Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information

Theoretical study on the effect of N-substitution on the electronic structures and photophysical properties of phosphorescent Ir(III) complexes

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Table S1 Optimized geometry parameters for the complex **1** in the ground at PBE0, B3LYP, M062X and BP86 Levels respectively, together with the experimental data

	PBE0	**B3LYP**	**M062X**	**BP86**	Exp.[22]
Bond Length					
Ir-N1	2.040	2.065	2.060	2.055	2.031
Ir-C1	1.980	1.998	1.972	1.992	1.970
Ir-C2	1.979	1.998	1.972	1.992	1.969
Ir-N2	2.040	2.065	2.060	2.051	2.027
Ir-O1	2.233	2.266	2.275	2.264	2.210
Ir-O2	2.234	2.267	2.274	2.265	2.194
Bond Angle					
N1-Ir-C1	80.9	80.6	81.0	80.9	80.6
N1-Ir-C2	95.9	96.4	95.6	96.0	93.9
N1-Ir-N2	175.5	175.6	175.2	175.6	172.9
N1-Ir-O1	91.7	91.6	90. 9	91.0	92.2
N1-Ir-O2	92.0	91.5	92. 6	92.6	93.3
C1-Ir-C2	92.5	93.1	90. 8	93.2	93.4
C1-Ir-N2	96.1	96.4	95.6	96.1	95.4
C1-Ir-O1	172.5	172.0	171.8	171.8	172.2
C1-Ir-O2	89.2	89. 4	90.9	88.8	87.3
C2-Ir-N2	80.8	80.6	81.0	80.9	80.4
C2-Ir-O1	89.3	89.4	91.1	88.6	90.0
C2-Ir-O2	172.1	172.0	171.8	171.4	172.8
N2-Ir-O1	91.3	91.5	92. 6	92.1	92.1
N2-Ir-O2	91.3	91.6	90.9	90.6	92. 4
O1-Ir-O2	90.0	89.1	88.4	90.5	90.2

Table S2 Molecular orbital composition (%) of **1** in the ground state

MO	Energy (eV)	Compositions (%)				Bond type
		Ir	tpip	tfmppy1	tfmppy2	
L+5	-0.68	0	97	1	2	π*(tpip)
L+4	-0.73	0	95	1	4	π*(tpip)
L+3	-0.75	2	5	44	50	π*(tfmppy)
L+2	-0.88	3	4	51	42	π*(tfmppy)
L+1	-1.42	4	2	39	55	π*(tfmppy)
LUMO	-1.50	4	2	55	40	π*(tfmppy)
HOMO	-5.39	45	5	25	25	d(Ir)+π(tfmppy)
H-1	-6.08	64	13	10	13	d(Ir)+π(tpip+tfmppy)
H-2	-6.13	66	14	12	8	d(Ir)+π(tpip+tfmppy)
H-3	-6.46	4	3	46	46	π(tfmppy)
H-4	-6.64	2	95	2	1	π(tpip)
H-5	-6.71	4	3	48	45	π(tfmppy)

Table S3 Molecular orbital composition (%) of **2** in the ground state

MO	Energy (eV)	Compositions (%)				Bond type
		Ir	tpip	dfppy1	dfppy2	
L+12	0.43	8	5	45	42	π*(dfppy)
L+7	-0.07	0	99	0	1	π*(tpip)
L+5	-0.53	1	5	41	53	π*(dfppy)
L+4	-0.65	1	54	34	11	π*(tpip+dfppy)
L+3	-0.66	1	44	21	33	π*(tpip+dfppy)
L+2	-0.7 0	0	96	2	2	π*(tpip)
L+1	-1.21	5	2	37	56	π*(dfppy)
LUMO	-1.26	5	3	55	37	π*(dfppy)
HOMO	-5.41	44	5	25	26	d(Ir)+π(dfppy)
H-1	-6.02	48	10	20	23	d(Ir)+π(tpip+dfppy)
H-2	-6.08	57	13	18	13	d(Ir)+π(tpip+dfppy)
H-3	-6.29	19	7	34	40	d(Ir)+π(dfppy)
H-4	-6.35	14	4	43	39	d(Ir)+π(dfppy)
H-5	-6.62	2	85	7	6	π(tpip)

Table S4 Molecular orbital composition (%) of **1a** in the ground state

MO	Energy (eV)	Compositions (%)				Bond type
		Ir	tpip	tfmppy1	tfmppy2	
L+5	-0.47	0	100	0	0	π*(tpip)
L+4	-0.52	0	99	0	0	π*(tpip)
L+3	-1.42	1	0	49	49	π*(tfmppy)
L+2	-1.53	1	1	49	49	π*(tfmppy)
L+1	-1.79	6	1	46	47	π*(tfmppy)
LUMO	-1.83	5	1	47	47	π*(tfmppy)
HOMO	-5.52	47	6	23	23	d(Ir)+π(tfmppy)
H-1	-6.18	50	34	8	8	d(Ir)+π(tpip)
H-2	-6.20	53	31	8	8	d(Ir)+π(tpip)
H-3	-6.45	9	83	4	4	π(tpip)
H-4	-6.69	3	6	46	46	π(tfmppy)
H-5	-6.79	6	86	4	4	π(tpip)

Table S5 Molecular orbital composition (%) of **1b** in the ground state

MO	Energy (eV)	Compositions (%)				Bond type
		Ir	tpip	tfmppy1	tfmppy2	
L+5	-0.70	0	99	0	0	π*(tpip)
L+4	-0.76	0	97	1	1	π*(tpip)
L+3	-1.06	2	1	45	51	π*(tfmppy)
L+2	-1.16	3	3	50	44	π*(tfmppy)
L+1	-1.89	4	1	44	50	π*(tfmppy)
LUMO	-1.98	3	1	51	45	π*(tfmppy)
HOMO	-5.71	46	6	24	24	d(Ir)+π(tfmppy)
H-1	-6.34	61	20	10	10	d(Ir)+π(tpip+tfmppy)
H-2	-6.37	61	21	9	9	d(Ir)+π(tpip)
H-3	-6.71	3	95	1	1	π(tpip)
H-4	-6.87	2	6	46	46	π(tfmppy)
H-5	-6.98	5	91	2	2	π(tpip)
H-8	-7.16	0	42	35	23	π(tfmppy+tpip)
H-9	-7.17	0	75	6	19	π(tpip+tfmppy)
H-10	-7.2	0	98	1	1	π(tpip)
H-11	-7.26	1	77	11	11	π(tpip+tfmppy)
H-12	-7.28	1	60	18	21	π(tpip+tfmppy)

Table S6 Molecular orbital composition (%) of **1c** in the ground state

MO	Energy (eV)	Compositions (%)				Bond type
		Ir	tpip	tfmppy1	tfmppy2	
L+5	-0.82	0	95	4	1	π*(tpip)
L+4	-0.89	0	95	3	2	π*(tpip)
L+3	-1.19	1	24	30	45	π*(tpip+tfmppy)
L+2	-1.35	2	21	31	46	π*(tpip+tfmppy)
L+1	-1.96	6	14	40	40	π*(tpip+tfmppy)
LUMO	-2.01	5	16	39	40	π*(tpip+tfmppy)
HOMO	-5.74	44	9	23	24	d(Ir)+π(tfmppy)
H-1	-6.50	54	19	13	14	d(Ir)+π(tpip+tfmppy)
H-2	-6.54	59	21	10	10	d(Ir)+π(tpip+tfmppy)
H-3	-6.76	4	33	30	33	π(tpip+tfmppy)
H-4	-6.83	7	75	8	10	π(tpip+tfmppy)
H-5	-6.99	4	24	34	38	π(tpip+tfmppy)
H-6	-7.11	9	81	5	5	π(tpip)
H-7	-7.11	2	11	43	44	π(tfmppy)

Table S7 Molecular orbital composition (%) of **1d** in the ground state

MO	Energy (eV)	Compositions (%)				Bond type
		Ir	tpip	tfmppy1	tfmppy2	
L+5	-0.81	0	99	1	1	π*(tpip)
L+4	-0.88	0	98	1	1	π*(tpip)
L+3	-1.30	1	1	46	52	π*(tfmppy)
L+2	-1.39	3	1	51	45	π*(tfmppy)
L+1	-1.65	5	2	43	50	π*(tfmppy)
LUMO	-1.71	3	2	51	44	π*(tfmppy)
HOMO	-5.58	45	5	25	25	d(Ir)+π(tfmppy)
H-1	-6.29	61	13	13	13	d(Ir)+π(tpip+tfmppy)
H-2	-6.33	63	15	11	11	d(Ir)+π(tpip+tfmppy)
H-3	-6.70	3	3	47	47	π(tfmppy)
H-4	-6.79	1	97	1	1	π(tpip)
H-5	-6.96	4	4	53	39	π(tfmppy)
H-6	-7.01	4	4	39	53	π(tfmppy)

Table S8 Molecular orbital composition (%) of **2a** in the ground state

MO	Energy (eV)	Compositions (%)				Bond type
		Ir	tpip	dfppy1	dfppy2	
L+5	-0.39	0	99	0	0	π*(tpip)
L+4	-0.45	0	99	0	0	π*(tpip)
L+3	-1.19	1	1	58	41	π*(dfppy)
L+2	-1.27	0	1	41	58	π*(dfppy)
L+1	-1.64	6	1	85	8	π*(dfppy)
LUMO	-1.65	6	1	8	86	π*(dfppy)
HOMO	-5.54	47	7	23	23	d(Ir)+π(dfppy)
H-1	-6.12	48	25	12	15	d(Ir)+π(tpip+dfppy)
H-2	-6.15	49	28	14	9	d(Ir)+π(tpip+dfppy)
H-3	-6.39	2	83	7	8	π tpip)
H-4	-6.58	4	15	31	51	π(tpip+dfppy)
H-5	-6.60	11	15	48	25	π(tpip+dfppy)

Table S9 Molecular orbital composition (%) of **2b** in the ground state

MO	Energy (eV)	Compositions (%)				Bond type
		Ir	tpip	dfppy1	dfppy2	
L+5	-0.67	0	99	0	0	π*(tpip)
L+4	-0.72	0	97	2	1	π*(tpip)
L+3	-0.88	2	1	41	56	π*(dfppy)
L+2	-0.97	3	3	54	40	π*(dfppy)
L+1	-1.67	4	2	41	52	π*(dfppy)
LUMO	-1.72	4	2	52	42	π*(dfppy)
HOMO	-5.74	46	6	24	24	d(Ir)+π(dfppy)
H-1	-6.30	57	19	10	14	d(Ir)+π(tpip+dfppy)
H-2	-6.34	58	21	13	8	d(Ir)+π(tpip+dfppy)
H-3	-6.67	0	62	20	18	π(tpip+dfppy)
H-4	-6.73	5	14	64	17	π(dfppy)
H-5	-6.74	6	27	8	59	π(tpip+dfppy)
H-6	-6.94	3	45	24	28	π(tpip+dfppy)
H-7	-6.95	4	49	26	20	π(tpip+dfppy)
H-8	-7.04	1	96	1	2	π(tpip)
H-9	-7.11	0	98	1	0	π(tpip)

Table S10 Molecular orbital composition (%) of **2c** in the ground state

MO	Energy (eV)	Compositions (%)				Bond type
		Ir	tpip	dfppy1	dfppy2	
L+6	-0.22	1	98	1	0	π*(tpip)
L+5	-0.79	0	98	1	1	π*(tpip)
L+4	-0.85	0	98	1	1	π*(tpip)
L+3	-0.96	1	8	46	45	π*(dfppy)
L+2	-1.08	1	6	50	43	π*(dfppy)
L+1	-1.79	6	8	44	43	π*(dfppy)
LUMO	-1.83	6	8	48	38	π*(dfppy)
HOMO	-5.76	42	7	26	25	d(Ir)+π(dfppy)
H-1	-6.38	28	11	31	29	d(Ir)+π(dfppy)
H-2	-6.45	37	15	25	23	d(Ir)+π(tpip+dfppy)
H-3	-6.65	28	27	23	22	d(Ir)+π(tpip+dfppy)
H-4	-6.69	27	15	30	28	d(Ir)+π(tpip+dfppy)
H-5	-6.81	8	84	4	4	π(tpip)

Table S11 Molecular orbital composition (%) of **2d** in the ground state

MO	Energy (eV)	Compositions (%)				Bond type
		Ir	tpip	dfppy1	dfppy2	
L+6	-0.21	1	98	1	0	π*(tpip)
L+5	-0.78	0	97	1	1	π*(tpip)
L+4	-0.84	0	97	1	1	π*(tpip)
L+3	-1.11	1	3	48	49	π*(dfppy)
L+2	-1.20	1	2	49	48	π*(dfppy)
L+1	-1.45	5	2	45	47	π*(dfppy)
LUMO	-1.48	5	3	47	45	π*(dfppy)
HOMO	-5.60	44	5	25	25	d(Ir)+π(dfppy)
H-1	-6.20	47	10	21	22	d(Ir)+π(dfppy)
H-2	-6.24	48	12	21	20	d(Ir)+π(dfppy)
H-3	-6.57	19	6	37	38	d(Ir)+π(dfppy)
H-4	-6.59	16	8	38	37	d(Ir)+π(dfppy)
H-5	-6.69	2	6	46	46	π(dfppy)

Table S12 Selected calculated wavelength (nm)/energies (eV), oscillator strength (*f*), major contribution and transition characters for **1**-**1d** and **2**-**2d** in CH_2Cl_2 media

	state	λ_{cal}/E	*f*	configuration	nature	Exp.[22]
1	S_1	486/2.55	0.0530	H->L (96%)	MLCT/ ILCT	464
	S_3	394/3.14	0.0021	H-2->L (60%)	MLCT/ILCT/LLCT	412
				H-1->L (35%)	MLCT/ILCT/LLCT	
	S_7	349/3.55	0.0358	H-2->L+1 (91%)	MLCT/ILCT/LLCT	350
	S_{27}	277/4.48	0.1107	H-5->L+1 (23%)	ILCT	
				H-2->L+3 (16%)	MLCT/ILCT/LLCT	
				H-2->L+4 (10%)	MLCT/LLCT/ILCT	
				H-1->L+5 (10%)	MLCT/LLCT/ILCT	
2	S_1	403/3.07	0.0379	H->L(95%)	MLCT/ILCT	388
	S_{19}	278/4.46	0.1440	H-5->L+1 (15%)	LLCT	
				H-1->L+4 (14%)	MLCT/LLCT/ILCT	
				H-1->L+5 (25%)	MLCT/ILCT/LLCT	
	S_{29}	268/4.63	0.1756	H->L+7 (12%)	MLCT/LLCT	
				H->L+12 (29%)	MLCT/ILCT	
	S_{50}	248/4.99	0.0034	H-4->L+2 (46%)	MLCT/ILCT	240
				H-4->L+3 (13%)	MLCT/LLCT/ILCT	
				H-3->L+4 (21%)	MLCT/LLCT/ILCT	
1a	S_1	473/2.62	0.0152	H->L (97%)	MLCT/ILCT	
	S_7	369/3.36	0.1606	H-2->L (47%)	MLCT/ILCT	
				H-1->L+1 (49%)	MLCT/ILCT	
1b	S_1	464/2.67	0.0498	H->L (97%)	MLCT/ILCT	
	S_{27}	280/4.43	0.1351	H-9->L (37%)	MLCT/ILCT	
				H-8->L+1 (18%)	MLCT/LLCT	
	S_{30}	277/4.48	0.1010	H-12->L (21%)	LLCT/ILCT	
				H-11->L+1 (15%)	LLCT/ILCT	
				H-10->L (17%)	LLCT	
				H-9->L+1 (21%)	LLCT/ILCT	
1c	S_1	473/2.62	0.0260	H->L (97%)	MLCT/ILCT	
	S_6	361/3.43	0.1346	H-2->L (32%)	MLCT/LLCT/ILCT	
				H-1->L+1 (34%)	MLCT/ILCT/LLCT	
				H->L+2 (30%)	MLCT/ILCT/LLCT	
	S_{27}	287/4.32	0.1377	H-7->L+1 (29%)	ILCT/LLCT	
				H-6->L (20%)	LLCT/ILCT	
				H-1->L+3 (17%)	MLCT/ILCT/LLCT	
1d	S_1	441/2.81	0.0435	H->L (95%)	MLCT/ILCT	
	S_{21}	280/4.42	0.1049	H-6->L (65%)	ILCT	
2a	S_1	446/2.78	0.0078	HOMO->L (79%)	MLCT/ILCT	
				H->L+1 (18%)	MLCT/ILCT	
	S_7	357/3.47	0.1913	H-2->L (42%),	MLCT/LLCT/ILCT	
				H-2->L+1 (12%),	MLCT/LLCT/ILCT	

				H-1->L (11%),	MLCT/ILCT/LLCT
				H-1->L+1 (27%)	MLCT/ILCT/LLCT
	S_{17}	301/4.11	0.1006	H-5->L (16%),	ILCT/LLCT/MLCT
				H-4->L+1 (54%)	ILCT/LLCT
2b	S_1	427/2.90	0.0436	H->L (96%)	ILCT/MLCT
	S_{23}	283/4.38	0.1953	H-4->L+1 (11%),	ILCT/LLCT
				H-2->L+2 (16%),	MLCT/LLCT/ILCT
				H-1->L+3 (18%)	MLCT/ILCT/LLCT
	S_{25}	279/4.44	0.1094	H-9->L (26%),	LLCT
				H-8->L+1 (14%)	LLCT
2c	S_1	446/2.78	0.0201	H->L (97%)	MLCT/ILCT
	S_{27}	282/4.39	0.1645	H-1->L+3 (62%)	MLCT/ILCT /LLCT
	S_{45}	260/4.77	0.1591	H-3->L+3 (48%),	MLCT/ILCT /LLCT
				H->L+6 (18%)	MLCT/LLCT
2d	S_1	411/3.02	0.0294	H->L (96%)	MLCT/ILCT
	S_7	339/3.66	0.1147	H-2->L (50%),	MLCT/ILCT/LLCT
				H-1->L+1 (45%)	MLCT/ILCT/LLCT
	S_{21}	286/4.34	0.1896	H-5->L+1 (62%),	ILCT
				H-4->L (12%)	MLCT/ILCT

Table S13 Calculated phosphorescent emission wavelength (nm)/energies (eV), of the complexes **1** and **2** in CH_2Cl_2 media with the TDDFT method at the B3LYP, M062X and PBE0 level, respectively, together with the experimental values

	λ_{cal}/E(eV) (M062X)	λ_{cal}/E(eV) (B3LYP)	λ_{cal}/E(eV) (PBE0)	Exp.[22]
1	496/2.50	594/2.08	598/ 2.07	524
2	472/2.63	544/2.28	551/2.25	485

Table S14 Optimized S_0 structure for $Ir(tfmppy)_2(tpip)$ (**1**)

Ir	0.69045400	0.01294100	-0.02144800	C	0.91298500	-0.41523100	-4.79861100
P	-2.32843500	1.41914200	-0.45043900	H	0.98773500	-0.48800700	-5.87987000
P	-2.38563300	-1.20902900	0.64559700	C	-3.11132800	5.28535700	0.60562100
N	0.73310800	-0.22471000	-2.04690600	H	-2.55302100	6.21464900	0.68209900
C	-3.56275100	0.48761600	-2.79199200	C	1.77334200	-0.53370800	4.03522700
H	-4.16134200	-0.12837200	-2.12623400	H	2.43265000	-1.22476300	4.54874500
N	0.80708900	0.24948000	2.00157600	C	-5.57732700	-3.42331400	-0.66067100
C	2.00706100	-1.40812600	0.38618600	H	-6.65117600	-3.29230200	-0.76562400
C	-2.46157800	-1.38521900	2.45283800	C	0.25024300	1.31741400	4.05923000
O	-0.82702800	1.64161500	-0.19166800	H	-0.30860000	2.09106200	4.57404000
C	2.64238300	-2.27881100	-0.50506100	C	-4.53797000	2.89666900	0.42784300
H	2.46241100	-2.18962100	-1.57202200	H	-5.08089900	1.95703100	0.37284300
C	-3.41546200	-2.54853200	-0.02183200	C	-3.39995800	-0.75911300	4.59097600
O	-0.94914600	-1.49207100	0.17204900	H	-4.07527800	-0.14059600	5.17657600
C	2.10879600	1.32106700	-0.46205200	C	-4.79787200	-2.38688500	-0.15618100
C	1.62808500	-0.61949800	2.64935500	H	-5.25357600	-1.44112400	0.12571100
C	3.51138900	-3.26831200	-0.05091500	C	0.02851400	-1.22699100	-4.09260400
C	-3.17949000	2.92272800	0.09925900	H	-0.61117000	-1.94453400	-4.59419000
N	-3.07870000	0.18928100	0.26093400	C	-2.82163300	-3.75706700	-0.39759300
C	2.37848000	1.45944000	-1.84706600	H	-1.74517400	-3.87286200	-0.30305400
C	-2.58022400	1.32091100	-2.25090100	C	-4.46651000	5.25602800	0.92640900
C	3.78367100	3.03710500	-0.05874400	H	-4.96800200	6.16456200	1.24970000
C	1.60466000	0.57694700	-2.71495200	C	-5.17880800	4.06110600	0.83900700
C	2.84157900	2.12818000	0.41524300	H	-6.23453700	4.03672300	1.09629900
H	2.68282000	2.04935600	1.48597300	C	1.08118900	0.43509700	4.74520200
C	3.78183700	-3.41837700	1.31002700	H	1.19142500	0.50445900	5.82357800
H	4.46570900	-4.18863600	1.64967500	F	5.21871000	-4.81676700	-0.57092800
C	-3.32916700	-0.59389200	3.21039800	C	-2.60409400	-1.71335900	5.22058500
H	-3.93095300	0.15854900	2.70781000	H	-2.66103400	-1.84312800	6.29840000
C	4.03109200	3.16866300	-1.42692100	F	4.44708400	-3.60306000	-2.19003600
H	4.77416000	3.87456500	-1.78258200	F	3.24904300	-5.20009300	-1.37190200
C	2.29980400	-1.56705400	1.76497900	C	-1.73166000	-2.50002400	4.47002200
C	-1.66052700	-2.33892500	3.08983900	H	-1.10454900	-3.23923700	4.96155600
H	-0.97126300	-2.93927300	2.50163800	C	-3.60383600	-4.79179800	-0.90419600
C	3.17448900	-2.56141200	2.21457800	H	-3.13699300	-5.72754600	-1.20028500
H	3.39104900	-2.67374500	3.27392600	C	-4.98084400	-4.62659500	-1.03399800
C	-0.03085100	-1.10079700	-2.71468500	H	-5.59031000	-5.43516000	-1.42911700
H	-0.69022700	-1.69818200	-2.09374100	C	4.11203100	-4.21873300	-1.04329300
C	-2.46762600	4.12229700	0.19103800	F	5.72013300	4.27997800	0.46324300
H	-1.40710900	4.13116400	-0.04596900	F	3.82341800	5.07805500	1.11731400
C	-1.78998200	2.10016700	-3.10327500	C	-1.98430900	2.04683400	-4.47945700
H	-1.01320700	2.73314600	-2.68251000	H	-1.36549600	2.65127600	-5.13746400

C	3.32656500	2.37473100	-2.31713000	C	-3.75462600	0.43467400	-4.17046700
H	3.52542500	2.47150400	-3.38146300	H	-4.51786100	-0.21817400	-4.58605900
C	1.70309600	0.48811500	-4.10503000	C	-2.96819700	1.21573900	-5.01373700
H	2.40411500	1.12441500	-4.63396900	H	-3.12027700	1.17658900	-6.08946000
C	0.14120900	1.19149600	2.68423800	C	4.50027000	3.93188000	0.90814700
H	-0.47858700	1.84279100	2.07686000	F	4.66175800	3.35406800	2.11017500

Table S15 Optimized S_0 structure for $Ir(dfppy)_2(tpip)$ (**2**)

C	1.27832800	3.87418000	0.16919200	C	-3.89978500	1.91559300	-2.53933900
H	0.56031300	3.79550800	-0.64294800	C	-1.92950500	-2.49951300	-1.23767400
C	1.48420800	-3.72339300	-0.37136600	C	-3.12259700	-1.00115700	1.95587900
H	0.72125600	-3.80727800	0.39806500	H	-2.96499000	-0.12118900	2.56966500
C	2.11229400	2.78960200	0.46049600	C	-2.65836800	2.33156100	-0.09785700
C	3.01561900	2.87799100	1.52316000	C	-2.09761900	3.47935800	2.12121800
H	3.64145400	2.02061700	1.75564800	H	-2.76253400	4.30643000	1.91658700
C	5.17146400	1.71913900	-3.16266300	C	-2.02398300	-3.52299500	-2.18817900
H	6.24418100	1.54438000	-3.15529800	H	-2.71054600	-4.34075300	-2.02077900
C	4.55499400	2.22982300	-4.30369300	C	-1.96938800	2.45130300	1.18003000
H	5.14775600	2.45503400	-5.18647800	C	3.03259900	1.64906200	-2.03713600
C	-2.41984200	-1.19965700	0.76410200	C	2.63711100	-4.63042400	-2.28657100
C	2.89448300	-1.75016400	2.26358000	H	2.78500500	-5.43712400	-3.00015600
C	1.35141000	5.03542500	0.93208000	C	2.20491400	-2.45835100	3.25211000
H	0.69648800	5.87292800	0.70669200	H	1.14550900	-2.66100200	3.12004800
C	-2.36865000	1.15337900	-0.84396900	C	-4.19453800	3.07975300	-1.84187100
C	2.26003100	5.12198200	1.98553100	H	-4.89128900	3.81499600	-2.22520600
H	2.31854200	6.03122300	2.57852300	C	-1.37651500	3.42575000	3.30386500
C	3.08923400	4.04250900	2.28237700	H	-1.47595200	4.22440900	4.03360900
H	3.79220700	4.10668000	3.10899800	C	3.40754800	-3.47358000	-2.37366200
C	-2.68280400	-2.37396600	0.00256100	H	4.15461300	-3.37335400	-3.15686000
C	-3.56103800	3.25853900	-0.62695700	C	4.25102500	-1.46160900	2.43738500
C	-0.37310300	-2.40678100	-3.52860600	H	4.77597400	-0.89449100	1.67351300
H	0.25793600	-2.33515400	-4.40740500	C	4.22228700	-2.59197600	4.56863300
C	-3.01255900	0.96102300	-2.06957000	H	4.73985200	-2.91931800	5.46664300
H	-2.83449800	0.07838200	-2.67388100	C	3.22057200	-2.44136700	-1.45758300
C	-0.44037700	1.35507800	2.58480400	H	3.80678900	-1.52883700	-1.52559800
H	0.18884400	0.47813600	2.69537900	C	4.91221400	-1.88280400	3.58688000
C	1.67383700	-4.75385000	-1.28611600	H	5.96649600	-1.65451700	3.71996200
H	1.06568800	-5.65231400	-1.22272000	C	3.17921900	2.44804100	-4.31434000
C	-4.04194400	-1.94703500	2.37883100	H	2.69684200	2.84049600	-5.20572100
C	-1.24488200	-3.47448300	-3.33364000	F	-4.50485600	1.71861400	-3.71826900
H	-1.31992500	-4.26814700	-4.07180200	F	-3.84873100	4.38861000	0.04804700
C	2.25839400	-2.56039200	-0.45140500	F	-4.70350700	-1.74538900	3.52614700
C	-4.31319500	-3.10729400	1.66537400	F	-3.88551600	-4.41828900	-0.20650800
H	-5.03575200	-3.83573400	2.01217600	Ir	-1.02398700	-0.02918300	-0.00402200

C	-3.62089300	-3.29184000	0.48387500	N	-1.06839400	-1.46580200	-1.45055800
C	2.86884700	-2.87638700	4.40228200	N	-1.13347600	1.40752400	1.43903200
H	2.32799400	-3.42155200	5.17135300	N	2.74983600	0.10293900	0.24452100
C	2.41850200	2.16061400	-3.18407300	C	-0.53273900	2.34566700	3.54741900
H	1.34297000	2.31603200	-3.18653500	H	0.04937700	2.26742600	4.45894100
C	4.41336000	1.42936300	-2.03226500	O	0.52139400	-1.17183400	1.12904000
H	4.88385200	1.01926100	-1.14231200	O	0.58621100	1.09962400	-1.06105700
C	-0.31585600	-1.42075800	-2.55860900	P	2.01665900	-1.22799600	0.76566700
H	0.33333700	-0.55462300	-2.63319800	P	2.03082300	1.29092500	-0.56472700