Supporting Information

Cyclometalated Ir(III) complexes of deprotonated *N*-methylbipyridinium ligands: effects of quaternised N centre position on luminescence

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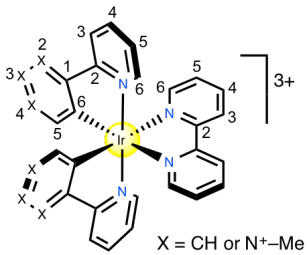
1. ^{13}C NMR Spectroscopic Data

Table S1 ^{13}C NMR data for complex salts **1P**, **4P** and **7P** in CD_3CN[a]

Environment:	pyridyl ring					cyclometalating ring						bpy rings					Me
Position:	2	3	4	5	6	1	2	3	4	5	6[b]	2	3	4	5	6	
Salt (isomer)[c]																	
1P (2)	157.16	130.02	141.47	129.98	153.64	149.91	---	144.70	127.28	149.91	157.05	156.23	126.55	141.91	129.87	152.44	50.88
4P (3)	161.69	123.35	142.22	128.61	151.91	147.43	138.94	---	142.41	132.23	175.08	156.07	126.55	142.10	130.13	152.22	48.14
7P (4)	161.59	126.46	141.76	130.14	152.41	143.79	122.31	141.68	---	147.02	161.66	156.43	126.46	141.92	129.90	152.58	48.44

[a] Signals assigned by using HMQC and HMBC measurements. [b] The position of the cyclometalating C atom. [c] Denotes the position with respect to the quaternised N atom of the N-coordinated 2′-pyridyl ring.

Numbering scheme:



2. Additional UV–vis Absorption Data

Table S2 UV–vis absorption data for complex salts **1C**–**9C** in water[a]

Salt (isomer)[b]	λ_{max}, nm (ε, 10^3 M^{-1} cm^{-1})	E_{max} (eV)	Assignment
1C (2)	209 (52.0)	5.93	$\pi \rightarrow \pi^*$
	255 (33.4)	4.86	$\pi \rightarrow \pi^*$
	300 (32.4)	4.13	$\pi \rightarrow \pi^*$
	354 (9.3)	3.50	d $\rightarrow \pi^*$
	438sh (2.6)	2.83	d $\rightarrow \pi^*$
2C (2)	212 (45.6)	5.85	$\pi \rightarrow \pi^*$
	262 (29.7)	4.73	$\pi \rightarrow \pi^*$
	296 (27.6)	4.19	$\pi \rightarrow \pi^*$
	350sh (9.4)	3.54	d $\rightarrow \pi^*$
	425sh (3.0)	2.92	d $\rightarrow \pi^*$
3C (2)	213 (66.7)	5.82	$\pi \rightarrow \pi^*$
	257 (38.3)	4.82	$\pi \rightarrow \pi^*$
	299 (37.0)	4.15	$\pi \rightarrow \pi^*$
	312sh (31.3)	3.97	d $\rightarrow \pi^*$
	355 (9.5)	3.49	d $\rightarrow \pi^*$
	446sh (2.3)	2.78	d $\rightarrow \pi^*$
4C (3)	237 (48.3)	5.23	$\pi \rightarrow \pi^*$
	255sh (42.4)	4.86	$\pi \rightarrow \pi^*$
	302 (22.8)	4.11	$\pi \rightarrow \pi^*$
	312 (21.8)	3.97	d $\rightarrow \pi^*$
	353sh (4.8)	3.51	d $\rightarrow \pi^*$
5C (3)	236 (47.4)	5.25	$\pi \rightarrow \pi^*$
	257 (43.2)	4.82	$\pi \rightarrow \pi^*$
	308 (21.6)	4.03	$\pi \rightarrow \pi^*$
	316 (20.9)	3.92	d $\rightarrow \pi^*$
	350sh (5.4)	3.54	d $\rightarrow \pi^*$
6C (3)	236 (51.8)	5.25	$\pi \rightarrow \pi^*$
	259sh (44.9)	4.79	$\pi \rightarrow \pi^*$
	299 (23.9)	4.15	$\pi \rightarrow \pi^*$
	311 (23.2)	3.99	d $\rightarrow \pi^*$
	356sh (4.5)	3.48	d $\rightarrow \pi^*$
7C (4)	254 (44.2)	4.88	$\pi \rightarrow \pi^*$
	277sh (31.6)	4.48	$\pi \rightarrow \pi^*$
	300 (28.4)	4.13	$\pi \rightarrow \pi^*$
	308 (28.2)	4.03	$\pi \rightarrow \pi^*$
	358 (6.7)	3.46	d $\rightarrow \pi^*$
	392sh (3.6)	3.16	d $\rightarrow \pi^*$
	439sh (1.7)	2.82	d $\rightarrow \pi^*$
8C (4)	252 (42.4)	4.92	$\pi \rightarrow \pi^*$
	296 (29.6)	4.19	$\pi \rightarrow \pi^*$
	307 (29.5)	4.04	$\pi \rightarrow \pi^*$
	348 (7.2)	3.56	d $\rightarrow \pi^*$
	388 (4.5)	3.20	d $\rightarrow \pi^*$
	427sh (2.2)	2.90	d $\rightarrow \pi^*$
9C (4)	233 (44.9)	5.32	$\pi \rightarrow \pi^*$
	256 (49.5)	4.84	$\pi \rightarrow \pi^*$
	298 (31.6)	4.16	$\pi \rightarrow \pi^*$
	309 (30.1)	4.01	$\pi \rightarrow \pi^*$
	357 (7.0)	3.47	d $\rightarrow \pi^*$
	395sh (3.6)	3.14	d $\rightarrow \pi^*$
	447sh (1.6)	2.77	d $\rightarrow \pi^*$

[a] Solutions ca. $1 \times 10^{-5} - 2 \times 10^{-4}$ M; ε values are the averages from measurements made at three or more different concentrations (with ε showing no significant variation). [b] Denotes the position with respect to the quaternised N atom of the N-coordinated 2′-pyridyl ring.

3. Luminescence Spectra

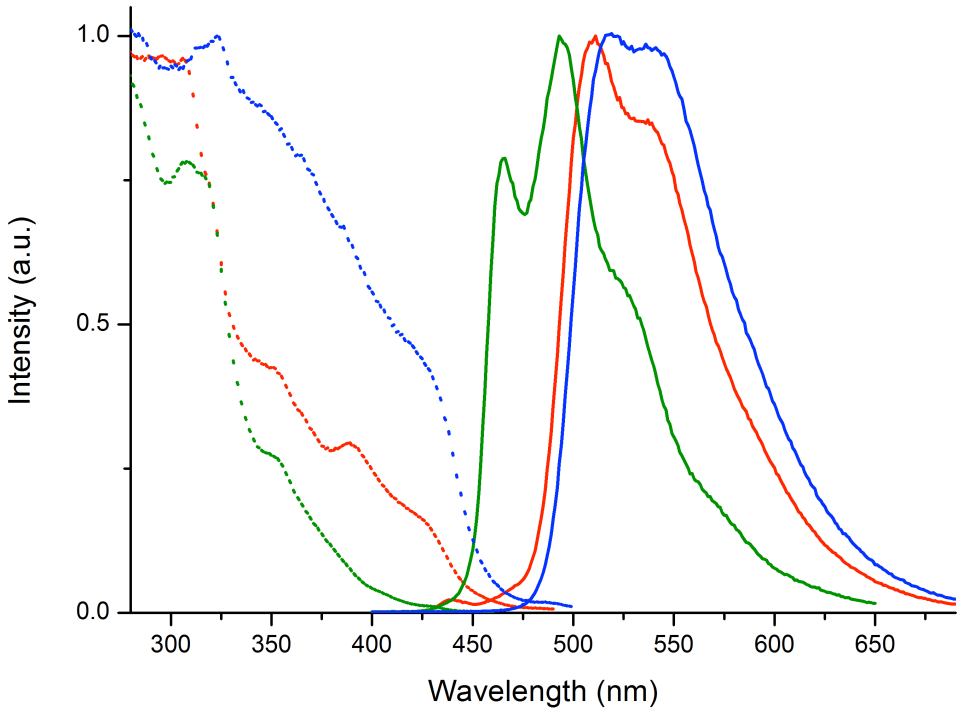


Fig. S1 Emission (full lines; excitation at 350 nm) and excitation (dashed lines) spectra of the 4,4′-$(CF_3)_2$bpy-containing complex salts **2P** (blue), **5P** (green) and **8P** (red) (top) recorded in acetonitrile at 295 K.

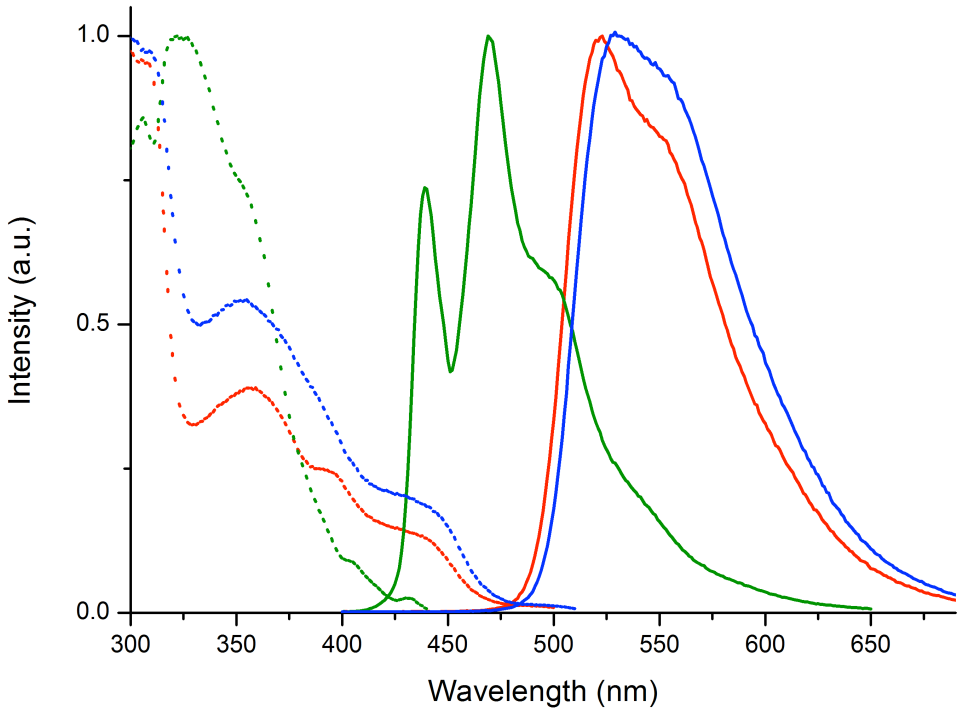
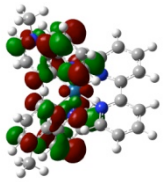
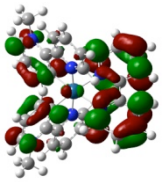
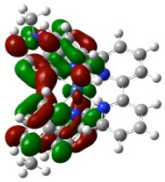


Fig. S2 Emission (full lines; excitation at 350 nm) and excitation (dashed lines) spectra of the 4,4′-(^{t}Bu)$_2$bpy-containing complex salts **3P** (blue), **6P** (green) and **9P** (red) (top) recorded in acetonitrile at 295 K.

4. Theoretical Studies

Table S3 Structural parameters obtained from the X-ray crystallographic studies on **1P–3P** and **7P**, and the geometries in the ground (S_0) and triplet excited (T_1) states optimised by DFT calculations on the complexes **1**–**3** and **7** ($[Ir^{III}(C^N)_2(N^N)]^{3+}$)

Complex:	**1**			**2**			**3**			**7**		
	Distances (Å)											
	X-ray	S_0	T_1	X-ray	S_0	T_1	X-ray	S_0	T_1	X-ray	S_0	T_1
Ir–C	2.002(4)	2.015	2.021	2.017(5)	2.016	1.965	1.993(3)	2.016	2.023	2.010(6)	2.026	1.963
Ir–C	2.003(4)	2.015	1.964	2.005(5)	2.016	2.020	2.002(3)	2.016	1.963	2.014(6)	2.026	2.030
Ir–N_{C^N}	2.043(3)	2.069	2.076	2.047(4)	2.070	2.063	2.041(3)	2.066	2.073	2.050(5)	2.077	2.066
Ir–N_{C^N}	2.044(3)	2.069	2.060	2.047(4)	2.070	2.075	2.042(3)	2.066	2.061	2.052(5)	2.077	2.090
Ir–N_{N^N}	2.128(3)	2.185	2.200	2.135(4)	2.180	2.204	2.113(3)	2.166	2.188	2.123(5)	2.166	2.172
Ir–N_{N^N}	2.133(3)	2.185	2.174	2.138(4)	2.180	2.181	2.129(3)	2.166	2.164	2.141(5)	2.166	2.202
	Angles (˚)											
C–Ir–C	87.3(2)	87.90	89.48	86.5(2)	87.87	89.13	88.5(1)	88.19	89.55	86.7(2)	87.84	91.08
C–Ir–N_{N^N}	97.3(2)	98.17	96.94	97.2(2)	98.25	98.23	100.0(1)	98.07	96.77	96.4(2)	98.14	96.53
C–Ir–N_{N^N}	172.1(1)	173.53	172.06	173.7(2)	173.46	178.19	175.7(1)	173.23	171.88	172.8(2)	173.37	171.56
C–Ir–N_{N^N}	99.0(1)	98.17	98.35	176.3(2)	173.46	172.55	170.6(1)	173.23	173.44	176.3(2)	173.37	172.27
C–Ir–N_{N^N}	175.3(1)	173.53	173.28	99.7(2)	98.25	97.33	95.3(1)	98.07	98.49	100.0(2)	98.14	97.25
C–Ir–N_{C^N}	79.9(2)	79.12	79.27	79.8(2)	79.08	81.32	80.0(1)	79.09	79.30	79.5(2)	79.77	81.65
C–Ir–N_{C^N}	97.1(2)	96.06	95.63	95.1(2)	96.11	95.16	96.5(1)	96.34	96.06	95.7(2)	96.69	96.21
C–Ir–N_{C^N}	97.6(1)	96.06	94.90	95.1(2)	96.11	96.02	96.2(1)	96.34	96.09	96.1(2)	96.69	96.12
C–Ir–N_{C^N}	79.3(1)	79.12	81.36	79.6(2)	79.08	79.21	79.6(1)	79.09	81.44	80.1(2)	81.44	79.93
N_{C^N}–Ir–N_{C^N}	175.8(1)	173.38	175.76	171.4(2)	173.40	174.16	174.7(1)	173.71	174.28	174.1(2)	175.14	175.50
N_{C^N}–Ir–N_{N^N}	94.5(1)	97.91	98.62	98.2(1)	97.86	95.82	97.5(1)	97.55	98.71	96.4(2)	96.63	96.06
N_{C^N}–Ir–N_{N^N}	84.4(1)	87.32	88.24	87.5(2)	87.38	86.23	89.4(1)	87.43	88.39	86.8(2)	87.21	86.33
N_{C^N}–Ir–N_{N^N}	88.8(1)	87.32	86.91	87.7(1)	87.38	88.17	86.2(1)	87.43	86.33	87.87(19)	87.21	86.61
N_{C^N}–Ir–N_{N^N}	99.0(1)	97.91	95.99	100.1(2)	97.86	98.92	95.2(1)	97.55	95.50	98.1(2)	96.63	97.86
N_{N^N}–Ir–N_{N^N}	76.5(1)	75.85	75.29	76.6(1)	75.74	75.35	76.5(1)	75.80	75.45	77.0(2)	76.02	75.18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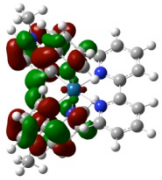	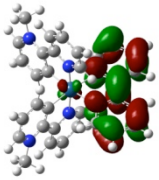	
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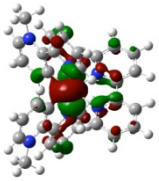	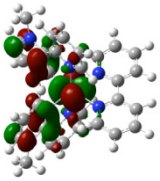	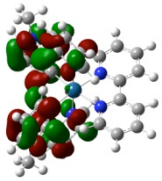
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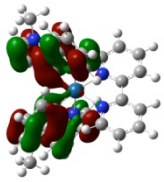	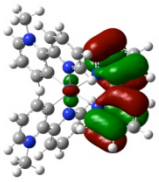	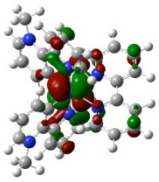
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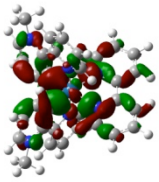
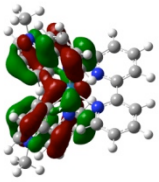
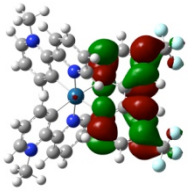
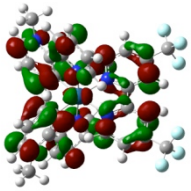
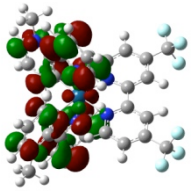
		
HOMO–6	HOMO–5	

Figure S3. M06/Def2-QZVP/SVP-derived contour surface diagrams of the frontier MOs for complex **1**.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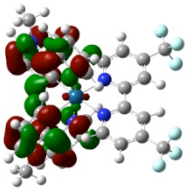	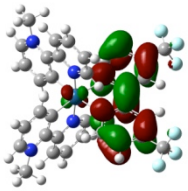	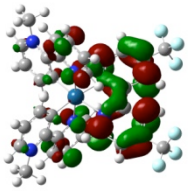
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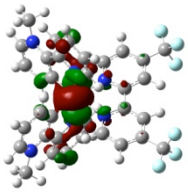	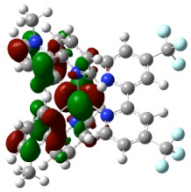	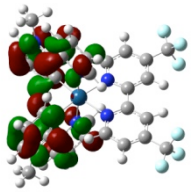
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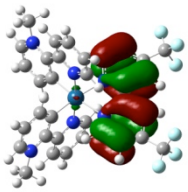	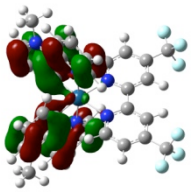	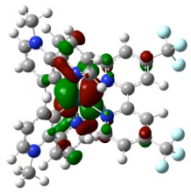
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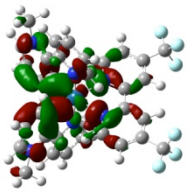
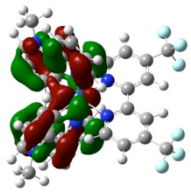
		
HOMO–6	HOMO–5	

Figure S4. M06/Def2-QZVP/SVP-derived contour surface diagrams of the frontier MOs for complex **2**.

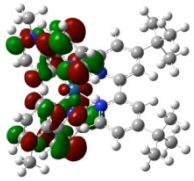
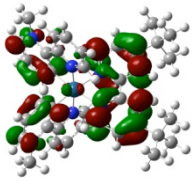
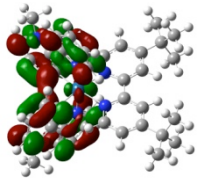
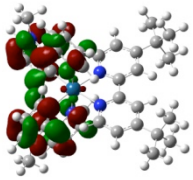
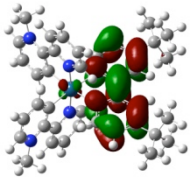
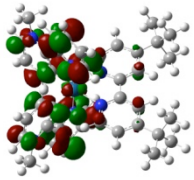
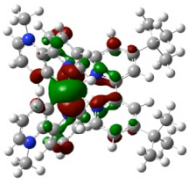
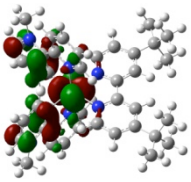
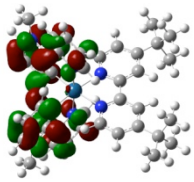
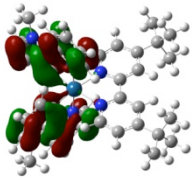
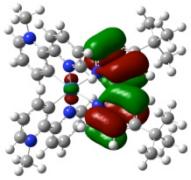
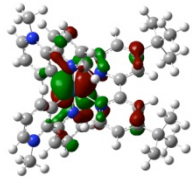
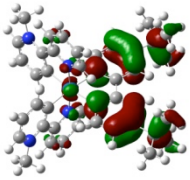
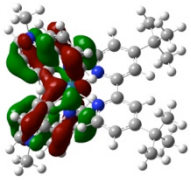
		
LUMO+4	LUMO+5	LUMO+6
		
LUMO+1	LUMO+2	LUMO+3
		
HOMO–1	HOMO	LUMO
		
HOMO–4	HOMO–3	HOMO–2
		
HOMO–6	HOMO–5	

Figure S5. M06/Def2-QZVP/SVP-derived contour surface diagrams of the frontier MOs for complex **3**.

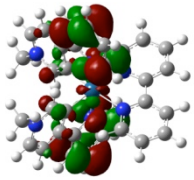
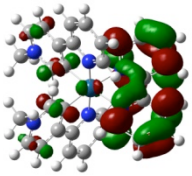
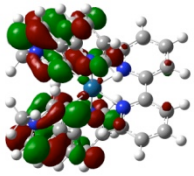
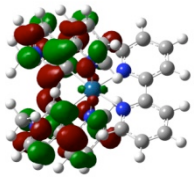
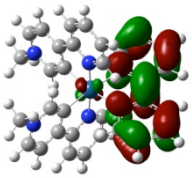
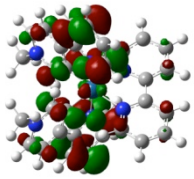
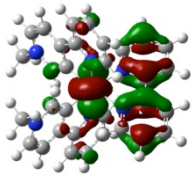
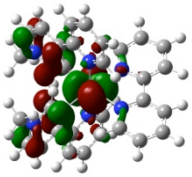
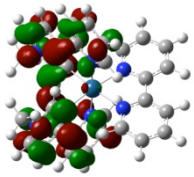
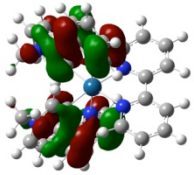
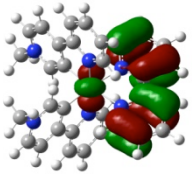
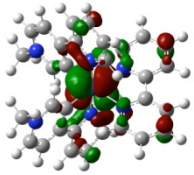
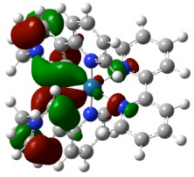
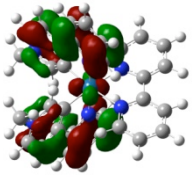
		
LUMO+4	LUMO+5	LUMO+6
		
LUMO+1	LUMO+2	LUMO+3
		
HOMO–1	HOMO	LUMO
		
HOMO–4	HOMO–3	HOMO–2
		
HOMO–6	HOMO–5	

Figure S6. M06/Def2-QZVP/SVP-derived contour surface diagrams of the frontier MOs for complex **7**.

Table S4 Contributions (%) in terms of metal and ligands to the frontier MOs computed by M06/Def2-QZVP/SVP for complexes **1**–**3** and **7**

	1			**2**			**3**			**7**		
MO	Ir	C^N	N^N	Ir	C^N	N^N	Ir	C^N	N^N	Ir	C^N	N^N
LUMO+10	48	47	5	21	54	25	1	99	0	1	98	1
LUMO+9	3	93	4	3	45	51	3	94	2	2	97	1
LUMO+8	1	1	99	2	94	4	1	1	98	5	94	1
LUMO+7	2	72	26	3	96	0	2	69	29	2	96	1
LUMO+6	4	96	0	7	92	2	4	96	1	1	1	98
LUMO+5	4	35	61	5	64	31	4	38	59	4	22	74
LUMO+4	6	93	1	1	2	98	6	93	1	4	96	0
LUMO+3	4	84	12	3	34	64	4	85	11	4	73	23
LUMO+2	3	1	97	3	2	95	3	1	97	3	0	97
LUMO+1	2	98	0	2	98	1	2	98	0	2	97	0
LUMO	2	97	1	2	96	2	2	98	1	3	97	1
HOMO	49	48	2	47	51	2	50	47	2	55	43	3
HOMO–1	69	21	10	72	22	6	67	21	12	70	20	11
HOMO–2	71	18	11	71	19	9	68	16	16	72	17	11
HOMO–3	3	1	95	2	97	1	3	1	96	3	1	95
HOMO–4	1	98	1	1	1	98	1	98	1	1	98	1
HOMO–5	17	82	1	18	81	1	17	81	2	4	96	0
HOMO–6	8	54	38	8	66	26	3	10	87	2	94	4
HOMO–7	2	33	66	2	79	19	5	35	60	7	49	44
HOMO–8	0	77	23	6	57	37	8	30	62	2	41	58
HOMO–9	1	11	87	2	88	10	1	50	49	2	11	87
HOMO–10	10	38	52	2	32	66	9	32	59	17	54	29

Table S5 Selected TD-DFT-calculated data for the complexes **1**–**3** and **7**[a]

Complex	ΔE (eV)	λ (nm)	f_{os}	major contributions
1	2.95	421	0.066	H → L (93%)
	3.08	403	0.014	H → L+1 (93%)
	3.26	380	0.063	H–1 → L (90%)
	3.43	361	0.051	H–2 → L+1 (94%)
	3.90	318	0.192	H–4 → L (26%), H–2 → L+2 (69%)
	3.91	317	0.037	H–4 → L+1 (27%), H → L+3 (62%)
	4.08	304	0.237	H–4 → L+1 (63%), H → L+3 (29%)
	4.22	294	0.022	H → L+4 (82%)
	4.22	294	0.321	H–3 → L+2 (73%), H–1 → L+3 (18%)
	4.29	289	0.076	H–3 → L+2 (14%), H–1 → L+3 (66%)
	4.43	280	0.046	H–5 → L (59%), H → L+5 (21%)
	4.44	279	0.041	H–5 → L (21%), H → L+5 (64%)
	4.53	274	0.157	H–2 → L+4 (62%), H–2 → L+6 (10%), H–2 → L+10 (11%)
	4.54	273	0.057	H–5 → L+1 (68%)
	4.66	266	0.023	H–6 → L (35%), H–1 → L+4 (–21%), H → L+6 (17%)
	4.66	266	0.046	H–6 → L (42%), H → L+6 (20%)
	4.66	266	0.066	H → L+7 (83%)
	4.75	261	0.119	H–6 → L+1 (11%), H–1 → L+5 (66%)
	4.77	260	0.046	H–10 → L (12%), H–6 → L+1 (56%), H–1 → L+5 (11%)
	4.84	256	0.092	H–1 → L+6 (71%)
	4.86	255	0.104	H–2 → L+4 (13%), H–2 → L+6 (67%)
	4.90	253	0.020	H–4 → L+3 (63%)
	4.94	251	0.036	H–3 → L+3 (46%), H–1 → L+7 (27%)
	4.98	249	0.016	H–3 → L+3 (36%), H–1 → L+7 (44%)
	4.98	249	0.018	H–6 → L+2 (17%), H–1 → L+8 (61%)
	5.06	245	0.013	H–10 → L (11%), H–7 → L (25%), H–4 → L+4 (15%), H–2 → L+10 (11%)
	5.08	244	0.143	H–2 → L+8 (86%)
	5.12	242	0.055	H–6 → L+2 (21%), H–2 → L+7 (25%), H–1 → L+8 (11%)
	5.21	238	0.026	H–8 → L (65%)
	5.21	238	0.025	H–7 → L+2 (10%), H–3 → L+5 (63%)
	5.23	237	0.011	H–3 → L+4 (89%)
	5.32	233	0.017	H–11 → L (15%), H–10 → L+1 (15%), H–4 → L+5 (30%), H–4 → L+7 (11%)
	5.39	230	0.030	H–8 → L+1 (46%), H–4 → L+6 (15%)
	5.44	228	0.023	H–10 → L (23%), H–7 → L (32%), H–4 → L+6 (17%)
	5.54	224	0.064	H–12 → L (27%), H–9 → L+1 (12%), H–5 → L+3 (41%)
	5.54	224	0.016	H–9 → L+1 (47%), H–8 → L+1 (18%), H–5 → L+3 (18%)
	5.61	221	0.183	H–12 → L (39%), H–9 → L+1 (27%), H–4 → L+6 (15%)
	5.64	220	0.018	H–12 → L+1 (15%), H → L+9 (43%)
	5.64	220	0.015	H–1 → L+13 (74%)
	5.69	218	0.106	H–12 → L+1 (10%), H–9 → L+2 (28%), H–6 → L+3 (16%), H–5 → L+4 (12%)
	5.71	217	0.160	H–11 → L+1 (66%), H–4 → L+6 (15%)

	5.71	217	0.041	H–16 → L (42%), H–9 → L+2 (18%)
	5.77	215	0.117	H–16 → L+1 (11%), H–14 → L (17%), H → L+11 (52%)
	5.82	213	0.024	H–16 → L+1 (23%), H–14 → L (19%), H–6 → L+4 (10%), H → L+11 (22%)
	5.82	213	0.150	H–12 → L+1 (14%), H–9 → L+2 (10%), H–8 → L+2 (39%), H–4 → L+7 (10%)
	5.85	212	0.018	H–12 → L+1 (11%), H–8 → L+2 (38%)
	5.85	212	0.013	H–16 → L+1 (26%), H–13 → L+1 (44%)
	5.88	211	0.052	H–15 → L (30%), H–14 → L+1 (13%), H–5 → L+6 (14%), H–1 → L+9 (16%)
	5.90	210	0.018	H–10 → L+3 (11%), H–6 → L+4 (31%), H–6 → L+6 (11%)
	5.93	209	0.013	H–5 → L+5 (39%), H–2 → L+9 (24%)
	5.99	207	0.032	H–5 → L+5 (20%), H–2 → L+9 (63%)
	5.99	207	0.015	H–11 → L+2 (16%), H–6 → L+5 (40%)
	6.02	206	0.049	H–11 → L+2 (42%), H–6 → L+5 (20%)
	6.05	205	0.018	H–17 → L (21%), H–15 → L+1 (12%), H–5 → L+5 (17%), H–5 → L+7 (13%), H–1 → L+11 (10%)
	6.08	204	0.013	H → L+12 (59%)
	6.08	204	0.020	H–15 → L (15%), H–5 → L+6 (30%), H–2 → L+11 (12%), H → L+12 (27%)
	6.08	204	0.014	H–15 → L+1 (15%), H–1 → L+11 (68%)
2	3.01	412	0.075	H → L (92%)
	3.14	395	0.014	H → L+1 (93%)
	3.33	372	0.065	H–1 → L (92%)
	3.41	364	0.014	H–2 → L (91%)
	3.53	351	0.038	H–2 → L+1 (80%), H–1 → L+2 (17%)
	3.69	336	0.093	H–2 → L+2 (90%)
	3.90	318	0.090	H–3 → L (93%)
	3.92	316	0.031	H–3 → L+1 (23%), H → L+3 (53%), H → L+5 (16%)
	4.07	305	0.185	H–3 → L+1 (60%), H → L+3 (31%)
	4.17	297	0.308	H–4 → L+2 (61%), H–1 → L+3 (15%)
	4.22	294	0.024	H → L+3 (14%), H → L+5 (66%)
	4.28	290	0.016	H → L+6 (74%)
	4.28	290	0.025	H → L+4 (80%)
	4.32	287	0.076	H–4 → L+2 (13%), H–1 → L+3 (56%), H–1 → L+5 (19%)
	4.44	279	0.085	H–5 → L (83%)
	4.53	274	0.077	H–1 → L+3 (20%), H–1 → L+5 (57%)
	4.58	271	0.136	H–5 → L+1 (11%), H–2 → L+5 (35%), H–1 → L+4 (14%), H → L+7 (18%)
	4.59	270	0.116	H–2 → L+6 (52%)
	4.61	269	0.033	H–2 → L+5 (22%), H–1 → L+4 (51%)
	4.64	267	0.072	H → L+8 (78%)
	4.70	264	0.101	H–5 → L+2 (62%), H–2 → L+4 (25%)
	4.71	263	0.154	H–5 → L+2 (33%), H–2 → L+4 (54%)
	4.88	254	0.044	H–3 → L+3 (50%), H–1 → L+7 (10%)
	4.92	252	0.022	H–6 → L+2 (15%), H–1 → L+7 (62%)
	4.94	251	0.070	H–2 → L+6 (13%), H–2 → L+7 (58%), H–1 → L+8 (10%)
	4.96	250	0.073	H–1 → L+8 (57%)

	5.00	248	0.084	H–4 → L+3 (71%)
	5.04	246	0.015	H–3 → L+6 (17%), H–2 → L+10 (22%), H–2 → L+11 (23%)
	5.06	245	0.016	H–3 → L+3 (10%), H–2 → L+8 (40%), H–1 → L+11 (10%)
	5.08	244	0.031	H–4 → L+4 (11%), H–2 → L+8 (10%), H–1 → L+11 (11%), H → L+11 (10%)
	5.10	243	0.020	H–3 → L+6 (37%), H–2 → L+7 (21%)
	5.12	242	0.014	H–4 → L+4 (45%), H–3 → L+5 (24%)
	5.23	237	0.034	H–7 → L (64%), H–3 → L+5 (16%)
	5.25	236	0.013	H → L+13 (67%)
	5.41	229	0.013	H–12 → L (12%), H–11 → L+1 (10%), H–9 → L+1 (20%), H–3 → L+8 (27%)
	5.41	229	0.029	H–7 → L+1 (49%), H–3 → L+7 (20%)
	5.49	226	0.036	H–9 → L (10%), H–5 → L+3 (66%)
	5.54	224	0.021	H–7 → L+2 (48%), H–4 → L+6 (36%)
	5.58	222	0.226	H–11 → L (12%), H–9 → L (38%), H–3 → L+7 (15%)
	5.61	221	0.050	H–12 → L (14%), H–10 → L (38%), H–10 → L+2 (13%)
	5.61	221	0.030	H–11 → L (11%), H–3 → L+7 (12%), H–1 → L+13 (53%)
	5.64	220	0.045	H–11 → L (40%), H–8 → L (12%), H–1 → L+13 (22%)
	5.64	220	0.015	H–10 → L (19%), H–10 → L+2 (14%), H–2 → L+13 (10%), H → L+9 (24%)
	5.64	220	0.043	H–10 → L+2 (24%), H → L+9 (27%)
	5.66	219	0.043	H–5 → L+5 (74%)
	5.77	215	0.145	H–12 → L+1 (29%), H–10 → L+1 (41%), H–3 → L+7 (11%)
	5.79	214	0.026	H–12 → L+1 (45%), H–10 → L+1 (26%)
	5.82	213	0.101	H–11 → L+1 (16%), H–8 → L+1 (11%), H–6 → L+3 (10%), H–5 → L+6 (10%)
	5.82	213	0.044	H–16 → L+1 (20%), H → L+12 (42%)
	5.85	212	0.010	H–13 → L (48%), H → L+10 (13%), H → L+11 (12%)
	5.88	211	0.121	H–16 → L+1 (13%), H → L+12 (11%)
	5.88	211	0.098	H–16 → L+1 (18%), H → L+12 (17%)
	5.90	210	0.012	H–11 → L+2 (25%), H–9 → L+2 (28%), H–4 → L+8 (40%)
	5.93	209	0.013	H–6 → L+4 (47%)
	5.93	209	0.020	H–6 → L+5 (62%)
	6.02	206	0.013	H–14 → L (38%), H–6 → L+6 (16%), H–2 → L+9 (10%)
	6.08	204	0.014	H–17 → L (24%), H–13 → L+1 (20%), H–5 → L+8 (13%), H–2 → L+9 (11%), H–1 → L+12 (10%)
	6.17	201	0.022	H–15 → L+2 (54%), H–10 → L+3 (12%)
3	2.92	424	0.060	H → L (93%)
	3.05	406	0.013	H → L+1 (93%)
	3.22	385	0.060	H–1 → L (90%)
	3.25	381	0.008	H–2 → L (92%)
	3.37	368	0.053	H–2 → L+1 (93%)
	3.87	320	0.051	H–4 → L (91%)
	3.90	318	0.025	H–4 → L+1 (21%), H–1 → L+2 (15%), H → L+3

			(55%)
3.99	311	0.181	H–2 → L+2 (88%)
4.03	308	0.022	H–3 → L+1 (94%)
4.07	305	0.245	H–4 → L+1 (66%), H → L+3 (27%)
4.20	295	0.019	H → L+4 (81%)
4.23	293	0.160	H–3 → L+2 (26%), H–1 → L+3 (64%)
4.29	289	0.234	H–3 → L+2 (59%), H–1 → L+3 (20%)
4.41	281	0.027	H–5 → L (55%), H–2 → L+4 (10%), H → L+5 (21%)
4.44	279	0.031	H–5 → L (17%), H → L+5 (62%)
4.49	276	0.177	H–5 → L (15%), H–2 → L+4 (54%), H–2 → L+6 (11%)
4.54	273	0.060	H–5 → L+1 (65%)
4.64	267	0.081	H–1 → L+4 (28%), H → L+6 (36%)
4.66	266	0.061	H → L+7 (80%)
4.71	263	0.011	H–10 → L (12%), H–8 → L+1 (14%), H–7 → L+1 (46%)
4.73	262	0.194	H–1 → L+5 (65%)
4.79	259	0.105	H–2 → L+4 (12%), H–2 → L+6 (61%)
4.81	258	0.112	H–1 → L+6 (69%)
4.88	254	0.028	H–8 → L (10%), H–6 → L+1 (12%), H–4 → L+3 (41%)
4.88	254	0.037	H–6 → L (21%), H–3 → L+3 (49%)
4.94	251	0.029	H–3 → L+3 (15%), H–1 → L+7 (66%)
5.00	248	0.012	H–2 → L+6 (10%), H–2 → L+11 (63%)
5.02	247	0.021	H–6 → L+1 (12%), H–1 → L+8 (56%)
5.04	246	0.013	H–2 → L+7 (58%)
5.06	245	0.184	H–2 → L+8 (80%)
5.08	244	0.012	H–10 → L (44%), H–7 → L+1 (13%), H–6 → L (12%)
5.10	243	0.021	H–8 → L (53%), H–6 → L+1 (26%)
5.12	242	0.033	H–6 → L+2 (15%), H–3 → L+5 (42%)
5.14	241	0.018	H–7 → L+2 (29%), H–3 → L+4 (48%)
5.17	240	0.034	H–7 → L+2 (27%), H–3 → L+4 (46%)
5.21	238	0.034	H–10 → L+1 (56%), H–6 → L+1 (11%)
5.37	231	0.017	H–11 → L (66%)
5.39	230	0.024	H–9 → L+1 (55%)
5.51	225	0.012	H–11 → L+1 (67%), H–9 → L+1 (13%)
5.54	224	0.039	H–14 → L (15%), H–11 → L+1 (14%), H–5 → L+3 (49%)
5.58	222	0.077	H–10 → L+2 (26%), H–6 → L+2 (25%), H–3 → L+7 (30%)
5.61	221	0.220	H–14 → L (39%), H–4 → L+6 (24%)
5.66	219	0.012	H–22 → L (34%), H–13 → L (16%), H–7 → L+3 (12%)
5.69	218	0.010	H–7 → L+3 (23%), H–2 → L+13 (31%)
5.69	218	0.347	H–8 → L+2 (17%), H–3 → L+8 (11%), H–2 → L+13 (17%)
5.71	217	0.107	H–8 → L+2 (23%), H–2 → L+13 (21%)
5.71	217	0.018	H–12 → L (54%)
5.74	216	0.015	H–17 → L (17%), H–15 → L (18%), H–14 → L+1 (16%)
5.74	216	0.133	H–16 → L (16%), H–12 → L (17%), H → L+10 (23%)
5.74	216	0.043	H–11 → L+2 (28%), H–9 → L+2 (10%)
5.77	215	0.012	H–22 → L (17%), H–13 → L (16%), H–7 → L+3

				(13%)
	5.77	215	0.016	H–16 → L (14%), H → L+10 (47%)
	5.79	214	0.020	H–22 → L+1 (37%), H–12 → L (15%)
	5.82	213	0.024	H–17 → L+1 (20%), H–15 → L+1 (54%)
	5.85	212	0.095	H–14 → L+1 (15%), H–4 → L+7 (26%)
	5.85	212	0.010	H–13 → L+1 (10%), H–7 → L+4 (17%)
	5.88	211	0.054	H–6 → L+3 (29%), H–5 → L+5 (10%)
	5.90	210	0.112	H–6 → L+3 (33%), H–5 → L+5 (11%), H–2 → L+9 (21%)
	5.93	209	0.018	H–22 → L+1 (12%), H–13 → L+1 (38%), H–6 → L+3 (11%)
	5.93	209	0.012	H–13 → L+1 (12%), H–2 → L+9 (49%)
	5.99	207	0.063	H–5 → L+5 (41%)
7	2.98	416	0.053	H → L (95%)
	3.27	379	0.051	H–1 → L (92%)
	3.42	363	0.047	H–2 → L+1 (95%)
	3.43	362	0.012	H–1 → L+1 (83%)
	3.87	320	0.086	H–2 → L+2 (95%)
	4.07	305	0.084	H–4 → L (86%)
	4.08	304	0.089	H–5 → L (12%), H–4 → L+1 (29%), H → L+3 (47%)
	4.22	294	0.185	H–4 → L+1 (24%), H–3 → L+2 (45%), H → L+3 (20%)
	4.25	292	0.373	H–4 → L+1 (20%), H–3 → L+2 (42%), H → L+3 (24%)
	4.34	286	0.065	H–5 → L (70%), H–4 → L+1 (17%)
	4.35	285	0.059	H–6 → L (29%), H–5 → L+1 (34%), H → L+4 (18%)
	4.43	280	0.033	H–5 → L+1 (12%), H–2 → L+3 (11%), H → L+4 (70%)
	4.46	278	0.134	H–1 → L+3 (80%)
	4.49	276	0.024	H–2 → L+3 (66%)
	4.58	271	0.023	H–6 → L+1 (29%), H → L+5 (51%)
	4.71	263	0.136	H–2 → L+4 (51%), H–2 → L+11 (30%)
	4.79	259	0.053	H–2 → L+4 (20%), H–2 → L+11 (36%), H → L+7 (15%)
	4.82	257	0.054	H–10 → L (15%), H–7 → L+1 (32%), H → L+7 (19%)
	4.86	255	0.184	H–7 → L+1 (18%), H–1 → L+5 (38%), H → L+7 (14%)
	4.88	254	0.051	H–5 → L+2 (62%), H → L+7 (12%)
	4.88	254	0.038	H–5 → L+2 (33%), H–2 → L+4 (11%), H–1 → L+5 (23%), H → L+7 (12%)
	4.90	253	0.134	H–2 → L+5 (23%), H–1 → L+11 (34%), H → L+8 (21%)
	4.92	252	0.044	H–2 → L+5 (33%), H–1 → L+6 (10%), H → L+11 (28%)
	4.98	249	0.036	H–7 → L+2 (14%), H–6 → L+2 (13%), H–2 → L+5 (11%), H–1 → L+6 (49%)
	5.02	247	0.058	H–3 → L+3 (42%), H–2 → L+6 (35%)
	5.02	247	0.075	H–7 → L+2 (25%), H–6 → L+2 (30%), H–1 → L+6 (27%)
	5.06	245	0.025	H–8 → L (27%), H–7 → L+1 (13%), H–3 → L+3 (11%), H–1 → L+7 (10%)
	5.06	245	0.105	H–8 → L (12%), H–3 → L+3 (23%), H–2 → L+6

			(41%)
5.10	243	0.048	H–1 → L+7 (57%)
5.17	240	0.029	H–2 → L+7 (58%), H–1 → L+8 (11%)
5.21	238	0.039	H–10 → L+1 (16%), H–8 → L+1 (15%), H–1 → L+8 (23%), H → L+8 (10%)
5.23	237	0.021	H–2 → L+8 (35%), H → L+13 (16%)
5.30	234	0.023	H–3 → L+5 (33%), H → L+13 (28%)
5.32	233	0.099	H–3 → L+5 (34%), H–2 → L+8 (12%), H → L+13 (20%)
5.32	233	0.075	H–11 → L (42%), H–10 → L (14%)
5.32	233	0.016	H–7 → L+2 (22%), H–6 → L+2 (22%), H–3 → L+6 (29%)
5.39	230	0.031	H → L+8 (13%), H → L+9 (59%)
5.46	227	0.035	H–11 → L (23%), H–10 → L (13%), H–8 → L (33%)
5.54	224	0.017	H → L+10 (83%)
5.61	221	0.012	H–11 → L+1 (34%), H–8 → L+1 (18%), H–1 → L+9 (10%)
5.61	221	0.016	H–16 → L (13%), H–12 → L (51%)
5.64	220	0.020	H–1 → L+7 (10%), H–1 → L+13 (70%)
5.64	220	0.022	H–5 → L+3 (43%), H–4 → L+4 (48%)
5.71	217	0.100	H–9 → L+2 (33%), H–6 → L+3 (11%), H–4 → L+5 (31%)
5.74	216	0.019	H–16 → L+1 (41%), H–2 → L+9 (13%)
5.85	212	0.010	H–4 → L+6 (66%)
5.96	208	0.058	H–12 → L+2 (11%), H–3 → L+8 (71%)
5.96	208	0.146	H–13 → L (19%), H–6 → L+4 (13%), H–4 → L+8 (22%)
5.96	208	0.138	H–12 → L+2 (29%), H–7 → L+3 (10%), H–3 → L+8 (14%)
5.99	207	0.016	H–15 → L (36%), H–7 → L+3 (13%)
5.99	207	0.012	H–15 → L (11%), H–12 → L+2 (20%), H–7 → L+3 (22%)
6.02	206	0.020	H–6 → L+4 (57%), H–4 → L+8 (23%)
6.05	205	0.054	H–17 → L (16%), H–15 → L+1 (25%), H–6 → L+8 (14%), H–4 → L+8 (18%)
6.05	205	0.029	H–7 → L+3 (10%), H–5 → L+6 (47%)
6.08	204	0.088	H–5 → L+6 (28%), H–4 → L+7 (30%)
6.11	203	0.032	H–14 → L+1 (77%)
6.20	200	0.034	H–15 → L+1 (19%), H–10 → L+3 (10%), H–8 → L+3 (10%), H–7 → L+4 (13%)

[a] Geometry optimizations and TD-DFT calculations used the M06 functional with the Def2-QZVP/Def2-SVP mixed basis set, and a CPCM acetonitrile solvent model was included for TD-DFT. Only the transitions with $f_{os} \geq 0.01$ are included. H = HOMO, L = LUMO.

Table S6 DFT-optimised coordinates for the complexes **1**–**3** and **7** in the singlet and triplet states

1 S_0 state			
atom	x	y	z
C	1.90241700	1.75418100	1.88225800
C	2.49139300	2.87998700	2.44158700
C	2.07245200	4.13377800	2.00640600
C	1.08217200	4.21209200	1.03365100
C	0.52957700	3.04110200	0.51356100
C	-0.52970000	3.04108800	-0.51347000
C	-1.08235900	4.21207000	-1.03351500
C	-2.07263600	4.13373900	-2.00627100
C	-2.49149200	2.87994000	-2.44151700
C	-1.90244600	1.75414800	-1.88224200
C	-1.77306700	0.71972100	2.34497000
C	-2.81435200	0.55576400	3.24889700
C	-3.76086700	-0.42337100	2.98289300
C	-3.65694700	-1.17205100	1.81248000
C	-2.60914700	-0.94565400	0.91484700
C	-2.31019100	-1.64464200	-0.35380400
C	-1.51503700	-2.96914100	-2.66287700
C	-0.67067400	-2.03556000	-2.08085800
C	-1.05116400	-1.34121600	-0.92246000
C	1.77307500	0.71989300	-2.34491900
C	2.81442100	0.55609500	-3.24880000
C	3.76102800	-0.42294800	-2.98279300
C	3.65710800	-1.17171900	-1.81243800
C	2.60922600	-0.94549800	-0.91485000
C	2.31024900	-1.64460400	0.35374300
C	1.51509300	-2.96914400	2.66281500
C	0.67074300	-2.03553900	2.08082200
C	1.05123500	-1.34118400	0.92243000
H	2.20167600	0.75084400	2.20298300
H	3.26314400	2.77068900	3.20638300
H	2.51079800	5.04527300	2.42093200
H	0.74458400	5.18909800	0.68355300
H	-0.74482700	5.18908300	-0.68338500
H	-2.51103900	5.04522300	-2.42076000
H	-3.26322700	2.77063500	-3.20632700
H	-2.20162700	0.75080500	-2.20302300
H	-0.98390100	1.45466500	2.52900100
H	-2.86145400	1.17516700	4.14690800
H	-4.58233300	-0.61243800	3.67852400
H	-4.40008300	-1.94315300	1.63688700
H	-1.23884400	-3.52528800	-3.56137100
H	0.30250500	-1.84331000	-2.54643200
H	0.98384300	1.45476800	-2.52894900
H	2.86149600	1.17554200	-4.14678300
H	4.58255000	-0.61188700	-3.67839200
H	4.40031700	-1.94274700	-1.63685500
H	1.23890800	-3.52529300	3.56130900
H	-0.30243900	-1.84330500	2.54639500
Ir	-0.00000100	0.10960200	0.00000000
N	0.94713200	1.82531200	0.94352200
N	-0.94717200	1.82529300	-0.94349400
N	-1.66070100	-0.00985700	1.22741100
N	1.66072200	-0.00975400	-1.22740600

C	-2.76098200	-3.17519800	-2.10220000
H	-3.48487300	-3.86298000	-2.54417400
C	2.76099700	-3.17526200	2.10207200
H	3.48484900	-3.86313000	2.54397500
N	-3.15623400	-2.52617100	-0.98580000
N	3.15624700	-2.52623400	0.98567100
C	4.53812200	-2.79573700	0.54881700
H	4.54574200	-3.44471800	-0.33804500
H	5.06314300	-1.85330700	0.34857700
H	5.06563900	-3.31537800	1.35606600
C	-4.53819100	-2.79545500	-0.54906100
H	-4.54600600	-3.44468700	0.33762000
H	-5.06294900	-1.85293900	-0.34854400
H	-5.06581300	-3.31473800	-1.35647300

1 T_1 state

atom	x	y	z
C	1.68776900	2.08523700	1.75335400
C	2.09919200	3.30442700	2.27445600
C	1.46330600	4.46137500	1.83362000
C	0.44402300	4.35429300	0.89344400
C	0.07669300	3.09709900	0.41224400
C	-0.99499900	2.89519700	-0.58329100
C	-1.75479600	3.94005000	-1.11034300
C	-2.73665300	3.66999300	-2.05757000
C	-2.93873300	2.35427000	-2.46393300
C	-2.15405500	1.35916500	-1.89805700
C	-1.78633100	0.55176900	2.38335000
C	-2.80281300	0.27494900	3.29579700
C	-3.62182200	-0.84049500	3.06083700
C	-3.43470300	-1.59296000	1.92177500
C	-2.41643400	-1.24752300	0.98402800
C	-2.10131700	-1.87992200	-0.23478700
C	-1.05855900	-3.36290800	-2.37345400
C	-0.32727200	-2.25519500	-1.91042200
C	-0.82348300	-1.49113700	-0.85569400
C	1.61435600	0.79131100	-2.45837400
C	2.64180900	0.69955600	-3.39023300
C	3.71268000	-0.13240800	-3.09952700
C	3.74683100	-0.80265300	-1.87752500
C	2.70862500	-0.64559600	-0.95594900
C	2.54997200	-1.27914900	0.37205400
C	2.02341200	-2.51291800	2.80955700
C	1.03024500	-1.76819300	2.18876500
C	1.27790000	-1.12892100	0.96726700
H	2.15898400	1.15204000	2.07949600
H	2.90204400	3.34211600	3.01355100
H	1.75709500	5.44183400	2.21732400
H	-0.05916200	5.25575400	0.53956800
H	-1.58650500	4.96886500	-0.78745700
H	-3.33586600	4.48257200	-2.47620300
H	-3.69246200	2.09780000	-3.21123600
H	-2.27324200	0.31242000	-2.19675200
H	-1.09675300	1.38484700	2.55543900
H	-2.92845900	0.90550700	4.17786800
H	-4.39919300	-1.11715000	3.77737100
H	-4.05342200	-2.47278500	1.75632700
H	-0.68465300	-4.01017500	-3.16909900

H	0.62592800	-2.00446100	-2.38620100
H	0.72940600	1.40335900	-2.65740300
H	2.58208800	1.25550000	-4.32818500
H	4.52680900	-0.26709300	-3.81632600
H	4.58674800	-1.46178800	-1.68173000
H	1.85846000	-3.02898400	3.75790600
H	0.04807700	-1.68497800	2.66705200
Ir	-0.00271700	0.08464100	-0.01891600
N	0.70491200	1.97845000	0.84782500
N	-1.20921700	1.61705600	-0.98042900
N	-1.57486800	-0.17585200	1.28727200
N	1.63449000	0.13089100	-1.29537900
C	-2.31947800	-3.60882200	-1.85834000
H	-2.94282200	-4.41480200	-2.25829200
C	3.26975700	-2.57326000	2.21843400
H	4.10161600	-3.10531900	2.68536300
N	-2.88815700	-2.85977700	-0.87730600
N	3.53553300	-1.96703700	1.03877600
C	4.93242500	-2.06393800	0.57453900
H	5.02033300	-2.79298500	-0.24315600
H	5.29891400	-1.07815300	0.26231900
H	5.55372800	-2.40917900	1.40807500
C	-4.31399100	-3.05599700	-0.60315900
H	-4.48329600	-3.75525900	0.23024300
H	-4.79084600	-2.09092300	-0.38392600
H	-4.79452800	-3.47223800	-1.49789100

2 S_0 state

atom	x	y	z
C	0.84286600	2.53006200	-0.86944200
C	1.96862800	3.30494700	-1.12254500
C	3.21755500	2.73299100	-0.91506400
C	3.29923400	1.41765200	-0.46780300
C	2.12973600	0.69925100	-0.23434400
C	2.12963500	-0.69957700	0.23417100
C	3.29902900	-1.41810800	0.46776000
C	3.21715600	-2.73346700	0.91493000
C	1.96814000	-3.30531300	1.12218400
C	0.84249100	-2.53029400	0.86899200
C	-0.18884800	-0.58169000	-2.88206300
C	-0.34727600	-1.12905600	-4.14866600
C	-1.33203800	-2.09058400	-4.32478200
C	-2.09130500	-2.49700400	-3.22959900
C	-1.86753000	-1.94420800	-1.96517100
C	-2.56746900	-2.22698300	-0.69428800
C	-3.87631000	-2.53569100	1.73755000
C	-2.94205100	-1.52225900	1.58312700
C	-2.25885100	-1.34867600	0.37000300
C	-0.18830700	0.58147500	2.88195000
C	-0.34674400	1.12861200	4.14865100
C	-1.33147500	2.09014800	4.32494300
C	-2.09062400	2.49688600	3.22979800
C	-1.86676300	1.94436800	1.96526500
C	-2.56669400	2.22750200	0.69446300
C	-3.87607700	2.53657700	-1.73701200
C	-2.94206100	1.52287400	-1.58283900
C	-2.25859500	1.34909900	-0.36989700
H	-0.15994100	2.94016400	-1.02808600

H	1.87299700	4.33432700	-1.47596000
H	4.28277800	0.96899900	-0.30541800
H	4.28263200	-0.96952400	0.30553900
H	1.87236200	-4.33471100	1.47550900
H	-0.16037800	-2.94030300	1.02748200
H	0.54978100	0.20486400	-2.70270500
H	0.28105700	-0.78944000	-4.97465600
H	-1.51648200	-2.53065600	-5.30826600
H	-2.86671000	-3.23802700	-3.39621700
H	-4.42362500	-2.68658200	2.67053100
H	-2.73863400	-0.85827700	2.43051100
H	0.55024500	-0.20512700	2.70247400
H	0.28153600	0.78879200	4.97459800
H	-1.51596400	2.52996400	5.30853300
H	-2.86602900	3.23790400	3.39646500
H	-4.42365100	2.68757000	-2.66982400
H	-2.73905900	0.85883300	-2.43027500
Ir	-0.80694800	0.00002300	-0.00007400
N	0.91416400	1.26455200	-0.43823100
N	0.91398000	-1.26475600	0.43788400
N	-0.92656900	-0.95941800	-1.83016100
N	-0.92595600	0.95947000	1.83009500
C	-4.09257800	-3.40207700	0.68309100
H	-4.78231700	-4.24489000	0.76227600
C	-4.09165700	3.40315900	-0.68257700
H	-4.78101600	4.24629600	-0.76164100
N	-3.44994000	-3.26362300	-0.49656400
N	-3.44869800	3.26455600	0.49689500
C	-3.72489000	4.31143700	1.49814300
H	-4.37934900	3.92630600	2.29263300
H	-2.78530300	4.69441000	1.91581000
H	-4.24171100	5.14077500	1.00297300
C	-3.72705800	-4.31010700	-1.49795300
H	-4.38091900	-3.92417800	-2.29254100
H	-2.78778200	-4.69405100	-1.91544400
H	-4.24488300	-5.13893400	-1.00298600
C	4.50690000	-3.49546700	1.16837100
C	4.50742400	3.49480700	-1.16841900
F	5.17930400	-2.89731900	2.13755400
F	4.25919700	-4.74312500	1.51204000
F	5.24371000	-3.47980300	0.07044900
F	5.24425800	3.47886000	-0.07051300
F	5.17970400	2.89666900	-2.13769200
F	4.25993300	4.74255500	-1.51191100

2 T_1 state

atom	x	y	z
C	-0.92329400	-2.44809900	-0.96331500
C	-2.07912700	-3.17653000	-1.21525500
C	-3.30416600	-2.56061200	-0.99157800
C	-3.33342700	-1.24549400	-0.53671200
C	-2.13699000	-0.57195700	-0.30718500
C	-2.08207600	0.82621700	0.16171900
C	-3.22274000	1.59027200	0.39321400
C	-3.08945200	2.90533600	0.83015400
C	-1.81911900	3.43321300	1.02374600
C	-0.72476300	2.61309100	0.77560800
C	0.44692100	0.58074400	-2.93369600

C	0.71009100	1.13242600	-4.18184000
C	1.73428300	2.06256600	-4.27917000
C	2.43257600	2.43478600	-3.13111300
C	2.10722100	1.87685200	-1.89179600
C	2.73590400	2.11779700	-0.57347200
C	3.91061500	2.32776000	1.94098600
C	2.93473800	1.36618900	1.71803100
C	2.32502600	1.24878100	0.46230900
C	0.02638100	-0.55493400	2.86103600
C	0.07278700	-1.16698800	4.11276100
C	0.95160600	-2.24575800	4.29473900
C	1.70215900	-2.69641400	3.23062700
C	1.59135900	-2.07524800	1.95082400
C	2.26011300	-2.41279100	0.75910500
C	3.95295600	-2.62475000	-1.46200300
C	3.03928900	-1.55673400	-1.42108300
C	2.17737500	-1.42764400	-0.33462300
H	0.06260900	-2.89332300	-1.13485500
H	-2.02211300	-4.20490500	-1.57916500
H	-4.29932600	-0.76326000	-0.36535600
H	-4.22316000	1.17806200	0.23735100
H	-1.68392300	4.46244700	1.36504900
H	0.29286700	2.98827600	0.92658500
H	-0.32768000	-0.18172800	-2.81000700
H	0.13040200	0.81952100	-5.05284500
H	1.99955700	2.50484500	-5.24300400
H	3.24013800	3.15170000	-3.23919800
H	4.41109200	2.43780800	2.90557400
H	2.64754400	0.69797100	2.53713600
H	-0.61481400	0.31737800	2.69575900
H	-0.54888200	-0.78854500	4.92647000
H	1.04880800	-2.72175300	5.27385900
H	2.40557200	-3.51341700	3.38085300
H	4.67740000	-2.73440000	-2.27138900
H	3.01608400	-0.83871900	-2.24646300
Ir	0.83515600	-0.02915200	-0.01456800
N	-0.94558300	-1.18409800	-0.51847500
N	-0.84617500	1.34612500	0.36087400
N	1.12407900	0.92676700	-1.83326400
N	0.75530200	-0.96395300	1.82329300
C	4.23412100	3.19058700	0.91229500
H	4.96394600	3.99250800	1.04405100
C	3.89197900	-3.61114900	-0.49089400
H	4.53319600	-4.49658000	-0.54901500
N	3.65851800	3.10192900	-0.30790400
N	3.02112300	-3.58421800	0.55020900
C	2.86118400	-4.80582600	1.34408900
H	3.49139800	-4.80112900	2.24675000
H	1.80713200	-4.93877900	1.62340500
H	3.15465300	-5.66820400	0.73163900
C	4.05819000	4.13864700	-1.27821600
H	4.73326400	3.71921300	-2.03742500
H	3.16973100	4.58299600	-1.74403200
H	4.59511700	4.92958600	-0.74335700
C	-4.34880200	3.71720000	1.08501700
C	-4.62488900	-3.27180200	-1.23785400
F	-5.05309500	3.13179600	2.03921400
F	-4.05164700	4.94705600	1.45104100
F	-5.07476900	3.74945900	-0.01905000

F	-5.35588100	-3.21964100	-0.13704300
F	-5.27437500	-2.65093400	-2.20754000
F	-4.42875000	-4.52986600	-1.57534000

3 S_0 state

atom	x	y	z
C	0.81968400	2.53400600	-0.83830300
C	1.94523200	3.30373000	-1.08977300
C	3.22218600	2.75863800	-0.90622700
C	3.26261900	1.42579600	-0.46914200
C	2.10040800	0.70237300	-0.22942000
C	2.10049400	-0.70187200	0.22997100
C	3.26278900	-1.42516600	0.46966500
C	3.22251100	-2.75798900	0.90681100
C	1.94562600	-3.30320100	1.09048100
C	0.81998600	-2.53361500	0.83900300
C	-0.20564800	-0.52001600	-2.88647000
C	-0.35313200	-1.04927100	-4.16196700
C	-1.32369700	-2.02111700	-4.35733300
C	-2.08183200	-2.45484500	-3.27243400
C	-1.87144600	-1.91792600	-1.99865600
C	-2.57499300	-2.22632100	-0.73596000
C	-3.90093200	-2.57621800	1.68052700
C	-2.97215800	-1.55516000	1.54699900
C	-2.27852500	-1.36061700	0.34255400
C	-0.20693900	0.52021300	2.88685000
C	-0.35543000	1.04920000	4.16234500
C	-1.32673700	2.02038500	4.35737400
C	-2.08449200	2.45388100	3.27212000
C	-1.87296000	1.91737400	1.99836100
C	-2.57591000	2.22574100	0.73534900
C	-3.90106100	2.57538800	-1.68156500
C	-2.97206900	1.55455400	-1.54775000
C	-2.27881600	1.36014700	-0.34307000
H	-0.18085500	2.95411800	-0.98932300
H	1.81507500	4.33214400	-1.43171900
H	4.23126800	0.94629500	-0.31390500
H	4.23139200	-0.94558800	0.31436400
H	1.81560800	-4.33159900	1.43252900
H	-0.18050500	-2.95381400	0.99009100
H	0.52251300	0.27200400	-2.68905100
H	0.27324800	-0.68786200	-4.97990500
H	-1.49840700	-2.44821500	-5.34814900
H	-2.84589800	-3.20379600	-3.45413100
H	-4.45527900	-2.74287100	2.60655400
H	-2.77951400	-0.90011200	2.40398800
H	0.52179400	-0.27135300	2.68970400
H	0.27074000	0.68806000	4.98056400
H	-1.50229100	2.44713400	5.34818900
H	-2.84919700	3.20229100	3.45344800
H	-4.45515400	2.74189700	-2.60777100
H	-2.77895100	0.89958200	-2.40469200
Ir	-0.83065000	-0.00001800	0.00003400
N	0.87872400	1.26335400	-0.41859100
N	0.87887900	-1.26298600	0.41919500
N	-0.94352000	-0.92388000	-1.84476900
N	-0.94449500	0.92379900	1.84482000
C	-4.10227100	-3.43055200	0.61360900

H	-4.78570800	-4.27967200	0.67573500
C	-4.10288100	3.42973300	-0.61474500
H	-4.78639800	4.27877200	-0.67713000
N	-3.45146600	-3.27156300	-0.55906500
N	-3.45240200	3.27090100	0.55813400
C	-3.71421400	4.30505700	1.57458900
H	-4.36239800	3.91297300	2.37073100
H	-2.76908800	4.67797900	1.98885600
H	-4.23167500	5.14313500	1.09516000
C	-3.71303200	-4.30557300	-1.57571700
H	-4.36045500	-3.91315200	-2.37230300
H	-2.76777400	-4.67892400	-1.98931400
H	-4.23123500	-5.14341400	-1.09668700
C	4.50668400	-3.52935000	1.15725200
C	4.50626200	3.53013500	-1.15675500
C	5.29754200	-2.81482200	2.26101100
H	5.58635300	-1.78828800	1.98219300
H	4.72589100	-2.77058100	3.20278200
H	6.22786200	-3.36903600	2.46335400
C	5.32598400	-3.55660400	-0.13941400
H	4.77486800	-4.05133300	-0.95615600
H	5.62116000	-2.55071600	-0.47977400
H	6.25452600	-4.12537400	0.02674500
C	4.22949300	-4.96306100	1.59644800
H	3.67149100	-5.00950500	2.54656700
H	3.67689700	-5.53391300	0.83153100
H	5.18269600	-5.48805900	1.76109800
C	5.32574900	3.55737700	0.13979200
H	4.77469400	4.05196500	0.95666100
H	5.62111100	2.55150100	0.48002300
H	6.25419300	4.12628000	-0.02645800
C	5.29703100	2.81577000	-2.26069000
H	5.58603000	1.78926200	-1.98197100
H	4.72522100	2.77149900	-3.20236400
H	6.22724200	3.37011800	-2.46317300
C	4.22887100	4.96385200	-1.59579600
H	3.67081000	5.01032300	-2.54587900
H	3.67624900	5.53455800	-0.83078800
H	5.18200100	5.48898200	-1.76044900

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atom	x	y	z
C	-0.69110600	2.62228600	0.71055100
C	-1.78159200	3.44287600	0.95292500
C	-3.08193900	2.94708700	0.79250300
C	-3.18008000	1.60978600	0.37600500
C	-2.05040100	0.83527400	0.14144000
C	-2.11088700	-0.57038400	-0.31030800
C	-3.30220100	-1.24645700	-0.54189300
C	-3.31828200	-2.57960800	-0.98046800
C	-2.06587300	-3.17578200	-1.17635900
C	-0.90813100	-2.45620000	-0.92847200
C	0.01581000	-0.48355300	2.86207900
C	0.05341900	-1.06222800	4.12855300
C	0.92941700	-2.13621500	4.34482200
C	1.68561900	-2.61833300	3.29780800
C	1.58266300	-2.03122600	2.00426300
C	2.25890000	-2.40453000	0.82367500

C	3.97563600	-2.68420800	-1.36967000
C	3.07053000	-1.60758000	-1.36454500
C	2.19551500	-1.44648300	-0.28978600
C	0.50293900	0.48205100	-2.95627500
C	0.79605500	0.98627700	-4.21795800
C	1.82711100	1.90725600	-4.32911400
C	2.49979000	2.32316200	-3.18122500
C	2.14345800	1.81396400	-1.92971600
C	2.74668200	2.10464400	-0.61043400
C	3.89086000	2.40255200	1.90786000
C	2.93146400	1.42043500	1.70181200
C	2.33591900	1.25995600	0.44440600
H	0.32600100	3.00635300	0.84628300
H	-1.60405900	4.47142700	1.27180500
H	-4.16827100	1.16809600	0.23113400
H	-4.25065400	-0.73029400	-0.38003000
H	-1.98113500	-4.20688300	-1.52448400
H	0.07416900	-2.91519200	-1.08732800
H	-0.62247500	0.38429800	2.66477100
H	-0.57216400	-0.66137200	4.92810700
H	1.02055600	-2.58513500	5.33715100
H	2.38676100	-3.43251100	3.47334500
H	4.70996100	-2.81636600	-2.16657500
H	3.06195000	-0.90876600	-2.20679700
H	-0.27705100	-0.27246000	-2.81766500
H	0.23445500	0.64231100	-5.08886400
H	2.11753600	2.30821000	-5.30360100
H	3.31388800	3.03185500	-3.29662600
H	4.38083600	2.54546800	2.87344000
H	2.64456100	0.76982900	2.53529500
Ir	0.85494500	-0.03852800	-0.01652700
N	-0.80561200	1.34635100	0.31939100
N	-0.91495100	-1.18379400	-0.50366900
N	0.75424000	-0.92283000	1.84272200
N	1.16027400	0.86598200	-1.85708100
C	3.89525800	-3.64503300	-0.37933700
H	4.53227300	-4.53492400	-0.40358500
C	4.20793700	3.24498900	0.86070300
H	4.92012500	4.06462000	0.97826000
N	3.00589800	-3.58666900	0.65089800
N	3.64632900	3.11401500	-0.36243200
C	4.03012300	4.13584200	-1.35346600
H	4.74326600	3.72305100	-2.08100200
H	3.13844400	4.52625700	-1.85933100
H	4.51787100	4.96508700	-0.82941500
C	2.81478800	-4.78940600	1.46322300
H	3.45807500	-4.79612800	2.35716400
H	1.76162400	-4.87540200	1.76343200
H	3.06443300	-5.67165500	0.85920000
C	-4.63295200	-3.29906600	-1.22217300
C	-4.33088100	3.77347600	1.04335000
C	-5.40402800	-2.55055100	-2.31759200
H	-5.65154900	-1.51480800	-2.03317800
H	-4.83863100	-2.52487000	-3.26374800
H	-6.35611100	-3.06876700	-2.51377800
C	-5.44129100	-3.29749900	0.08190700
H	-4.90217600	-3.81391700	0.89321800
H	-5.69653700	-2.28206400	0.42624200
H	-6.39168200	-3.83111500	-0.07720900

C	-4.41485400	-4.74126300	-1.66721500
H	-3.86811000	-4.80636500	-2.62277500
H	-3.87706900	-5.33487400	-0.90903800
H	-5.38887000	-5.22910500	-1.82385400
C	-5.15785600	3.81991400	-0.24819700
H	-4.59366600	4.28420300	-1.07375200
H	-5.49567000	2.82325800	-0.57577600
H	-6.06130200	4.42733600	-0.08069400
C	-5.14149300	3.10206600	2.16011300
H	-5.47505900	2.08596000	1.89334000
H	-4.56512300	3.04356600	3.09822600
H	-6.04667400	3.69594400	2.36385000
C	-3.99299400	5.19917900	1.46544100
H	-3.42365200	5.23282900	2.40933400
H	-3.42799000	5.74149400	0.68898000
H	-4.92343700	5.76200100	1.63491000

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atom	x	y	z
C	1.77262300	-2.14307300	1.59753300
C	2.89552200	-2.81019700	2.06814100
C	4.15114400	-2.33914900	1.69656500
C	4.23451200	-1.22236700	0.87241400
C	3.06663300	-0.59596400	0.43556100
C	3.06664800	0.59582900	-0.43565200
C	4.23454100	1.22219900	-0.87251200
C	4.15119900	2.33898300	-1.69666400
C	2.89558700	2.81006300	-2.06823500
C	1.77267300	2.14297100	-1.59761900
C	0.81332000	1.47487600	2.57709000
C	0.73100800	2.48937500	3.52481600
C	-0.16980200	3.52946900	3.31956500
C	-0.95945300	3.51752200	2.17336400
C	-0.83375400	2.47379200	1.25975300
C	-1.60679300	2.33861000	0.02276500
C	-2.03945800	1.04280700	-1.93413000
C	-1.31713600	1.18476300	-0.75607200
C	0.81314000	-1.47496200	-2.57713600
C	0.73071600	-2.48946200	-3.52485200
C	-0.17016600	-3.52948600	-3.31956300
C	-0.95977000	-3.51747400	-2.17333200
C	-0.83396000	-2.47374500	-1.25973400
C	-1.60693700	-2.33851400	-0.02271400
C	-2.03943700	-1.04268900	1.93420000
C	-1.31717500	-1.18468500	0.75611100
H	0.76745000	-2.48262500	1.86741100
H	2.78293600	-3.68302500	2.71444700
H	5.06042000	-2.83626400	2.04403300
H	5.21419400	-0.84739300	0.57133900
H	5.21421400	0.84719800	-0.57144200
H	5.06048700	2.83607300	-2.04413700
H	2.78302200	3.68289200	-2.71454300
H	0.76750800	2.48254900	-1.86749400
H	1.50929200	0.64020900	2.70316000
H	1.37159300	2.45796700	4.40881300
H	-0.25811800	4.34315600	4.04387700
H	-1.67399500	4.32385000	1.99210000
H	-1.90379700	0.19670300	-2.61738600

H	1.50917600	-0.64035200	-2.70323800
H	1.37127500	-2.45810900	-4.40887100
H	-0.25856900	-4.34317000	-4.04386900
H	-1.67436400	-4.32374700	-1.99202600
H	-1.90369800	-0.19659600	2.61745600
Ir	0.14219000	-0.00000700	-0.00001500
N	1.84911000	-1.06367400	0.80546000
N	1.84913500	1.06357400	-0.80554200
N	0.05412600	1.46249700	1.47282200
N	0.05398300	-1.46251500	-1.47284300
C	-3.23240300	3.04354900	-1.59415300
H	-3.98705600	3.73364600	-1.97871100
C	-3.23251000	-3.04336500	1.59427900
H	-3.98718000	-3.73342300	1.97887200
C	-2.56268900	3.26130400	-0.40359700
H	-2.80429900	4.16182900	0.16666500
C	-2.56286600	-3.26115200	0.40368900
H	-2.80455500	-4.16166100	-0.16656700
C	-3.69123500	1.71807800	-3.59551900
H	-4.35247000	0.84705000	-3.48528300
H	-4.29420800	2.59857400	-3.84522200
H	-2.97027200	1.53523000	-4.40346400
C	-3.69108800	-1.71790800	3.59572200
H	-4.35186400	-0.84650000	3.48576400
H	-4.29451300	-2.59816200	3.84518100
H	-2.97000200	-1.53567400	4.40370000
N	-2.96654500	-1.95161900	2.33548300
N	-2.96653600	1.95178600	-2.33536800

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atom	x	y	z
C	-1.66029500	-2.33875600	-1.46196100
C	-2.74821100	-3.10241500	-1.86282100
C	-4.02365000	-2.68292200	-1.49613800
C	-4.16153500	-1.51760600	-0.74972900
C	-3.02638000	-0.79335400	-0.38411100
C	-3.08321600	0.45539600	0.39958200
C	-4.27923000	1.06596300	0.77650800
C	-4.24946700	2.24736200	1.51026400
C	-3.01779800	2.79560600	1.85484200
C	-1.86358900	2.14030400	1.44974100
C	-0.87565700	1.30138300	-2.64337500
C	-0.85455700	2.28408400	-3.62722400
C	-0.01984400	3.40006900	-3.44987500
C	0.75263100	3.49102900	-2.31085300
C	0.69733500	2.46749700	-1.33031400
C	1.42026200	2.43908700	-0.12056800
C	1.85667100	1.20346600	1.96640700
C	1.18727000	1.26946500	0.74462200
C	-0.67406300	-1.45296700	2.63949900
C	-0.51754700	-2.43665200	3.61133700
C	0.44484900	-3.42268200	3.42001600
C	1.21762900	-3.39413900	2.26161900
C	1.01547700	-2.38455600	1.32431200
C	1.75476900	-2.24693800	0.06627100
C	2.06548200	-0.99841600	-1.95351800
C	1.38647900	-1.14781300	-0.75296200
H	-0.64094200	-2.63612300	-1.72909800

H	-2.59322800	-4.00939200	-2.45081800
H	-4.90637800	-3.25834300	-1.78695300
H	-5.15602100	-1.18144700	-0.45093100
H	-5.23880100	0.62936300	0.49391100
H	-5.18158900	2.73462100	1.80774800
H	-2.94627600	3.72035000	2.43124500
H	-0.87582300	2.53873600	1.70287800
H	-1.50997200	0.41528600	-2.75013000
H	-1.48231200	2.17648800	-4.51382900
H	0.01772200	4.18823200	-4.20595800
H	1.40844000	4.35056400	-2.15514100
H	1.72777800	0.36584600	2.66025500
H	-1.41665200	-0.65683600	2.75557300
H	-1.14750800	-2.42184700	4.50347900
H	0.59320300	-4.20916500	4.16452000
H	1.97733800	-4.16062300	2.09104000
H	1.86152600	-0.18254500	-2.65567300
Ir	-0.11016800	-0.00391500	0.00428200
N	-1.79032600	-1.21376700	-0.74435300
N	-1.88985600	0.99895900	0.74341300
N	-0.13260200	1.37587400	-1.53370200
N	0.07153100	-1.42344400	1.52770800
C	2.94469200	3.28629500	1.54662100
H	3.64996100	4.01868800	1.94787100
C	3.39001300	-2.90233700	-1.56188600
H	4.18185800	-3.55624500	-1.93564600
C	2.34076000	3.43222400	0.34338900
H	2.57486700	4.32320200	-0.24418700
C	2.76053200	-3.12145600	-0.35050100
H	3.07401100	-3.98329000	0.24384400
C	3.40121700	2.12392900	3.65411100
H	4.49115200	2.13716300	3.49598000
H	3.12908800	2.99655300	4.26907100
H	3.12899400	1.20881900	4.19358400
C	3.74318900	-1.61889100	-3.61445700
H	4.41298300	-0.75326500	-3.51022200
H	4.33410400	-2.50244500	-3.88222200
H	3.00658100	-1.42476200	-4.40494900
N	3.04258700	-1.85783200	-2.34001400
N	2.70774100	2.17539900	2.37437000