Supporting Information

A theoretical study on the electronic and photophysical properties of two series of iridium(III) complexes with different substituted N^N ligand[†]

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MO	Energy		Сс	ontribution (%	b)	Assignment
		Ir	C^N	pyrapy	mbiphpyrapy	
L+8	-2.31	2	12	8	78	π^* (mbiphpyrapy)
L+7	-2.68	1	4	78	17	π^* (pyrapy)
L+6	-2.88	0	5	8	87	π^* (mbiphpyrapy)
L+5	-3.24	2	95	1	3	π*(C^N)
L+4	-3.35	2	91	6	1	π*(C^N)
L+3	-3.82	1	16	83	0	$\pi^*(C^N+pyrapy)$
L+2	-3.87	4	87	9	1	π*(C^N)
L+1	-4.01	5	92	3	0	π*(C^N)
L	-4.56	3	2	95	1	$\pi^*(\text{ pyrapy})$
Н	-7.41	0	0	0	100	π (mbiphpyrapy)
H-1	-8.14	0	0	0	100	π (mbiphpyrapy)
Н-2	-8.18	0	0	0	100	π (mbiphpyrapy)
Н-3	-8.34	0	2	0	97	π (mbiphpyrapy)
H-4	-8.47	31	66	1	1	$d(Ir)+\pi(C^N)$
Н-5	-8.81	4	91	1	5	π(C^N)
H-6	-8.85	0	3	0	97	π (mbiphpyrapy)
H-7	-8.91	8	89	1	3	π(C^N)
H-8	-8.98	0	0	0	99	π (mbiphpyrapy)

Table S1Frontier molecular orbital energies (eV) and compositions (%) in theground state for complex 1

MO	Energy		С	ontribution (%)	Assignment
		Ir	C^N	pyrapy	mbiphpyrapy	
L+8	-2.26	1	3	8	87	π^* (mbiphpyrapy)
L+7	-2.60	1	2	81	15	$\pi^*(\text{ pyrapy})$
L+6	-2.85	0	6	4	89	π^* (mbiphpyrapy)
L+5	-3.22	2	94	0	4	π*(C^N)
L+4	-3.34	2	88	9	1	π*(C^N)
L+3	-3.73	1	26	73	0	$\pi^*(C^N+pyrapy)$
L+2	-3.77	4	80	16	1	$\pi^*(C^N+pyrapy)$
L+1	-3.91	5	91	4	0	π*(C^N)
L	-4.46	3	2	95	1	$\pi^*(\text{ pyrapy})$
Н	-7.40	0	0	0	100	π (mbiphpyrapy)
H-1	-8.14	0	0	0	100	π (mbiphpyrapy)
Н-2	-8.19	0	0	0	99	π (mbiphpyrapy)
H-3	-8.24	28	68	1	3	$d(Ir)+\pi(C^N)$
H-4	-8.33	1	2	0	96	π (mbiphpyrapy)
Н-5	-8.61	3	95	0	1	π(C^N)
Н-6	-8.85	0	2	0	97	π (mbiphpyrapy)
H-7	-8.88	14	79	1	6	$d(Ir)+\pi(C^N)$
H-8	-8.99	0	0	0	99	π (mbiphpyrapy)

Table S2Frontier molecular orbital energies (eV) and compositions (%) in theground state for complex 1a

MO	Energy		(Contribution (%)	Assignment
		Ir	C^N	CF ₃ -pyrapy	mbiphpyrapy	
L+8	-2.35	1	5	5	89	π^* (mbiphpyrapy)
L+7	-2.76	1	2	79	17	$\pi^*(CF_3$ -pyrapy+mbiphpyrapy)
L+6	-2.92	1	6	9	84	π^* (mbiphpyrapy)
L+5	-3.31	2	94	0	4	π*(C^N)
L+4	-3.45	2	93	4	1	π*(C^N)
L+3	-3.85	4	94	1	1	π*(C^N)
L+2	-3.99	4	86	10	0	$\pi^*(C^N)$
L+1	-4.11	2	11	87	0	$\pi^*(CF_3$ -pyrapy)
L	-4.81	3	1	95	1	$\pi^*(CF_3$ -pyrapy)
Н	-7.43	0	0	0	100	π(mbiphpyrapy)
H-1	-8.17	0	0	0	100	π(mbiphpyrapy)
Н-2	-8.22	0	0	0	100	π(mbiphpyrapy)
Н-3	-8.34	24	63	1	13	$d(Ir)+\pi(C^N)$
H-4	-8.39	4	10	0	86	π(mbiphpyrapy)
Н-5	-8.71	3	95	0	1	π(C^N)
H-6	-8.88	0	0	0	100	π(mbiphpyrapy)
H-7	-8.98	13	82	1	3	$d(Ir) + \pi(C^N)$
H-8	-9.03	0	0	0	100	π(mbiphpyrapy)

Table S3Frontier molecular orbital energies (eV) and compositions (%) in theground state for complex 1b

MO	Energy			Contribution	(%)	Assignment
		Ir	C^N	CF ₃ -pyrapy	mbiphpyrapy	
L+8	-2.40	4	20	6	71	$\pi^*(C^N+mbiphpyrapy)$
L+7	-2.82	1	2	70	26	$\pi^*(CF_3$ -pyrapy+mbiphpyrapy)
L+6	-2.96	1	5	18	76	$\pi^*(CF_3$ -pyrapy+mbiphpyrapy)
L+5	-3.33	2	95	1	3	π*(C^N)
L+4	-3.45	2	94	4	1	π*(C^N)
L+3	-3.96	4	94	1	1	π*(C^N)
L+2	-4.10	4	85	10	0	π*(C^N)
L+1	-4.19	2	11	87	0	π*(CF ₃ -pyrapy)
L	-4.90	3	1	95	1	π*(CF ₃ -pyrapy)
Н	-7.44	0	0	0	100	π(mbiphpyrapy)
H-1	-8.16	0	0	0	100	π(mbiphpyrapy)
H-2	-8.21	0	0	0	100	π(mbiphpyrapy)
H-3	-8.38	0	2	0	98	π(mbiphpyrapy)
H-4	-8.57	30	68	1	1	$d(Ir)+\pi(C^N)$
H-5	-8.87	0	3	0	96	π(mbiphpyrapy)
H-6	-8.90	4	90	0	6	$\pi(C^N)$
H-7	-9.01	8	88	1	4	$\pi(C^N)$
H-8	-9.02	0	2	0	98	π (mbiphpyrapy)

Table S4Frontier molecular orbital energies (eV) and compositions (%) in theground state for complex 1c

MO	Energy		Сс	ontribution (%	ó)	Assignment
		Ir	C^N	triapy	mphtriapy	
L+8	-2.96	0	1	2	97	π^* (mphtriapy)
L+7	-2.97	0	5	7	88	π^* (mphtriapy)
L+6	-3.08	2	91	3	4	π*(C^N)
L+5	-3.16	0	2	6	92	π^* (mphtriapy)
L+4	-3.35	1	11	78	11	$\pi^*(\text{triapy})$
L+3	-3.49	4	86	8	2	π*(C^N)
L+2	-3.74	4	84	11	1	π*(C^N)
L+1	-3.75	2	13	81	3	$\pi^*(\text{triapy})$
L	-4.35	2	0	96	1	π^* (triapy)
Н	-8.09	29	69	1	0	$d(Ir)+\pi(C^N)$
H-1	-8.43	6	93	0	0	$\pi(C^N)$
Н-2	-8.62	5	94	0	0	$\pi(C^N)$
Н-3	-8.92	3	96	1	0	$\pi(C^N)$
H-4	-9.00	1	0	0	99	π (mphtriapy)
H-5	-9.07	68	26	5	1	$d(Ir)+\pi(C^N)$
H-6	-9.18	66	26	8	1	$d(Ir)+\pi(C^N)$
H-7	-9.71	0	0	0	100	π (mphtriapy)
H-8	-9.84	0	0	5	95	π (mphtriapy)

Table S5Frontier molecular orbital energies (eV) and compositions (%) in theground state for complex 2

МО	Energy		Сс	ontribution (%	ó)	Assignment
		Ir	C^N	triapy	mphtriapy	
L+8	-2.82	0	1	17	81	$\pi^*(triapy+mphtriapy)$
L+7	-2.94	2	94	1	4	π*(C^N)
L+6	-2.98	0	5	2	93	π^* (mphtriapy)
L+5	-3.03	2	79	8	11	π*(C^N)
L+4	-3.13	1	5	60	35	π^* (triapy+mphtriapy)
L+3	-3.46	3	46	50	1	$\pi^*(C^N+\text{triapy})$
L+2	-3.50	3	61	36	1	$\pi^*(C^N+\text{triapy})$
L+1	-3.60	5	93	2	0	π*(C^N)
L	-4.09	3	2	96	0	π^* (triapy)
Н	-7.86	29	70	1	0	$d(Ir) + \pi(C^N)$
H-1	-8.29	4	95	0	0	π(C^N)
Н-2	-8.55	11	89	1	0	π(C^N)
Н-3	-8.70	0	0	0	100	π (mphtriapy)
H-4	-8.89	23	73	4	0	$d(Ir) + \pi(C^N)$
Н-5	-8.92	68	25	6	0	$d(Ir)+\pi(C^N)$
Н-6	-9.02	47	47	6	0	$d(Ir)+\pi(C^N)$
H-7	-9.32	0	0	0	100	π (mphtriapy)
H-8	-9.73	1	2	86	11	π (triapy)

Table S6Frontier molecular orbital energies (eV) and compositions (%) in theground state for complex 2a

МО	Energy		Сс	ontribution (%)	Assignment
		Ir	C^N	CF ₃ -triapy	mphtriapy	
L+8	-2.89	1	2	18	79	$\pi^*(CF_3$ -triapy+mphtriapy)
L+7	-2.99	0	0	2	97	π^* (mphtriapy)
L+6	-3.06	2	96	1	2	$\pi^*(C^N)$
L+5	-3.14	2	74	15	9	$\pi^*(C^N)$
L+4	-3.28	1	22	63	13	$\pi^*(C^N+CF_3-triapy)$
L+3	-3.60	4	95	1	0	π*(C^N)
L+2	-3.72	4	94	2	0	$\pi^*(C^N)$
L+1	-3.88	1	5	94	1	$\pi^*(CF_3$ -triapy)
L	-4.52	3	0	96	0	$\pi^*(CF_3$ -triapy)
Н	-8.00	28	71	1	0	$d(Ir)+\pi(C^N)$
H-1	-8.41	4	96	0	0	$\pi(C^N)$
Н-2	-8.51	0	0	0	100	π (mphtriapy)
Н-3	-8.67	10	89	1	0	$\pi(C^N)$
H-4	-9.02	14	82	3	0	$\pi(C^N)$
Н-5	-9.08	69	25	6	0	$d(Ir)+\pi(C^N)$
H-6	-9.13	0	0	0	100	π (mphtriapy)
H-7	-9.18	56	38	7	0	$d(Ir)+\pi(C^N)$
H-8	-9.73	0	0	0	100	π (mphtriapy)

Table S7Frontier molecular orbital energies (eV) and compositions (%) in theground state for complex 2b

МО	Energy		С	ontribution (%	⁄0)	Assignment
		Ir	C^N	CF ₃ -triapy	mphtriapy	
L+8	-2.94	0	2	17	80	$\pi^*(CF_3$ -triapy+mphtriapy)
L+7	-3.03	0	0	2	97	π^* (mphtriapy)
L+6	-3.09	2	96	0	2	$\pi^*(C^N)$
L+5	-3.16	2	86	7	5	$\pi^*(C^N)$
L+4	-3.35	1	11	73	15	$\pi^*(CF_3$ -triapy+ mphtriapy)
L+3	-3.71	4	94	2	0	$\pi^*(C^N)$
L+2	-3.83	4	93	2	0	$\pi^*(C^N)$
L+1	-3.98	1	5	94	1	$\pi^*(CF_3-triapy)$
L	-4.62	3	0	96	0	$\pi^*(CF_3$ -triapy)
Н	-8.22	30	68	1	0	$d(Ir)+\pi(C^N)$
H-1	-8.54	0	0	0	100	π (mphtriapy)
H-2	-8.59	5	95	0	0	$\pi(C^N)$
Н-3	-8.72	5	95	0	0	$\pi(C^N)$
H-4	-9.04	3	95	1	0	$\pi(C^N)$
Н-5	-9.16	0	0	0	100	π (mphtriapy)
H-6	-9.22	69	24	6	0	$d(Ir)+\pi(C^N)$
H-7	-9.31	65	26	8	0	$d(Ir)+\pi(C^N)$
H-8	-9.77	0	0	0	100	π (mphtriapy)

Table S8Frontier molecular orbital energies (eV) and compositions (%) in theground state for complex 2c

Table S9 Selected calculated wavelength (nm)/energies (eV), oscillator strength (f), major contribution and transition characters for **1-1c** in CH₂Cl₂ media, along with the experimental data for **1**

$\begin{array}{c} 1 & S_1 \\ & S_2 \\ & S_3 \end{array}$	1 22 27	366/3.38 277/4.47	0.002	H→L(96%)	[-(mhinhayanany)=*(ayanany)] II CT	
S_2 S_2	22	277/4.47	0.105	· /	$[\pi(1101pnpy1apy) \rightarrow \pi^{*}(pyrapy)]$ ILC I	363
Sa	27		0.195	H→L+4(65%)	$[\pi(\text{mbiphpyrapy}) \rightarrow \pi^*(C^N)]$ LLCT	
2		269/4.59	0.743	H-7→L (56%)	$[\pi(C^N) \rightarrow \pi^*(\text{ pyrapy})]$ LLCT	
S	31	263/4.70	0.339	H-1→L+6 (79%)	$[\pi(mbiphpyrapy) \rightarrow \pi^*(mbiphpyrapy)]$ ILCT	
S_2	40	252/4.91	0.176	H-1→L+7(58%)	$[\pi(\text{mbiphpyrapy}) \rightarrow \pi^*(\text{pyrapy})]$ ILCT	
S ₂	44	251/4.93	0.205	H-5→L+3(50%)	$[\pi(C^N) \rightarrow \pi^*(C^N+ pyrapy)]$ LLCT/ILCT	
S	54	244/5.07	0.132	$H\rightarrow L+5(49\%)$	$[\pi(\text{mbiphpyrapy}) \rightarrow \pi^*(C^N)]$ LLCT	
1a S ₁	1	381/3.25	0.002	H→L(97%)	$[\pi(\text{mbiphpyrapy}) \rightarrow \pi^*(\text{pyrapy})]$ ILCT	
S_2	21	279/4.43	0.088	H-6→L+2(51%)	$[\pi(mbiphpyrapy) \rightarrow \pi^*(C^N+pyrapy)]LLCT /ILCT$	
S_2	26	270/4.58	0.263	H→L+6(51%)	$[\pi(\text{mbiphpyrapy}) \rightarrow \pi^*(\text{mbiphpyrapy})]$ ILCT	
S	31	263/4.71	0.405	H-1→L+6(43%)	$[\pi(\text{mbiphpyrapy}) \rightarrow \pi^*(\text{mbiphpyrapy})]$ ILCT	
S	36	257/4.81	0.128	H-8→L(49%)	$[\pi(\text{mbiphpyrapy}) \rightarrow \pi^*(\text{pyrapy})]$ ILCT	
S ₂	42	251/4.92	0.173	H-1→L+7 (47%)	$[\pi(\text{mbiphpyrapy}) \rightarrow \pi^*(\text{pyrapy})]$ ILCT	
S	50	247/5.00	0.102	H-1→L+4 (66%)	$[\pi(\text{mbiphpyrapy}) \rightarrow \pi^*(C^N)]$ LLCT	
1b S ₁	1	417/2.96	0.002	H→L(97%)	$[\pi(mbiphpyrapy) \rightarrow \pi^*(CF_3-pyrapy)]$ ILCT	
S_2	27	275/4.49	0.152	H-6→L (43%)	$[\pi(mbiphpyrapy) \rightarrow \pi^*(CF_3-pyrapy)]$ ILCT	
S	34	267/4.63	0.441	H-1→L+4 (56%)	$[\pi(\text{mbiphpyrapy}) \rightarrow \pi^*(C^N)]$ LLCT	
S	38	263/4.70	0.206	H-6→L+3 (66%)	$[\pi(\text{mbiphpyrapy}) \rightarrow \pi^*(C^N)]$ LLCT	
S_2	43	257/4.82	0.236	H-3→L+5(74%)	$[d(Ir)+\pi(C^N) \rightarrow \pi^*(C^N)] MLCT/LLCT/ILCT$	
\mathbf{S}_{4}	45	252/4.91	0.268	H-1→L+7 (54%)	$[\pi(mbiphpyrapy) \rightarrow \pi^*(CF_3-pyrapy+mbiphpyrapy)]$ ILCT	
$\mathbf{S}_{\mathbf{S}}$	54	247/5.01	0.128	H→L+7 (46%)	$[\pi(mbiphpyrapy) \rightarrow \pi^*(CF_3-pyrapy+mbiphpyrapy)]$ ILCT	
$1c S_1$	1	399/3.10	0.001	H→L(73%)	$[\pi(\text{mbiphpyrapy}) \rightarrow \pi^*(\text{ CF}_3\text{-pyrapy})]$ ILCT	
S_2	25	277/4.46	0.178	H-2→L+4 (61%)	$[\pi(\text{mbiphpyrapy}) \rightarrow \pi^*(C^N)]$ LLCT	
S_2	28	275/4.50	0.170	H-8→L+1 (49%)	$[\pi(\text{mbiphpyrapy}) \rightarrow \pi^*(\text{ CF}_3\text{-pyrapy})]$ ILCT	
S	35	267/4.63	0.667	H-5→L+5 (55%)	$[\pi(\text{mbiphpyrapy}) \rightarrow \pi^*(C^N)]$ LLCT	
S	39	262/4.73	0.261	H-2→L+4 (51%)	$[\pi(\text{mbiphpyrapy}) \rightarrow \pi^*(C^N)]$ LLCT	
\mathbf{S}_{2}	45	252/4.91	0.416	H-2→L+5 (45%)	$[\pi(\text{mbiphpyrapy}) \rightarrow \pi^*(C^N)]$ LLCT	
$\mathbf{S}_{\mathbf{S}}$	57	244/5.06	0.182	H→L+8 (43%)	$[\pi(mbiphpyrapy) \rightarrow \pi^*(C^N+mbiphpyrapy)]$ LLCT/ILCT	

^a From ref. 19

Table S10Selected calculated wavelength (nm)/energies (eV), oscillator strength(f), major contribution and transition characters for 2-2c in CH₂Cl₂ media, along withthe experimental data for 2

	State	λ/Ε	f	Configuration	Assignment	Exptla
2	S_1	371/3.33	0.002	H→L(96%)	$[d(Ir)+\pi(C^N)\rightarrow\pi^*(triapy)]MLCT/LLCT$	361
	S_{12}	293/4.22	0.170	H-1→L+2 (73%)	$[\pi(C^N) \rightarrow \pi^*(C^N)]$ LLCT/ILCT	
	S_{18}	278/4.45	0.100	H-5→L+1(53%)	$[d(Ir)+\pi(C^N)\rightarrow\pi^*(triapy)]$ MLCT/LLCT	
	S_{28}	260/4.75	0.084	H-2→L+3 (45%)	$[\pi(C^N) \rightarrow \pi^*(C^N)]$ LLCT/ILCT	
	S ₃₄	251/4.92	0.100	H-1→L+6(72%)	$[\pi(C^N) \rightarrow \pi^*(C^N)]$ LLCT/ILCT	
	S ₃₉	248/4.98	0.154	H-2→L+6(60%)	$[\pi(C^N) \rightarrow \pi^*(C^N)]$ LLCT/ILCT	
	S ₄₄	244/5.07	0.123	H-1→L+7 (48%)	$[\pi(C^N) \rightarrow \pi^*(\text{ mphtriapy})]$ LLCT	
2a	\mathbf{S}_1	378/3.27	0.001	H→L(97%)	$[d(Ir)+\pi(C^N)\rightarrow\pi^*(triapy)]$ MLCT/LLCT	
	\mathbf{S}_{10}	295/4.18	0.083	H-2→L+1(57%)	$[\pi(C^N) \rightarrow \pi^*(C^N)]$ LLCT/ILCT	
	S ₁₉	278/4.44	0.158	H-5→L+2 (47%)	$[d(Ir)+\pi(C^N)\rightarrow\pi^*(C^N+triapy)]$ MLCT/LLCT/ILCT	
	S_{27}	259/4.76	0.114	H-7→L(67%)	$[\pi(mphtriapy) \rightarrow \pi^*(triapy)]$ ILCT	
	S ₃₉	249/4.96	0.425	H-3→L+4(45%)	$[\pi(mphtriapy) \rightarrow \pi^*(triapy+mphtriapy)]$ ILCT	
	S_{42}	246/5.03	0.146	H→L+8 (41%)	$[d(Ir)+\pi(C^N)\rightarrow\pi^*(triapy+mphtriapy)]$ MLCT/LLCT	
	S_{55}	235/5.25	0.137	H-5→L+7(60%)	$[d(Ir)+\pi(C^N)\rightarrow\pi^*(C^N)]$ MLCT/LLCT /ILCT	
2b	\mathbf{S}_1	420/2.94	0.001	H→L(97%)	$[d(Ir)+\pi(C^N)\rightarrow\pi^*(CF_3-triapy)]$ MLCT/LLCT	
	S_8	316/3.91	0.113	H-5→L (70%)	$[d(Ir)+\pi(C^N)\rightarrow\pi^*(CF_3-triapy)]$ MLCT/LLCT	
	\mathbf{S}_{23}	276/4.48	0.143	H-4→L+2(45%)	$[\pi(C^N) \rightarrow \pi^*(C^N)]$ MLCT/LLCT/ILCT	
	S_{28}	263/4.71	0.108	H-6→L+1(49%)	$[\pi(mphtriapy) \rightarrow \pi^*(CF_3-triapy)]$ ILCT	
	S_{35}	256/4.84	0.256	H-1→L+6 (45%)	$[\pi(C^N) \rightarrow \pi^*(C^N)]$ LLCT/ILCT	
	\mathbf{S}_{41}	251/4.93	0.374	H-2→L+5(70%)	$[\pi(mphtriapy) \rightarrow \pi^*(C^N)] LLCT/ILCT$	
	S_{46}	246/5.02	0.107	H→L+2 (43%)	$[d(Ir)+\pi(C^N) \rightarrow \pi^*(C^N)] MLCT/LLCT/ILCT$	
2c	\mathbf{S}_1	402/3.07	0.003	H→L(97%)	$[d(Ir)+\pi(C^N)\rightarrow\pi^*(CF_3-triapy)]$ MLCT/LLCT	
	S_9	311/3.98	0.139	H-6→L (63%)	$[d(Ir)+\pi(C^N)\rightarrow\pi^*(CF_3-triapy)]$ MLCT/LLCT	
	S ₂₃	273/4.52	0.135	H-4→L+2 (73%)	$[\pi(C^N) \rightarrow \pi^*(C^N)]$ LLCT/ILCT	
	S ₃₉	251/4.93	0.298	H-2→L+5 (55%)	$[\pi(C^N) \rightarrow \pi^*(C^N)]$ LLCT/ILCT	

^a From ref. 19

Table S11 Calculated phosphorescent emission wavelength (λ , in nm) for 1 and 2 in CH₂Cl₂ media with the TDDFT method at M062X, M052X, PBE0, B3LYP, CAM-B3LYP and BP86 level, respectively, together with the experimental values

	Exptl ^a	M062X	M052X	PBE0	B3LYP	CAM-B3LYP	BP86
1	454	479	511	555	540	567	553
2	454	476	507	552	538	561	556

^a From ref. 19

	MO	E	MC	composition	n (%)	Assignment
1			Ir	C^N	N^N	
	L	-4.55	3	3	94	π*(N^N)
	Н	-7.40	0	0	100	$\pi(N^N)$
1 a			Ir	C^N	N^N	
	L	-4.88	4	1	95	π*(N^N)
	Н	-7.39	0	0	100	$\pi(N^N)$
1b			Ir	C^N	N^N	
	L	-5.26	4	2	94	π*(N^N)
	Н	-7.40	0	0	100	$\pi(N^N)$
1c			Ir	C^N	N^N	
	L	-5.32	4	1	95	π*(N^N)
	H	-7.35	0	0	100	$\pi(N^N)$
2			Ir	C^N	N^N	
	L	-4.35	2	1	97	$\pi^*(N^N)$
	H	-8.02	26	72	2	$d(Ir) + \pi(C^N)$
2a			Ir	C^N	N^N	
	L	-4.08	2	2	96	$\pi^*(N^N)$
	Н	-7.78	25	74	1	$d(Ir)+\pi(C^N)$
2b			Ir	C^N	N^N	
	L	-5.03	4	1	95	$\pi^*(N^N)$
	Н	-7.88	28	70	2	$d(Ir) + \pi(C^N)$
2c			Ir	C^N	N^N	
	L	-5.10	4	1	95	π*(N^N)
	Н	-8.08	30	67	3	$d(Ir)+\pi(C^N)$

Table S12 Frontier molecular orbital energies (eV) and composition (%) of 1-1cand 2-2c in the lowest lying triplet excited state (L and H represent)

Table S13 The xyz coordinates for the optimized structures for 1 in the S_0 and T_1 states at PBE0/6-31G* level

		So			T ₁	
Ir	-3.36056800	0.18187000	-0.09182900	-3.35420400	0.18088900	-0.08269400
F	-7.67405900	-2.56696300	1.11376100	-7.69030000	-2.60592700	1.10335700
F	-4.60874200	-2.15429800	4.59633600	-4.59669600	-2.21537000	4.57884100
F	0.73634500	-3.01545300	0.73623300	0.73079700	-3.04659400	0.67730800
F	-2.32012100	-4.57898100	-2.41146700	-2.35611800	-4.54731800	-2.47115600
Ν	-1.74517200	0.42998100	1.15259100	-1.72199300	0.41081300	1.15705400
C	-0.83080100	-0.58169200	1.15273900	-0.81562400	-0.60712900	1.13814700
C	0.29692200	-0.49304600	1.97834500	0.32016900	-0.53574700	1.95405000
Н	1.02197700	-1.29354500	1.97305600	1.03939400	-1.34128500	1.93502300
C	0.47686200	0.61490700	2.78928900	0.51638200	0.56400600	2.77261400
Н	1.35131500	0.67782800	3.43025600	1.39747800	0.61430400	3.40556600
C	-0.46862800	1.63798100	2.77305200	-0.42016700	1.59542900	2.77375000
Н	-0.36924800	2.52108700	3.39455000	-0.30695400	2.47245900	3.40145600
C	-1.56192400	1.50278700	1.93739900	-1.52282800	1.47599100	1.94764300
Н	-2.33375400	2.26167100	1.88494100	-2.28984500	2.24078000	1.90817500
C	-2.36038000	-1.50759200	-0.49901500	-2.36393500	-1.50465700	-0.51575500
C	-1.16384100	-1.67181600	0.24768600	-1.16351600	-1.68375200	0.22138700
C	-0.40427000	-2.83210300	0.05520900	-0.41306800	-2.84623800	0.00685900
C	-0.76846600	-3.82477900	-0.83500700	-0.79021200	-3.82347200	-0.89495000
Н	-0.16389000	-4.71516600	-0.95888900	-0.19129600	-4.71513800	-1.03636700
C	-1.94451100	-3.63550200	-1.54800800	-1.97010200	-3.61798500	-1.59778200
C	-2.73890100	-2.50596600	-1.39882600	-2.75670600	-2.48623900	-1.42745700
Н	-3.65029600	-2.43871000	-1.98344400	-3.67230900	-2.40137700	-2.00287300
Ν	-4.97363200	-0.29357200	-1.27726200	-4.94751700	-0.24953500	-1.26687400
C	-5.94373100	-1.04558600	-0.68324300	-5.95831500	-1.04661400	-0.64790600
C	-7.06786100	-1.43261700	-1.42443400	-7.10400200	-1.43087500	-1.42760300
Н	-7.83241100	-2.03202800	-0.95155200	-7.85683300	-2.05062700	-0.96058400
C	-7.18752000	-1.05496300	-2.75165600	-7.23714300	-1.03147900	-2.72370900
Η	-8.05752700	-1.36054500	-3.32516400	-8.10152000	-1.32743200	-3.30825500
C	-6.18380100	-0.28825200	-3.33969400	-6.21714400	-0.22284100	-3.30189600
Η	-6.23547400	0.02502300	-4.37650600	-6.27792600	0.11954500	-4.32855800
C	-5.09639900	0.06882000	-2.56372400	-5.11160800	0.12452200	-2.53160400
Н	-4.28071200	0.65826200	-2.96567700	-4.31268900	0.72511600	-2.95415000
C	-4.42275300	-0.89080800	1.21373100	-4.40150100	-0.87209800	1.22481100
C	-5.66008000	-1.37140700	0.70689700	-5.68048600	-1.36872100	0.67538400
C	-6.49620900	-2.10533800	1.55805300	-6.51812400	-2.14585100	1.56033700
C	-6.16750400	-2.38172500	2.87124400	-6.16589100	-2.42549800	2.84276200
Н	-6.83314900	-2.95377000	3.50621200	-6.81570800	-3.01100900	3.48325200
C	-4.95060000	-1.90102800	3.33396600	-4.92763400	-1.93809200	3.32090800
C	-4.08061000	-1.16665800	2.53726800	-4.06204700	-1.18222600	2.52947500
Н	-3.14361500	-0.83424000	2.97053100	-3.12276300	-0.85909000	2.96569100
Ν	-4.36481400	2.08677700	0.33538800	-4.36268600	2.10028700	0.36308000
C	-4.07114800	3.12187800	-0.48461300	-4.07387500	3.13384300	-0.45872900
C	-4.70505700	4.35651400	-0.35849800	-4.70890800	4.36791500	-0.32981900
H	-4.448/9800	5.16802000	-1.03129000	-4.45587/00	5.18093500	-1.00199300
C	-5.66057000	4.52751100	0.63425400	-5.66270900	4.53583100	0.66515300
H	-6.16640/00	5.48129800	0./4919000	-6.17054500	5.48842600	0.78136200
	-5.95652500	3.45963200	1.4/630800	-5.954/1300	3.46/42900	1.50816800
	-0.09463100	3.54862800	2.2000/400	-0.092/9000	3.33438300	2.2981/900
	-5.28/73900	2.25/40900	1.29112800	-5.28102/00	2.26808800	1.32185800
	-3.4808/200	1.39303300	1.91843000	-3.4035/000	1.40340100	1.952/9100
	-2.49230900	1.02033300	-1.47000300	-2.490/1100	1.04013300	-1.40123000 2 48600100
I TN	-1.00508100	1.02400300	-2.42210200	-1.00039000	1.040/9300	-2.40009100

C	-1.57597300	2.82495400	-3.12117500	-1.58870200	2.84974200	-3.10648500
Н	-0.90145600	3.00226900	-3.94693600	-0.91909500	3.03201300	-3.93515200
C	-2.49334200	3.64645700	-2.50249300	-2.50819300	3.66494900	-2.48263700
H	-2 72697700	4 66861200	-2 76018300	-2 74940600	4 68581400	-2 73838000
C	-3 04645000	2.85121500	-1 48497500	-3 05236700	2 86546000	-1 46371600
C	-0 70354400	0 50850800	-2 72558400	-0.70565500	0 53572200	-2 72281700
н	-0.48323000	0.50467800	-3 79934400	-0.48672000	0.54151700	-3 79680200
н	-1 25868300	-0.40618100	-2 49872300	-1 25998500	-0 38145400	-2 50423500
	0 570/6900	0 57571500	-1.91264500	0 56925700	0.59681000	-1 91100700
	1 36381100	-0.57128000	-1.91204500 -1.83037500	1 36/38800	-0 5/969300	-1 83950000
	1.03058200	1 48007800	2 31/53600	1.04146300	1 46437700	2 33210100
	2 55201700	-1.48777800	-2.31433000	2 55420700	-1.40437700	1 12561200
	2.33291700	-0.33993100	-1.11311/00 1.02727100	2.33439700	-0.34272300	-1.12301200
	2.00512200	-1.4/310600	-1.03/3/100	2.00577000	-1.433/4/00	-1.03038000
	2.99313300	1.74508800	-0.40301000	2.99377900	0.01304000	-0.40413000
	2.19497000	1./4308800	-0.33034/00	2.19425700	1.73722900	-0.34/62000
Н	2.52577700	2.00/80500	-0.08800900	2.524/1600	2.6/6/4500	-0.07268100
	0.99955600	1./3429/00	-1.26803900	0.99/9//00	1./50/5300	-1.25/84300
H	0.40920700	2.645/9100	-1.3198/300	0.40658700	2.6619/000	-1.30231800
C	4.26201100	0.61335000	0.29818400	4.262/4300	0.62048600	0.29/04100
C	4.38485800	1.34860200	1.48256800	4.38573300	1.34835400	1.48601500
H	3.53043000	1.90333400	1.86285400	3.53183300	1.90200200	1.86903300
C	5.58286900	1.36717600	2.18911400	5.58334400	1.36157800	2.19334500
H	5.65521700	1.94658700	3.10730600	5.65570500	1.93544200	3.11501700
C	6.68882200	0.64872100	1.73638700	6.68895000	0.64497400	1.73684800
C	6.57268800	-0.08989200	0.55574200	6.57287100	-0.08594600	0.55141000
H	7.43589300	-0.63810000	0.18738400	7.43587000	-0.63245500	0.18005900
C	5.37877900	-0.10557000	-0.15135400	5.37932900	-0.09626600	-0.15644600
H	5.32043400	-0.65980900	-1.08446400	5.32130800	-0.64443500	-1.09314800
C	7.98543400	0.65277700	2.51530900	7.98488900	0.64286500	2.51695200
Η	7.95748100	1.41944000	3.29617200	7.95762500	1.40595000	3.30133700
Н	8.14544600	-0.31373000	3.00384400	8.14236700	-0.32622000	3.00121500
Ν	9.77293200	-0.15115700	1.12091000	9.77173700	-0.15818500	1.12018600
Ν	9.14915500	0.88608300	1.69065200	9.14992400	0.87763700	1.69470800
C	9.65903400	2.08040000	1.29402400	9.66339000	2.07275200	1.30510100
Η	9.25845200	3.01380600	1.66446100	9.26485800	3.00520600	1.68013100
C	10.68726200	1.80461100	0.42526700	10.69187900	1.79893300	0.43605600
Н	11.34507200	2.49300100	-0.08213000	11.35205800	2.48830800	-0.06690600
C	10.71703500	0.39449100	0.35096000	10.71810400	0.38914800	0.35423300
N	12.50270100	0.23489600	-1.21455900	12.50502800	0.23345900	-1.21020900
C	11.63956300	-0.43092800	-0.43582800	11.63949600	-0.43438200	-0.43588200
C	11.60519800	-1.82834600	-0.36450000	11.60174900	-1.83205100	-0.37185200
Н	10.88801400	-2.31289200	0.28982300	10.88276000	-2.31831400	0.27921000
C	12.50140700	-2.55501000	-1.13516100	12.49704400	-2.55681400	-1.14536900
H	12.50153800	-3.64131100	-1.10024600	12.49458000	-3.64327800	-1.11613200
C	13.40069800	-1.87039300	-1.94831600	13.39879800	-1.87009400	-1.95400400
H	14.12094500	-2.39726200	-2.56657000	14.11844200	-2.39543000	-2.57425700
C	13.35565700	-0.47881300	-1.94594500	13.35707400	-0.47843300	-1.94441100
H	14.04384700	0.09413000	-2.56590600	14.04727700	0.09610200	-2.56064000
						

					1		
Ir -1.52191800 -0.04680800 -0.19851600 -1.51670800 -0.05692500 -0.6853000 N -0.1884700 1.64848200 -0.6957500 1.34701600 -1.33473100 C 1.88674100 2.31345000 -1.69779500 1.87763000 2.23574100 -1.73030500 R 2.8355800 2.03544000 -2.1696000 3.6878500 -1.24744800 R 2.890700 4.4345500 -1.71889100 3.2578100 -4.7744800 R 2.27844500 -0.47392200 2.9131550 -0.60414900 0.12313200 4.99971600 -0.60712700 C -0.47392200 2.9131550 -0.60414800 0.12582800 0.712700 -4.4382800 0.60744900 0.12582700 -2.1673100 -1.3805500 N 1.78474100 -2.1052700 -1.85042500 1.7948300 -2.1173100 -3.8700500 N 0.5522700 -2.18246500 -1.5248600 1.79478300 -5.1572400 -1.3499100 N 1.84174100 -1.52418600 1.79478300 -1.53434000 1.717707 -1.65			S_0			T ₁	
N -0.18984700 1.64486200 -0.69577500 -0.17327500 1.6555060 -0.63730800 C 0.9721500 1.33713000 -1.33730800 -1.334730800 C 2.8355800 2.03544000 -2.1696000 2.8077400 2.32574100 -1.73630500 H 2.8335300 3.64600300 -1.44402400 2.80774400 2.32574100 -1.47744800 C 0.38491000 3.9611100 -0.82174400 0.3351200 -9.8258300 -0.60712700 C 0.447392200 2.93157500 -0.46146800 -0.45289700 2.182800 0.08561700 N 0.5527000 2.1824500 -1.5324600 0.179243300 -2.1731300 -1.53490100 N 0.5527000 -2.18246500 -1.52418600 1.1697700 -0.0946300 -2.01715300 N 0.5327000 -2.1852000 -2.17612900 -2.15711800 -2.15711800 C 2.22140500 -0.59375900 -1.1693000 0.57292100 -2.1834500 -2.15711800 Z 2.2144500	Ir	-1.52191800	-0.04680800	-0.19851600	-1.51670800	-0.05692500	-0.18551000
C 0.97155900 1.33597000 -1.31712900 0.97221500 1.34701600 -1.73630300 I 2.82355800 2.03544000 -2.16960000 2.80374400 2.20935500 -2.22963000 C 1.58853300 3.64600300 -1.44402400 1.88706300 -1.4744800 L 2.9409700 4.42345500 -1.71889100 2.27844500 -1.37743100 C 0.38491000 3.96151100 -0.82174400 0.32351200 3.97228300 -0.60712700 H 0.11115700 4.9889800 -0.60744900 0.12313300 -1.38282800 0.60712700 N 1.7847100 -2.13025700 -1.85042500 -1.35282800 0.4375100 -1.37524000 N 1.7847100 -2.13025700 -1.4804200 1.7977700 -0.4791200 -1.3752400 C 1.17677700 -0.9946300 -1.5752400 1.27943300 -1.5752400 C 2.2163500 -6.3544600 3.1992200 -3.52478200 -2.17143100 L 3.151500 -6.3544500	Ν	-0.18984700	1.64486200	-0.69577500	-0.17327500	1.65550600	-0.68730800
C 1.887674100 2.31345000 -1.69779500 1.87763000 2.32574100 -1.73630500 H 2.2355800 2.03544000 -2.16960000 2.80374400 2.4035500 -2.2296300 C 1.58853300 3.64600300 -1.44402400 1.58190600 3.65785000 -1.47744800 C 0.38491000 3.96151100 0.82174400 0.3351200 3.97228300 0.82383600 C -0.47392200 2.93157500 -0.46146800 -0.45289700 2.94002100 -0.44338100 N 1.78474100 -2.13025700 -1.85046200 1.79483300 -2.11733100 -1.87003500 N 0.18416900 -0.95375900 -1.5484600 0.7292100 -2.17612900 -1.34909100 C 2.104050 -0.85940600 -1.9826190 2.21905700 -8.832400 -2.01716300 C 2.50371300 -3.24770400 -3.23486400 3.31999200 -3.23478200 -3.23419600 C 2.50371300 -3.8544000 -3.234770400 -3.23478200 -3.23819600	C	0.97155900	1.33597000	-1.31712900	0.97221500	1.34701600	-1.33473100
H 2.82355800 2.03544000 -2.16960000 2.80374400 2.04935500 -1.222963000 C 1.58853300 3.66603300 -1.44402400 1.58190660 3.65785000 -1.47744800 H 2.29409700 4.42345500 -1.71881100 2.27844500 4.4363700 -1.77043100 C 0.38491000 3.95151100 -0.82174400 0.3231200 3.97228300 -0.607112700 C -0.47392200 2.93157500 -0.46146800 -0.45289700 2.94002100 -0.44338100 H -1.4882800 3.12104400 0.03751300 -1.38246000 3.12582800 0.088617000 N 0.55227000 -2.81246500 -1.35042500 2.17612900 -1.54344000 C 1.1693000 -0.99018080 -2.19905700 -0.84392400 -2.1715200 C 2.21405500 -0.85940600 -1.98261900 2.51950300 -3.32445500 -1.5438400 C 2.2140500 -3.52478200 -3.17151800 1.37171800 -1.68423900 H 9.17	C	1.88674100	2.31345000	-1.69779500	1.87763000	2.32574100	-1.73630500
C 1.58853300 3.6460300 -1.44402400 1.58190600 3.65785000 -1.77043100 C 0.38491000 3.96151100 -0.82174400 0.39351200 3.97228300 -0.8283600 H 0.11115700 4.98898800 -0.60744900 0.12313200 4.99971600 -0.60712700 C 0.47392200 2.93157500 -0.46146800 0.12313200 -2.1773100 -1.87005500 N 1.78474100 -2.13227000 -1.8246500 1.79483300 -2.1173100 -1.34909100 N 0.52227000 -2.18246500 -1.35288000 0.57292100 -2.17612900 -1.34909100 C 2.2140500 -0.8594600 -1.98261900 2.21905700 -0.84392400 -2.01716300 C 2.2140500 -0.8594600 -2.13236200 2.5195300 -3.52478200 -2.19711800 C 2.2140500 -0.8594600 -2.1323620 2.5995300 -3.25478200 -2.39445500 H 2.48880600 -3.54770400 -3.21260200 2.50609300 -3.25478200	Η	2.82355800	2.03544000	-2.16960000	2.80374400	2.04935500	-2.22963000
H 2.29409700 4.42345500 -1.71889100 2.27844500 4.43683700 -1.77043100 C 0.38491000 3.96151100 -0.82174400 0.3935120 3.97228300 -0.82583600 H 0.11115700 4.98898800 -0.60744900 0.12313200 4.99971600 -0.60712700 C -0.47392200 2.33157500 -0.46146800 -1.3828000 3.1282800 0.048561700 N 1.78474100 -2.13025700 -1.85042500 1.79483300 -2.17612900 -1.349091000 N 0.55227000 -2.18246500 -1.52820800 0.57292100 -2.17612900 -1.34909100 C 1.16693000 -0.9900800 -1.52418600 1.1767700 -0.6746300 -2.3944500 C 2.2105700 -3.837000 -3.3249400 -2.15711800 -1.68423900 H 1.91174300 -4.15717900 -1.6552400 1.93049900 -1.44455700 -1.68423900 N 5.34019800 3.15066800 -0.42150300 5.32827200 3.8337600 -0.3558500	C	1.58853300	3.64600300	-1.44402400	1.58190600	3.65785000	-1.47744800
C 0.38491000 3.96151100 -0.82174400 0.39351200 3.97228300 -0.82838600 H 0.11115700 4.9898800 -0.60744900 0.12313200 4.99971600 -0.60712700 C -0.47392200 2.93157500 -1.68042500 1.79483300 2.1733100 -1.87003500 N 1.78474100 -2.18246500 -1.3520800 0.57292100 -2.17612900 -1.37524000 N 0.5227000 -2.18246500 -1.98261900 2.21905700 -0.84392400 -2.01716300 C 2.2140500 -0.85946600 -2.3386400 3.19992200 -0.59954600 -2.39445500 C 2.2140500 -0.85946600 -3.21260200 2.50609300 -3.52478200 -3.23819600 H 2.48880600 -3.54770400 -2.13326200 1.534344000 5.32877200 -3.1837600 -0.36959500 K 3.4019800 3.15066800 -42133030 -3.14485700 -1.68423900 K 3.435500 0.42150300 5.38287600 3.376409337660 -2.34655300	Н	2.29409700	4.42345500	-1.71889100	2.27844500	4.43683700	-1.77043100
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$ \begin{array}{c} C & -0.47392200 & 2.93157500 & -0.46146800 & -0.45289700 & 2.94002100 & -0.44338100 \\ H & -1.41882800 & 3.12104400 & 0.03751300 & -1.38246000 & 3.12582800 & 0.08561700 \\ N & 0.55227000 & -2.18246500 & -1.3520800 & 0.57292100 & -2.17612900 & -1.34909100 \\ N & 0.18416900 & -0.95375900 & -1.16093000 & 0.19904800 & -0.94917000 & -1.54344000 \\ C & 1.17609300 & -0.09000800 & -1.52418600 & 1.17677700 & -0.7946300 & -1.54344000 \\ C & 2.221405500 & -0.85940600 & -1.98261900 & 2.21905700 & -0.84392400 & -2.07116300 \\ H & 3.21136550 & -0.62015400 & -2.3386400 & 3.1992200 & -0.59954600 & -2.33445500 \\ C & 2.50371300 & -3.37005000 & -2.13236200 & 2.51950300 & -3.52478200 & -3.23819600 \\ H & 1.91174300 & -4.15717900 & -1.65524000 & 1.93049900 & -4.14435700 & -1.68423900 \\ N & 5.34019800 & 3.15066800 & -0.42150300 & 5.32827200 & 3.18337600 & 0.36595000 \\ C & 4.65561700 & 2.83305500 & 0.68697800 & 4.62123200 & 2.84328700 & 0.72144900 \\ C & 3.94583000 & 3.77253900 & 1.44168300 & 3.8808100 & 3.76409900 & 1.46971700 \\ H & 3.41735400 & 3.45515900 & 2.33463400 & 3.33626800 & 5.49238400 & 2.34655300 \\ C & 4.68050100 & 5.44262900 & -0.11169100 & 4.62808600 & 5.4409900 & 1.64325300 \\ C & 4.68050100 & 5.44262900 & -0.11169100 & 4.6759800 & 6.49360500 & -0.38156900 \\ S .524718700 & -0.62997400 & 1.41436900 & 5.23911400 & -0.62216200 & 1.41464970 \\ N & 3.84151000 & 0.86598900 & 1.97942900 & 3.80758000 & 0.38156900 \\ N & 5.24718700 & -0.62997400 & 1.41436900 & 5.23911400 & -0.62216200 & 1.41464900 \\ C & 5.1027900 & 4.46596700 & -0.7713900 & 5.30758000 & 0.38156900 \\ C & 5.1027900 & -1.46159600 & 0.77813500 & 2.18435200 & 1.43420800 & 1.1721900 \\ C & 4.70970100 & 1.42820900 & 1.9693100 & 5.23911400 & -0.62216200 & 0.7365200 \\ D & 5.24718700 & -0.62997400 & 1.41636900 & 5.23911400 & -0.62216200 & 0.7365200 \\ C & 5.81027900 & -1.96399100 & 1.3694200 & 5.81411800 & 1.95669400 & 0.7374500 \\ C & 5.81027900 & -1.96399100 & 1.5486800 & 3.42374200 & -2.8866700 & 0.17374500 \\ C & 5.6119900 & -0.6218500 & 0.4797500 & 6.6703300 & -3.24787000 $	Н	0.11115700	4.98898800	-0.60744900	0.12313200	4.99971600	-0.60712700
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N 1.78474100 -2.13025700 -1.85042500 1.79483300 -2.11733100 -1.87003500 N 0.55227000 -2.18246500 -1.35280800 0.57292100 -2.17612900 -1.3572400 C 1.17609300 -0.09000800 -1.5824800 0.57292100 -0.7946300 -1.3524400 C 2.2140500 -0.85940600 -1.98261900 2.21905700 -0.84392400 -2.17711800 H 3.21136500 -0.62015400 -2.33886400 3.19992200 -0.59954600 -2.39445500 C 2.50371300 -3.37005000 -2.13206200 2.5069300 -3.52478200 -2.15711800 H 1.9174300 -4.15717900 -1.65524000 1.9349900 -1.44435700 -0.68423900 C 3.9458000 3.77253900 1.4416300 3.888100 3.76409000 1.446971700 C 3.94583000 3.77253900 1.44163800 3.33626800 3.464778700 C 3.9458300 5.4726390 0.1169100 4.62808600 5.446390700 0.72748900 </td <td>Н</td> <td>-1.41882800</td> <td>3.12104400</td> <td>0.03751300</td> <td>-1.38246000</td> <td>3.12582800</td> <td>0.08561700</td>	Н	-1.41882800	3.12104400	0.03751300	-1.38246000	3.12582800	0.08561700
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$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Н	3.21136500	-0.62015400	-2.33886400	3.19992200	-0.59954600	-2.39445500
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$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Н	3.41735400	3.45515900	2.33463400	3.33626800	3.42938400	2.34655300
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	С	3.96261100	5.09939000	1.03153700	3.88834800	5.09556800	1.07478700
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Н	3.43619500	5.85816000	1.60425400	3.33780700	5.84029900	1.64325300
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	С	4.68050100	5.44262900	-0.11169100	4.62808600	5.46190000	-0.04699600
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	Н	4.73569300	6.46978700	-0.45897200	4.67659800	6.49360500	-0.38156900
H5.923542004.65747600-1.692931005.920943004.71271900-1.60562900N5.24718700-0.629974001.414369005.23911400-0.622162001.41464900N4.16505400-0.375835002.164983004.14174500-0.389927002.14985100N3.841510000.865989001.979429003.807580000.850852001.97504100C4.709701001.428209001.094317004.684352001.434208001.11248900C5.618432000.461596000.716070005.610053000.482596000.73736200H6.465073000.487805000.047980006.467063000.526823000.08361100C5.81027900-1.969991001.386942005.316111800-1.956694001.37544800H5.35611400-2.492158002.234302005.36603800-2.490401002.21886800C3.92092800-3.32644000-1.615128003.93593300-3.30478600-1.63781100C4.21075600-2.73928100-0.384492004.22105500-2.72020700-0.40489900H3.41621300-2.303434000.218686003.42374200-2.88667000.19768300C6.54797800-3.24063000-0.675027006.56033300-3.82657000-1.90997300H7.06203100-4.29433400-2.478995007.58583500-3.8575600-2.49787700C6.26119900-3.88475000-2.368955004.97355900-3.8575600-2.49787700C <td>C</td> <td>5.34810600</td> <td>4.42916900</td> <td>-0.79713900</td> <td>5.32700900</td> <td>4.46596700</td> <td>-0.72696200</td>	C	5.34810600	4.42916900	-0.79713900	5.32700900	4.46596700	-0.72696200
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	Н	5.92354200	4.65747600	-1.69293100	5.92094300	4.71271900	-1.60562900
N 4.16505400 -0.37583500 2.16498300 4.14174500 -0.38992700 2.149851000 N 3.84151000 0.86598900 1.97942900 3.80758000 0.85085200 1.97504100 C 4.70970100 1.42820900 1.09431700 4.68435200 1.43420800 1.11248900 C 5.61843200 0.46159600 0.71607000 5.61005300 0.48259600 0.73736200 H 6.46507300 0.48780500 0.04798000 6.46706300 0.52682300 0.08361100 C 5.81027900 -1.96999100 1.38694200 5.81411800 -1.95669400 1.37544800 H 5.35611400 -2.49215800 2.23430200 5.36603800 -2.49040100 2.21886800 C 3.92092800 -3.32644000 -1.61512800 3.93593300 -3.30478600 -1.63781100 C 4.21075600 -2.73928100 -0.38449200 4.22105500 -2.72020700 -0.40489900 H 3.41621300 -2.67342100 0.08161900 5.53239400 -2.65277900	Ν	5.24718700	-0.62997400	1.41436900	5.23911400	-0.62216200	1.41464900
N 3.84151000 0.86598900 1.97942900 3.80758000 0.85085200 1.97504100 C 4.70970100 1.42820900 1.09431700 4.68435200 1.43420800 1.11248900 C 5.61843200 0.46159600 0.71607000 5.61005300 0.48259600 0.73736200 H 6.46507300 0.48780500 0.04798000 6.46706300 0.52682300 0.08361100 C 5.81027900 -1.96999100 1.38694200 5.81411800 -1.95669400 1.37544800 H 5.35611400 -2.49215800 2.23430200 5.36603800 -2.49040100 2.21886800 H 6.88692900 -1.90348900 1.56909400 6.89023700 -1.88144300 1.55696400 C 3.20292800 -3.32644000 -1.61512800 3.93593300 -3.30478600 -1.63781100 C 4.21075600 -2.73928100 -0.38449200 4.22105500 -2.72020700 -0.40489900 H 3.41621300 -2.67342100 0.08161900 5.53239400 -2.65277900	Ν	4.16505400	-0.37583500	2.16498300	4.14174500	-0.38992700	2.14985100
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Ν	3.84151000	0.86598900	1.97942900	3.80758000	0.85085200	1.97504100
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C	4.70970100	1.42820900	1.09431700	4.68435200	1.43420800	1.11248900
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	С	5.61843200	0.46159600	0.71607000	5.61005300	0.48259600	0.73736200
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Н	6.46507300	0.48780500	0.04798000	6.46706300	0.52682300	0.08361100
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	C	5.81027900	-1.96999100	1.38694200	5.81411800	-1.95669400	1.37544800
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Н	5.35611400	-2.49215800	2.23430200	5.36603800	-2.49040100	2.21886800
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Н	6.88692900	-1.90348900	1.56909400	6.89023700	-1.88144300	1.55696400
C4.21075600-2.73928100-0.384492004.22105500-2.72020700-0.40489900H3.41621300-2.303434000.218686003.42374200-2.288667000.19768300C5.52352100-2.673421000.081619005.53239400-2.652779000.06492500C6.54797800-3.24063000-0.675027006.56033300-3.21423300-0.69130400H7.57448900-3.19524200-0.319425007.58583500-3.16735700-0.33299000C6.26119900-3.85657500-1.890772006.27832800-3.82657000-1.90997300H7.06203100-4.29433400-2.478995007.08193900-4.25963600-2.49787700C4.95527800-3.88475000-2.368955004.97355900-3.85754600-2.39115600H4.74112600-4.34111900-3.332474004.76295900-4.31172800-3.35648900N-0.64493500-0.562158001.59021900-0.64174700-0.594775001.60737400C-1.16474900-1.662186002.20775500-1.17127300-1.697548002.21021100C-0.63713300-2.073623003.43843700-0.65112200-2.127918003.43720700H-1.05962300-2.937492003.93098500-1.08201200-2.993404003.91953600	C	3.92092800	-3.32644000	-1.61512800	3.93593300	-3.30478600	-1.63781100
H3.41621300-2.303434000.218686003.42374200-2.288667000.19768300C5.52352100-2.673421000.081619005.53239400-2.652779000.06492500C6.54797800-3.24063000-0.675027006.56033300-3.21423300-0.69130400H7.57448900-3.19524200-0.319425007.58583500-3.16735700-0.33299000C6.26119900-3.85657500-1.890772006.27832800-3.82657000-1.90997300H7.06203100-4.29433400-2.478995007.08193900-4.25963600-2.49787700C4.95527800-3.88475000-2.368955004.97355900-3.85754600-2.39115600H4.74112600-4.34111900-3.332474004.76295900-4.31172800-3.35648900N-0.64493500-0.562158001.59021900-0.64174700-0.594775001.60737400C-1.16474900-1.662186002.20775500-1.17127300-1.697548002.21021100C-0.63713300-2.073623003.43843700-0.65112200-2.127918003.43720700H-1.05962300-2.937492003.93098500-1.08201200-2.993404003.91953600	С	4.21075600	-2.73928100	-0.38449200	4.22105500	-2.72020700	-0.40489900
C5.52352100-2.673421000.081619005.53239400-2.652779000.06492500C6.54797800-3.24063000-0.675027006.56033300-3.21423300-0.69130400H7.57448900-3.19524200-0.319425007.58583500-3.16735700-0.33299000C6.26119900-3.85657500-1.890772006.27832800-3.82657000-1.90997300H7.06203100-4.29433400-2.478995007.08193900-4.25963600-2.49787700C4.95527800-3.88475000-2.368955004.97355900-3.85754600-2.39115600H4.74112600-4.34111900-3.332474004.76295900-4.31172800-3.35648900N-0.64493500-0.562158001.59021900-0.64174700-0.594775001.60737400C-1.16474900-1.662186002.20775500-1.17127300-1.697548002.21021100C-0.63713300-2.073623003.43843700-0.65112200-2.127918003.43720700H-1.05962300-2.937492003.93098500-1.08201200-2.993404003.91953600	Н	3.41621300	-2.30343400	0.21868600	3.42374200	-2.28866700	0.19768300
C6.54797800-3.24063000-0.675027006.56033300-3.21423300-0.69130400H7.57448900-3.19524200-0.319425007.58583500-3.16735700-0.33299000C6.26119900-3.85657500-1.890772006.27832800-3.82657000-1.90997300H7.06203100-4.29433400-2.478995007.08193900-4.25963600-2.49787700C4.95527800-3.88475000-2.368955004.97355900-3.85754600-2.39115600H4.74112600-4.34111900-3.332474004.76295900-4.31172800-3.35648900N-0.64493500-0.562158001.59021900-0.64174700-0.594775001.60737400C-1.16474900-1.662186002.20775500-1.17127300-1.697548002.21021100C-0.63713300-2.073623003.43843700-0.65112200-2.127918003.43720700H-1.05962300-2.937492003.93098500-1.08201200-2.993404003.91953600	С	5.52352100	-2.67342100	0.08161900	5.53239400	-2.65277900	0.06492500
H7.57448900-3.19524200-0.319425007.58583500-3.16735700-0.33299000C6.26119900-3.85657500-1.890772006.27832800-3.82657000-1.90997300H7.06203100-4.29433400-2.478995007.08193900-4.25963600-2.49787700C4.95527800-3.88475000-2.368955004.97355900-3.85754600-2.39115600H4.74112600-4.34111900-3.332474004.76295900-4.31172800-3.35648900N-0.64493500-0.562158001.59021900-0.64174700-0.594775001.60737400C-1.16474900-1.662186002.20775500-1.17127300-1.697548002.21021100C-0.63713300-2.073623003.43843700-0.65112200-2.127918003.43720700H-1.05962300-2.937492003.93098500-1.08201200-2.993404003.91953600	C	6.54797800	-3.24063000	-0.67502700	6.56033300	-3.21423300	-0.69130400
C6.26119900-3.85657500-1.890772006.27832800-3.82657000-1.90997300H7.06203100-4.29433400-2.478995007.08193900-4.25963600-2.49787700C4.95527800-3.88475000-2.368955004.97355900-3.85754600-2.39115600H4.74112600-4.34111900-3.332474004.76295900-4.31172800-3.35648900N-0.64493500-0.562158001.59021900-0.64174700-0.594775001.60737400C-1.16474900-1.662186002.20775500-1.17127300-1.697548002.21021100C-0.63713300-2.073623003.43843700-0.65112200-2.127918003.43720700H-1.05962300-2.937492003.93098500-1.08201200-2.993404003.91953600	H	7.57448900	-3.19524200	-0.31942500	7.58583500	-3.16735700	-0.33299000
H7.06203100-4.29433400-2.478995007.08193900-4.25963600-2.49787700C4.95527800-3.88475000-2.368955004.97355900-3.85754600-2.39115600H4.74112600-4.34111900-3.332474004.76295900-4.31172800-3.35648900N-0.64493500-0.562158001.59021900-0.64174700-0.594775001.60737400C-1.16474900-1.662186002.20775500-1.17127300-1.697548002.21021100C-0.63713300-2.073623003.43843700-0.65112200-2.127918003.43720700H-1.05962300-2.937492003.93098500-1.08201200-2.993404003.91953600	C	6.26119900	-3.85657500	-1.89077200	6.27832800	-3.82657000	-1.90997300
C4.95527800-3.88475000-2.368955004.97355900-3.85754600-2.39115600H4.74112600-4.34111900-3.332474004.76295900-4.31172800-3.35648900N-0.64493500-0.562158001.59021900-0.64174700-0.594775001.60737400C-1.16474900-1.662186002.20775500-1.17127300-1.697548002.21021100C-0.63713300-2.073623003.43843700-0.65112200-2.127918003.43720700H-1.05962300-2.937492003.93098500-1.08201200-2.993404003.91953600	H	7.06203100	-4.29433400	-2.47899500	7.08193900	-4.25963600	-2.49787700
H4.74112600-4.34111900-3.332474004.76295900-4.31172800-3.35648900N-0.64493500-0.562158001.59021900-0.64174700-0.594775001.60737400C-1.16474900-1.662186002.20775500-1.17127300-1.697548002.21021100C-0.63713300-2.073623003.43843700-0.65112200-2.127918003.43720700H-1.05962300-2.937492003.93098500-1.08201200-2.993404003.91953600	C	4.95527800	-3.88475000	-2.36895500	4.97355900	-3.85754600	-2.39115600
N-0.64493500-0.562158001.59021900-0.64174700-0.594775001.60737400C-1.16474900-1.662186002.20775500-1.17127300-1.697548002.21021100C-0.63713300-2.073623003.43843700-0.65112200-2.127918003.43720700H-1.05962300-2.937492003.93098500-1.08201200-2.993404003.91953600	H	4.74112600	-4.34111900	-3.33247400	4.76295900	-4.31172800	-3.35648900
C -1.16474900 -1.66218600 2.20775500 -1.17127300 -1.69754800 2.21021100 C -0.63713300 -2.07362300 3.43843700 -0.65112200 -2.12791800 3.43720700 H -1.05962300 -2.93749200 3.93098500 -1.08201200 -2.99340400 3.91953600	N	-0.64493500	-0.56215800	1.59021900	-0.64174700	-0.59477500	1.60737400
C -0.63713300 -2.07362300 3.43843700 -0.65112200 -2.12791800 3.43720700 H -1.05962300 -2.93749200 3.93098500 -1.08201200 -2.99340400 3.91953600	C	-1.16474900	-1.66218600	2,20775500	-1.17127300	-1.69754800	2.21021100
H -1.05962300 -2.93749200 3.93098500 -1.08201200 -2.99340400 3.91953600	Ċ	-0.63713300	-2.07362300	3.43843700	-0.65112200	-2.12791800	3.43720700
	Н	-1.05962300	-2.93749200	3.93098500	-1.08201200	-2.99340400	3.91953600

Table S14 The xyz coordinates for the optimized structures for 2 in the S_0 and T_1 states at PBE0/6-31G* level

C	0.41865700	-1.38084600	4.00814800	0.41063600	-1.45119300	4.01577800
Η	0.82770600	-1.70586700	4.96029900	0.81452700	-1.79020200	4.96526600
C	0.95362600	-0.27799900	3.34735900	0.95871900	-0.34768400	3.36716700
Н	1.80241800	0.27724500	3.72821000	1.81259000	0.19454700	3.75526100
C	0.38537300	0.09663800	2.14381100	0.39548600	0.04668500	2.16713300
Н	0.76184600	0.94853200	1.59068200	0.78207200	0.90014100	1.62306700
C	-2.58690100	-1.68468500	0.23315900	-2.58109800	-1.69629600	0.22290800
C	-2.24185300	-2.29859600	1.46515700	-2.24678300	-2.32092600	1.45277700
C	-2.92913400	-3.45461300	1.85495500	-2.94301000	-3.47713600	1.82516900
C	-3.92885800	-4.02300800	1.08987900	-3.93671800	-4.03466100	1.04406500
Η	-4.44495200	-4.91708400	1.41777500	-4.45838000	-4.93041900	1.35851500
C	-4.24142300	-3.39617000	-0.10800000	-4.23586000	-3.39752600	-0.15223600
C	-3.59744800	-2.24694100	-0.54508200	-3.58434800	-2.24665300	-0.57289800
Н	-3.90727200	-1.81409000	-1.48988600	-3.88000400	-1.80116800	-1.51602800
F	-2.62727500	-4.06360400	3.01279800	-2.65623200	-4.09704700	2.98064000
F	-5.20389400	-3.92427100	-0.86621200	-5.19174100	-3.91698900	-0.92340800
Ν	-2.59810600	0.40059000	-1.88930600	-2.54330900	0.39472400	-1.87495200
C	-3.69687300	1.18690400	-1.70576100	-3.69127800	1.22103100	-1.68163500
C	-4.49435300	1.52524000	-2.80708100	-4.48887200	1.56620800	-2.82531200
Н	-5.36592300	2.14635400	-2.65804000	-5.36396500	2.18280900	-2.67266600
C	-4.17033100	1.05431300	-4.06859300	-4.15993400	1.12088800	-4.07083100
Η	-4.79377000	1.31264700	-4.91941000	-4.76890200	1.38012900	-4.93015600
C	-3.04891400	0.24353900	-4.23161600	-3.00734500	0.29674100	-4.22489200
Н	-2.76637700	-0.15505900	-5.19963600	-2.71194600	-0.08985600	-5.19354300
C	-2.29309800	-0.05708300	-3.11335700	-2.25481800	-0.02858500	-3.10252100
Η	-1.41918500	-0.69584300	-3.17104600	-1.38573100	-0.67339800	-3.18696100
C	-2.97636100	1.05298500	0.61674700	-2.93858500	1.04632000	0.63513500
C	-3.91174900	1.57361600	-0.31887400	-3.90173800	1.57699000	-0.35277600
C	-4.94827400	2.39191000	0.14806200	-4.96921100	2.40607800	0.15143200
C	-5.09944000	2.71519700	1.48254700	-5.10600400	2.69788100	1.47198700
Н	-5.91259400	3.34811800	1.81665100	-5.91954300	3.32348700	1.82150700
C	-4.17148800	2.18837900	2.37093800	-4.16562900	2.16050000	2.38268700
C	-3.12271600	1.37279600	1.96681600	-3.10877000	1.35077700	1.97630300
H	-2.44285200	0.99416600	2.72226000	-2.43611100	0.96439300	2.73464300
F	-5.84352400	2.90470200	-0.70998600	-5.86031000	2.91417900	-0.71211900
F	-4.29665100	2.48590300	3.66428300	-4.31351300	2.46101200	3.67115900