

Theoretical study on the influence of ancillary and cyclometalated
ligands on the electronic structures and optoelectronic properties of
heteroleptic iridium(III) complexes

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Table S1. Optimized geometry parameters for the complex **3** at DFT/PBE0/LANL2DZ and DFT/B3LYP/LANL2DZ Levels respectively, together with the experimental data

	S0 (PBE0)	S0 (B3LYP)	Exptl	Δ (PBE0)	Δ (B3LYP)
Bond Length/Å					
Ir-N1	2.031	2.057	2.043	0.012	-0.014
Ir-N3	2.033	2.060	2.030	-0.003	-0.030
Ir-C1	2.022	2.043	2.018	-0.005	-0.026
Ir-C2	2.022	2.043	2.038	0.016	-0.005
Ir-S1	2.511	2.564	2.477	-0.033	-0.087
Ir-S2	2.514	2.568	2.488	-0.025	-0.080
Bond Angle/deg					
S1-Ir-S2	80.2	79.2	79.7	-0.5	0.5
C2-Ir-N3	79.5	79.2	78.9	-0.6	-0.3
C1-Ir-N1	79.5	79.3	79.5	0.0	0.2
S1-Ir-N1	96.7	96.7	98.8	2.2	2.2
S1-Ir-N3	90.4	90.5	89.8	-0.6	-0.7
S1-Ir-C1	172.7	171.9	174.6	1.9	2.7
C1-Ir-C2	92.8	93.4	91.6	-1.2	-1.8
N1-Ir-N3	170.7	170.6	169.0	-1.7	-1.6
C2-Ir-S2	172.8	172.1	172.8	0.0	0.7
S1-P-S2	107.0	107.3	106.0	-1.0	-1.3
O3-P-O4	94.2	94.1	95.2	1.0	1.1
P-O4-C4	119.6	121.0	121.5	1.9	0.5
P-O3-C6	120.6	121.7	124.7	4.1	3.0
Dihedral Angle/deg					
C3-C4-O4-P	170.5	172.1	177.5	7.0	5.4
C5-C6-O3-P	-105.0	-109.1	-102.3	2.7	6.8

^a Experimental data²⁰

Table S2. Mulliken and NBO charge on different fragments of the complexes in the ground states

	Mulliken charge				NBO charge			
	Ir	dox _A	dox _B	acac	Ir	dox _A	dox _B	acac
1a	1.143	-0.411	-0.411	-0.321	0.388	0.004	0.004	-0.396
	Ir	fox _A	fox _B	C ^a	Ir	fox _A	fox _B	C ^a
1b	1.155	-0.422	-0.422	-0.312	0.392	-0.002	-0.002	-0.387
2	0.517	-0.396	-0.396	0.276	-0.131	0.016	0.016	0.099
3	0.489	-0.364	-0.358	0.234	-0.127	0.037	0.038	0.052
	Ir	pypz ₁	pypz ₂	acac	Ir	pypz ₁	pypz ₂	acac
4a	1.229	-0.491	-0.482	-0.257	0.670	-0.223	-0.177	-0.270
4b	1.224	-0.490	-0.482	-0.253	0.674	-0.225	-0.184	-0.266
4c	1.234	-0.496	-0.487	-0.252	0.674	-0.226	-0.184	-0.265
	Ir	bptz ₁	bptz ₂	acac	Ir	bptz ₁	bptz ₂	acac
5	1.198	-0.472	-0.468	-0.258	0.671	-0.222	-0.182	-0.267

^aC=acac(**1b**); Et₂dtc(**2**); Et₂ntp(**3**)

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

MO	Energy/eV	Composition(%)				Assign
		Ir	dox _A	dox _B	acac	
L+10	1.37	84	7	7	3	d(Ir)
L+9	1.33	50	23	23	3	d(Ir)+ $\pi^*(dox)$
L+8	0.60	8	45	45	1	$\pi^*(dox)$
L+7	0.45	4	47	48	1	$\pi^*(dox)$
L+6	-0.32	1	25	24	50	$\pi^*(dox + acac)$
L+5	-0.33	0	50	50	0	$\pi^*(dox)$
L+4	-0.34	1	26	26	47	$\pi^*(dox + acac)$
L+3	-0.78	4	47	47	2	$\pi^*(dox)$
L+2	-0.82	4	48	48	1	$\pi^*(dox)$
L+1	-1.58	1	49	49	0	$\pi^*(dox)$
LUMO	-1.64	1	50	50	0	$\pi^*(dox)$
Gap		3.36				
HOMO	-5.00	46	24	24	6	d(Ir)+ $\pi(dox)$
H-1	-5.15	27	5	5	63	d(Ir)+ $\pi(acac)$
H-2	-5.73	46	24	24	6	d(Ir)+ $\pi(dox)$
H-3	-5.76	9	34	34	23	$\pi(dox + acac)$
H-4	-6.17	6	32	32	31	$\pi(dox + acac)$
H-5	-6.40	5	21	21	53	$\pi(dox + acac)$
H-6	-6.42	31	32	32	5	d(Ir)+ $\pi(dox)$
H-7	-6.62	34	27	27	12	d(Ir)+ $\pi(dox)$
H-8	-6.96	7	32	32	29	$\pi(dox + acac)$
H-9	-7.14	3	37	37	22	$\pi(dox + acac)$
H-10	-7.17	1	49	49	0	$\pi(dox)$

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

MO	Energy/eV	Composition(%)				Assign
		Ir	<i>fox</i> _A	<i>fox</i> _B	<i>acac</i>	
L+10	1.18	83	7	7	3	d(Ir)
L+9	1.08	52	23	23	3	d(Ir)+ $\pi^*(fox)$
L+8	0.25	8	45	45	1	$\pi^*(fox)$
L+7	0.09	4	48	48	1	$\pi^*(fox)$
L+6	-0.52	2	1	1	96	$\pi^*(acac)$
L+5	-0.68	1	49	50	1	$\pi^*(fox)$
L+4	-0.69	0	50	50	0	$\pi^*(fox)$
L+3	-0.92	3	47	48	2	$\pi^*(fox)$
L+2	-0.96	4	48	48	1	$\pi^*(fox)$
L+1	-1.70	1	49	49	0	$\pi^*(fox)$
LUMO	-1.75	1	50	50	0	$\pi^*(fox)$
Gap			3.53			
HOMO	-5.28	45	25	25	5	d(Ir)+ $\pi(fox)$
H-1	-5.35	26	6	6	62	d(Ir)+ $\pi(acac)$
H-2	-5.88	5	36	36	23	$\pi(fox + acac)$
H-3	-5.92	38	28	28	7	d(Ir)+ $\pi(fox)$
H-4	-6.47	4	21	21	53	$\pi(fox + acac)$
H-5	-6.53	42	26	26	5	d(Ir)+ $\pi(fox)$
H-6	-6.68	20	22	22	36	d(Ir)+ $\pi(fox + acac)$
H-7	-6.81	23	34	34	8	d(Ir)+ $\pi(fox)$
H-8	-7.07	2	48	48	2	$\pi(fox)$
H-9	-7.14	2	49	49	1	$\pi(fox)$
H-10	-7.30	6	22	22	51	$\pi(fox+ acac)$

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

MO	Energy/eV	Composition(%)				Assign
		Ir	<i>fox</i> _A	<i>fox</i> _B	<i>Et₂dtc</i>	
L+10	1.00	37	24	24	16	d(Ir)+ $\pi^*(fox + Et_2dtc)$
L+9	0.85	39	21	21	19	d(Ir)+ $\pi^*(fox + Et_2dtc)$
L+8	0.26	9	43	43	5	$\pi^*(fox)$
L+7	0.07	7	44	44	5	$\pi^*(fox)$
L+6	-0.27	5	0	0	94	$\pi^*(Et_2dtc)$
L+5	-0.62	1	49	50	0	$\pi^*(fox)$
L+4	-0.63	0	50	49	0	$\pi^*(fox)$
L+3	-0.83	3	48	48	1	$\pi^*(fox)$
L+2	-0.89	4	47	47	2	$\pi^*(fox)$
L+1	-1.62	1	49	50	0	$\pi^*(fox)$
LUMO	-1.69	1	50	49	0	$\pi^*(fox)$
Gap		3.53				
HOMO	-5.22	33	11	11	45	d(Ir)+ $\pi(Et_2dtc)$
H-1	-5.42	30	21	21	28	d(Ir)+ $\pi(fox + Et_2dtc)$
H-2	-5.43	37	15	15	32	d(Ir)+ $\pi(fox + Et_2dtc)$
H-3	-5.87	2	15	15	69	$\pi(fox + Et_2dtc)$
H-4	-5.97	10	35	35	21	$\pi(fox + Et_2dtc)$
H-5	-6.01	2	35	35	29	$\pi(fox + Et_2dtc)$
H-6	-6.74	2	45	46	7	$\pi(fox)$
H-7	-6.76	33	25	25	18	d(Ir)+ $\pi(fox + Et_2dtc)$
H-8	-7.01	24	26	26	24	d(Ir)+ $\pi(fox + Et_2dtc)$
H-9	-7.02	9	36	36	19	$\pi(fox + Et_2dtc)$
H-10	-7.07	23	28	28	22	d(Ir)+ $\pi(fox + Et_2dtc)$

Table S6. Frontier molecular orbital energies (eV) and compositions (%) of different fragments in the ground state for complex **3**

MO	Energy/eV	Composition(%)				Assign
		Ir	fox_A	fox_B	Et_2dtp	
L+10	0.93	16	23	31	30	d(Ir)+ $\pi^*(fox + Et_2dtp)$
L+9	0.74	51	8	8	32	d(Ir)+ $\pi^*(Et_2dtp)$
L+8	0.40	35	25	25	15	d(Ir)+ $\pi^*(fox + Et_2dtp)$
L+7	0.04	22	20	19	39	d(Ir)+ $\pi^*(fox + Et_2dtp)$
L+6	-0.13	12	39	38	11	$\pi^*(fox)$
L+5	-0.79	7	43	44	6	$\pi^*(fox)$
L+4	-0.81	1	91	8	0	$\pi^*(fox_A)$
L+3	-1.06	0	8	91	0	$\pi^*(fox_B)$
L+2	-1.11	4	57	37	2	$\pi^*(fox)$
L+1	-1.82	4	37	57	2	$\pi^*(fox)$
LUMO	-1.89	1	57	42	0	$\pi^*(fox)$
Gap		3.60				
HOMO	-5.49	38	18	18	27	d(Ir)+ $\pi(fox + Et_2dtp)$
H-1	-5.67	40	21	16	23	d(Ir)+ $\pi(fox + Et_2dtp)$
H-2	-5.72	29	14	18	40	d(Ir)+ $\pi(fox + Et_2dtp)$
H-3	-6.23	9	34	39	19	$\pi(fox + Et_2dtp)$
H-4	-6.27	5	36	31	29	$\pi(fox + Et_2dtp)$
H-5	-6.34	4	19	18	59	$\pi(fox + Et_2dtp)$
H-6	-6.94	1	42	43	14	$\pi(fox)$
H-7	-7.00	31	25	24	20	d(Ir)+ $\pi(oxd + Et_2dtp)$
H-8	-7.21	8	45	28	19	$\pi(fox + Et_2dtp)$
H-9	-7.25	1	41	56	2	$\pi(fox)$
H-10	-7.27	25	20	24	31	d(Ir)+ $\pi(fox + Et_2dtp)$

Table S7. Frontier molecular orbital energies (eV) and compositions (%) of different fragments in the ground state for complex **4a**

MO	Energy/eV	Composition(%)				Assign
		Ir	<i>pypz</i> ₁	<i>pypz</i> ₂	<i>acac</i>	
L+10	0.82	57	23	12	8	d(Ir)+ $\pi^*(pypz_1)$
L+9	0.51	58	6	21	15	d(Ir)+ $\pi^*(pypz_2)$
L+8	0.22	0	0	100	0	$\pi^*(pypz_2)$
L+7	0.13	0	100	0	0	$\pi^*(pypz_1)$
L+6	-0.14	1	0	99	0	$\pi^*(pypz)$
L+5	-0.22	1	99	0	0	$\pi^*(pypz_1)$
L+4	-0.78	1	7	86	6	$\pi^*(pypz_2)$
L+3	-0.91	3	3	5	89	$\pi^*(acac)$
L+2	-1.01	1	90	9	1	$\pi^*(pypz_1)$
L+1	-1.35	4	1	94	1	$\pi^*(pypz_2)$
LUMO	-1.52	3	94	1	1	$\pi^*(pypz_1)$
Gap		3.54				
HOMO	-5.06	16	11	72	1	d(Ir)+ $\pi(pypz_2)$
H-1	-5.19	18	63	15	4	d(Ir)+ $\pi(pypz)$
H-2	-5.61	15	9	42	35	d(Ir)+ $\pi(pypz_2+acac)$
H-3	-5.87	16	58	12	15	d(Ir)+ $\pi(pypz_1+acac)$
H-4	-5.96	8	24	45	23	$\pi(pypz+acac)$
H-5	-6.10	1	3	96	0	$\pi(pypz_2)$
H-6	-6.16	0	96	3	1	$\pi(pypz_1)$
H-7	-6.41	36	38	17	10	d(Ir)+ $\pi(pypz)$
H-8	-6.59	34	25	35	7	d(Ir)+ $\pi pypz$
H-9	-6.73	17	5	67	10	d(Ir)+ $\pi(pypz_2)$
H-10	-6.81	6	82	3	9	$\pi(pypz_1)$

Table S8. Frontier molecular orbital energies (eV) and compositions (%) of different fragments in the ground state for complex **4b**

MO	Energy/eV	Composition(%)				Assign
		Ir	<i>Opyrz</i> ₁	<i>Opyrz</i> ₂	<i>acac</i>	
L+10	0.54	57	23	13	7	d(Ir)+ $\pi^*(Opyrz_1)$
L+9	0.38	1	0	99	0	$\pi^*(Opyrz_2)$
L+8	0.28	50	21	17	12	d(Ir)+ $\pi^*(Opyrz)$
L+7	0.25	9	85	3	2	$\pi^*(Opyrz_1)$
L+6	-0.45	1	0	99	0	$\pi^*(Opyrz_2)$
L+5	-0.56	1	98	1	0	$\pi^*(Opyrz_1)$
L+4	-0.90	1	9	88	2	$\pi^*(Opyrz_2)$
L+3	-1.10	2	53	1	44	$\pi^*(Opyrz_1 + acac)$
L+2	-1.12	1	40	10	50	$\pi^*(Opyrz_1 + acac)$
L+1	-1.50	4	2	93	0	$\pi^*(Opyrz_2)$
LUMO	-1.66	3	94	2	1	$\pi^*(Opyrz_1)$
Gap		3.63				
HOMO	-5.29	15	12	72	1	d(Ir)+ $\pi(Opyrz_2)$
H-1	-5.39	18	57	20	5	d(Ir)+ $\pi(Opyrz)$
H-2	-5.62	7	13	72	8	$\pi(Opyrz_2)$
H-3	-5.80	9	85	4	3	$\pi(Opyrz_1)$
H-4	-6.05	15	4	20	61	d(Ir)+ $\pi(Opyrz_2 + acac)$
H-5	-6.51	0	0	99	1	$\pi(Opyrz_2)$
H-6	-6.60	12	71	15	3	$\pi(Opyrz)$
H-7	-6.61	17	59	18	6	d(Ir)+ $\pi(Opyrz)$
H-8	-6.78	8	23	64	5	$\pi(Opyrz)$
H-9	-6.87	39	16	34	10	d(Ir)+ $\pi(Opyrz)$
H-10	-7.01	10	77	8	5	$\pi(Opyrz_1)$

Table S9. Frontier molecular orbital energies (eV) and compositions (%) of different fragments in the ground state for complex **4c**

MO	Energy/eV	Composition(%)				Assign
		Ir	<i>Spypz</i> ₁	<i>Spypz</i> ₂	<i>acac</i>	
L+10	0.51	32	48	16	4	d(Ir)+ $\pi^*(Spypz)$
L+9	0.28	56	11	19	14	d(Ir)+ $\pi^*(Spypz_2)$
L+8	0.08	1	0	99	0	$\pi^*(Spypz_2)$
L+7	-0.03	0	99	0	0	$\pi^*(Spypz_1)$
L+6	-0.44	1	0	99	0	$\pi^*(Spypz_2)$
L+5	-0.54	1	99	1	0	$\pi^*(Spypz_1)$
L+4	-0.90	1	9	88	3	$\pi^*(Spypz_2)$
L+3	-1.09	3	14	1	82	$\pi^*(acac)$
L+2	-1.12	0	78	11	10	$\pi^*(Spypz_1)$
L+1	-1.51	4	2	94	0	$\pi^*(Spypz_2)$
LUMO	-1.67	3	94	2	1	$\pi^*(Spypz_1)$
Gap		3.63				
HOMO	-5.30	11	14	73	1	$\pi(Spypz_2)$
H-1	-5.39	17	6	70	6	d(Ir)+ $\pi(Spypz_2)$
H-2	-5.46	8	64	27	1	$\pi(Spypz)$
H-3	-5.55	7	85	6	1	$\pi(Spypz_1)$
H-4	-5.99	17	5	11	67	d(Ir)+ $\pi(acac)$
H-5	-6.47	0	0	99	0	$\pi(Spypz_2)$
H-6	-6.54	0	99	0	0	$\pi(Spypz_1)$
H-7	-6.59	17	16	61	6	d(Ir)+ $\pi(Spypz)$
H-8	-6.71	20	40	35	6	d(Ir)+ $\pi(Spypz)$
H-9	-6.79	24	49	20	7	d(Ir)+ $\pi(Spypz)$
H-10	-6.87	34	40	19	7	d(Ir)+ $\pi(Spypz)$

Table S10. Frontier molecular orbital energies (eV) and compositions (%) of different fragments in the ground state for complex **5**

MO	Energy/eV	Composition(%)				Assign
		Ir	<i>bptz</i> ₁	<i>bptz</i> ₂	<i>acac</i>	
L+10	1.62	14	81	2	2	$\pi^*(bptz_1)$
L+9	1.43	74	17	2	7	d(Ir)+ $\pi^*(bptz_1)$
L+8	1.41	79	2	13	6	d(Ir)
L+7	1.33	73	12	1	13	d(Ir)
L+6	0.50	58	23	12	8	d(Ir)+ $\pi^*(bptz_1)$
L+5	0.18	59	6	20	15	d(Ir)+ $\pi^*(bptz_2)$
L+4	-0.96	1	13	85	2	$\pi^*(bptz_2)$
L+3	-1.15	1	85	10	3	$\pi^*(bptz_1)$
L+2	-1.21	3	3	4	90	$\pi^*(acac)$
L+1	-1.59	4	2	93	0	$\pi^*(bptz_2)$
LUMO	-1.72	3	93	2	1	$\pi^*(bptz_1)$
Gap				3.80		
HOMO	-5.52	22	26	50	2	d(Ir)+ $\pi(bptz)$
H-1	-5.61	19	45	29	6	d(Ir)+ $\pi(bptz)$
H-2	-6.02	17	10	16	56	d(Ir)+ $\pi(acac)$
H-3	-6.41	35	48	8	10	d(Ir)+ $\pi(bptz_1)$
H-4	-6.57	30	7	54	8	d(Ir)+ $\pi(bptz_2)$
H-5	-6.74	1	1	95	2	$\pi(bptz_2)$
H-6	-6.81	1	95	4	0	$\pi(bptz_1)$
H-7	-6.94	40	11	22	27	d(Ir)+ $\pi(bptz_2 + acac)$
H-8	-7.49	8	56	5	31	$\pi(bptz_1 + acac)$
H-9	-7.53	11	63	12	14	$\pi(bptz_1)$
H-10	-7.66	22	7	52	20	d(Ir)+ $\pi(bptz_2 + acac)$

Table S11. Selected calculated wavelength (nm)/energies (eV), oscillator strength (f), major contribution, transition characters, and the experimental wavelength (nm) for **1a**, **1b**, **2** and **3** in CH₂Cl₂ media

	state	λ /E	Oscillator	Configuration	Assignment	Nature	Exptl. ^a
1a	S ₁	429/2.89	0.1753	HOMO→LUMO(95%)	d(Ir)+ $\pi(dox) \rightarrow \pi^*(dox)$	MLCT/ LLCT/IL	424
	S ₁₁	325/3.82	0.3387	H-3→L+1 (76%),	$\pi(dox+acac) \rightarrow \pi^*(dox)$	LLCT/IL	355
	S ₁₂	322/3.86	0.2954	H-1→L+3 (75%)	d(Ir)+ $\pi(acac) \rightarrow \pi^*(dox)$	MLCT/ LLCT	
	S ₁₇	290/4.28	0.4636	H-2→L+2 (53%)	d(Ir)+ $\pi(dox) \rightarrow \pi^*(dox)$	MLCT/ LLCT/IL	298
	S ₁₉	284/4.37	0.117	H-5→LUMO (61%)	$\pi(dox+acac) \rightarrow \pi^*(dox)$	LLCT/IL	
	S ₃₁	263/4.71	0.1792	HOMO→L+7(63%)	d(Ir)+ $\pi(dox) \rightarrow \pi^*(dox)$	MLCT/ LLCT/IL	246
1b	S ₁	408/3.04	0.2087	HOMO→LUMO(94%)	d(Ir)+ $\pi(fox) \rightarrow \pi^*(fox)$	MLCT/ LLCT/IL	369
	S ₁₀	323/3.83	0.6028	H-2→L+1 (88%)	$\pi(fox+acac) \rightarrow \pi^*(fox)$	LLCT/IL	312
	S ₁₂	317/3.91	0.1139	H-1→L+3 (90%)	d(Ir)+ $\pi(acac) \rightarrow \pi^*(fox)$	MLCT/ LLCT	
	S ₁₅	288/4.31	0.4419	H-4→LUMO (68%),	$\pi(fox+acac) \rightarrow \pi^*(fox)$	LLCT/IL	
	S ₃₃	263/4.71	0.1562	H-7→L+1 (57%),	d(Ir)+ $\pi(fox) \rightarrow \pi^*(fox)$	MLCT/ LLCT/IL	
	S ₄₀	252/ 4.91	0.1512	H-8→LUMO (64%),	$\pi(fox) \rightarrow \pi^*(fox)$	LLCT/IL	230
2	S ₁	401/3.10	0.1698	HOMO→LUMO (95%)	d(Ir)+ $\pi(C) \rightarrow \pi^*(fox)$	MLCT/ LLCT	402
	S ₄	373/3.33	0.1058	H-2→LUMO (82%)	d(Ir)+ $\pi(fox+C) \rightarrow \pi^*(fox)$	MLCT/ LLCT/IL	
	S ₁₀	317/3.91	0.3174	H-4→LUMO (47%)	$\pi(fox+C) \rightarrow \pi^*(fox)$	LLCT/IL	323
	S ₁₁	316/3.93	0.293	H-4→LUMO (41%)	$\pi(fox+C) \rightarrow \pi^*(fox)$	LLCT/IL	
				H-3→L+1 (37%)	$\pi(fox+C) \rightarrow \pi^*(fox)$	LLCT/IL	
	S ₁₄	309/4.01	0.3051	H-5→L+1 (47%)	$\pi(fox+C) \rightarrow \pi^*(fox)$	LLCT/IL	
				H-3→L+1 (31%)	$\pi(fox+C) \rightarrow \pi^*(fox)$	LLCT/IL	
	S ₂₉	268/4.63	0.1537	H-4→L+2 (51%)	$\pi(fox+C) \rightarrow \pi^*(fox)$	LLCT/IL	
	S ₄₇	251/4.93	0.1557	H-8→LUMO (44%)	d(Ir)+ $\pi(fox+C) \rightarrow \pi^*(fox)$	MLCT/ LLCT/IL	238
S ₅₅	245/5.06	0.098	H-8→L+1 (20%)	d(Ir)+ $\pi(fox+C) \rightarrow \pi^*(fox)$	MLCT/ LLCT/IL		
3	S ₁	392/3.16	0.2184	HOMO→LUMO (94%)	d(Ir)+ $\pi(fox+C) \rightarrow \pi^*(fox)$	MLCT/ LLCT/IL	397
	S ₄	359/3.45	0.1607	H-1→L+1 (72%)	d(Ir)+ $\pi(fox+C) \rightarrow \pi^*(fox)$	MLCT/ LLCT/IL	
	S ₉	310/4.00	0.6498	H-3→LUMO (65%)	$\pi(fox+C) \rightarrow \pi^*(fox)$	LLCT/IL	313
	S ₁₀	309/4.02	0.1095	H-4→LUMO (64%)	$\pi(fox+C) \rightarrow \pi^*(fox)$	LLCT/IL	
	S ₁₄	300/4.13	0.1803	H-4→L+1 (84%)	$\pi(fox+C) \rightarrow \pi^*(fox)$	LLCT/IL	
	S ₄₉	243/5.10	0.127	H-1→L+8 (26%)	d(Ir)+ $\pi(fox+C) \rightarrow d(Ir)+\pi^*(fox+C)$	MLCT/ LLCT/IL	241

^a C= Et₂dtp(2); Et₂dtp(3)

Table S12. Selected calculated wavelength (nm)/energies (eV), oscillator strength (*f*), major contribution and transition characters for **4a-4c** and **5** in CH₂Cl₂ media

	state	λ/E	Oscillator	Configuration	Assignment	Nature	
4a	S ₁	385/3.22	0.0616	HOMO→LUMO(72%)	d(Ir)+ π (pypz ₂)→ π^* (pypz ₁)	MLCT/ LLCT	
	S ₉	322/3.86	0.1474	HOMO→L+3 (73%)	d(Ir)+ π (pypz ₂)→ π^* (acac)	MLCT/ LLCT	
	S ₁₂	310/4.00	0.1378	H-3→LUMO(57%)	d(Ir)+ π (pypz ₁ +acac)→ π^* (pypz ₁)	MLCT/ LLCT/IL	
	S ₁₃	305/4.07	0.1537	H-3→L+1 (54%)	d(Ir)+ π (pypz ₁ +acac)→ π^* (pypz ₂)	MLCT/ LLCT	
	S ₁₆	298/4.17	0.1343	H-4→LUMO (83%)	π (pypz +acac)→ π^* (pypz ₁)	LLCT/IL	
	S ₁₇	295/4.20	0.2323	H-4→L+1 (66%)	π (pypz +acac)→ π^* (pypz ₂)	LLCT/IL	
	S ₁₉		288/4.30	0.1808	HOMO→L+5 (26%)	d(Ir)+ π (pypz ₂)→ π^* (pypz ₁)	MLCT/ LLCT
					HOMO→L+6 (26%)	d(Ir)+ π (pypz ₂)→ π^* (pypz ₂)	MLCT/IL
	S ₂₂	284/4.37	0.2045	HOMO→L+6(33%)	d(Ir)+ π (pypz ₂)→ π^* (pypz ₂)	MLCT/IL	
	S ₃₇		264/4.70	0.1558	H-1→L+9(16%)	d(Ir)+ π (pypz)→d(Ir)+ π^* (pypz ₂)	MLCT/ LLCT/IL
HOMO→L+9 (14%)					d(Ir)+ π (pypz ₂)→d(Ir)+ π^* (pypz ₂)	MLCT/ LLCT/IL	
4b	S ₁	378/3.28	0.0432	HOMO→LUMO(82%)	d(Ir)+ π (Opypz ₂)→ π^* (Opypz ₁)	MLCT/ LLCT	
	S ₈	329/3.77	0.1512	H-2→L+1 (79%)	π (Opypz ₂)→ π^* (Opypz ₂)	IL	
	S ₁₀	320/3.87	0.1405	H-3→L+1 (58%)	π (Opypz ₁)→ π^* (Opypz ₂)	LLCT	
	S ₁₆	300/4.13	0.1325	HOMO→L+4 (57%)	d(Ir)+ π (Opypz ₂)→ π^* (Opypz ₂)	MLCT/ IL	
	S ₁₉	294/4.22	0.4826	HOMO→L+5 (50%)	d(Ir)+ π (Opypz ₂)→ π^* (Opypz ₁)	MLCT/ LLCT	
	S ₂₀	290/4.28	0.1463	HOMO→L+6 (31%)	d(Ir)+ π (Opypz ₂)→ π^* (Opypz ₂)	MLCT/ IL	
	S ₂₆	281/4.41	0.1057	H-3→L+3 (78%)	π (Opypz ₁)→ π^* (Opypz ₁ +acac)	LLCT/IL	
	S ₅₇	278/4.45	0.1338	H-2→L+4 (69%)	π (Opypz ₂)→ π^* (Opypz ₂)	IL	
	S ₄₄	253/4.90	0.1089	H-6→L+1 (30%)	π (Opypz)→ π^* (Opypz ₂)	LLCT/IL	
	S ₅₃	247/5.02	0.1793	HOMO→L+7 (48%)	d(Ir)+ π (Opypz ₂)→ π^* (Opypz ₁)	MLCT/ LLCT	
	S ₅₄		246/5.05	0.1458	H-1→L+8(25%)	d(Ir)+ π (Opypz)→d(Ir)+ π^* (Opypz)	MLCT/ LLCT/IL
HOMO→L+8 (22%)					d(Ir)+ π (Opypz ₂)→d(Ir)+ π^* (Opypz)	MLCT/ LLCT/IL	
4c	S ₁	378/3.28	0.0581	HOMO→LUMO(78%)	π (Spypz ₂)→ π^* (Spypz ₁)	LLCT	
	S ₇	342/3.62	0.1751	H-3→LUMO (62%)	π (Spypz ₁)→ π^* (Spypz ₁)	IL	
	S ₁₄	312/3.97	0.1238	HOMO→L+3 (65%)	π (Spypz ₂)→ π^* (acac)	LLCT	
	S ₂₁	293/4.23	0.2631	HOMO→L+5 (45%)	π (Spypz ₂)→ π^* (Spypz ₁)	LLCT	
	S ₂₆		287/4.32	0.3384	H-2→L+6 (23%)	π (Spypz)→ π^* (Spypz ₂)	LLCT/IL
					H-1→L+6 (22%)	d(Ir)+ π (Spypz ₂)→ π^* (Spypz ₂)	MLCT/IL
	S ₄₁	260/4.76	0.2737	HOMO→L+7 (57%)	π (Spypz ₂)→ π^* (Spypz ₁)	LLCT	
	S ₄₃		258/4.81	0.2368	H-1→L+8(22%)	d(Ir)+ π (Spypz ₂)→ π^* (Spypz ₂)	MLCT/IL
					HOMO→L+8 (26%)	π (Spypz ₂)→ π^* (Spypz ₂)	IL
	S ₄₅	257/4.83	0.1333	H-10→LUMO (30%),	d(Ir)+ π (Spypz)→ π^* (Spypz ₁)	MLCT/ LLCT/IL	
S ₄₇	255/4.87	0.191	HOMO→L+8 (20%)	π (Spypz ₂)→ π^* (Spypz ₂)	IL		
5	S ₁	370/3.35	0.0659	HOMO→LUMO(82%)	d(Ir)+ π (bptz)→ π^* (bptz ₁)	MLCT/ LLCT/IL	
	S ₁₆	286/4.34	0.1084	H-3→L+1 (52%)	d(Ir)+ π (bptz ₁)→ π^* (bptz ₂)	MLCT/ LLCT	
	S ₁₈	279/4.45	0.1505	H-4→LUMO (40%)	d(Ir)+ π (bptz ₂)→ π^* (bptz ₁)	MLCT/ LLCT	
	S ₃₃	246/5.04	0.1708	H-3→L+4 (62%)	d(Ir)+ π (bptz ₁)→ π^* (bptz ₂)	MLCT/ LLCT	
	S ₂₇	261/4.75	0.0912	H-5→LUMO (40%)	d(Ir)+ π (bptz ₁)→ π^* (bptz ₁)	MLCT/ IL	

Table S13. Single-electron transitions according to TDDFT calculations for the absorption of the complexes in CH₂Cl₂ Media

state	λ/E	Oscillator	Configuration	Assignment	Nature	Exptl. ^a	
1a	T ₁	481/2.58	0	HOMO→LUMO (60%)	d(Ir)+ π(<i>dox</i>)→π*(<i>dox</i>)	MLCT/ LLCT/IL	465
	T ₂	476/2.61	0	HOMO→L+1 (47%)	d(Ir)+ π(<i>dox</i>)→π*(<i>dox</i>)	MLCT/ LLCT/IL	
	T ₃	427/2.90	0	H-2→LUMO(20%)	d(Ir)+ π(<i>dox</i>)→π*(<i>dox</i>)	MLCT/ LLCT/IL	
				H-1→L+1(27%)	d(Ir)+ π(<i>acac</i>)→π*(<i>dox</i>)	MLCT/ LLCT	
				HOMO→LUMO (24%)	d(Ir)+ π(<i>dox</i>)→π*(<i>dox</i>)	MLCT/ LLCT/IL	
T ₄	426/2.91	0	H-1→LUMO(31%)	d(Ir)+ π(<i>acac</i>)→π*(<i>dox</i>)	MLCT/ LLCT		
			HOMO→L+1 (33%)	d(Ir)+ π(<i>dox</i>)→π*(<i>dox</i>)	MLCT/ LLCT/IL		
T ₅	407/3.04	0	H-1→L+4 (74%)	d(Ir)+ π(<i>acac</i>)→π*(<i>dox+acac</i>)	MLCT/ LLCT/IL		
1b	T ₁	469/2.64	0	HOMO→LUMO (47%)	d(Ir)+ π(<i>fox</i>)→π*(<i>fox</i>)	MLCT/ LLCT/IL	468
	T ₂	466/2.66	0	HOMO→L+1 (37%)	d(Ir)+ π(<i>fox</i>)→π*(<i>fox</i>)	MLCT/ LLCT/IL	
	T ₃	410/3.03	0	HOMO→LUMO (31%)	d(Ir)+ π(<i>fox</i>)→π*(<i>fox</i>)	MLCT/ LLCT/IL	432
	T ₄	407/3.05	0	HOMO→L+1 (42%)	d(Ir)+ π(<i>fox</i>)→π*(<i>fox</i>)	MLCT/ LLCT/IL	
	T ₅	406/3.05	0	H-1→L+4 (64%)	d(Ir)+ π(<i>acac</i>)→π*(<i>fox</i>)	MLCT/ LLCT	
2	T ₁	467/2.66	0	HOMO→LUMO (43%)	d(Ir)+ π(C)→π*(<i>fox</i>)	MLCT/ LLCT	472
	T ₂	464/2.67	0	H-1→LUMO (35%)	d(Ir)+ π(<i>fox</i> +C)→π*(<i>fox</i>)	MLCT/ LLCT/IL	
				HOMO→L+1 (31%)	d(Ir)+ π(C)→π*(<i>fox</i>)	MLCT/ LLCT	
	T ₃	402/3.09	0	HOMO→LUMO (23%)	d(Ir)+ π(C)→π*(<i>fox</i>)	MLCT/ LLCT	436
	T ₄	394/3.14	0	HOMO→L+1 (37%)	d(Ir)+ π(C)→π*(<i>fox</i>)	MLCT/ LLCT	
T ₅	389/3.19	0	H-1→L+2 (25%)	d(Ir)+ π(<i>fox</i> +C)→π*(<i>fox</i>)	MLCT/ LLCT/IL		
3	T ₁	463/2.68	0	HOMO→LUMO (44%)	d(Ir)+ π(<i>fox</i> +C)→π*(<i>fox</i>)	MLCT/ LLCT/IL	469
				H-1→L+1 (29%)	d(Ir)+ π(<i>fox</i> +C)→π*(<i>fox</i>)	MLCT/ LLCT/IL	
	T ₂	462/2.69	0	H-1→LUMO (40%)	d(Ir)+ π(<i>fox</i> +C)→π*(<i>fox</i>)	MLCT/ LLCT/IL	
				HOMO→L+1 (32%)	d(Ir)+ π(<i>fox</i> +C)→π*(<i>fox</i>)	MLCT/ LLCT/IL	
	T ₃	396/3.13	0	HOMO→L+2 (25%)	d(Ir)+ π(<i>fox</i> +C)→π*(<i>fox</i>)	MLCT/ LLCT/IL	434
T ₄	391/3.17	0	HOMO→L+3 (29%)	d(Ir)+ π(<i>fox</i> +C)→π*(<i>fox_B</i>)	MLCT/ LLCT/IL		
T ₅	385/3.22	0	HOMO→L+1 (35%)	d(Ir)+ π(<i>fox</i> +C)→π*(<i>fox</i>)	MLCT/ LLCT/IL		
4a	T ₁	440/2.82	0	HOMO→L+1 (44%)	d(Ir)+ π(<i>pypz</i> ₂)→π*(<i>pypz</i> ₂)	MLCT/ IL	
	T ₂	439/2.82	0	H-1→LUMO (32%)	d(Ir)+ π(<i>pypz</i>)→π*(<i>pypz</i> ₁)	MLCT/ LLCT/IL	
	T ₃	415/2.99	0	H-2→L+2 (56%)	d(Ir)+ π(<i>pypz</i> ₂ + <i>acac</i>)→π*(<i>pypz</i> ₁)	MLCT/ LLCT	
	T ₄	399/3.11	0	H-1→L+1 (56%)	d(Ir)+ π(<i>pypz</i>)→π*(<i>pypz</i> ₂)	MLCT/ LLCT/IL	
	T ₅	391/3.17	0	H-3→LUMO(44%)	d(Ir)+ π(<i>pypz</i> ₁ + <i>acac</i>)→π*(<i>pypz</i> ₁)	MLCT/ LLCT/IL	
4b	T ₁	445/2.79	0	HOMO→L+1 (40%)	d(Ir)+ π(<i>Oppyz</i> ₂)→π*(<i>Oppyz</i> ₂)	MLCT/ IL	
	T ₂	443/2.80	0	H-1→LUMO(23%)	d(Ir)+π(<i>Oppyz</i>)→π*(<i>Oppyz</i> ₁)	MLCT/ LLCT/IL	
				HOMO→LUMO (27%)	d(Ir)+ π(<i>Oppyz</i> ₂)→π*(<i>Oppyz</i> ₁)	MLCT/ LLCT	
	T ₃	413/3.00	0	H-4→L+2 (45%)	d(Ir)+ π(<i>Oppyz</i> ₂ + <i>acac</i>)→π*(<i>Oppyz</i> ₁ + <i>acac</i>)	MLCT/ LLCT/IL	
T ₄	400/3.10	0	H-3→LUMO(46%)	π(<i>Oppyz</i> ₁)→π*(<i>Oppyz</i> ₁)	IL		

4c	T ₅	398/3.11	0	H-1→L+1 (44%)	d(Ir)+ π(<i>Opyyz</i>)→π*(<i>Opyyz</i> ₂)	MLCT/ LLCT/IL
	T ₁	451/2.75	0	HOMO→L+1 (58%)	π(<i>Spyyz</i> ₂)→π*(<i>Spyyz</i> ₂)	IL
	T ₂	448/2.77	0	H-1→LUMO (32%)	d(Ir)+ π(<i>Spyyz</i> ₂)→π*(<i>Spyyz</i> ₁)	MLCT/ LLCT
	T ₃	413/3.01	0	H-4→L+2 (61%)	d(Ir)+ π(<i>acac</i>)→π*(<i>Spyyz</i> ₁)	MLCT/ LLCT
	T ₄	405/3.06	0	H-3→LUMO(49%) HOMO→LUMO (33%)	π(<i>Spyyz</i> ₁)→π*(<i>Spyyz</i> ₁) π(<i>Spyyz</i> ₂)→π*(<i>Spyyz</i> ₁)	IL LLCT
5	T ₅	399/3.11	0	H-2→L+1 (44%) H-1→L+1 (38%)	π(<i>Spyyz</i>)→π*(<i>Spyyz</i> ₂) d(Ir)+ π(<i>Spyyz</i> ₂)→π*(<i>Spyyz</i> ₂)	LLCT/IL MLCT/IL
	T ₁	444/2.80	0	HOMO→LUMO (58%)	d(Ir)+ π(<i>bptz</i>)→π*(<i>bptz</i> ₁)	MLCT/ LLCT/IL
	T ₂	437/2.84	0	HOMO→L+1 (39%)	d(Ir)+ π(<i>bptz</i>)→π*(<i>bptz</i> ₂)	MLCT/ LLCT/IL
	T ₃	411/3.02	0	H-2→L+2 (62%)	d(Ir)+ π(<i>acac</i>)→π*(<i>acac</i>)	MLCT/ IL
	T ₄	382/3.24	0	H-1→L+1 (48%)	d(Ir)+ π(<i>bptz</i>)→π*(<i>bptz</i> ₂)	MLCT/ LLCT/IL
	T ₅	364/3.40	0	H-1→LUMO (37%)	d(Ir)+ π(<i>bptz</i>)→π*(<i>bptz</i> ₁)	MLCT/ LLCT/IL

C= *Et*₂*dte*(**2**); *Et*₂*dtp*(**3**)

Table S14. The coordinates of optimized geometries at ground states and lowest triplet states of the studied complexes

1a S0				1a T1					
1	C	-1.513933	-1.656215	-1.831866	1	C	1.409243	-1.478359	1.933256
2	C	-0.181112	-1.354024	-1.434362	2	C	0.103949	-1.101885	1.503675
3	C	0.823250	-2.043333	-2.126188	3	C	-0.973069	-1.634759	2.219646
4	H	1.866653	-1.853355	-1.888851	4	H	-1.988014	-1.362604	1.947216
5	C	0.516621	-2.959122	-3.129332	5	C	-0.758286	-2.517019	3.275301
6	C	-0.807509	-3.231216	-3.490701	6	C	0.536658	-2.882644	3.663832
7	H	-1.026010	-3.948831	-4.276081	7	H	0.682231	-3.571004	4.491331
8	C	-1.836372	-2.572174	-2.838316	8	C	1.632598	-2.358743	2.997523
9	H	-2.875038	-2.757924	-3.100623	9	H	2.645229	-2.618629	3.293514
10	C	-2.449687	-0.893738	-1.068863	10	C	2.406578	-0.802374	1.176575
11	C	-4.126269	0.039609	-0.143261	11	C	4.154663	0.005570	0.261081
12	C	-5.526408	0.332530	0.097826	12	C	5.570331	0.201647	0.033863
13	C	-5.869156	1.266217	1.084628	13	C	5.986031	1.083080	-0.974628
14	H	-5.080078	1.752942	1.649404	14	H	5.238203	1.600323	-1.567661
15	C	-7.204923	1.555195	1.325344	15	C	7.340088	1.280751	-1.201067
16	H	-7.468053	2.279617	2.090799	16	H	7.659403	1.963549	-1.983169
17	C	-8.205468	0.920379	0.589507	17	C	8.288429	0.606802	-0.430677
18	C	-7.864750	-0.007736	-0.391570	18	C	7.875741	-0.269360	0.570880
19	H	-8.641493	-0.503710	-0.966602	19	H	8.611552	-0.795858	1.171938
20	C	-6.530019	-0.304469	-0.640729	20	C	6.522235	-0.475266	0.807049
21	H	-6.261652	-1.027118	-1.405017	21	H	6.198764	-1.157349	1.587064
22	C	1.514141	-1.654895	1.832804	22	C	-1.265856	-1.693570	-1.851952
23	C	0.181336	-1.353101	1.434973	23	C	0.044603	-1.275486	-1.437699
24	C	-0.823041	-2.041942	2.127235	24	C	1.135012	-1.859282	-2.051324
25	H	-1.866436	-1.852224	1.889662	25	H	2.142043	-1.547740	-1.787382
26	C	-0.516429	-2.956942	3.131104	26	C	0.972915	-2.849335	-3.048877
27	C	0.807691	-3.228672	3.492783	27	C	-0.302074	-3.261245	-3.420498
28	H	1.026176	-3.945673	4.278727	28	H	-0.425567	-4.032356	-4.176775
29	C	1.836564	-2.570060	2.839979	29	C	-1.429612	-2.694719	-2.830265
30	H	2.875221	-2.755531	3.102520	30	H	-2.427034	-3.017228	-3.115876
31	C	2.449866	-0.89288	1.069308	31	C	-2.272727	-0.976164	-1.194828
32	C	4.126415	0.039895	0.143073	32	C	-4.038113	-0.158430	-0.258867
33	C	5.526547	0.332684	-0.098218	33	C	-5.438624	0.009417	-0.003099
34	C	5.869267	1.265787	-1.085582	34	C	-5.875370	0.957886	0.942691
35	H	5.080172	1.752176	-1.650625	35	H	-5.137035	1.556684	1.467149
36	C	7.205027	1.554621	-1.326509	36	C	-7.227752	1.118074	1.192503
37	H	7.468136	2.278590	-2.092400	37	H	-7.553386	1.853076	1.923985
38	C	8.205593	0.920240	-0.590325	38	C	-8.172822	0.344202	0.512343

39	C	7.864903	-0.007294	0.391311	39	C	-7.745311	-0.595377	-0.424642
40	H	8.641663	-0.502928	0.966613	40	H	-8.473362	-1.200841	-0.958149
41	C	6.530179	-0.303879	0.640686	41	C	-6.392537	-0.767351	-0.685701
42	H	6.261834	-1.026076	1.405407	42	H	-6.061753	-1.499349	-1.415526
43	Ir	0.000069	0.042201	-0.000138	43	Ir	0.027728	0.180592	-0.028298
44	N	-2.017948	-0.066045	-0.144561	44	N	2.045844	0.049582	0.239108
45	N	-3.082625	0.534212	0.450906	45	N	3.150663	0.564869	-0.350718
46	N	2.018087	-0.065821	0.144452	46	N	-1.934476	0.000447	-0.310960
47	N	3.082754	0.534070	-0.451417	47	N	-3.029058	0.480564	0.281270
48	O	-3.787869	-0.868161	-1.111827	48	O	3.742957	-0.867742	1.238285
49	O	3.788045	-0.867225	1.112255	49	O	-3.624923	-1.093460	-1.206956
50	C	0.032439	2.817088	1.255760	50	C	-0.206379	2.903692	-1.350731
51	C	-0.033352	2.816842	-1.256537	51	C	-0.539639	2.951414	1.122982
52	C	-0.000490	3.442712	-0.000446	52	C	-0.622779	3.516530	-0.163576
53	H	-0.000605	4.526889	-0.000553	53	H	-0.939292	4.551045	-0.227863
54	C	-0.043415	3.684655	-2.492490	54	C	-0.903870	3.792742	2.317669
55	H	-0.911867	3.429241	-3.109090	55	H	-0.075571	3.787504	3.033621
56	H	-0.066910	4.752170	-2.260697	56	H	-1.148146	4.823434	2.050778
57	H	0.848761	3.466665	-3.090024	57	H	-1.766056	3.337502	2.817704
58	C	0.042348	3.685137	2.491551	58	C	-0.181136	3.700326	-2.627694
59	H	0.065008	4.752619	2.259530	59	H	-0.563688	4.714970	-2.496122
60	H	-0.849373	3.466607	3.089550	60	H	0.847521	3.747514	-3.001521
61	H	0.911296	3.430496	3.107792	61	H	-0.775845	3.183400	-3.388116
62	O	0.055282	1.572475	1.495910	62	O	0.208270	1.705405	-1.469670
63	O	-0.055963	1.572187	-1.496464	63	O	-0.152316	1.776747	1.395868
64	H	-9.249938	1.149822	0.781327	64	H	9.347817	0.764730	-0.612028
65	H	1.324044	-3.473269	-3.646342	65	H	-1.611134	-2.930401	3.807659
66	H	9.250058	1.149567	-0.782313	66	H	-9.232547	0.474618	0.712544
67	H	-1.323857	-3.470750	3.648443	67	H	1.849219	-3.290971	-3.514927

1b S0				1b T1					
1	C	1.434742	-1.558382	1.889990	1	C	1.335847	-1.455856	1.941895
2	C	0.117074	-1.251718	1.439570	2	C	0.031676	-1.159758	1.453244
3	C	-0.921229	-1.931098	2.082724	3	C	-1.029926	-1.787944	2.105933
4	H	-1.961066	-1.755587	1.825632	4	H	-2.061510	-1.614740	1.817284
5	C	-0.636543	-2.840513	3.090756	5	C	-0.777768	-2.648635	3.165334
6	C	0.656455	-3.134398	3.521786	6	C	0.502326	-2.936529	3.635097
7	H	0.808469	-3.856891	4.315952	7	H	0.629261	-3.619157	4.467943
8	C	1.708394	-2.476447	2.908317	8	C	1.575432	-2.325331	3.009906
9	H	2.732493	-2.670582	3.216056	9	H	2.590503	-2.517938	3.346492
10	C	2.401758	-0.797543	1.168365	10	C	2.332464	-0.741811	1.210896
11	C	4.117215	0.135003	0.315591	11	C	4.085690	0.140416	0.382107
12	C	5.525274	0.425197	0.133497	12	C	5.501933	0.409367	0.236318
13	C	5.911446	1.357348	-0.839782	13	C	5.930556	1.291341	-0.765567
14	H	5.149072	1.844598	-1.439292	14	H	5.194640	1.756217	-1.413879
15	C	7.252198	1.650790	-1.031699	15	C	7.279946	1.563667	-0.924136
16	H	7.575098	2.368121	-1.778746	16	H	7.635957	2.241787	-1.692414
17	C	8.199433	1.006411	-0.244669	17	C	8.192732	0.948528	-0.075231
18	C	7.843681	0.079664	0.725389	18	C	7.794390	0.071475	0.924231
19	H	8.615945	-0.399952	1.317315	19	H	8.540944	-0.386515	1.564242
20	C	6.499098	-0.210245	0.912985	20	C	6.441390	-0.197491	1.078308
21	H	6.202613	-0.932170	1.667094	21	H	6.111927	-0.880605	1.854553
22	C	-1.434941	-1.558705	-1.889747	22	C	-1.467313	-1.722577	-1.798522
23	C	-0.117244	-1.251985	-1.439446	23	C	-0.110875	-1.342111	-1.403519
24	C	0.921012	-1.931522	-2.082506	24	C	0.934595	-2.019958	-2.003699
25	H	1.960865	-1.755982	-1.825496	25	H	1.969871	-1.782021	-1.779677
26	C	0.636257	-2.841145	-3.090334	26	C	0.672646	-3.027748	-2.935027
27	C	-0.656767	-3.135088	-3.521242	27	C	-0.624790	-3.408453	-3.307546
28	H	-0.808838	-3.857744	-4.315249	28	H	-0.751721	-4.204090	-4.034778
29	C	-1.708662	-2.476977	-2.907867	29	C	-1.701850	-2.762739	-2.745981
30	H	-2.732779	-2.671148	-3.215524	30	H	-2.717354	-3.031123	-3.019506
31	C	-2.401907	-0.797686	-1.168241	31	C	-2.412192	-0.954091	-1.163485
32	C	-4.117296	0.135087	-0.315581	32	C	-4.103226	0.100108	-0.340826
33	C	-5.525337	0.425361	-0.133483	33	C	-5.460325	0.443506	-0.113853
34	C	-5.911438	1.357671	0.839673	34	C	-5.787417	1.488814	0.781523
35	H	-5.149025	1.844976	1.439086	35	H	-4.987356	2.019757	1.286998
36	C	-7.252173	1.651196	1.031589	36	C	-7.107267	1.826392	1.007865
37	H	-7.575020	2.368650	1.778542	37	H	-7.379342	2.624388	1.690891
38	C	-8.199459	1.006739	0.244686	38	C	-8.110380	1.123328	0.342039
39	C	-7.843778	0.079834	-0.725247	39	C	-7.822417	0.091129	-0.544186
40	H	-8.616081	-0.399837	-1.317076	40	H	-8.635602	-0.428593	-1.040200
41	C	-6.499212	-0.210157	-0.912845	41	C	-6.500122	-0.249539	-0.772977

42	H	-6.202780	-0.932205	-1.666857	42	H	-6.255178	-1.051673	-1.460946
43	F	-1.655338	-3.473565	3.688409	43	F	-1.816014	-3.235600	3.772292
44	F	9.492311	1.288318	-0.427743	44	F	9.493383	1.209874	-0.226177
45	F	1.655010	-3.474351	-3.687896	45	F	1.706028	-3.668729	-3.501229
46	F	-9.492320	1.288726	0.427761	46	F	-9.387525	1.453096	0.563316
47	Ir	-0.000039	0.143601	-0.000072	47	Ir	-0.041435	0.152387	-0.074449
48	N	2.010676	0.033696	0.229390	48	N	1.983412	0.051861	0.226367
49	N	3.100735	0.633482	-0.320148	49	N	3.096307	0.621303	-0.308043
50	N	-2.010756	0.033737	-0.229459	50	N	-1.992430	0.041812	-0.284983
51	N	-3.100771	0.633662	0.320011	51	N	-3.022451	0.669232	0.205870
52	O	3.737372	-0.774905	1.267519	52	O	3.663207	-0.727064	1.355938
53	O	-3.737525	-0.775045	-1.267327	53	O	-3.780608	-0.926377	-1.213114
54	C	0.023662	2.912860	-1.256428	54	C	0.222446	2.797403	-1.537270
55	C	-0.022833	2.913050	1.255904	55	C	0.023030	3.015684	0.958597
56	C	0.000640	3.538487	-0.000307	56	C	0.196259	3.524753	-0.339313
57	H	0.000938	4.622577	-0.000387	57	H	0.294541	4.600744	-0.426423
58	C	-0.064583	3.779539	2.491438	58	C	-0.045177	3.987128	2.111197
59	H	0.780655	3.527537	3.140859	59	H	0.700338	3.711466	2.864507
60	H	-0.036373	4.847144	2.261097	60	H	0.117475	5.022389	1.802727
61	H	-0.977940	3.557495	3.054393	61	H	-1.028066	3.905755	2.588553
62	C	0.065727	3.779148	-2.492090	62	C	0.398819	3.545536	-2.834931
63	H	0.037964	4.846797	-2.261884	63	H	0.485048	4.625274	-2.693035
64	H	0.978973	3.556640	-3.055039	64	H	1.296151	3.174692	-3.342187
65	H	-0.779655	3.527438	-3.141442	65	H	-0.450946	3.334577	-3.493043
66	O	0.013446	1.667367	-1.496404	66	O	0.104982	1.539311	-1.679393
67	O	-0.013373	1.667585	1.496052	67	O	-0.096659	1.799179	1.294778

2				2					
S0				T1					
1	C	1.377476	-1.891201	1.916836	1	C	1.414815	-1.945972	1.904858
2	C	0.070013	-1.546843	1.465766	2	C	0.073540	-1.563928	1.480926
3	C	-0.989412	-2.196976	2.105719	3	C	-0.987196	-2.184770	2.112326
4	H	-2.023361	-1.990827	1.846716	4	H	-2.017526	-1.944482	1.867673
5	C	-0.732925	-3.116801	3.111503	5	C	-0.749338	-3.137318	3.109548
6	C	0.550811	-3.448728	3.543431	6	C	0.535404	-3.514970	3.517602
7	H	0.680765	-4.177361	4.335953	7	H	0.644699	-4.262395	4.296775
8	C	1.622253	-2.819552	2.933879	8	C	1.626398	-2.923392	2.920543
9	H	2.639830	-3.044139	3.242733	9	H	2.636133	-3.189073	3.217701
10	C	2.366838	-1.151180	1.205327	10	C	2.379957	-1.245939	1.221280
11	C	4.112320	-0.254541	0.378829	11	C	4.103627	-0.260716	0.380953
12	C	5.528617	0.000643	0.207514	12	C	5.465722	0.052499	0.165059
13	C	5.944126	0.923893	-0.762157	13	C	5.825451	1.045208	-0.779274
14	H	5.197448	1.429094	-1.366654	14	H	5.042346	1.556768	-1.329427
15	C	7.292966	1.184863	-0.944517	15	C	7.153470	1.353974	-0.995352
16	H	7.638445	1.894185	-1.689147	16	H	7.449757	2.110199	-1.714945
17	C	8.218815	0.517195	-0.151563	17	C	8.134439	0.676393	-0.271495
18	C	7.833904	-0.401406	0.815013	18	C	7.815237	-0.303356	0.663019
19	H	8.590142	-0.900118	1.411860	19	H	8.611811	-0.804722	1.203042
20	C	6.481308	-0.658868	0.992914	20	C	6.485129	-0.616339	0.882401
21	H	6.161974	-1.373909	1.744271	21	H	6.216411	-1.377352	1.607209
22	C	-1.377387	-1.891832	-1.916377	22	C	-1.329763	-1.942369	-1.857852
23	C	-0.069956	-1.547255	-1.465375	23	C	-0.025704	-1.588381	-1.412777
24	C	0.989518	-2.197551	-2.105085	24	C	1.039154	-2.255250	-2.021593
25	H	2.023453	-1.991243	-1.846150	25	H	2.070990	-2.043904	-1.759521
26	C	0.733108	-3.117738	-3.110556	26	C	0.788610	-3.206410	-3.000373
27	C	-0.550598	-3.449887	-3.542405	27	C	-0.492543	-3.550044	-3.429461
28	H	-0.680494	-4.178804	-4.334674	28	H	-0.618172	-4.302921	-4.199655
29	C	-1.622087	-2.820553	-2.933101	29	C	-1.567623	-2.902288	-2.846734
30	H	-2.639644	-3.045299	-3.241907	30	H	-2.583288	-3.136434	-3.154113
31	C	-2.366806	-1.151628	-1.205143	31	C	-2.326063	-1.179510	-1.180331
32	C	-4.112357	-0.254710	-0.379086	32	C	-4.082022	-0.246504	-0.419612
33	C	-5.528666	0.000543	-0.207977	33	C	-5.499915	0.018610	-0.281511
34	C	-5.944249	0.924075	0.761394	34	C	-5.928241	0.972293	0.652493
35	H	-5.197617	1.429440	1.365811	35	H	-5.190548	1.492604	1.255162
36	C	-7.293102	1.185115	0.943562	36	C	-7.278872	1.243280	0.803196
37	H	-7.638638	1.894655	1.687958	37	H	-7.634655	1.975651	1.520100
38	C	-8.218891	0.517230	0.150719	38	C	-8.193341	0.554727	0.014749
39	C	-7.833906	-0.401652	-0.815562	39	C	-7.795413	-0.394394	-0.916619
40	H	-8.590097	-0.900526	-1.412332	40	H	-8.543196	-0.908730	-1.510791
41	C	-6.481297	-0.659181	-0.993271	41	C	-6.441090	-0.661710	-1.063043

42	H	-6.161906	-1.374441	-1.744396	42	H	-6.111838	-1.400815	-1.786294
43	C	-0.075913	4.890267	1.241148	43	C	-0.209363	4.862249	1.306586
44	H	0.499727	5.810895	1.090782	44	H	0.340911	5.801642	1.180605
45	H	0.425278	4.317467	2.026812	45	H	0.289361	4.297355	2.099349
46	C	-1.509545	5.206656	1.644187	46	C	-1.662435	5.129369	1.673438
47	H	-2.024635	5.784000	0.868242	47	H	-2.174962	5.696270	0.888255
48	H	-1.521149	5.794699	2.568324	48	H	-1.716137	5.709663	2.600828
49	H	-2.066128	4.280688	1.816324	49	H	-2.194311	4.185396	1.824850
50	C	0.076003	4.890317	-1.241115	50	C	0.011182	4.898015	-1.170964
51	H	-0.425354	4.317653	-2.026763	51	H	-0.451214	4.322028	-1.977637
52	H	-0.499421	5.811050	-1.090659	52	H	-0.594989	5.799237	-1.024272
53	C	1.509677	5.206457	-1.644241	53	C	1.446309	5.260106	-1.526757
54	H	2.024960	5.783635	-0.868288	54	H	1.921295	5.841743	-0.728898
55	H	1.521338	5.794601	-2.568310	55	H	1.467611	5.860239	-2.442750
56	H	2.066079	4.280399	-1.816463	56	H	2.034843	4.353197	-1.693698
57	F	-1.770239	-3.722770	3.706200	57	F	-1.800625	-3.719656	3.705257
58	F	9.519737	0.767844	-0.325479	58	F	9.420317	0.979330	-0.483295
59	F	1.770474	-3.723854	-3.705016	59	F	1.828580	-3.830270	-3.567276
60	F	-9.519825	0.767943	0.324453	60	F	-9.495519	0.814745	0.158259
61	Ir	-0.000032	-0.148744	0.000005	61	Ir	0.048534	-0.153720	0.026381
62	N	2.003716	-0.297895	0.274013	62	N	1.991497	-0.295117	0.275086
63	N	3.114797	0.277955	-0.258954	63	N	3.038717	0.292742	-0.220319
64	N	-2.003762	-0.298063	-0.274057	64	N	-1.976742	-0.295901	-0.274733
65	N	-3.114889	0.277949	0.258646	65	N	-3.093162	0.305543	0.215230
66	O	3.702149	-1.164015	1.316971	66	O	3.745525	-1.237606	1.298814
67	O	-3.702112	-1.164498	-1.316889	67	O	-3.658330	-1.192008	-1.315767
68	S	0.103684	1.85871	-1.446205	68	S	0.130858	1.870792	-1.410716
69	S	-0.103857	1.858705	1.446141	69	S	-0.146052	1.831957	1.480111
70	C	-0.000057	2.788023	-0.000026	70	C	-0.036696	2.779685	0.041529
71	N	-0.000001	4.127384	-0.000017	71	N	-0.077253	4.116134	0.058654

3				3					
S0				T1					
1	C	-1.376437	-2.030035	-1.829034	1	C	-1.385604	-2.126964	-1.707219
2	C	-0.068472	-1.644361	-1.417662	2	C	-0.056947	-1.674429	-1.384688
3	C	0.992238	-2.309955	-2.037394	3	C	1.012505	-2.323852	-1.994310
4	H	2.026239	-2.072371	-1.808329	4	H	2.039879	-2.028025	-1.809888
5	C	0.735257	-3.285124	-2.990041	5	C	0.764750	-3.358868	-2.886903
6	C	-0.549209	-3.657810	-3.384572	6	C	-0.525099	-3.801744	-3.202590
7	H	-0.679187	-4.428320	-4.136356	7	H	-0.645992	-4.615779	-3.909758
8	C	-1.621405	-3.013367	-2.792929	8	C	-1.609520	-3.187007	-2.609933
9	H	-2.639629	-3.268166	-3.074656	9	H	-2.620995	-3.509872	-2.837071
10	C	-2.365296	-1.270065	-1.139225	10	C	-2.360418	-1.385460	-1.022796
11	C	-4.114824	-0.377888	-0.315458	11	C	-4.099499	-0.352845	-0.315363
12	C	-5.532700	-0.145162	-0.127049	12	C	-5.499814	-0.073823	-0.145147
13	C	-5.952286	0.784151	0.835406	13	C	-5.905702	0.965136	0.712048
14	H	-5.209140	1.305926	1.430310	14	H	-5.153799	1.536059	1.247726
15	C	-7.302888	1.027752	1.028164	15	C	-7.249908	1.249425	0.879308
16	H	-7.651388	1.740366	1.768185	16	H	-7.584097	2.044093	1.538102
17	C	-8.226596	0.335442	0.253796	17	C	-8.190123	0.490829	0.188450
18	C	-7.837661	-0.591100	-0.703839	18	C	-7.819104	-0.542911	-0.661201
19	H	-8.592368	-1.109306	-1.285769	19	H	-8.584922	-1.110351	-1.179481
20	C	-6.483455	-0.830392	-0.892827	20	C	-6.471241	-0.825079	-0.827278
21	H	-6.161335	-1.550231	-1.638367	21	H	-6.164261	-1.628609	-1.488641
22	C	1.400267	-1.831138	1.950914	22	C	1.409300	-1.951992	1.821875
23	C	0.090526	-1.496489	1.502516	23	C	0.077421	-1.542747	1.459464
24	C	-0.966583	-2.104417	2.184758	24	C	-0.986863	-2.140911	2.127347
25	H	-2.001952	-1.897844	1.933078	25	H	-2.016572	-1.871290	1.917521
26	C	-0.704438	-2.978181	3.229856	26	C	-0.731017	-3.086039	3.112841
27	C	0.581940	-3.301837	3.660003	27	C	0.562012	-3.487278	3.467410
28	H	0.715949	-3.992915	4.484738	28	H	0.689621	-4.230650	4.247455
29	C	1.650556	-2.712472	3.007741	29	C	1.641480	-2.921669	2.819006
30	H	2.670117	-2.931291	3.313798	30	H	2.655540	-3.213650	3.074673
31	C	2.385055	-1.133005	1.193705	31	C	2.378654	-1.265653	1.074617
32	C	4.131228	-0.293958	0.308973	32	C	4.109416	-0.271341	0.294265
33	C	5.547778	-0.057402	0.115983	33	C	5.506940	0.013921	0.112839
34	C	5.967014	0.784311	-0.924084	34	C	5.907496	0.976040	-0.832308
35	H	5.224644	1.236300	-1.574436	35	H	5.154219	1.481583	-1.428334
36	C	7.316624	1.029307	-1.122245	36	C	7.249179	1.266417	-1.009842
37	H	7.665216	1.674905	-1.921343	37	H	7.579012	2.002374	-1.735611
38	C	8.239297	0.426267	-0.275345	38	C	8.192458	0.590419	-0.241813
39	C	7.850608	-0.412641	0.760051	39	C	7.826900	-0.367229	0.694960
40	H	8.604641	-0.862583	1.397013	40	H	8.594872	-0.871834	1.271759
41	C	6.497541	-0.653632	0.954214	41	C	6.481659	-0.655234	0.871654

42	H	6.175299	-1.305225	1.760009	42	H	6.179190	-1.399239	1.601210
43	C	2.536198	3.666275	-0.252401	43	C	2.544633	3.661642	-0.332988
44	H	2.993137	4.306741	-1.012981	44	H	2.958319	4.345166	-1.080231
45	H	2.633032	2.626306	-0.583141	45	H	2.625192	2.639619	-0.717410
46	C	3.173918	3.880144	1.102593	46	C	3.245717	3.807813	0.998526
47	H	3.064588	4.920849	1.423253	47	H	3.150610	4.829367	1.379439
48	H	4.243205	3.644029	1.049398	48	H	4.311013	3.578719	0.879778
49	H	2.709731	3.233605	1.853394	49	H	2.823362	3.118555	1.735672
50	C	-2.564987	3.548234	-0.304873	50	C	-2.569140	3.581069	-0.189821
51	H	-2.743114	3.038212	-1.259027	51	H	-2.796200	3.096649	-1.146214
52	H	-2.718144	2.824631	0.503516	52	H	-2.700612	2.841176	0.606532
53	C	-3.457418	4.756894	-0.149479	53	C	-3.427213	4.803820	0.030440
54	H	-3.271273	5.255441	0.806653	54	H	-3.193719	5.274561	0.990173
55	H	-4.508039	4.448181	-0.183219	55	H	-4.484235	4.516069	0.030645
56	H	-3.281824	5.476351	-0.955113	56	H	-3.269514	5.539078	-0.764466
57	F	1.772946	-3.904732	-3.567516	57	F	1.802678	-3.964140	-3.480492
58	F	-9.528399	0.568596	0.437818	58	F	-9.488210	0.765471	0.349829
59	F	-1.738809	-3.543498	3.865949	59	F	-1.764474	-3.640696	3.761325
60	F	9.540046	0.660767	-0.464626	60	F	9.488013	0.870759	-0.413406
61	Ir	0.006981	-0.177265	-0.027966	61	Ir	0.003877	-0.192057	-0.028579
62	N	-2.001998	-0.363256	-0.260217	62	N	-1.990387	-0.372652	-0.225152
63	N	-3.116177	0.208048	0.272602	63	N	-3.078335	0.282808	0.201583
64	N	2.018551	-0.320468	0.228234	64	N	2.000998	-0.334514	0.186707
65	N	3.130803	0.217655	-0.342344	65	N	3.083328	0.299730	-0.284882
66	O	-3.701932	-1.320336	-1.218282	66	O	-3.709244	-1.416553	-1.100049
67	O	3.721370	-1.154317	1.290965	67	O	3.727404	-1.268919	1.164826
68	O	1.150117	4.051768	-0.221103	68	O	1.157647	4.038476	-0.216171
69	O	-1.205181	4.007508	-0.279437	69	O	-1.197476	4.013857	-0.213736
70	P	-0.007068	2.937426	-0.19259	70	P	-0.007168	2.941074	-0.168195
71	S	-0.059305	1.82464	1.485677	71	S	-0.016495	1.806707	1.500923
72	S	0.067206	1.658065	-1.744386	72	S	0.006829	1.667215	-1.731375

4a					4a				
S0					T1				
1	Ir	-0.424794	-1.036331	0.026723	1	Ir	-0.540328	-0.977471	-0.021268
2	O	0.450136	-2.887657	0.344995	2	O	0.151181	-2.900762	0.253898
3	O	-0.097137	-1.127261	-1.981895	3	O	-0.229831	-1.067450	-2.030929
4	N	-1.451193	0.645826	-0.278623	4	N	-1.354733	0.787793	-0.275883
5	N	-1.104631	1.903732	-0.192425	5	N	-0.864443	1.985701	-0.189788
6	N	1.355286	-0.232197	0.431863	6	N	1.322332	-0.358649	0.414626
7	N	2.381074	0.028172	-0.334569	7	N	2.377366	-0.158649	-0.329824
8	C	-2.760352	0.499320	-0.639075	8	C	-2.753075	0.789191	-0.590319
9	C	-2.207745	2.623476	-0.517662	9	C	-1.909516	2.832315	-0.470172
10	C	1.589329	0.085029	1.733249	10	C	1.573067	-0.130882	1.732507
11	C	3.332710	0.550766	0.479500	11	C	3.366938	0.227511	0.515232
12	C	1.832865	-4.722593	-0.080263	12	C	1.360476	-4.848668	-0.192213
13	H	2.605385	-4.440899	0.644389	13	H	2.134070	-4.653766	0.559177
14	H	1.119635	-5.367481	0.443778	14	H	0.578933	-5.441250	0.294914
15	H	2.298928	-5.281635	-0.894406	15	H	1.797487	-5.425825	-1.009698
16	C	1.136170	-3.477340	-0.559964	16	C	0.786511	-3.537526	-0.655951
17	C	1.284051	-3.082182	-1.890024	17	C	0.972995	-3.136859	-1.979145
18	H	1.932735	-3.691105	-2.508796	18	H	1.559218	-3.794490	-2.609873
19	C	0.698887	-1.965986	-2.510964	19	C	0.480440	-1.968074	-2.580955
20	C	1.028529	-1.673125	-3.946669	20	C	0.806725	-1.690639	-4.020442
21	H	1.796242	-0.889622	-3.959090	21	H	1.603536	-0.937438	-4.046592
22	H	1.413960	-2.548904	-4.473868	22	H	1.149101	-2.582718	-4.549628
23	H	0.146646	-1.282006	-4.460841	23	H	-0.066340	-1.268020	-4.525125
24	C	-3.250002	-0.847759	-0.700467	24	C	-3.370986	-0.469119	-0.642144
25	C	-2.658919	-3.088873	-0.357140	25	C	-2.975751	-2.794810	-0.394804
26	H	-1.861179	-3.767060	-0.070703	26	H	-2.252978	-3.575932	-0.175633
27	C	-3.927786	-3.528155	-0.693785	27	C	-4.294553	-3.086051	-0.673999
28	C	-4.886798	-2.576126	-1.049443	28	C	-5.208259	-2.014030	-0.953863
29	H	-5.891770	-2.884948	-1.323219	29	H	-6.249190	-2.220023	-1.178943
30	C	-4.549380	-1.234469	-1.052908	30	C	-4.730067	-0.731737	-0.934433
31	H	-5.271281	-0.472527	-1.326844	31	H	-5.383128	0.111391	-1.144451
32	C	-2.186481	4.090588	-0.526302	32	C	-1.703194	4.273205	-0.471841
33	C	-3.155826	4.807919	-1.244095	33	C	-2.724589	5.134171	-0.908315
34	C	-3.126183	6.194559	-1.222301	34	C	-2.501512	6.503511	-0.898229
35	H	-3.867294	6.768545	-1.772958	35	H	-3.274592	7.189424	-1.233703
36	C	-2.125076	6.833383	-0.496914	36	C	-1.270998	6.976552	-0.455850
37	C	-1.201491	6.034371	0.172491	37	C	-0.318025	6.041464	-0.043324
38	H	-0.397661	6.493227	0.748010	38	H	0.657901	6.374423	0.307881
39	C	0.514824	-0.207151	2.635546	39	C	0.471032	-0.364462	2.619430
40	C	-1.647088	-1.091486	2.789873	40	C	-1.770803	-1.048330	2.731370
41	H	-2.478746	-1.534207	2.253544	41	H	-2.634940	-1.381132	2.167185

42	C	-1.695576	-0.870139	4.154371	42	C	-1.798255	-0.900531	4.106001
43	C	-0.586355	-0.291812	4.774390	43	C	-0.638978	-0.466061	4.752900
44	H	-0.590630	-0.099611	5.843452	44	H	-0.626200	-0.338165	5.831580
45	C	0.518951	0.039541	4.012972	45	C	0.495282	-0.198355	4.009243
46	H	1.395093	0.496894	4.459657	46	H	1.411045	0.142609	4.479833
47	C	4.636554	0.970158	-0.044180	47	C	4.710410	0.544427	0.020149
48	C	6.197142	0.876249	-1.716525	48	C	6.259898	0.404982	-1.659645
49	H	6.461429	0.476696	-2.695754	49	H	6.484915	0.048912	-2.665086
50	C	7.081838	1.715918	-1.045006	50	C	7.224539	1.099133	-0.934132
51	C	6.690342	2.203444	0.198455	51	C	6.880792	1.536709	0.341577
52	H	7.335639	2.872304	0.762525	52	H	7.590391	2.092678	0.949316
53	C	5.453369	1.832911	0.703447	53	C	5.609757	1.263071	0.823560
54	H	-3.906172	4.279531	-1.824579	54	H	-3.668939	4.731290	-1.258990
55	H	5.107573	2.220022	1.656979	55	H	5.303579	1.615411	1.803764
56	H	-2.056094	7.916182	-0.453176	56	H	-1.047541	8.038790	-0.430447
57	H	-4.155843	-4.588184	-0.680972	57	H	-4.621601	-4.119920	-0.682536
58	H	-2.584348	-1.141315	4.713130	58	H	-2.708112	-1.120293	4.653180
59	H	8.038509	1.980228	-1.485489	59	H	8.205565	1.291956	-1.357832
60	C	-3.285772	1.777199	-0.812572	60	C	-3.101975	2.127063	-0.729433
61	C	2.877172	0.608685	1.805065	61	C	2.904740	0.261558	1.839217
62	N	-0.577601	-0.777367	2.046245	62	N	-0.672897	-0.790150	2.006695
63	N	5.012128	0.501263	-1.243693	63	N	5.040492	0.123903	-1.210186
64	N	-2.328349	-1.791254	-0.356353	64	N	-2.489460	-1.545755	-0.358944
65	N	-1.221823	4.704993	0.173009	65	N	-0.513412	4.730883	-0.045043
66	H	-4.298378	2.049470	-1.075833	66	H	-4.078587	2.527756	-0.953865
67	H	3.407142	0.953104	2.681842	67	H	3.455770	0.507325	2.736068

4b					4b				
S0					T1				
1	Ir	-0.103004	-1.093461	-0.011393	1	Ir	-0.113497	-1.088784	-0.042460
2	O	1.107017	-2.762047	0.174381	2	O	1.078962	-2.766071	0.099391
3	O	-0.225767	-1.290475	-2.035141	3	O	-0.262768	-1.246175	-2.067288
4	N	-1.417046	0.402266	-0.149271	4	N	-1.391623	0.421132	-0.150090
5	N	-1.237547	1.701732	-0.219031	5	N	-1.202174	1.718656	-0.224468
6	N	1.572707	-0.004375	-0.062819	6	N	1.581299	-0.008064	-0.080873
7	N	2.336946	0.346487	-1.071613	7	N	2.345525	0.372998	-1.079114
8	C	-2.743216	0.014828	-0.183083	8	C	-2.769712	0.026556	-0.150832
9	C	-2.486702	2.213252	-0.311130	9	C	-2.479461	2.235038	-0.296423
10	C	2.023536	0.423762	1.164349	10	C	2.041335	0.374332	1.158650
11	C	3.343277	1.049434	-0.501939	11	C	3.360299	1.047298	-0.489607
12	C	2.615682	-4.420073	-0.483639	12	C	2.564372	-4.426809	-0.600197
13	H	3.481773	-3.974055	0.018523	13	H	3.428957	-4.003092	-0.076811
14	H	2.152745	-5.111820	0.227944	14	H	2.090266	-5.137847	0.084627
15	H	2.961193	-4.975165	-1.358234	15	H	2.912541	-4.956347	-1.489384
16	C	1.641765	-3.329450	-0.840299	16	C	1.599491	-3.320157	-0.929619
17	C	1.405671	-3.037734	-2.184932	17	C	1.351774	-3.003620	-2.266556
18	H	1.967299	-3.612451	-2.912005	18	H	1.897138	-3.573653	-3.009381
19	C	0.528055	-2.069374	-2.700218	19	C	0.471785	-2.024070	-2.754793
20	C	0.440106	-1.878038	-4.187616	20	C	0.353634	-1.818234	-4.238431
21	H	1.000314	-0.971646	-4.447272	21	H	0.877746	-0.890838	-4.498473
22	H	0.858199	-2.720585	-4.742879	22	H	0.788495	-2.641028	-4.810008
23	H	-0.600611	-1.715544	-4.481245	23	H	-0.697344	-1.689275	-4.512324
24	C	-3.007880	-1.383883	-0.069599	24	C	-3.049784	-1.332973	-0.027732
25	C	-2.003959	-3.479641	0.216215	25	C	-2.035672	-3.456366	0.219046
26	H	-1.064770	-4.010579	0.334863	26	H	-1.112715	-4.023035	0.304235
27	C	-3.229681	-4.122097	0.204198	27	C	-3.272867	-4.075049	0.250221
28	C	-4.384282	-3.349663	0.046311	28	C	-4.466486	-3.285549	0.134418
29	H	-5.362236	-3.822372	0.029626	29	H	-5.443498	-3.755503	0.152905
30	C	-4.277112	-1.977613	-0.090569	30	C	-4.334218	-1.931289	-0.003579
31	H	-5.151632	-1.347927	-0.216809	31	H	-5.202889	-1.284963	-0.097515
32	C	-3.229193	3.445173	-0.414728	32	C	-3.198101	3.467916	-0.388388
33	C	-4.584513	3.025757	-0.452487	33	C	-4.564124	3.067680	-0.399798
34	C	-5.611144	3.939043	-0.552802	34	C	-5.578550	4.003872	-0.484909
35	H	-6.652186	3.632891	-0.584194	35	H	-6.625422	3.717999	-0.496756
36	C	-5.218978	5.277169	-0.611105	36	C	-5.159309	5.327233	-0.553846
37	C	-3.861115	5.607287	-0.565606	37	C	-3.787072	5.638122	-0.533686
38	H	-3.561543	6.652929	-0.610553	38	H	-3.476324	6.679896	-0.587243
39	C	1.235584	0.040095	2.289965	39	C	1.258880	-0.039359	2.278067
40	C	-0.672313	-1.133878	2.961152	40	C	-0.655274	-1.220166	2.929189
41	H	-1.522448	-1.727231	2.644305	41	H	-1.511519	-1.795646	2.596060

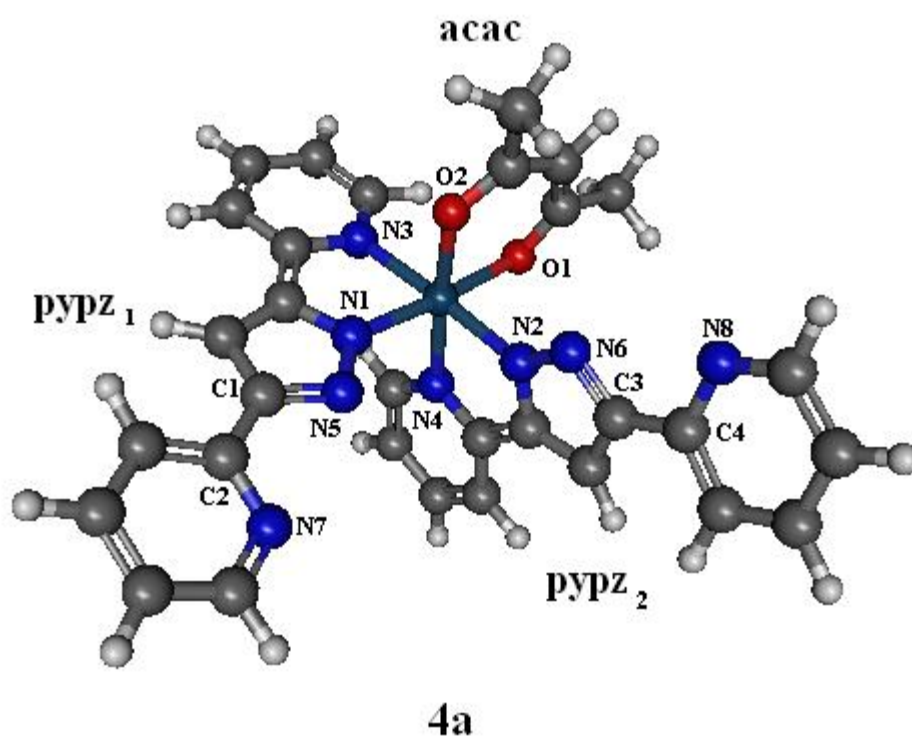
42	C	-0.451460	-0.828860	4.291819	42	C	-0.415445	-0.964812	4.266930
43	C	0.664376	-0.056307	4.623016	43	C	0.711729	-0.214690	4.612294
44	H	0.866086	0.204031	5.658033	44	H	0.928500	0.004671	5.653823
45	C	1.509957	0.379365	3.620396	45	C	1.551080	0.249082	3.616972
46	H	2.383209	0.986169	3.835282	46	H	2.434088	0.836973	3.844352
47	C	4.559504	1.768450	-0.787269	47	C	4.580760	1.767350	-0.754134
48	C	6.338408	2.742948	-1.778929	48	C	6.362720	2.765011	-1.717462
49	H	6.875574	2.957275	-2.701323	49	H	6.897694	3.008669	-2.633850
50	C	6.843065	3.213962	-0.563336	50	C	6.875753	3.188231	-0.487922
51	C	6.161441	2.942632	0.624055	51	C	6.196749	2.879044	0.691755
52	H	6.513144	3.286265	1.591870	52	H	6.554863	3.184795	1.669891
53	C	5.004846	2.206763	0.487541	53	C	5.034402	2.156786	0.533718
54	H	-5.962865	6.063733	-0.691485	54	H	-5.887246	6.129571	-0.623279
55	H	-3.277548	-5.199902	0.312592	55	H	-3.322973	-5.153061	0.356770
56	H	-1.141406	-1.186466	5.047886	56	H	-1.098331	-1.345299	5.018238
57	H	7.763535	3.789339	-0.548158	57	H	7.800611	3.755836	-0.455832
58	C	-3.446626	1.206696	-0.294886	58	C	-3.443434	1.246080	-0.260205
59	C	3.187953	1.123730	0.878883	59	C	3.210756	1.073994	0.893519
60	N	0.144392	-0.720048	1.982168	60	N	0.154852	-0.775113	1.957940
61	N	5.218571	2.030107	-1.914598	61	N	5.237246	2.065390	-1.874014
62	N	-1.892580	-2.150996	0.086940	62	N	-1.880611	-2.134581	0.091886
63	N	-2.865190	4.724828	-0.468952	63	N	-2.808599	4.745472	-0.452974
64	O	4.172884	1.816041	1.512559	64	O	4.203464	1.736174	1.547527
65	O	-4.727454	1.657383	-0.378255	65	O	-4.724758	1.716498	-0.319461

4c					4c				
S0					T1				
1	Ir	-0.133521	-1.200303	-0.011684	1	Ir	-0.136145	-1.197486	-0.046390
2	O	1.076366	-2.868906	0.173298	2	O	1.062264	-2.872240	0.069251
3	O	-0.211004	-1.363920	-2.040657	3	O	-0.252482	-1.293366	-2.077368
4	N	-1.451552	0.290188	-0.150408	4	N	-1.434315	0.307332	-0.134121
5	N	-1.283033	1.589551	-0.186404	5	N	-1.266197	1.608023	-0.169683
6	N	1.541502	-0.111645	-0.006473	6	N	1.554237	-0.113796	-0.024864
7	N	2.329758	0.256142	-0.986527	7	N	2.334990	0.297151	-0.994349
8	C	-2.772502	-0.089070	-0.218207	8	C	-2.793993	-0.081843	-0.175284
9	C	-2.528677	2.101888	-0.289123	9	C	-2.537121	2.126512	-0.253107
10	C	1.976293	0.293844	1.227464	10	C	2.005040	0.232917	1.221856
11	C	3.328301	0.942176	-0.388519	11	C	3.343669	0.949931	-0.376062
12	C	2.602729	-4.513163	-0.478373	12	C	2.557447	-4.512400	-0.656674
13	H	3.459799	-4.071897	0.043162	13	H	3.418137	-4.099611	-0.118297
14	H	2.128812	-5.213414	0.217435	14	H	2.079309	-5.238550	0.009193
15	H	2.963522	-5.057631	-1.353480	15	H	2.912223	-5.021964	-1.554900
16	C	1.633910	-3.419282	-0.838677	16	C	1.594320	-3.398907	-0.968324
17	C	1.426531	-3.106167	-2.183064	17	C	1.362419	-3.047963	-2.299450
18	H	2.005641	-3.667405	-2.906957	18	H	1.918155	-3.598027	-3.049690
19	C	0.559910	-2.129540	-2.701603	19	C	0.491982	-2.052924	-2.774246
20	C	0.508693	-1.910286	-4.186735	20	C	0.402095	-1.803504	-4.253215
21	H	1.086967	-1.006975	-4.416029	21	H	0.954064	-0.883166	-4.478855
22	H	0.929396	-2.747971	-4.747437	22	H	0.826149	-2.620819	-4.840700
23	H	-0.522627	-1.728683	-4.501289	23	H	-0.640663	-1.640233	-4.539465
24	C	-3.036968	-1.491710	-0.137553	24	C	-3.074447	-1.443630	-0.096127
25	C	-2.031707	-3.590554	0.133413	25	C	-2.055479	-3.569983	0.122247
26	H	-1.093023	-4.119807	0.263352	26	H	-1.132073	-4.135268	0.213108
27	C	-3.254293	-4.237746	0.084262	27	C	-3.291711	-4.195254	0.114911
28	C	-4.407556	-3.466643	-0.085558	28	C	-4.486810	-3.407602	-0.007905
29	H	-5.383396	-3.941688	-0.131935	29	H	-5.461869	-3.881601	-0.020565
30	C	-4.302068	-2.091896	-0.196414	30	C	-4.356595	-2.051259	-0.111842
31	H	-5.179960	-1.468771	-0.331673	31	H	-5.230215	-1.411565	-0.208382
32	C	-3.091560	3.426010	-0.366919	32	C	-3.083752	3.446806	-0.320401
33	C	-4.506521	3.347239	-0.454857	33	C	-4.504980	3.377238	-0.385931
34	C	-5.251917	4.514773	-0.540071	34	C	-5.242305	4.556156	-0.460744
35	H	-6.336083	4.493471	-0.609771	35	H	-6.327283	4.545707	-0.513800
36	C	-4.552933	5.716913	-0.532489	36	C	-4.530688	5.745338	-0.464369
37	C	-3.157824	5.693708	-0.439962	37	C	-3.127615	5.711693	-0.393069
38	H	-2.599799	6.628755	-0.432020	38	H	-2.565923	6.644372	-0.394457
39	C	1.164278	-0.105820	2.332438	39	C	1.205109	-0.209420	2.320205
40	C	-0.763845	-1.282382	2.944608	40	C	-0.724701	-1.398732	2.909912
41	H	-1.610133	-1.865365	2.599448	41	H	-1.578488	-1.960630	2.548404

42	C	-0.570755	-1.001062	4.285016	42	C	-0.506647	-1.180286	4.258271
43	C	0.541073	-0.240005	4.652281	43	C	0.617574	-0.445457	4.641370
44	H	0.722398	0.002527	5.695338	44	H	0.818816	-0.254127	5.691475
45	C	1.409389	0.208444	3.674687	45	C	1.474391	0.040759	3.671499
46	H	2.278154	0.808182	3.924785	46	H	2.353709	0.618969	3.935229
47	C	4.519541	1.617901	-0.833853	47	C	4.532707	1.642070	-0.801792
48	C	6.092316	2.405473	-2.269000	48	C	6.092360	2.493479	-2.215093
49	H	6.435331	2.489529	-3.299199	49	H	6.423999	2.626149	-3.243929
50	C	6.836060	2.989518	-1.239276	50	C	6.850204	3.024303	-1.167040
51	C	6.386948	2.872668	0.071735	51	C	6.415195	2.845792	0.141838
52	H	6.938819	3.312753	0.897899	52	H	6.978112	3.243282	0.982047
53	C	5.206647	2.172795	0.278481	53	C	5.234489	2.140995	0.327997
54	H	-5.079594	6.664073	-0.597127	54	H	-5.046716	6.698724	-0.521275
55	H	-3.300188	-5.317385	0.173356	55	H	-3.339062	-5.275525	0.196364
56	H	-1.278733	-1.367405	5.019894	56	H	-1.204038	-1.576744	4.987674
57	H	7.752179	3.526610	-1.465021	57	H	7.766127	3.568113	-1.377000
58	C	-3.503143	1.093388	-0.315835	58	C	-3.509694	1.136811	-0.265601
59	C	3.157023	0.998663	1.003024	59	C	3.187246	0.941741	1.018286
60	N	0.075580	-0.856837	1.990899	60	N	0.102933	-0.933250	1.964151
61	N	4.960041	1.731764	-2.089853	61	N	4.959558	1.815669	-2.055784
62	N	-1.922994	-2.260002	0.029399	62	N	-1.903175	-2.247482	0.026822
63	N	-2.428641	4.585158	-0.358022	63	N	-2.407279	4.602974	-0.322238
64	S	-5.126842	1.695303	-0.440216	64	S	-5.128517	1.741532	-0.360749
65	S	4.413834	1.869928	1.824566	65	S	4.457199	1.767664	1.866533

5					5				
S0					T1				
1	Ir	-0.182752	-0.760091	0.016675	1	Ir	-0.218666	-0.747337	-0.018852
2	O	0.827209	-2.538955	0.320079	2	O	0.713044	-2.563538	0.256396
3	O	-0.156868	-0.980498	-2.006922	3	O	-0.209302	-0.946370	-2.044840
4	N	-1.338562	0.846365	-0.247116	4	N	-1.267097	0.898744	-0.255646
5	N	-1.123263	2.147606	-0.349758	5	N	-0.996771	2.175002	-0.352897
6	N	1.591705	0.156267	0.119776	6	N	1.602058	0.101659	0.110786
7	N	2.534567	0.478096	-0.755393	7	N	2.565411	0.420231	-0.743715
8	C	-2.660146	0.616344	-0.372466	8	C	-2.678327	0.722012	-0.344073
9	C	-2.354983	2.663628	-0.541829	9	C	-2.231069	2.756866	-0.512647
10	C	1.995021	0.526153	1.345252	10	C	2.005840	0.419844	1.351139
11	C	3.488555	1.049432	0.003031	11	C	3.530312	0.934710	0.041183
12	C	2.197956	-4.360652	-0.189194	12	C	2.015155	-4.430020	-0.267411
13	H	3.059540	-3.998268	0.383095	13	H	2.876406	-4.108237	0.328962
14	H	1.605437	-4.987464	0.485439	14	H	1.388525	-5.050730	0.381643
15	H	2.556443	-4.964643	-1.025350	15	H	2.369280	-5.028080	-1.109551
16	C	1.378213	-3.181174	-0.638496	16	C	1.242531	-3.216477	-0.707050
17	C	1.282575	-2.894858	-2.002402	17	C	1.156285	-2.913430	-2.067696
18	H	1.830351	-3.545142	-2.674311	18	H	1.673855	-3.579405	-2.747859
19	C	0.553120	-1.853866	-2.599176	19	C	0.458036	-1.844415	-2.650431
20	C	0.586226	-1.697462	-4.093554	20	C	0.470713	-1.685028	-4.144801
21	H	1.222662	-0.838127	-4.335961	21	H	1.090885	-0.816806	-4.396585
22	H	0.981474	-2.582035	-4.597676	22	H	0.869225	-2.564573	-4.654803
23	H	-0.418038	-1.474670	-4.465038	23	H	-0.542290	-1.477505	-4.501911
24	C	-3.094321	-0.748858	-0.261330	24	C	-3.155807	-0.580793	-0.224222
25	C	-2.352303	-2.930477	0.120907	25	C	-2.476954	-2.821838	0.094509
26	H	-1.492709	-3.563573	0.316578	26	H	-1.654001	-3.514824	0.245729
27	C	-3.640741	-3.429749	0.025013	27	C	-3.790057	-3.257065	0.043739
28	C	-4.687769	-2.538457	-0.225813	28	C	-4.843860	-2.305307	-0.151637
29	H	-5.708482	-2.901114	-0.308006	29	H	-5.877686	-2.630985	-0.195736
30	C	-4.415597	-1.188662	-0.369501	30	C	-4.513811	-0.985705	-0.283480
31	H	-5.189284	-0.454132	-0.564815	31	H	-5.262816	-0.214361	-0.435885
32	C	1.087394	0.238968	2.422480	32	C	1.085005	0.127387	2.416723
33	C	-0.986446	-0.695161	2.941246	33	C	-1.021122	-0.761344	2.902796
34	H	-1.875746	-1.186739	2.563580	34	H	-1.922610	-1.211110	2.502138
35	C	-0.826165	-0.405995	4.285715	35	C	-0.848911	-0.530978	4.256929
36	C	0.344984	0.229877	4.701765	36	C	0.342727	0.050965	4.694563
37	H	0.497948	0.470375	5.749843	37	H	0.504749	0.242829	5.751349
38	C	1.308677	0.554777	3.762888	38	C	1.316829	0.382132	3.768587
39	H	2.235341	1.053702	4.024521	39	H	2.260548	0.836672	4.049410
40	H	-3.817313	-4.493278	0.142719	40	H	-4.002128	-4.315168	0.149926
41	H	-1.607809	-0.673233	4.988257	41	H	-1.636314	-0.803423	4.950935

42	N	-0.055929	-0.387813	2.027606	42	N	-0.080708	-0.442123	2.002805
43	N	-2.083448	-1.625563	-0.015558	43	N	-2.127822	-1.537446	-0.023697
44	N	3.196077	1.100656	1.320581	44	N	3.225535	0.954571	1.356733
45	N	-3.341992	1.747103	-0.562253	45	N	-3.272852	1.910967	-0.512032
46	C	-2.563875	4.147797	-0.716447	46	C	-2.345616	4.242954	-0.672621
47	C	-2.033117	4.877090	0.526461	47	C	-1.745803	4.912991	0.576112
48	C	-1.781807	4.618637	-1.951632	48	C	-1.530889	4.660383	-1.909696
49	C	-4.051519	4.447669	-0.898875	49	C	-3.808029	4.651350	-0.840260
50	H	-2.583768	4.572536	1.424255	50	H	-2.308760	4.641512	1.476320
51	H	-0.973448	4.653229	0.684458	51	H	-0.702643	4.615363	0.717935
52	H	-2.146814	5.961892	0.408460	52	H	-1.787422	6.002922	0.463722
53	H	-2.147936	4.123800	-2.858532	53	H	-1.937468	4.204691	-2.819344
54	H	-1.896018	5.701804	-2.083584	54	H	-1.571941	5.750007	-2.025238
55	H	-0.716695	4.389817	-1.846703	55	H	-0.484536	4.356863	-1.811261
56	H	-4.199556	5.526478	-1.028295	56	H	-3.875696	5.739208	-0.956003
57	H	-4.454053	3.933334	-1.777295	57	H	-4.252379	4.178925	-1.721592
58	H	-4.631591	4.118728	-0.030586	58	H	-4.404224	4.355703	0.028457
59	C	4.773384	1.597984	-0.564048	59	C	4.838412	1.458230	-0.495580
60	C	4.845862	1.346630	-2.070472	60	C	4.925159	1.239355	-2.006379
61	C	4.825722	3.107491	-0.285808	61	C	4.930486	2.958815	-0.181566
62	C	5.955195	0.913594	0.136989	62	C	5.990323	0.724672	0.205361
63	H	4.808084	0.275768	-2.296235	63	H	4.859975	0.175546	-2.257622
64	H	4.010107	1.823449	-2.592041	64	H	4.110966	1.751657	-2.528434
65	H	5.783322	1.752356	-2.469671	65	H	5.879441	1.626723	-2.383339
66	H	4.747917	3.304375	0.788205	66	H	4.843793	3.132841	0.895744
67	H	5.769925	3.530118	-0.651582	67	H	5.891435	3.362000	-0.524886
68	H	4.000874	3.625994	-0.787553	68	H	4.128077	3.512595	-0.68217
69	H	6.904601	1.327499	-0.224776	69	H	6.955858	1.118751	-0.135209
70	H	5.899467	1.061458	1.220038	70	H	5.924343	0.850624	1.290606
71	H	5.956342	-0.164896	-0.060072	71	H	5.963239	-0.348854	-0.015154



Figures S1. Optimized structures of complex **4a** in the ground state at DFT/PBE0/LANL2DZ level.