Theoretical Research on the Effect of Regulated π-conjugation on Photophysical Properties of Ir(III) Complexes

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Table SI1. Molecular orbital compositions in the ground states for complexes **A-D**

Complexes	Orbital	MO composition (%)			
		Ir	C^N1	C^C*	C^N2
A	L+5	3	2	94	1
	L	2	82	1	14
	H	38	25	5	32
	H-2	2	48	18	33
	H-9	20	7	35	37
B	L+3	3	65	18	15
	L	2	14	1	82
	H	39	30	6	24
	H-2	2	35	16	47
	H-3	26	13	54	7
	H-6	9	17	21	53
C	L+1	2	95	1	2
	L	2	2	1	95
	H	33	37	4	26
	H-2	4	33	16	47
	H-3	31	23	34	12
D	L+2	1	30	1	68
	L	3	12	1	85
	H	38	32	4	25
	H-4	14	30	37	19
	H-8	9	30	46	15
	H-10	5	29	17	49

Table SI2. Molecular orbital compositions in the lowest-lying triplet states for **A-D**

Complexes	Orbital	MO composition (%)			
		Ir	C^N1	C^C*	C^N2
A	L	2	2	1	94
	H	27	23	4	47
	H-1	4	39	15	42
B	L	2	2	1	95
	H	27	21	5	48
	H-1	6	39	26	30
	H-2	12	9	64	16
C	L	2	70	1	27
	H	22	57	4	17
	H-1	10	37	11	42
D	L	2	82	1	15
	H	25	56	4	15
	H-1	26	27	32	15

Table SI3. The main transitions, oscillator strengths and vertical excitation energy of complex **A**

States	oscillator strength	Energy(eV)	Transition (CI)
T_1	-	2.4846	H-L (0.61)
			H-1-L(0.27)
T_2	-	3.3150	H-L+1(0.40)
			H-1-L+1(0.35)
			H-5-L+1(0.29)
			H-2-L+1(0.20)
S^1	0.1750	3.3168	H-L(0.68)
S_2	0.0626	3.8660	H-L+1(0.60)
			H-1-L+1(0.23)
S_3	0.0284	3.9724	H-1-L(0.52)
			H-5-L(0.20)
S_4	0.0211	4.1467	H-2-L(0.54)
			H-1-L(0.24)
			H-4-L(0.23)
S_5	0.1038	4.2706	H-3-L(0.60)
S_6	0.0655	4.4249	H-4-L(0.34)
S_7	0.0429	4.4634	H-1-L+1(0.57)
			H-L+1(0.22)
S_8	0.1761	4.5516	H-2-L+1(0.36)
			H-1-L+1(0.26)
			H-4-L(0.24)
S_9	0.1012	4.5636	H-2-L+1(0.31)
			H-4-L(0.26)

Table SI4. The main transitions, oscillator strengths and vertical excitation energy of complex **B**

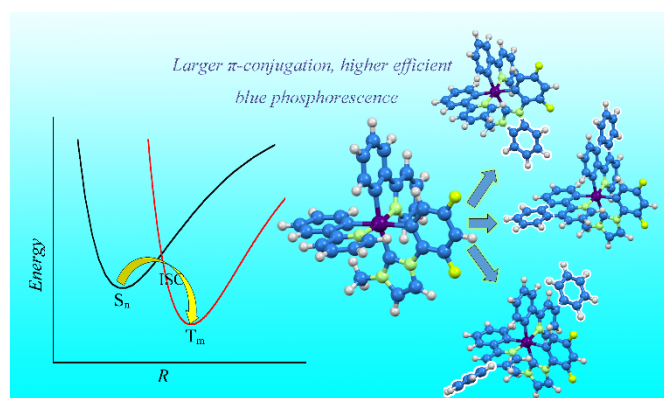| States	oscillator strength	Energy(eV)	Transition (CI)
T_1	-	2.4795	H-L(0.61)
			H-1-L(0.20)
			H-2-L(0.20)
T_2	-	3.3301	H-L+1(0.37)
			H-1-L+1(0.34)
			H-2-L+1(0.24)
			H-5-L+1(0.23)
S_1	0.1666	3.3284	H-L(0.68)
S_2	0.0527	3.9030	H-L+1(0.56)
			H-1-L+1(0.22)
			H-1-L(0.24)
S_3	0.0248	3.9665	H-1-L(0.48)
			H-3-L(0.23)
			H-L+1(0.22)
S_4	0.0116	4.1777	H-2-L(0.51)
			H-4-L(0.24)
			H-3-L(0.21)
S_5	0.1867	4.3080	H-3-L(0.46)
			H-4-L(0.38)
			H-1-L(0.26)
S_7	0.0512	4.4640	H-1-L+1(0.54)
			H-L+1(0.24)
S_8	0.1117	4.4942	H-5-L(0.20)
S_9	0.1053	4.5805	H-2-L+1(0.41)
			H-3-L+1(0.32)
			H-4-L+1(0.22)
S_{10}	0.0929	4.6042	H-5-L(0.24)
			H-4-L(0.20)

Table SI5. The main transitions, oscillator, strengths and vertical excitation energy of complex **C**

States	oscillator strength	Energy(eV)	Transition (CI)
T_1	-	2.6549	H-L(0.56)
			H-1-L(0.29(
T_2	-	3.2655	H-L(0.32)
			H-3-L(0.30)
			H-2-L(0.24)
			H-L+2(0.21)
S_1	0.1307	3.3008	H-L(0.66)
S_3	0.0007	3.9589	H-L+2(0.39)
			H-2-L(0.32)
			H-3-L(0.23)
S_4	0.4534	4.1112	H-L+2(0.47)
			H-1-L(0.30)
			H-2-L(0.29)
S_5	0.0112	4.1563	H-2-L(0.39)
			H-1-L(0.27)
S_6	0.0495	4.1883	H-1-L(0.33)
S_8	0.0297	4.3232	H-3-L(0.49)
			H-1-L(0.23)
S_{10}	0.0189	4.4596	H-5-L(0.56)
			H-4-L(0.21)

Table SI6. The main transitions, oscillator strengths and vertical excitation energy of complex **D**

States	oscillator strength	Energy(eV)	Transition (CI)
T_1	-	2.4938	H-L(0.57)
			H-2-L(0.23)
T_2	-	3.2610	H-L+1(0.36)
			H-2-L+1(0.34)
			H-5-L+1(0.22)
S_1	0.2225	3.2380	H-L(0.68)
S_2	0.1095	3.7326	H-L+1(0.61)
			H-2-L+1(0.22)
S_3	0.1685	3.9481	H-1-L(0.60)
			H-3-L(0.22)
S_4	0.0710	4.1123	H-2-L(0.61)
S_5	0.0052	4.2065	H-3-L(0.44)
			H-4-L(0.23)
			H-1-L(0.21)
S_6	0.0982	4.2501	H-3-L(0.39)
S_7	0.1000	4.3035	H-2-L+1(0.45)
			H-3-L+1(0.29)
			H-4-L+1(0.23)
S_8	0.0207	4.3438	H-1-L+1(0.62)
S_9	0.0862	4.4132	H-3-L+1(0.32)
S_{10}	0.3344	4.4703	H-4-L(0.51)

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Larger π-skeleton-conjugation in host ligands of Ir(III) carbene complexes can attain remarkably blue-shifted emission and effectively improve the quantum efficiency.