Electronic Supplementary Material (ESI) for Dalton Transactions.

Vibrational circular dichroism and chiroptical properties of chiral Ir(III) luminescent complexes

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Electronic Supplementary Information

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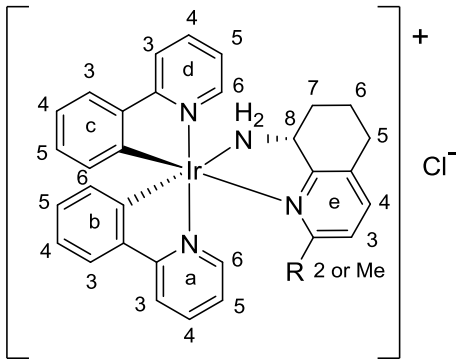
1. Complexes NMR

Figure ESI-1 Labels used in ^{1}H-NMR assignment.



ΔR

$^{\Delta S}$Ir-Me-Campy

Yellow solid soluble in CH_2Cl_2/MeOH, yield 23 mg (46%). ^{1}H NMR (300 MHz, $CDCl_3/CD_3OD$, 3:1 v/v) δ 9.26 (d, *J* = 5.2 Hz, 1H, a6), 7.93 (d, *J* = 8.1 Hz, 1H, d3), 7.88 – 7.71 (m, 3H, a3/d4/a4), 7.58 – 7.47 (m, 2H, c3/b3), 7.46 – 7.35 (m, 2H, d6/a5), 7.26 (m, 1H, e4), 7.07 – 6.94 (m, 2H, d4/e2), 6.81 (d, *J* = 2.8 Hz, 2H, b4/c4), 6.67 (dd, *J* = 7.9, 7.4 Hz, 2H, b5/c5), 6.11 (d, *J* = 7.8 Hz, 1H, b6), 6.07 (d, *J* = 7.4 Hz, 1H, d6), 5.98 (s, 1H, NH), 4.75 (s, 1H, e8), 3.05(m, 1H, NH), 2.77 (s, 2H, e7/e5), 2.68 (m, 1H, e5), 1.93 (s, 2H, e5/e6), 1.82 (s, 3H, Me), 1.59 (s, 1H, e5). ^{13}C-NMR (75 MHz, $CDCl_3$) δ 169.30, 169.24, 161.72, 160.31, 155.27, 153.03, 148.18, 144.06, 143.98, 143.05, 139.69, 138.22, 137.93, 133.69, 132.44, 131.75, 130.58, 130.13, 126.23, 124.61, 124.41, 123.64, 123.11, 122.38, 121.51, 120.11, 119.25, 58.66, 33.67, 28.45, 28.21, 21.64. CHN calculated: C 55.04%, H 4.33%, N 8.02% found: C 54.92%, H 4.33%, N 8.00%.

$^{\Delta S}$Ir-Me-Campy

Yellow solid soluble in CH_2Cl_2, yield 22 mg (44%). ^{1}H-NMR (300 MHz, $CDCl_3$) δ: 9.91 (d, *J* = 6.4 Hz, 1H, a6), 8.03 (d, *J* = 5.8 Hz, 1H, d6), 7.99 – 7.75 (m, 4H, d3/a3/d4/a4), 7.60 (d, *J* = 7.1 Hz, 1H, b3), 7.53 (d, *J* = 6.8 Hz, 1H, c3), 7.45 (d, *J* = 7.8 Hz, 1H, e4), 7.38 (t, *J* = 5.9 Hz, 1H, a5), 7.14 (t, *J* = 6.6 Hz, 1H, d5), 6.92 (d, *J* = 7.9 Hz, 1H, e3), 6.84 (t, *J* = 7.5 Hz, 2H, b4/c4), 6.70 (m, 2H, b5/c5), 6.49 (t, *J* = 12.1 Hz, 1H, NH), 6.11 (d, *J* = 7.7 Hz, 1H, b6), 6.00 (d, *J* = 7.8 Hz, 1H, c6), 3.77 (m, 1H, e8), 3.22 (d, *J* = 12.1 Hz, NH), 3.02 (m, 2H, e5/e7), 2.72 (d, *J* = 16.7 Hz, H, e5'), 2.17 – 2.10 (m, 1H, e7'), 1.99 (m, 1H, e6), 1.71 (s, 3H, Me), 1.58 (m, 1H, e6').^{13}C-NMR (75 MHz, $CDCl_3$) δ: 169.22, 168.23, 160.99, 160.20, 154.33, 153.76, 149.51, 144.71, 144.49, 143.10, 139.71, 138.19, 137.81, 134.31, 132.62, 131.04, 130.82, 129.95, 125.48, 124.93, 124.57, 123.63, 123.27, 122.61, 121.26, 120.33, 118.84, 58.69, 32.78, 28.82, 26.52, 22.18. CHN calculated: C 55.04%, H 4.33%, N 8.02% found: C 54.8%, H 4.33%, N 7.98%.

$^{\Lambda S}$Ir-Me-Campy

Yellow solid soluble in CH_2Cl_2/MeOH, yield 23 mg (46%). ^{1}H-NMR (300 MHz, $CDCl_3$) δ: 10.13 (d, *J* = 5.5 Hz, 1H, a6), 7.92 (d, *J* = 8.3 Hz, 1H, d3), 7.78 (m, 3H, a3/d4/a4), 7.58 (m, 3H,c3/b3/e2), 7.46 (m, 2H, a5/e4), 7.09 (m, 2H, e3/d6), 7.04 – 6.90 (m, d5/c4/NH), 6.90 – 6.74 (m, 3H, b4/b5/c5), 6.51 (d, *J* = 6.7 Hz, 1H, c6), 6.18 (d, *J* = 7.2 Hz, 1H, b6), 4.65 (m, 1H, e8), 3.50 (m, 1H, NH), 2.77 (m, 3H, e5/e5'/e7), 2.04 – 1.6 (m, 3H, e7', e6, e6'). ^{13}C-NMR (75 MHz, $CDCl_3$) δ 168.49, 162.52, 154.96, 153.66, 148.20, 148.04, 147.53, 144.81, 143.57, 138.12, 138.00, 137.57, 136.90, 133.03, 132.04, 130.60, 130.52, 125.20, 124.45, 124.45, 124.32, 122.71, 122.01, 121.94, 119.86, 118.99, 58.96, 32.51, 28.26, 22.47. CHN calculated: C 54.41%, H 4.12%, N 8.19% found: C 54.7%, H 4.18%, N 8.22%.

$^{\Lambda R}$Ir-Me-Campy

Yellow solid soluble in CH_2Cl_2, yield 22 mg (44%). ^{1}H-NMR (300 MHz, $CDCl_3$) δ: 10.08 (d, *J* = 4.8Hz, 1H, a6), 7.99 (d, *J* = 8.0 Hz, 1H, d3), 7.88 (m, 3H, a3/d6/d4), 7.78 (t, *J* = 7.5 Hz, 1H, a4), 7.69 (d, *J* = 7.6 Hz, 1H,

b3), 7.62 (d, *J* = 7.7 Hz, 1H, c3), 7.51 (d, *J* = 7.6 Hz, 1H, e4), 7.45 (d, *J* = 5.1 Hz, 1H, e2), 7.39 (m, 1H, a5), 7.10 (t, *J* = 6.2 Hz, 1H, d5), 7.03 – 6.93 (m, 2H, e3/b4), 6.89 (t, *J* = 7.2 Hz, 1H, c4), 6.78 (t+m, *J* = 7.4 Hz, 3H, b5/c5/NH), 6.31 (d, *J* = 7.5 Hz, 1H, c6), 6.18 (d, *J* = 7.5 Hz, 1H, b6), 3.92 (m, 1H, e8), 3.30 (m, 1H, NH), 3.00 (m, 2H, e7/e5), 2.75 (m, 1H, e5'), 2.30 (m, 1H, e7'), 2.06 (m, 1H, e6), 1.64 (m,1H, e6'). ^{13}C-NMR (75 MHz, $CDCl_3$) d 170.12, 167.20, 160.54, 154.04, 151.97, 148.97, 148.32, 147.23, 144.57, 143.57, 138.43, 138.21, 137.79, 137.68, 133.92, 131.78, 130.80, 129.98, 124.96, 124.73, 124.12, 122.72, 122.35, 122.09, 120.13, 119.03, 58.38, 31.84, 28.42, 22.55. CHN calculated: C 54.41%, H 4.12%, N 8.19% found: C 53.96%, H 4.22%, N 8.07%.

2. Details of data and structure refinements of complex $^{\Delta R}$Ir-Me-Campy

Table ESI-1. Crystal data and selected structure refinement parameters for $^{\Delta R}$**Ir-Me-Campy**.

Compound	**Δ*R*-Ir-Me-Campy**
empirical formula	$C_{23}H_{23}ClIrN_4O$
Crystal system	Orthorombic
Space group	$P2_12_12_1$
Z	4
fw	716.27
a , Å	10.662(3)
b , Å	14.595(3)
c , Å	18.403(5)
α, β, γ, deg	90, 90, 90
V, Å^3	2863.7(12)
d_c, g cm^{-3}	1.661
μ, mm^{-1}	4.788
Independent reflections [R(int)]	5716 [0.0404]
Data/restraints/parameters	5421 / 3 / 354
Goodness-of-fit on F^2	0.957
Absolute structure parameter	-0.003(5)
[a]R1 [I > 2 σ (I)]	0.0183
[b,c]wR2	0.0457

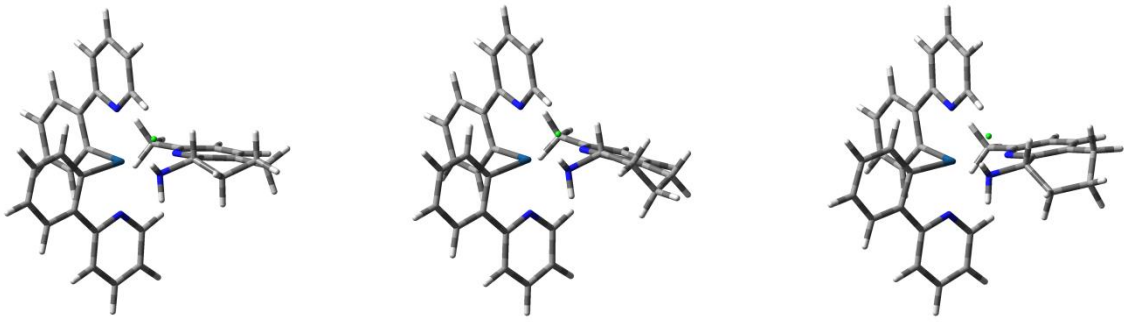
$^a R1 = \sum ||F_o|-|F_c|| / \sum |F_o|$. $^b wR2 = \{ \sum [w(F_o^2-F_c^2)^2] / [(w(F_o^2)^2]\}^{1/2}$. $^c w = 1/[\sigma^2(F_o^2) + (aP)^2+bP]$ with $P = [F_o^2+2F_c^2]/3$, $a = 0.0245$ and $b = 0$.

3. DFT-Analysis

The input geometry for $^{\Lambda S}$Ir-Me-Campy was taken from the X-ray diffraction data, while the one for $^{\Delta S}$Ir-Me-Campy was obtained by inversion of the metal chirality. A conformational search was carried out starting from the obtained structures and modifying the input geometries in the tetrahydroquinoline moiety conformation. All the obtained structures were optimized at the B3LYP/6-31+G(d,p) level of theory with LANL2DZ pseudo-potential on Ir atom, in the PCM polarizable continuum approximation and the presence of one Cl^- counterion was allowed. The lowest energy three conformers are shown in figure SI-2, the energies and the relative populations are reported in table SI-2.

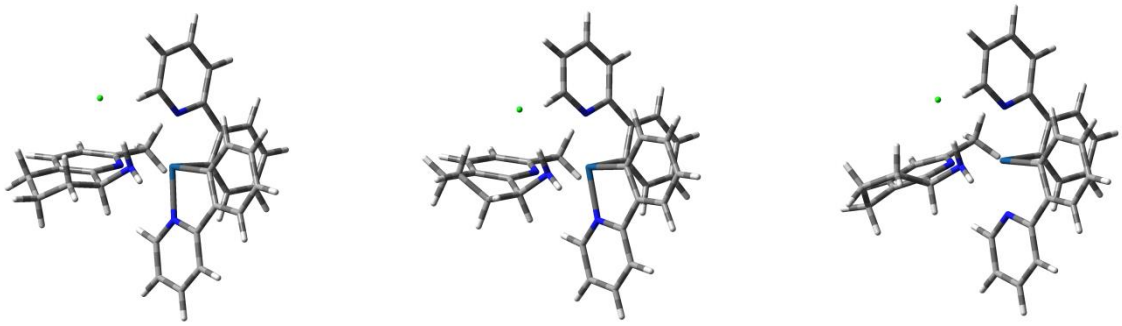
Figure ESI-2 Calculated structures of the three conformers lower in energy of $^{\Lambda S}$Ir-Me-Campy (top) and $^{\Delta S}$Ir-Me-Campy (bottom).

$^{\Lambda S}$Ir-Me-Campy



half-chair on (C24) half-chair on (C25) boat

$^{\Delta S}$Ir-Me-Campy



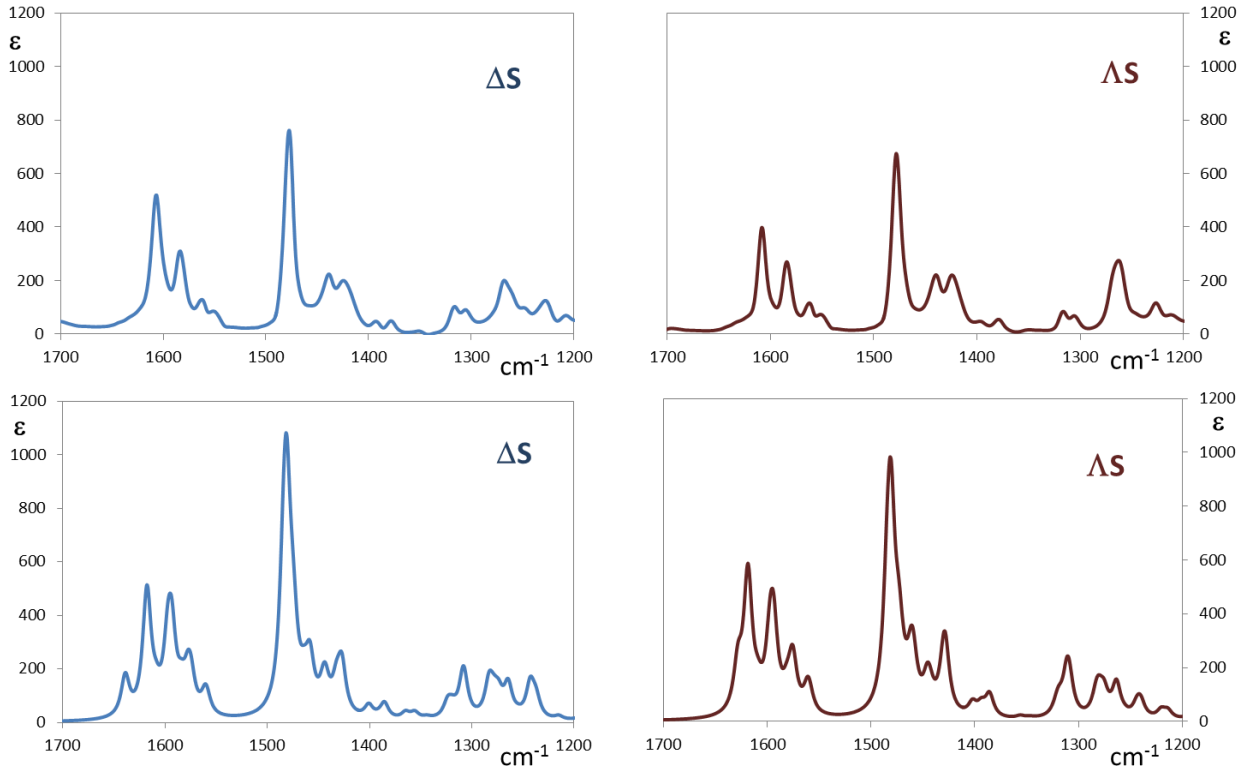
half-chair on (C24) half-chair on (C25) boat

Table ESI-2. Energy values and population factors for the three reported conformers. Electronic energy, zero-point energy, energy-evaluated populations, free energy and free energy populations.

$^{\Lambda S}$Ir-Me-Campy					
	E_{elec}	ΔE_0 (kcal/mol)	pop- ΔE_0	ΔG(kcal/mol)	pop- ΔG
half-chair (C24)	-2021.636857	0	0.903769	0	0.804877
half-chair (C25)	-2021.632337	2.710213	0.009321	2.619225	0.009679
boat	-2021.634325	1.387423	0.08691	0.869728	0.185445
$^{\Delta S}$Ir-Me-Campy					
	E_{elec}	ΔE_0 (kcal/mol)	pop- ΔE_0	ΔG(kcal/mol)	pop- ΔG
half-chair (C24)	-2021.637237	0	0.975609	0	0.95687
half-chair (C25)	-2021.633955	2.205068	0.023602	2.591614	0.012056
boat	-2021.630397	4.218746	0.000789	2.030621	0.031074

4. IR spectra

Figure ESI-3: Comparison of calculated (lower) and experimental (top) IR spectra for $^{\Delta S}$Ir-Me-Campy (left in blue) and $^{\Lambda S}$Ir-Me-Campy (right in red).



5. Normal Mode assignments

Tables ESI-3: Normal Mode assignments for $^{\Delta S}$Ir-Me-Campy. In brackets is specified the ring involved in the normal mode (see figure SI-1). Units for dipole strength and rotatory strength are 10^{-40} esu^{2}cm^2 and 10^{-44} esu^{2}cm^2 respectively.

#	Frequencies (cm^{-1})	Dipole strength	Rotatory strength	Normal Mode Descriptions
120	1200	11	-12	CC stretching (e), CH2 e5/e6/e7 twisting, CC/CN stretching (e)
121	1221	6	9	CC stretching (e), C*H bending out of HCN plane, NH2/CH2 e5/e6/e7 twisting, CC/CN stretching (e7 ring)
122	1240	15	-14	CC stretching (e), C*H bending out of HCN plane, NH2/CH2 e5/e6/e7 twisting, CC/CN stretching (e)
123	1262	67	20	Symmetric CC stretching (c/d), NH2 wagging, CH2 e5/e6/e7 twisting
124	1264	12	6	C*H bending in-plane HCN, NH2 wagging, CH e5/e6/e7 twisting
125	1268	142	-32	C*H bending in-plane HCN, NH2 wagging, CH e5/e6/e7 twisting
126	1281	10	-4	C*H bending out of HCN plane, CC stretching (e), CH2 e5/e6/e7 twisting
127	1290	133	1	CC stretching (e), CH e5/e7 twisting
128	1300	63	-7	CC stretching (d), CN stretching (e), N-Ir-C (c/d) rocking
129	1301	15	15	Symmetric CC stretching (e/a), NH/bending in-plane HCN, C*H bending out of HCN plane, CH2 e6 twisting, in-plane aromatic CH bending (a)
130	1304	48	97	Anti-symmetric CC stretching (a/b and c/d), NH/ C*H bending out of HCN plane, in-plane aromatic CH bending (b)
131	1308	28	-94	Symmetric CC stretching (c/d)
132	1309	121	57	Symmetric CC stretching (a/b), NH/ C*H bending in-plane HCN, in-plane aromatic CH bending (a)
133	1334	56	-83	Symmetric CC stretching (a/b/c/d), in-plane aromatic CH bending (c)
134	1335	149	100	Symmetric CC stretching (a/b/c/d), in-plane aromatic CH bending (b)
135	1346	31	-3	Anti-symmetric CC stretching (c/d), in-plane aromatic CH bending (d)
136	1350	23	8	Anti-symmetric CC stretching (a/b/e ring), C*H bending orthogonal to HCN plane in-plane aromatic CH bending (a)
137	1351	40	-21	CH2 e5 rocking, CH2 e6 twisting, C*H bending orthogonal to HCN plane
138	1371	8	13	NH/CH e5/e7 bending, CH2 e6 rocking, CH e8 bending (in-plane HCN)
139	1384	26	17	C*H bending orthogonal to HCN plane, NH2/CH2 e5/6 rocking, CH2 e7 twisting
140	1393	26	-44	NH/CH e7/CH e6 bending
141	1414	60	29	C*H bending orthogonal to HCN plane, NH2 rocking, CH3 wagging, CC stretching (e), CH2 e5 wagging
142	1421	4	-9	C*H bending in-plane HCN, NH2 twisting, CH3 wagging, CC stretching (e), CH2 e5 wagging
143	1429	46	-33	CH e8 bending in-plane HCN, NH2 twisting, CH3 wagging
144	1456	182	-24	Symmetric CC stretching ppy (c/d), in-plane aromatic CH bending (d/c)
145	1462	97	-3	Symmetric CC stretching ppy (a/b), CH CH3 bending, in-plane aromatic CH bending (b/a)
146	1472	33	11	Anti-Symmetric CC stretching ppy (a/b), CH3 asymmetrical bending, in-plane aromatic CH bending (b/a)
147	1473	62	-11	CH3 asymmetrical bending, CH2 e5 scissoring, Symmetric CC stretching ppy (a/b), in-plane aromatic CH bending (b)
148	1474	27	-13	Symmetric CC stretching ppy (c/d), IrC-IrN rocking, in-plane aromatic CH bending (c)
149	1475	29	-7	CHe5 scissoring
150	1488	138	-37	CH3 asymmetrical bending
151	1489	43	36	CH3 asymmetrical bending, anti-symmetric CC stretching ppy (c/d)
152	1494	28	-62	CH2 e6 scissoring, anti-symmetric CC stretching ppy (a/b)
153	1494	42	45	CH2 e6 scissoring
154	1504	174	-68	CH2 e7/e5 scissoring, CC stretching (e)
155	1507	87	4	CH2 e7 scissoring
156	1511	677	739	Anti-symmetric rings stretching (d/a)
157	1514	308	-585	Symmetric rings stretching (a/d)
158	1591	63	5	Symmetric ring stretching (c/d)
159	1593	31	-6	Symmetric ring stretching (b/a)
160	1607	96	-5	Anti-symmetric ring stretching (d/c)

161	1610	99	6	Anti-symmetric ring stretching (a/b)
162	1616	63	11	Ring stretching (e-ring)
163	1626	237	46	Symmetric ring stretching (b/c)
164	1630	196	-42	Anti-symmetric rings stretching (b/c)
165	1642	45	-10	Ring stretching (e-ring)
166	1650	192	24	Ring stretching (d-ring)
167	1651	220	29	Ring stretching (a-ring)
168	1672	130	-28	NH2 scissoring

Tables ESI-4: Normal Mode assignments $^{\Lambda S}$Ir-Me-Campy. Units for dipole strength and rotatory strength are 10^{-40} esu^{2}cm^2 and 10^{-44} esu^{2}cm^2 respectively.

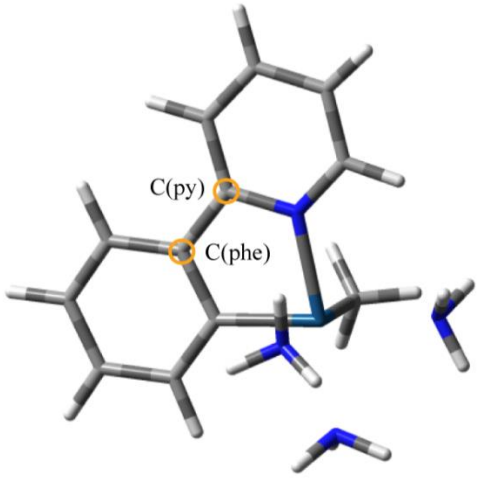
#	Frequencies (cm-^{1})	Dipole strength	Rotatory strength	Normal Mode Descriptions
120	1207	156	-37	C*H bending in-plane HCN, NH2 wagging, CH2 e6/e5 twisting, CC stretching (e)
121	1235	29	51	C*H bending out of HCN plane, NH2 twisting, CH2 e6 twisting, CC stretching (e)
122	1249	19	6	C*H bending out of HCN plane, NH2 twisting, CH2 e6 twisting, CC stretching (e)
123	1254	144	91	C*H bending out of HCN plane, NH2 wagging, CH2 e6 twisting, CC stretching (e)
124	1264	71	-29	CC stretching (c/d/b/a), in-plane CH stretching (c)
125	1267	61	46	CC stretching (c/d/b/a), in-plane CH stretching (b)
126	1282	5	7	C*H bending out of HCN plane, CH2 e5/e7 twisting
127	1289	184	-45	CC stretching (e), NH2/CH2 e7/e5 twisting
128	1296	11	18	C*H bending out of HCN plane, NH2/CH2 e7/e6/e5 twisting, CC stretching (e)
129	1302	42	-4	CCN anti-symmetric stretching a6, CN stretching a2, in-plane aromatic CH bending (a)
130	1304	56	-23	CN anti-symmetric stretching (a), CC stretching (c), in-plane aromatic CH bending (d)
131	1307	97	39	Symmetric rings stretching (b/a), in-plane aromatic CH bending (a)
132	1308	45	-79	CN anti-symmetric stretching (d), CC stretching (d)
133	1335	45	154	Symmetric rings stretching (b/c)
134	1336	195	-153	Symmetric rings stretching (b/c)
135	1348	37	45	Anti-symmetric rings stretching (d/c), C*H bending out of HCN plane, CH2 e7 twisting, in-plane aromatic CH bending (d ring)
136	1348	34	-18	Anti-symmetric rings stretching (a/b), C*H bending out of HCN plane, CH2 e7 twisting, in-plane aromatic CH bending (a)
137	1349	8	-31	C*H bending out of HCN plane, CH2 e7 twisting, CH2 e5, CC stretching (e)
138	1370	1	-2	C*H bending in-plane HCN, NH2/CH2 e5 twisting, CH2 e7/e6 wagging, CC e7/e6 stretching
139	1376	8	14	C*H bending (out of HCN plane), CH2 e7/e6 twisting, NH2/CH2 e5 wagging
140	1385	15	-8	CC e6/e7 stretching, CH2 e6/e7 wagging
141	1414	84	-11	CH3 wagging, CH2 e5 wagging, C*H bending out of HCN plane, CC stretching (e)
142	1425	48	-88	C*H bending in-plane HCN, NH2 twisting, CH3 wagging, CH2 e5 wagging
143	1435	63	-51	C*H bending in-plane HCN, NH2 twisting, CH3 wagging
144	1457	207	44	Symmetric rings stretching (c/d), in-plane aromatic CH bending (d/c)
145	1460	98	-40	Symmetric rings stretching (b/a), in-plane aromatic CH bending (a/b)
146	1472	25	14	CH2 e5 scissoring
147	1473	31	-3	Anti-symmetric rings stretching (b/a), in-plane aromatic CH bending (b)
148	1474	24	16	Anti-symmetric rings stretching (c/d), in-plane aromatic CH bending (c)
149	1480	59	4	CH3 asymmetrical bending
150	1489	83	75	CH3 asymmetrical bending Anti-symmetric rings stretching (d/c)
151	1490	118	-72	CH3 asymmetrical bending, Anti-symmetric rings stretching (d/c)
152	1493	34	33	CH2 e6/e7 scissoring, CC stretching (a/b)
153	1493	9	-46	CH2 >e7/e6 scissoring
154	1499	128	99	CH2 e5/e6/e7 scissoring, CC stretching (e)
155	1502	114	57	CH2 >e6/e7 scissoring
156	1512	695	-714	Anti-symmetric rings stretching (d/a)
157	1514	253	572	Symmetric rings stretching (a/d)
158	1591	60	-66	Symmetric rings stretching (b/a)

159	1592	37	75	Symmetric rings stretching (c/d)
160	1607	100	33	Anti-symmetric rings stretching (d/c)
161	1609	102	-37	Anti-symmetric rings stretching (a/b-ring)
162	1616	69	12	Ring stretching (e)
163	1626	232	-54	Symmetric ring stretching (b/c)
164	1630	211	43	Anti-symmetric rings stretching (c/b)
165	1640	52	0	Ring stretching (e)
166	1651	162	25	Ring stretching (d)
167	1651	246	-71	Ring stretching (a)
168	1666	84	36	NH_2 scissoring

6. *ppy*-model

In order to isolate the dipole strength of the *ppy*-moiety few models were tested; here we report the one which provided frequencies and dipole strength values closest to what observed for Ir-Me-Campy and thus the best fitting with experiments (see Table 2): the *ppy* was coordinated to an octahedral Ir(III) whose coordination sphere was saturated with three NH_3 molecules and a CH_3 *cis* to the orthometallated phenyl ring.

Figure ESI-4: the simulated *ppy*-model for building Table 2.



7. XYZ coordinates of optimized structures

7.1. $^{\Lambda S}$Ir-Me-Campy half-chair (C24)

Center Number	Atom	Coordinates (Angstroms) X	Y	Z
1	Ir	-0.296301	-0.050855	-0.039659
2	Cl	1.488156	0.506283	4.342651
3	N	-0.353277	1.973154	0.464615
4	N	-0.460496	-2.064157	-0.543624
5	N	1.336717	-0.682084	1.327674
6	H	1.174578	-0.422832	2.316317
7	H	1.375658	-1.701772	1.309035
8	N	1.684469	0.262271	-1.274076
9	C	0.354641	2.548824	1.459612
10	H	0.950957	1.893277	2.083024
11	C	0.296596	3.910285	1.728967
12	H	0.884127	4.315996	2.544624
13	C	-0.532185	4.715179	0.942714
14	H	-0.59709	5.784541	1.118125
15	C	-1.292533	4.121247	-0.057681

16	H	-1.961716	4.721786	-0.662011
17	C	-1.210052	2.738631	-0.28242
18	C	-2.010241	1.98621	-1.250937
19	C	-2.985445	2.579721	-2.073624
20	H	-3.162941	3.650866	-2.040638
21	C	-3.744932	1.793773	-2.937453
22	H	-4.499215	2.25064	-3.571263
23	C	-3.533363	0.407759	-2.967261
24	H	-4.13198	-0.215377	-3.627633
25	C	-2.560039	-0.179244	-2.153964
26	H	-2.421899	-1.25572	-2.207112
27	C	-1.757315	0.588453	-1.289508
28	C	0.102643	-4.037473	-1.792645
29	H	0.703206	-4.490206	-2.573345
30	C	0.257471	-2.689441	-1.500303
31	H	0.970585	-2.076428	-2.035393
32	C	-0.833472	-4.776041	-1.060602
33	H	-0.982187	-5.832853	-1.25878
34	C	-1.574288	-4.137972	-0.073722
35	H	-2.304651	-4.692633	0.502924
36	C	-1.383673	-2.770333	0.181425
37	C	-2.102035	-1.977534	1.179342
38	C	-3.074641	-2.516933	2.041945
39	H	-3.330162	-3.57164	1.99776
40	C	-3.718906	-1.699883	2.96665
41	H	-4.467804	-2.115566	3.633991
42	C	-3.388598	-0.338679	3.027898
43	H	-3.885494	0.305213	3.74919
44	C	-2.422842	0.199787	2.173212
45	H	-2.189947	1.256775	2.251484
46	C	-1.751874	-0.600869	1.233209
47	C	2.662596	-0.140127	0.956211
48	C	3.818888	-0.91709	1.59815
49	H	3.688108	-0.885434	2.683912
50	H	3.77309	-1.970597	1.286192
51	C	5.158172	-0.306239	1.180638
52	H	5.986846	-0.811822	1.687001
53	H	5.190266	0.745413	1.49379
54	C	5.336281	-0.408152	-0.337406
55	H	6.168213	0.220886	-0.673847
56	H	5.611467	-1.439657	-0.60051
57	C	4.090741	-0.046055	-1.127531
58	C	4.190781	0.216296	-2.496403
59	C	3.051321	0.511325	-3.228193
60	C	1.799332	0.521137	-2.601765
61	C	2.810505	0.006429	-0.550628
62	H	2.693714	0.876468	1.368312
63	H	5.163202	0.192665	-2.981818
64	H	3.114234	0.729955	-4.288648
65	C	0.576137	0.819153	-3.421057
66	H	-0.126415	-0.017712	-3.411857
67	H	0.038152	1.686298	-3.031757
68	H	0.861729	1.021368	-4.45572

7.2. $^{\Lambda S}$Ir-Me-Campy half-chair (C25)

Center Number	Atom	Coordinates (Angstroms) X	Y	Z
1	Ir	0.26853	-0.051847	0.029089
2	C	1.752848	-0.062144	1.40445
3	C	2.245565	-1.154853	2.141389
4	C	2.375988	1.195723	1.624333
5	C	3.27556	-1.00574	3.074957
6	H	1.816437	-2.142397	1.996273
7	C	3.408002	1.34884	2.568011
8	C	3.856646	0.250438	3.298873
9	H	3.629353	-1.870984	3.630689
10	H	3.870227	2.317894	2.733458
11	H	4.655134	0.367279	4.025624
12	C	1.590528	-0.759169	-1.30781
13	C	2.511378	-0.027	-2.07683
14	C	1.548881	-2.166193	-1.502905
15	C	3.344617	-0.65721	-3.004857
16	H	2.580817	1.049731	-1.963216
17	C	2.388517	-2.79762	-2.439686

18	C	3.286644	-2.045531	-3.191461
19	H	4.042044	-0.062694	-3.589568
20	H	2.344668	-3.872793	-2.586944
21	H	3.933574	-2.531327	-3.91565
22	N	0.907791	1.927999	-0.106376
23	C	1.883016	2.290637	0.785313
24	C	0.457834	2.831298	-1.003012
25	C	2.352326	3.612505	0.811522
26	C	0.901103	4.147734	-1.024534
27	H	-0.242404	2.477665	-1.751465
28	C	1.855453	4.550167	-0.086428
29	H	3.113151	3.89545	1.529026
30	H	0.507253	4.828764	-1.770293
31	H	2.218898	5.57293	-0.067226
32	N	-0.148938	-2.090842	0.16596
33	C	-1.055935	-2.651863	0.993378
34	C	0.586955	-2.8881	-0.670764
35	C	-1.28542	-4.020123	1.038153
36	H	-1.603218	-1.972393	1.633015
37	C	0.387663	-4.27812	-0.667081
38	C	-0.547981	-4.849161	0.186119
39	H	-2.024306	-4.418314	1.724145
40	H	0.971025	-4.903206	-1.332182
41	H	-0.70036	-5.923884	0.190387
42	N	-1.633559	0.542972	1.303881
43	C	-1.76915	0.524369	2.651308
44	C	-2.754039	0.57597	0.527098
45	C	-3.039814	0.455923	3.242266
46	C	-4.045659	0.439277	1.053062
47	C	-4.170406	0.372167	2.445614
48	H	-3.12014	0.442021	4.323885
49	H	-5.153761	0.263555	2.896083
50	C	-5.257981	0.323659	0.153736
51	C	-2.532218	0.856046	-0.951774
52	H	-2.184641	1.893336	-1.002626
53	N	-1.395826	0.04512	-1.455011
54	H	-1.713106	-0.906105	-1.645201
55	H	-1.115415	0.43905	-2.370132
56	C	-3.806769	0.754825	-1.82497
57	H	-4.241139	1.757154	-1.922645
58	H	-3.509066	0.454277	-2.833366
59	C	-4.868172	-0.177719	-1.238878
60	H	-5.746054	-0.204375	-1.892728
61	H	-4.48967	-1.206763	-1.169619
62	H	-5.987464	-0.342572	0.627957
63	H	-5.747654	1.303872	0.061506
64	C	-0.552428	0.579687	3.531209
65	H	0.021212	-0.35	3.485618
66	H	0.119414	1.383158	3.223561
67	H	-0.851514	0.74852	4.568236
68	Cl	-0.9481	1.712725	-4.216142

7.3. $^{\Lambda S}$Ir-Me-Campy (boat)

Center Number	Atom	Coordinates (Angstroms) X	Y	Z
1	Ir	-0.317211	-0.049207	-0.044732
2	N	-0.084666	1.80649	0.875542
3	C	-0.857399	2.815332	0.362691
4	C	0.746322	2.062642	1.908102
5	C	-0.742964	4.115527	0.87714
6	C	0.886841	3.331367	2.45653
7	H	1.283423	1.221484	2.330467
8	C	0.135384	4.380941	1.921302
9	H	-1.349213	4.910787	0.460479
10	H	1.565645	3.4784	3.288793
11	H	0.223329	5.386768	2.320201
12	N	-0.74438	-1.867131	-0.955965
13	C	-0.121036	-2.347147	-2.052311
14	C	-1.734399	-2.601323	-0.358683
15	C	-0.445033	-3.571279	-2.620738
16	H	0.656575	-1.717948	-2.465899
17	C	-2.095873	-3.848086	-0.893991
18	C	-1.454746	-4.336148	-2.026052

19	H	0.084327	-3.911283	-3.503518
20	H	-2.878938	-4.427444	-0.419935
21	H	-1.735679	-5.299344	-2.440354
22	N	1.63394	0.355156	-1.242112
23	C	1.787172	0.989022	-2.438158
24	C	2.745324	-0.032351	-0.571653
25	C	3.060569	1.261388	-2.948148
26	C	4.05075	0.228496	-1.022427
27	C	4.198201	0.89139	-2.237604
28	H	3.147446	1.765016	-3.904812
29	H	5.188761	1.109272	-2.628036
30	C	5.201229	-0.220643	-0.159065
31	C	2.642912	-0.778629	0.739583
32	H	2.988445	-0.105327	1.53475
33	N	1.252691	-1.151472	1.087117
34	H	1.111385	-2.14048	0.882899
35	H	1.16704	-1.064485	2.113752
36	C	3.578916	-2.011813	0.737531
37	H	3.562402	-2.437087	1.745391
38	H	3.141801	-2.760156	0.064934
39	C	5.03043	-1.68865	0.294209
40	H	5.731475	-1.890032	1.109652
41	H	5.312451	-2.346729	-0.534077
42	H	6.148189	-0.090898	-0.691761
43	H	5.252308	0.424873	0.7291
44	C	-1.711916	1.02109	-1.048591
45	C	-1.780313	2.395809	-0.694418
46	C	-2.630075	0.565377	-2.01291
47	C	-2.694152	3.268736	-1.313849
48	C	-3.541945	1.429818	-2.624353
49	H	-2.633213	-0.481464	-2.304362
50	C	-3.57252	2.789889	-2.283219
51	H	-2.731592	4.319402	-1.040452
52	H	-4.23437	1.044595	-3.369266
53	H	-4.27957	3.462317	-2.760004
54	C	-1.8021	-0.68787	1.153364
55	C	-2.345454	-0.040046	2.275792
56	C	-2.326893	-1.966866	0.819747
57	C	-3.355202	-0.632928	3.03894
58	H	-1.977384	0.938297	2.568116
59	C	-3.343331	-2.561655	1.590419
60	C	-3.858915	-1.896619	2.699579
61	H	-3.751788	-0.108819	3.904886
62	H	-3.733704	-3.541682	1.331755
63	H	-4.642232	-2.355279	3.295486
64	C	0.575911	1.392325	-3.231163
65	H	-0.132498	0.56733	-3.329733
66	H	0.039229	2.213481	-2.748549
67	H	0.876369	1.718475	-4.229535
68	Cl	1.839268	-0.611585	4.220963

7.4. $^{\Delta S}$Ir-Me-Campy half-chair (C24)

Center Number	Atom	Coordinates (Angstroms) X	Y	Z
1	Ir	0.329754	-0.06794	-0.011237
2	N	0.491963	1.958239	0.47408
3	N	0.449849	-2.07669	-0.526022
4	N	-1.388533	-0.60984	1.315882
5	H	-1.092146	-1.36654	1.931963
6	H	-1.732128	0.12402	1.956358
7	N	-1.591507	0.360797	-1.270204
8	C	-0.31821	2.627046	1.321041
9	H	-1.125567	2.075764	1.78841
10	C	-0.136577	3.97051	1.626826
11	H	-0.818006	4.450656	2.319825
12	C	0.926649	4.656995	1.036272
13	H	1.10153	5.706147	1.25383
14	C	1.763671	3.973089	0.161956
15	H	2.594253	4.485332	-0.308424
16	C	1.539669	2.616948	-0.11754
17	C	2.338496	1.797693	-1.031337
18	C	3.446962	2.292142	-1.742731
19	H	3.770314	3.32199	-1.621217
20	C	4.146878	1.462235	-2.615843

21	H	5.003071	1.843713	-3.164291
22	C	3.734275	0.131926	-2.773677
23	H	4.275793	-0.524788	-3.450552
24	C	2.63445	-0.359683	-2.06404
25	H	2.35045	-1.397685	-2.210311
26	C	1.90044	0.454113	-1.180398
27	C	-0.029781	-3.98304	-1.904757
28	H	-0.549223	-4.387409	-2.766051
29	C	-0.169626	-2.639842	-1.585161
30	H	-0.78634	-1.976691	-2.179541
31	C	0.786347	-4.780592	-1.094593
32	H	0.916711	-5.836468	-1.309863
33	C	1.438926	-4.201118	-0.013328
34	H	2.086672	-4.79921	0.616245
35	C	1.273222	-2.834253	0.262029
36	C	1.935313	-2.086562	1.332903
37	C	2.792736	-2.681272	2.277268
38	H	2.987824	-3.749542	2.253334
39	C	3.400543	-1.901378	3.257632
40	H	4.061194	-2.359549	3.987472
41	C	3.149699	-0.52251	3.292971
42	H	3.620562	0.092181	4.056054
43	C	2.297293	0.070968	2.357179
44	H	2.121929	1.140414	2.416945
45	C	1.665441	-0.690308	1.359125
46	C	-2.516467	-1.093449	0.480874
47	C	-3.795523	-1.359168	1.286806
48	H	-3.608781	-2.195252	1.970493
49	H	-4.022041	-0.483077	1.905436
50	C	-4.967895	-1.665441	0.351622
51	H	-5.860144	-1.92305	0.931663
52	H	-4.732517	-2.536517	-0.275282
53	C	-5.254294	-0.448294	-0.532495
54	H	-5.985883	-0.693263	-1.310711
55	H	-5.710265	0.3426	0.079564
56	C	-4.006521	0.112663	-1.187381
57	C	-4.109296	0.927797	-2.319077
58	C	-2.963596	1.430057	-2.915899
59	C	-1.704939	1.132516	-2.378486
60	C	-2.719572	-0.144731	-0.693063
61	H	-2.189326	-2.048025	0.049975
62	H	-5.088075	1.155207	-2.733547
63	H	-3.027118	2.05	-3.803671
64	Cl	-2.781169	1.430487	3.586593
65	C	-0.47075	1.662658	-3.050942
66	H	0.020758	2.42263	-2.437825
67	H	0.257828	0.867996	-3.223009
68	H	-0.732704	2.117734	-4.00878

7.5. $^{\Delta S}$Ir-Me-Campy half-chair (C25)

Center Number	Atom	Coordinates (Angstroms) X	Y	Z
1	Ir	0.337609	-0.06442	-0.050063
2	C	1.662673	-0.595354	1.366384
3	C	2.044174	0.131187	2.506884
4	C	2.222545	-1.891867	1.198403
5	C	2.934097	-0.402928	3.443369
6	H	1.641278	1.124376	2.678014
7	C	3.117193	-2.42728	2.143744
8	C	3.474354	-1.684464	3.266038
9	H	3.207302	0.181552	4.318343
10	H	3.535507	-3.420831	2.010191
11	H	4.163521	-2.096954	3.996749
12	C	1.844124	0.916174	-0.984374
13	C	2.807846	0.391517	-1.866015
14	C	1.959866	2.292926	-0.651573
15	C	3.822944	1.188764	-2.403125
16	H	2.773211	-0.656768	-2.147641
17	C	2.983223	3.095048	-1.189017
18	C	3.915733	2.546444	-2.066696
19	H	4.548493	0.75065	-3.084539
20	H	3.060384	4.146429	-0.927098
21	H	4.706254	3.165154	-2.481008
22	N	0.906353	-1.920411	-0.783453

23	C	1.809679	-2.602075	-0.013608
24	C	0.492352	-2.4448	-1.956889
25	C	2.273414	-3.859794	-0.431494
26	C	0.929358	-3.678839	-2.41766
27	H	-0.204629	-1.840708	-2.525582
28	C	1.833277	-4.403134	-1.632193
29	H	2.983987	-4.399317	0.183011
30	H	0.567483	-4.056978	-3.367002
31	H	2.193922	-5.373897	-1.957496
32	N	0.022027	1.868177	0.676566
33	C	-0.973416	2.236336	1.510111
34	C	0.93245	2.804438	0.258095
35	C	-1.122682	3.539928	1.967648
36	H	-1.654971	1.465355	1.848378
37	C	0.822918	4.133126	0.694109
38	C	-0.206211	4.507793	1.550485
39	H	-1.9383	3.77346	2.642398
40	H	1.545852	4.866761	0.358603
41	H	-0.290016	5.535909	1.888971
42	N	-1.536243	0.207683	-1.42698
43	C	-1.718105	1.119867	-2.409248
44	C	-2.616534	-0.467815	-0.937728
45	C	-3.006453	1.419208	-2.875993
46	C	-3.9299	-0.182017	-1.327753
47	C	-4.108772	0.794601	-2.315539
48	H	-3.125957	2.155819	-3.663439
49	H	-5.112324	1.052714	-2.643981
50	C	-5.114689	-0.875	-0.689005
51	C	-2.299727	-1.607669	0.01893
52	H	-1.752251	-2.350757	-0.570434
53	N	-1.325199	-1.117609	1.029432
54	H	-1.813284	-0.597207	1.777692
55	H	-0.92403	-1.922988	1.509712
56	C	-3.541449	-2.31745	0.608029
57	H	-3.782305	-3.175338	-0.033175
58	H	-3.278257	-2.723482	1.590109
59	C	-4.769795	-1.410635	0.702591
60	H	-5.617032	-1.972292	1.110344
61	H	-4.568703	-0.582462	1.391998
62	H	-5.952744	-0.17046	-0.642982
63	H	-5.444356	-1.70469	-1.331748
64	Cl	-2.877536	0.121359	3.686652
65	C	-0.530932	1.812199	-3.01696
66	H	-0.172075	2.623482	-2.376662
67	H	0.3017	1.121211	-3.156078
68	H	-0.805288	2.243994	-3.982501

7.6. $^{\Delta S}$Ir-Me-Campy (boat)

Center Number	Atom	Coordinates (Angstroms) X	Y	Z
1	Ir	0.295466	0.071407	0.010612
2	N	0.031343	2.120085	0.283591
3	C	0.764571	2.917084	-0.554199
4	C	-0.750562	2.684383	1.22804
5	C	0.6666	4.314155	-0.452603
6	C	-0.871755	4.058929	1.37657
7	H	-1.281722	1.999699	1.876676
8	C	-0.153254	4.889887	0.509934
9	H	1.243102	4.940882	-1.122245
10	H	-1.513216	4.460775	2.15256
11	H	-0.225957	5.969838	0.59139
12	N	0.82174	-1.936179	-0.225898
13	C	0.196638	-2.817023	-1.034568
14	C	1.909689	-2.344839	0.502326
15	C	0.608269	-4.138026	-1.163245
16	H	-0.637126	-2.452921	-1.621908
17	C	2.363777	-3.668167	0.403574
18	C	1.71436	-4.572191	-0.429344
19	H	0.070503	-4.796102	-1.8361
20	H	3.224012	-3.981954	0.982469
21	H	2.066275	-5.596272	-0.506769
22	N	-1.59613	-0.489764	1.231158
23	C	-1.68178	-1.025067	2.479151

24	C	-2.734463	-0.07087	0.62547
25	C	-2.910729	-1.102917	3.142483
26	C	-3.986301	-0.066964	1.262301
27	C	-4.063874	-0.604932	2.545085
28	H	-2.947597	-1.541354	4.133805
29	H	-5.014813	-0.63428	3.070274
30	C	-5.155259	0.552612	0.541387
31	C	-2.689073	0.489833	-0.782833
32	H	-2.756259	1.582157	-0.688997
33	N	-1.39587	0.191935	-1.451504
34	H	-1.500211	-0.631913	-2.063979
35	H	-1.185667	0.946821	-2.102982
36	C	-3.88834	-0.004418	-1.632309
37	H	-3.90874	0.591	-2.550497
38	H	-3.668137	-1.029099	-1.943669
39	C	-5.260365	0.048643	-0.911403
40	H	-5.957197	0.689676	-1.460158
41	H	-5.699275	-0.954325	-0.901649
42	H	-6.083299	0.356391	1.087228
43	H	-5.02297	1.644343	0.535275
44	C	1.608862	0.769252	-1.344166
45	C	1.627416	2.18423	-1.482085
46	C	2.445291	0.026755	-2.195488
47	C	2.440071	2.813103	-2.444028
48	C	3.253745	0.654036	-3.147616
49	H	2.466156	-1.056163	-2.126742
50	C	3.253488	2.050068	-3.277343
51	H	2.441704	3.894347	-2.547228
52	H	3.886216	0.052017	-3.795229
53	H	3.87996	2.533881	-4.020631
54	C	1.83446	-0.052809	1.320913
55	C	2.350488	0.961321	2.149491
56	C	2.493669	-1.310819	1.358421
57	C	3.45249	0.739671	2.98137
58	H	1.890844	1.945275	2.154251
59	C	3.604833	-1.533335	2.191476
60	C	4.086564	-0.510176	3.005512
61	H	3.822771	1.545258	3.611098
62	H	4.099079	-2.500466	2.21109
63	H	4.945211	-0.681367	3.648008
64	Cl	-1.798541	-2.101462	-3.880729
65	C	-0.441715	-1.539457	3.152947
66	H	0.04199	-2.310211	2.548238
67	H	0.288805	-0.741515	3.305575
68	H	-0.694621	-1.972163	4.123368

7.7. $^{\Lambda S}$Ir-H-Campy half-chair (C24)

Center Number	Atom	Coordinates (Angstroms) X	Y	Z
1	Ir	-0.302327	-0.036703	-0.046589
2	Cl	1.636267	0.21767	4.322302
3	N	-0.153173	1.966802	0.505838
4	N	-0.668806	-2.01115	-0.595886
5	N	1.303707	-0.859154	1.28596
6	H	1.205175	-0.627569	2.289457
7	H	1.266239	-1.877232	1.226167
8	N	1.557879	0.167028	-1.258379
9	C	0.512102	2.426868	1.586497
10	H	0.9598	1.688208	2.243838
11	C	0.598906	3.781104	1.88577
12	H	1.143253	4.095939	2.768803
13	C	-0.028944	4.698216	1.038603
14	H	0.023687	5.764106	1.237689
15	C	-0.740454	4.224582	-0.057939
16	H	-1.253946	4.916797	-0.714451
17	C	-0.809683	2.847009	-0.312468
18	C	-1.57581	2.216255	-1.39167
19	C	-2.328465	2.941561	-2.333048
20	H	-2.349622	4.027338	-2.308828
21	C	-3.062396	2.270406	-3.309231
22	H	-3.644799	2.830067	-4.035144
23	C	-3.044175	0.869021	-3.340003
24	H	-3.620256	0.337943	-4.094062

25	C	-2.291862	0.148163	-2.406955
26	H	-2.299361	-0.936872	-2.460068
27	C	-1.53119	0.795251	-1.415537
28	C	-0.27296	-4.012299	-1.86562
29	H	0.299538	-4.510891	-2.639463
30	C	0.006746	-2.690975	-1.546506
31	H	0.786798	-2.144017	-2.059792
32	C	-1.29616	-4.664608	-1.168799
33	H	-1.54251	-5.699042	-1.386868
34	C	-1.99789	-3.968742	-0.192831
35	H	-2.79562	-4.455459	0.355113
36	C	-1.681367	-2.629643	0.089569
37	C	-2.352594	-1.78131	1.074101
38	C	-3.414728	-2.228823	1.882575
39	H	-3.776641	-3.250308	1.808143
40	C	-4.01452	-1.36094	2.790644
41	H	-4.83332	-1.704515	3.415663
42	C	-3.549261	-0.041522	2.889017
43	H	-4.01234	0.642049	3.59641
44	C	-2.493913	0.403159	2.08843
45	H	-2.15886	1.430136	2.195188
46	C	-1.862277	-0.448967	1.164432
47	C	2.648069	-0.388613	0.865248
48	C	3.797516	-1.267958	1.371342
49	H	3.759894	-1.293962	2.464422
50	H	3.66349	-2.296834	1.007737
51	C	5.136164	-0.70603	0.878217
52	H	5.968326	-1.286558	1.289209
53	H	5.254517	0.320199	1.249365
54	C	5.20758	-0.718609	-0.654894
55	H	6.049724	-0.112475	-1.007221
56	H	5.406951	-1.743197	-1.000033
57	C	3.933666	-0.246325	-1.331325
58	C	3.929913	0.087297	-2.691372
59	C	2.74491	0.469911	-3.315389
60	C	1.572879	0.484781	-2.566237
61	H	0.61688	0.745453	-3.006143
62	C	2.714182	-0.169014	-0.637396
63	H	2.767649	0.599374	1.328394
64	H	4.857542	0.045723	-3.256301
65	H	2.719347	0.741436	-4.365129

7.7. $^{\Delta S}$Ir-H-Campy half-chair (C24)

Center Number	Atom	Coordinates (Angstroms) X	Y	Z
1	Ir	0.32975	-0.046778	-0.022027
2	N	0.219421	1.971461	0.506621
3	N	0.680718	-2.016477	-0.579947
4	N	-1.361703	-0.843036	1.239632
5	H	-1.033646	-1.654207	1.762943
6	H	-1.734877	-0.209173	1.965662
7	N	-1.483629	0.280028	-1.264723
8	C	-0.570176	2.48234	1.47431
9	H	-1.186314	1.792077	2.039883
10	C	-0.60296	3.83967	1.771629
11	H	-1.25403	4.191276	2.563871
12	C	0.210452	4.708726	1.040962
13	H	0.210057	5.774974	1.245293
14	C	1.027805	4.185828	0.04521
15	H	1.670552	4.839959	-0.531484
16	C	1.030221	2.807705	-0.215296
17	C	1.854589	2.136674	-1.223643
18	C	2.748808	2.818135	-2.06993
19	H	2.860556	3.896696	-2.006475
20	C	3.506404	2.112284	-3.001706
21	H	4.19784	2.637664	-3.653816
22	C	3.367905	0.719845	-3.084917
23	H	3.958842	0.160717	-3.80647
24	C	2.478933	0.042836	-2.244522
25	H	2.402882	-1.036527	-2.335482
26	C	1.694446	0.726188	-1.296111
27	C	0.375231	-3.9518	-1.968893
28	H	-0.122067	-4.403698	-2.819547
29	C	0.095891	-2.63628	-1.627233

30	H	-0.606364	-2.041248	-2.198709
31	C	1.302149	-4.659393	-1.194731
32	H	1.54407	-5.691579	-1.427844
33	C	1.919382	-4.020291	-0.126865
34	H	2.650461	-4.547321	0.474286
35	C	1.609569	-2.683566	0.17326
36	C	2.216695	-1.878522	1.234288
37	C	3.174081	-2.381791	2.135236
38	H	3.491694	-3.419473	2.085847
39	C	3.724786	-1.548492	3.105193
40	H	4.462222	-1.935031	3.802292
41	C	3.317517	-0.208054	3.171724
42	H	3.745058	0.448241	3.925794
43	C	2.364763	0.291903	2.279708
44	H	2.069398	1.333451	2.362603
45	C	1.782253	-0.524795	1.293829
46	C	-2.466714	-1.279341	0.339948
47	C	-3.78901	-1.557116	1.066615
48	H	-3.64803	-2.402004	1.749544
49	H	-4.054968	-0.690338	1.682752
50	C	-4.899233	-1.853764	0.051941
51	H	-5.823803	-2.12537	0.571436
52	H	-4.617296	-2.717175	-0.566017
53	C	-5.149502	-0.633652	-0.843179
54	H	-5.813928	-0.891035	-1.675635
55	H	-5.671764	0.13958	-0.262261
56	C	-3.873026	-0.02717	-1.392638
57	C	-3.904164	0.838761	-2.493378
58	C	-2.727083	1.4121	-2.967207
59	C	-1.532724	1.113198	-2.319006
60	H	-0.588241	1.539943	-2.637486
61	C	-2.625782	-0.287472	-0.803311
62	H	-2.131586	-2.21945	-0.117713
63	H	-4.853444	1.059647	-2.974271
64	H	-2.726685	2.082705	-3.819635
65	Cl	-2.655299	0.78333	3.830464

7.8. *ppy*-model

Center Number	Atom	Coordinates (Angstroms) X	Y	Z
1	Ir	0.375158	-0.580254	-0.351338
2	N	-0.187958	1.393767	-0.254494
3	N	2.489726	-0.245459	-1.094605
4	H	2.530288	0.471823	-1.816651
5	H	3.150413	0.021368	-0.347446
6	N	1.136921	-0.466663	1.781734
7	C	0.625301	2.443377	-0.498192
8	H	1.652953	2.207915	-0.741318
9	C	0.193771	3.761214	-0.434686
10	H	0.892314	4.564185	-0.640515
11	C	-1.141309	4.011531	-0.101494
12	H	-1.517797	5.028069	-0.045715
13	C	-1.980421	2.936765	0.165501
14	H	-3.015573	3.109456	0.434848
15	C	-1.494781	1.621644	0.092589
16	C	-2.26147	0.407472	0.377875
17	C	-3.613163	0.420804	0.76629
18	H	-4.154358	1.358126	0.860881
19	C	-4.276973	-0.774442	1.034749
20	H	-5.320602	-0.76584	1.33474
21	C	-3.580953	-1.985168	0.910668
22	H	-4.090682	-2.923905	1.114937
23	C	-2.23769	-1.996632	0.522365
24	H	-1.74822	-2.96403	0.431208
25	C	-1.529052	-0.80911	0.244625
26	Cl	4.348032	0.360663	1.558157
27	C	-0.247447	-0.694696	-2.34591
28	H	0.582772	-0.485023	-3.037338
29	H	-0.639936	-1.691876	-2.600929
30	H	-1.048422	0.022358	-2.569479
31	N	0.824932	-2.670708	-0.409843
32	H	1.823109	-2.881625	-0.418039

33	H	0.438803	-3.172213	0.388763
34	H	2.876999	-1.080412	-1.533105
35	H	0.426784	-3.099708	-1.246049
36	H	0.625331	0.247478	2.297033
37	H	1.015806	-1.332801	2.303381
38	H	2.136123	-0.21818	1.8293
