→8

7 10 Excited State: Triplet
3.2680 eV 379.39 nm 26358.cm-1 f=0.0000
160 →167 2.80 % -6→0
163 →167 2.27 % -3→0
165 →167 91.63 % -1→0

8 12 Excited State: Triplet
3.4520 eV 359.14 nm 27844.cm-1 f=0.0000
154 →167 4.83 % -12→0
155 →167 5.99 % -11→0
156 →167 5.97 % -10→0
158 →167 36.13 % -8→0
158 →168 2.42 % -8→1
159 →172 3.21 % -7→5
159 →173 2.07 % -7→6
160 →173 5.93 % -6→6
164 →167 3.74 % -2→0

9 14 Excited State: Triplet
3.6160 eV 342.88 nm 29165.cm-1 f=0.0000
162 →167 87.70 % -4→0
166 →169 2.82 % 0→2

10 16 Excited State: Triplet
3.6420 eV 340.38 nm 29379.cm-1 f=0.0000
161 →169 3.37 % -5→2
161 →170 2.50 % -5→3
161 →175 3.72 % -5→8
162 →167 7.94 % -4→0
162 →169 7.11 % -4→2
164 →169 6.42 % -2→2
166 →169 24.12 % 0→2
166 →170 6.32 % 0→3
166 →172 2.66 % 0→5
166 →175 3.33 % 0→8

11 17 Excited State: Triplet
3.6730 eV 337.55 nm 29625.cm-1 f=0.0000
159 →167 63.57 % -7→0
159 →173 4.40 % -7→6
160 →167 3.59 % -6→0
161 →167 19.98 % -5→0

12 18 Excited State: Triplet
3.6990 eV 335.12 nm 29840.cm-1 f=0.0000
160 →174 2.58 % -6→7
161 →170 2.97 % -5→3
161 →174 4.31 % -5→7
162 →169 2.20 % -4→2
162 →170 3.87 % -4→3

163 →169 3.09 % -3→2
163 →170 3.24 % -3→3
164 →170 2.92 % -2→3
166 →168 8.15 % 0→1
166 →169 11.35 % 0→2
166 →170 23.44 % 0→3
166 →174 4.77 % 0→7

13 19 Excited State: Triplet
3.7180 eV 333.40 nm 29994.cm-1 f=0.0000
160 →169 5.17 % -6→2
160 →170 2.37 % -6→3
162 →169 2.37 % -4→2
163 →170 7.26 % -3→3
164 →168 2.14 % -2→1
164 →169 47.96 % -2→2
164 →170 4.04 % -2→3
166 →169 5.32 % 0→2
166 →170 2.23 % 0→3

14 21 Excited State: Triplet
3.7650 eV 329.29 nm 30368.cm-1 f=0.0000
157 →170 3.27 % -9→3
163 →169 17.33 % -3→2
163 →170 20.71 % -3→3
164 →170 23.06 % -2→3
166 →168 4.44 % 0→1
166 →170 5.02 % 0→3

15 23 Excited State: Triplet
3.8320 eV 323.52 nm 30910.cm-1 f=0.0000
159 →167 19.25 % -7→0
160 →167 18.72 % -6→0
161 →167 39.95 % -5→0
166 →168 9.81 % 0→

5a "free" cation/D95(d)/SDD/M06/DCM level of theory

07058_Ir_2PhPzol_PyImmino_Ph_SDD_D95d_M06_DCM_TD15.out
HOMO is orbital 131 and LUMO is orbital 132

>>>> Singlet states <<<<

eV nm cm-1 f
2.2790; 543.83; 18388.1;
0.0016
2.7370; 452.96; 22077.0;
0.0045
3.0360; 408.35; 24488.8;
0.1185
3.0440; 407.20; 24558.0;
0.0060
3.3760; 367.25; 27229.4;
0.0058
3.4980; 354.41; 28215.9;
0.2469
3.5760; 346.66; 28846.7;
0.0020
3.7210; 333.14; 30017.4;
0.0095
3.7790; 328.04; 30484.1;
0.0766
3.8620; 321.03; 31149.7;
0.0134
3.8990; 317.98; 31448.5;
0.0034
4.2110; 294.39; 33968.5;
0.0127
4.3120; 287.53; 34779.0;
0.0463
4.3250; 286.61; 34890.6;
0.0063
4.3720; 283.57; 35264.7;
0.0814

1 1 Excited State: Single
2.2790 eV 543.83 nm
18388.cm-1 f=0.0016
131 → 132 97.89 % 0 → 0

2 2 Excited State: Single
2.7370 eV 452.96 nm
22077.cm-1 f=0.0045
128 → 132 4.01 % -3 → 0
129 → 132 94.18 % -2 → 0

3 3 Excited State: Single
3.0360 eV 408.35 nm
24489.cm-1 f=0.1185
128 → 132 93.24 % -3 → 0
129 → 132 3.66 % -2 → 0

4 4 Excited State: Single
3.0440 eV 407.20 nm
24558.cm-1 f=0.0060
130 → 132 99.06 % -1 → 0

5 5 Excited State: Single
3.3760 eV 367.25 nm
27229.cm-1 f=0.0058
127 → 132 96.32 % -4 → 0

6 6 Excited State: Single
3.4980 eV 354.41 nm
28216.cm-1 f=0.2469
125 → 132 90.74 % -6 → 0
126 → 132 3.29 % -5 → 0

7 7 Excited State: Single
3.5760 eV 346.66 nm
28847.cm-1 f=0.0020
125 → 132 3.16 % -6 → 0
126 → 132 93.95 % -5 → 0

8 8 Excited State: Single
3.7210 eV 333.14 nm
30017.cm-1 f=0.0095
131 → 133 89.02 % 0 → 1
131 → 134 5.90 % 0 → 2

9 9 Excited State: Single
3.7790 eV 328.04 nm
30484.cm-1 f=0.0766
131 → 133 6.63 % 0 → 1
131 → 134 85.30 % 0 → 2

10 10 Excited State: Single
3.8620 eV 321.03 nm
31150.cm-1 f=0.0134
124 → 132 96.32 % -7 → 0

11 11 Excited State: Single
3.8990 eV 317.98 nm
31449.cm-1 f=0.0034
131 → 135 91.00 % 0 → 3

12 12 Excited State: Single
4.2110 eV 294.39 nm
33969.cm-1 f=0.0127
122 → 132 3.78 % -9 → 0
123 → 132 7.23 % -8 → 0
129 → 133 81.31 % -2 → 1

13 13 Excited State: Single
4.3120 eV 287.53 nm
34779.cm-1 f=0.0463
129 → 133 3.35 % -2 → 1
129 → 134 79.31 % -2 → 2
129 → 139 2.15 % -2 → 7
130 → 135 4.05 % -1 → 3

14 14 Excited State: Single
4.3250 eV 286.61 nm
34891.cm-1 f=0.0063
120 → 132 2.02 % -11 → 0
122 → 132 8.01 % -9 → 0
123 → 132 16.26 % -8 → 0
128 → 133 54.31 % -3 → 1
129 → 133 6.10 % -2 → 1

15 15 Excited State: Single
4.3720 eV 283.57 nm
35265.cm-1 f=0.0814
121 → 132 22.30 % -10 → 0
122 → 132 22.51 % -9 → 0
123 → 132 7.14 % -8 → 0
128 → 133 6.88 % -3 → 1
128 → 134 2.54 % -3 → 2
129 → 133 2.25 % -2 → 1
129 → 135 13.03 % -2 → 3
130 → 133 6.66 % -1 → 1
130 → 134 8.19 % -1 → 2

Table S7: TD-DFT results for Structure 8a iPr at/D95(d)/SDD/M06/DCM level of theory .

8a-PF_6^- Phenylpyrazoleside.

07016_Ir_2PhPzol_PF6_PyImminoiPr_SDD_D95d_M06_DCM_TD15.out
HOMO is orbital 158 and LUMO is orbital 159

>>>> Singlet states <<<<

eV	nm	cm-1	f
2.4445;	507.19;	19716.5;	0.0001
2.8987;	427.72;	23379.8;	0.0020
3.2093;	386.33;	25884.6;	0.0978
3.2443;	382.16;	26167.1;	0.0218
3.5614;	348.13;	28724.9;	0.0007
3.6992;	335.17;	29835.6;	0.0005
3.7580;	329.92;	30310.4;	0.0685
3.7916;	327.00;	30581.0;	0.0015
3.9344;	315.13;	31732.9;	0.0242
3.9536;	313.60;	31887.8;	0.0140
3.9751;	311.90;	32061.6;	0.0317
4.0307;	307.60;	32509.8;	0.0089
4.1512;	298.67;	33481.8;	0.0357
4.1928;	295.71;	33816.9;	0.0053
4.2138;	294.23;	33987.0;	0.0201

Excited State: 2
2.4445 eV 507.19 nm 19716.cm-1
f=0.0001
158 →159 97.42 % 0→0

Excited State: 5
2.8987 eV 427.72 nm 23380.cm-1
f=0.0020
155 →159 4.06 % -3→0
156 →159 93.83 % -2→0

Excited State: 8
3.2093 eV 386.33 nm 25885.cm-1
f=0.0978
155 →159 76.96 % -3→0
156 →159 4.41 % -2→0
157 →159 16.29 % -1→0

Excited State: 10
3.2443 eV 382.16 nm 26167.cm-1
f=0.0218
155 →159 16.54 % -3→0
157 →159 82.11 % -1→0

Excited State: 13
3.5614 eV 348.13 nm 28725.cm-1
f=0.0007
154 →159 97.61 % -4→0

Excited State: 16
3.6992 eV 335.17 nm 29836.cm-1
f=0.0005
158 →160 95.02 % 0→1

Excited State: 20
3.7580 eV 329.92 nm 30310.cm-1
f=0.0685
158 →161 90.29 % 0→2

Excited State: 22
3.7916 eV 327.00 nm 30581.cm-1
f=0.0015
153 →159 96.35 % -5→0

Excited State: 24
3.9344 eV 315.13 nm 31733.cm-1
f=0.0242
158 →162 90.99 % 0→3

Excited State: 25
3.9536 eV 313.60 nm 31888.cm-1
f=0.0140
152 →159 6.35 % -6→0
156 →160 87.93 % -2→1

Excited State: 26
3.9751 eV 311.90 nm 32062.cm-1
f=0.0317
155 →160 4.00 % -3→1
156 →161 84.70 % -2→2
156 →164 2.43 % -2→5

Excited State: 27
4.0307 eV 307.60 nm 32510.cm-1
f=0.0089
149 →159 2.90 % -9→0
150 →159 3.51 % -8→0
151 →159 7.97 % -7→0
152 →159 34.40 % -6→0
155 →160 38.77 % -3→1
156 →160 7.23 % -2→1

Excited State: 28
4.1512 eV 298.67 nm 33482.cm-1
f=0.0357
149 →159 4.25 % -9→0
151 →159 26.17 % -7→0
152 →159 10.69 % -6→0
155 →160 40.66 % -3→1
156 →161 4.98 % -2→2
157 →160 4.85 % -1→1

Excited State: 29
4.1928 eV 295.71 nm 33817.cm-1
f=0.0053
151 →159 2.34 % -7→0
155 →160 3.78 % -3→1
157 →160 87.11 % -1→1

Excited State: 30
4.2138 eV 294.23 nm 33987.cm-1
f=0.0201
154 →161 3.30 % -4→2
155 →161 32.91 % -3→2
157 →160 2.75 % -1→1
157 →161 47.69 % -1→2

>>>> Triplet states <<<<

eV	nm	cm-1	f
2.4137;	513.66;	19468.1;	0.0000
2.6080;	475.40;	21034.9;	0.0000
2.8977;	427.88;	23371.0;	0.0000
3.1246;	396.80;	25201.6;	0.0000
3.1483;	393.82;	25392.3;	0.0000
3.2289;	383.99;	26042.3;	0.0000
3.2896;	376.90;	26532.2;	0.0000
3.5569;	348.57;	28688.6;	0.0000
3.6455;	340.10;	29403.1;	0.0000
3.6624;	338.53;	29539.5;	0.0000
3.7038;	334.75;	29873.0;	0.0000
3.7445;	331.11;	30201.4;	0.0000
3.7518;	330.47;	30259.9;	0.0000
3.7801;	327.99;	30488.7;	0.0000
3.8273;	323.94;	30869.9;	0.0000

Excited State: 1
2.4137 eV 513.66 nm 19468.cm-1
f=0.0000
158 →159 97.02 % 0→0

Excited State: 3
2.6080 eV 475.40 nm 21035.cm-1
f=0.0000
151 →159 5.48 % -7→0
152 →159 11.76 % -6→0
155 →159 4.15 % -3→0
156 →159 72.07 % -2→0

Excited State: 4
2.8977 eV 427.88 nm 23371.cm-1
f=0.0000
155 →159 91.26 % -3→0
156 →159 3.59 % -2→0

Excited State: 6
3.1246 eV 396.80 nm 25202.cm-1
f=0.0000
153 →161 2.92 % -5→2
153 →165 2.92 % -5→6
154 →161 11.22 % -4→2

157 →161 10.79 % -1→2
157 →162 12.05 % -1→3
158 →161 31.71 % 0→2
158 →162 4.80 % 0→3
158 →164 5.28 % 0→5

Excited State: 7
3.1483 eV 393.82 nm 25392.cm-1
f=0.0000
153 →161 2.01 % -5→2
153 →164 3.87 % -5→5
154 →162 9.50 % -4→3
154 →165 2.14 % -4→6
157 →159 2.02 % -1→0
157 →161 16.00 % -1→2
157 →162 11.87 % -1→3
158 →162 28.96 % 0→3
158 →165 6.82 % 0→6

Excited State: 9
3.2289 eV 383.99 nm 26042.cm-1
f=0.0000
152 →159 2.41 % -6→0
156 →159 3.26 % -2→0
157 →159 88.09 % -1→0

Excited State: 11
3.2896 eV 376.90 nm 26532.cm-1
f=0.0000
148 →159 7.07 % -10→0
150 →159 3.97 % -8→0
151 →159 21.61 % -7→0
152 →159 30.53 % -6→0
156 →159 17.82 % -2→0
157 →159 6.61 % -1→0

Excited State: 12
3.5569 eV 348.57 nm 28689.cm-1
f=0.0000
152 →162 4.22 % -6→3
155 →160 4.71 % -3→1
155 →161 7.65 % -3→2

154 →159 96.25 % -4→0

Excited State: 14
3.6455 eV 340.10 nm 29403.cm-1
f=0.0000
153 →161 4.87 % -5→2
153 →164 4.81 % -5→5
154 →161 3.27 % -4→2
155 →160 5.60 % -3→1
158 →160 33.06 % 0→1
158 →161 22.06 % 0→2
158 →164 3.24 % 0→5

Excited State: 15
3.6624 eV 338.53 nm 29539.cm-1
f=0.0000
144 →160 4.94 % -14→1
145 →160 2.90 % -13→1
150 →160 4.18 % -8→1
151 →160 4.20 % -7→1
152 →159 2.89 % -6→0
152 →160 9.18 % -6→1
153 →159 2.36 % -5→0
153 →161 2.13 % -5→2
155 →160 32.21 % -3→1
156 →162 4.89 % -2→3
158 →161 4.98 % 0→2

Excited State: 17
3.7038 eV 334.75 nm 29873.cm-1
f=0.0000
153 →159 2.32 % -5→0
153 →162 2.18 % -5→3
153 →165 3.05 % -5→6
154 →161 3.74 % -4→2
154 →162 2.79 % -4→3
154 →164 2.23 % -4→5
158 →160 45.25 % 0→1
158 →161 14.48 % 0→2
155 →162 2.88 % -3→3
156 →161 2.25 % -2→2
156 →162 40.00 % -2→3

158 →162 4.19 % 0→3
158 →164 2.01 % 0→5

Excited State: 18
3.7445 eV 331.11 nm 30201.cm-1
f=0.0000
153 →164 4.96 % -5→5
154 →162 6.12 % -4→3
154 →165 4.50 % -4→6
155 →161 8.38 % -3→2
156 →162 9.32 % -2→3
158 →160 9.44 % 0→1
158 →162 30.23 % 0→3
158 →165 6.34 % 0→6

Excited State: 19
3.7518 eV 330.47 nm 30260.cm-1
f=0.0000
145 →161 2.11 % -13→2
150 →161 2.25 % -8→2
153 →159 2.75 % -5→0
153 →161 2.49 % -5→2
155 →161 30.28 % -3→2
155 →162 5.02 % -3→3
156 →161 31.32 % -2→2
158 →161 4.22 % 0→2

Excited State: 21
3.7801 eV 327.99 nm 30489.cm-1
f=0.0000
153 →159 84.67 % -5→0
158 →160 5.49 % 0→1

Excited State: 23
3.8273 eV 323.94 nm 30870.cm-1
f=0.0000

158 →162 9.41 % 0→3

8a-PF_6^- Pyridineimine side .

07016_Ir_2PhPzol_PyImminoiPr_PF6_SDD_D95d_M06_DC M_TD15.out
HOMO is orbital 158 and LUMO is orbital 159

>>>>Singletstates<<<<
eV nm cm-1 f
2.6701 464.35 21535.5 0.0009
3.1225 397.07 25184.5 0.0014
3.4088 363.72 27493.7 0.1174
3.5062 353.62 28278.9 0.0019
3.749 330.72 30237.1 0.0772
3.8374 323.1 30950.2 0.0011
3.8396 322.91 30968.4 0.0031
3.9427 314.46 31800.5 0.011
3.998 310.11 32246.6 0.002
4.0505 306.09 32670.1 0.0621
4.196 295.48 33843.2 0.0108
4.2369 292.63 34172.8 0.0258
4.3061 287.92 34731.9 0.0307
4.3302 286.32 34926.0 0.0246
4.4073 281.32 35546.7 0.0200

ExcitedState:2
158 →15997.46 % 0 →0

ExcitedState:5
156 →15995.44 % -2 →0

ExcitedState:8
155 →15993.73 % -3 →0

ExcitedState:11
157 →15995.68 % -1 →0

ExcitedState:15
158 →16192.24 % 0 →2

ExcitedState:18
154 →15966.05 % -4 →0
158 →16023 % 0 →1
158 →1627.91 % 0 →3

ExcitedState:19
154 →15931.44 % -4 →0
158 →16041.09 % 0 →1
158 →16223.8 % 0 →3

ExcitedState:21
3.9427eV314.46nm31801.cm-1f0.011
158 →16033.12 % 0 →1
158 →16260.99 % 0 →3

ExcitedState:24
151 →1592.75 % -7 →0
152 →1593.15 % -6 →0
153 →15991.91 % -5 →0

ExcitedState:25
156 →16186.66 % -2 →2
156 →1642.44 % -2 →5

ExcitedState:26
151 →1599.86 % -7 →0
152 →15942.09 % -6 →0
153 →1594.57 % -5 →0
156 →16034.78 % -2 →1

ExcitedState:27
151 →15910.22 % -7 →0
152 →15917.85 % -6 →0
155 →1602.42 % -3 →1
155 →1615.49 % -3 →2
156 →16037.14 % -2 →1
156 →16216.78 % -2 →3

ExcitedState:28
155 →1605.33 % -3 →1
155 →16144.97 % -3 →2
156 →1627.6 % -2 →3
157 →16123.37 % -1 →2
158 →1653.62 % 0 →6

ExcitedState:29
151 →1596.04 % -7 →0
155 →16115.74 % -3 →2
156 →16018.9 % -2 →1
156 →16247.51 % -2 →3
157 →1622.48 % -1 →3

ExcitedState:30
151 →1595.3 % -7 →0
155 →16047.56 % -3 →1
155 →16220.59 % -3 →3
157 →1612.32 % -1 →2
157 →1628.56 % -1 →3

>>>>Triplet states<<<<
eV nm cm-1 f
2.60 41 476.11 21003.5 0
2.7693 447.71 22335.9 0
3.0852 401.87 24883.7 0
3.1303 396.08 25247.4 0
3.1543 393.07 25440.8 0
3.4129 363.28 27527 0
3.4953 354.71 28192 0
3.6518 339.52 29453.3 0
3.6936 335.68 29790.3 0
3.7478 330.82 30227.9 0
3.787 5327.3 530548.30
3.835 323.3 309310
3.892 6318.5 131396.20
3.962 4312.9 31959.10
3.965 7312.6 431985.70

ExcitedState:1
152 →159 5.86 % -6 →0
155 →159 2.13 % -3 →0
156 →159 12.24 % -2 →0
158 →159 74.4 % 0 →0

ExcitedState:3
151 →1594.37 % -7 →0
152 →15912.19 % -6 →0
155 →1597.83 % -3 →0
156 →15944.21 % -2 →0
158 →15922.83 % 0 →0

ExcitedState:4
155 →15982.45 % -3 →0
156 →15910.67 % -2 →0

ExcitedState:6
153 →1622.06 % -5 →3
153 →1653.86 % -5 →6
154 →16111.98 % -4 →2
157 →16219.92 % -1 →3
158 →16136.79 % 0 →2
158 →1646.04 % 0 →5

ExcitedState:7
153 →1612.68 % -5 →2
153 →1644.96 % -5 →5
154 →16211.1 % -4 →3
157 →16127.16 % -1 →2
158 →1602.71 % 0 →1
158 →16225.63 % 0 →3
158 →1656.67 % 0 →6

ExcitedState:9
148 →1593.56 % -10 →0
151 →15910.81 % -7 →0
152 →15937.16 % -6 →0
152 →1603.59 % -6 →1
155 →1602.33 % -3 →1
156 →15927.48 % -2 →0

ExcitedState:10
156 →1592.35 % -2 →0
157 →15994.4 % -1 →0

ExcitedState:12
153 →1612.68 % -5 →2
153 →1625.1 % -5 →3
153 →1657.5 % -5 →6
154 →16110.87 % -4 →2
154 →1644.1 % -4 →5
158 →16142.87 % 0 →2
158 →1648.61 % 0 →5

ExcitedState:13
153 →1614.34-5 →2

153 →1649.79-5 →5
154 →1626.68-4 →3
154 →1652.73-4 →6
158 →16013.580 →1
158 →16232.460 →3
158 →1656.710 →6

ExcitedState:14
145 →1612.07-13 →2
152 →1612.68-6 →2
155 →1616.23-3 →2
155 →16210.09-3 →3
156 →16153.09-2 →2
156 →1622.07-2 →3

ExcitedState:16
150 →1622.89-8 →3
155 →16119.82-3 →2
155 →16213.54-3 →3
156 →1603.4-2 →1
156 →16231.77-2 →3
158 →1602.720 →1

ExcitedState:17
154 →15995.5-4 →0

ExcitedState:20

158 →16071.770 →1
158 →16215.330 →3

ExcitedState:22
152 →1593.93-6 →0
153 →1593.6-5 →0
153 →1622.23-5 →3
154 →16110.95-4 →2
155 →1604.31-3 →1
157 →16211.18-1 →3
157 →1655.77-1 →6
158 →1602.210 →1
158 →16433.840 →5
158 →1652.050 →6

ExcitedState:23
146 →1602.34 -12 →1
150 →1603.65 -8 →1
151 →1594.79 -7 →0
152 →15916.01 -6 →0
152 →1606.51 -6 →1
153 →15921.17 -5 →0
154 →1612.82 -4 →2
155 →16011.56 -3 →1
157 →1622.29 -1 →3
158 →1648.68 0 → 5

Electronic Supplementary Material (ESI) for Dalton Transactions
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8a "free" cation in DCM

07016_Ir_2PhPyzol_PyImminoiPr_SDD_D95d_M06_DCM_TD46.out
HOMO is orbital 123 and LUMO is orbital 124

>>>> Singlet states <<<<

eV	nm	cm-1	f
2.4927;	497.40;	20104.5;	0.0001
2.9373;	422.10;	23691.1;	0.0002
3.2566;	380.71;	26266.7;	0.0769
3.2709;	379.05;	26381.7;	0.0397
3.6101;	343.44;	29117.2;	0.0006
3.7441;	331.15;	30197.8;	0.0006
3.7833;	327.71;	30514.8;	0.0823
3.8197;	324.59;	30808.1;	0.0010
3.9344;	315.13;	31732.9;	0.0084
4.2363;	292.67;	34168.2;	0.0174
4.3226;	286.83;	34863.9;	0.0585
4.3805;	283.04;	35330.7;	0.0065
4.4163;	280.74;	35620.1;	0.0190
4.4385;	279.34;	35798.7;	0.0556
4.4728;	277.20;	36075.0;	0.0196
4.4837;	276.52;	36163.7;	0.0607
4.5350;	273.40;	36576.4;	0.0091
4.5502;	272.48;	36699.9;	0.0397
4.5620;	271.78;	36794.5;	0.0322
4.5700;	271.30;	36859.6;	0.0323
4.6457;	266.88;	37470.0;	0.1806
4.6972;	263.95;	37886.0;	0.0397
4.7196;	262.70;	38066.2;	0.1276
4.7581;	260.58;	38375.9;	0.0122
4.7735;	259.73;	38501.5;	0.0141
4.7794;	259.42;	38547.5;	0.0649
4.7971;	258.46;	38690.7;	0.0106
4.8387;	256.23;	39027.4;	0.2195
4.8807;	254.03;	39365.4;	0.0207
4.9652;	249.71;	40046.5;	0.0009
5.0054;	247.70;	40371.4;	0.0050
5.0159;	247.18;	40456.3;	0.0113
5.1014;	243.04;	41145.5;	0.0243
5.1062;	242.81;	41184.5;	0.0124
5.1622;	240.17;	41637.2;	0.0122
5.1872;	239.02;	41837.5;	0.0704
5.2494;	236.19;	42338.8;	0.0028
5.2732;	235.12;	42531.5;	0.1132
5.3003;	233.92;	42749.7;	0.0301
5.3199;	233.06;	42907.4;	0.0063
5.3493;	231.78;	43144.4;	0.0116
5.3623;	231.22;	43248.9;	0.0957
5.3921;	229.94;	43489.6;	0.1330
5.4048;	229.40;	43592.0;	0.0162
5.4652;	226.86;	44080.0;	0.0076
5.4920;	225.75;	44296.8;	0.0294

1 1 Excited State: Singlet
2.4927 eV 497.40 nm
20105.cm-1 f=0.0001
123→124 0.69777 97.38 % 0 → 0

2 2 Excited State: Singlet
2.9373 eV 422.10 nm
23691.cm-1 f=0.0002
121 →124 0.69837 97.54 % -2 → 0

3 3 Excited State: Singlet
3.2566 eV 380.71 nm
26267.cm-1 f=0.0769
120 →124 0.57898 67.04 % -3 → 0
122 →124 -0.39299 30.89 % -1 → 0

4 4 Excited State: Singlet
3.2709 eV 379.05 nm
26382.cm-1 f=0.0397
120 →124 0.38861 30.20 % -3 → 0
122 →124 0.58040 67.37 % -1 → 0

5 5 Excited State: Singlet
3.6101 eV 343.44 nm
29117.cm-1 f=0.0006
119 →124 0.69611 96.91 % -4 → 0

6 6 Excited State: Singlet
3.7441 eV 331.15 nm
30198.cm-1 f=0.0006
123 →125 0.68321 93.36 % 0 → 1

7 7 Excited State: Singlet
3.7833 eV 327.71 nm
30515.cm-1 f=0.0823
123 →126 0.67473 91.05 % 0 → 2

8 8 Excited State: Singlet
3.8197 eV 324.59 nm
30808.cm-1 f=0.0010
118 →124 0.69136 95.60 % -5 → 0

9 9 Excited State: Singlet
3.9344 eV 315.13 nm
31733.cm-1 f=0.0084
122 →126 -0.10224 2.09 % -1 → 2
123 →125 -0.10674 2.28 % 0 → 1
123 →127 0.66943 89.63 % 0 → 3

10 10 Excited State: Singlet
4.2363 eV 292.67 nm
34168.cm-1 f=0.0174
117 →124 0.19673 7.74 % -6 → 0
121 →125 0.65812 86.62 % -2 → 1

11 11 Excited State: Singlet
4.3226 eV 286.83 nm
34864.cm-1 f=0.0585
120 →125 -0.12702 3.23 % -3 → 1
121 →126 0.63145 79.75 % -2 → 2
121 →129 -0.11121 2.47 % -2 → 5
122 →126 0.14101 3.98 % -1 → 2
122 →127 0.11914 2.84 % -1 → 3

12 12 Excited State: Singlet
4.3805 eV 283.04 nm
35331.cm-1 f=0.0065
117 →124 0.23565 11.11 % -6 → 0
120 →125 0.61671 76.07 % -3 → 1
121 →125 -0.12134 2.94 % -2 → 1
121 →126 0.14077 3.96 % -2 → 2

13 13 Excited State: Singlet
4.4163 eV 280.74 nm
35620.cm-1 f=0.0190
121 →126 -0.11481 2.64 % -2 → 2
122 →125 0.65023 84.56 % -1 → 1
122 →126 0.14124 3.99 % -1 → 2

14 14 Excited State: Singlet
4.4385 eV 279.34 nm
35799.cm-1 f=0.0556
117 →124 -0.12888 3.32 % -6 → 0
120 →126 -0.15875 5.04 % -3 → 2
121 →127 -0.29487 17.39 % -2 → 3
122 →125 0.19708 7.77 % -1 → 1
122 →126 -0.51957 53.99 % -1 → 2
123 →127 -0.12289 3.02 % 0 → 3

15 15 Excited State: Singlet

4.4728 eV 277.20 nm
36075.cm-1 f=0.0196
116 →124 -0.19554 7.65 % -7 → 0
117 →124 -0.18856 7.11 % -6 → 0
120 →125 0.10390 2.16 % -3 → 1
120 →126 0.35327 24.96 % -3 → 2
121 →127 -0.42929 36.86 % -2 → 3
122 →126 0.19643 7.72 % -1 → 2

16 16 Excited State: Singlet
4.4837 eV 276.52 nm
36164.cm-1 f=0.0607
114 →124 0.16167 5.23 % -9 → 0
115 →124 0.13469 3.63 % -8 → 0
116 →124 -0.29748 17.70 % -7 → 0
117 →124 -0.36388 26.48 % -6 → 0
120 →125 0.19566 7.66 % -3 → 1
120 →126 -0.24921 12.42 % -3 → 2
121 →125 0.10060 2.02 % -2 → 1
121 →127 0.27273 14.88 % -2 → 3

17 17 Excited State: Singlet
4.5350 eV 273.40 nm
36576.cm-1 f=0.0091
116 →124 -0.10373 2.15 % -7 → 0
120 →126 0.38091 29.02 % -3 → 2
120 →127 -0.14399 4.15 % -3 → 3
121 →127 0.26642 14.20 % -2 → 3
121 →132 -0.11452 2.62 % -2 → 8
122 →126 -0.26092 13.62 % -1 → 2
123 →129 -0.16488 5.44 % 0 → 5
123 →130 -0.21323 9.09 % 0 → 6

18 18 Excited State: Singlet
4.5502 eV 272.48 nm
36700.cm-1 f=0.0397
116 →124 0.12133 2.94 % -7 → 0
119 →126 0.16643 5.54 % -4 → 2
120 →126 0.15357 4.72 % -3 → 2
120 →127 0.38038 28.94 % -3 → 3
122 →126 -0.15241 4.65 % -1 → 2
122 →127 0.40514 32.83 % -1 → 3
123 →129 0.16119 5.20 % 0 → 5

19 19 Excited State: Singlet
4.5620 eV 271.78 nm
36794.cm-1 f=0.0322
114 →124 -0.20233 8.19 % -9 → 0
116 →124 -0.12110 2.93 % -7 → 0
118 →127 0.13668 3.74 % -5 → 3
120 →127 0.15993 5.12 % -3 → 3
122 →127 0.23016 10.59 % -1 → 3
123 →128 0.13712 3.76 % 0 → 4
123 →129 -0.46372 43.01 % 0 → 5
123 →138 -0.10852 2.36 % 0 →14

20 20 Excited State: Singlet
4.5700 eV 271.30 nm
36860.cm-1 f=0.0323
114 →124 -0.40528 32.85 % -9 → 0
115 →124 0.13976 3.91 % -8 → 0
116 →124 -0.40611 32.99 % -7 → 0
117 →124 0.14882 4.43 % -6 → 0
123 →129 0.24399 11.91 % 0 → 5

21 21 Excited State: Singlet
4.6457 eV 266.88 nm
37470.cm-1 f=0.1806
114 →124 0.21482 9.23 % -9 → 0
116 →124 -0.10219 2.09 % -7 → 0
117 →124 0.12704 3.23 % -6 → 0
120 →127 -0.43102 37.16 % -3 → 3
122 →127 0.42493 36.11 % -1 → 3

22 22 Excited State: Singlet
4.6972 eV 263.95 nm
37886.cm-1 f=0.0397
114 →124 0.19689 7.75 % -9 → 0
116 →124 -0.12834 3.29 % -7 → 0
117 →124 0.12187 2.97 % -6 → 0
118 →126 0.11273 2.54 % -5 → 2
120 →126 0.17680 6.25 % -3 → 2
120 →127 0.16057 5.16 % -3 → 3
123 →128 -0.30841 19.02 % 0 → 4
123 →129 -0.15775 4.98 % 0 → 5
123 →130 0.21252 9.03 % 0 → 6
123 →132 -0.32011 20.49 % 0 → 8
123 →134 0.14921 4.45 % 0 →10

23 23 Excited State: Singlet
4.7196 eV 262.70 nm
38066.cm-1 f=0.1276
114 →124 0.31742 20.15 % -9 → 0
115 →124 0.16136 5.21 % -8 → 0
116 →124 -0.16271 5.29 % -7 → 0
117 →124 0.33601 22.58 % -6 → 0
120 →125 -0.14548 4.23 % -3 → 1
120 →127 0.14457 4.18 % -3 → 3
122 →127 -0.15372 4.73 % -1 → 3
123 →128 0.26997 14.58 % 0 → 4
123 →132 0.13239 3.51 % 0 → 8

24 24 Excited State: Singlet
4.7581 eV 260.58 nm
38376.cm-1 f=0.0122
115 →124 0.26648 14.20 % -8 → 0
118 →125 -0.17021 5.79 % -5 → 1
118 →126 -0.13852 3.84 % -5 → 2
119 →125 0.49190 48.39 % -4 → 1
119 →127 0.18169 6.60 % -4 → 3
123 →128 -0.17713 6.28 % 0 → 4
123 →130 -0.11195 2.51 % 0 → 6

25 25 Excited State: Singlet
4.7735 eV 259.73 nm
38502.cm-1 f=0.0141
115 →124 0.21408 9.17 % -8 → 0
118 →125 0.11966 2.86 % -5 → 1
119 →125 -0.30866 19.05 % -4 → 1
119 →126 -0.16427 5.40 % -4 → 2
123 →128 -0.39489 31.19 % 0 → 4
123 →130 -0.16591 5.51 % 0 → 6
123 →132 0.24794 12.29 % 0 → 8

26 26 Excited State: Singlet
4.7794 eV 259.42 nm
38548.cm-1 f=0.0649
115 →124 -0.49635 49.27 % -8 → 0
116 →124 -0.23152 10.72 % -7 → 0
118 →126 -0.17877 6.39 % -5 → 2
119 →127 0.17358 6.03 % -4 → 3
123 →128 -0.20142 8.11 % 0 → 4
123 →130 -0.13223 3.50 % 0 → 6

27 27 Excited State: Singlet
4.7971 eV 258.46 nm
38691.cm-1 f=0.0106
118 →126 0.27766 15.42 % -5 → 2
119 →125 0.28653 16.42 % -4 → 1
119 →127 -0.24272 11.78 % -4 → 3
121 →132 -0.25895 13.41 % -2 → 8
121 →134 0.13277 3.53 % -2 →10
122 →129 0.14440 4.17 % -1 → 5
123 →128 -0.13859 3.84 % 0 → 4
123 →132 0.24949 12.45 % 0 → 8

28 28 Excited State: Singlet

4.8387 eV 256.23 nm
39027.cm-1 f=0.2195
118 →127 -0.11714 2.74 % -5 → 3
119 →126 0.55242 61.03 % -4 →
2
123 →126 -0.10168 2.07 % 0 → 2
123 →128 -0.18334 6.72 % 0 → 4
123 →129 -0.20598 8.49 % 0 → 5
123 →138 -0.12774 3.26 % 0
→14

29 29 Excited State: Singlet
4.8807 eV 254.03 nm
39365.cm-1 f=0.0207
118 →126 -0.17413 6.06 % -5 → 2
119 →127 0.14623 4.28 % -4 → 3
120 →126 -0.10425 2.17 % -3 → 2
121 →127 -0.13795 3.81 % -2 → 3
121 →130 0.17586 6.19 % -2 → 6
121 →132 -0.45208 40.88 % -2 →
8
121 →134 0.20205 8.16 % -2
→10
123 →132 -0.23062 10.64 % 0 →
8
123 →134 0.10727 2.30 % 0 →10

30 30 Excited State: Singlet
4.9652 eV 249.71 nm
40046.cm-1 f=0.0009
118 →125 0.60896 74.17 % -5 →
1
118 →126 0.11555 2.67 % -5 → 2
118 →127 0.10098 2.04 % -5 → 3
119 →125 0.18857 7.11 % -4 → 1
119 →126 0.13729 3.77 % -4 → 2
119 →127 0.15941 5.08 % -4 → 3

31 31 Excited State: Singlet
5.0054 eV 247.70 nm
40371.cm-1 f=0.0050
120 →127 -0.15431 4.76 % -3 → 3
120 →130 0.20363 8.29 % -3 → 6
120 →132 -0.45731 41.83 % -3 →
8
120 →134 0.23103 10.67 % -3
→10
121 →129 -0.26000 13.52 % -2 →
5
121 →138 -0.13131 3.45 % -2
→14

32 32 Excited State: Singlet
5.0159 eV 247.18 nm
40456.cm-1 f=0.0113
118 →125 -0.23010 10.59 % -5 →
1
118 →126 0.36392 26.49 % -5 →
2
119 →125 -0.11346 2.57 % -4 → 1
119 →126 0.13573 3.68 % -4 → 2
119 →127 0.48392 46.84 % -4 →
3
122 →126 -0.11140 2.48 % -1 → 2

33 33 Excited State: Singlet
5.1014 eV 243.04 nm
41145.cm-1 f=0.0243
112 →124 -0.11524 2.66 % -11 →
0
113 →124 -0.37505 28.13 % -10 →
0
118 →127 0.41786 34.92 % -5 →
3
119 →126 0.14961 4.48 % -4 → 2
119 →127 -0.14668 4.30 % -4 → 3
121 →129 0.10804 2.33 % -2 → 5
122 →130 -0.10950 2.40 % -1 → 6

34 34 Excited State: Singlet
5.1062 eV 242.81 nm
41184.cm-1 f=0.0124
112 →124 0.14529 4.22 % -11 →
0
113 →124 0.45966 42.26 % -10 →
0
114 →124 -0.10783 2.33 % -9 → 0
118 →126 -0.11545 2.67 % -5 → 2
118 →127 0.35736 25.54 % -5 →
3
119 →126 0.12769 3.26 % -4 → 2

35 35 Excited State: Singlet
5.1622 eV 240.17 nm
41637.cm-1 f=0.0122
113 →124 0.20253 8.20 % -10 →
0
120 →127 -0.10643 2.27 % -3 → 3
120 →130 0.18031 6.50 % -3 → 6
120 →132 -0.20151 8.12 % -3 → 8
120 →134 0.10205 2.08 % -3
→10
121 →128 -0.15676 4.91 % -2 → 4
121 →129 0.50121 50.24 % -2 →
5
121 →138 0.12226 2.99 % -2
→14

36 36 Excited State: Singlet
5.1872 eV 239.02 nm
41838.cm-1 f=0.0704
118 →126 -0.13312 3.54 % -5 → 2
122 →129 -0.29166 17.01 % -1 →
5
123 →129 -0.14053 3.95 % 0 → 5
123 →130 0.46353 42.97 % 0 → 6
123 →132 0.22099 9.77 % 0 → 8
123 →134 -0.10721 2.30 % 0
→10
123 →138 0.13210 3.49 % 0 →14

37 37 Excited State: Singlet
5.2494 eV 236.19 nm
42339.cm-1 f=0.0028
110 →124 -0.16066 5.16 % -13 →
0
111 →124 0.19594 7.68 % -12 →
0
112 →124 -0.51790 53.64 % -11 →
0
113 →124 0.19736 7.79 % -10 →
0
117 →125 0.11940 2.85 % -6 → 1
121 →129 -0.14469 4.19 % -2 → 5
123 →131 0.20588 8.48 % 0 → 7

38 38 Excited State: Singlet
5.2732 eV 235.12 nm
42531.cm-1 f=0.1132
118 →127 -0.23421 10.97 % -5 →
3
122 →128 0.42919 36.84 % -1 →
4
123 →129 -0.14264 4.07 % 0 → 5
123 →130 -0.19306 7.45 % 0 → 6
123 →133 -0.22468 10.10 % 0 →
9
123 →135 0.20745 8.61 % 0 →11
123 →136 -0.12166 2.96 % 0
→12
123 →138 0.20103 8.08 % 0 →14

39 39 Excited State: Singlet
5.3003 eV 233.92 nm
42750.cm-1 f=0.0301
118 →127 -0.13528 3.66 % -5 → 3
122 →128 -0.49996 49.99 % -1 →
4
123 →129 -0.14396 4.14 % 0 → 5
123 →131 -0.14393 4.14 % 0 → 7
123 →133 -0.15810 5.00 % 0 → 9
123 →135 0.16792 5.64 % 0 →11
123 →138 0.25901 13.42 % 0
→14

40 40 Excited State: Singlet
5.3199 eV 233.06 nm
42907.cm-1 f=0.0063
120 →126 0.10174 2.07 % -3 → 2
120 →128 -0.16559 5.48 % -3 → 4
120 →129 0.51164 52.36 % -3 →
5
120 →138 0.14076 3.96 % -3
→14
121 →128 -0.28477 16.22 % -2 →
4
121 →129 -0.12606 3.18 % -2 → 5
123 →131 0.13377 3.58 % 0 → 7

41 41 Excited State: Singlet

5.3493 eV 231.78 nm
43144.cm-1 f=0.0116
120 →129 0.27073 14.66 % -3 →
5
121 →128 0.56662 64.21 % -2 →
4
121 →129 0.13932 3.88 % -2 → 5
121 →132 -0.14363 4.13 % -2 → 8
122 →129 0.13536 3.66 % -1 → 5

42 42 Excited State: Singlet
5.3623 eV 231.22 nm
43249.cm-1 f=0.0957
111 →124 -0.12058 2.91 % -12 →
0
123 →136 -0.12166 2.96 % 0
→12
123 →138 0.20103 8.08 % 0 →14

39 39 Excited State: Singlet
5.3003 eV 233.92 nm
42750.cm-1 f=0.0301
118 →127 -0.13528 3.66 % -5 → 3
122 →128 -0.49996 49.99 % -1 →
4
123 →129 -0.14396 4.14 % 0 → 5
123 →131 -0.14393 4.14 % 0 → 7
123 →133 -0.15810 5.00 % 0 → 9
123 →135 0.16792 5.64 % 0 →11
123 →138 0.25901 13.42 % 0
→14

40 40 Excited State: Singlet
5.3199 eV 233.06 nm
42907.cm-1 f=0.0063
120 →126 0.10174 2.07 % -3 → 2
120 →128 -0.16559 5.48 % -3 → 4
120 →129 0.51164 52.36 % -3 →
5
120 →138 0.14076 3.96 % -3
→14
121 →128 -0.28477 16.22 % -2 →
4
121 →129 -0.12606 3.18 % -2 → 5
123 →131 0.13377 3.58 % 0 → 7

41 41 Excited State: Singlet
5.3493 eV 231.78 nm
43144.cm-1 f=0.0116
120 →129 0.27073 14.66 % -3 →
5
121 →128 0.56662 64.21 % -2 →
4
121 →129 0.13932 3.88 % -2 → 5
121 →132 -0.14363 4.13 % -2 → 8
122 →129 0.13536 3.66 % -1 → 5

42 42 Excited State: Singlet
5.3623 eV 231.22 nm
43249.cm-1 f=0.0957
111 →124 -0.12058 2.91 % -12 →
0
117 →125 -0.12101 2.93 % -6 → 1
118 →126 0.17389 6.05 % -5 → 2
120 →129 -0.10439 2.18 % -3 → 5
121 →128 0.17031 5.80 % -2 → 4
121 →130 0.10030 2.01 % -2 → 6
122 →128 -0.16675 5.56 % -1 → 4
122 →129 -0.30243 18.29 % -1 →
5
123 →131 0.40655 33.06 % 0 → 7
123 →137 -0.11732 2.75 % 0
→13

43 43 Excited State: Singlet
5.3921 eV 229.94 nm
43490.cm-1 f=0.1330
112 →124 -0.10360 2.15 % -11 →
0
118 →126 0.21682 9.40 % -5 → 2
122 →129 -0.30138 18.17 % -1 →
5
123 →131 -0.46625 43.48 % 0 →
7
123 →134 0.10774 2.32 % 0 →10
123 →137 -0.12548 3.15 % 0
→13

44 44 Excited State: Singlet
5.4048 eV 229.40 nm
43592.cm-1 f=0.0162
109 →124 0.22987 10.57 % -14 →
0
110 →124 -0.10478 2.20 % -13 →
0
111 →124 0.35438 25.12 % -12 →
0
112 →124 0.35232 24.83 % -11 →
0
115 →124 -0.11994 2.88 % -8 → 0
116 →125 -0.11696 2.74 % -7 → 1
117 →125 0.30455 18.55 % -6 →
1
123 →131 0.10705 2.29 % 0 → 7

45 45 Excited State: Singlet
5.4652 eV 226.86 nm
44080.cm-1 f=0.0076
121 →130 -0.62534 78.21 % -2 →
6
121 →132 -0.19350 7.49 % -2 → 8

46 46 Excited State: Singlet
5.4920 eV 225.75 nm
44297.cm-1 f=0.0294
118 →127 0.17217 5.93 % -5 → 3
119 →129 -0.21844 9.54 % -4 → 5
122 →130 0.44175 39.03 % -1 →
6
123 →129 -0.11014 2.43 % 0 → 5
123 →133 0.22526 10.15 % 0 → 9
123 →135 0.13708 3.76 % 0 →11
123 →136 -0.20152 8.12 % 0
→12
123 →138 0.13194 3.48 % 0 →14

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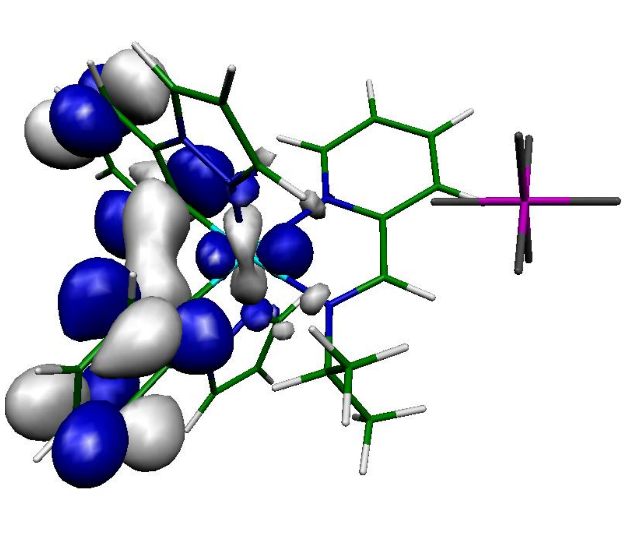
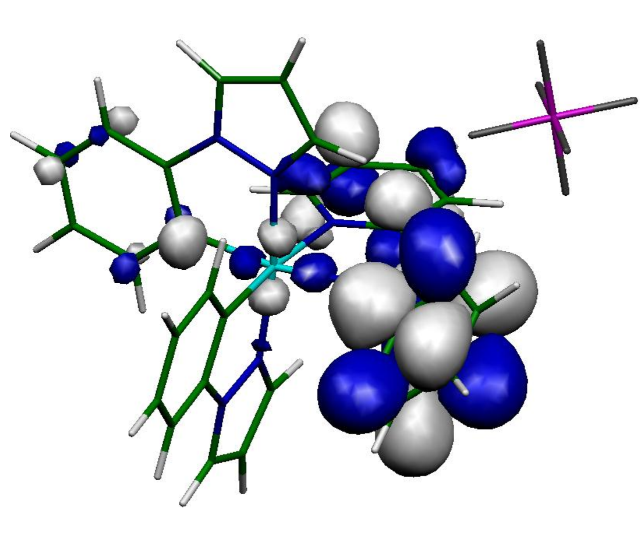
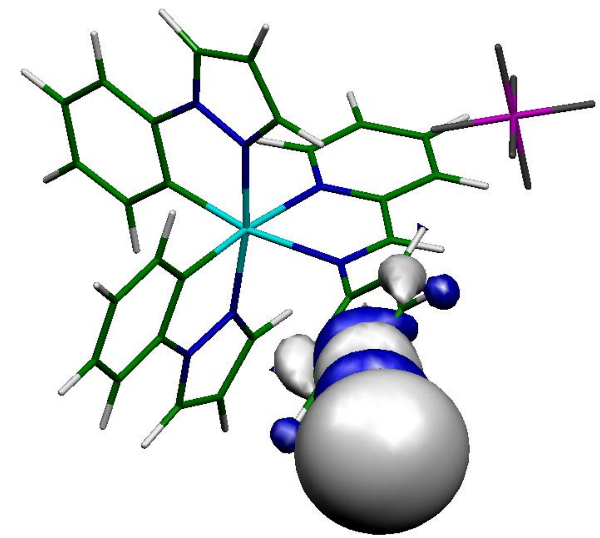
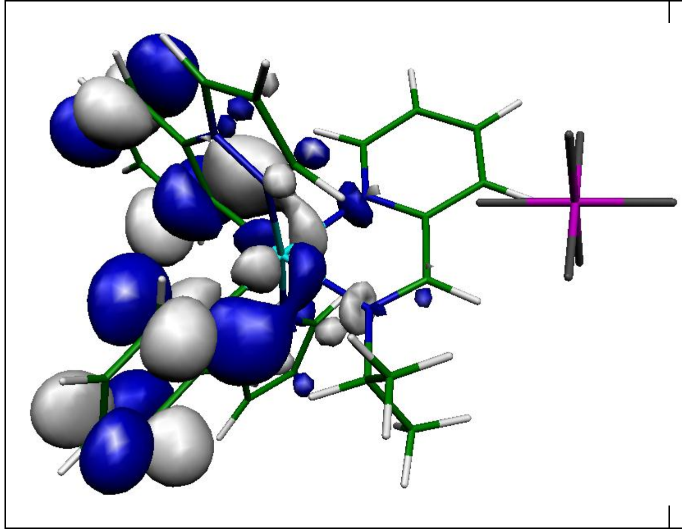
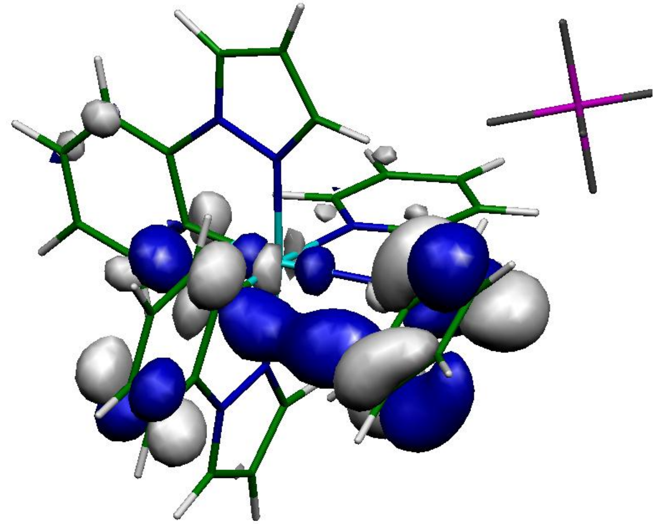
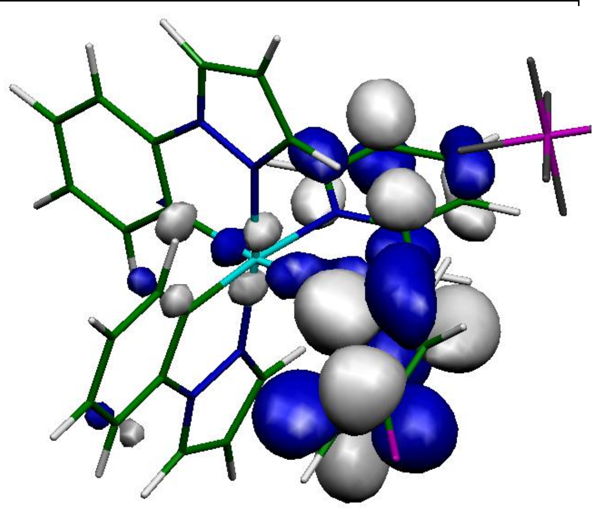
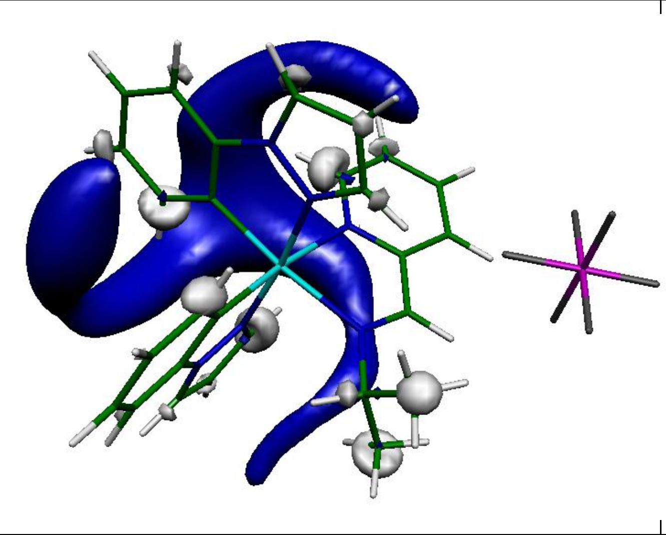
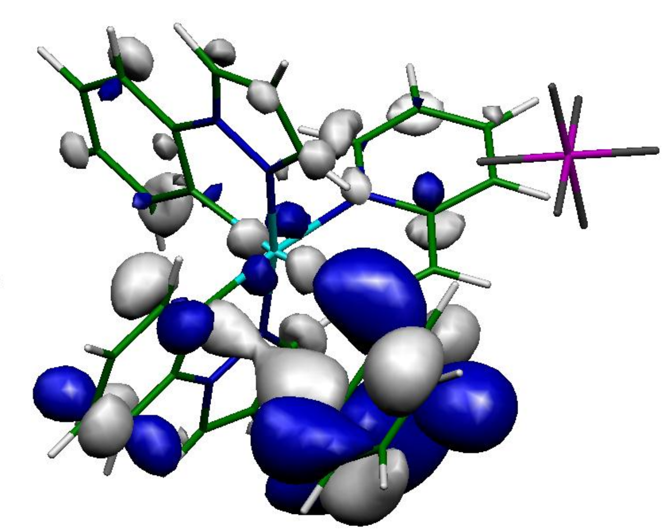
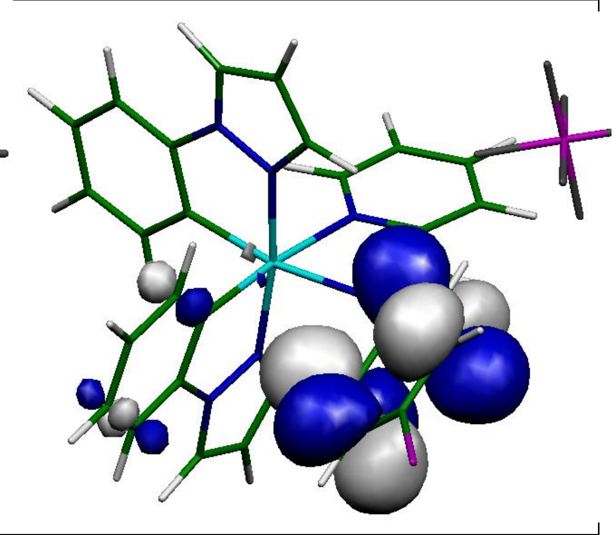
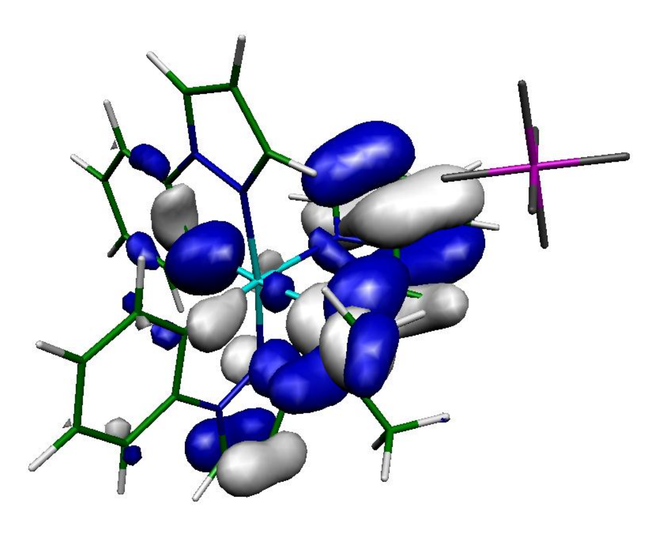
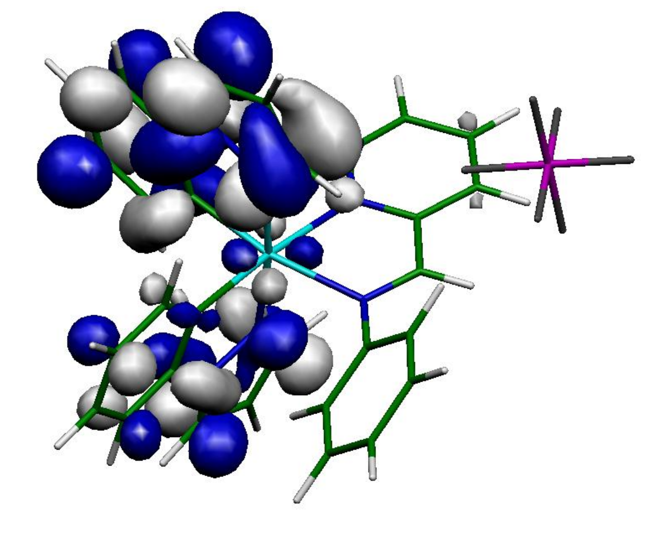
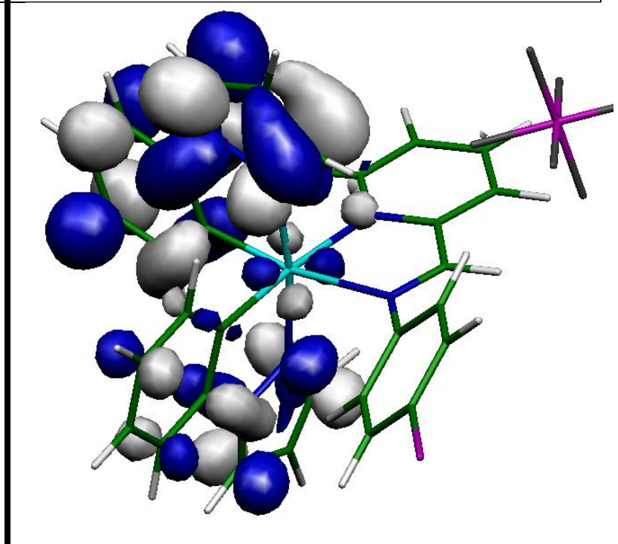
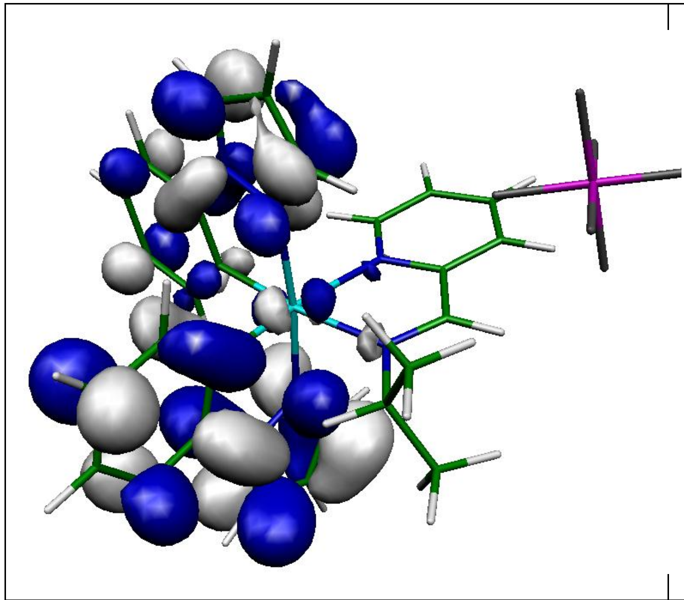
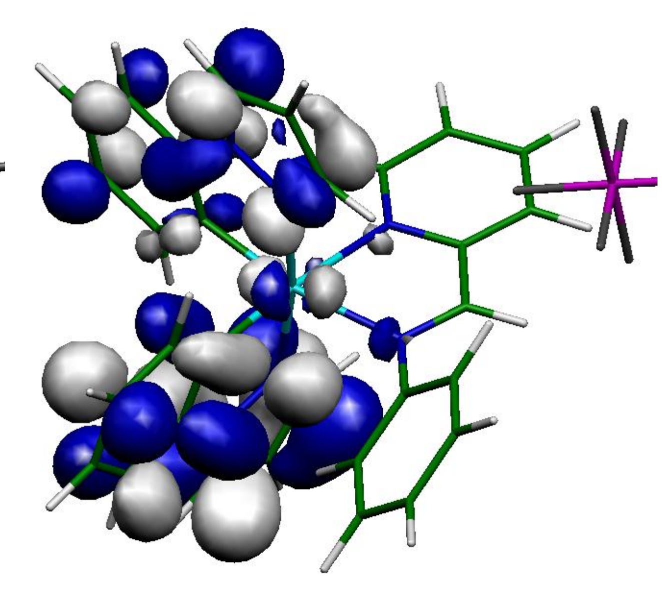
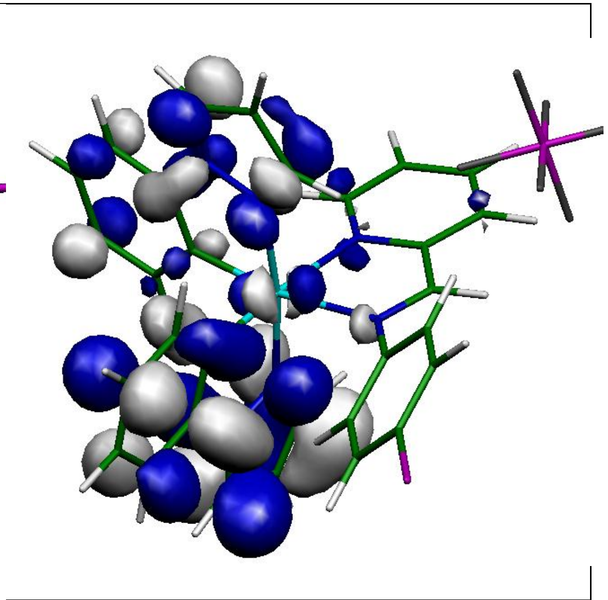
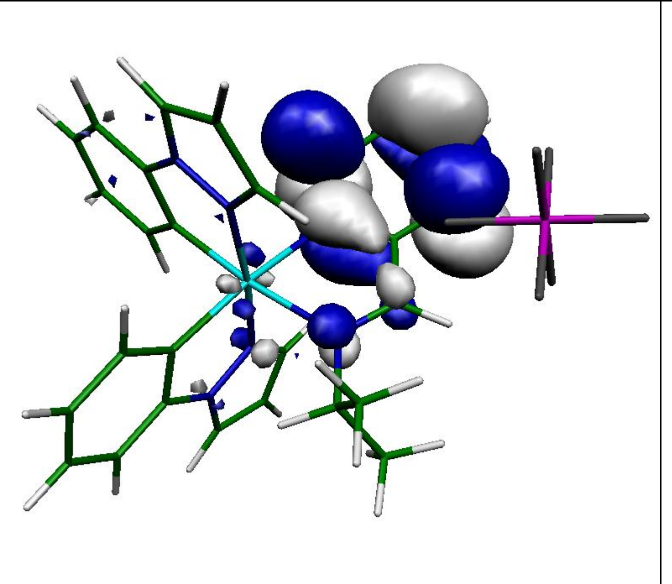
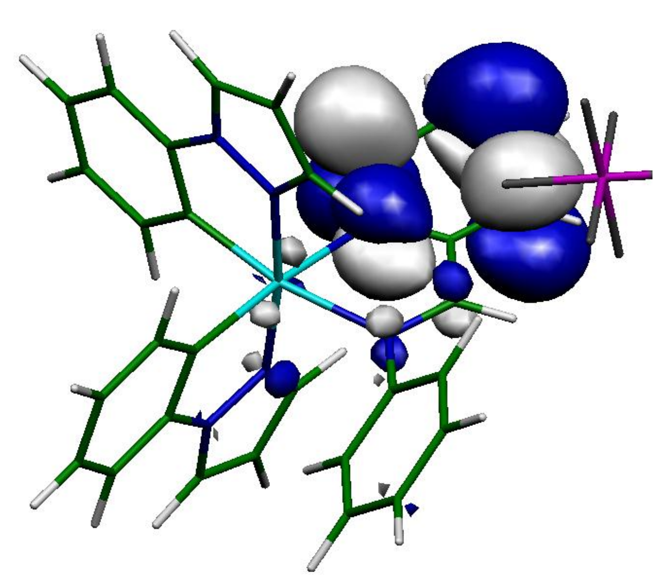
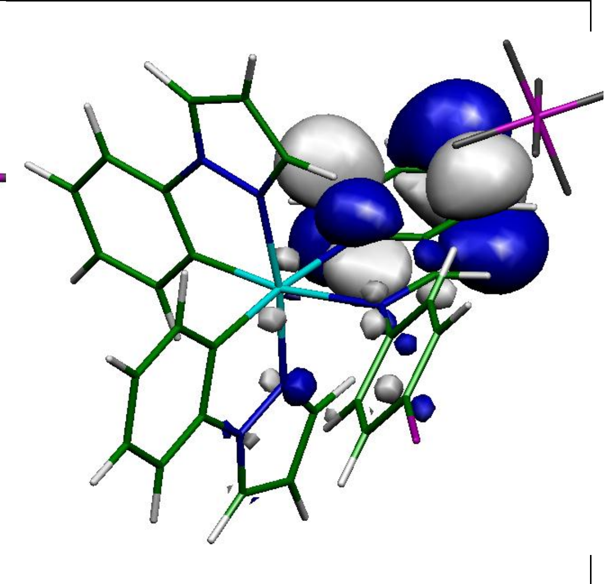
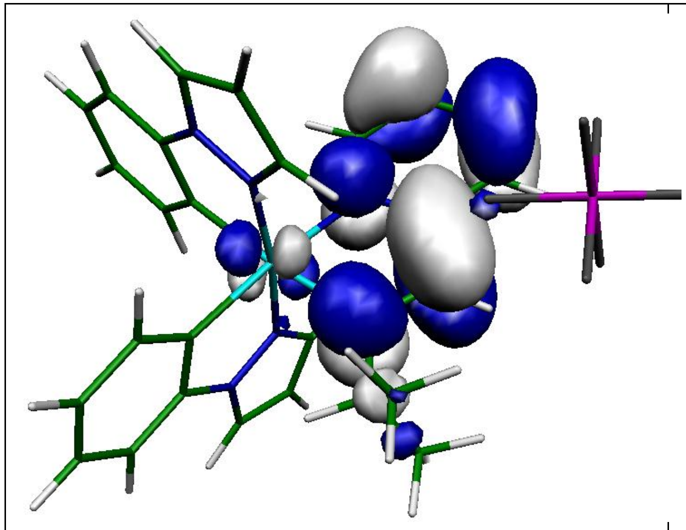
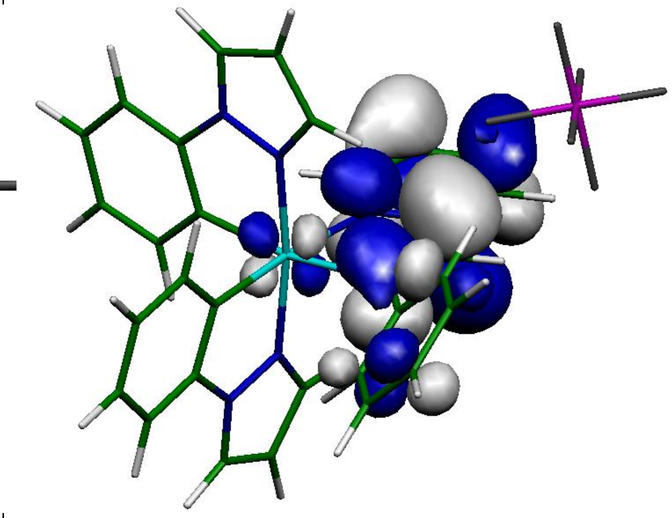
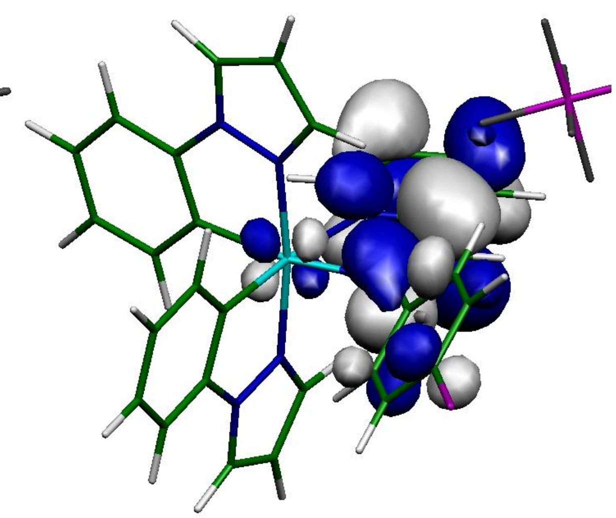
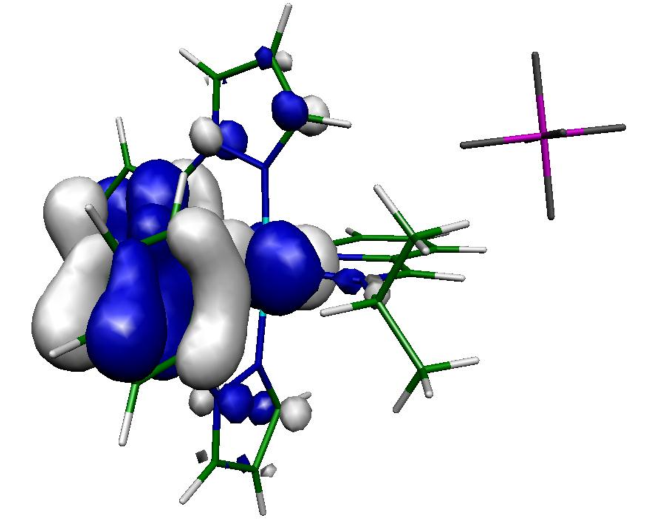
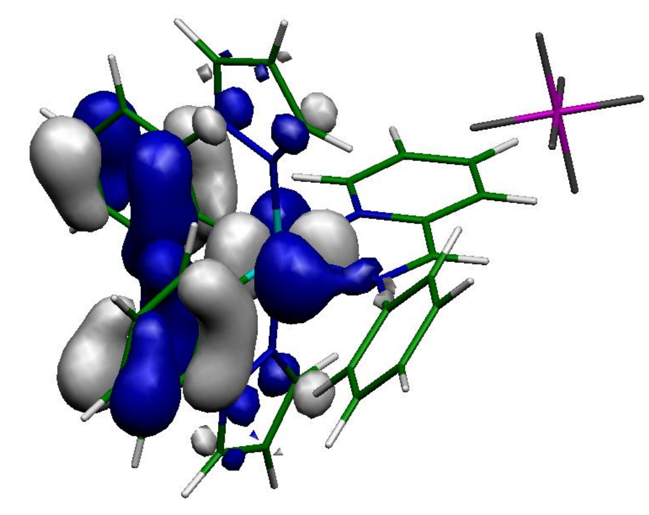
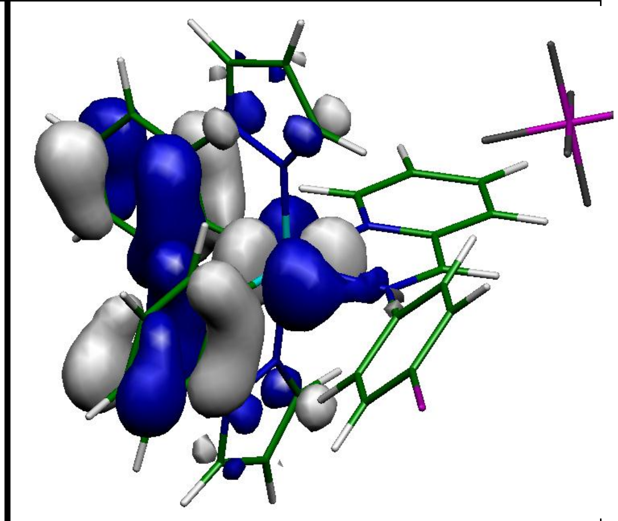
Figure S9 : Most relevant MO's involved in the most intense transitions of: 4a, 5a,8a p-Br, p-H, iPr at /D95(d)/SDD/M06/DCM level of theory

8a (i-Pr)	5a (p-H)	4a (p-Br)
		
MO 165(LUMO+6)	MO 173(LUMO+6)	MO 176(LUMO+6)
		

MO 164 (LUMO+5)	MO 172(LUMO+5)	MO 175(LUMO+5)
		
MO 163 (LUMO+4)	MO 171(LUMO+4)	MO 174(LUMO+4)
		
MO 162 (LUMO+3)	MO 170(LUMO+3)	MO 173(LUMO+3)

		
MO 161 (LUMO+2)	MO 169(LUMO+2)	MO 172(LUMO+2)
		
MO 160 (LUMO+1)	MO 168 (LUMO+1)	MO 171 (LUMO+1)

		
MO 159 (LUMO)	**MO 167 (LUMO)**	**MO 170 (LUMO)**
		
MO 158(HOMO)	**MO 166 (HOMO)**	**MO 169 (HOMO)**

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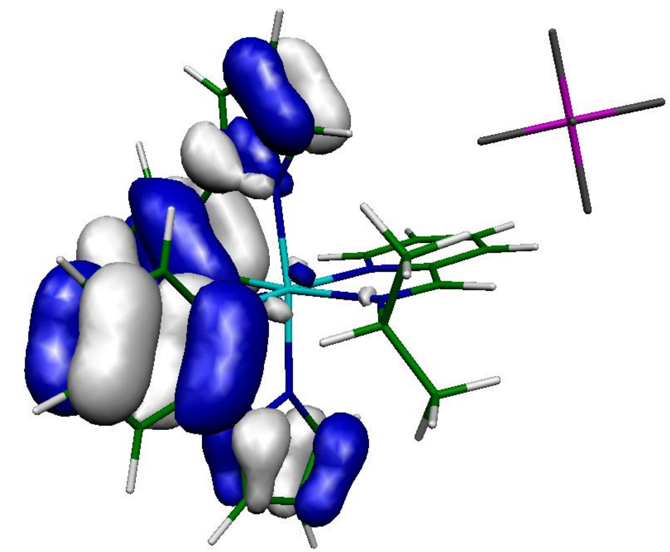
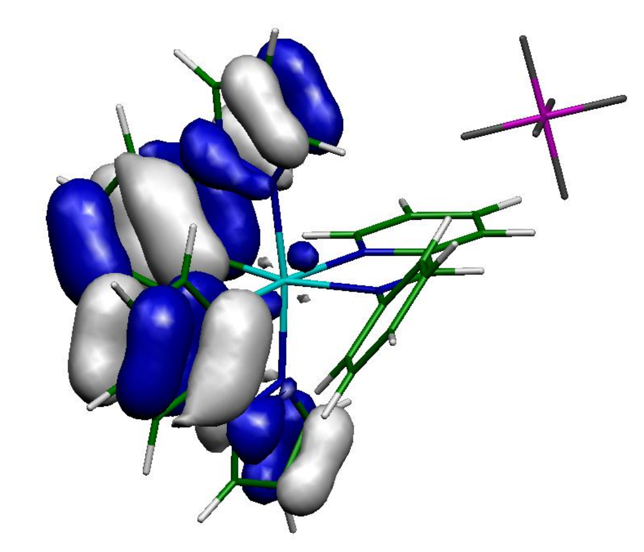
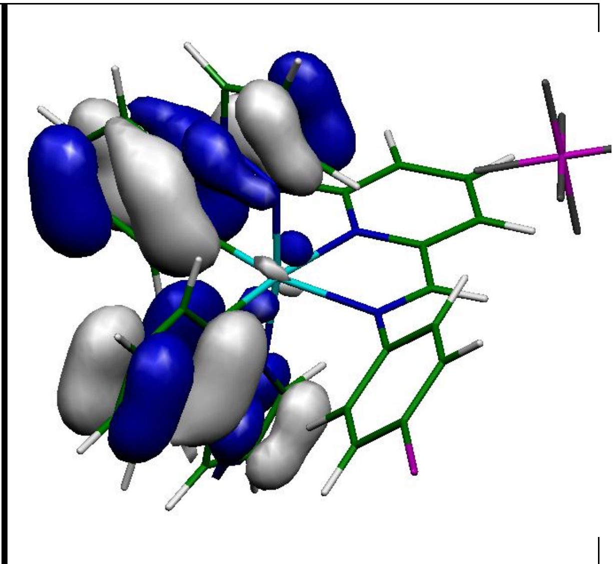
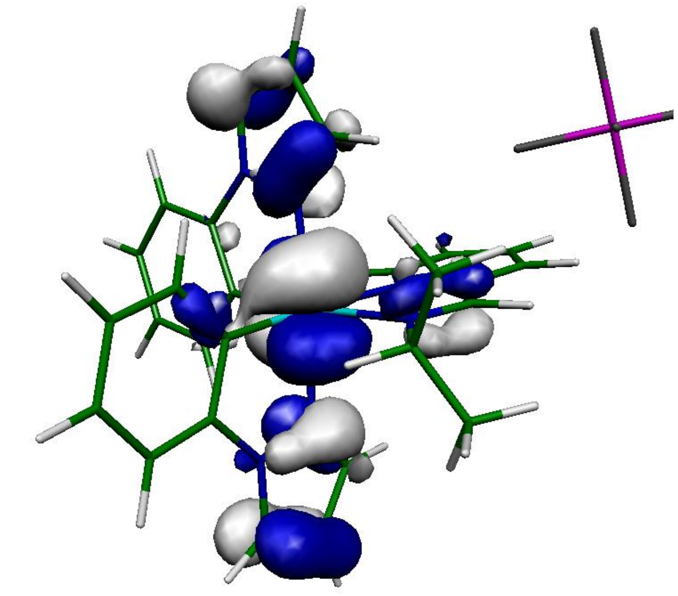
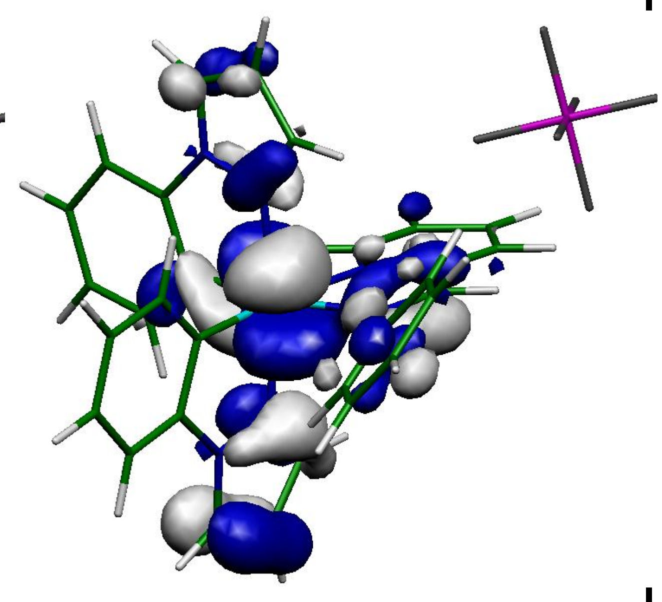
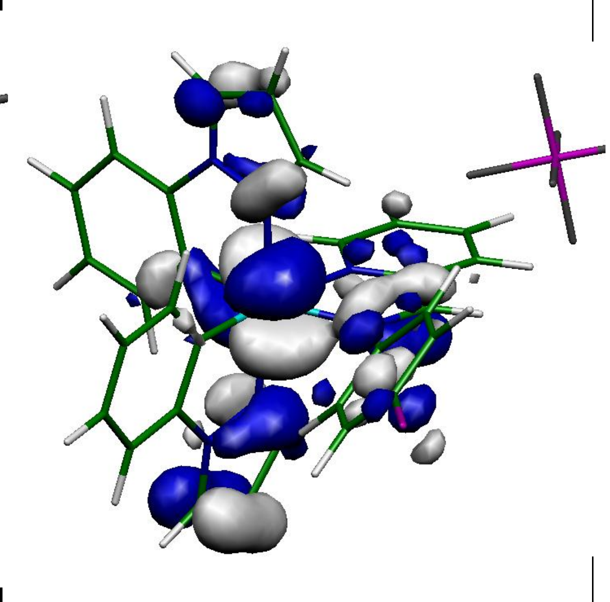
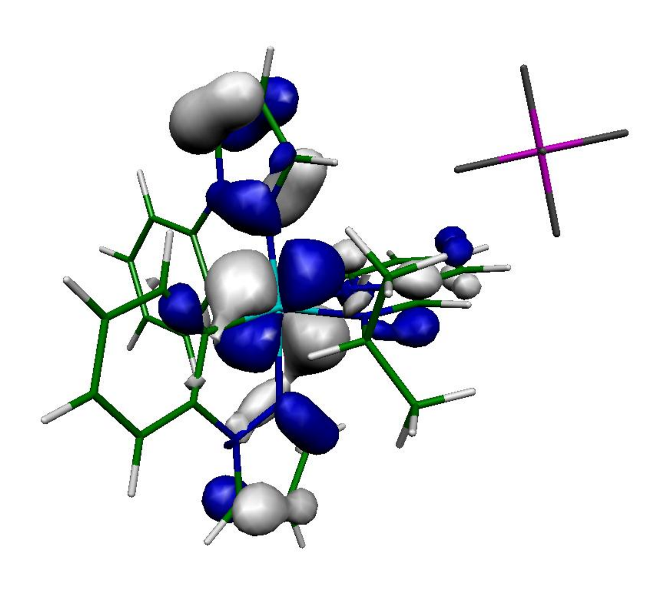
		
157(HOMO-1)	MO 165 (HOMO-1)	MO 168 (HOMO-1)
		
MO 156 (HOMO-2)	MO 164 (HOMO-2)	MO 167 (HOMO-2)



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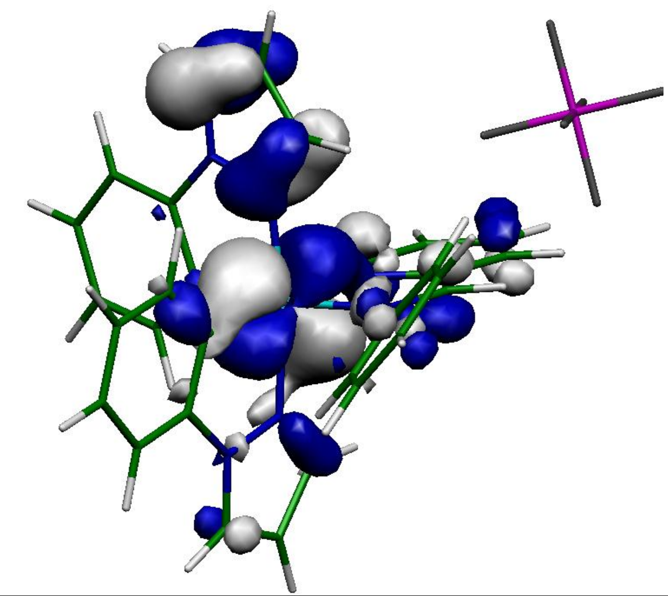

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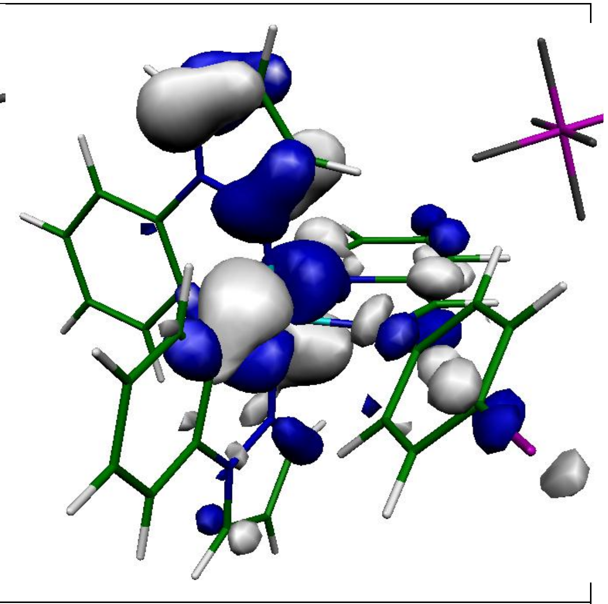

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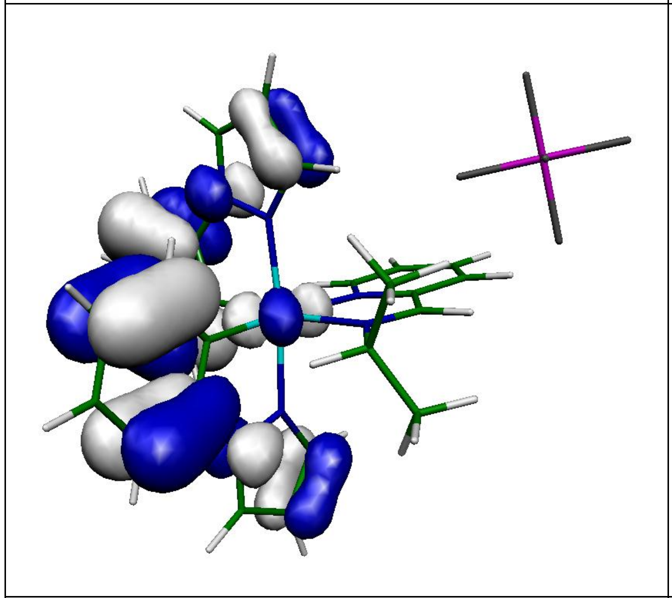
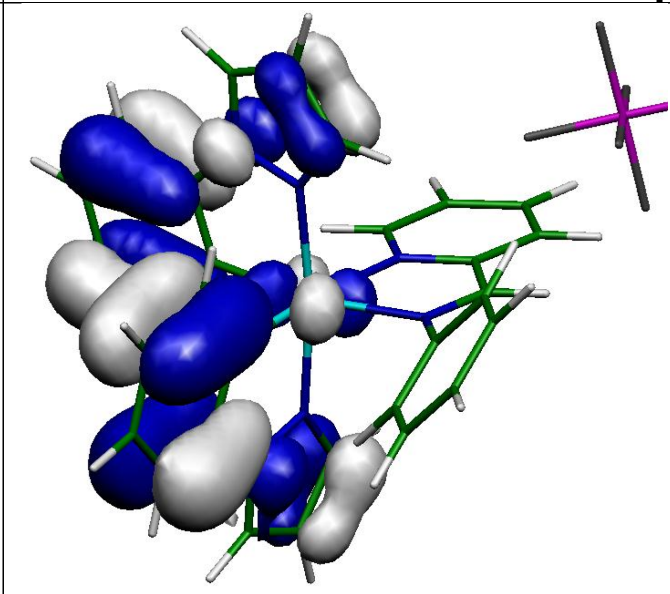
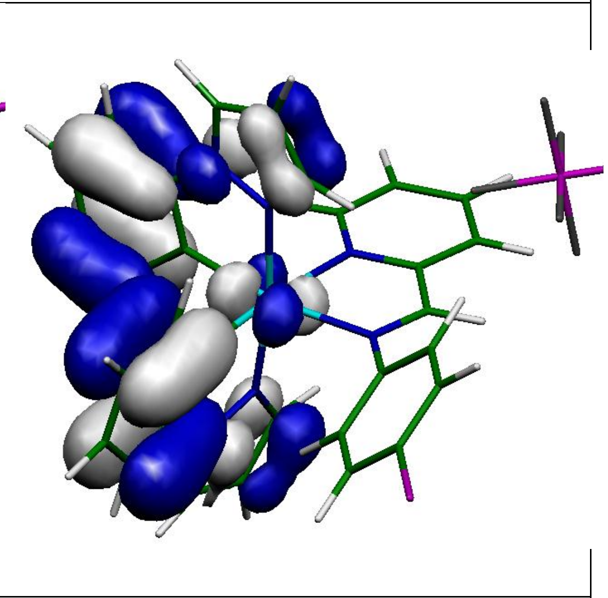


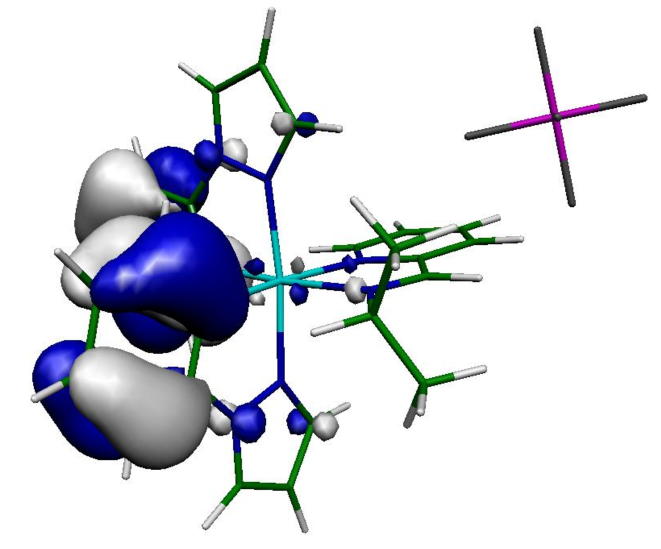
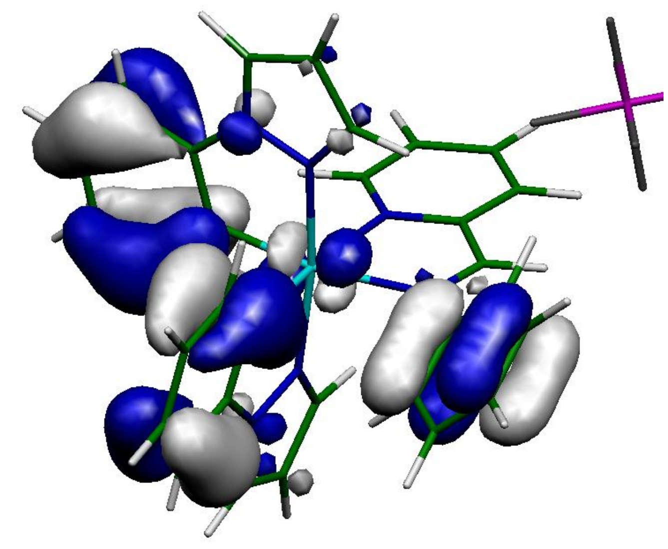
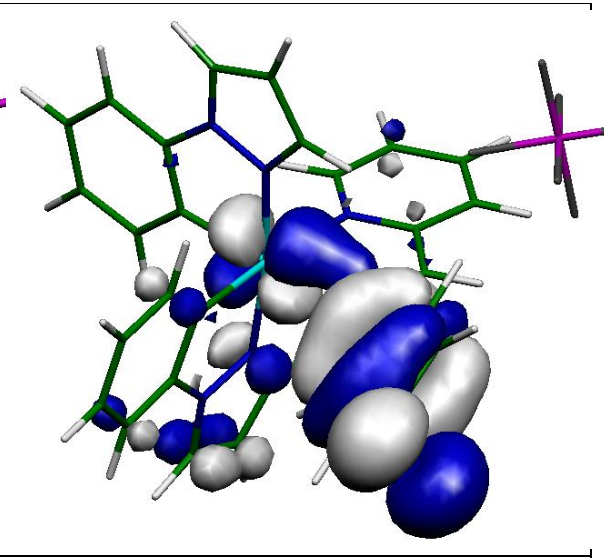
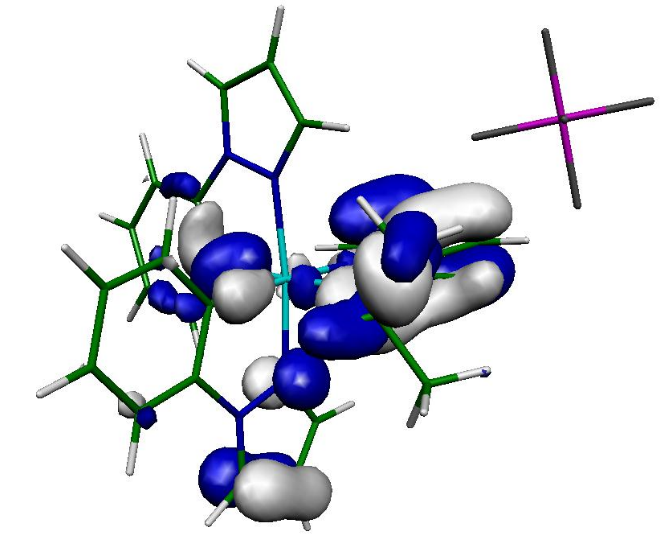
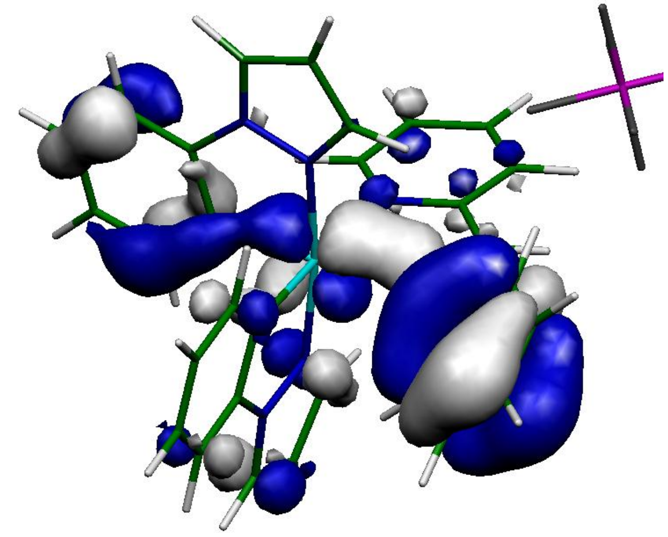
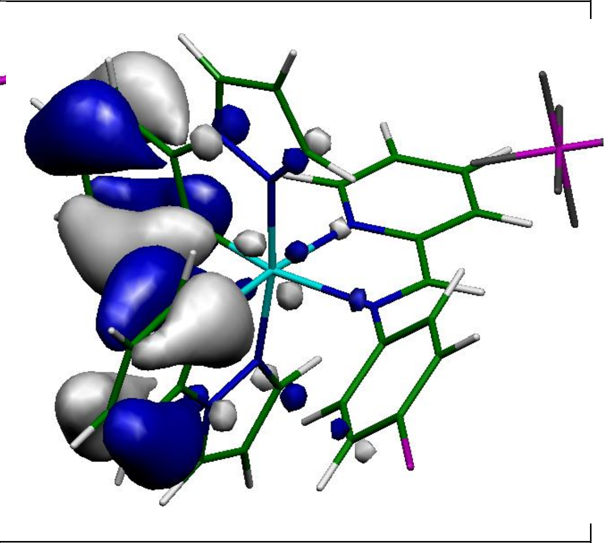
MO 154 (HOMO-4)

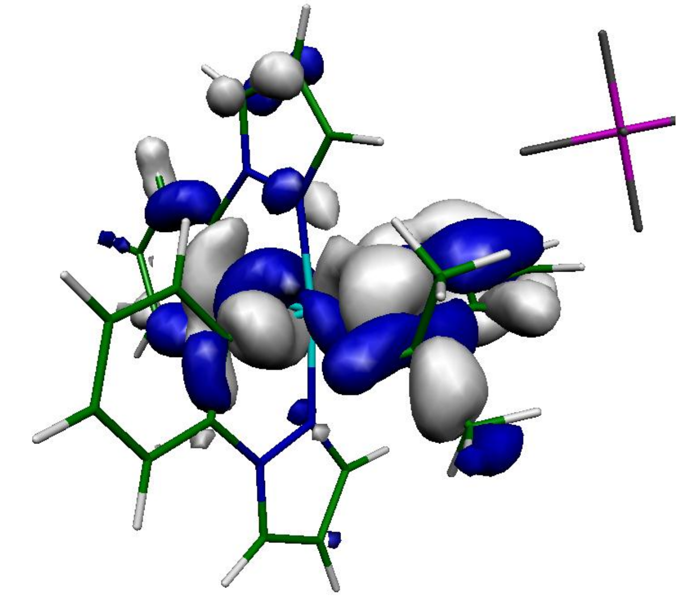
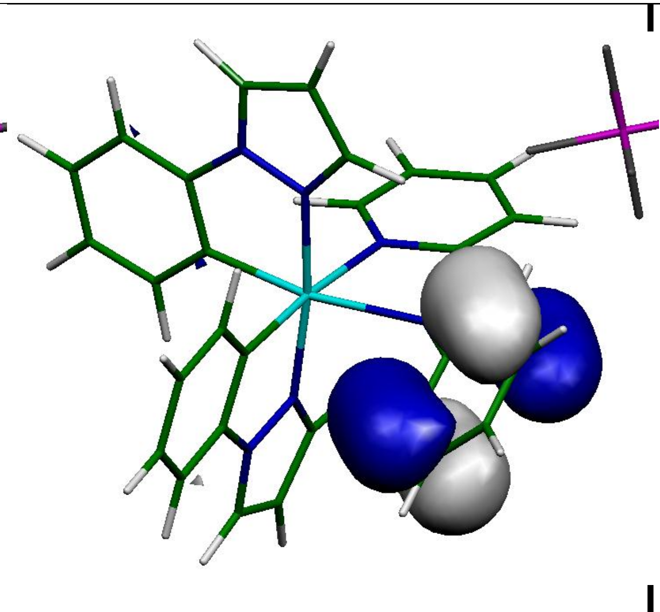
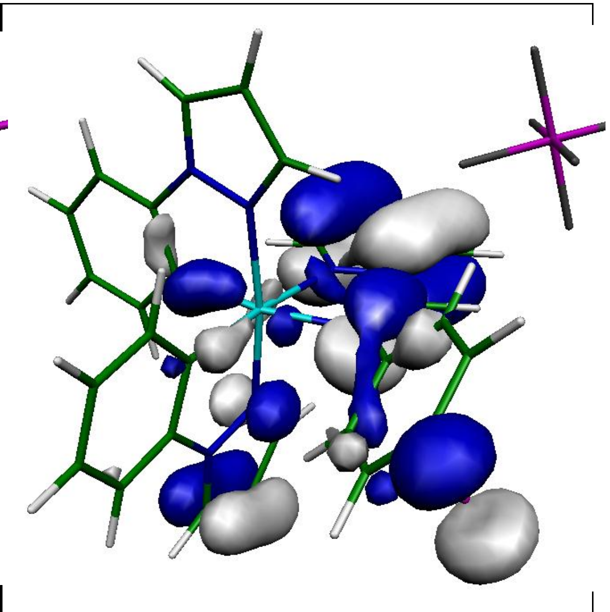
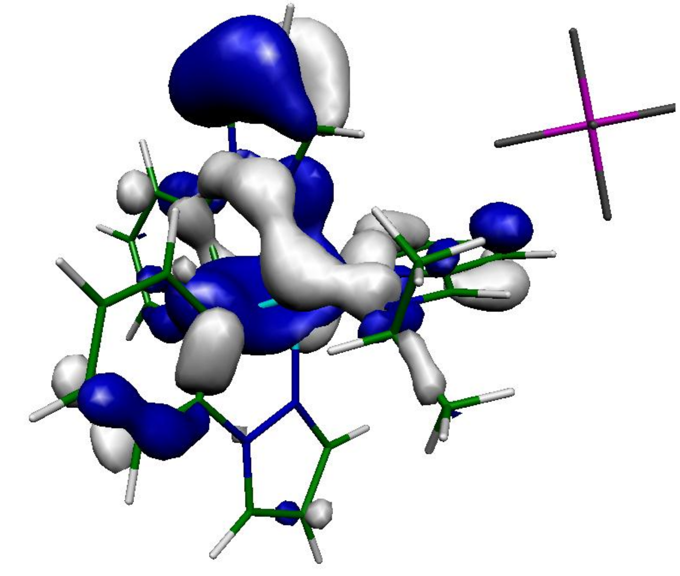
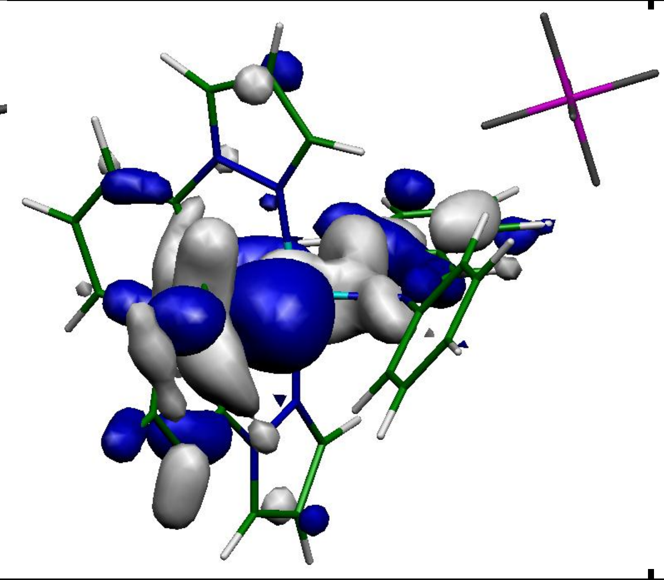
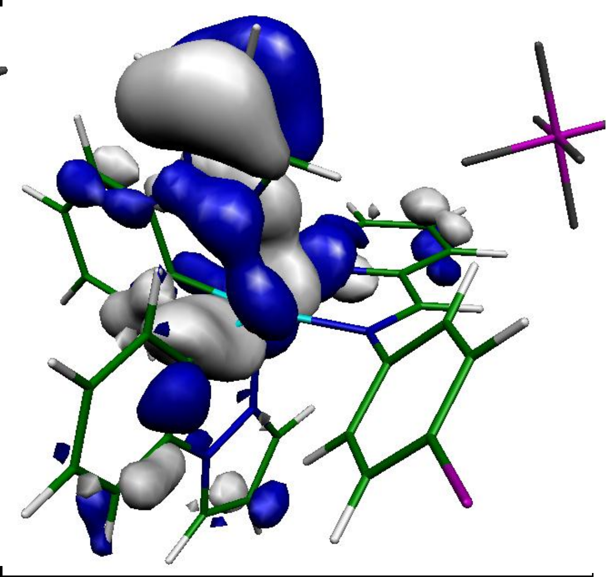


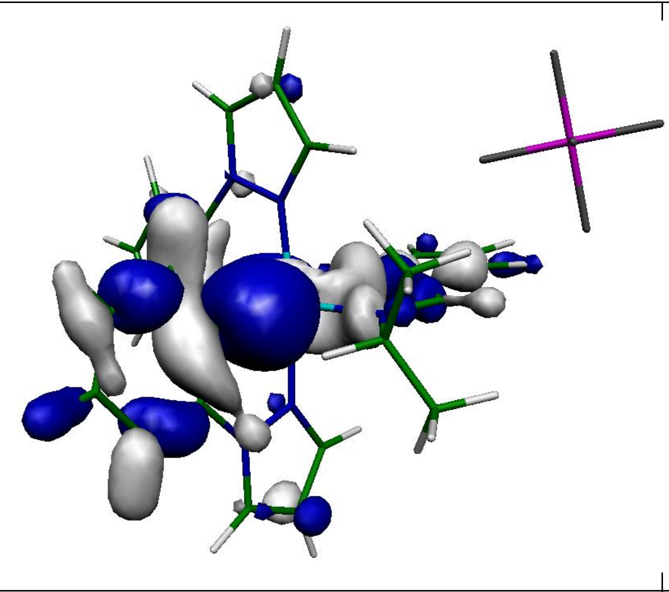
MO 162 (HOMO-4)



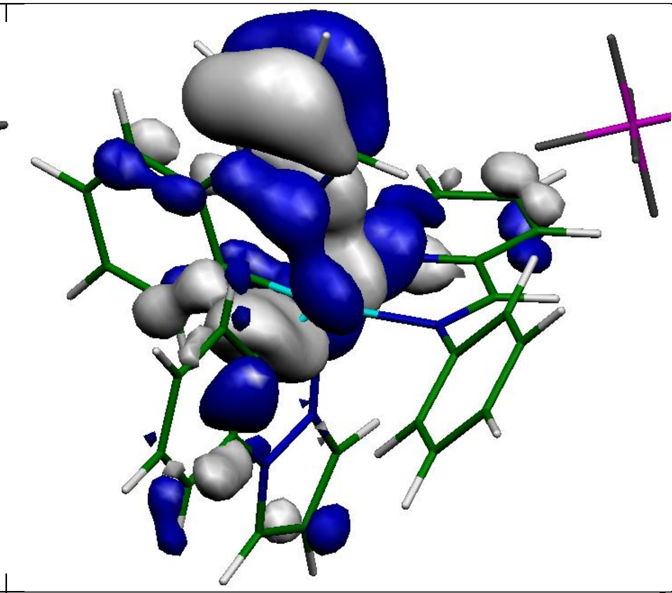
MO 165 (HOMO-4)

		
MO 153 (HOMO-5)	MO 161 (HOMO-5)	MO 164 (HOMO-5)
		
MO **152 (HOMO-6)**	MO 160 (HOMO-6)	MO 163 (HOMO-6)

		
MO 151 (HOMO-7)	MO 159 (HOMO-7)	MO 161 (HOMO-7)
		
150 (HOMO-8)	MO 158 (HOMO-8)	MO 160 (HOMO-8)



MO 149 (HOMO-9)



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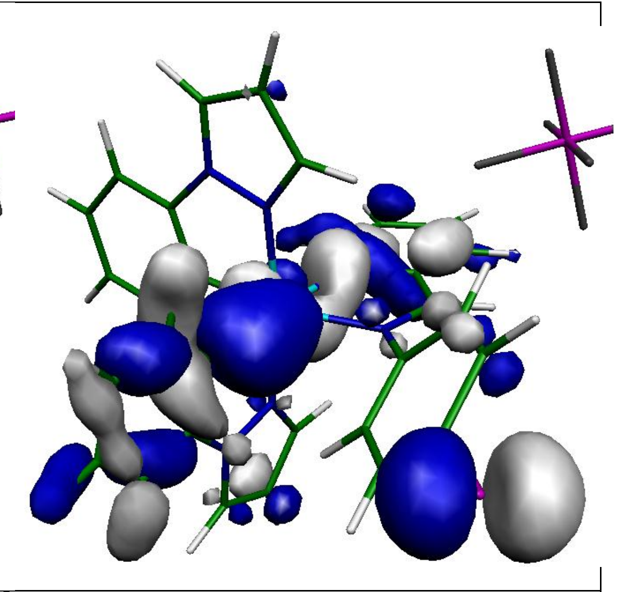

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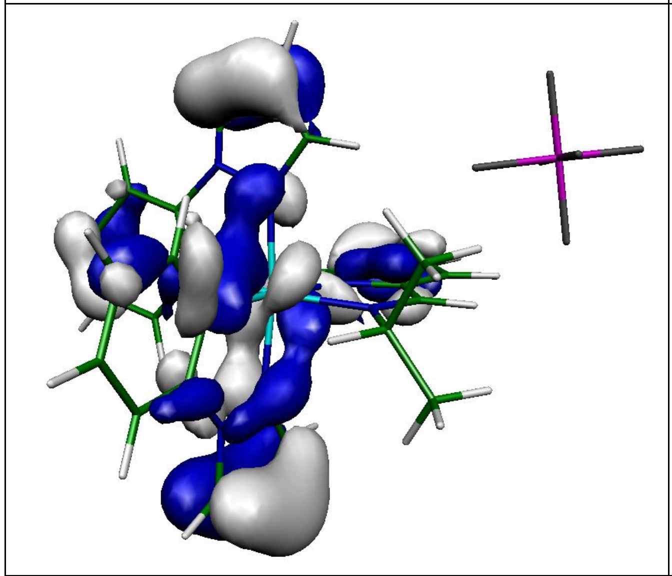
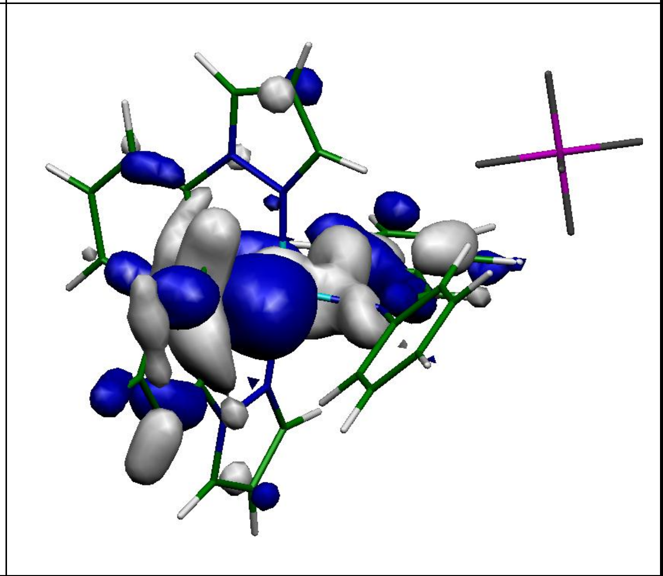
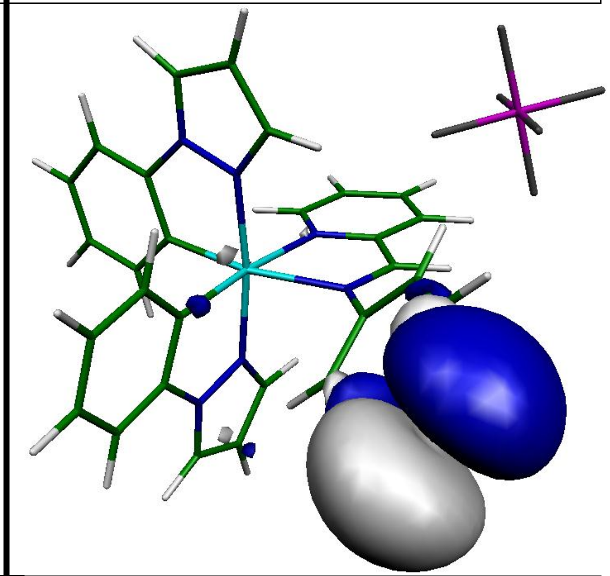


MO 148 (HOMO-10)



MO 156 (HOMO-10)



MO 158 (HOMO-10)

Spin Orbit Coupling

The intensity of the transition from the excited state Ψ_κ to the ground state singlet Ψ_0 can be computed according to the perturbation theory by the equation

$$f = \frac{8m\pi^2}{3he^2}\tilde{\nu}_{em}|\langle\Psi_0|\,\hat{\mu}\,|\Psi_k\rangle|^2 \qquad (1)$$

where m and e are the mass and charge of the electron, h the Plank's constant, $\tilde{\nu}_{em}$ the energy of the emission in wavenumbers and $\hat{\mu}$ the electric dipole moment operator.

Because of Spin Orbit (SO) coupling Hamiltonian ($\mathcal{H}_{SO}$) the Ψ_k electronic state can be obtained (K.Nozaki *Journal of the Chinese Chemical Society*, **2006**, *53*, 101-112) as eigenfunction of the secular equation whose matrix elements are

$$\langle {}^M\Psi_i' |\mathcal{H}_{SO}| {}^N\Psi_i' \rangle \cong \sum_{p=1}^{occ}\sum_{q=occ+1}\sum_{r=occ+1} a_{pqk}a_{prl}\langle\mathcal{D}(p\to q)|\mathcal{H}_{SO}|\mathcal{D}(p\to r)\rangle + \sum_{p=1}^{occ}\sum_{r=1}^{occ}\sum_{q=occ+1} a_{pqk}a_{prl}\langle\mathcal{D}(p\to q)|\mathcal{H}_{SO}|\mathcal{D}(r\to q)\rangle \qquad (2)$$

and described as a mixture of pure singlet and triplet states ${}^M\Psi_i'$ (M=1 or 3 respectively):

$$\Psi_k = \sum_i \left({}^1c_{ki}\,{}^1\Psi_i' + {}^3c_{ki}\,{}^3\Psi_i'' \right)$$

where ${}^M\Psi_i'$ represent the excited state wavefunctions described by a combination of Slater's determinants $\mathcal{D}$ relative to the opportune mono excitation from a p-th occupied MO and q-th virtual MO giving rise to the given multiplicity M

$${}^M\Psi_i' = \sum_{p=1}^{occ}\sum_{q=occ+1} a_{pq}\mathcal{D}(p\to q)$$

The SO interaction matrix elements in eq. 2 are then approximated by the sum of one-electron one-centre spin-orbit integrals between these electronic configuration. In the LCAO approximation each MO's can be described by a linear combination of natural atomic orbitals (NAO) χ_i

$$\varphi_j = \sum_i b_{ji}\chi_i$$

Than the matrix elements of the SO coupling became

$$\langle {}^{M}\Psi_i' | \mathcal{H}_{SO} | {}^{N}\Psi_i' \rangle \cong \sum_{p=1}^{occ} \sum_{q=occ+1} \sum_{r=occ+1} a_{pqk} a_{prl} \sum_m \sum_n \mathrm{b}_{qm}\, \mathrm{b}_{rn}\, \Theta_{\mathrm{V}}(\chi_m, \chi_n, \omega_k, \omega_l) + \sum_{p=1}^{occ} \sum_{r=1}^{occ} \sum_{q=occ+1} a_{pqk} a_{prl} \sum_m \sum_m \mathrm{b}_{pm} \mathrm{b}_{rn}\, \Theta_{\mathrm{O}}(\chi_m, \chi_n, \omega_k, \omega_l)$$

where the $\Theta_{\mathrm{V}}(\chi_m, \chi_n, \omega_k, \omega_l)$, $\Theta_{\mathrm{O}}(\chi_m, \chi_n, \omega_k, \omega_l)$ represent the integrals between those NAO's and ω_k and ω_l are the singlet or triplet spin functions.

The SO perturbation in one centre approximation is maximal when a change of magnetic angular quantum number involves orbitals on the atoms that have large effective nuclear charge: in our case the Ir atom. Because the NAO's resemble Slater orbitals the one centre integrals can be replaced by integrals between spin-orbitals χ_m^α relative to this atom discarding the contribution from lighter atoms so that the Θ's can be reduced to integral of the kind

$$\left\langle \chi_{d_{xy}}^{\alpha} \middle| \mathcal{H}_{SO} \middle| \chi_{d_{xz}}^{\beta} \right\rangle \approx \zeta_c \left\langle \chi_{d_{xy}}^{\alpha} \middle| \hat{\ell}\hat{s} \middle| \chi_{d_{xz}}^{\beta} \right\rangle = \frac{1}{2}\zeta_c$$

where ζ_c is the integral related to the radial part of the orbital and assumed a constant for a given atom.

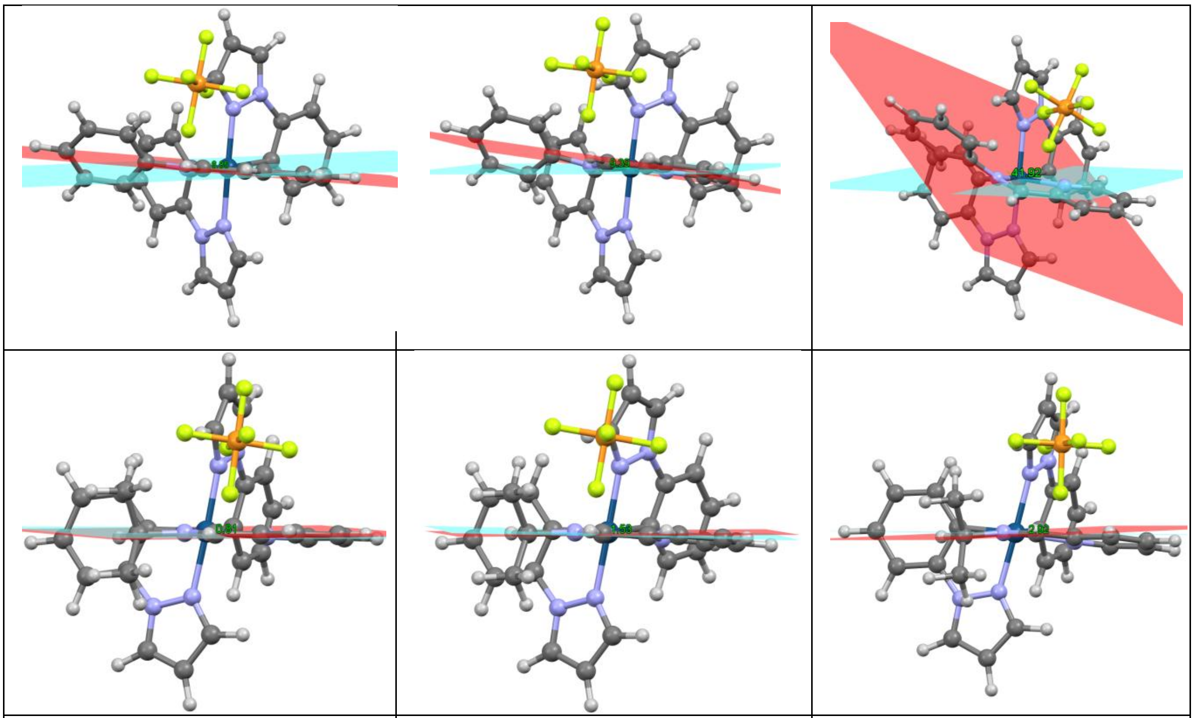
If the ground state Ψ_0 is a singlet state than the equation (1) become

$$f = \frac{8m\pi^2}{3he^2} \tilde{\nu}_{em} \left| \sum_i c_{kj} \langle \Psi_0 | \hat{\mu} | {}^{1}\Psi_i' \rangle \right|^2$$

where the ${}^{1}\Psi_i'$ are the singlet states contribution to the Ψ_k with ${}^{3}c_{ki} \geq {}^{1}c_{ki}$

Electronic Supplementary Material (ESI) for Dalton Transactions

Figure S.10 : Minimum energy structures of 5a-PF6PI (above) and 8a-PF6PI (below) in the ground (S_0), first singlet (S_1) and first triplet state (T_1) computed at the D95/SDD/M06/DCM level of theory



S0	S1	T1

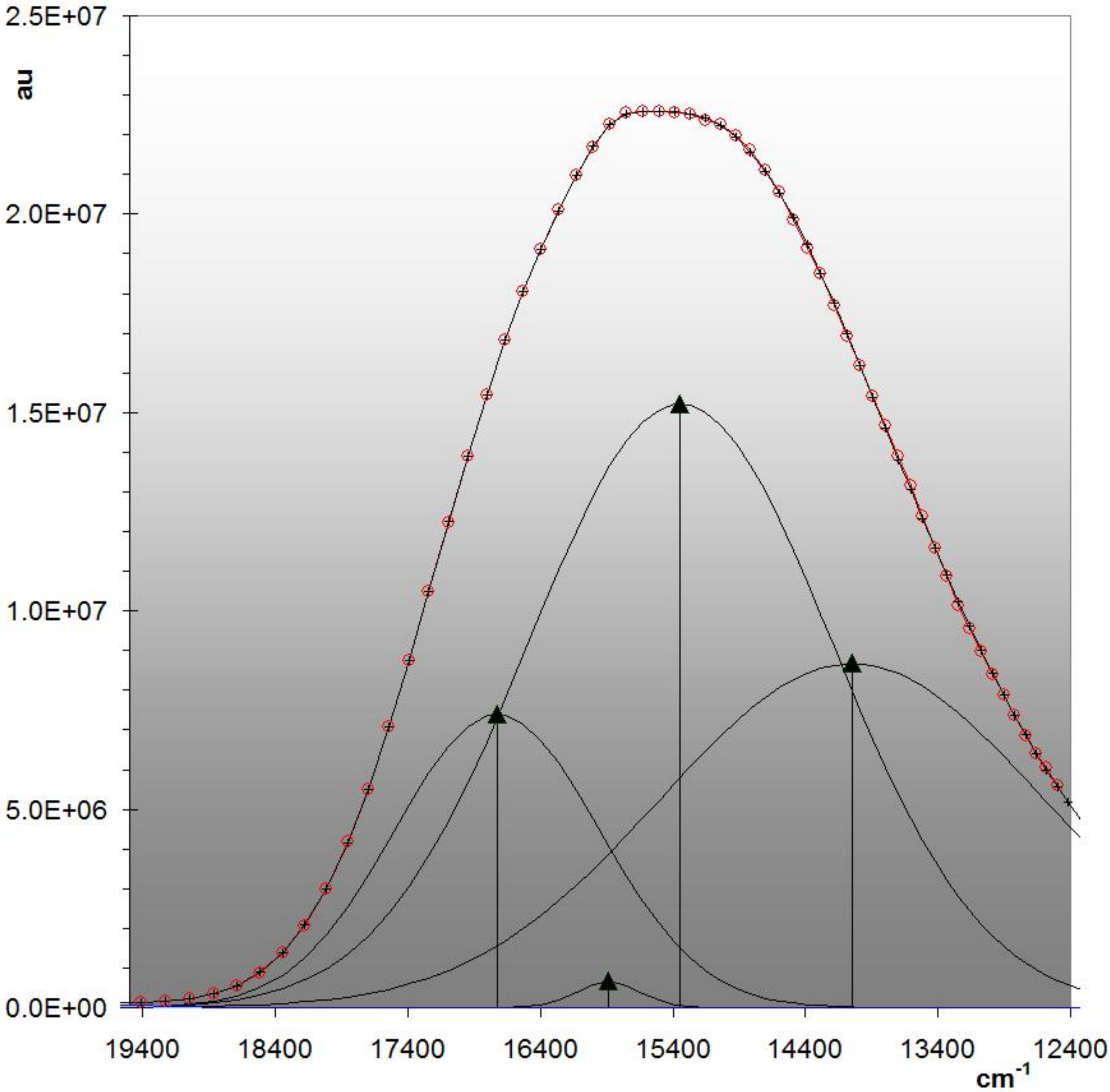
Figure 10: Minimum energy structures of **5a** (above) and **8a** (below) in the ground (S_0), first singlet (S_1) and first triplet state (T_1) computed at the D95/SDD/M06/DCM level of theory.

The "out of plane" bending of the N(im)-C(aryl) bond is defined by the dihedral ϕ between the planes identified by the atoms C(im)-Ir-N(im) (light blue) and Ir-N(im)-C(aryl/alkyl) (red). The dihedral is positive if the rotation looking from the C(im) atom toward the Ir atom is clockwise for superimposing the "light blue" to the "red plane".

In the case of **5a-**PF6PI the ground state S_0, S_1 and T_1 have minimum energy equilibrium geometries characterized by angles ϕ of 6.9, 9.4 and 41.9 ° respectively, hence the geometry of the first triplet excited state (Figure 11) is considerably different than in the ground state reducing the FC factors. Similar behaviour is shown by the other aryl derivative **4a**. On the other hand in case of **8a-**PF6PI the angles are -0.8, -1.5, and -2.9 °respectively and the ground and T_1 states have closer equilibrium geometries as in case of **8a** so these effects are not very relevant.

Figure S.11 Decomposition of the 8a/8aPF6FI emission band.

Emission spectrum of 8a/8aPF6FI. (o) Experimental data and (+) fitting data(▲) Position of fitting Gaussian functions.



Position (nm,cm^{-1}), intensity(a.u.) and Δ_i (cm^{-1}) of each Gaussian function used for the fitting

λ_i	$\tilde{\nu}_i$	$\epsilon(\tilde{\nu}_i)$	Δ_i
598	16726	7394718	909
630	15884	662161	280
652	15344	15219690	1344
712	14049	8673379	1701

Table S8 ΔE(T1→S0) computed at the unrestricted DFT SDD/D95(d)/M06/DCM level of theory for ion pairs

Table 5 ΔE(T1→S0) computed at the unrestricted DFT SDD/D95(d)/M06/DCM level of theory for ion pairs

	ΔSCF		Exp
	a	b	
4aPF6PI	658	1098	780
5aPF6PI	646	997	715
8aPF6PI	534	646	640

We suggest that in case of the emission the long half-life of the triplet state together with the new charge distribution and a possible change in the complex geometry allows the modification of the counter ion position. Then the emitting species (cation + anion) will undertake a fast radiationless decay that quenches mainly the emission due to the ion pair leaving predominantly the contribution of "free" ion species which is also present in solution as suggested by the absorption spectra. In fact decomposition of the broad emission band of **8a** (see Fig above) suggests that the emission has two contributions one more intense due to the "free" ion at longer wavelength (652, 713 nm) corresponding to a computed value of 682 nm (see Table 5) and a less intense contribution at (598, 630 nm) corresponding to the computed value of 646 nm of **8a-**PF6PI.

Table S9 Cartesian coordinates of the studied complexes

7a Ir 2PhPyrazole Pyridin Immino Phenyl_pOH M06 SDD D95 (d) in Acetonitrile

C30H24Ir1N6O1(1+)1,1
Ir,0,-0.9669063637,0.09089533,-0.0820976242
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2.0260743649
N,0,-0.5763299074,-1.826547718,-2.2171371974
N,0,-1.0021508812,0.4718603085,1.9345105137
N,0,-2.0568618206,-0.0679775782,2.5950142134
N,0,0.778464381,1.426374698,-0.4496900718
N,0,-1.8525466084,2.0473539543,-0.4800439295
C,0,-1.5086131701,-0.134729213,-3.1969199467
H,0,-1.9329803982,0.8595966061,-3.2840481292
C,0,-1.3604698259,-1.1410880955,-4.1668118264
H,0,-1.6474439691,-1.1005831159,-5.2088392375
C,0,-0.7635869613,-2.2021271837,-3.5031031818
H,0,-0.4646314175,-3.1812846531,-3.8563636027
C,0,-0.0150756117,-2.4716687359,-1.0833076014
C,0,0.5822526707,-3.7272032311,-1.1779763115
H,0,0.6176299957,-4.2687990297,-2.1227170494
C,0,1.1484024541,-4.2793798669,-0.0268972878
H,0,1.6209125243,-5.2584120195,-0.0748488722
C,0,1.1044504937,-3.5706654882,1.1789762991
H,0,1.5459125349,-4.002175024,2.0764818958
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C,0,-0.0691148373,-1.7172278667,0.106879481
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C,0,-5.0461978724,-1.9880424027,1.518334438
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C,0,2.6285525793,-0.1160638008,-0.8000210028
H,0,1.9503923855,-0.7862609363,-1.3239242841
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H,0,6.3689182011,-0.7248534851,-0.2430745586

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Quadrupole=-4.6879016,6.9544077,-2.2665061,-
14.2368196,-3.0004553,4.1313246
PG=C01 [X(C30H24Ir1N6O1)]

4a Ir 2PhPyrazole Pyridin Immino Phenyl_p-Br M06 SDD D95 (d) in Acetonitrile

C30H23Br1Ir1N6(1+)
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Ir,0,3.5844380944,13.7314759868,4.0088263151
Br,0,9.4541942876,9.2158595495,2.1304458981
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C,0,0.4530948876,11.0636676758,2.8142058001
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C,0,6.7729076062,10.1212613979,2.6627595165
H,0,6.605496765,9.1108926732,3.0308583109
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Quadrupole=-6.8061898,7.6763834,-
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PG=C01 [X(C30H23Br1Ir1N6)]

6a Ir 2PhPyrazole Pyridin Immino Phenyl_pCOOH M06 SDD D95 (d) in Acetonitrile

C31H24Ir1N6O2(1+)

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Ir,0,-0.9729076936,0.1114756477,-0.070312448
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N,0,-2.0592174028,-0.0775335079,2.6062611376
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N,0,-1.8701907716,2.0626009147,-0.4828404834
C,0,-1.5077882399,-0.1259023426,-3.1861894598
H,0,-1.9427590363,0.8635009829,-3.2769796835
C,0,-1.3453095106,-1.1319814597,-4.1536856595
H,0,-1.6305864723,-1.0965486752,-5.1963244429
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C,0,-0.8139188466,0.9114397283,4.1404577478
H,0,-0.4328417515,1.2777158851,5.0841075415
C,0,-1.9610042434,0.1607710444,3.9339958521
H,0,-2.6986155605,-0.2124790021,4.6336750642
C,0,-2.9977141213,-0.7841776295,1.8113794255
C,0,-4.1435889914,-1.352484186,2.3634870689
H,0,-4.3566997052,-1.2771793799,3.4290063478
C,0,-5.0254022005,-2.0247787461,1.5150985522
H,0,-5.9275863782,-2.4755374774,1.9235987526
C,0,-4.7469088198,-2.1089441762,0.1468644506
H,0,-5.4358371686,-2.6326107304,-0.5145166116
C,0,-3.5874721568,-1.5278790539,-0.3801525841
H,0,-3.3947452978,-1.6099716906,-1.4523000507
C,0,-2.6787590775,-0.8467258804,0.4394422381
C,0,-3.1753097063,2.341109719,-0.5177671881
H,0,-3.854686106,1.518940767,-0.2911351089
C,0,-3.6585404618,3.6143949897,-0.8305736352
H,0,-4.7305901871,3.7896374451,-0.8454575116
C,0,-2.7515083837,4.6331918382,-1.1138025886
H,0,-3.0983712009,5.6334942373,-1.3610072197
C,0,-1.3865046762,4.3458054918,-1.0767513253
H,0,-0.6390304108,5.1071636012,-1.288663719
C,0,-0.9835588135,3.0504265088,-0.7585734091
C,0,0.4256567408,2.6806932621,-0.7050156734
H,0,1.175094345,3.4564412608,-0.8903037777
C,0,2.1295691692,1.1296758774,-0.3128206326
C,0,2.9940407238,1.9606069613,0.415527601
H,0,2.6138541678,2.8657138049,0.888341827
C,0,4.3339991106,1.6126004503,0.5571917217
H,0,5.0040722144,2.251434208,1.1280201489
C,0,4.8180432858,0.4353971478,-0.0264690999
C,0,3.9496117938,-0.394325324,-0.7482473714
H,0,4.3366121385,-1.3070376935,-1.1980775686
C,0,2.6094188183,-0.0576718116,-0.8829542878
H,0,1.9358812475,-0.6943157777,-1.4516902198
C,0,6.2389803555,0.0250804325,0.0969673303
O,0,6.7085156509,-0.9861658025,-0.390756734
O,0,6.9733558649,0.8934407631,0.8104019818
H,0,7.8827563793,0.5424189925,0.8333497943

State=1-A
HF=-1778.0896701
PG=C01 [X(C31H24Ir1N6O2)]

5a_Ir_2PhPzol_PyImmino_Ph_SDD_D95d_M06 structure in ACN

C30H24Ir1N6(1+)

1,1
Ir,0,6.2391093484,10.3337616061,10.8841026333
N,0,5.2405971137,8.9069452891,9.801341595
N,0,5.4874670112,7.6287661003,10.1808506816
N,0,7.1776183642,11.5971106924,12.200070974
N,0,6.5146624474,11.7960884513,13.3675906107
N,0,5.5564379956,11.9855670642,9.5801653565
N,0,7.7719319996,10.4733402547,9.3260190472
C,0,4.3266155402,8.860230801,8.8305391881
H,0,3.9643552813,9.7758313123,8.3743894044
C,0,3.9726588784,7.524386976,8.5747978779
H,0,3.2617885835,7.1570554305,7.8471102392
C,0,4.732912953,6.7711541525,9.4560717373
H,0,4.7833122222,5.7003585251,9.6091584258
C,0,6.4276596386,7.4543425553,11.2296998406
C,0,6.8047645996,6.1869225243,11.6685986338
H,0,6.3882149018,5.2852883981,11.2210498986
C,0,7.7382702203,6.0930689673,12.7026938442
H,0,8.0476011292,5.1142157287,13.0634368826
C,0,8.2694915287,7.2570986599,13.2679481156
H,0,8.997562878,7.1840822823,14.0747595287
C,0,7.8719024375,8.5172832592,12.8061504141
H,0,8.3031605248,9.4086651726,13.2673339457
C,0,6.9392581596,8.6527021244,11.7695175348
C,0,4.856024876,10.4142506632,12.3627971093
C,0,3.589053062,9.8210538816,12.4243872008
H,0,3.2394588121,9.2002986783,11.5961522527
C,0,2.7456745673,10.0175483667,13.524096479
H,0,1.7616419261,9.5504987318,13.5398084095
C,0,3.1552412083,10.8093822625,14.6026629338
H,0,2.4976644852,10.9645827611,15.4556105674
C,0,4.4173157714,11.40698634,14.5847143803
H,0,4.7436938683,12.0279342401,15.4183597434
C,0,5.2338321875,11.1918277559,13.4763598226
C,0,7.2492032082,12.5724316822,14.1969462222
H,0,6.8897413404,12.8488681934,15.1804578303
C,0,8.4297964234,12.8858954572,13.5409911684
H,0,9.243252685,13.4930516478,13.9143835189
C,0,8.3379350946,12.2500939588,12.2908492974
H,0,9.0427935088,12.2306476997,11.4668932958
C,0,4.2992883228,12.6413881898,9.6549635851
C,0,3.8691926211,13.1643614436,10.880715536
H,0,4.5149047894,13.097105111,11.7546486988
C,0,2.6312962912,13.7981054602,10.963884143
H,0,2.3077437834,14.2170015586,11.9149909997
C,0,1.8052282117,13.8885401066,9.8376655438
H,0,0.8323718103,14.370713857,9.9114261012
C,0,2.2286497429,13.3482930794,8.6207656109
H,0,1.5867852078,13.4013324307,7.7435612234
C,0,3.4742762875,12.7266646285,8.5238554461
H,0,3.7950688468,12.2868502379,7.5789382753
C,0,6.324768164,12.213174903,8.567564582
H,0,6.0780696476,12.9689510265,7.8155223555
C,0,7.5563904189,11.4483969388,8.4098798679
C,0,8.4494805367,11.7046158248,7.3713889488
H,0,8.2339268274,12.4971027918,6.6581378852
C,0,9.6061881666,10.9301389535,7.275382753
H,0,10.3245076583,11.1074191382,6.4787126828
C,0,9.8222530832,9.9277883475,8.2192654712
H,0,10.7059993968,9.2969287306,8.1838495713
C,0,8.8778520937,9.7313302744,9.2297894167
H,0,9.0104313104,8.9582283195,9.9871546607

State=1-A
HF=-1589.5490298
PG=C01 [X(C30H24Ir1N6)]

8a Ir 2PhPyrazole Pyridin Immino i-Propyl M06 SDD D95 (d) in Acetonitrile

C27H26Ir1N6(1+)

1,1
Ir,0,-0.0793807104,-0.1195473993,0.0361313923
N,0,0.9047974993,-1.0040837421,-1.5265187844
N,0,2.2519252844,-0.8510262589,-1.5212178872
N,0,-0.9129656213,0.975858669,1.5618281398
N,0,-1.0486619766,2.3011557091,1.3035731943
N,0,-0.4518887324,-2.1177680184,0.9400238933
N,0,-2.0997858267,-0.6484056217,-
0.6127219944
C,0,0.5898333414,-1.6986439695,-2.6213511534
H,0,-0.4458907316,-1.9386185323,-
2.8367643374
C,0,1.757782166,-2.0043939758,-3.3411808999
H,0,1.8355119251,-2.5555812625,-4.2685326424
C,0,2.7949613543,-1.4486398127,-2.6069897703
H,0,3.8629926631,-1.4418375073,-2.7855736179
C,0,2.7995349669,-0.1537800409,-0.4124448661
C,0,4.1721589609,0.0521957993,-0.2861807489
H,0,4.871207639,-0.3097964926,-1.0392803215
C,0,4.6392320569,0.7394790345,0.8357474656
H,0,5.7065680647,0.913191051,0.9568443936
C,0,3.7302272592,1.2046145737,1.7924687428
H,0,4.0917573409,1.7469463781,2.6652793386
C,0,2.3575509817,0.9814972261,1.6367098673
H,0,1.6704542933,1.3594563471,2.3978750931
C,0,1.8489215233,0.2810528498,0.5346580867
C,0,-1.3816712834,0.7681312044,2.793275688
H,0,-1.375809551,-0.2311917551,3.2143004994
C,0,-1.8231101316,1.9812973263,3.3481777895
H,0,-2.2515950629,2.1409967111,4.3283475093
C,0,-1.5939328673,2.9338479417,2.3675909957
H,0,-1.7832235004,4.0002286253,2.3582267135
C,0,-0.6255646597,2.7393843995,0.0222375543
C,0,-0.7636344772,4.0666037195,-0.3780530214
H,0,-1.1923087317,4.8158290481,0.2864334907
C,0,-0.341514027,4.4202540283,-1.6611902412
H,0,-0.4401922853,5.4503685145,-1.9974896169
C,0,0.2020208396,3.4470423769,-2.5063935968
H,0,0.529155352,3.7217026231,-3.5084005949
C,0,0.3285275369,2.1210669311,-2.07559493
H,0,0.752853158,1.3832020687,-2.7603076874
C,0,-0.0846454627,1.727161994,-0.7962727648
C,0,-2.893967863,0.0858429752,-1.3972202219
H,0,-2.4818422675,1.0291269065,-1.7576158783
C,0,-4.1820633815,-0.3247163436,-
1.7451019648
H,0,-4.789545499,0.3080802796,-2.386122795
C,0,-4.6606304209,-1.5392055689,-
1.2570834755
H,0,-5.6604687346,-1.8842133802,-
1.5090728154
C,0,-3.8314780494,-2.3082947008,-
0.4390683492
H,0,-4.1577266944,-3.2651086712,-
0.0371540801
C,0,-2.5578928349,-1.830309847,-0.1399434449
C,0,-1.6214191236,-2.588054325,0.690589571
H,0,-1.9460425818,-3.5608815416,1.0763767981
C,0,0.4595868538,-2.9451698431,1.7498253398
H,0,-0.0712142565,-3.8715031897,2.0224712081
C,0,0.8407922955,-2.200859724,3.0205247866
H,0,1.2995333583,-1.2323446694,2.7781704439
H,0,1.5686042219,-2.7947003103,3.5859923451
H,0,-0.0319701016,-2.0333293903,3.6634789009
C,0,1.6861386305,-3.311161336,0.9247583127
H,0,1.4033800482,-3.778309788,-0.0275308245
H,0,2.300190464,-4.0218311498,1.4902686614
H,0,2.2963737886,-2.4224600036,0.718754161

State=1-A
HF=-1476.5170976
PG=C01 [X(C27H26Ir1N6)]

4b_Ir_2PhMe_Pzol_PyImminoPh_pBr_SDD_D95d_M06_ACN M06 SDD D95 (d) in Acetonitrile

C32H27Br1Ir1N6(1+)

1,1
Ir,0,-0.9812564018,0.1111702018,-0.0967414872
Br,0,6.60379475,-0.3046121027,0.0406304546
N,0,-1.0473575729,-0.5622705905,-2.0333557341
N,0,-0.5819906321,-1.8251745977,-2.213354675
N,0,-1.0283992747,0.5004487113,1.9196594023
N,0,-2.0811211253,-0.0443756274,2.5790148785
N,0,0.7579141357,1.4362761804,-0.4681679816
N,0,-1.8560905802,2.0787706074,-0.4891491069
C,0,-1.5370552081,-0.1526309325,-3.2052314139
H,0,-1.9689761696,0.8377299102,-3.299865204
C,0,-1.3861335214,-1.1679942251,-4.1651166757
H,0,-1.6807121484,-1.1422105178,-5.2055220446
C,0,-0.7739037649,-2.2160916014,-3.4941836089
H,0,-0.4668675221,-3.1951704375,-3.840757218
C,0,0.0073773319,-2.4449124798,-1.0787811083
C,0,0.6428235471,-3.6813200592,-1.1719327731
H,0,0.6795814887,-4.2267347154,-2.1163392042
C,0,1.2507306462,-4.2244727513,-0.0340719463
C,0,1.2045077519,-3.486652649,1.1579652849
H,0,1.681774029,-3.8930851198,2.0513382853
C,0,0.5627628095,-2.2451720385,1.2245968546
H,0,0.5583255051,-1.7049044974,2.1742330754
C,0,-0.0522864156,-1.6790881936,0.1016635774
C,0,-0.2696243154,1.1123142884,2.8306894387
H,0,0.6412716864,1.6204601291,2.5339866012
C,0,-0.839415343,0.9602752012,4.1062902503
H,0,-0.463364352,1.340378806,5.0464957826
C,0,-1.9916212392,0.2167788166,3.9029841359
H,0,-2.7395698616,-0.134723345,4.602873251
C,0,-3.0226546038,-0.7525008621,1.787542771
C,0,-4.1730567009,-1.3040933622,2.3427408696
H,0,-4.3847587641,-1.2141047532,3.4096734938
C,0,-5.074589121,-1.9861396404,1.5151818892
C,0,-4.7775116383,-2.0821365599,0.1498494086
H,0,-5.470399514,-2.6089969354,-0.5079180598
C,0,-3.6128651491,-1.518811315,-0.386393443
H,0,-3.4261002438,-1.6204330575,-1.4577519901
C,0,-2.696612877,-0.832621472,0.4182655576
C,0,-3.1578305224,2.3706500139,-0.5391353296
H,0,-3.8477637396,1.5437866577,-0.3688784559
C,0,-3.6235026278,3.6617447499,-0.7992230495
H,0,-4.6933955062,3.8480768257,-0.8286371919
C,0,-2.7011172666,4.6840315668,-1.0131125219
H,0,-3.0340682307,5.6987218334,-1.21679922
C,0,-1.3398051219,4.3816624008,-0.9646370182
H,0,-0.5821669766,5.1442493402,-1.1311923045
C,0,-0.9541343608,3.068472371,-0.701506694
C,0,0.4501153833,2.6765051931,-0.6545905629
H,0,1.2142740665,3.4465743204,-0.8002331418
C,0,2.1215749936,1.0642863212,-0.3543544375
C,0,3.014058659,1.8086991184,0.4283630643
H,0,2.6709767815,2.6922666043,0.9658465586
C,0,4.3441052047,1.4056943606,0.5496519814
H,0,5.0348528954,1.9768244903,1.1664028498
C,0,4.7660421257,0.2615372166,-0.1239516731
C,0,3.8925904096,-0.4902348565,-0.9103394569
H,0,4.2386880574,-1.3776638209,-1.4363332964
C,0,2.5638362359,-0.0901373907,-1.0123611735
H,0,1.8745346785,-0.6585486058,-1.6324245598
C,0,1.914984109,-5.5712042374,-0.0880447266
H,0,1.2029420271,-6.3714198737,0.1549090543
H,0,2.3142998422,-5.7829785308,-1.0870121931
H,0,2.738371641,-5.6389668397,0.6325872481
C,0,-6.3255989598,-2.5877594373,2.0906081139
H,0,-6.0936109359,-3.3089533292,2.8847044755
H,0,-6.9705465199,-1.8182233076,2.5343604794
H,0,-6.9059857933,-3.1087466281,1.3208794541

State=1-A
HF=-1680.8811413
PG=C01 [X(C32H27Br1Ir1N6)]

4c_Ir_2PhPzol2Me_PyImminoPh_pBr_SDD_D95d_M06_ACNM06 SDD D95 (d) in Acetonitrile

C34H31Br1Ir1N6(1+)

1,1
Ir,0,-0.8695549167,-0.0158870773,0.1582763766
Br,0,6.7652673991,-0.5817918591,-0.553729724
N,0,-0.3626924416,1.5707971321,1.3763138768
N,0,0.2194350217,2.6335476519,0.732297017
N,0,-1.5119603472,-1.3315161897,-1.3040231847
N,0,-2.684085176,-0.9799257616,-1.9243810818
N,0,0.8746179889,-1.1580590658,1.0194816204
N,0,-1.7487126322,-1.3966292914,1.6269552643
C,0,-0.5737169324,1.9389376673,2.6446353697
C,0,-0.1141643296,3.2536137713,2.8226786819
H,0,-0.1411176786,3.8361104415,3.7357511954
C,0,0.3816723987,3.6737802527,1.5975981638
C,0,0.5126038272,2.4319177737,-0.6449138311
C,0,1.2265099104,3.3527754788,-1.4149512532
H,0,1.5834681269,4.2922645821,-1.0044197606
C,0,1.4981727303,3.0502164783,-2.7515624034
H,0,2.0543692879,3.7623026936,-3.3581700277
C,0,1.0610272013,1.8408411724,-3.2970441016
H,0,1.2722432887,1.6035385008,-4.3390087417
C,0,0.3538302918,0.9297766059,-2.5045399689
H,0,0.022576211,-0.011938647,-2.9473324325
C,0,0.0716295799,1.1936903135,-1.1585858088
C,0,-1.0521978425,-2.426805779,-1.9159441715
C,0,-1.9370437791,-2.7857887068,-2.9451450573
H,0,-1.8423992765,-3.6254829685,-3.6231932029
C,0,-2.9618725553,-1.8526445759,-2.9329645463
C,0,-3.3175863375,0.1879209383,-1.4223436154
C,0,-4.5628621999,0.6375075303,-1.8677426843
H,0,-5.1208999186,0.1103866118,-2.634221866
C,0,-5.1077684232,1.7941361349,-1.3054883864
H,0,-6.0759313216,2.1509017573,-1.6516342372
C,0,-4.4135752186,2.4793637017,-0.3066385387
H,0,-4.8366009079,3.3816970929,0.1330508372
C,0,-3.1722871562,2.0079442116,0.1331551184
H,0,-2.6491383555,2.5559281877,0.91957254
C,0,-2.5952068264,0.8522638185,-0.4084538969
C,0,-3.0482218824,-1.5241194742,1.9044558242
H,0,-3.7262802252,-0.8594720323,1.3673429843
C,0,-3.5269331698,-2.4395755976,2.845065328
H,0,-4.5942259034,-2.4971380286,3.0397356104
C,0,-2.6200214168,-3.2565197321,3.5173625714
H,0,-2.9629696878,-3.9738137973,4.2588156611
C,0,-1.2624919497,-3.1389621209,3.2169665669
H,0,-0.5156924403,-3.7588938029,3.7081368554
C,0,-0.8657423272,-2.2025962321,2.2632156721
C,0,0.5383186708,-2.0275256945,1.9114501182
H,0,1.2827675438,-2.6359894978,2.4354698122
C,0,2.246161566,-1.0422596088,0.6722264395
C,0,3.0183970686,-2.1803970894,0.4015359786
H,0,2.5714176226,-3.1730923734,0.4527926942
C,0,4.3588532416,-2.050920058,0.0385117756
H,0,4.9526198464,-2.9343836144,-0.1868819814
C,0,4.9144816269,-0.7761184409,-0.0415794423
C,0,4.1655068282,0.3669267038,0.2360163434
H,0,4.6168656125,1.3554621833,0.1833216777
C,0,2.8247415311,0.229052337,0.5844964891
H,0,2.2409299191,1.1116149602,0.8354017032
C,0,-4.1388167491,-1.7892507815,-3.8399684397
H,0,-4.0452769832,-2.5845528011,-4.5847769522
H,0,-5.0827493216,-1.9428878799,-3.3032003058
H,0,-4.1946162526,-0.8325144647,-4.3726317302
C,0,0.9706961544,4.9976939281,1.2637593503
H,0,0.8963148895,5.6430268992,2.1435536131
H,0,2.0313257584,4.9204392733,0.9958467829
H,0,0.4396059919,5.4867735698,0.4385314674
C,0,0.2190811741,-3.0894635674,-1.5251021668
H,0,0.505344153,-3.8253592646,-2.2819521014
H,0,1.0294112391,-2.3551736638,-1.4309509579
H,0,0.115531261,-3.6158999556,-0.567222187
C,0,-1.2416501043,1.0557738104,3.6377058085
H,0,-0.6780415573,0.1292973705,3.8041516042
H,0,-1.3313508588,1.5750231307,4.5961343439
H,0,-2.2494941124,0.7832331385,3.2975380885

State=1-A
HF=-1759.4736023

4a DCM PF6- Py_Immine side

06075 in DCM PF6- Py_Immine side
C30H23Br1F6Ir1N6P1

0,1
Ir,3.5402977289,13.6556449019,3.7969509897
Br,9.2132903908,8.9329121201,1.8444696313
N,2.0805921557,12.2484702196,3.4859990784
N,2.145104996,11.1713636958,4.3090187661
N,4.9496754283,15.0179284585,4.3946959347
N,4.5966237664,15.7642484855,5.4714004887
N,4.6967424876,13.0622064849,2.000732304
N,2.8699307656,15.0367631781,2.235739995
C,0.9764423934,12.1136078954,2.7486180908
H,0.7146118712,12.868329541,2.0150407629
C,0.3117893818,10.9257180998,3.0987492871
H,-0.6061804868,10.534975598,2.6810457704
C,1.0879976579,10.3547148465,4.0961719134
H,0.9597270876,9.4369400222,4.6566908992
C,3.2651110623,11.1118375504,5.181485453
C,3.5024722561,10.0021834403,5.9901560221
H,2.8201365223,9.1526761222,6.0024151872
C,4.6484922696,9.9982132882,6.7881292483
H,4.8572030085,9.1433015053,7.4281699534
C,5.5204633241,11.0923193804,6.7579513986
H,6.4146426897,11.0883127171,7.3800127217
C,5.2552449835,12.1911137993,5.9330264967
H,5.9560956769,13.0290937926,5.9239156112
C,4.1226126354,12.2282232249,5.1106001503
C,6.1938741562,15.3655497433,4.0639666014
H,6.6877335542,14.8972496358,3.2190394839
C,6.6601131202,16.3556996804,4.9461730343
H,7.6250407786,16.8439955293,4.9368051572
C,5.6141976472,16.5814191407,5.8273478674
H,5.5294992437,17.2601111032,6.6670229927
C,3.2944102953,15.5448186255,5.9899938277
C,2.7949688806,16.295041869,7.0522474543
H,3.3919624729,17.0744974178,7.5245419904
C,1.5003685611,16.0292722771,7.5026353696
H,1.0891819508,16.6027450904,8.3309725785
C,0.7409173944,15.0303200151,6.8850059488
H,-0.269152965,14.8227644671,7.2361031627
C,1.2694081216,14.2922109257,5.8194334834
H,0.6538217888,13.5169024295,5.3571048305
C,2.5630202077,14.5304467484,5.3384179473
C,1.94780386,15.9948360759,2.3579091795
H,1.4756657682,16.0927488336,3.3361532163
C,1.5997279776,16.8327326326,1.2961999507
H,0.8439783814,17.5989976399,1.4460833389
C,2.2407830862,16.6740802624,0.068524196
H,1.9988448723,17.3203581294,-0.7718268293
C,3.205251814,15.6750603962,-0.0620082589
H,3.7526758018,15.5186778616,-0.9895723205
C,3.4863386062,14.8716093603,1.0410615278
C,4.4820359685,13.8087114908,0.968898757
H,5.0265683793,13.6770699137,0.029908899
C,5.7482197375,12.1110491949,1.946101963
C,6.9806768723,12.4394140367,1.3633303184
H,7.1517207404,13.4364410705,0.9549624102
C,8.0099697627,11.4988241403,1.3329751063
H,8.970246366,11.7543932975,0.889504299
C,7.7908059316,10.2385085337,1.8841683785
C,6.5733578325,9.897251242,2.4733488024
H,6.4184349061,8.9089103843,2.9015503151
C,5.5552537336,10.8457064292,2.5129379253
H,4.5974568309,10.5938154757,2.9639080636
P,7.1362786939,16.195875152,-0.5913133957
F,8.3192815598,15.0728980089,-0.4184113043
F,6.5165525492,15.7394166607,0.8757167587
F,8.068833376,17.3081127394,0.1542129413
F,5.9307552848,17.2918161711,-0.7479229707
F,7.7390497375,16.6270870884,-2.0437523782
F,6.1851421587,15.0593966924,-1.3216130239

State=1-A
HF=-2542.9047994

5a DCM PF6- Py_Immine side

07058 in DCM PF6- Py_Immine side
C30H24F6Ir1N6P1

0,1
Ir,3.5268516357,13.64758547,3.7999038395
N,2.0662434779,12.2420637067,3.486570452
N,2.1340352723,11.1596111779,4.302325216
N,4.940242226,15.0049303973,4.3975219029
N,4.5903715769,15.75235088,5.4740895619
N,4.6889534655,13.0693291012,2.0043739633
N,2.8611841982,15.0417337052,2.248624253
C,0.9609151123,12.1106445958,2.7504596836
H,0.6966970116,12.8702547469,2.022812411
C,0.2988671771,10.9191772665,3.0935801105
H,-0.6191137271,10.5295770506,2.6748236262
C,1.0778551502,10.3426494797,4.0856669779
H,0.9516285058,9.4207356542,4.6399126905
C,3.254593592,11.0974551031,5.1736743306
C,3.4932392831,9.9851995736,5.9781842664
H,2.8121298986,9.1347028658,5.9867600366
C,4.6390159526,9.9796587137,6.77643497
H,4.8488432469,9.1225515554,7.4132238833
C,5.5090861176,11.0754924337,6.7509046797
H,6.4029815948,11.0706573379,7.3734575746
C,5.2424939453,12.1769436041,5.9302977043
H,5.9424697713,13.0157039577,5.9250738965
C,4.110459092,12.2153995643,5.1071258121
C,6.1868363305,15.3451767586,4.0683605448
H,6.6792606419,14.8714389027,3.2255510612
C,6.6580995366,16.3317716843,4.952018851
H,7.6261954937,16.8137968742,4.944733313
C,5.612615584,16.5627953721,5.8324073795
H,5.5312771217,17.2392578846,6.6743004729
C,3.2880074806,15.5370098983,5.9934838559
C,2.7915836956,16.2936497669,7.0523917244
H,3.391001091,17.0754729522,7.5177930908
C,1.497460182,16.0321359561,7.5065813613
H,1.0882016813,16.6104691675,8.3324961786
C,0.7359399637,15.0304774324,6.8956894648
H,-0.2735711316,14.8254997142,7.249974176
C,1.2611945849,14.2869970246,5.8320861069
H,0.6439335581,13.5103814079,5.3741774806
C,2.553918453,14.5215505107,5.3462274172
C,1.9368114869,15.9973761336,2.3751254974
H,1.4506089201,16.0766762946,3.3482127907
C,1.6049228996,16.855577438,1.3249915819
H,0.8468439779,17.6189347094,1.4781196405
C,2.2662088534,16.7213332899,0.1048962159
H,2.0383850581,17.3849486371,-0.7258815263
C,3.2321319172,15.724354581,-0.0303281802
H,3.7949484769,15.585567153,-0.9517570411
C,3.4953785198,14.8985287665,1.0608367866
C,4.4890746812,13.8337525835,0.9829739266
H,5.0446962236,13.7171873567,0.0483990607
C,5.7400228298,12.1145889055,1.9474181835
C,6.9798466866,12.4517476546,1.3843209352
H,7.151322359,13.4552511536,0.9919326758
C,8.0042764486,11.5046174073,1.358891689
H,8.9680505195,11.7730248464,0.9295868682
C,7.7995907246,10.2269321547,1.8867298665
C,6.5613350207,9.8982036582,2.4494783098
H,6.3930852313,8.9055529974,2.8638326349
C,5.5365952167,10.8408002836,2.4920088837
H,4.5695970559,10.5876466771,2.9232210048
P,7.1754066067,16.1954591138,-0.6422795082
F,8.3336672805,15.0529312227,-0.4347011772
F,6.5543983506,15.8098351994,0.8418573626
F,8.1392027882,17.3134898672,0.0548240222
F,5.9956368255,17.313925396,-0.8356486881
F,7.7804108731,16.5580185544,-2.1136185675
F,6.1932323613,15.0566795803,-1.328098122
H,8.6029475631,9.4926697159,1.8669031829

State=1-A

8a DCM PF6- Py_Immine side

07016 iPr in DCM PF6- Py_Immine side
C27H26F6Ir1N6P1

0,1
Ir,1.1020508276,-0.3170714267,-0.104169471
N,2.1257724017,0.3416055373,-1.7531853986
N,3.021943433,1.3314069365,-1.5171080231
N,0.2873261255,-0.9804301332,1.6589909876
N,1.0352280753,-1.8928273418,2.3296524449
N,-0.5538640146,0.9402447861,-0.7269876297
N,-0.2633914021,-1.6963871814,-1.1180982935
C,2.181504466,0.0609510706,-3.0561716983
H,1.5438642862,-0.7106356397,-3.4741416496
C,3.1365331563,0.8836726781,-3.6788635769
H,3.4151757938,0.898339533,-4.7238647394
C,3.6491962017,1.6784624098,-2.6642027169
H,4.4048207441,2.4540592858,-2.6855686466
C,3.1141248253,1.786342731,-0.174575313
C,3.9728167081,2.8212479332,0.1892951492
H,4.6123339877,3.3118333082,-0.5439175374
C,3.9961487496,3.2229279748,1.5263032002
H,4.6576481792,4.0295550944,1.8359494439
C,3.168796572,2.585908316,2.4577459489
H,3.1875055074,2.8992640452,3.5008957141
C,2.3183049598,1.5475850168,2.0614590019
H,1.6837896987,1.0664668538,2.8095473841
C,2.2617423065,1.1187338355,0.7287571399
C,-0.8146539152,-0.767770723,2.3803193502
H,-1.5798252529,-0.0853827305,2.0244911035
C,-0.774875487,-1.5478097855,3.5494318992
H,-1.5183426771,-1.5973795929,4.3333618893
C,0.4181667138,-2.2501127363,3.4790319688
H,0.8569679153,-2.9723158531,4.1565460555
C,2.2445795136,-2.2975065916,1.7064014083
C,3.0740081458,-3.2601641456,2.2777997442
H,2.82661271,-3.7278621044,3.2303539483
C,4.2395499226,-3.6191445736,1.5977190913
H,4.9032812828,-4.3693090862,2.023120524
C,4.5455719353,-3.0117540167,0.3750472961
H,5.4558214402,-3.290400081,-0.1547655381
C,3.6930167847,-2.0450376183,-0.170955332
H,3.9589275514,-1.5823358051,-1.1245411341
C,2.5114873725,-1.661147336,0.4773358885
C,-0.1010497003,-3.0107458612,-1.2903772911
H,0.8507526455,-3.4287289867,-0.9606606065
C,-1.0903155193,-3.8133144829,-1.8612834935
H,-0.9119224683,-4.8783510014,-1.9826110632
C,-2.2924881743,-3.2271764668,-2.2550717359
H,-3.0859701911,-3.8291120874,-2.6918627744
C,-2.4655618856,-1.854600856,-2.0735798829
H,-3.3903980153,-1.3486492755,-2.345009051
C,-1.4265962165,-1.1213924919,-1.5060635736
C,-1.5235042579,0.3263217072,-1.302530446
H,-2.4266439096,0.8318188043,-1.6569468024
P,-5.1537752756,0.0808589786,0.1290485611
F,-5.1312933381,1.6328011699,0.6501409986
F,-3.5805662724,-0.0918151655,0.6039298493
F,-5.6512132102,-0.4199647957,1.6022526805
F,-5.1518013088,-1.4683462719,-0.4073292823
F,-6.7028598485,0.2555772414,-0.3577663437
F,-4.6324047839,0.5821226343,-1.3572619267
C,-0.6082932185,2.4085714064,-0.5613372773
C,-1.6575776595,2.7795560486,0.477697928
C,-0.8269736223,3.1106086889,-1.8950982572
H,0.3800686127,2.6953935691,-0.1772412777
H,-1.4409105519,2.2976407976,1.4404363003
H,-1.6573646995,3.8652498576,0.6310295548
H,-2.6626932637,2.4734502511,0.1557845046
H,-0.0876293349,2.7780000526,-2.6362780055
H,-1.8327407035,2.9260285566,-2.2950928238
H,-0.7172464434,4.1929321355,-1.7601610261

State=1-A
HF=-2417.1224997

References

[i] Daniel C.Harris and Michael D. Bertolucci " Symmetry and Spectroscopy: An introduction to Vibrational and Electronic Spectroscopy" Dover, Mineola, N.Y. (1989)