Supporting Information

Phosphorescent Ir(III) Complexes Bearing Double Benzyldiphenylphosphine Cyclometalates; Strategic Synthesis, Fundamental and Integration for White OLED Fabrication

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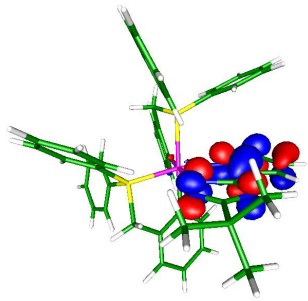
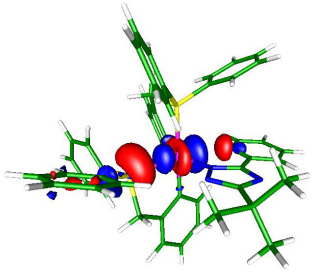
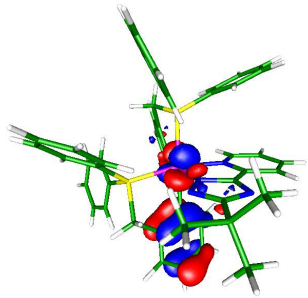
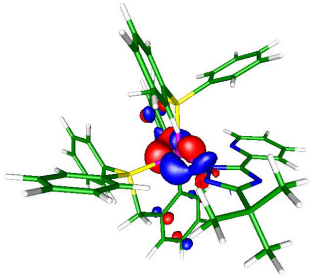
^{3}MLCT (net spin value located on Ir = 0.155)	^{3}MC (net spin value located on Ir = 1.285)
SOMO	SOMO
	
SOMO-1	SOMO-1
	

Figure S1. The frontier orbital distributions and net spin values located on central metal for ^{3}MLCT and ^{3}MC state geometries of complex **3**. (The singly occupied molecular orbital (SOMO) for the triplet electronic state is similar to the LUMO of ground state; while SOMO-1 is like HOMO.)

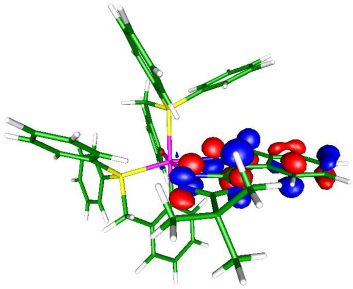
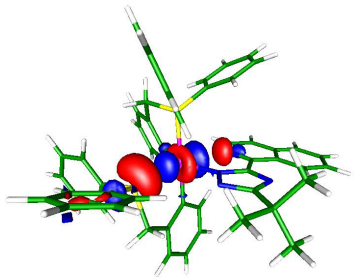
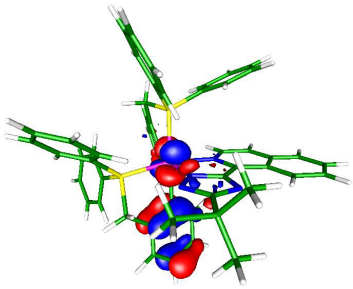
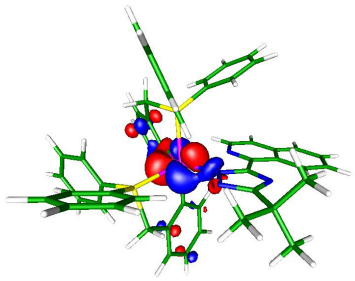
^{3}MLCT (net spin value located on Ir = 0.076)	^{3}MC (net spin value located on Ir = 1.295)
SOMO	SOMO
	
SOMO-1	SOMO-1
	

Figure S2. The frontier orbital distributions and net spin values located on central metal for ^{3}MLCT and ^{3}MC state geometries of complex **4**. (The singly occupied molecular orbital (SOMO) for the triplet electronic state is similar to the LUMO of ground state; while SOMO-1 is like HOMO.)

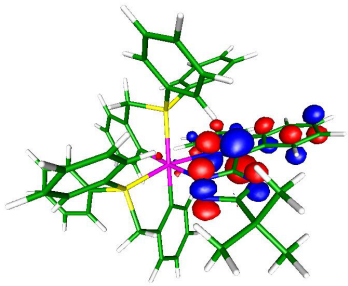
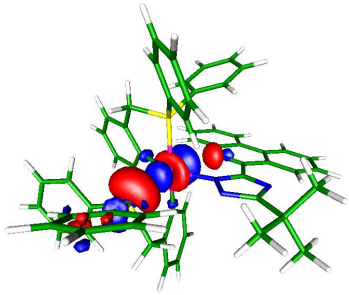
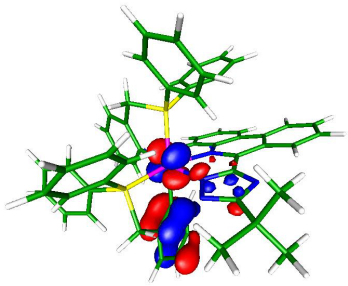
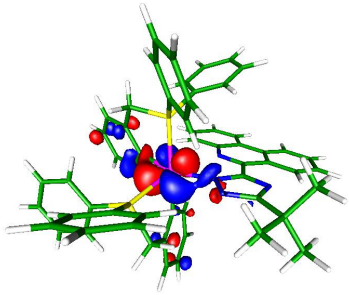
^{3}MLCT (net spin value located on Ir = 0.106)	^{3}MC (net spin value located on Ir = 1.316)
SOMO	SOMO
	
SOMO-1	SOMO-1
	

Figure S3. The frontier orbital distributions and net spin values located on central metal for ^{3}MLCT and ^{3}MC state geometries of complex **5**. (The singly occupied molecular orbital (SOMO) for the triplet electronic state is similar to the LUMO of ground state; while SOMO-1 is like HOMO.)

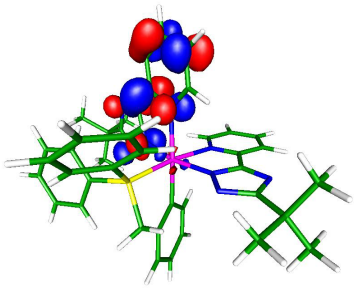
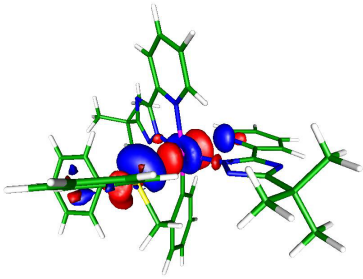
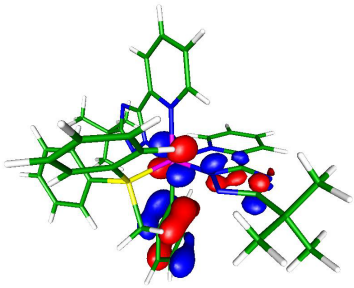
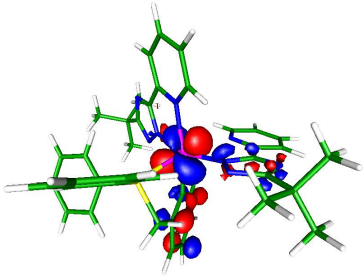
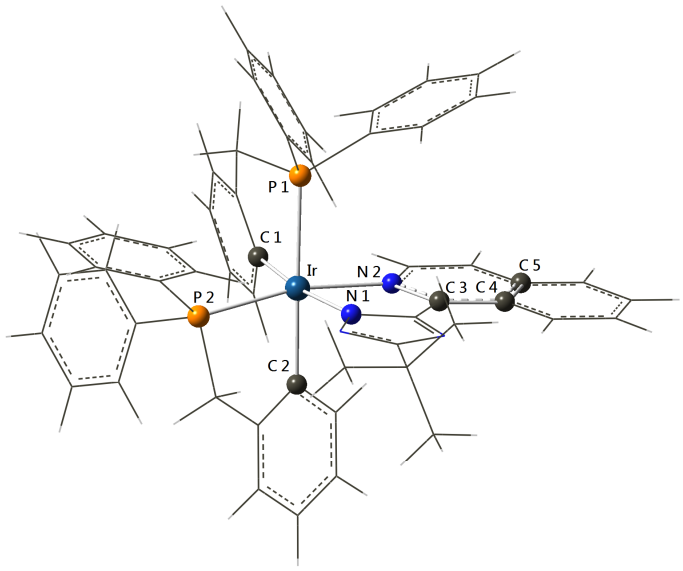
^{3}MLCT (net spin value located on Ir = 0.083)	^{3}MC (net spin value located on Ir = 1.230)
SOMO	SOMO
	
SOMO-1	SOMO-1
	

Figure S4. The frontier orbital distributions and net spin values located on central metal for ^{3}MLCT and ^{3}MC state geometries of complex **6**. (The singly occupied molecular orbital (SOMO) for the triplet electronic state is similar to the LUMO of ground state; while SOMO-1 is like HOMO.)

4



degree	Dihedral Angle (N_2-C_3-C_4-C_5)	Angle (P_1-Ir-N_2)	Angle (P_1-Ir-N_1)	Angle (P_1-Ir-C_1)	Angle (P_1-Ir-P_2)
	0.89	89.12	96.75	80.42	102.78

Figure S5. Structures and selected geometrical parameters of the lowest triplet state (T_1) for **4**.

5

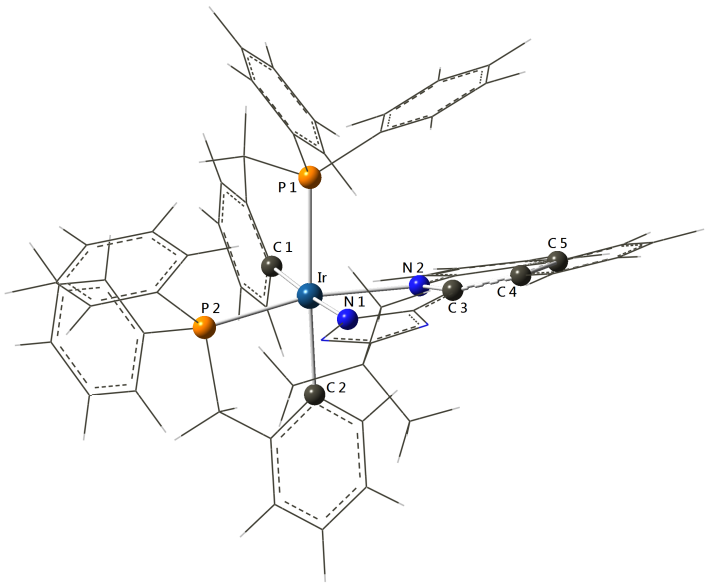


Figure S6. Structures and selected geometrical parameters of the lowest triplet state (T_1) for **5** respectively.

degree	Dihedral Angle (N_2-C_3-C_4-C_5)	Angle (P_1-Ir-N_2)	Angle (P_1-Ir-N_1)	Angle (P_1-Ir-C_1)	Angle (P_1-Ir-P_2)
	-5.63	85.40	97.17	79.52	104.61