Supporting information

Modification of C^N Cyclometalated Ligands: Theoretical Design of Structurally Diverse Ir(III) Complexes for Two-Photon Photodynamic Therapy

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Table S1. OPA characteristics of the complexes [Ir(ppy)$_2$(sip)](PF$_6$) and [Ir(ppy)$_2$(osip)](PF$_6$) under various functionals (basis sets：6-31G*/LANL2DZ)

Functionals	**[Ir(ppy)$_2$(sip)](PF$_6$)**			
	$\boldsymbol{\lambda}_{S_n}^{Exp}$**/nm**	$\boldsymbol{\lambda}_{S_n}^{Calc}$**/nm**	$\boldsymbol{f}_{S_n}$	$\mathbf{E}_{S_n}$**/eV**
M06	470	466.1	0.0003	2.66
	416	412.9	0.3018	3.00
	357	364.8	0.8878	3.40
TPSSH	470	536.8	0.0004	2.31
	416	469.5	0.1135	2.64
	357	396.2	0.3334	3.13
B3LYP	470	479.3	0.0002	2.59
	416	429.8	0.1861	2.89
	357	372.5	0.6757	3.33
PBE0	470	448.1	0.0003	2.77
	416	408.1	0.2444	3.04
	357	356.4	0.6193	3.48
CAM-B3LYP	470	344.6	0.0009	3.60
	416	342.0	0.6592	3.62
	357	313.6	0.8894	3.95
WB97XD	470	339.0	0.0011	3.66
	416	337.0	0.7632	3.68
	357	309.4	0.8082	4.00

Functionals	**[Ir(ppy)$_2$(osip)](PF$_6$)**			
	$\boldsymbol{\lambda}_{S_n}^{Exp}$**/nm**	$\boldsymbol{\lambda}_{S_n}^{Calc}$**/nm**	$\boldsymbol{f}_{S_n}$	$\mathbf{E}_{S_n}$**/eV**
M06	468	462.2	0.0003	2.68
	421	428.9	0.2646	2.89
	396	377.8	0.8130	3.28

	344	353.3	0.6649	3.51
TPSSH	468	533.5	0.0004	2.32
	421	515.5	0.0855	2.40
	396	430.8	0.2591	2.88
	344	388.7	1.1076	3.19
B3LYP	468	477.0	0.0002	2.60
	421	458.6	0.1539	2.70
	396	394.2	0.5389	3.14
	344	364.8	0.6483	3.40
PBE0	468	446.2	0.0003	2.78
	421	432.2	0.2109	2.87
	396	375.0	0.7046	3.31
	344	353.0	1.0092	3.51
CAM-B3LYP	468	349.5	0.7992	3.55
	421	325.0	0.1404	3.81
	396	321.5	0.9799	3.86
	344	300.9	0.2744	4.12
WB97XD	468	342.9	0.9662	3.62
	421	326.4	0.1345	3.80
	396	316.1	0.8379	3.92
	344	293.9	0.1664	4.22

Table S2. OPA characteristics of the complexes $[Ir(ppy)_2(sip)](PF_6)$ and $[Ir(ppy)_2(osip)](PF_6)$ under various basis sets (DFT functional:M06)

Basis Sets	**$[Ir(ppy)_2(sip)](PF_6)$**			
	$\boldsymbol{\lambda_{S_n}^{Exp}}$**/nm**	$\boldsymbol{\lambda_{S_n}^{Calc}}$**/nm**	$\boldsymbol{f}_{S_n}$	$\mathbf{E}_{S_n}$**/eV**
6-31G*	470	466.1	0.0003	2.66
	416	412.9	0.3018	3.00
	357	364.8	0.8878	3.40

6-31G**	470	466.9	0.0003	2.66
	416	413.4	0.2976	3.00
	357	365.6	0.8951	3.39
6-31+G*	470	469.9	0.0003	2.64
	416	417.9	0.2580	2.97
	357	371.4	1.1248	3.34
6-311G*	470	472.0	0.0003	2.63
	416	418.0	0.2734	2.97
	357	369.1	0.6147	3.36
6-311+G*	470	475.8	0.0003	2.61
	416	421.0	0.2419	2.94
	357	373.6	0.8784	3.32

Basis Sets	**[Ir(ppy)$_2$(osip)](PF$_6$)**			
	$\boldsymbol{\lambda}_{S_n}^{Exp}$**/nm**	$\boldsymbol{\lambda}_{S_n}^{Calc}$**/nm**	$\boldsymbol{f}_{S_n}$	$\mathbf{E}_{S_n}$**/eV**
6-31G*	468	462.2	0.0003	2.68
	421	428.9	0.2646	2.89
	396	377.8	0.8130	3.28
	344	353.3	0.6649	3.51
6-31G**	468	463.0	0.0003	2.68
	421	429.6	0.2598	2.89
	396	378.7	0.8142	3.27
	344	354.0	0.6661	3.50
6-31+G*	468	466.3	0.0003	2.66
	421	433.5	0.2119	2.86
	396	383.2	0.9930	3.24
	344	362.7	0.3705	3.42
6-311G*	468	468.2	0.0003	2.65
	421	434.1	0.2334	2.86

	396	379.9	0.5386	3.26
	344	358.1	0.6318	3.46
6-311+G*	468	472.1	0.0003	2.63
	421	436.2	0.1975	2.84
	396	383.5	0.7652	3.23
	344	364.4	0.4719	3.40

Table S3. Calculated OPA wavelengths for the molecules $[Ir(ppy)_2(sip)](PF_6)$ and $[Ir(ppy)_2(osip)](PF_6)$ in aqueous environment, using the M06/6-31G*/LANL2DZ method and compared them with experimentals

MOL.	$\boldsymbol{\lambda}_{S_n}^{Exp}$**/nm**	$\boldsymbol{\lambda}_{S_n}^{Calc}$**/nm**	f	$\mathbf{E}_{S_n}$**/eV**
$[Ir(ppy)_2(sip)](PF_6)$	470	466.1	0.0003	2.66
	416	412.9	0.3018	3.00
	357	364.8	0.8878	3.40
$[Ir(ppy)_2(osip)](PF_6)$	468	462.2	0.0003	2.68
	421	428.9	0.2646	2.89
	396	377.8	0.8130	3.28
	344	353.3	0.6649	3.51

Table S4. Calculated phosphorescence wavelengths for the molecules $[Ir(ppy)_2(sip)](PF_6)$ and $[Ir(ppy)_2(osip)](PF_6)$ in aqueous environment, using the M06/6-31G*/LANL2DZ method and compared them with experimentals

MOL.	$\boldsymbol{\lambda}_{T_1}^{Exp}$**/nm**	$\boldsymbol{\lambda}_{T_1}^{Calc}$**/nm**	$\mathbf{E}_{T_1}$**/eV**
$[Ir(ppy)_2(sip)](PF_6)$	608	569.4	2.18
$[Ir(ppy)_2(osip)](PF_6)$	769	731.1	1.70

Table S5. The key dihedral angles for part 1 (φ1） and part 3 (φ2, φ3) of the complexes

	φ_1 [deg]			φ_2 [deg]			φ_3 [deg]		
MOL.	S_0	S_1	T_1	S_0	S_1	T_1	S_0	S_1	T_1
0	3.41	1.26	3.44	179.47	179.69	179.88	179.57	179.79	179.87
1	9.13	5.16	9.14	179.65	179.88	179.96	179.65	179.34	179.91
2	2.07	0.60	2.07	178.54	178.11	179.35	178.55	177.73	179.35
3	2.80	2.36	2.79	178.60	179.38	179.43	179.47	179.45	179.64
4	2.02	1.84	2.03	179.34	179.88	179.71	178.83	179.49	179.79
5	16.22	16.18	16.17	179.96	179.75	179.95	179.95	179.66	179.94

Table S6. Analysis of the bond lengths, bond angles, and dihedral angles for part 2 of the complexes

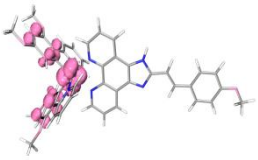
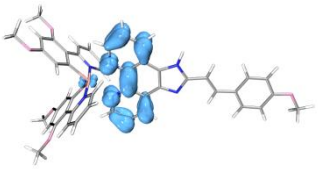
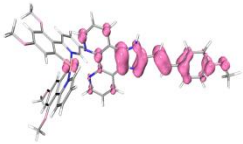
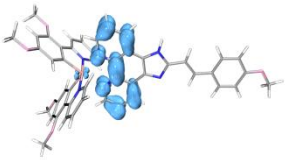
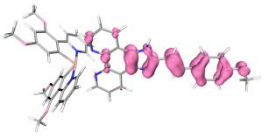
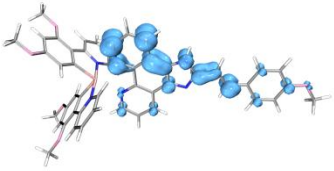
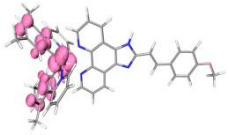
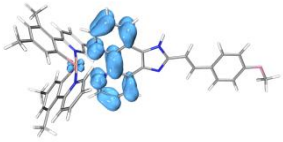
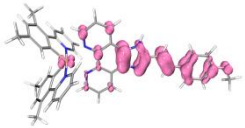
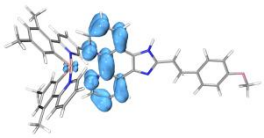
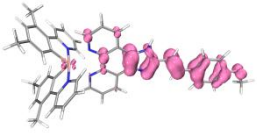
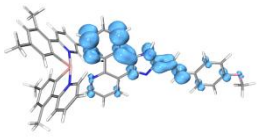
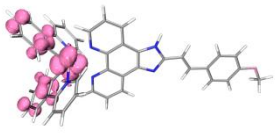
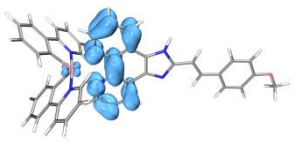
	0			**1**			**2**		
	S_0	S_1	T_1	S_0	S_1	T_1	S_0	S_1	T_1
Bond length[Å]									
M-C_1	2.006	1.988	2.006	2.006	1.984	2.006	2.009	1.988	2.009
M-N_1	2.066	2.065	2.066	2.062	2.601	2.063	2.071	2.071	2.071
M-N_2	2.206	2.190	2.206	2.213	2.196	2.213	2.206	2.192	2.206
Bond angle[deg]									
C_1-M-N_1	79.94	80.79	79.94	79.57	80.36	79.57	80.14	80.98	80.15
N_1-M-N_2	87.29	86.60	87.25	87.18	86.49	87.11	87.85	86.82	87.84
Dihedral angle[deg]									
C_1-M-N_1-N_2	98.31	94.91	98.34	98.24	94.82	98.26	98.28	94.19	98.33
	3			**4**			**5**		
	S_0	S_1	T_1	S_0	S_1	T_1	S_0	S_1	T_1
Bond length[Å]									
M-C_1	2.007	2.009	2.007	2.007	2.009	2.007	2.005	2.007	2.005
M-N_1	2.070	2.067	2.070	2.068	2.063	2.067	2.062	2.058	2.062

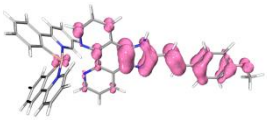
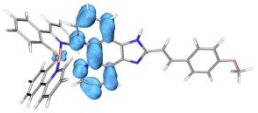
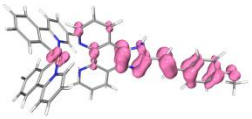
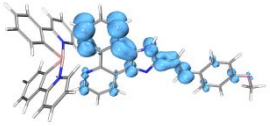
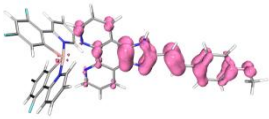
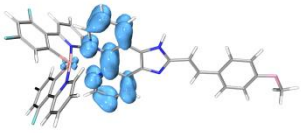
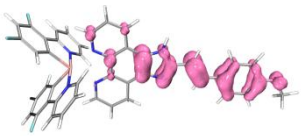
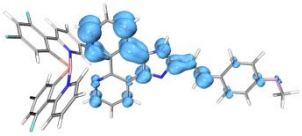
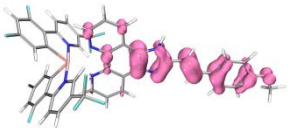
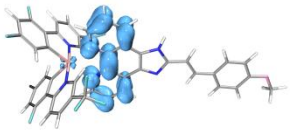
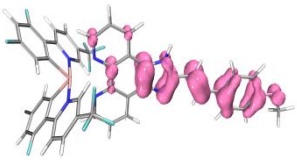
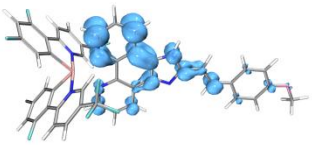
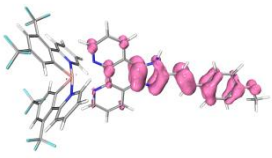
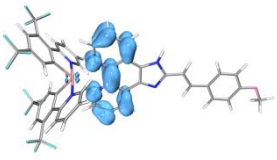
M-N_2	2.199	2.177	2.199	2.197	2.174	2.198	2.202	2.178	2.202
Bond angle[deg]									
C_1-M-N_1	80.19	80.18	80.19	80.14	80.13	80.14	79.40	79.40	79.40
N_1-M-N_2	87.15	87.72	87.11	87.46	87.99	87.43	87.36	88.20	87.36
Dihedral angle[deg]									
C_1-M-N_1-N_2	98.22	97.63	98.25	98.19	97.55	98.25	98.81	97.02	98.85

Table S7. Calculated OPA properties of the studied complexes, including absorption wavelengths, vertical excitation energies (E), oscillator strengths (*f*), and corresponding transition nature by M06/6-31G*/LANL2DZ in water

Mol.	λ_{abs}/nm	f	E/eV		Transition character		Assignment
0	458.3	0.0003	2.71	$S_0 \rightarrow S_1$	HOMO-1→LUMO	91.82%	MLCT/LLCT
	427.9	0.3001	2.90	$S_0 \rightarrow S_2$	HOMO→LUMO	92.38%	MLCT/ILCT
	377.0	0.9424	3.29	$S_0 \rightarrow S_7$	HOMO→LUMO+1	91.64%	ILCT
1	475.5	0.0004	2.61	$S_0 \rightarrow S_1$	HOMO→LUMO	96.53%	MLCT/LLCT
	427.3	0.2896	2.90	$S_0 \rightarrow S_2$	HOMO-1→LUMO	92.76%	MLCT/ILCT
	377.0	0.9813	3.29	$S_0 \rightarrow S_7$	HOMO-1→LUMO+1	89.14%	MLCT/ILCT
2	462.2	0.0003	2.68	$S_0 \rightarrow S_1$	HOMO-1→LUMO	96.31%	MLCT/LLCT
	428.9	0.2646	2.89	$S_0 \rightarrow S_2$	HOMO→LUMO	93.07%	MLCT/ILCT
	377.8	0.8146	3.28	$S_0 \rightarrow S_6$	HOMO→LUMO+1	79.66%	MLCT/ILCT
3	434.4	0.2253	2.85	$S_0 \rightarrow S_1$	HOMO→LUMO	94.48%	MLCT/ILCT
	380.3	0.8142	3.26	$S_0 \rightarrow S_3$	HOMO→LUMO+1	92.28%	ILCT
4	440.5	0.1992	2.81	$S_0 \rightarrow S_1$	HOMO→LUMO	94.66%	MLCT/ILCT
	383.2	0.7058	3.24	$S_0 \rightarrow S_4$	HOMO→LUMO+2	38.96%	ILCT
					HOMO→LUMO+3	53.68%	ILCT
5	438.5	0.2113	2.83	$S_0 \rightarrow S_1$	HOMO→LUMO	88.37%	MLCT/ILCT
	384.8	0.4741	3.22	$S_0 \rightarrow S_6$	HOMO→LUMO+2	45.01%	ILCT
					HOMO→LUMO+3	44.46%	ILCT/LLCT
	372.5	0.3808	3.33	$S_0 \rightarrow S_7$	HOMO→LUMO+2	47.45%	MLCT/ILCT/ LLCT
					HOMO→LUMO+3	45.19%	MLCT/ILCT/ LLCT

Table S8. The distribution of holes (pink) and electrons (blue) in the singlet excited state of the complex（Isovalue：0.001721）

Mol.	States	Hole	Electron
0	S_1		
	S_2		
	S_7		
1	S_1		
	S_2		
	S_7		
2	S_1		

	S_2		
	S_6		
3	S_1		
	S_3		
4	S_1		
	S_4		
5	S_1		

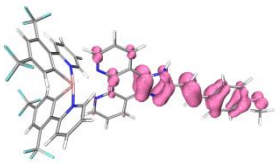
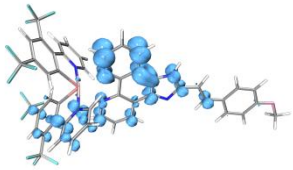
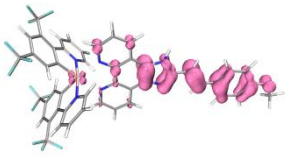
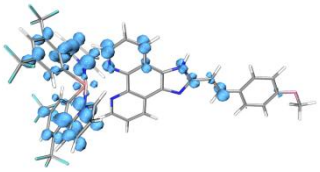
	S_6		
	S_7		

Table S9. Calculated two-photon absorption transition matrix elements for studied compounds by CAM-B3LYP/ 6-31G*/ LANL2DZ

Mol.	Ex.states	TPA tensor elements(in a.u.)					
		S_{xx}	S_{yy}	S_{zz}	S_{xy}	S_{xz}	S_{yz}
0	1	-174.6	6.1	1.4	3.7	0.9	5.9
1	1	-174.2	3.5	-0.6	3.6	1.8	5.9
2	1	179.2	-1.2	-2.4	4.4	2.4	-6.3
3	1	194.5	-4.9	-1.8	-4.6	-4.1	-5.5
4	1	-213.9	-3.2	9.6	-0.8	-6.8	2.2
5	1	181.3	-8.7	1.7	-12.2	-3.7	-5.0

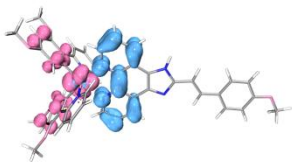
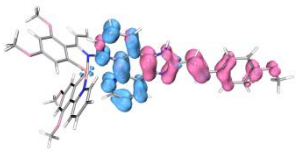
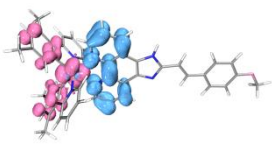
Table S10. The $\langle \mathbf{S_1}|\widehat{\boldsymbol{H}}_{\boldsymbol{SOC}}|\mathbf{T_n}\rangle$ and intersystem crossing rate (k_{isc}) of the studied complexes (Foscan：$\langle \mathbf{S_1}|\widehat{\boldsymbol{H}}_{\boldsymbol{SOC}}|\mathbf{T_1}\rangle$=0.96 cm^{-1})

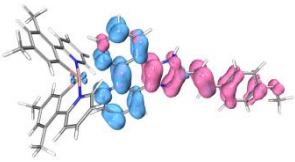
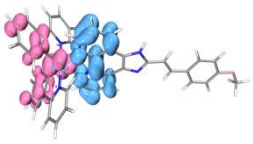
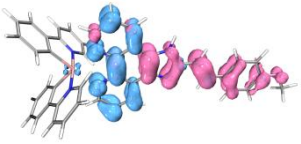
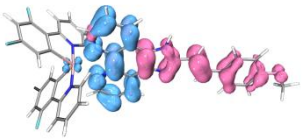
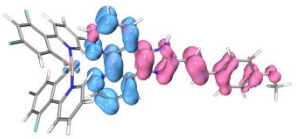
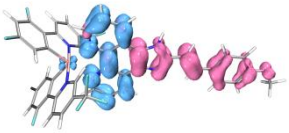
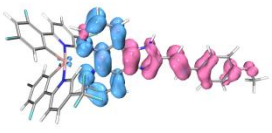
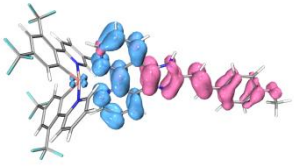
MOL.	Triplet states	$\langle S_1\|\widehat{H}_{SOC}\|T_n\rangle$/cm	ΔE_{ST}/eV	k_{isc}/s^{-1}	λ/cm
0	T_1	130.65	0.438	2.61×10^{12}	
	T_2	61.62	-0.234	9.10×10^{6}	5333.9
	T_3	422.40	-0.497	1.51×10^{5}	
1	T_1	41.50	0.331	1.05×10^{11}	
	T_2	120.58	-0.342	1.60×10^{6}	5387.6
	T_3	378.57	-0.570	9.07×10^{3}	
2	T_1	112.05	0.402	1.45×10^{12}	
	T_2	67.45	-0.257	5.68×10^{6}	5353.7
	T_3	350.37	-0.527	3.56×10^{4}	
3	T_1	4.33	0.522	7.40×10^{8}	
	T_2	6.26	-0.092	1.89×10^{8}	2102.9
	T_3	71.62	-0.389	3.77×10^{5}	
4	T_1	3.07	0.479	1.14×10^{9}	
	T_2	5.31	-0.094	1.07×10^{8}	2252.8
	T_3	45.37	-0.411	6.01×10^{4}	
5	T_1	3.27	0.495	8.26×10^{8}	
	T_2	5.40	-0.093	1.28×10^{8}	2160.6
	T_3	49.66	-0.398	1.22×10^{5}	

Table S11. The fluorescence properties of the studied complexes, including fluorescence emission wavelength (λ_{ems}), oscillator strength (f), vertical excitation energy (E), transition characteristics, and fluorescence rate (k_f)

Mol.	λ_{ems}/nm	f	E/eV	Transition nature		k_f/s
0	546.9	0.0004	2.267	$S_1 \rightarrow S_0$	H→L (97.00%)	8.92×10^4
1	575.5	0.0006	2.154	$S_1 \rightarrow S_0$	H→L (98.14%)	1.21×10^5
2	559.8	0.0004	2.215	$S_1 \rightarrow S_0$	H→L (98.28%)	8.51×10^4
3	534.5	0.3358	2.320	$S_1 \rightarrow S_0$	H→L (96.33%)	7.84×10^7
4	545.4	0.2960	2.273	$S_1 \rightarrow S_0$	H→L (96.53%)	6.64×10^7
5	541.5	0.3090	2.290	$S_1 \rightarrow S_0$	H→L (96.14%)	7.03×10^7

Table S12. The distribution of holes (pink) and electrons (blue) in the S_1 and T_1 states of the studied complex (Isovalue：0.001721)

Mol.	States	Hole-Electron	Assignment
0	S_1		^{1}MLCT/^{1}LLCT
	T_1		^{3}MLCT/^{3}ILCT
1	S_1		^{1}MLCT/^{1}LLCT

	T_1		^{3}MLCT/^{3}ILCT
2	S_1		^{1}MLCT/^{1}LLCT
	T_1		^{3}MLCT/^{3}ILCT
3	S_1		^{1}MLCT/^{1}ILCT
	T_1		^{3}MLCT/^{3}ILCT
4	S_1		^{1}MLCT/^{1}ILCT
	T_1		^{3}MLCT/^{3}ILCT
5	S_1		^{1}MLCT/^{1}ILCT

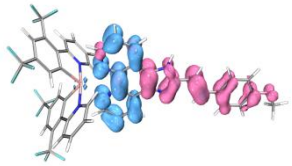
	T_1		^{3}MLCT/^{3}ILCT

Table S13. The overlap integral (S_{H-L}/a.u.) and spatial transfer distance (D_{H-L}/Å) of the HOMO and LUMO orbitals of the studied complex in the S_1 state

MOL.	S_{H-L}/a.u.	D_{H-L}/Å
0	0.203	3.751
1	0.200	3.807
2	0.201	3.769
3	0.497	4.864
4	0.483	4.975
5	0.486	4.986

Table S14. In the S_1 state, the contribution of the metal Ir(III) atom to the dominant frontier orbitals and the proportion of the MLCT transition (MLCT%)

	MO	Ir(III) contribution (%)	MLCT%
0	**H**	36.4 (24.3d_{x2-y2}+7.5d_{yz}+2.9d_{z2}+1.2d_{xy})	**32.9**
	L	2.5 (1.9d_{xz})	
1	**H**	36.0 (22.0d_{x2-y2}+7.9d_{yz}+4.4d_{z2}+1.1d_{xy})	**33.1**
	L	2.3 (1.6d_{xz})	
2	**H**	38.0 (18.4d_{x2-y2}+10.2d_{z2}+7.5d_{yz}+1.0d_{xy})	**35.0**
	L	2.4 (1.2d_{xz})	
3	**H**	0.3 (0.2d_{xz})	**1.8**
4	**H**	0.2(0.2d_{xy})	**1.7**
	L	2.0 (1.6d_{xy})	
5	**H**	0.2 (0.2d_{xz})	**1.5**
	L	1.8 (1.2d_{xz})	

Table S15. Calculated the emission energies, emission wavelengths and transition natures of T_1 states for studied complexes by M06/6-31G*/ LANL2DZ

MOL.	States	E(T_1)/eV	λ/nm	Transition character (contribution larger than 10%)	Assignment
0	T_1	1.69	731.9	HOMO→LUMO(56.25%) HOMO→LUMO+1(33.88%)	^{3}ILCT
1	T_1	1.69	731.8	HOMO→LUMO(56.52%) HOMO→LUMO+1(33.61%)	^{3}ILCT
2	T_1	1.70	731.1	HOMO→LUMO(52.80%) HOMO→LUMO+1(37.15%)	^{3}ILCT
3	T_1	1.70	728.8	HOMO→LUMO(42.98%) HOMO→LUMO+1(46.22%)	^{3}ILCT
4	T_1	1.71	727.2	HOMO→LUMO(35.48%) HOMO→LUMO+1(52.21%)	^{3}ILCT
5	T_1	1.70	727.8	HOMO→LUMO(33.35%) HOMO→LUMO+2(28.09%) HOMO→LUMO+3(19.03%)	^{3}ILCT

Table S16. Cartesian coordinates of optimized structures

0 (S_0)

Ir	-1.80327300	-0.01884000	-0.01557800
C	-5.10115200	-2.19119200	-1.77415300
C	-5.47223400	-3.05626300	-0.74200300
C	-4.06060100	-1.27462600	-1.59988600
C	-4.79531200	-2.99666400	0.47676600
C	-3.74225700	-2.07391300	0.67501900
C	-2.96130300	-1.92241000	1.89516300
N	-1.87488100	0.99102600	-1.81641300
N	0.07716600	1.05930400	0.39443900
N	-0.21470200	-1.45787600	-0.54713700
N	-1.95612900	-0.99963600	1.79596600
C	-3.14364300	-2.58504000	3.11825300
C	-3.65261100	1.64825300	1.71045100
C	-3.32370800	2.39562100	-0.58045700
C	-2.66828000	2.10528300	-1.84845600
C	-1.21564100	0.58434200	-2.91321500
C	0.18023100	2.30722300	0.83878000
C	1.20577000	0.35055700	0.12934400
C	1.04950100	-1.00062100	-0.35934400
C	-0.40650200	-2.69471100	-0.99321200
C	-1.15762100	-0.73691100	2.84309200
C	-2.32036500	-2.30572600	4.19520100
C	-4.47402900	2.75276600	1.95109300
C	-4.15585300	3.50783300	-0.31547000
C	-2.77915200	2.81435500	-3.05403600
C	-1.29747300	1.25037300	-4.12031800
C	1.41597400	2.92886100	1.05517900
C	2.48672300	0.90714600	0.32985600
C	2.17601600	-1.81117000	-0.64123300
C	0.65571900	-3.55645300	-1.28919400
C	-1.30147800	-1.36512600	4.06457300
C	-4.72852700	3.68742800	0.94431400
C	-2.09921100	2.38766900	-4.18159800
C	2.57388000	2.22591900	0.80246600
C	3.61879300	0.08369000	0.04099000
C	1.94881100	-3.11505300	-1.11613100
C	3.44851700	-1.21793800	-0.41885800
N	4.93918300	0.39975200	0.16089100
N	4.72214200	-1.69825500	-0.57909400
C	5.58826400	-0.69273500	-0.21952800
C	7.01747300	-0.87340000	-0.27460600

C	7.87787100	0.10685200	0.06480800
H	-6.27842700	-3.76652400	-0.88369800
H	-3.81351500	-0.62281300	-2.43820200
H	-3.94010300	-3.31129600	3.21031800
H	-3.48985800	0.94950400	2.53140200
H	-0.61556400	-0.31658400	-2.80015200
H	-0.75807500	2.82603900	1.03374900
H	-1.44306800	-3.00373600	-1.12437800
H	-0.39005400	0.01687100	2.67812900
H	-2.47592600	-2.82235000	5.14002900
H	-3.40735600	3.69470000	-3.09130000
H	-0.74956400	0.88342000	-4.98313300
H	1.44387600	3.95119100	1.42127500
H	0.44837100	-4.55799500	-1.65462400
H	-0.63508500	-1.11835200	4.88573300
H	-5.36548100	4.54291200	1.13687600
H	-2.19715700	2.94352700	-5.11179000
H	3.55520500	2.66820200	0.96123300
H	2.78752200	-3.76851000	-1.34769500
H	7.44475600	1.05719500	0.38740100
H	4.99399200	-2.62029700	-0.89966000
H	7.36848500	-1.85039700	-0.60841900
C	9.32737600	0.04901900	0.05075400
C	10.05581100	1.18214000	0.43223300
C	10.05332000	-1.09595900	-0.33013400
C	11.44563300	1.19704200	0.44082500
H	9.51567500	2.08073800	0.73129300
C	11.43229400	-1.09777200	-0.32693700
H	9.52798200	-2.00042700	-0.63381000
C	12.14315600	0.04943000	0.05860400
H	11.96973800	2.09945900	0.74408700
H	11.99684700	-1.98067400	-0.62067900
C	-3.07082600	1.46042100	0.46245300
C	-3.37380700	-1.20831200	-0.39357400
O	13.48820000	-0.05625000	0.02658100
C	14.25212600	1.07211500	0.40429000
H	14.05070700	1.36079800	1.44519100
H	15.29981600	0.77921100	0.30749600
H	14.05241200	1.92850200	-0.25457700
O	-4.98787000	2.84432700	3.19710700
O	-4.36751300	4.38611600	-1.32150400
C	-5.18840400	5.51479700	-1.09228500
H	-4.77524300	6.15485600	-0.30123100
H	-5.20797600	6.06994500	-2.03256100

H	-6.21127700	5.21709400	-0.82523900
C	-5.82889700	3.93803700	3.50382400
H	-6.12643000	3.81207400	4.54733700
H	-5.30001300	4.89477000	3.39195800
H	-6.72669300	3.94375000	2.87030200
O	-5.11276500	-3.81708900	1.50368800
O	-5.70230800	-2.17700600	-2.98383100
C	-6.15458900	-4.75927900	1.33899000
H	-5.92752600	-5.46829800	0.53160500
H	-6.22517000	-5.29992900	2.28527100
H	-7.11247900	-4.26361100	1.13187600
C	-6.76264600	-3.08028200	-3.22332900
H	-7.60090900	-2.90657200	-2.53440200
H	-7.09549400	-2.89696200	-4.24749600
H	-6.42912300	-4.12342400	-3.13310500

1 (S_0)

Ir	-2.23172600	0.01410800	0.00353300
C	-5.50596800	-1.84777800	-2.12469300
C	-5.83658800	-2.87976500	-1.24385300
C	-4.48394900	-0.97334000	-1.76363300
C	-5.20718200	-3.04935700	-0.01331700
C	-4.18792800	-2.13302500	0.35186400
C	-3.42210200	-2.14333000	1.60244400
N	-2.29496300	1.28345800	-1.62071000
N	-0.33891100	1.01005400	0.57004200
N	-0.64152400	-1.34139900	-0.73033700
N	-2.40262300	-1.23181700	1.63764800
C	-3.64061300	-2.93024100	2.74081400
C	-4.06293900	1.42449700	1.96256000
C	-3.72794600	2.51923700	-0.18110900
C	-3.09906800	2.38298200	-1.49867400
C	-1.64870100	1.02209300	-2.76755100
C	-0.22971400	2.17775600	1.19447000
C	0.78621600	0.34311700	0.20233600
C	0.62433000	-0.92066300	-0.48067000
C	-0.83870600	-2.49982600	-1.35050300
C	-1.61037100	-1.11950100	2.71507000
C	-2.82810500	-2.80531000	3.85644100
C	-4.84256600	2.48939500	2.40830400
C	-4.49330200	3.62515300	0.26884500
C	-3.26329700	3.20663100	-2.62003500
C	-1.76739000	1.82140000	-3.88837200
C	1.00882300	2.75459700	1.50043200

C	2.06976700	0.85795000	0.48241800
C	1.74767400	-1.68497600	-0.88086400
C	0.21971200	-3.31333800	-1.77072900
C	-1.78111400	-1.89041400	3.84887300
C	-5.02794800	3.57800200	1.55369900
C	-2.60409800	2.92895000	-3.80676400
C	2.16334600	2.09132200	1.14571300
C	3.19809900	0.08295900	0.07164600
C	1.51475900	-2.90560500	-1.53913000
C	3.02294100	-1.13455200	-0.57779800
N	4.51954500	0.37539600	0.23231000
N	4.29506500	-1.58699100	-0.81379800
C	5.16464600	-0.64814500	-0.31135600
C	6.59330300	-0.81928800	-0.40091900
C	7.45503200	0.09759700	0.08195600
H	-6.61811500	-3.58589000	-1.53132200
H	-4.21053900	-0.17789500	-2.46115300
H	-4.46017700	-3.63463900	2.77006900
H	-3.89868500	0.58229700	2.63909200
H	-1.03313400	0.12471000	-2.77262600
H	-1.16551400	2.66731900	1.46404400
H	-1.87691900	-2.78355800	-1.52145200
H	-0.82781300	-0.36582100	2.65326300
H	-3.01852900	-3.42203600	4.73195300
H	-3.92333900	4.06174400	-2.57908500
H	-1.22852600	1.56990200	-4.79692000
H	1.04146700	3.71120400	2.01406000
H	0.00809200	-4.25119800	-2.27597800
H	-1.11858900	-1.76330200	4.69973100
H	-5.61302800	4.42955700	1.90654900
H	-2.74948700	3.57802100	-4.66738500
H	3.14688300	2.50030500	1.36766000
H	2.35057700	-3.52264000	-1.86272700
H	7.02206800	0.98509100	0.55082800
H	4.56463900	-2.44781300	-1.27530900
H	6.94137300	-1.73325900	-0.88328500
C	8.90446200	0.04674900	0.05238800
C	9.63175900	1.10154300	0.61682900
C	9.63153300	-1.01496300	-0.51958600
C	11.02151200	1.11911700	0.62276100
H	9.09076200	1.93485100	1.06571600
C	11.01056400	-1.01270200	-0.52220200
H	9.10707600	-1.85617500	-0.97075700
C	11.72032600	0.05502500	0.04911300

H	11.54425700	1.95898500	1.07244600
H	11.57602800	-1.83107300	-0.96379200
C	-3.48662700	1.42066000	0.69028900
C	-3.80557400	-1.10057200	-0.54931500
O	13.06547900	-0.03916300	-0.00600500
C	13.82845200	1.01187400	0.55319700
H	13.63098800	1.12074300	1.62861400
H	14.87636100	0.74252900	0.40443700
H	13.62402900	1.96629000	0.04853700
C	-4.75458000	4.87397000	-0.52541200
H	-3.83206300	5.32323000	-0.91633800
H	-5.42377400	4.69731200	-1.37920700
H	-5.24032600	5.62588000	0.10684700
C	-5.47717500	2.47386200	3.76580200
H	-5.45190000	3.46635500	4.23377200
H	-6.53431100	2.17828600	3.70392000
H	-4.97862300	1.76353800	4.43647000
C	-6.24442800	-1.69022800	-3.41915300
H	-6.44692800	-2.66179400	-3.88808500
H	-7.21810800	-1.20460900	-3.26176000
H	-5.68308100	-1.07390300	-4.13177500
C	-5.65116600	-4.22075100	0.81677400
H	-4.81306700	-4.86308500	1.11830200
H	-6.17708200	-3.91281900	1.73139300
H	-6.34864900	-4.84317800	0.24480000

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Ir	-2.65153800	0.03798500	0.02710900
C	-6.04976000	-1.43874800	-2.26342100
C	-6.35432600	-2.61591900	-1.57827600
C	-5.00732800	-0.61827800	-1.83753100
C	-5.61036500	-2.96801300	-0.46150700
C	-4.56259400	-2.14623200	-0.03040900
C	-3.73285100	-2.44748200	1.13079600
N	-2.76605800	1.63317200	-1.28850300
N	-0.76565200	0.90044600	0.77817000
N	-1.07088100	-1.07773000	-1.04056300
N	-2.74448900	-1.54043600	1.36514100
C	-3.88437000	-3.54220700	1.98386100
C	-4.50828900	0.98647100	2.28372600
C	-4.19051800	2.46865900	0.41217700
C	-3.55299800	2.66870200	-0.88443800
C	-2.13367300	1.68668200	-2.47213400
C	-0.65533000	1.88458700	1.66423500

C	0.35885600	0.34808900	0.25168800
C	0.19579200	-0.71583800	-0.71282600
C	-1.26847700	-2.05187000	-1.92231700
C	-1.91993500	-1.69605300	2.41410500
C	-3.03374400	-3.70115000	3.06484200
C	-5.32684600	1.93825400	2.88770700
C	-5.01340600	3.42240800	1.02254100
C	-3.69672300	3.78935000	-1.70465100
C	-2.24622200	2.77188300	-3.32146000
C	0.58365200	2.37850100	2.08983300
C	1.64264900	0.78838100	0.63749800
C	1.31842500	-1.35023600	-1.29849200
C	-0.21029700	-2.72629600	-2.54216400
C	-2.03016300	-2.76096200	3.28895900
C	-5.58134500	3.15894800	2.26052100
C	-3.04405100	3.84316800	-2.92473900
C	1.73735900	1.82661500	1.57723000
C	2.77043000	0.14043200	0.04557700
C	1.08491500	-2.37538800	-2.23239200
C	2.59390800	-0.88266300	-0.88016100
N	4.09211200	0.38690400	0.26873900
N	3.86535900	-1.26096900	-1.22424800
C	4.73596400	-0.47358400	-0.50887300
C	6.16417800	-0.62427200	-0.63387900
C	7.02765200	0.12171400	0.08331800
H	-7.16927200	-3.25377200	-1.91490400
H	-4.79427200	0.29671100	-2.39315500
H	-4.67489600	-4.26445600	1.79767800
H	-4.32898600	0.04052000	2.79795700
H	-1.52981200	0.81932600	-2.73151700
H	-1.59013700	2.28813300	2.05258800
H	-2.30657200	-2.29719900	-2.14434600
H	-1.16031400	-0.92789400	2.54462700
H	-3.15205400	-4.55186300	3.73194800
H	-4.32564200	4.61535900	-1.38299500
H	-1.71941300	2.77245600	-4.27100800
H	0.61713100	3.18360200	2.81827300
H	-0.42271800	-3.51383500	-3.25925100
H	-1.34358700	-2.84617400	4.12593400
H	-6.22105000	3.89958300	2.73650200
H	-3.15707700	4.71433600	-3.56588200
H	2.72137900	2.17560800	1.88344800
H	1.92057700	-2.88641400	-2.70644000
H	6.59625500	0.85375200	0.77101500

H	4.13470800	-1.98659400	-1.87808300
H	6.50972900	-1.38167200	-1.33826200
C	8.47681900	0.06389000	0.05482000
C	9.20637900	0.90608300	0.90256200
C	9.20144300	-0.80357800	-0.78509800
C	10.59592000	0.89913400	0.93164400
H	8.66745800	1.58723900	1.56145400
C	10.58024600	-0.82218400	-0.76914300
H	8.67521700	-1.47400400	-1.46323300
C	11.29217500	0.02870300	0.09065800
H	11.12077700	1.56952300	1.60693200
H	11.14384200	-1.49083600	-1.41699900
C	-3.91633900	1.22772500	1.03834900
C	-4.23562800	-0.95134200	-0.71786800
O	12.63685600	-0.06816500	0.03038200
C	13.40069500	0.76522000	0.87985200
H	13.18211300	0.56445100	1.93784200
H	14.44821500	0.53199800	0.67715200
H	13.21752200	1.82759100	0.66726400
H	-6.63353800	-1.15763900	-3.13965000
H	-5.84949500	-3.88848900	0.07077900
H	-5.21297600	4.37667500	0.53539200
H	-5.77357200	1.72694500	3.85899000

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Ir	-2.22564900	0.00458000	0.01438500
C	-5.53858500	-1.65806800	-2.20087600
C	-5.97494600	-2.69429200	-1.38880000
C	-4.48236000	-0.82799700	-1.86012500
C	-5.30799600	-2.87902500	-0.19250100
C	-4.23686400	-2.07533100	0.21121900
C	-3.48924400	-2.21630300	1.45617200
N	-2.20374900	1.35834100	-1.55151800
N	-0.35209300	0.93078000	0.69672100
N	-0.65440200	-1.32606000	-0.75884600
N	-2.46413400	-1.32500900	1.58247900
C	-3.73414900	-3.13106400	2.48431000
C	-4.12950600	1.35231500	1.97910300
C	-3.67523200	2.51236900	-0.10763700
C	-2.97149300	2.47366200	-1.38504100
C	-1.50982800	1.17422000	-2.68617400
C	-0.24358500	2.05201000	1.40177100
C	0.77386600	0.28517100	0.29251100
C	0.61226600	-0.92988500	-0.47106000

C	-0.85282400	-2.44365800	-1.44984800
C	-1.69435500	-1.32633400	2.68256900
C	-2.93925500	-3.12588600	3.61903500
C	-4.93188600	2.41581900	2.36174300
C	-4.49679300	3.55261800	0.33812300
C	-3.02931200	3.42604000	-2.40665800
C	-1.53634200	2.08495400	-3.72573400
C	0.99496100	2.60162500	1.75375800
C	2.05666100	0.77694600	0.61234100
C	1.73469400	-1.67308700	-0.91058100
C	0.20518300	-3.23724700	-1.90726100
C	-1.89734000	-2.20957100	3.72657600
C	-5.13476800	3.53200900	1.56382900
C	-2.31262900	3.23022600	-3.57618100
C	2.14946100	1.96232000	1.35827300
C	3.18491800	0.03020900	0.15308600
C	1.50013600	-2.85129000	-1.64204300
C	3.00982400	-1.14461200	-0.57140700
N	4.50578000	0.31436200	0.32879800
N	4.28193100	-1.57920800	-0.83769900
C	5.15120800	-0.67133100	-0.28078600
C	6.57957200	-0.82972600	-0.39210100
C	7.44068600	0.06848000	0.12594000
H	-6.80341000	-3.33544100	-1.67331500
H	-4.20062800	-0.03569400	-2.55255200
H	-4.54946300	-3.83712800	2.39061500
H	-4.02096400	0.51125800	2.66283000
H	-0.92932800	0.25615400	-2.74839200
H	-1.17794600	2.52599600	1.70038500
H	-1.88955200	-2.71053200	-1.65082100
H	-0.90196000	-0.58134500	2.71201600
H	-3.13459300	-3.83594500	4.41925000
H	-3.64013800	4.31124000	-2.28036500
H	-0.96255500	1.89394100	-4.62755000
H	1.02678200	3.51993700	2.33285100
H	-0.00759000	-4.14203200	-2.46890900
H	-1.25281900	-2.17316400	4.59966300
H	-5.76608900	4.35606900	1.88107200
H	-2.36287700	3.97074000	-4.37107400
H	3.13268400	2.35349100	1.61117300
H	2.33488200	-3.45282100	-1.99596400
H	7.00713500	0.92901500	0.64207400
H	4.55235900	-2.40847000	-1.35333900
H	6.92751100	-1.71469300	-0.92584700

C	8.88976000	0.03124800	0.07518700
C	9.61585000	1.07155700	0.66745900
C	9.61760500	-1.00191500	-0.54603600
C	11.00522100	1.10294000	0.65231000
H	9.07410700	1.88245200	1.15483700
C	10.99629300	-0.98588600	-0.56961500
H	9.09412200	-1.83179500	-1.01878700
C	11.70483900	0.06763900	0.02901800
H	11.52707800	1.93098100	1.12435100
H	11.56251800	-1.78218500	-1.04896800
C	-3.48524700	1.38764000	0.74055000
C	-3.81294000	-1.02784100	-0.65077200
F	-5.73194300	-3.88456300	0.58620700
F	-6.17012600	-1.45910100	-3.36121600
F	-4.69430400	4.63508900	-0.42763200
F	-5.54055200	2.37285800	3.55016400
O	13.04966400	-0.01055100	-0.05065500
C	13.81109900	1.02734200	0.53473500
H	13.62879200	1.09545300	1.61614700
H	14.85912700	0.77406600	0.36078100
H	13.58975200	1.99711800	0.06791400

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Ir	2.16140400	0.00332300	0.03181900
C	5.51363900	-1.03974200	-2.48350000
C	5.89128200	0.17790600	-3.03178300
C	4.46689600	-1.17058800	-1.58414700
C	5.17377700	1.29128700	-2.64244600
C	4.10667000	1.22684600	-1.73807300
C	3.31105800	2.35874400	-1.28961900
N	2.21599700	-2.00725700	0.51061200
N	0.28836900	0.12457100	1.17454400
N	0.58849200	-0.12974700	-1.50062500
N	2.31139800	2.01462200	-0.42186000
C	3.48267800	3.70207400	-1.63940400
C	4.03806500	1.19048200	2.12233800
C	3.66113800	-1.20811700	2.19789400
C	2.99224700	-2.34426800	1.58424100
C	1.55275400	-2.94880600	-0.16948100
C	0.18124500	0.23386600	2.49506400
C	-0.83817800	0.05229000	0.41640600
C	-0.67810000	-0.06979300	-1.01349600
C	0.78523500	-0.23960500	-2.81042500
C	1.50755300	2.95126500	0.09148900

C	2.64903900	4.67004000	-1.10863600
C	4.85135300	1.06651400	3.23807400
C	4.49291400	-1.26555500	3.32284700
C	3.08375300	-3.68593300	1.97040800
C	1.61679300	-4.28716300	0.17501200
C	-1.05683100	0.28392100	3.14642600
C	-2.12022100	0.10223100	1.00225500
C	-1.80161100	-0.13503400	-1.87296900
C	-0.27445200	-0.30120200	-3.72234300
C	1.64369900	4.29180000	-0.22411600
C	5.09785300	-0.14807600	3.86250300
C	2.39504600	-4.65790400	1.26855300
C	-2.21161100	0.21990700	2.39805300
C	-3.24939200	0.03004100	0.13007900
C	-1.56872600	-0.25122000	-3.25533800
C	-3.07562000	-0.08094200	-1.24596800
N	-4.56975700	0.05373500	0.46435700
N	-4.34763900	-0.12544800	-1.75283700
C	-5.21619300	-0.04198900	-0.69027200
C	-6.64440000	-0.06517500	-0.88139700
C	-7.50701500	0.02893000	0.15001300
H	6.71422300	0.25845200	-3.73494900
H	4.23672200	-2.16324000	-1.19956900
H	4.27363000	3.98261800	-2.32310900
H	3.89810200	2.18100400	1.69184200
H	0.96863800	-2.61075800	-1.02329400
H	1.11533300	0.29042400	3.05259300
H	1.82134300	-0.28635300	-3.14263700
H	0.74342200	2.60856900	0.78737100
H	2.78358400	5.71510000	-1.37532200
H	3.70037300	-3.96077900	2.81671800
H	-1.08782300	0.37548900	4.22816500
H	-0.06274000	-0.39108800	-4.78361000
H	5.73792300	-0.22317300	4.73589100
H	2.46924600	-5.70164500	1.56340800
H	-3.19447400	0.25944200	2.86284800
H	-2.40502300	-0.30147600	-3.94975500
H	-7.07610000	0.13017900	1.14948300
H	-4.61746500	-0.20552400	-2.72633300
H	-6.99193900	-0.16388900	-1.91001800
C	-8.95607200	0.01212400	0.08866100
C	-9.68749900	0.14744500	1.27477700
C	-9.67872400	-0.13620700	-1.11087600
C	-11.07722800	0.13999500	1.28898600

H	-9.14987200	0.26280700	2.21617200
C	-11.05755300	-0.14644200	-1.11400200
H	-9.15085200	-0.24777400	-2.05698800
C	-11.77158900	-0.00821100	0.08657800
H	-11.60355200	0.24895600	2.23347500
H	-11.61963700	-0.26215500	-2.03874800
C	3.42678300	0.05509000	1.58835400
C	3.74484500	-0.03924000	-1.20105100
F	5.53797200	2.46494000	-3.17346700
F	6.19503200	-2.12841800	-2.84372300
F	4.72971300	-2.43617900	3.92733200
F	5.42774900	2.15910200	3.74119400
O	-13.11610700	-0.03189200	-0.02517900
C	-13.88294400	0.10035300	1.15556700
H	-13.69128000	1.06238500	1.65057100
H	-14.92982300	0.05528600	0.84772500
H	-13.67602300	-0.71735600	1.85977400
C	0.67770600	5.27117800	0.36387100
C	0.80843500	-5.28247100	-0.59568800
F	-0.46116200	-5.31250200	-0.17050600
F	0.77474400	-4.98279100	-1.89884800
F	1.29858100	-6.51726300	-0.47034000
F	-0.52944000	5.16378300	-0.20632400
F	0.50522000	5.05807300	1.67380800
F	1.08779500	6.52976100	0.20307300

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Ir	-1.26282600	-0.05904700	-0.00532300
C	-4.52000000	-2.28174100	-1.75168600
C	-4.82291000	-3.19395500	-0.75151700
C	-3.52514800	-1.33534700	-1.55652000
C	-4.16930700	-3.13283100	0.47464600
C	-3.20945500	-2.12158900	0.71902800
C	-2.48955200	-1.84602000	1.98003600
N	-1.31333700	0.86653700	-1.84706300
N	0.61685200	1.02336500	0.37363500
N	0.31370000	-1.53376900	-0.44908300
N	-1.46106800	-0.95925000	1.83780100
C	-2.79575400	-2.31019600	3.26047700
C	-3.11389400	1.70201100	1.61640700
C	-2.70561500	2.39689500	-0.67351500
C	-2.11845800	1.96329100	-1.95822300
C	-0.69957300	0.35058700	-2.92283700
C	0.72619600	2.28774500	0.76835200

C	1.74229000	0.29915500	0.13610000
C	1.58044000	-1.07109900	-0.28956300
C	0.11624000	-2.79151100	-0.83026700
C	-0.70421300	-0.60665500	2.88796400
C	-2.02447000	-1.93141100	4.34948400
C	-3.84857900	2.85708300	1.84099600
C	-3.38867000	3.60628800	-0.40157900
C	-2.36659000	2.48159700	-3.23029300
C	-0.87639800	0.86557400	-4.19394700
C	1.96474300	2.91257800	0.95550200
C	3.02546100	0.85945800	0.30821800
C	2.70321200	-1.89768700	-0.53751900
C	1.17475500	-3.67017900	-1.08610700
C	-0.94239900	-1.08145400	4.16459700
C	-3.96303000	3.81803300	0.84734400
C	-1.74645500	1.93688600	-4.34512800
C	3.11880100	2.19635600	0.72555500
C	4.15379200	0.02208600	0.04884200
C	2.46938500	-3.22376100	-0.94347600
C	3.97821400	-1.29831400	-0.35255300
N	5.47460500	0.34104100	0.14581300
N	5.24979600	-1.78710200	-0.50080200
C	6.11976500	-0.76800500	-0.19171200
C	7.54819600	-0.95177300	-0.24961200
C	8.41017000	0.03962300	0.05195300
H	-5.56065400	-3.96782900	-0.93305600
H	-3.27602200	-0.66002600	-2.37650500
H	-3.65135900	-2.94746000	3.42899200
H	-3.00212000	0.98509000	2.43146300
H	-0.07219700	-0.51983400	-2.74472800
H	-0.20656700	2.82153800	0.94756500
H	-0.91997100	-3.10821300	-0.94239400
H	0.09712700	0.09976000	2.68369800
H	-2.27800000	-2.29872100	5.34088600
H	-3.06504100	3.29351600	-3.37044500
H	-0.36402100	0.41493000	-5.03838800
H	1.99667900	3.94831200	1.28075100
H	0.96228600	-4.68855400	-1.39759500
H	-0.30844300	-0.76720200	4.98800000
H	-4.48835400	4.74459300	1.05158100
H	-1.95246900	2.34939100	-5.32970500
H	4.10222800	2.64144100	0.86124900
H	3.30511400	-3.89084100	-1.14442200
H	7.97821700	0.99977600	0.34574200

H	5.51873300	-2.72221900	-0.78418000
H	7.89687000	-1.93966200	-0.55193500
C	9.85933400	-0.01779200	0.03216400
C	10.58856600	1.12589900	0.37927500
C	10.58424900	-1.17239900	-0.32075300
C	11.97829900	1.14171800	0.38165300
H	10.04908400	2.03199600	0.65601000
C	11.96314800	-1.17333700	-0.32345800
H	10.05816800	-2.08489900	-0.59791400
C	12.67487600	-0.01563000	0.02787800
H	12.50312900	2.05229000	0.65802800
H	12.52707700	-2.06347700	-0.59569000
C	-2.51024100	1.46262500	0.38054700
C	-2.83832300	-1.25255700	-0.34373000
O	14.01963900	-0.12142000	-0.00692200
C	14.78465500	1.01697200	0.33740800
H	14.58725000	1.33315600	1.37103300
H	15.83203900	0.72187300	0.24419900
H	14.58182200	1.85530600	-0.34332100
C	-3.50716900	4.75316600	-1.37042400
C	-4.47231800	3.05289200	3.18744000
C	-5.23196800	-2.30746800	-3.06815400
C	-4.52198800	-4.22503000	1.44931900
F	-3.43218900	-4.77784400	1.99734500
F	-5.29499000	-3.77996500	2.45768700
F	-5.20332400	-5.21699800	0.87134400
F	-4.36981000	-2.43912400	-4.08670600
F	-6.11400500	-3.30623000	-3.15832800
F	-5.89836700	-1.16332800	-3.27912200
F	-3.54748900	3.03778500	4.15838900
F	-5.13657900	4.20720200	3.28598400
F	-5.33546700	2.06654100	3.46877200
F	-3.90163700	5.87994500	-0.77285700
F	-2.34084700	5.02595300	-1.96911400
F	-4.40839100	4.51089700	-2.34089000