Supporting Information

An 18+ δ Iridium Dimer Releasing Metalloradical Spontaneously

Tsun-Ren Chen,*[, a] Hsiu-Pen Lee,[a] Jhy-Der Chen[b] and Kelvin H.-C. Chen [a]

[a] *Department of Chemical Biology, National Pingtung University of Education, Pingtung, Taiwan,90003, R.O.C., and* [b] *Department of Chemistry, Chung-Yuan Christian University, Chung-Li,*

* To whom correspondence should be addressed. Fax: 886-8-723-0305 Phone: 886-8-722-6141-6316. Email: trchen@mail.npue.edu.tw

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Contents

Notation and formulas

dfpboH $C_{13}H_7F_2NO$
[(dfpbo)$_2$Ir(μ-Cl)]$_2$ $C_{52}H_{24}F_8Cl_2Ir_2N_4O_4$
1 $C_{52}H_{24}N_4O_4ClF_8Ir_2$
4 $C_{41}H_{23}F_4IrN_2O_4$
5 $C_{33}H_{15}N_2O_3Br_2F_4Ir$

Experimental

General

2,4-Difluorobenzoic acid was purchased from Matrix, and $IrCl_3.nH_2O$ was from Seedchem Co. All other chemicals were purchased from Acros and used as received. NMR spectra were measured on a Bruker Advance-400 MHz or a Mercury 300 MHz NMR spectrometer. Elemental analyses (CHN) were obtained from an Elementar vario EL Ⅲ analyzer. Mass spectra were taken with a Finnigan/Thermo Quest MAT 95XL instrument with electron impact ionization for organic compounds or fast atom bombardment for metal complexes. X-ray absorption spectroscopy data were collected at the wiggler beam line 17C of National Synchrotron Radiation Research Center (NSRRC) in Hsinchu. A Si(111) double crystal monochromator was employed for energy scanning. All samples were loaded into aluminum holders covered with sheets of Kapton. Fluorescence data were obtained at room temperature using an

Ar-filled ionization chamber detector. Typically, each sample was scanned 3 times for averaging. Data reduction included energy calibration, pre-edge background subtraction using a linear function, and normalization with respect to the edge jump step.

Synthesis

Synthesis of 2-(3.5-difluorophenyl)benzoxazole, (dfpboH):

The benzoxazole derivative ligand, dfpboH**,** was prepared by Philips' condensation[1] (as shown in Scheme S 1) as follows: one equiv of 3.5-difluorobenzoic acid and 1.05 equiv of an 2-aminophenol were added to polyphosphoric acid (10 g/mmol of 3.5-difluorobenzoic acid), and then the mixture was stirred at 200 ℃ for 5 hours. After cooling to room temperature, the mixture was slowly poured into pure water and well stirred; the precipitate was collected by filtration, washed with pure water (3 × 100 mL), and dried to yield a crude product. The crude product was purified by column chromatography over silica gel using n-hexane-CH_2Cl_2 (1:1~1:5) as eluent to obtain the pure product.

Yield: 85%. ^{1}H NMR (300 MHz, $CDCl_3$, 298 K; δ (ppm)): 7.74−7.80 (m, 3H), 7.56−7.59 (m, 1H), 7.36−7.41 (m, 2H), 6.96−7.00 (m, 1H). ^{13}C NMR (75 MHz, $CDCl_3$, 298 K; δ (ppm)): 165.1, 164.9, 161.8, 161.7, 160.9, 151.0, 141.9, 130.4, 130.3, 130.1, 126.1, 125.2, 120.6, 110.9, 110.8, 110.7, 110.6, 107.3, 107.0, 106.7. Anal. Calcd for $C_{13}H_7F_2NO$ (MW = 231.20): C, 67.53; H, 3.05; N, 6.06. Found: C, 67.50; H, 3.08; N, 5.99%. MS (FAB; m/z): 231.0496

Synthesis of $[(dfpbo)_2Ir(\mu\text{-}Cl)]_2$:

The cyclometalated Ir(III) chloro-bridged dimer,$[(dfpbo)_2Ir(\mu\text{-}Cl)]_2$, was synthesized according to previous papers.[2,3] A mixture of 2-ethoxylethanol and water (3:1, v/v) was added to a flask containing iridium trichloride ($IrCl_3 \cdot 3H_2O$, 2 mmol) and dfpboH (5 mmol), and then the mixture was refluxed

for 24 hours under nitrogen. After cooling to room temperature, the mixture was poured into 20 mL of pure water, and the dimer precipitate was filtered off, washed with deionized water, and followed by drying at 60℃ in a vacuum oven.

Yield: 75%. ^{1}H NMR (300 MHz, DMSO-d^{6}, 298 K; δ (ppm)): 8.18 (d, *J* = 8.18, 8.1 Hz, 4H), 7.31 (dd, *J* = 7.6, 2.7 Hz, 4H), 7.12−7.22 (m, 8H), 6.99 (dt, *J* = 7.1, 1.5 Hz, 4H), 6.14 (dt, *J* = 9.6, 2.7 Hz, 4H). ^{13}C NMR (75 MHz, $CDCl_3$, 298 K; δ (ppm)): 174.9, 169.2, 169.1, 167.5, 167.4, 160.3, 160.2, 158.7, 158.6, 149.1, 140.8, 133.6, 133.5, 133.4, 133.3, 125.1, 124.4, 118.0, 115.3, 115.0, 110.9, 108.6, 108.4, 107.2, 107.0, 106.8, 31.8, 31.1, 22.8, 14.3. Anal. Calcd for $C_{52}H_{24}F_8Cl_2Ir_2N_4O_4$ (MW = 1376.12): C, 45.38; H, 1.76; N, 4.07. Found: C, 44.89; H, 1.70; N, 3.98%. MS (FAB; m/z): 1376.0319

Synthesis of compound 1, $[(dfpbo)_2Ir]_2(\mu\text{-}Cl)$:

A flask was charged with 500 mg of [(fpbo)2Ir (μ-Cl)]2 (0.363 mmol) and 55 mg of anhydrous potassium carbonate (0.40 mmol). Toluene (15 ml) and ethoxyethanol (0.5 ml) were added to give a clear yellow solution, and the solution was stirred under N2 and warmed to 100℃ for 24 h. After cooling to room temperature, the reaction mixture was filtered through silica gel. The filtrate was purified via column chromatography over silica gel using n-hexane-toluene (3:1 ratio) as eluent to obtain the pure product.

Experimental data For **1**: Yield: 293 mg (60% based on iridium). Anal. Calcd for $C_{52}H_{24}N_4O_4ClF_8Ir_2\cdot CH_2Cl_2$: C, 44.65; H, 1.84; N, 3.93. Found: C, 44.75; H, 1.67; N, 3.78%. MS (FAB; m/z): 1341.0605

Synthesis of compound 4, $[(dfpbo)_2Ir(dbm)]$ (dbm = dibenzoylmethanate):

A mixture of chalcone (312 mg, 1.5 mmol) and compound **1** (50 mg, 0.037 mmol) in toluene (30 ml) was stirred under N_2 at 110 ℃ for 2 d. The final

solution was taken to dryness in vacuo. The residue was purified via column chromatography.

Experimental data For **4**: Yield: 14 mg (43% based on iridium). 1H NMR (300 MHz, $CDCl_3$, 298 K; δ (ppm)): 7.84−7.87 (m, 4H), 7.60 (d, *J* = 8.1 Hz, 2H), 7.32−7.45 (m, 12H), 7.15−7.20 (m, 2H), 6.71 (s, 1H), 6.29−6.36 (m, 2H). ^{13}C NMR (75 MHz, $CDCl_3$, 298 K; δ (ppm)): 179.9, 149.9, 140.1, 139.5, 130.8, 128.6, 127.2, 126.3, 125.5, 117.2, 111.7, 108.8, 108.4, 107.1, 106.8, 106.7, 106.4, 95.6. Anal. Calcd for $C_{41}H_{23}F_4IrN_2O_4$ (MW = 875.85): C, 56.22; H, 2.65; N, 3.20. Found: C, 56.25 H, 2.66; N, 3.21%. MS (FAB; m/z): 876.3012

Synthesis of compound 5, $[(dfpbo)_2Ir(dbp)(CO)]$ (dbp = 3,5-dibromophenyl):

A mixture of 3,5-dibromobenzaldehyde (396 mg, 1.5 mmol) and compound **1** (50 mg, 0.037 mmol) in toluene (30 ml) was stirred under N_2 at 110 ℃ for 2 d. The final solution was taken to dryness in vacuo. The residue was purified via column chromatography. Yield: 16 mg (47% based on iridium). 1H NMR (300 MHz, $CDCl_3$, 298 K; δ (ppm)): 7.2−7.23 (m, 5H), 7.12−7.16 (m, 3H), 7.08−7.10 (m, 7H). Anal. Calcd for $C_{33}H_{15}N_2O_3Br_2F_4Ir$: C, 43.29; H, 1.65; N, 3.06. Found: C, 43.32; H, 1.66; N, 3.07%.; IR (KBr pellet): ν(CO) 2360 cm^{-1}. MS (FAB; m/z): 916.02

X-Ray Structure Determinations

The diffraction data of complexes **1**, **4** and **5** were collected on a Bruker SMART APEX CCD diffractometer with graphite-monochromatized Mo Kα X-ray radiation (λ = 0.71073 Å) at room temperature. All the calculations for the structure determination were carried out using SHELXTL package (version 5.1).[5] The positions of the heavy atoms, including the iridium atoms were located by the direct method. The remaining atoms were found in a series of alternating difference Fourier maps and least-square refinement.[6]

Crystal data for compound **1**: formula $C_{52}H_{24}N_4O_4ClF_8Ir_2$, M =1340.67, orthorhombic, space group A b a 2, a = 21.8706(4), b = 14.4783(3), c = 16.9835(3) Å, V = 5377.81(18) $Å^3$, Z = 4, ρ_{calc} = 2.075 gcm^{-3}, F(000) = 3228, T =100(2) K, $2\theta_{max}$ = 58.5°, 25544 reflections collected, 6320 unique, GooF = 1.192, R1 = 0.0317, wR_2 = 0.0637. For **4**: formula $C_{41}H_{23}F_4IrN_2O_4$, M = 875.85, triclinic, space group P-1, a = 12.0381(3), b = 14.6705(4), c = 19.5320(5) Å, = 102.358(2), = 95.205(2), = 94.203(2)°, V = 3340.35(15) $Å^3$, Z = 4, ρ_{calc} = 1.742 gcm^{-3}, F(000) = 1712, T =120(2) K, $2\theta_{max}$ = 58.7°, 29949 reflections collected, 15412 unique, GooF = 1.132, R1 = 0.0516, wR_2 = 0.1161. For **5**. formula $C_{33}H_{15}N_2O_3Br_2F_4Ir$, M = 915.52, monoclinic, space group P 21/n, a = 14.5053(3), b = 12.1682(3), c = 16.3047(3) Å, = 102.514(2)°, V = 2809.47(10) $Å^3$, Z = 4, ρ_{calc} = 2.164 gcm^{-3}, F(000) = 1736, T =110(2) K, $2\theta_{max}$ = 58.4°, 13799 reflections collected, 6500 unique, GooF = 1.023, R1 = 0.0246, wR_2 = 0.0484. Basic information pertaining to crystal parameters and structure refinement are summarized in Table S1. Selected bond distances and angles are listed in Table S2.

References

DFT (B3LYP/LANL2DZ level) calculation: Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A.; Vreven, Jr. T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson,G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Omperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; G. Liu; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, A. Gaussian 03, Revision B.04, Gaussian, Inc: Pittsburgh PA, **2003**.

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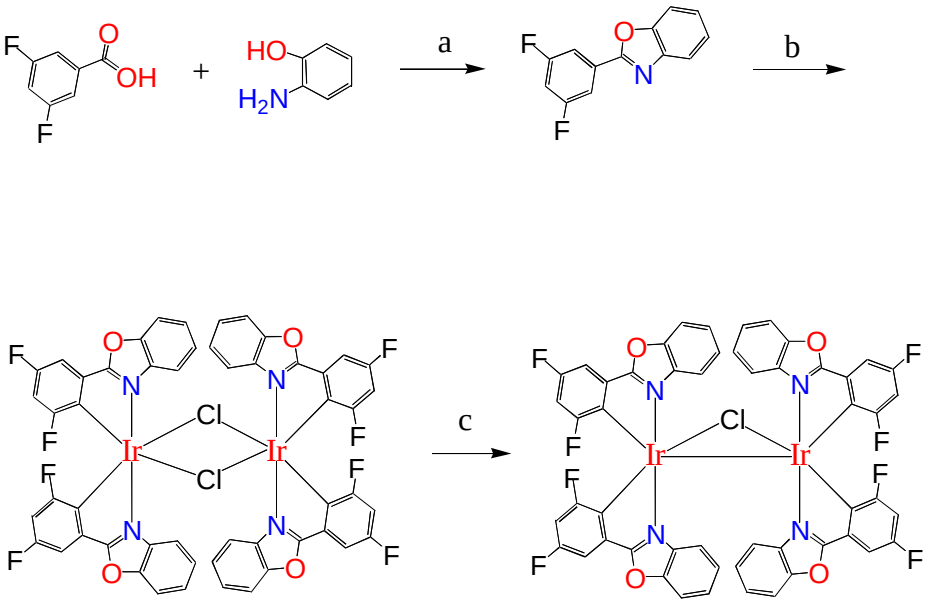
Scheme S1



1

a. PPA (polyphosphoric acid)/ 200 ℃ / 8 h; b. $IrCl_3$/2-ethoxylethanol-H_2O (3:1, v/v)/ 100 ℃ / 24 h; c. K_2CO_3/ toluene-ethoxyethanol (30:1, v/v)/ 100 ℃/ 24 h

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Table S1. Crystal data for Compound **1**, **4**, and **5**

	1	**4**	**5**
empirical formula	$C_{52}H_{24}N_4O_4ClF_8Ir_2$	$C_{41}H_{23}F_4IrN_2O_4$	$C_{33}H_{15}N_2O_3Br_2F_4Ir$
fw	1340.67	875.85	915.52
temp [K]	100 (2)	120(2)	110(2))
radiated used (λ[Å])	0.71073	0.71073	0.71073
cryst size [mm^3]	0.52 x 0.36 x 0.28	0.44 x 0.28 x 0.26	0.74 x 0.56 x 0.44
cryst syst	orthorhombic	triclinic	monoclinic
space group	A b a 2	P-1	P 21/n
a [Å]	21.8706(4)	12.0381(3)	14.5053(3)
b [Å]	14.4783(3)	14.6705(4)	12.1682(3)
c [Å]	16.9835(3)	19.5320(5)	16.3047(3)
α [deg]	90	102.358(2)	90
β [deg]	90	95.205(2)	102.514(2)
γ [deg]	90	94.203(2)	90
V [$Å^3$], Z	5377.81(18), 4	3340.35(15), 4	2809.47(10), 4
ρ_{calcd} [$g.cm^{-3}$]	2.075	1.742	2.164
μ [mm^{-1}]	5.473	4.067	7.664
F(000)	3228	1712	1736
scan rang θ [deg]	2.62 to 29.28	2.77 to 29.38	2.88 to 29.20
no. of total refins	25544	29949	13799
no. of unique refins	6320 [R(int) = 0.0343]	15412 [R(int) = 0.0362]	6500 [R(int) = 0.0276]
no. of data/restraints/ params	6320 / 1 / 375	15412 / 0 / 911	6500 / 0 / 400
goodness-of-fit on F^2	1.192	1.132	1.023
R_1, wR_2 [$I>\sigma 2(I)$]	0.0317 and 0.0637	0.0516 and 0.1161	0.0246 and 0.0484
R_1, wR_2 (all data)	0.0367 and 0.0647	0.0874 and 0.1225	0.0366 and 0.0494

Table S2. Selected Bond Distance (Å) and Bond Angles for Compound **1**, **4**, and **5**

1			
Ir-N(1)	2.030(4)	Ir-C(26)	2.036(5)
Ir-C(13)	2.055(6)	Ir-N(2)	2.062(4)
Ir-Cl(1)	2.4658(14)	Ir-Ir(1)	3.0433(3)
Cl(1)-Ir(1)	2.4658(14)	N(1)-Ir-C(26)	95.1(2)
N(1)-Ir-C(13)	79.7(2)	C(26)-Ir-C(13)	89.1(2)
N(1)-Ir-N(2)	172.91(16)	C(26)-Ir-N(2)	80.1(2)
C(13)-Ir-N(2)	95.0(2)	N(1)-Ir-Cl(1)	95.53(13)
C(26)-Ir-Cl(1)	169.40(16)	C(13)-Ir-Cl(1)	93.10(15)
N(2)-Ir-Cl(1)	89.42(16)	N(1)-Ir-Ir(1)	91.88(11)
C(26)-Ir-Ir(1)	127.37(15)	C(13)-Ir-Ir(1)	143.30(15)
N(2)-Ir-Ir(1)	95.17(12)	Cl(1)-Ir-Ir(1)	51.90(3)
4			
Ir(1)-C(26)	2.005(7)	Ir(1)-C(13)	2.010(6)
Ir(1)-N(1)	2.039(5)	Ir(1)-N(2)	2.050(5)
Ir(1)-O(3)	2.087(5)	Ir(1)-O(4)	2.130(4)
C(26)-Ir(1)-C(13)	92.2(2)	C(26)-Ir(1)-N(1)	97.9(2)
C(13)-Ir(1)-N(1)	79.5(2)	C(26)-Ir(1)-N(2)	79.4(2)
C(13)-Ir(1)-N(2)	100.4(2)	N(1)-Ir(1)-N(2)	177.3(2)
5			
Ir-C(33)	1.906(4)	Ir-N(1)	2.047(3)
Ir-N(2)	2.065(3)	Ir-C(13)	2.090(4)
Ir-C(27)	2.114(3)	Ir-C(26)	2.128(3)
C(33)-Ir-N(1)	96.30(14)	C(33)-Ir-N(2)	89.58(14)
N(1)-Ir-N(2)	171.23(12)	C(33)-Ir-C(13)	173.60(15)
N(1)-Ir-C(13)	78.26(13)	N(2)-Ir-C(13)	96.22(13)
C(33)-Ir-C(27)	90.51(15)	N(1)-Ir-C(27)	88.91(12)
N(2)-Ir-C(27)	97.56(12)	C(13)-Ir-C(27)	86.05(13)
C(33)-Ir-C(26)	97.77(15)	N(1)-Ir-C(26)	94.56(13)
N(2)-Ir-C(26)	78.16(13)	C(13)-Ir-C(26)	86.10(13)
C(27)-Ir-C(26)	170.60(14)		

```
[ Elemental Composition ]
Data  : FAB-H-1102                        Date : 02-Sep-98 12:54
Sample: Ir2F4cl(NBA)
Note : *
Inlet : Direct                            Ion Mode : FAB+
RT : 11.42 min                            Scan#: (67,72)
Elements : C 57/0, 1H 80/0, D 0/0, O 4/1, N 4/0, Cl 1/0, F 8/0, Ir 2/0
Mass Tolerance      : 10ppm, 5mmu if m/z < 500, 20mmu if m/z > 2000
Unsaturation (U.S.) : -0.5 - 40.0

Observed m/z Int%   Err[ppm / mmu]    U.S.  Composition
 1341.0605    29.6     -0.9 /  -1.2   39.5  C 52 1H 24 O 4 N 4 Cl F 8 Ir 2
```

```
[ Mass Spectrum ]
Data  : FAb-1564                          Date : 11-Aug-98 10:44
Sample: Ir2F4Cl(NBA)
Note : *
Inlet : Direct                            Ion Mode : FAB+
Spectrum Type : Regular [MF-Linear]
RT : 4.00 min          Scan# : (23,28)                Temp : 15.3 deg.C
BP : m/z 654.0000      Int.  : 1357.47
Output m/z range : 45.0000 to 1406.1500   Cut Level : 0.00 %
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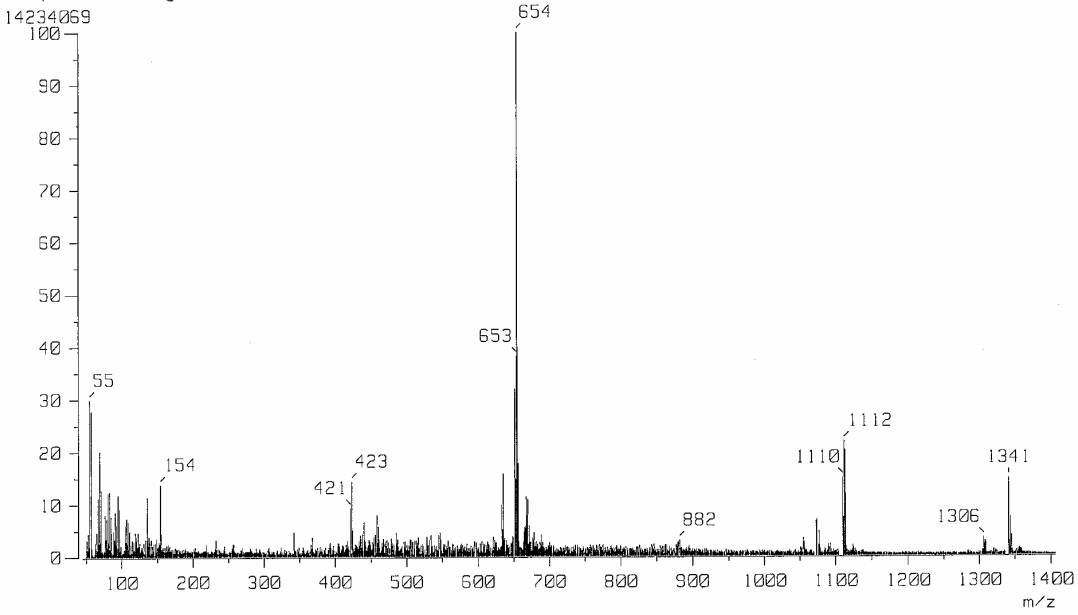

Figure S1. Mass spectrum of **1** with fast atom bombardment

Table S3. Mass Data of Compound **1**

[Mass Spectrum]
Data : FAb-1564 Date : 11-Aug-98 10:44
Sample: Ir2F4Cl(NBA)
Note : *
Inlet : Direct Ion Mode : FAB+
Spectrum Type : Regular [MF-Linear]
RT : 4.00 min Scan# : (23,28) Temp : 15.3 deg.C
BP : m/z 654.0000 Int. : 1357.47
Output m/z range : 45.0000 to 1406.1500 Cut Level : 1.00 %

m/z	Int.	Norm.	m/z	Int.	Norm.
590.0000	28.45	2.10	646.0000	34.81	2.56
591.0000	20.73	1.53	647.0000	38.55	2.84
592.0000	22.82	1.68	648.0000	51.76	3.81
593.0000	26.17	1.93	649.0000	50.50	3.72
595.0000	39.95	2.94	651.0000	434.64	32.02
597.0000	37.02	2.73	652.0000	203.90	15.02
598.0000	22.16	1.63	653.0000	519.01	38.23
599.0000	16.97	1.25	654.0000	1357.47	100.00
600.0000	20.21	1.49	655.0000	542.27	39.95
601.0000	23.80	1.75	656.0000	240.80	17.74
1073.0000	91.49	6.74			
1074.0000	95.94	7.07			
1076.0000	29.72	2.19			
1077.0000	64.92	4.78			
1078.0000	28.84	2.12			
1079.0000	18.49	1.36			
1085.0000	19.87	1.46			
1086.0000	17.02	1.25			
1089.0000	14.55	1.07			
1090.0000	30.25	2.23			
1091.0000	23.19	1.71			
1093.0000	32.12	2.37			
1094.0000	16.57	1.22			
1097.0000	17.05	1.26			
1101.0000	14.38	1.06			
1103.0000	15.76	1.16			
1110.0000	203.39	14.98			
1111.0000	100.03	7.37			
1112.0000	296.86	21.87			
1113.0000	275.33	20.28			
1114.0000	161.56	11.90			
1115.0000	26.42	1.95			
1116.0000	16.79	1.24			
1121.0000	13.73	1.01			
1123.0000	17.44	1.28			
1124.0000	28.06	2.07			
1125.0000	22.55	1.66			
1127.0000	18.30	1.35			
1137.0000	14.24	1.05			
1138.0000	14.22	1.05			
1304.0000	14.79	1.09			
1305.0000	14.26	1.05			
1306.0000	46.26	3.41			
1307.0000	29.39	2.17			
1308.0000	38.52	2.84			
1309.0000	33.42	2.46			
1320.0000	16.70	1.23			
1322.0000	14.10	1.04			
1341.0000	200.39	14.76			
1342.0000	37.36	2.75			

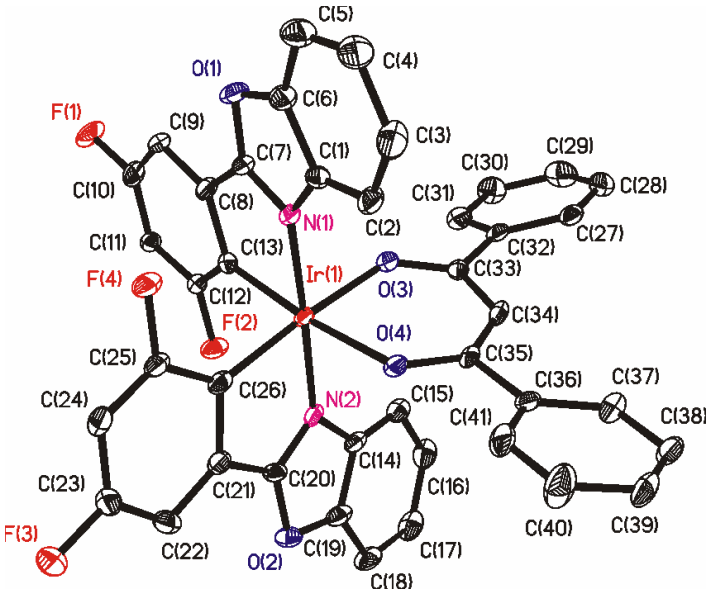

Figure S2. ORTEP plots of **4**. Thermal ellipsoids are drawn at the 30% probability level and hydrogen atoms are omitted for clarity.

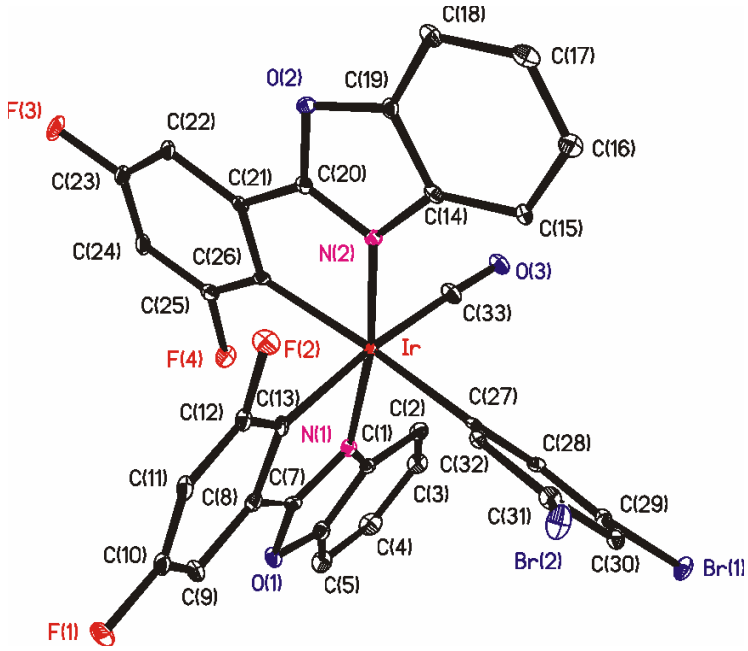

Figure S3. ORTEP plots of **5**. Thermal ellipsoids are drawn at the 30% probability level and hydrogen atoms are omitted for clarity.

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Table S4 Cartesian coordinates for Compound **1**

Atom	coordinate			Atom	coordinate		
Ir1	21.73063	5.72472	12.32153	C33	20.1122	2.856569	15.87448
Cl2	21.8706	7.23915	10.38201	C34	21.47256	2.98253	15.77258
F3	23.25282	0.893311	8.736312	C35	21.99964	3.813584	14.81471
F4	19.78852	3.337248	10.67922	C36	21.24291	4.528812	13.8959
F5	19.5895	2.051575	16.82555	H37	24.09265	7.191372	14.75357
F6	23.3578	3.887424	14.75526	H38	26.18786	7.538851	15.68087
O7	25.57548	4.405747	11.82901	H39	28.07966	6.55867	14.82829
O8	17.74799	4.929861	12.95332	H40	27.9725	5.055822	13.00766
N9	23.73398	5.47135	12.51854	H41	24.75752	2.542389	10.01857
N10	19.67698	5.727615	12.15	H42	20.86893	1.541939	9.329037
C11	24.80126	5.921625	13.29638	H43	19.38391	7.320228	9.780798
C12	24.86687	6.770053	14.39521	H44	17.30621	7.839999	8.884069
C13	26.10256	6.964062	14.9285	H45	15.31598	7.06541	9.914967
C14	27.24202	6.363213	14.42578	H46	15.4144	5.669702	11.80353
C15	27.20047	5.487276	13.35582	H47	18.31225	3.412535	15.07116
C16	25.9276	5.294714	12.83613	H48	22.04556	2.50185	16.35851
C17	24.25231	4.569351	11.71352	Ir49	22.01057	8.75358	12.32153
C18	23.36436	3.726714	10.93058	F50	20.48838	13.58499	8.736312
C19	23.82802	2.697307	10.14594	F51	23.95268	11.14105	10.67922
C20	22.85915	1.895209	9.55152	F52	24.1517	12.42672	16.82555
C21	21.51411	2.10804	9.736641	F53	20.3834	10.59088	14.75526
C22	21.12919	3.166404	10.53317	O54	18.16572	10.07255	11.82901
C23	22.00401	4.043789	11.17175	O55	25.99321	9.548439	12.95332
C24	18.62938	6.193817	11.3195	N56	20.00722	9.00695	12.51854
C25	18.58782	6.995915	10.18331	N57	24.06422	8.750685	12.15
C26	17.36307	7.299959	9.66531	C58	18.93994	8.556675	13.29638
C27	16.158	6.819279	10.28011	C59	18.87433	7.708247	14.39521
C28	16.20174	6.007047	11.39083	C60	17.63864	7.514238	14.9285
C29	17.45274	5.717481	11.85958	C61	16.49918	8.115087	14.42578
C30	19.08647	4.999357	13.06371	C62	16.54073	8.991024	13.35582
C31	19.8585	4.313086	14.04875	C63	17.8136	9.183586	12.83613

An 18+ δ Iridium Dimer Releasing Metalloradical Spontaneously

(Continued) Cartesian coordinates

Atom	coordinate			Atom	coordinate		
C32	19.25706	3.508092	15.01172	C64	19.48889	9.908949	11.71352
C65	20.37684	10.75159	10.93058	C81	22.26864	11.49577	15.77258
C66	19.91318	11.78099	10.14594	C82	21.74156	10.66472	14.81471
C67	20.88205	12.58309	9.55152	C83	22.49829	9.949488	13.8959
C68	22.22709	12.37026	9.736641	H84	19.64855	7.286928	14.75357
C69	22.61201	11.3119	10.53317	H85	17.55334	6.939449	15.68087
C70	21.73719	10.43451	11.17175	H86	15.66154	7.91963	14.82829
C71	25.11182	8.284483	11.3195	H87	15.7687	9.422478	13.00766
C72	25.15338	7.482385	10.18331	H88	18.98368	11.93591	10.01857
C73	26.37813	7.178341	9.66531	H89	22.87227	12.93636	9.329037
C74	27.5832	7.659021	10.28011	H90	24.35729	7.158072	9.780798
C75	27.53946	8.471253	11.39083	H91	26.43499	6.638301	8.884069
C76	26.28846	8.760819	11.85958	H92	28.42522	7.41289	9.914967
C77	24.65473	9.478943	13.06371	H93	28.3268	8.808598	11.80353
C78	23.8827	10.16521	14.04875	H94	25.42895	11.06576	15.07116
C79	24.48414	10.97021	15.01172	H95	21.69564	11.97645	16.35851
C80	23.629	11.62173	15.87448				

Table S5 SOMO and LUMO orbital compositions for Compound **1**

			256 (SOMO)	257 (LUMO)		256 (SOMO)	257 (LUMO)
EIGENVALUES			-0.31366	-0.28066		-0.31366	-0.28066
atom		orbital			orbital		
1	Ir	1S	-0.0003	0.05104	2S	-0.00088	0.01079
		3S	-0.01528	-0.11315	4PX	-0.00031	0.05043
		4PY	0.00295	-0.0522	4PZ	0.01066	-0.07791
		5PX	0.00311	-0.10718	5PY	0.01863	0.04226
		5PZ	-0.00562	-0.01556	6PX	-0.00184	0.00765
		6PY	0.00141	0.00696	6PZ	-0.01223	0.02043
		7D 0	0.02558	-0.06604	7D+1	-0.03177	0.19353
		7D-1	0.01607	-0.20861	7D+2	0.00194	-0.00504
		7D-2	0.00867	0.23305	8D 0	-0.0053	0.00211
		8D+1	-0.00836	0.04483	8D-1	0.00355	-0.02568
		8D+2	-0.00841	0.00186	8D-2	0.00967	0.03202
2	Cl	1S	0.00754	-0.00911	2S	0.01452	0.02592
		3PX	0.03147	0	3PY	-0.02709	0
		3PZ	-0.01434	0.00316	4PX	0.01962	0
		4PY	-0.02063	0	4PZ	-0.0171	-0.02465
3	F	1S	0.00006	-0.00118	2S	-0.00021	0.00401
		3S	-0.00005	0.00163	4PX	-0.00595	0.00095
		4PY	0.00466	-0.00427	4PZ	-0.00836	-0.01278
		5PX	-0.00324	0.00303	5PY	0.00173	0.00049
		5PZ	-0.00397	-0.00672			
4	F	1S	-0.00061	0.00368			
		2S	0.00143	-0.00733	3S	0.003	-0.02312
		4PX	0.00868	-0.01437	4PY	-0.00236	-0.04744
		4PZ	0.00169	-0.00866	5PX	0.00452	-0.00875
		5PY	-0.0003	-0.03348	5PZ	0.001	-0.00596
5	F	1S	-0.00005	0.00039	2S	0.00021	-0.00133
		3S	-0.00015	-0.00034	4PX	-0.01008	0.02848
		4PY	0.00821	-0.02326	4PZ	0.01153	-0.03626
		5PX	-0.0053	0.01643	5PY	0.00346	-0.00897
		5PZ	0.00596	-0.02071			
6	F	1S	0.00038	-0.00146			
		2S	-0.00099	0.00393	3S	-0.00137	0.00491
		4PX	0.00922	-0.03197	4PY	-0.00406	0.00807
		4PZ	-0.00978	0.03156	5PX	0.00587	-0.0211
		5PY	-0.0015	-0.00031	5PZ	-0.00516	0.01614

7	O	1S	0	-0.00057	2S	-0.00022	0.00076
		3S	0.00218	0.00112	4PX	0.01068	-0.00671
		4PY	-0.00267	0.01014	4PZ	0.00946	0.0098
		5PX	0.0038	-0.00154	5PY	-0.00121	0.00815
		5PZ	0.00395	0.00585			
8	O	1S	0.00036	0.00205			
		2S	-0.00077	-0.00528	3S	-0.00276	-0.01155
		4PX	-0.00276	-0.05539	4PY	0.00796	0.01676
		4PZ	0.00659	0.0289	5PX	-0.00121	-0.03023
		5PY	0.00123	0.01561	5PZ	0.00326	0.00904
9	N	1S	0.00011	0.01362	2S	0.00066	-0.0288
		3S	-0.00918	-0.05597	4PX	-0.00189	0.04697
		4PY	-0.00166	0.07374	4PZ	-0.00139	0.01434
		5PX	0.00771	0.03678	5PY	0.00671	0.0358
		5PZ	-0.00683	0.01559			
10	N	1S	-0.00107	0.01453			
		2S	0.00291	-0.03082	3S	0.00457	-0.06144
		4PX	0.02687	-0.03549	4PY	-0.02585	-0.072
		4PZ	-0.02653	-0.02654	5PX	0.01154	-0.0026
		5PY	-0.01466	-0.05567	5PZ	-0.00715	0.02559
11	C	1S	0.00033	-0.00672	2S	-0.00321	0.02132
		3S	0.00197	-0.00696	4PX	-0.00497	-0.03263
		4PY	0.00161	-0.02412	4PZ	-0.01023	0.00783
		5PX	0.00187	-0.02923	5PY	0.01918	-0.02266
		5PZ	0.00943	0.00448			
12	C	1S	-0.00001	-0.00321			
		2S	0.00097	0.01351	3S	-0.0026	0.01554
		4PX	0.00262	-0.01547	4PY	-0.00113	0.00077
		4PZ	0.00236	0.00038	5PX	-0.01006	0.00357
		5PY	0.00082	-0.00134	5PZ	0.00213	-0.00442
13	C	1S	-0.00005	0.00047	2S	0.00038	-0.00358
		3S	0.00539	0.00138	4PX	0.02353	0.00178
		4PY	-0.01337	0.00105	4PZ	0.01959	-0.00235
		5PX	0.00645	-0.00538	5PY	-0.00833	0.00196
		5PZ	0.00525	0.0051			
14	C	1S	0.00052	-0.00091			
		2S	-0.00165	0.00134	3S	0.0006	0.01154
		4PX	0.00703	0.00742	4PY	-0.00231	-0.00524
		4PZ	0.00551	0.00813	5PX	0.00517	-0.00017
		5PY	0.00057	-0.00065	5PZ	0.00047	0.00502
15	C	1S	0.00011	-0.00262	2S	0.00014	0.00525

		3S	-0.0054	0.0244	4PX	-0.024	-0.00854
		4PY	0.01418	-0.01278	4PZ	-0.0212	0.00597
		5PX	-0.00858	-0.01064	5PY	-0.00062	0.0022
		5PZ	-0.01211	0.01614			
16	C	1S	0.0007	0.00537			
		2S	-0.00157	-0.01843	3S	-0.01486	0.00429
		4PX	-0.01615	-0.00154	4PY	0.01045	0.02634
		4PZ	-0.01409	-0.00302	5PX	0.00254	-0.01214
		5PY	0.0083	-0.02465	5PZ	0.00118	-0.00324
17	C	1S	-0.00071	0.00803	2S	0.00196	-0.02309
		3S	0.00663	-0.00366	4PX	0.00467	0.0452
		4PY	-0.00466	0.0045	4PZ	0.00868	-0.02202
		5PX	-0.0072	-0.02334	5PY	-0.00602	-0.00176
		5PZ	0.00679	0.01365			
18	C	1S	-0.00074	0.01095			
		2S	0.00209	-0.02425	3S	-0.00021	-0.04787
		4PX	-0.00551	0.02024	4PY	-0.00203	0.06191
		4PZ	-0.00672	0.00317	5PX	-0.00214	-0.05043
		5PY	-0.01219	0.06261	5PZ	-0.00803	0.06021
19	C	1S	0.00044	-0.00829	2S	-0.00122	0.02585
		3S	0.00046	0.00623	4PX	0.00254	0.0261
		4PY	-0.00009	-0.04648	4PZ	0.00913	-0.03858
		5PX	0.00904	-0.01977	5PY	-0.00288	-0.00341
		5PZ	-0.00165	0.00768			
20	C	1S	0.0003	-0.00266			
		2S	-0.00075	0.01144	3S	-0.00385	0.02123
		4PX	0.00576	0.00937	4PY	-0.00374	-0.01601
		4PZ	0.00989	0.00224	5PX	0.00878	-0.03946
		5PY	0.0075	-0.0299	5PZ	-0.00151	0.01266
21	C	1S	0.0003	-0.00952	2S	-0.00093	0.03046
		3S	0.00338	-0.00985	4PX	0.00459	0.04279
		4PY	-0.00337	-0.04985	4PZ	0.01292	-0.032
		5PX	0.00167	0.02256	5PY	0.00846	-0.04842
		5PZ	0.00913	-0.02949			
22	C	1S	-0.00038	0.01087			
		2S	0.0026	-0.03519	3S	-0.01689	0.05471
		4PX	0.00145	-0.08483	4PY	0.00332	-0.02226
		4PZ	-0.00587	0.02552	5PX	-0.01152	0.00923
		5PY	0.00235	0.01109	5PZ	0.00561	-0.00712
23	C	1S	0.003	-0.05702	2S	-0.00587	0.11032
		3S	-0.01047	0.26788	4PX	-0.01793	0.13981

		4PY	0.02015	-0.20095	4PZ	-0.00779	-0.20517
		5PX	-0.03097	0.18282	5PY	-0.00285	-0.12614
		5PZ	0.01377	-0.17373			
24	C	1S	-0.00028	-0.00403			
		2S	0.00352	0.0146	3S	-0.01049	-0.04378
		4PX	-0.00535	0.02435	4PY	0.00247	0.00772
		4PZ	0.00253	-0.02589	5PX	0.00671	0.01013
		5PY	0.0065	-0.03839	5PZ	0.01404	0.03263
25	C	1S	0.00052	-0.00074	2S	-0.00126	0.00548
		3S	-0.0057	-0.01281	4PX	-0.01219	-0.01007
		4PY	0.00431	0.00693	4PZ	0.00459	0.00069
		5PX	-0.00154	0.01769	5PY	-0.00496	0.02017
		5PZ	-0.00008	0.00266			
26	C	1S	-0.00029	-0.00053			
		2S	0.00138	-0.00039	3S	-0.00466	0.02057
		4PX	-0.00322	-0.01117	4PY	0.00343	0.01338
		4PZ	0.00194	0.01125	5PX	-0.00155	-0.0092
		5PY	0.00078	0.00306	5PZ	0.00298	0.00074
27	C	1S	-0.00016	-0.00067	2S	0.00087	0.00105
		3S	-0.00087	0.00816	4PX	0.01068	0.00496
		4PY	-0.00838	-0.00455	4PZ	-0.01041	-0.00932
		5PX	0.00502	-0.00228	5PY	0.00068	-0.00081
		5PZ	-0.00218	-0.01025			
28	C	1S	0.00013	-0.00094			
		2S	-0.00013	0.00123	3S	-0.0036	0.02298
		4PX	0.01128	0.01531	4PY	-0.00735	-0.00268
		4PZ	-0.00837	-0.01128	5PX	0.00023	-0.00303
		5PY	-0.00926	0.00693	5PZ	-0.00517	-0.01679
29	C	1S	-0.00055	0.00277	2S	0.00132	-0.01113
		3S	0.01464	0.00512	4PX	-0.00421	-0.02007
		4PY	0.0075	-0.00302	4PZ	0.00842	-0.00284
		5PX	-0.00344	0.00936	5PY	-0.00066	0.03948
		5PZ	0.01004	-0.01763			
30	C	1S	-0.00001	-0.00724			
		2S	-0.00033	0.01759	3S	0.01184	0.01395
		4PX	0.00788	0.05507	4PY	-0.00837	-0.03666
		4PZ	-0.00574	-0.04063	5PX	0.00061	0.05507
		5PY	-0.01026	-0.00305	5PZ	0.00061	0.02211
31	C	1S	0.00042	-0.00445	2S	-0.00052	0.00903
		3S	-0.00136	0.00866	4PX	-0.01209	0.0602
		4PY	0.00517	-0.03591	4PZ	0.0097	-0.0412

		5PX	-0.01716	0.06039	5PY	0.00483	-0.04441
		5PZ	-0.00961	0.06753			
32	C	1S	-0.0004	0.00273			
		2S	0.00129	-0.00815	3S	-0.00227	0.00455
		4PX	0.01474	-0.07313	4PY	-0.00959	0.0507
		4PZ	-0.00972	0.04581	5PX	0.00079	-0.00153
		5PY	-0.00025	-0.01218	5PZ	-0.01082	0.05945
33	C	1S	-0.00023	0.00035	2S	0.00069	-0.00286
		3S	0.00348	-0.00246	4PX	0.01455	-0.05351
		4PY	-0.01092	0.03639	4PZ	-0.01406	0.05072
		5PX	0.0058	-0.03393	5PY	0.00983	-0.0504
		5PZ	-0.00598	0.03613			
34	C	1S	-0.00044	0.00236			
		2S	0.00127	-0.00855	3S	-0.0047	0.02967
		4PX	0.00947	0.00011	4PY	-0.00632	-0.00571
		4PZ	-0.00514	-0.02525	5PX	0.01296	-0.04203
		5PY	0.00109	-0.02352	5PZ	0.00416	-0.03896
35	C	1S	0.00056	-0.00304	2S	-0.00307	0.0145
		3S	0.0195	-0.08277	4PX	-0.01197	0.04706
		4PY	0.01368	-0.05795	4PZ	0.00968	-0.03689
		5PX	-0.00174	0.00525	5PY	-0.00756	0.03876
		5PZ	0.01247	-0.03714			
36	C	1S	-0.00282	0.01569			
		2S	0.00474	-0.02849	3S	0.01235	-0.06209
		4PX	-0.01058	-0.02471	4PY	0.0169	-0.02229
		4PZ	0.03501	-0.09585	5PX	0.00871	-0.07834
		5PY	-0.02212	0.08026	5PZ	0.04029	-0.19556
37	H	1S	0.00293	-0.00246	2S	0.00444	-0.00914
38	H	1S	0.00083	-0.00067	2S	-0.00097	0.00425
39	H	1S	-0.00009	-0.00013	2S	-0.00261	0.00288
40	H	1S	0.00076	-0.00458	2S	0.00442	-0.01005
41	H	1S	0.00115	-0.01534	2S	0.00018	-0.01015
42	H	1S	0.00137	-0.02045	2S	-0.00065	-0.00414
43	H	1S	-0.00282	-0.00247	2S	0.0035	-0.01933
44	H	1S	0.00022	-0.00023	2S	0.00005	0.00092
45	H	1S	0.00038	0	2S	0.00201	0.00191
46	H	1S	-0.00051	-0.00373	2S	-0.00372	-0.00915
47	H	1S	-0.00091	0.00276	2S	-0.00069	-0.0024
48	H	1S	-0.00125	0.00567	2S	0.00174	-0.00415
49	Ir	1S	-0.00501	0.05104	2S	-0.00094	0.01079
		3S	0.03612	-0.11315	4PX	0.00702	-0.05043

		4PY	-0.00708	0.0522	4PZ	0.00914	-0.07791
		5PX	0.00778	0.10718	5PY	0.03275	-0.04226
		5PZ	-0.01437	-0.01556	6PX	0.00123	-0.00765
		6PY	0.00869	-0.00696	6PZ	0.00594	0.02043
		7D 0	0.03013	-0.06604	7D+1	0.04624	-0.19353
		7D-1	-0.0169	0.20861	7D+2	-0.0819	-0.00504
		7D-2	-0.03553	0.23305	8D 0	0.0034	0.00211
		8D+1	0.00056	-0.04483	8D-1	-0.00202	0.02568
		8D+2	0.01303	0.00186	8D-2	-0.00581	0.03202
50	F	1S	0.00027	-0.00118	2S	-0.00073	0.00401
		3S	-0.00109	0.00163	4PX	0.07872	-0.00095
		4PY	-0.0649	0.00427	4PZ	-0.12194	-0.01278
		5PX	0.03954	-0.00303	5PY	-0.03195	-0.00049
		5PZ	-0.06015	-0.00672			
51	F	1S	0.00059	0.00368			
		2S	-0.00202	-0.00733	3S	-0.0007	-0.02312
		4PX	-0.03961	0.01437	4PY	0.02921	0.04744
		4PZ	0.10474	-0.00866	5PX	-0.02269	0.00875
		5PY	0.01486	0.03348	5PZ	0.05258	-0.00596
52	F	1S	-0.00007	0.00039	2S	0.00037	-0.00133
		3S	-0.00042	-0.00034	4PX	-0.05341	-0.02848
		4PY	0.04184	0.02326	4PZ	-0.05444	-0.03626
		5PX	-0.02621	-0.01643	5PY	0.02063	0.00897
		5PZ	-0.02684	-0.02071			
53	F	1S	0.00023	-0.00146			
		2S	-0.00053	0.00393	3S	-0.00063	0.00491
		4PX	0.0307	0.03197	4PY	-0.0189	-0.00807
		4PZ	0.05058	0.03156	5PX	0.01525	0.0211
		5PY	-0.01191	0.00031	5PZ	0.02446	0.01614
54	O	1S	0.00119	-0.00057	2S	-0.0031	0.00076
		3S	-0.00467	0.00112	4PX	-0.02121	0.00671
		4PY	0.00267	-0.01014	4PZ	0.01911	0.0098
		5PX	-0.00759	0.00154	5PY	0.00542	-0.00815
		5PZ	0.0115	0.00585			
55	O	1S	-0.00067	0.00205			
		2S	0.00154	-0.00528	3S	0.00347	-0.01155
		4PX	0.0182	0.05539	4PY	-0.01812	-0.01676
		4PZ	0.01934	0.0289	5PX	0.00895	0.03023
		5PY	-0.00823	-0.01561	5PZ	0.0096	0.00904
56	N	1S	0.00171	0.01362	2S	-0.00533	-0.0288
		3S	-0.00399	-0.05597	4PX	-0.14676	-0.04697

		4PY	0.05515	-0.07374	4PZ	0.13137	0.01434
		5PX	-0.03709	-0.03678	5PY	0.02533	-0.0358
		5PZ	0.07199	0.01559			
57	N	1S	-0.0011	0.01453			
		2S	0.00263	-0.03082	3S	0.00444	-0.06144
		4PX	0.09904	0.03549	4PY	-0.1034	0.072
		4PZ	0.09514	-0.02654	5PX	0.03261	0.0026
		5PY	-0.03174	0.05567	5PZ	0.05309	0.02559
58	C	1S	-0.00053	-0.00672	2S	0.00033	0.02132
		3S	0.02243	-0.00696	4PX	0.09982	0.03263
		4PY	-0.04242	0.02412	4PZ	-0.07918	0.00783
		5PX	0.03044	0.02923	5PY	0.01426	0.02266
		5PZ	-0.0149	0.00448			
59	C	1S	0.00061	-0.00321			
		2S	-0.00203	0.01351	3S	-0.00972	0.01554
		4PX	0.0836	0.01547	4PY	-0.04241	-0.00077
		4PZ	-0.07187	0.00038	5PX	0.02005	-0.00357
		5PY	-0.02898	0.00134	5PZ	-0.02378	-0.00442
60	C	1S	-0.00028	0.00047	2S	0.00079	-0.00358
		3S	-0.00512	0.00138	4PX	-0.0682	-0.00178
		4PY	0.03471	-0.00105	4PZ	0.05895	-0.00235
		5PX	-0.01955	0.00538	5PY	0.00613	-0.00196
		5PZ	0.01659	0.0051			
61	C	1S	0.00025	-0.00091			
		2S	-0.00046	0.00134	3S	-0.00631	0.01154
		4PX	-0.11843	-0.00742	4PY	0.06003	0.00524
		4PZ	0.10733	0.00813	5PX	-0.03117	0.00017
		5PY	0.01877	0.00065	5PZ	0.03364	0.00502
62	C	1S	-0.0003	-0.00262	2S	0.00073	0.00525
		3S	-0.00203	0.0244	4PX	0.01689	0.00854
		4PY	-0.00722	0.01278	4PZ	-0.01468	0.00597
		5PX	0.00635	0.01064	5PY	-0.00036	-0.0022
		5PZ	-0.00973	0.01614			
63	C	1S	0.00035	0.00537			
		2S	-0.00195	-0.01843	3S	0.00829	0.00429
		4PX	0.11721	0.00154	4PY	-0.05541	-0.02634
		4PZ	-0.11136	-0.00302	5PX	0.03308	0.01214
		5PY	-0.01912	0.02465	5PZ	-0.02686	-0.00324
64	C	1S	-0.00174	0.00803	2S	0.00483	-0.02309
		3S	-0.03666	-0.00366	4PX	-0.07471	-0.0452
		4PY	0.03504	-0.0045	4PZ	0.0994	-0.02202

		5PX	-0.03499	0.02334	5PY	0.0118	0.00176
		5PZ	0.01567	0.01365			
65	C	1S	-0.0007	0.01095			
		2S	0.00027	-0.02425	3S	0.00936	-0.04787
		4PX	0.06854	-0.02024	4PY	-0.04442	-0.06191
		4PZ	-0.11076	0.00317	5PX	-0.00784	0.05043
		5PY	-0.02949	-0.06261	5PZ	-0.0516	0.06021
66	C	1S	0.00031	-0.00829	2S	-0.00052	0.02585
		3S	-0.00179	0.00623	4PX	-0.06965	-0.0261
		4PY	0.05199	0.04648	4PZ	0.12389	-0.03858
		5PX	-0.02091	0.01977	5PY	0.02288	0.00341
		5PZ	0.04666	0.00768			
67	C	1S	0.00016	-0.00266			
		2S	-0.00112	0.01144	3S	0.00126	0.02123
		4PX	-0.09586	-0.00937	4PY	0.07649	0.01601
		4PZ	0.15613	0.00224	5PX	-0.01195	0.03946
		5PY	0.00891	0.0299	5PZ	0.01596	0.01266
68	C	1S	0.00096	-0.00952	2S	-0.00287	0.03046
		3S	-0.00189	-0.00985	4PX	-0.06858	-0.04279
		4PY	0.04863	0.04985	4PZ	0.12745	-0.032
		5PX	-0.02239	-0.02256	5PY	0.01968	0.04842
		5PZ	0.04167	-0.02949			
69	C	1S	-0.0007	0.01087			
		2S	0.00169	-0.03519	3S	-0.00192	0.05471
		4PX	0.06019	0.08483	4PY	-0.05179	0.02226
		4PZ	-0.11934	0.02552	5PX	0.01347	-0.00923
		5PY	-0.00858	-0.01109	5PZ	-0.02808	-0.00712
70	C	1S	0.00193	-0.05702	2S	0.00039	0.11032
		3S	0.00023	0.26788	4PX	0.17935	-0.13981
		4PY	-0.14082	0.20095	4PZ	-0.27759	-0.20517
		5PX	0.05185	-0.18282	5PY	-0.0657	0.12614
		5PZ	-0.05468	-0.17373			
71	C	1S	0.0012	-0.00403			
		2S	-0.00222	0.0146	3S	-0.01768	-0.04378
		4PX	-0.07923	-0.02435	4PY	0.07968	-0.00772
		4PZ	-0.07472	-0.02589	5PX	0.00202	-0.01013
		5PY	0.03116	0.03839	5PZ	-0.01676	0.03263
72	C	1S	-0.00056	-0.00074	2S	0.00162	0.00548
		3S	0.00857	-0.01281	4PX	-0.06062	0.01007
		4PY	0.04794	-0.00693	4PZ	-0.05471	0.00069
		5PX	-0.02622	-0.01769	5PY	0.00675	-0.02017

		5PZ	-0.0232	0.00266			
73	C	1S	0.00032	-0.00053			
		2S	-0.00094	-0.00039	3S	0.0032	0.02057
		4PX	0.06913	0.01117	4PY	-0.05312	-0.01338
		4PZ	0.06087	0.01125	5PX	0.01562	0.0092
		5PY	-0.01765	-0.00306	5PZ	0.01999	0.00074
74	C	1S	0	-0.00067	2S	-0.00025	0.00105
		3S	0.00257	0.00816	4PX	0.10527	-0.00496
		4PY	-0.08157	0.00455	4PZ	0.09832	-0.00932
		5PX	0.02902	0.00228	5PY	-0.02334	0.00081
		5PZ	0.03071	-0.01025			
75	C	1S	0.00029	-0.00094			
		2S	-0.00088	0.00123	3S	0.0038	0.02298
		4PX	-0.01301	-0.01531	4PY	0.01254	0.00268
		4PZ	-0.0132	-0.01128	5PX	-0.00535	0.00303
		5PY	0.00644	-0.00693	5PZ	-0.00483	-0.01679
76	C	1S	-0.00025	0.00277	2S	0.00167	-0.01113
		3S	-0.00929	0.00512	4PX	-0.10615	0.02007
		4PY	0.08303	0.00302	4PZ	-0.09501	-0.00284
		5PX	-0.02651	-0.00936	5PY	0.01847	-0.03948
		5PZ	-0.03022	-0.01763			
77	C	1S	0.00077	-0.00724			
		2S	-0.00057	0.01759	3S	0.0163	0.01395
		4PX	0.07527	-0.05507	4PY	-0.07298	0.03666
		4PZ	0.08287	-0.04063	5PX	0.01776	-0.05507
		5PY	-0.02919	0.00305	5PZ	0.01239	0.02211
78	C	1S	0.00025	-0.00445	2S	0.00056	0.00903
		3S	-0.00353	0.00866	4PX	-0.05943	-0.0602
		4PY	0.05029	0.03591	4PZ	-0.06168	-0.0412
		5PX	-0.02556	-0.06039	5PY	0.00135	0.04441
		5PZ	-0.03	0.06753			
79	C	1S	-0.00003	0.00273			
		2S	0.00011	-0.00815	3S	-0.00152	0.00455
		4PX	0.02297	0.07313	4PY	-0.01849	-0.0507
		4PZ	0.02551	0.04581	5PX	0.01081	0.00153
		5PY	-0.00436	0.01218	5PZ	0.01738	0.05945
80	C	1S	0.00029	0.00035	2S	-0.0004	-0.00286
		3S	0.00183	-0.00246	4PX	0.06613	0.05351
		4PY	-0.05369	-0.03639	4PZ	0.06918	0.05072
		5PX	0.00879	0.03393	5PY	-0.00128	0.0504
		5PZ	0.00674	0.03613			

81	C	1S	-0.00063	0.00236			
		2S	0.00221	-0.00855	3S	0.00209	0.02967
		4PX	0.07174	-0.00011	4PY	-0.05715	0.00571
		4PZ	0.08303	-0.02525	5PX	0.02634	0.04203
		5PY	-0.02274	0.02352	5PZ	0.02287	-0.03896
82	C	1S	0.00052	-0.00304	2S	-0.00101	0.0145
		3S	-0.00974	-0.08277	4PX	-0.04033	-0.04706
		4PY	0.02311	0.05795	4PZ	-0.0476	-0.03689
		5PX	-0.00366	-0.00525	5PY	0.00793	-0.03876
		5PZ	-0.01605	-0.03714			
83	C	1S	0.00045	0.01569			
		2S	-0.00525	-0.02849	3S	-0.01083	-0.06209
		4PX	-0.13696	0.02471	4PY	0.11457	0.02229
		4PZ	-0.13729	-0.09585	5PX	-0.04465	0.07834
		5PY	0.00579	-0.08026	5PZ	-0.03777	-0.19556
84	H	1S	-0.00138	-0.00246	2S	0.01187	-0.00914
85	H	1S	0.0007	-0.00067	2S	0.00187	0.00425
86	H	1S	-0.00007	-0.00013	2S	0.004	0.00288
87	H	1S	0.00038	-0.00458	2S	0.00358	-0.01005
88	H	1S	0.00175	-0.01534	2S	0.00446	-0.01015
89	H	1S	0.00164	-0.02045	2S	0.00174	-0.00414
90	H	1S	0.00153	-0.00247	2S	-0.00592	-0.01933
91	H	1S	-0.00018	-0.00023	2S	-0.00212	0.00092
92	H	1S	0.00039	0	2S	-0.00096	0.00191
93	H	1S	0.00072	-0.00373	2S	-0.00069	-0.00915
94	H	1S	-0.00007	0.00276	2S	-0.00144	-0.0024
95	H	1S	-0.00126	0.00567	2S	-0.00609	-0.00415