Electronic Supplementary Material (ESI) for Dalton Transactions.

The Influence of Numbers and Ligation Positions of Triphenylamine Unit on the Photophysical and Electroluminescent Properties of Homoleptic Iridium(III) Complexes: A Theoretical Perspective

Yuqi Liu,[a] Xiaobo Sun,[b] Ying Wang,*[a] and Zhijian Wu*[a]

[a] State Key Laboratory of Rare Earth Resource Utilization, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun 130022，People's Republic of China.

[b] Department of Applied Chemistry, Qingdao Agricultural University, Qingdao 266109, People's Republic of China.

* Corresponding authors. Email: ywang_2012@ciac.jl.cn (YW), zjwu@ciac.jl.cn (ZJW); *Tel: +86-431-85682801*

The method for calculating the MLCT contribution in T_1 state:

The MLCT contribution in T_1 state in our work was calculated according to Chou's work [Inorg. Chem., 2007, **46**, 10276, Ref.54]. In that study, the CT character in the HOMO-x→LUMO+y transitions is expressed as follows:

$$CT(M) = \%(M)HOMO\text{-}x - \%(M)LUMO+y \qquad (1)$$

where %(M)HOMO-x and %(M)LUMO+y are electronic densities on the metal in orbitals HOMO-x and LUMO+y. If the excited state is formed by more than one one-electron excitation, then the metal charge transfer (CT) character of this excited-state can be calculated as a sum of CT characters of each participating excitation, $i \rightarrow j$:

$$CT_I(M) = \sum[C_I(i \rightarrow j)]^2(\%(M)_i - \%(M)_j) \qquad (2)$$

where $C_I(i \rightarrow j)$ is the appropriate coefficient of the Ith eigenvector of the CT matrix. Therefore, one can use the MO compositions in terms of fragment orbital contributions to probe the nature of electronic transitions.

Table S1 Frontier molecular orbital energies (eV) and compositions (%) of different fragments in the ground state for complex **Ir(ppy)$_3$**

MO[a]	Energy/eV	MO composition(%)[b]				Assign
		Ir	ppy_1	ppy_2	ppy_3	
L+10	1.57	2	29	7	63	$\pi^*[ppy_1+ppy_3]$
L+9	1.43	2	33	33	33	π^*[ppy]
L+8	1.10	5	59	30	6	$\pi^*[ppy_1+ppy_2]$
L+7	1.10	5	4	33	57	$\pi^*[ppy_2+ppy_3]$
L+6	0.95	3	32	33	32	π^*[ppy]
L+5	-0.48	2	50	48	0	$\pi^*[ppy_1+ppy_2]$
L+4	-0.48	2	15	18	65	π^*[ppy]
L+3	-0.74	2	33	33	33	π^*[ppy]
L+2	-0.99	5	45	50	1	$\pi^*[ppy_1+ppy_2]$
L+1	-0.99	5	19	14	63	π^*[ppy]
L	-1.09	1	33	33	33	π^*[ppy]
H	-5.12	48	17	17	17	d(Ir)+π[ppy]
H-1	-5.25	40	35	8	18	d(Ir)+$\pi[ppy_1+ppy_3]$
H-2	-5.26	40	5	33	22	d(Ir)+$\pi[ppy_2+ppy_3]$
H-3	-6.11	3	7	30	60	$\pi[ppy_2+ppy_3]$
H-4	-6.11	3	58	35	4	$\pi[ppy_1+ppy_2]$
H-5	-6.22	2	32	33	32	π[ppy]
H-6	-6.77	22	26	26	26	d(Ir)+π[ppy]
H-7	-6.90	31	9	22	38	d(Ir)+$\pi[ppy_2+ppy_3]$
H-8	-6.90	31	37	24	8	d(Ir)+$\pi[ppy_1+ppy_2]$
H-9	-7.00	15	29	28	28	d(Ir)+π[ppy]
H-10	-7.42	13	12	38	38	d(Ir)+π[ppy]

[a] H = HOMO; L= LUMO; ppy_1, ppy_2 and ppy_3 are the same ligands, but in different positions, Figure 1.

Table S2 Frontier molecular orbital energies (eV) and compositions (%) of different fragments in the ground state for complex **1a**

MO[a]	Energy/eV	MO composition(%)[b]				Assign
		Ir	$(C^N)_1$	$(C^N)_2$	$(C^N)_3$	
L+10	-0.15	1	89	0	10	$\pi^*[(C^N)_1]$
L+9	-0.18	1	10	1	88	$\pi^*[(C^N)_3]$
L+8	-0.34	0	4	95	0	$\pi^*[(C^N)_2]$
L+7	-0.36	0	69	3	28	$\pi^*[(C^N)_1+(C^N)_3]$
L+6	-0.37	0	25	4	70	$\pi^*[(C^N)_1+(C^N)_3]$
L+5	-0.49	1	17	75	8	$\pi^*[(C^N)_1+(C^N)_2]$
L+4	-0.56	1	53	2	44	$\pi^*[(C^N)_1+(C^N)_3]$
L+3	-0.75	1	31	19	49	$\pi^*[(C^N)]$
L+2	-1.13	4	22	68	7	$\pi^*[(C^N)_1+(C^N)_2]$
L+1	-1.15	4	51	5	40	$\pi^*[(C^N)_1+(C^N)_3]$
L	-1.21	1	24	25	50	$\pi^*[(C^N)]$
H	-5.01	47	17	23	13	$d(Ir)+\pi[(C^N)]$
H-1	-5.11	40	29	27	5	$d(Ir)+\pi[(C^N)_1+(C^N)_2]$
H-2	-5.13	41	11	11	36	$d(Ir)+\pi[(C^N)]$
H-3	-5.26	1	0	98	1	$\pi[(C^N)_2]$
H-4	-5.42	0	100	0	0	$\pi[(C^N)_1]$
H-5	-5.43	0	0	0	100	$\pi[(C^N)_3]$
H-6	-5.97	3	24	70	3	$\pi[(C^N)_1+(C^N)_2]$
H-7	-6.01	3	54	14	30	$\pi[(C^N)]$
H-8	-6.12	3	19	15	63	$\pi[(C^N)]$
H-9	-6.62	19	27	32	22	$d(Ir)+\pi[(C^N)]$
H-10	-6.67	16	12	55	18	$d(Ir)+\pi[(C^N)]$

[a] H = HOMO; L= LUMO; [b] $(C^N)_1$, $(C^N)_2$ and $(C^N)_3$ are the same ligands, but in different positions, Figure 1.

Table S3 Frontier molecular orbital energies (eV) and compositions (%) of different fragments in the ground state for complex **1b**

MO[a]	Energy/eV	MO composition(%)[b]				Assign
		Ir	$(C^N)_1$	$(C^N)_2$	$(C^N)_3$	
L+10	-0.25	0	0	0	100	$\pi^*[(C^N)_3]$
L+9	-0.25	0	0	100	0	$\pi^*[(C^N)_2]$
L+8	-0.33	0	57	0	43	$\pi^*[(C^N)_1+(C^N)_3]$
L+7	-0.33	0	43	1	56	$\pi^*[(C^N)_1+(C^N)_3]$
L+6	-0.36	0	1	99	1	$\pi^*[(C^N)_2]$
L+5	-0.54	1	50	48	0	$\pi^*[(C^N)_1+(C^N)_2]$
L+4	-0.55	1	15	18	66	$\pi^*[(C^N)]$
L+3	-0.77	2	34	32	32	$\pi^*[(C^N)]$
L+2	-1.24	4	61	5	31	$\pi^*[(C^N)_1+(C^N)_3]$
L+1	-1.24	4	5	56	35	$\pi^*[(C^N)_2+(C^N)_3]$
L	-1.30	1	31	36	32	$\pi^*[(C^N)]$
H	-5.01	48	17	17	18	$d(Ir)+\pi[(C^N)]$
H-1	-5.13	40	6	22	32	$d(Ir)+\pi[(C^N)_2+(C^N)_3]$
H-2	-5.13	40	34	19	7	$d(Ir)+\pi[(C^N)_1+(C^N)_2]$
H-3	-5.34	0	99	0	1	$\pi[(C^N)_1]$
H-4	-5.35	0	1	2	97	$\pi[(C^N)_3]$
H-5	-5.35	0	0	97	2	$\pi[(C^N)_2]$
H-6	-6.01	3	31	5	61	$\pi[(C^N)_1+(C^N)_3]$
H-7	-6.01	3	31	61	5	$\pi[(C^N)_1+(C^N)_2]$
H-8	-6.12	3	35	32	31	$\pi[(C^N)]$
H-9	-6.58	15	30	25	29	$d(Ir)+\pi[(C^N)]$
H-10	-6.62	15	21	17	47	$d(Ir)+\pi[(C^N)]$

[a] H = HOMO; L= LUMO; [b] $(C^N)_1$, $(C^N)_2$ and $(C^N)_3$ are the same ligands, but in different positions, Figure 1.

Table S4 Frontier molecular orbital energies (eV) and compositions (%) of different fragments in the ground state for complex **1c**

MO[a]	Energy/eV	MO composition(%)[b]				Assign
		Ir	$(C^N)_1$	$(C^N)_2$	$(C^N)_3$	
L+10	-0.28	0	0	98	2	$\pi^*[(C^N)_2]$
L+9	-0.28	0	0	2	98	$\pi^*[(C^N)_3]$
L+8	-0.36	0	84	8	8	$\pi^*[(C^N)_1]$
L+7	-0.37	0	0	51	48	$\pi^*[(C^N)_2+(C^N)_3]$
L+6	-0.38	0	15	41	44	$\pi^*[(C^N)]$
L+5	-0.50	1	48	51	0	$\pi^*[(C^N)_1+(C^N)_2]$
L+4	-0.51	1	20	15	65	$\pi^*[(C^N)]$
L+3	-0.71	1	32	33	34	$\pi^*[(C^N)]$
L+2	-1.21	4	69	23	5	$\pi^*[(C^N)_1+(C^N)_2]$
L+1	-1.22	4	5	43	48	$\pi^*[(C^N)_2+(C^N)_3]$
L	-1.28	1	24	31	44	$\pi^*[(C^N)]$
H	-4.94	47	19	16	18	$d(Ir)+\pi[(C^N)]$
H-1	-5.04	38	33	18	11	$d(Ir)+\pi[(C^N)]$
H-2	-5.04	38	8	25	29	$d(Ir)+\pi[(C^N)_2+(C^N)_3]$
H-3	-5.35	1	48	28	23	$\pi[(C^N)]$
H-4	-5.37	2	45	41	12	$\pi[(C^N)]$
H-5	-5.37	2	6	29	63	$\pi[(C^N)_2+(C^N)_3]$
H-6	-5.95	3	65	18	14	$\pi[(C^N)]$
H-7	-5.96	3	2	46	50	$\pi[(C^N)_2+(C^N)_3]$
H-8	-6.06	3	31	33	34	$\pi[(C^N)]$
H-9	-6.58	19	27	27	26	$d(Ir)+\pi[(C^N)]$
H-10	-6.65	21	29	10	40	$d(Ir)+\pi[(C^N)]$

[a] H = HOMO; L= LUMO; [b] $(C^N)_1$, $(C^N)_2$ and $(C^N)_3$ are the same ligands, but in different positions, Figure 1.

Table S5 Frontier molecular orbital energies (eV) and compositions (%) of different fragments in the ground state for complex **2a**

MO[a]	Energy/eV	MO composition(%)[b]				Assign
		Ir	$(C^N)_1$	$(C^N)_2$	$(C^N)_3$	
L+10	-0.13	1	21	2	77	$\pi^*[(C^N)_1+(C^N)_3]$
L+9	-0.16	0	79	2	19	$\pi^*[(C^N)_1+(C^N)_3]$
L+8	-0.29	0	0	99	1	$\pi^*[(C^N)_2]$
L+7	-0.33	0	0	1	99	$\pi^*[(C^N)_3]$
L+6	-0.38	0	100	0	0	$\pi^*[(C^N)_1]$
L+5	-0.59	1	26	71	3	$\pi^*[(C^N)_1+(C^N)_2]$
L+4	-0.62	1	27	3	69	$\pi^*[(C^N)_1+(C^N)_3]$
L+3	-0.85	1	46	25	28	$\pi^*[(C^N)]$
L+2	-1.23	4	1	6	89	$\pi^*[(C^N)_3]$
L+1	-1.28	4	24	69	3	$\pi^*[(C^N)_1+(C^N)_2]$
L	-1.40	2	72	22	4	$\pi^*[(C^N)_1+(C^N)_2]$
H	-5.10	9	5	84	1	$\pi[(C^N)_2]$
H-1	-5.12	14	79	4	3	$d(Ir)+\pi[(C^N)_1]$
H-2	-5.17	23	8	16	53	$d(Ir)+\pi[(C^N)_2+(C^N)_3]$
H-3	-5.23	0	2	78	19	$\pi[(C^N)_2+(C^N)_3]$
H-4	-5.27	17	12	32	39	$d(Ir)+\pi[(C^N)]$
H-5	-5.34	1	1	0	97	$\pi[(C^N)_3]$
H-6	-5.39	28	50	15	7	$d(Ir)+\pi[(C^N)_1+(C^N)_2]$
H-7	-5.40	34	7	25	34	$d(Ir)+\pi[(C^N)_2+(C^N)_3]$
H-8	-5.48	5	92	2	1	$\pi[(C^N)_1]$
H-9	-6.24	5	4	68	23	$\pi[(C^N)_2+(C^N)_3]$
H-10	-6.28	6	31	12	52	$\pi[(C^N)]$

[a] H = HOMO; L= LUMO; [b] $(C^N)_1$, $(C^N)_2$ and $(C^N)_3$ are the same ligands, but in different positions, Figure 1.

Table S6 Frontier molecular orbital energies (eV) and compositions (%) of different fragments in the ground state for complex **2b**

MO[a]	Energy/eV	MO composition(%)[b]				Assign
		Ir	$(C^N)_1$	$(C^N)_2$	$(C^N)_3$	
L+17	0.17	0	1	48	51	$\pi^*[(C^N)_2+(C^N)_3]$
L+16	0.16	0	1	96	3	$\pi^*[(C^N)_2]$
L+15	0.14	0	96	1	3	$\pi^*[(C^N)_1]$
L+7	-0.42	0	35	39	26	$\pi^*[(C^N)]$
L+6	-0.42	0	34	27	38	$\pi^*[(C^N)]$
L+5	-0.72	0	37	9	54	$\pi^*[(C^N)_1+(C^N)_3]$
L+4	-0.74	2	26	47	26	$\pi^*[(C^N)]$
L+3	-0.96	0	38	24	37	$\pi^*[(C^N)]$
L+2	-1.38	1	7	39	53	$\pi^*[(C^N)_2+(C^N)_3]$
L+1	-1.40	3	38	41	18	$\pi^*[(C^N)]$
L	-1.45	2	37	36	25	$\pi^*[(C^N)]$
H	-4.65	0	12	51	37	$\pi[(C^N)]$
H-1	-4.67	0	39	37	24	$\pi[(C^N)]$
H-2	-4.71	0	64	23	13	$\pi[(C^N)]$
H-3	-5.40	0	27	18	55	$\pi[(C^N)]$
H-4	-5.40	0	57	25	18	$\pi[(C^N)]$
H-5	-5.40	0	23	51	25	$\pi[(C^N)]$
H-6	-5.56	0	22	62	16	$\pi[(C^N)]$
H-7	-5.68	0	18	62	20	$\pi[(C^N)]$
H-8	-5.70	0	30	55	15	$\pi[(C^N)]$
H-9	-6.23	0	11	47	41	$\pi[(C^N)]$
H-10	-6.24	0	59	23	18	$\pi[(C^N)]$

[a] H = HOMO; L= LUMO; [b] $(C^N)_1$, $(C^N)_2$ and $(C^N)_3$ are the same ligands, but in different positions, Figure 1.

Table S7 Frontier molecular orbital energies (eV) and compositions (%) of different fragments in the ground state for complex **2c**

MO[a]	Energy/eV	MO composition(%)[b]				Assign
		Ir	$(C^N)_1$	$(C^N)_2$	$(C^N)_3$	
L+13	0.12	1	42	27	31	π*[(C^N)]
L+12	0.07	1	17	61	21	π*[(C^N)]
L+8	-0.35	0	39	4	57	$\pi^*[(C^N)_1+(C^N)_3]$
L+7	-0.39	0	65	1	34	$\pi^*[(C^N)_1+(C^N)_3]$
L+6	-0.41	0	1	94	5	$\pi^*[(C^N)_2]$
L+5	-0.53	1	59	6	34	$\pi^*[(C^N)_1+(C^N)_3]$
L+4	-0.55	1	15	41	43	π*[(C^N)]
L+3	-0.77	2	24	55	20	π*[(C^N)]
L+2	-1.19	3	30	5	61	$\pi^*[(C^N)_1+(C^N)_3]$
L+1	-1.2	3	51	10	36	π*[(C^N)]
L	-1.28	2	6	86	6	$\pi^*[(C^N)_2]$
H	-4.64	4	60	12	24	π[(C^N)]
H-1	-4.66	4	46	11	39	π[(C^N)]
H-2	-4.69	1	39	53	7	$\pi[(C^N)_1+(C^N)_2]$
H-3	-5.08	42	27	12	19	d(Ir)+π[(C^N)]
H-4	-5.16	36	12	26	27	d(Ir)+π[(C^N)]
H-5	-5.17	34	26	18	23	d(Ir)+π[(C^N)]
H-6	-5.36	6	20	24	50	π[(C^N)]
H-7	-5.38	7	37	29	27	π[(C^N)]
H-8	-5.4	6	7	51	37	$\pi[(C^N)_2+(C^N)_3]$
H-9	-6.28	1	39	46	14	π[(C^N)]
H-10	-6.31	1	32	51	16	π[(C^N)]

[a] H = HOMO; L= LUMO; [b] $(C^N)_1$, $(C^N)_2$ and $(C^N)_3$ are the same ligands, but in different positions, Figure 1.

Table S8 Selected calculated wavelength (λ, in nm)/energies (E, in eV), oscillator strength (f), major contribution and transition characters for the studied complexes in toluene media, along with the experimental data for **2b** and **2c**

	state	λ/E	f	Configuration[a]	Assignment	Exptl[b]
Ir(ppy)$_3$	S_1	398/3.11	0.0172	H→L(95%)	d(Ir)+π[ppy]→π*[ppy]/MLCT/LLCT/IL	
	S_4	371/3.34	0.0626	H-1→L(91%)	d(Ir)+π[ppy$_1$+ppy$_3$]→π*[ppy]/MLCT/LLCT/IL	
	S_5	371/3.34	0.0624	H-2→L(91%)	d(Ir)+π[ppy$_2$+ppy$_3$]→π*[ppy]/MLCT/LLCT/IL	
	S_7	362/3.43	0.0628	H-1→L+1(40%)	d(Ir)+π[ppy$_1$+ppy$_3$]→π*[ppy]/MLCT/LLCT/IL	
				H-2→L+2(39%)	d(Ir)+π[ppy$_2$+ppy$_3$]→π*[ppy$_1$+ppy$_2$]/MLCT/LLCT/IL	
	S_8	362/3.43	0.0627	H-1→L+2(40%)	d(Ir)+π[ppy$_1$+ppy$_3$]→π*[ppy$_1$+ppy$_2$]/MLCT/LLCT/IL	
				H-2→L+1(39%)	d(Ir)+π[ppy$_2$+ppy$_3$]→π*[ppy]/MLCT/LLCT/IL	
	S_{10}	338/3.67	0.0885	H→L+3(60%)	d(Ir)+π[ppy]→π*[ppy]/MLCT/LLCT/IL	
	S_{19}	283/4.38	0.0817	H-3→L(78%)	π[ppy$_2$+ppy$_3$]→π*[ppy]/LLCT/IL	
	S_{20}	283/4.39	0.0816	H-4→L(78%)	π[ppy$_1$+ppy$_2$]→π*[ppy]/LLCT/IL	
	S_{21}	278/4.45	0.4597	H-4→L+1(23%)	π[ppy$_1$+ppy$_2$]→π*[ppy]/LLCT/IL	
				H-3→L+2(23%)	π[ppy$_2$+ppy$_3$]→π*[ppy$_1$+ppy$_2$]/LLCT/IL	
	S_{22}	277/4.48	0.0619	H-3→L+1(36%)	π[ppy$_2$+ppy$_3$]→π*[ppy]/LLCT/IL	
				H-4→L+2(35%)	π[ppy$_1$+ppy$_2$]→π*[ppy$_1$+ppy$_2$]/LLCT/IL	
	S_{23}	277/4.48	0.0619	H-4→L+1(36%)	π[ppy$_1$+ppy$_2$]→π*[ppy]/LLCT/IL	
				H-3→L+2(35%)	π[ppy$_2$+ppy$_3$]→π*[ppy$_1$+ppy$_2$]/LLCT/IL	
	S_{31}	257/4.83	0.0515	H-6→L+1(74%)	d(Ir)+π[ppy]→π*[ppy]/MLCT/LLCT/IL	
	S_{32}	257/4.83	0.0506	H-6→L+2(74%)	d(Ir)+π[ppy]→π*[ppy$_1$+ppy$_2$]/MLCT/LLCT/IL	
	S_{33}	255/4.85	0.0880	H-5→L+3(60%)	π[ppy]→π*[ppy]/LLCT/IL	
1a	S_1	415/2.99	0.0052	H→L(90%)	d(Ir)+π[(C^N)]→π*[(C^N)]/MLCT/LLCT/IL	
	S_4	391/3.17	0.1110	H-1→L(64%)	d(Ir)+π[(C^N)$_1$+(C^N)$_2$]→π*[(C^N)]/MLCT/LLCT/IL	
				H-2→L(21%)	d(Ir)+π[(C^N)]→π*[(C^N)]/MLCT/LLCT/IL	
	S_5	389/3.18	0.1252	H-2→L(66%)	d(Ir)+π[(C^N)]→π*[(C^N)]/MLCT/LLCT/IL	
				H-1→L(23%)	d(Ir)+π[(C^N)$_1$+(C^N)$_2$]→π*[(C^N)]/MLCT/LLCT/IL	
	S_7	383/3.24	0.0746	H-2→L+2(50%)	d(Ir)+π[(C^N)]→π*[(C^N)$_1$+(C^N)$_2$]/MLCT/LLCT/IL	
				H-1→L+1(21%)	d(Ir)+π[(C^N)$_1$+(C^N)$_2$]→π*[(C^N)$_1$+(C^N)$_3$]/MLCT/LLCT/IL	
	S_8	381/3.26	0.0825	H-1→L+2(49%)	d(Ir)+π[(C^N)$_1$+(C^N)$_2$]→π*[(C^N)$_1$+(C^N)$_2$]/MLCT/LLCT/IL	
				H-2→L+1(38%)	d(Ir)+π[(C^N)]→π*[(C^N)$_1$+(C^N)$_3$]/MLCT/LLCT/IL	
	S_9	378/3.28	0.0503	H-3→L+2(40%)	π[(C^N)$_2$]→π*[(C^N)$_1$+(C^N)$_2$]/LLCT/IL	
				H-3→L(32%)	π[(C^N)$_2$]→π*[(C^N)]/LLCT/IL	
	S_{13}	349/3.56	0.0937	H→L+3(75%)	d(Ir)+π[(C^N)]→π*[(C^N)]/MLCT/LLCT/IL	
	S_{19}	330/3.76	0.0678	H→L+5(84%)	d(Ir)+π[(C^N)]→π*[(C^N)$_1$+(C^N)$_2$]/MLCT/LLCT/IL	
	S_{27}	318/3.90	0.0557	H-3→L+3(48%)	π[(C^N)$_2$]→π*[(C^N)/LLCT/IL	
				H-3→L+5(27%)	π[(C^N)$_2$]→π*[(C^N)$_1$+(C^N)$_2$]/LLCT/IL	
	S_{31}	310/4.00	0.0688	H-3→L+6(74%)	π[(C^N)$_2$]→π*[(C^N)$_1$+(C^N)$_3$]/LLCT	
1b	S_1	422/2.94	0.0043	H→L(92%)	d(Ir)+π[(C^N)]→π*[(C^N)]/MLCT/LLCT/IL	
	S_4	396/3.13	0.1534	H-1→L(80%)	d(Ir)+π[(C^N)$_2$+(C^N)$_3$]→π*[(C^N)]/MLCT/LLCT/IL	

	S_5	396/3.13	0.1567	H-2→L(80%)	d(Ir)+π[(C^N)$_1$+(C^N)$_2$]→π*[(C^N)]/MLCT/LLCT/IL
	S_7	389/3.19	0.1047	H-1→L+1(34%)	d(Ir)+π[(C^N)$_2$+(C^N)$_3$]→π*[(C^N)$_2$+(C^N)$_3$]/MLCT/LLCT/IL
				H-2→L+2(31%)	d(Ir)+π[(C^N)$_1$+(C^N)$_2$]→π*[(C^N)$_1$+(C^N)$_3$]/MLCT/LLCT/IL
	S_8	389/3.19	0.1144	H-1→L+2(33%)	d(Ir)+π[(C^N)$_2$+(C^N)$_3$]→π*[(C^N)$_1$+(C^N)$_3$]/MLCT/LLCT/IL
				H-2→L+1(32%)	d(Ir)+π[(C^N)$_1$+(C^N)$_2$]→π*[(C^N)$_2$+(C^N)$_3$]/MLCT/LLCT/IL
	S_{13}	352/3.52	0.1278	H→L+3(79%)	d(Ir)+π[(C^N)]→π*[(C^N)]/MLCT/LLCT/IL
	S_{19}	335/3.70	0.0801	H→L+4(84%)	d(Ir)+π[(C^N)]→π*[(C^N)]/MLCT/LLCT/IL
	S_{21}	334/3.71	0.0790	H→L+5(83%)	d(Ir)+π[(C^N)]→π*[(C^N)$_1$+(C^N)$_2$]/MLCT/LLCT/IL
	S_{28}	311/3.99	0.1053	H-3→L+3(48%)	π[(C^N)$_1$]→π*[(C^N)]/LLCT/IL
	S_{29}	311/3.99	0.1169	H-4→L+3(31%)	π[(C^N)$_3$]→π*[(C^N)]/LLCT/IL
	S_{30}	310/4.00	0.1114	H-5→L+3(41%)	π[(C^N)$_2$]→π*[(C^N)]/LLCT/IL
	S_{31}	304/4.08	0.2649	H-5→L+6(46%)	π[(C^N)$_2$]→π*[(C^N)$_2$]/IL
				H-4→L+6(21%)	π[(C^N)$_3$]→π*[(C^N)$_2$]/LLCT
	S_{32}	303/4.09	0.3401	H-3→L+7(37%)	π[(C^N)$_1$]→π*[(C^N)$_1$+(C^N)$_3$]/LLCT/IL
	S_{33}	303/4.09	0.3263	H-4→L+8(27%)	π[(C^N)$_3$]→π*[(C^N)$_1$+(C^N)$_3$]/LLCT/IL
1c	S_1	423/2.93	0.0027	H→L(87%)	d(Ir)+π[(C^N)]→π*[(C^N)]/MLCT/LLCT/IL
	S_4	404/3.07	0.6873	H-2→L(47%)	d(Ir)+π[(C^N)$_2$+(C^N)$_3$]→π*[(C^N)]/MLCT/LLCT/IL
				H-1→L(27%)	d(Ir)+π[(C^N)]→π*[(C^N)]/MLCT/LLCT/IL
	S_5	403/3.07	0.6571	H-1→L(43%)	d(Ir)+π[(C^N)]→π*[(C^N)]/MLCT/LLCT/IL
				H-2→L(25%)	d(Ir)+π[(C^N)$_2$+(C^N)$_3$]→π*[(C^N)]/MLCT/LLCT/IL
	S_7	394/3.15	0.1112	H-1→L+2(35%)	d(Ir)+π[(C^N)]→π*[(C^N)$_1$+(C^N)$_2$]/MLCT/LLCT/IL
				H-2→L+1(33%)	d(Ir)+π[(C^N)$_2$+(C^N)$_3$]→π*[(C^N)$_2$+(C^N)$_3$]/MLCT/LLCT/IL
	S_8	393/3.15	0.0751	H-2→L+2(47%)	d(Ir)+π[(C^N)$_2$+(C^N)$_3$]→π*[(C^N)$_1$+(C^N)$_2$]/MLCT/LLCT/IL
				H-1→L+1(22%)	d(Ir)+π[(C^N)]→π*[(C^N)$_2$+(C^N)$_3$]/MLCT/LLCT/IL
	S_9	380/3.26	0.2702	H-1→L+2(28%)	d(Ir)+π[(C^N)]→π*[(C^N)$_1$+(C^N)$_2$]/MLCT/LLCT/IL
				H-2→L+1(26%)	d(Ir)+π[(C^N)$_2$+(C^N)$_3$]→π*[(C^N)$_2$+(C^N)$_3$]/MLCT/LLCT/IL
	S_{10}	363/3.42	0.4968	H-5→L(30%)	π[(C^N)$_2$+(C^N)$_3$]→π*[(C^N)]/LLCT/IL
	S_{11}	362/3.42	0.4867	H-4→L(27%)	π[(C^N)]→π*[(C^N)]/LLCT/IL
				H-3→L+2(26%)	π[(C^N)]→π*[(C^N)$_1$+(C^N)$_2$]/LLCT/IL
	S_{12}	362/3.42	0.4700	H-3→L(20%)	π[(C^N)]→π*[(C^N)]/LLCT/IL
				H→L+3(20%)	d(Ir)+π[(C^N)]→π*[(C^N)]/MLCT/LLCT/IL
	S_{16}	337/3.68	0.0394	H→L+4(72%)	d(Ir)+π[(C^N)]→π*[(C^N)]/MLCT/LLCT/IL
	S_{17}	336/3.69	0.0428	H→L+5(66%)	d(Ir)+π[(C^N)]→π*[(C^N)$_1$+(C^N)$_2$]/MLCT/LLCT/IL
2a	S_1	422/2.94	0.0013	H-1→L(40%)	d(Ir)+π[(C^N)$_1$]→π*[(C^N)$_1$+(C^N)$_2$]/MLCT/LLCT/IL
				H-4→L(22%)	d(Ir)+π[(C^N)]→π*[(C^N)$_1$+(C^N)$_2$]/MLCT/LLCT/IL
	S_2	412/3.01	0.0728	H→L(45%)	π[(C^N)$_2$]→π*[(C^N)$_1$+(C^N)$_2$]/LLCT/IL
				H-1→L+1(28%)	d(Ir)+π[(C^N)$_1$]→π*[(C^N)$_1$+(C^N)$_2$]/MLCT/LLCT/IL
	S_4	406/3.06	0.0840	H-2→L+1(31%)	d(Ir)+π[(C^N)$_2$+(C^N)$_3$]→π*[(C^N)$_1$+(C^N)$_2$]/MLCT/LLCT/IL
				H→L(22%)	π[(C^N)$_2$]→π*[(C^N)$_1$+(C^N)$_2$]/LLCT/IL
	S_8	388/3.19	0.1169	H-7→L(20%)	d(Ir)+π[(C^N)$_2$+(C^N)$_3$]→π*[(C^N)$_1$+(C^N)$_2$]/MLCT/LLCT/IL
				H-1→L+1(16%)	d(Ir)+π[(C^N)$_1$]→π*[(C^N)$_1$+(C^N)$_2$]/MLCT/LLCT/IL

	S_{12}	376/3.30	0.0845	H-5→L+2(31%)	π[(C^N)$_3$]→π*[(C^N)$_3$]/IL	
	S_{13}	375/3.31	0.0542	H-8→L(53%)	π[(C^N)$_1$]→π*[(C^N)$_1$+(C^N)$_2$]/LLCT/IL	
	S_{26}	344/3.60	0.0602	H-1→L+3(38%)	d(Ir)+π[(C^N)$_1$]→π*[(C^N)]/MLCT/LLCT/IL	
	S_{27}	341/3.63	0.0503	H-2→L+3(42%)	d(Ir)+π[(C^N)$_2$+(C^N)$_3$]→π*[(C^N)]/MLCT/LLCT/IL	
	S_{43}	308/4.03	0.0771	H-3→L+8(64%)	π[(C^N)$_2$+(C^N)$_3$]→π*[(C^N)$_2$]/LLCT/IL	
2b	S_1	470/2.64	0.0108	H→L(67%)	π[(C^N)]→π*[(C^N)]/LLCT/IL	
	S_4	449/2.76	0.0833	H→L+1(31%)	π[(C^N)]→π*[(C^N)]/LLCT/IL	424
				H-2→L(27%)	π[(C^N)]→π*[(C^N)]/LLCT/IL	
	S_5	448/2.77	0.0712	H-1→L(36%)	π[(C^N)]→π*[(C^N)]/LLCT/IL	
	S_{10}	396/3.13	0.0569	H→L+3(84%)	π[(C^N)]→π*[(C^N)]/LLCT/IL	
	S_{28}	344/3.61	0.1956	H-7→L(61%)	π[(C^N)]→π*[(C^N)]/LLCT/IL	
	S_{31}	341/3.64	0.1203	H-3→L+2(26%)	π[(C^N)]→π*[(C^N)$_2$+(C^N)$_3$]/LLCT/IL	
	S_{32}	340/3.64	0.0723	H-3→L+2(35%)	π[(C^N)]→π*[(C^N)$_2$+(C^N)$_3$]/LLCT/IL	
				H-8→L(25%)	π[(C^N)]→π*[(C^N)]/LLCT/IL	
	S_{36}	329/3.77	0.1543	H-8→L+2(52%)	π[(C^N)]→π*[(C^N)$_2$+(C^N)$_3$]/LLCT/IL	
				H-7→L+1(22%)	π[(C^N)]→π*[(C^N)]/LLCT/IL	
	S_{41}	311/3.98	0.0733	H→L+17(19%)	π[(C^N)]→π*[(C^N)$_2$+(C^N)$_3$]/LLCT/IL	
	S_{42}	311/3.98	0.0833	H→L+16(28%)	π[(C^N)]→π*[(C^N)$_2$]/LLCT/IL	
				H-1→L+16(18%)	π[(C^N)]→π*[(C^N)$_2$]/LLCT/IL	
	S_{43}	310/3.99	0.1185	H→L+7(16%)	π[(C^N)]→π*[(C^N)]/LLCT/IL	
				H-2→L+15(15%)	π[(C^N)]→π*[(C^N)$_1$]/LLCT/IL	
	S_{48}	307/4.03	0.1942	H-7→L+3(34%)	π[(C^N)]→π*[(C^N)]/LLCT/IL	307
	S_{49}	307/4.04	0.1095	H-1→L+7(36%)	π[(C^N)]→π*[(C^N)]/LLCT/IL	
	S_{50}	307/4.04	0.0822	H-1→L+7(15%)	π[(C^N)]→π*[(C^N)]/LLCT/IL	
2c	S_1	439/2.83	0.0748	H→L(39%)	π[(C^N)]→π*[(C^N)$_2$]/LLCT/IL	
				H-1→L(30%)	π[(C^N)]→π*[(C^N)$_2$]/LLCT/IL	
	S_2	431/2.88	0.1749	H→L+1(54%)	π[(C^N)]→π*[(C^N)]/LLCT/IL	
	S_3	431/2.88	0.1526	H→L+2(35%)	π[(C^N)]→π*[(C^N)$_1$+(C^N)$_3$]/LLCT/IL	
				H-1→L+2(28%)	π[(C^N)]→π*[(C^N)$_1$+(C^N)$_3$]/LLCT/IL	
	S_4	423/2.93	0.2992	H-2→L(71%)	π[(C^N)$_1$+(C^N)$_2$]→π*[(C^N)$_2$]/LLCT/IL	
	S_5	417/2.97	0.1100	H-1→L(43%)	π[(C^N)]→π*[(C^N)$_2$]/LLCT/IL	
	S_6	412/3.01	0.0949	H-1→L+2(35%)	π[(C^N)]→π*[(C^N)$_1$+(C^N)$_3$]/LLCT/IL	
	S_7	412/3.01	0.1591	H-1→L+1(40%)	π[(C^N)]→π*[(C^N)]/LLCT/IL	
				H-2→L+1(20%)	π[(C^N)$_1$+(C^N)$_2$]→π*[(C^N)]/LLCT/IL	
	S_9	397/3.12	0.0982	H-2→L+2(53%)	π[(C^N)$_1$+(C^N)$_2$]→π*[(C^N)$_1$+(C^N)$_3$]/LLCT/IL	
	S_{10}	394/3.14	0.3908	H-3→L(38%)	d(Ir)+π[(C^N)]→π*[(C^N)$_2$]/MLCT/LLCT/IL	
	S_{11}	388/3.20	0.2346	H-4→L(40%)	d(Ir)+π[(C^N)]→π*[(C^N)$_2$]/MLCT/LLCT/IL	
	S_{12}	386/3.21	0.3865	H-3→L+2(46%)	d(Ir)+π[(C^N)]→π*[(C^N)$_1$+(C^N)$_3$]/MLCT/LLCT/IL	376
	S_{13}	383/3.23	0.1700	H-5→L(22%)	d(Ir)+π[(C^N)]→π*[(C^N)$_2$]/MLCT/LLCT/IL	
	S_{14}	381/3.25	0.3516	H-4→L+1(16%)	d(Ir)+π[(C^N)]→π*[(C^N)]/MLCT/LLCT/IL	
				H-4→L+2(16%)	d(Ir)+π[(C^N)]→π*[(C^N)$_1$+(C^N)$_3$]/MLCT/LLCT/IL	

			H-3→L+1(15%)	d(Ir)+π[(C^N)]→π*[(C^N)]/MLCT/LLCT/IL	
S_{15}	378/3.28	0.1890	H-3→L+1(23%)	d(Ir)+π[(C^N)]→π*[(C^N)]/MLCT/LLCT/IL	
S_{16}	377/3.29	0.3301	H→L+3(49%)	π[(C^N)]→π*[(C^N)]/LLCT/IL	
S_{17}	375/3.31	0.0816	H-5→L+1(32%)	d(Ir)+π[(C^N)]→π*[(C^N)]/MLCT/LLCT/IL	
S_{18}	371/3.34	0.1839	H-1→L+3(38%)	π[(C^N)]→π*[(C^N)]/LLCT/IL	
			H→L+3(20%)	π[(C^N)]→π*[(C^N)]/LLCT/IL	
S_{19}	370/3.35	0.1504	H-4→L+2(17%)	d(Ir)+π[(C^N)]→π*[$(C^N)_1$+$(C^N)_3$]/MLCT/LLCT/IL	
S_{20}	369/3.36	0.1922	H-2→L+3(43%)	π[$(C^N)_1$+$(C^N)_2$]→π*[(C^N)]/LLCT/IL	
S_{21}	365/3.40	0.2480	H-5→L+2(48%)	d(Ir)+π[(C^N)]→π*[$(C^N)_1$+$(C^N)_3$]/MLCT/LLCT/IL	
S_{22}	358/3.46	0.2909	H-8→L(19%)	π[$(C^N)_2$+$(C^N)_3$]→π*[$(C^N)_2$]/LLCT/IL	
			H-2→L+3(19%)	π[$(C^N)_1$+$(C^N)_2$]→π*[(C^N)]/LLCT/IL	
S_{23}	357/3.48	0.2670	H-1→L+3(15%)	π[(C^N)]→π*[(C^N)]/LLCT/IL	
			H→L+5(14%)	π[(C^N)]→π*[$(C^N)_1$+$(C^N)_3$]/LLCT/IL	
S_{24}	354/3.51	0.1067	H-7→L+1(18%)	π[(C^N)]→π*[(C^N)]/LLCT/IL	
S_{45}	313/3.96	0.1875	H-1→L+12(55%)	π[(C^N)]→π*[(C^N)]/LLCT/IL	304
S_{48}	311/3.99	0.0517	H-5→L+7(16%)	d(Ir)+π[(C^N)]→π*[$(C^N)_1$+$(C^N)_3$]/MLCT/LLCT/IL	
S_{49}	310/3.99	0.1113	H→L+13(16%)	π[(C^N)]→π*[(C^N)]/LLCT/IL	

[a] H = HOMO; L= LUMO; [b] Experimental data from refs. 27-28

Table S9. The Cartesian coordinates for the optimized structures for **2a** in the ground states (S_0)

C	-2.77897600	-2.34478400	-3.61148200
C	-2.16268600	-1.23930900	-3.03843200
C	-1.19340600	-1.36895900	-2.03207700
C	-0.86955100	-2.68812700	-1.59289600
C	-1.45303700	-3.80856200	-2.22918300
C	-2.41225200	-3.62877800	-3.22116800
H	-3.53108800	-2.21156700	-4.38594900
H	-2.43351700	-0.24492400	-3.38096600
H	-2.85046400	-4.50691700	-3.68682400
C	0.05062400	-2.75311000	-0.44742300
C	0.40728700	-3.89425500	0.27992100
C	1.24083600	-3.82400600	1.39763700
H	0.03198000	-4.85353500	-0.04002300
C	1.33185200	-1.46625400	1.01789800
C	1.71209500	-2.56123200	1.77189500
H	1.67203200	-0.46935800	1.27837600
H	2.33904900	-2.41431900	2.64172600
N	0.52627400	-1.54523500	-0.04742600

C	-1.20564700	3.40645600	-3.81675500
C	-0.55600600	2.32275300	-3.24253400
C	-1.07903900	1.64675200	-2.12829600
C	-2.32746300	2.10129900	-1.60474800
C	-3.00230600	3.18023700	-2.22419500
C	-2.42955200	3.83450700	-3.30933800
H	-0.76769300	3.91706700	-4.67180800
H	0.39070800	1.99176700	-3.65865100
H	-2.96639200	4.66770400	-3.75451900
C	-2.77371700	1.41018200	-0.38503900
C	-3.96012500	1.63145600	0.32462600
C	-4.25230800	0.92967500	1.49348500
H	-4.67552500	2.34604100	-0.05179100
C	-2.15887700	-0.18188400	1.20888000
C	-3.30918800	0.00656800	1.95227400
H	-1.40535300	-0.89810800	1.51925700
H	-3.45456900	-0.55302100	2.86800400
C	1.77689800	3.01154500	1.52594600
C	0.85374800	2.22751100	0.86122200
C	2.40547000	1.54260900	-0.74563000
C	3.37955300	2.31557000	-0.10536700
C	3.08749000	3.05682500	1.03812500
H	1.48064600	3.56957800	2.40725600
H	-0.17261300	2.15274200	1.20632000
H	4.37605500	2.34841800	-0.51708700
C	2.58281900	0.71787200	-1.95201500
C	3.77935700	0.59727400	-2.69730600
C	3.82706200	-0.22764600	-3.81694300
C	1.51361200	-0.80858800	-3.50115400
C	2.69242900	-0.91994100	-4.22585600
H	4.76551500	-0.31177800	-4.35783200
H	0.63542400	-1.35616900	-3.82922700
H	2.73392600	-1.54899900	-5.11258300
N	-1.89215000	0.48583000	0.08099900
Ir	-0.18698000	0.13459000	-1.15080400
N	1.14966300	1.50441900	-0.22582500
C	1.42379800	-0.01507200	-2.34729300
C	4.16206000	3.82066400	1.71001000
C	5.40614200	3.20039300	1.89213900
C	3.99332700	5.13999900	2.18255100
C	6.45092900	3.83539500	2.55089600

H	5.53385600	2.18111100	1.53590900
C	5.05458600	5.77368400	2.84094000
C	6.26768600	5.12837400	3.03578500
H	7.39695000	3.32059000	2.69145700
H	4.91174100	6.79218500	3.18978200
H	7.07462800	5.64348400	3.54982100
C	-5.52377900	1.22060700	2.20052000
C	-6.48458200	0.23335700	2.49597600
C	-5.82075300	2.55389900	2.51550700
C	-7.70002100	0.60265300	3.07881200
C	-7.02559100	2.90935300	3.11014100
H	-5.08659800	3.32048700	2.28002900
C	-7.97347600	1.92877600	3.39057300
H	-8.43398900	-0.17518800	3.27121100
H	-7.22432100	3.95092500	3.34641900
H	-8.92264500	2.19417700	3.84783200
C	1.57337700	-5.07821800	2.11455400
C	2.87419800	-5.40664100	2.54759900
C	0.56038900	-6.03350700	2.29600600
C	3.12816200	-6.66741900	3.09437900
C	0.81696000	-7.27402600	2.86463600
H	-0.45116500	-5.78871900	1.98257700
C	2.11257000	-7.60076100	3.25670700
H	4.14747400	-6.89977200	3.39073500
H	0.00618600	-7.98548300	2.99368100
H	2.33032300	-8.57252500	3.69094000
N	2.78497100	5.85464200	1.98842800
N	-6.28145200	-1.13739200	2.15282200
N	3.97043700	-4.49800700	2.41623100
C	4.25555600	-3.61488200	3.47269200
C	5.07802300	-2.49476800	3.25722100
C	3.67418200	-3.78056600	4.73817100
C	5.32599800	-1.59400700	4.28376500
H	5.50986600	-2.32704900	2.27566700
C	3.92218500	-2.86186600	5.75500100
H	3.02673200	-4.63038700	4.92727200
C	4.75309100	-1.76740000	5.54329800
H	5.96428600	-0.73599900	4.08847500
H	3.45958400	-3.01580600	6.72658000
H	4.94635800	-1.05617500	6.34085400
C	4.94348000	-4.81738900	1.43410300

C	4.53132700	-5.09511000	0.12561300
C	6.30586600	-4.89473000	1.75064300
C	5.46628200	-5.43588500	-0.84542500
H	3.47773600	-5.03987200	-0.13212300
C	7.23478200	-5.22403300	0.76847700
H	6.63283200	-4.69489600	2.76681200
C	6.82261700	-5.49701200	-0.53407000
H	5.12215700	-5.63860400	-1.85578000
H	8.28819800	-5.28023500	1.03109700
H	7.55107000	-5.75268200	-1.29813100
C	2.26194500	6.02004400	0.68314500
C	3.10952200	6.04186500	-0.42850500
C	0.87834900	6.12337200	0.48505500
C	2.58012700	6.14694000	-1.71098900
H	4.18346100	5.95745600	-0.29218500
C	0.35979900	6.25020500	-0.79758300
H	0.21231700	6.09503900	1.34277400
C	1.20653300	6.25513100	-1.90448800
H	3.25694800	6.13732700	-2.56039500
H	-0.71629300	6.31910900	-0.93309400
H	0.79481200	6.32999400	-2.90657700
C	2.23854900	6.56288500	3.08060000
C	2.21793400	5.97613200	4.35372900
C	1.71611000	7.85365200	2.92315100
C	1.68810200	6.66560500	5.43825100
H	2.62808000	4.97887200	4.48714800
C	1.17412500	8.52788000	4.01134200
H	1.73644200	8.32109200	1.94362700
C	1.15697100	7.94302400	5.27571600
H	1.68161500	6.19238000	6.41672100
H	0.77477700	9.52873700	3.86871800
H	0.73708600	8.47655000	6.12348900
C	-5.55539200	-1.97250900	3.01843300
C	-4.92195900	-3.12422700	2.52125100
C	-5.39253600	-1.64854600	4.37205400
C	-4.15950600	-3.92524200	3.35974700
H	-5.02015900	-3.36843300	1.46760100
C	-4.61263600	-2.45319700	5.19982300
H	-5.87312200	-0.76148800	4.77300500
C	-3.99469300	-3.59729200	4.70614200
H	-3.67153500	-4.80608900	2.94902400

H	-4.49829500	-2.18010700	6.24579400
H	-3.38961800	-4.22263500	5.35592900
C	-7.10750400	-1.67305100	1.13352100
C	-7.76116600	-2.90129900	1.29669600
C	-7.29965700	-0.95219100	-0.05072900
C	-8.57078500	-3.40322200	0.28377200
H	-7.63134100	-3.46021500	2.21865700
C	-8.12359700	-1.45609400	-1.05046400
H	-6.79668600	-0.00001400	-0.19199700
C	-8.75975900	-2.68532000	-0.89453200
H	-9.06869600	-4.35895700	0.42648000
H	-8.24866300	-0.88130100	-1.96389800
H	-9.39457100	-3.08044600	-1.68253400
N	4.99881000	1.27394500	-2.34942600
N	-4.29277500	3.64848700	-1.79985300
N	-1.07068200	-5.15761700	-1.93083400
C	6.05370800	0.45801900	-1.88262400
C	7.39115200	0.68004700	-2.24044600
C	5.75280000	-0.64374600	-1.06574700
C	8.39281800	-0.16616200	-1.77576700
H	7.64524000	1.50651500	-2.89591700
C	6.75927900	-1.49597300	-0.62796800
H	4.71912500	-0.84386300	-0.79954100
C	8.08923200	-1.25953200	-0.96952000
H	9.42169400	0.02525900	-2.07073200
H	6.49780300	-2.36233600	-0.02535900
H	8.87301700	-1.92692100	-0.62293600
C	5.21676600	2.57290400	-2.85144000
C	6.10178600	3.44956000	-2.20059200
C	4.51915800	3.04037200	-3.97325500
C	6.30927000	4.73466200	-2.68594400
H	6.62932900	3.11629900	-1.31140800
C	4.72873600	4.33220500	-4.44546900
H	3.81869200	2.38367300	-4.47814900
C	5.63006600	5.18691600	-3.81647200
H	7.00494200	5.39007700	-2.16795100
H	4.18446400	4.66638400	-5.32522500
H	5.79913900	6.19022900	-4.19725400
C	0.15574500	-5.63312800	-2.43669600
C	0.83280400	-6.68996100	-1.80559500
C	0.75597600	-5.02044300	-3.54512600

C	2.05552300	-7.13584000	-2.29316500
H	0.39840000	-7.16175900	-0.92885500
C	1.98636200	-5.46609500	-4.01528100
H	0.25245100	-4.19427200	-4.03623500
C	2.64228700	-6.53104100	-3.40340600
H	2.55882200	-7.95619300	-1.78803600
H	2.43006500	-4.97575400	-4.87786200
H	3.59562000	-6.88571000	-3.78529100
C	-2.05280500	-6.01506000	-1.39692100
C	-2.16366200	-7.35702200	-1.78793700
C	-2.96874800	-5.50976000	-0.46023100
C	-3.15021400	-8.16939500	-1.24006200
H	-1.47983600	-7.75843100	-2.52901800
C	-3.96117200	-6.32796000	0.06724400
H	-2.90444700	-4.46588300	-0.16516200
C	-4.05626100	-7.66577900	-0.31017500
H	-3.21920600	-9.20552500	-1.56179700
H	-4.66919800	-5.91253100	0.78051900
H	-4.83052200	-8.30298100	0.10710100
C	-5.44178800	3.01989700	-2.31448500
C	-6.67162500	3.10861700	-1.63854800
C	-5.37423700	2.23661200	-3.47583800
C	-7.79927700	2.46650100	-2.13570700
H	-6.74126600	3.68316700	-0.71945700
C	-6.50783100	1.59031700	-3.95667800
H	-4.43101400	2.14276300	-4.00329200
C	-7.73104300	1.70640800	-3.30205700
H	-8.73820100	2.55470700	-1.59520100
H	-6.42972200	0.99634100	-4.86366100
H	-8.61697700	1.21358400	-3.69268500
C	-4.34443000	4.88652200	-1.12687000
C	-5.32204500	5.85012700	-1.41197900
C	-3.37379400	5.18049700	-0.15711600
C	-5.33638500	7.06076400	-0.72780700
H	-6.06611900	5.64883800	-2.17624300
C	-3.39139000	6.39930700	0.51240800
H	-2.60145700	4.44793100	0.05870300
C	-4.37534400	7.34675000	0.23888100
H	-6.10144900	7.79452600	-0.96872500
H	-2.63036400	6.60496200	1.26147700
H	-4.38914700	8.29587000	0.76668600

Table S10. The Cartesian coordinates for the optimized structures for **2b** in the ground states (S_0)

C	-3.21603900	-0.49118000	3.64031700
C	-1.96885000	-0.62409200	3.04443900
C	-1.59378600	0.12373200	1.91515600
C	-2.55477700	1.05269200	1.43422900
C	-3.80543300	1.20486800	2.04555900
C	-4.15231100	0.42456300	3.14198900
H	-1.26569100	-1.34149500	3.45797600
H	-4.53431200	1.91996200	1.67362700
C	-2.14986300	1.85153300	0.27825400
C	-2.91941500	2.84700000	-0.33075800
C	-2.43529100	3.56428200	-1.42303300
H	-3.89717200	3.08518000	0.07293700
C	-0.42883000	2.25974800	-1.23533700
C	-1.14508200	3.25325100	-1.87699700
H	0.57125600	1.98762700	-1.55817700
H	-0.71418000	3.76299700	-2.73261200
N	-0.90996600	1.56720200	-0.19612700
C	2.18493300	-2.74751200	3.54620100
C	1.73576700	-1.57337200	2.95664800
C	0.85783400	-1.57287100	1.85890600
C	0.45706800	-2.84938000	1.38123700
C	0.93294300	-4.03602500	1.95331900
C	1.79400500	-3.99617800	3.04360200
H	2.06035600	-0.62386900	3.37312400
H	0.63918800	-5.00758300	1.56525200
C	-0.47611900	-2.84798500	0.25553400
C	-1.07840100	-3.98062900	-0.30053000
C	-1.97977500	-3.87068900	-1.35764000
H	-0.87773100	-4.95544700	0.13021200
C	-1.62857900	-1.49858500	-1.25053400
C	-2.24780300	-2.58284800	-1.84371900
H	-1.81922800	-0.48560400	-1.59130700
H	-2.92031100	-2.42761800	-2.68076400
C	3.48768300	-0.52490700	-1.95785100
C	2.26950200	-0.62009900	-1.31119600
C	2.85424900	1.00338900	0.25127900
C	4.10620700	1.13558000	-0.35678800

C	4.44675700	0.37832400	-1.47583700
H	3.68102200	-1.13278800	-2.83574900
H	1.50394600	-1.31119300	-1.65030900
H	4.83666600	1.81232000	0.07267900
C	2.40161000	1.73888000	1.43106900
C	3.18763000	2.72338000	2.04351200
C	2.73290200	3.38034800	3.18051700
H	4.16504100	2.99088300	1.65120800
C	0.68244700	2.09096100	3.06434800
C	1.47107700	3.04628200	3.69117300
H	-0.29089400	1.85895100	3.48736100
N	-0.76774000	-1.61558800	-0.23283300
Ir	0.11508300	0.00854600	0.86696800
N	1.94856500	0.12170700	-0.24433500
C	1.11043200	1.40004200	1.91743100
C	5.76682300	0.51613200	-2.12591600
C	6.40947300	1.75887300	-2.19139700
C	6.39423400	-0.60405200	-2.67702300
C	7.65229800	1.86321100	-2.80660600
H	5.92428100	2.64340000	-1.78950500
C	7.63861400	-0.50034100	-3.30761900
C	8.26578700	0.75123000	-3.37024000
H	8.14271500	2.83079400	-2.86959000
H	9.22901600	0.84332000	-3.86225700
C	-2.64202400	-5.06384600	-1.92546300
C	-3.97254800	-4.98775500	-2.34650700
C	-1.95224200	-6.27564600	-2.05222700
C	-4.63231800	-6.10641400	-2.86694200
C	-2.59924200	-7.38457100	-2.58653400
H	-0.90907600	-6.34046500	-1.75711600
C	-3.92892300	-7.31339300	-2.98256400
H	-2.06404200	-8.32498400	-2.68609000
H	-4.43170500	-8.18976200	-3.37916000
C	-3.24831300	4.61192900	-2.07543100
C	-2.63417700	5.76259800	-2.57638900
C	-4.63716700	4.47304100	-2.19168700
C	-3.37943400	6.76482900	-3.20665900
C	-5.38216600	5.47242200	-2.80824300
H	-5.12609000	3.57373600	-1.82882900
C	-4.76729900	6.60775900	-3.32145700
H	-6.45754300	5.35636400	-2.91207900

H	-5.35411100	7.37655400	-3.81436800
H	-4.51972600	-4.05646900	-2.23691600
H	2.85272300	-2.71134200	4.40348100
H	-1.56441300	5.90150600	-2.45344900
H	-3.48150700	-1.09824300	4.50252100
H	5.92774500	-1.58085000	-2.59426700
H	1.11479700	3.55443100	4.58395500
N	8.24765200	-1.64040600	-3.86738700
N	3.53022200	4.37328200	3.81207200
N	-5.98251300	-6.02249700	-3.26051500
N	2.26509800	-5.19798100	3.63798800
N	-5.43690700	0.54816900	3.73872000
N	-2.74060100	7.91352800	-3.71330700
C	-6.58122200	0.47465000	2.92304700
C	-7.71364900	1.25852800	3.19016600
C	-6.60012800	-0.37344400	1.80551300
C	-8.83203300	1.18236400	2.36839900
H	-7.70869500	1.92940800	4.04385000
C	-7.71734400	-0.42922100	0.98083700
H	-5.72990500	-0.98574500	1.58921100
C	-8.84418700	0.34312500	1.25631200
H	-9.69743500	1.80047900	2.59438700
H	-7.70728500	-1.09613700	0.12202800
H	-9.71816100	0.29416600	0.61267000
C	-5.53120900	0.75580200	5.12856900
C	-6.57156800	0.18504200	5.87611200
C	-4.56452900	1.52186900	5.79480700
C	-6.64587600	0.39174900	7.24836900
H	-7.31775400	-0.42337400	5.37405400
C	-4.63971000	1.70812000	7.17012100
H	-3.75457000	1.96698000	5.22504800
C	-5.68148300	1.15098000	7.90783800
H	-7.45995200	-0.06095300	7.80891800
H	-3.87907400	2.30565000	7.66606100
H	-5.73959800	1.30327400	8.98173800
C	3.64510400	-5.36133000	3.86374500
C	4.11501100	-6.05827800	4.98670800
C	4.57881600	-4.80840900	2.97568400
C	5.47982900	-6.20736000	5.20119600
H	3.40234500	-6.47774300	5.69022400
C	5.94160500	-4.94957700	3.20959600

H	4.22606700	-4.26561300	2.10408600
C	6.40489000	-5.65331900	4.31867600
H	5.82152000	-6.75003600	6.07904300
H	6.64725800	-4.51190100	2.50794200
H	7.47079300	-5.76588500	4.49497400
C	1.34252400	-6.20910500	3.97177300
C	1.66205400	-7.56386500	3.80119100
C	0.07337500	-5.87339400	4.46427500
C	0.73988100	-8.55069600	4.13013800
H	2.63769600	-7.83586000	3.40974400
C	-0.84651000	-6.86768100	4.77474200
H	-0.18283400	-4.82706800	4.60023300
C	-0.52148300	-8.21318200	4.61558000
H	1.00863400	-9.59481900	3.99039400
H	-1.82376000	-6.58455200	5.15748300
H	-1.24120100	-8.98737700	4.86562900
C	-6.43465300	-6.74528700	-4.38988700
C	-7.65623200	-7.42787200	-4.35083300
C	-5.66938200	-6.78361900	-5.56183700
C	-8.10256500	-8.12749100	-5.46623400
H	-8.25008200	-7.40304800	-3.44201600
C	-6.11522600	-7.50136400	-6.66589200
H	-4.72496300	-6.24859200	-5.59897400
C	-7.33477600	-8.17356200	-6.62793300
H	-9.05305300	-8.65240700	-5.41982500
H	-5.50928100	-7.52158600	-7.56791800
H	-7.68361300	-8.72733800	-7.49478400
C	-6.89443900	-5.22045900	-2.53568100
C	-7.85276100	-4.45496700	-3.21193900
C	-6.85758900	-5.18289000	-1.13598400
C	-8.75912900	-3.67833900	-2.49936200
H	-7.88249900	-4.47665100	-4.29724900
C	-7.75428600	-4.38635100	-0.43290000
H	-6.12177000	-5.77920600	-0.60476800
C	-8.71474600	-3.63463300	-1.10737600
H	-9.49820800	-3.09309600	-3.04019600
H	-7.71051600	-4.36502100	0.65269600
H	-9.42170200	-3.02508400	-0.55169000
C	9.64671900	-1.82215000	-3.77096800
C	10.37155600	-2.31891700	-4.86110900
C	10.32498300	-1.51362500	-2.58538100

C	11.74509800	-2.50823800	-4.76036000
H	9.84999900	-2.55586000	-5.78369100
C	11.70163900	-1.68881400	-2.50102400
H	9.76659700	-1.13740400	-1.73325400
C	12.42017900	-2.19047500	-3.58390400
H	12.29274200	-2.89502400	-5.61573400
H	12.21265700	-1.44460400	-1.57347000
H	13.49447300	-2.33316000	-3.51140100
C	4.87718000	4.08977900	4.10968700
C	5.87063100	5.07047200	3.97450600
C	5.25243400	2.80531500	4.52921000
C	7.19673000	4.77344500	4.26729000
H	5.59521100	6.06548200	3.63819200
C	6.58341700	2.51522400	4.80340500
H	4.49102500	2.03882300	4.63690000
C	7.56601800	3.49543100	4.68041400
H	7.95021000	5.54925000	4.15584900
H	6.85066800	1.51310000	5.12896700
H	8.60430700	3.26618000	4.90250700
C	2.96668400	5.63498100	4.08217400
C	2.01070500	6.18337000	3.21540600
C	3.32816900	6.35724200	5.22910700
C	1.43454800	7.41743900	3.49263000
H	1.72185600	5.63178100	2.32598600
C	2.75747600	7.59765400	5.48737800
H	4.05584000	5.93696100	5.91678500
C	1.80503300	8.13783700	4.62558100
H	0.69474800	7.82247000	2.80673800
H	3.05115100	8.13911800	6.38317700
H	1.35607100	9.10421700	4.83637600
C	-3.35915300	9.18028900	-3.60172200
C	-3.30556000	10.08968300	-4.66510700
C	-4.02966300	9.54385100	-2.42741500
C	-3.90567400	11.33824700	-4.54876500
H	-2.79071000	9.81023700	-5.57951000
C	-4.64290000	10.78761700	-2.32809900
H	-4.06564300	8.84623300	-1.59590200
C	-4.58207200	11.69417700	-3.38403400
H	-3.85481700	12.03249800	-5.38340300
H	-5.15913300	11.05396600	-1.40958200
H	-5.05577800	12.66795300	-3.29980500

C	-1.46734200	7.80505100	-4.31895300
C	-0.47105100	8.75156600	-4.05200900
C	-1.18648800	6.75041600	-5.19711600
C	0.77615100	8.64510500	-4.65741800
H	-0.68231900	9.56861600	-3.36859000
C	0.06964200	6.64226800	-5.78295800
H	-1.95987100	6.02030100	-5.41759100
C	1.05759900	7.58923600	-5.52132200
H	1.53836600	9.38811700	-4.43821100
H	0.27024300	5.81891200	-6.46360300
H	2.03549700	7.50588500	-5.98660300
C	7.45615600	-2.61848000	-4.51321400
C	7.69974700	-3.98094200	-4.30310000
C	6.41956400	-2.23678100	-5.37452100
C	6.92412000	-4.93818900	-4.94767000
H	8.49991300	-4.28138100	-3.63323200
C	5.63792500	-3.20133500	-6.00019700
H	6.23481500	-1.18097200	-5.55013200
C	5.88627000	-4.55693200	-5.79492600
H	7.12585500	-5.99163800	-4.77266000
H	4.83877200	-2.88840500	-6.66716500
H	5.27830700	-5.30795900	-6.29097800

Table S11. The Cartesian coordinates for the optimized structures for **2c** in the ground states (S_0)

C	1.15018800	-3.36697800	3.22242800
C	1.08811700	-2.08971900	2.65170300
C	0.19392900	-1.77745800	1.61895800
C	-0.65841300	-2.82350000	1.16365500
C	-0.62091500	-4.09143900	1.76159400
C	0.26344400	-4.36682600	2.78443800
H	1.77346200	-1.32627900	3.00752100
H	-1.28967400	-4.88227500	1.42986400
H	0.28717200	-5.34933700	3.24441100
C	-1.52630800	-2.51192500	0.03786100
C	-2.47687000	-3.37470000	-0.52127700
C	-3.25385300	-2.98671500	-1.61061000
H	-2.63519500	-4.34965900	-0.07346600
C	-2.10245400	-0.88069600	-1.52131800
C	-3.04678500	-1.69361700	-2.11879500

H	-1.91732700	0.12615600	-1.88291800
H	-3.59647800	-1.33470500	-2.98257100
N	-1.35558700	-1.26773300	-0.48084300
C	2.30078000	2.49869500	3.33845100
C	1.26170700	1.74932800	2.77293900
C	1.44178700	0.96998600	1.62545100
C	2.75314600	0.91600000	1.07622300
C	3.79491100	1.66526100	1.64176900
C	3.57788900	2.46235000	2.74828100
H	0.28253400	1.77599700	3.23988300
H	4.79183700	1.64673500	1.20699700
H	4.38480400	3.05787800	3.16197800
C	2.93455500	0.03587500	-0.06780400
C	4.15170900	-0.23384100	-0.70470200
C	4.22755000	-1.12822400	-1.77051400
H	5.05871000	0.22801500	-0.32994300
C	1.86055900	-1.44595900	-1.51074400
C	3.03440400	-1.75098600	-2.17357600
H	0.91748200	-1.90446800	-1.79243600
H	3.01782800	-2.44445600	-3.00788700
C	0.07939300	3.40278500	-2.17694900
C	0.37336500	2.22232900	-1.52090200
C	-1.43265000	2.45466700	-0.06936600
C	-1.77469900	3.65915300	-0.69431600
C	-1.02892000	4.15830500	-1.76148700
H	0.69044400	3.71766400	-3.01632400
H	1.22184200	1.61229400	-1.81555100
H	-2.61253700	4.23348300	-0.31450200
C	-2.12620400	1.86090500	1.06695500
C	-3.29893600	2.40950800	1.60607400
C	-3.91616100	1.82569500	2.69550300
H	-3.73987000	3.30764700	1.17932200
C	-2.18344000	0.12676000	2.73050600
C	-3.35060900	0.67653200	3.26790000
H	-4.82278500	2.24811400	3.11768300
H	-1.77703400	-0.77017600	3.18944000
N	1.79733500	-0.57383700	-0.49780000
Ir	0.03973200	-0.04505500	0.60661900
N	-0.35607400	1.74929200	-0.50364700
C	-1.54545800	0.68099700	1.61292900
C	-1.38314200	5.42964200	-2.41645300

C	-2.71885700	5.83145300	-2.55512600
C	-0.39432700	6.28591100	-2.91991000
C	-3.05550300	7.02665500	-3.17075700
H	-3.51417100	5.17492000	-2.21179000
C	-0.71790800	7.49263400	-3.52009800
C	-2.05785500	7.88351500	-3.65911700
H	-4.09920100	7.30155600	-3.28706100
H	0.06992900	8.14967700	-3.87495500
C	5.51000100	-1.41962000	-2.43476200
C	5.80658300	-2.70470000	-2.90829200
C	6.48254100	-0.42581400	-2.60948800
C	7.02144100	-2.99311800	-3.51037800
C	7.69127400	-0.69621500	-3.23101400
H	6.27195500	0.59107500	-2.28838700
C	7.98704700	-1.99040700	-3.68551500
H	7.23601400	-4.00582000	-3.83684300
H	8.41559500	0.09926300	-3.37515200
C	-4.25564400	-3.89277600	-2.20218400
C	-5.45832100	-3.40027100	-2.72630500
C	-4.04208100	-5.27636200	-2.26181700
C	-6.40445900	-4.24507500	-3.28598300
C	-4.98476500	-6.13185700	-2.81109000
H	-3.11251100	-5.69235800	-1.88241400
C	-6.18424400	-5.62907100	-3.33526700
H	-7.32793200	-3.83672900	-3.68461300
H	-4.79417700	-7.20011300	-2.84151800
N	-3.97293000	0.07660300	4.39112500
N	2.08358800	3.29585900	4.48061100
N	2.10070300	-3.68308100	4.21642200
C	3.13147900	3.50137800	5.41019200
C	3.92402200	2.42980900	5.83786900
C	3.38354500	4.78204400	5.91686400
C	4.95587500	2.64408500	6.74506800
H	3.72291200	1.43191300	5.46035600
C	4.40592500	4.98303500	6.83751900
H	2.77046200	5.61434100	5.58350000
C	5.20220200	3.91791600	7.25333400
H	5.56231800	1.80065900	7.06577500
H	4.58908600	5.98347600	7.22109700
H	6.00546800	4.07912500	7.96691500
C	0.82062500	3.86950900	4.74612100

C	0.32538000	3.90727300	6.05660400
C	0.04809500	4.42115800	3.71570700
C	-0.91153100	4.48341400	6.32592600
H	0.91981600	3.48417500	6.86100700
C	-1.19530500	4.97664800	3.99203900
H	0.42268500	4.39680700	2.69722900
C	-1.68422000	5.01598100	5.29636500
H	-1.27839700	4.50195500	7.34905200
H	-1.78343800	5.38944000	3.17673100
H	-2.65518500	5.45467200	5.50761700
C	-3.20382600	-0.19468400	5.54280800
C	-3.37876900	-1.38956300	6.25301800
C	-2.25916400	0.73539200	5.99347300
C	-2.63378400	-1.63847500	7.39962500
H	-4.10219200	-2.11744300	5.89769000
C	-1.51308200	0.47245500	7.13668600
H	-2.12127700	1.66700700	5.45230600
C	-1.69609900	-0.71076800	7.85023400
H	-2.77930600	-2.57165000	7.93765900
H	-0.79449100	1.21435800	7.47610500
H	-1.11389300	-0.90967200	8.74570600
C	-5.35577300	-0.17768300	4.37047800
C	-5.98628700	-0.55527800	3.17555100
C	-6.13269400	-0.05389400	5.53185700
C	-7.35491200	-0.79370600	3.14775200
H	-5.39146300	-0.66303900	2.27357400
C	-7.49800400	-0.31094600	5.49472600
H	-5.65872100	0.24694100	6.46107100
C	-8.12244100	-0.67852600	4.30483400
H	-7.82209400	-1.08728200	2.21096700
H	-8.08093200	-0.20762200	6.40660600
H	-9.19093800	-0.87277200	4.28001400
C	2.50600800	-2.73486900	5.18100300
C	3.85074000	-2.65661400	5.56781100
C	1.57520800	-1.87797800	5.78168700
C	4.24943500	-1.75730500	6.54966800
H	4.57857800	-3.30985200	5.09620900
C	1.98852200	-0.96803800	6.74727600
H	0.52970100	-1.92739900	5.49275600
C	3.32234600	-0.90607900	7.14693800
H	5.29643100	-1.71704700	6.84011500

H	1.24952900	-0.31267100	7.19823400
H	3.63395000	-0.19774100	7.90955600
C	2.70592600	-4.96106100	4.21793400
C	3.14006100	-5.54473400	3.02099100
C	2.88493900	-5.66034000	5.41832100
C	3.72954500	-6.80367600	3.02807500
H	3.00924500	-5.00154900	2.08986400
C	3.49072700	-6.91151500	5.41769700
H	2.54692100	-5.21215800	6.34796100
C	3.91271900	-7.49408700	4.22438400
H	4.06164900	-7.24128500	2.09003600
H	3.62062500	-7.44057200	6.35835800
H	4.37963300	-8.47501600	4.22698200
H	-5.66628500	-2.33450100	-2.68105000
N	-7.14341700	-6.49112000	-3.89613900
C	-6.73708900	-7.63257200	-4.62626200
C	-7.39694100	-8.85511600	-4.45280900
C	-5.67662100	-7.55378500	-5.53737000
C	-7.00525700	-9.97148300	-5.18283200
H	-8.21708500	-8.92130200	-3.74414300
C	-5.28041100	-8.68032800	-6.24911300
H	-5.16758700	-6.60542600	-5.68229800
C	-5.94312400	-9.89414400	-6.08097500
H	-7.52774700	-10.91307600	-5.03608800
H	-4.45539400	-8.60235000	-6.95229900
H	-5.63538900	-10.77036400	-6.64428700
C	-8.52353200	-6.22786600	-3.72865200
C	-9.02221700	-5.80433300	-2.49068400
C	-9.40975200	-6.39629400	-4.79928100
C	-10.37915400	-5.54490300	-2.33496000
H	-8.34002700	-5.68127800	-1.65468100
C	-10.76768800	-6.15220300	-4.62845300
H	-9.02582400	-6.72126000	-5.76173200
C	-11.26093100	-5.72070100	-3.39913600
H	-10.75027400	-5.21732500	-1.36745200
H	-11.44257300	-6.28816700	-5.46940600
H	-12.32153900	-5.52437100	-3.27135900
H	0.65359500	6.02504000	-2.79722700
N	-2.39360700	9.10264600	-4.27117600
C	-1.61485300	9.60469000	-5.34079700
C	-1.27745400	10.96231500	-5.39234900

C	-1.17932600	8.75407100	-6.36411100
C	-0.52441800	11.45616400	-6.45141900
H	-1.61055400	11.62396500	-4.59833900
C	-0.41119000	9.25387800	-7.40951500
H	-1.44757000	7.70215000	-6.33262100
C	-0.08226200	10.60663200	-7.46311100
H	-0.27044200	12.51255000	-6.47668900
H	-0.08085600	8.58079600	-8.19627900
H	0.51179800	10.99482600	-8.28539500
C	-3.50079000	9.85336300	-3.80857600
C	-4.37022800	10.46337200	-4.72053100
C	-3.73535400	10.00405500	-2.43653600
C	-5.44814200	11.21354100	-4.26443900
H	-4.19237300	10.34600400	-5.78537400
C	-4.82649200	10.74098000	-1.99039300
H	-3.05730300	9.54115000	-1.72564300
C	-5.68682900	11.35340100	-2.89906500
H	-6.11397300	11.68102300	-4.98502000
H	-4.99469600	10.84896200	-0.92215400
H	-6.53404100	11.93456800	-2.54661500
H	5.09034300	-3.50849900	-2.75872100
N	9.22039700	-2.27194000	-4.29491600
C	10.39368600	-1.59361000	-3.88318000
C	10.66628100	-1.39762100	-2.52426300
C	11.30266900	-1.12211800	-4.83724900
C	11.82194600	-0.73089800	-2.13268500
H	9.96782900	-1.77087900	-1.78109100
C	12.46442800	-0.47265800	-4.43569600
H	11.09129800	-1.27200600	-5.89190100
C	12.72927500	-0.26828200	-3.08330900
H	12.02018200	-0.58640800	-1.07396300
H	13.16075900	-0.11243700	-5.18832600
H	13.63444000	0.24564800	-2.77291300
C	9.32050300	-3.26115800	-5.30191100
C	10.38774800	-4.16703200	-5.29309600
C	8.36621100	-3.34147600	-6.32337500
C	10.49821100	-5.12878200	-6.29060800
H	11.12789600	-4.10938600	-4.50059600
C	8.47549000	-4.31844500	-7.30663100
H	7.54195600	-2.63445900	-6.33941000
C	9.54209600	-5.21480700	-7.30002100

H	11.33267500	-5.82468700	-6.26905000
H	7.72688100	-4.36771900	-8.09298900
H	9.62748600	-5.97171300	-8.07435600

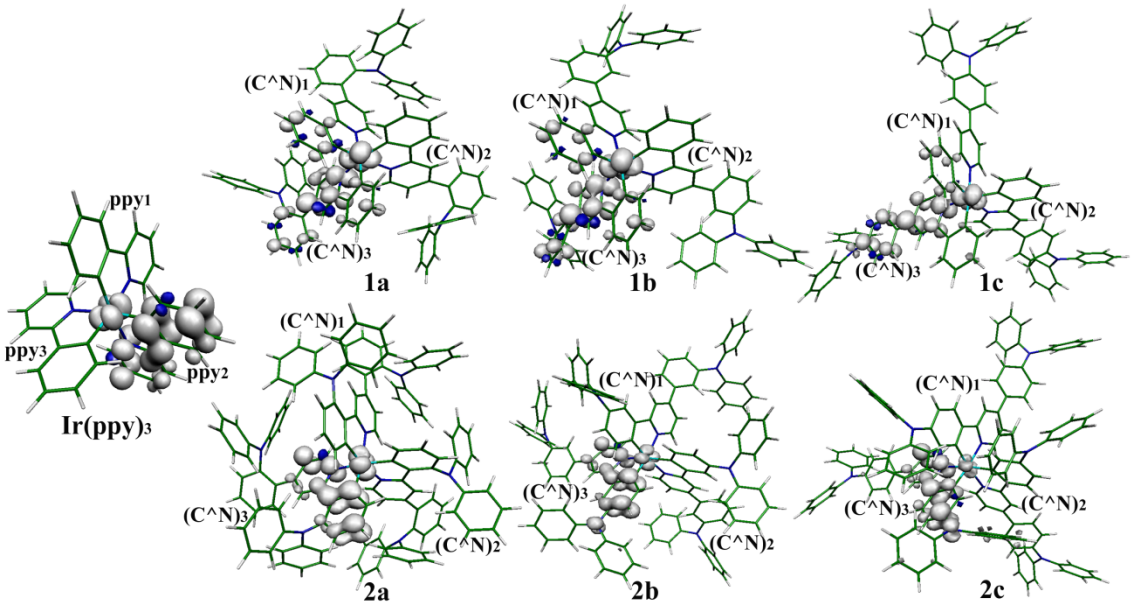

Figure S1. Spin-density contours of the studied complexes in the triplet electronic configuration.

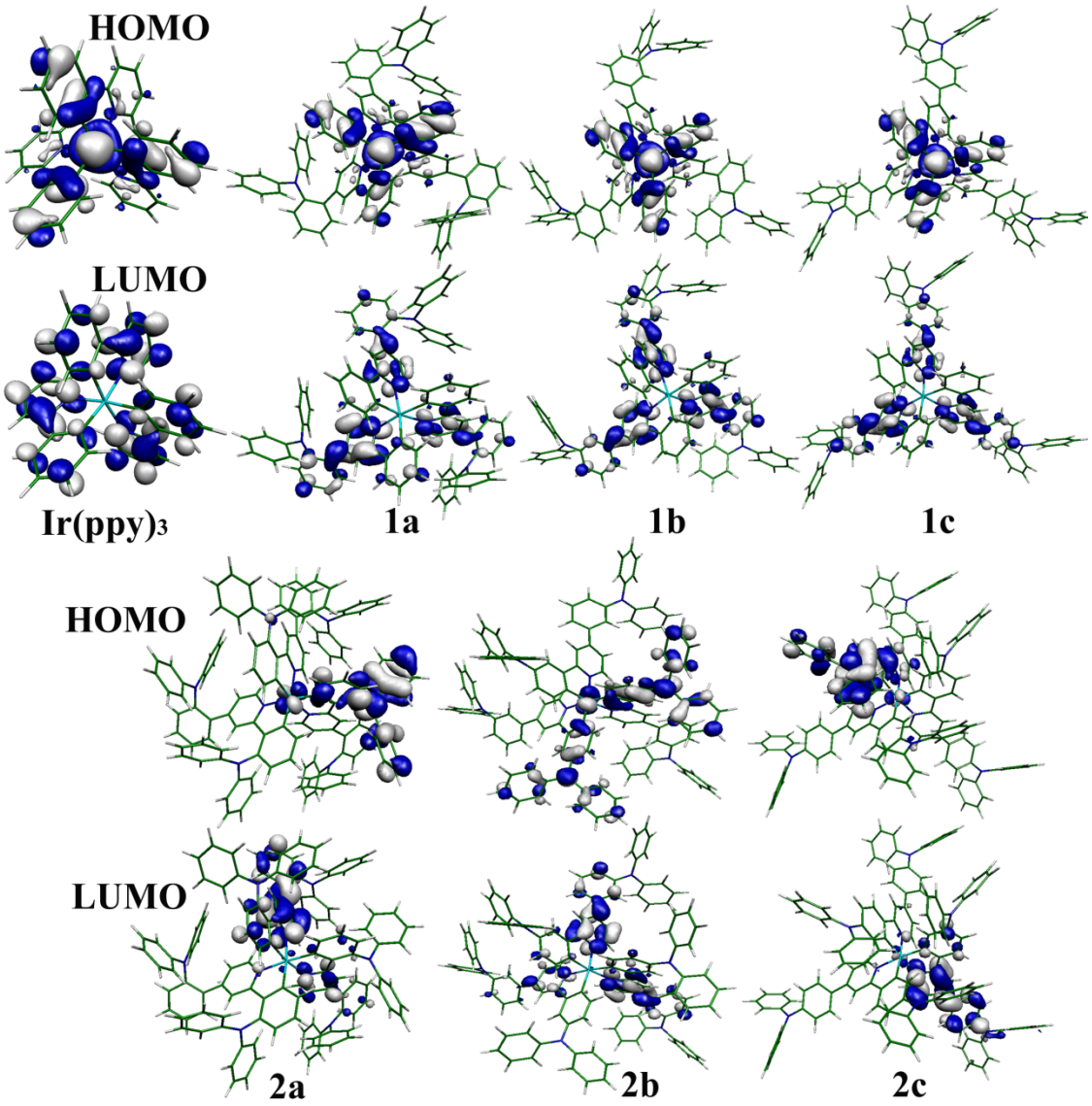

Figure S2. Contour plots of HOMO and LUMO for the studied complexes obtained from DFT calculations at their S_0 optimized geometries.