ESI for

A diphenylamino-substituted cationic cyclometalated Ir(III) complex: its aggregation-induced phosphorescent emission and oxygen sensing properties

Lei Wang,[a] Zhanming Gao,[a] Chun Liu,* [a] Xin Jin[b]

[a] State Key Laboratory of Fine Chemicals, Dalian University of Technology, Linggong Road 2, 116024, Dalian, China; E-mail: cliu@dlut.edu.cn

[b] Eco-chemical Engineering Cooperative Innovation Center of Shandong, Qingdao University of Science and Technology, Qingdao 266042, China.

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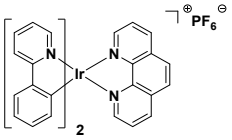
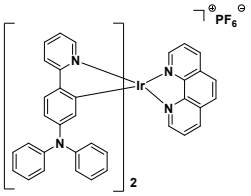


Ir1, Yield 71%, yellow solid; ^{1}H NMR (400 MHz, DMSO-d_6): δ 8.90 (d, J = 8.2 Hz, 2H), 8.39 (s, 2H), 8.26 (d, J = 8.1 Hz, 2H), 8.20 (d, J = 4.9 Hz, 2H), 8.05 (dd, J = 8.2, 5.1 Hz, 2H), 7.95 (d, J = 7.7 Hz, 2H), 7.87 (t, J = 7.8 Hz, 2H), 7.46 (d, J = 5.7 Hz, 2H), 7.06 (t, J = 7.5 Hz, 2H), 7.02 - 6.91 (m, 4H), 6.29 (d, J = 7.5 Hz, 2H).



Ir2, Yield 62%, yellow solid; ^{1}H NMR (400 MHz, DMSO-d_6): δ 8.89 (dd, J = 8.2, 1.2 Hz, 2H), 8.42 - 8.32 (m, 4H), 8.13 (dd, J = 8.2, 5.1 Hz, 2H), 7.80 (d, J = 8.3 Hz, 2H), 7.72 (d, J = 8.7 Hz, 2H), 7.49 - 7.42 (m, 2H), 7.25 (t, J = 7.9 Hz, 8H), 7.05 (t, J = 7.4 Hz, 6H), 6.98 (d, J = 7.6 Hz, 8H), 6.55 (dd, J = 8.6, 2.3 Hz, 2H), 6.53 - 6.46 (m, 2H), 5.88 (d, J = 2.3 Hz, 2H). ^{13}C NMR (126 MHz, DMSO-d_6): δ 171.49, 156.26, 153.60, 153.25, 151.46, 151.33, 142.86, 141.88, 136.27, 134.64, 133.50, 132.39, 130.96, 130.85, 130.61, 129.06, 127.26, 127.15, 124.15, 124.03, 119.09. HRMS (MALDI-TOF, m/z): calcd for $C_{58}H_{42}N_6Ir$ $[M - PF_6]^+$ 1015.3100, found: 1015.3111.

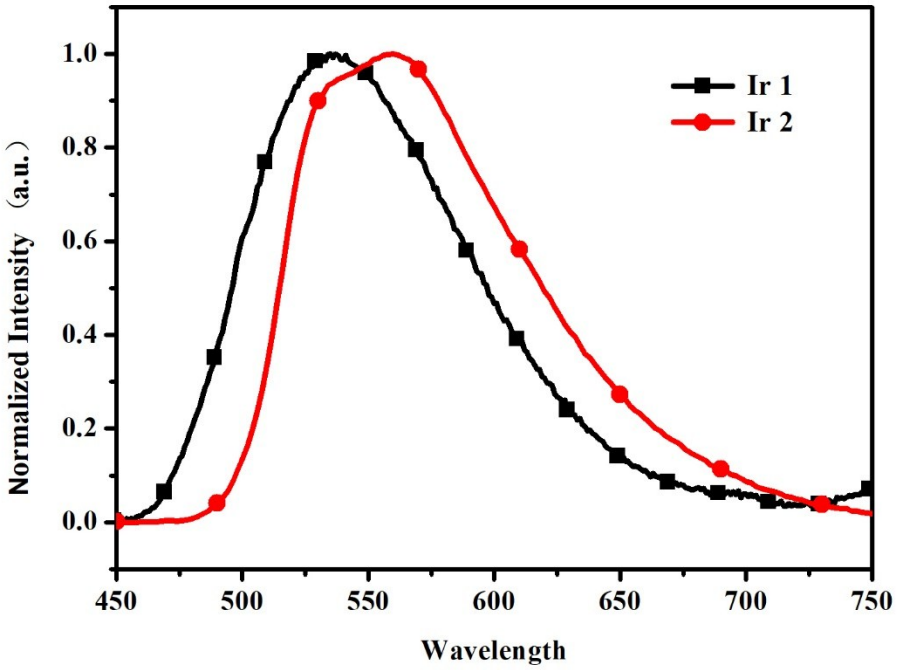


Fig. S1 Emission spectra of Ir(III) complexes **Ir1** and **Ir2** in EC film at room temperature (λ_{ex}= 410 nm).

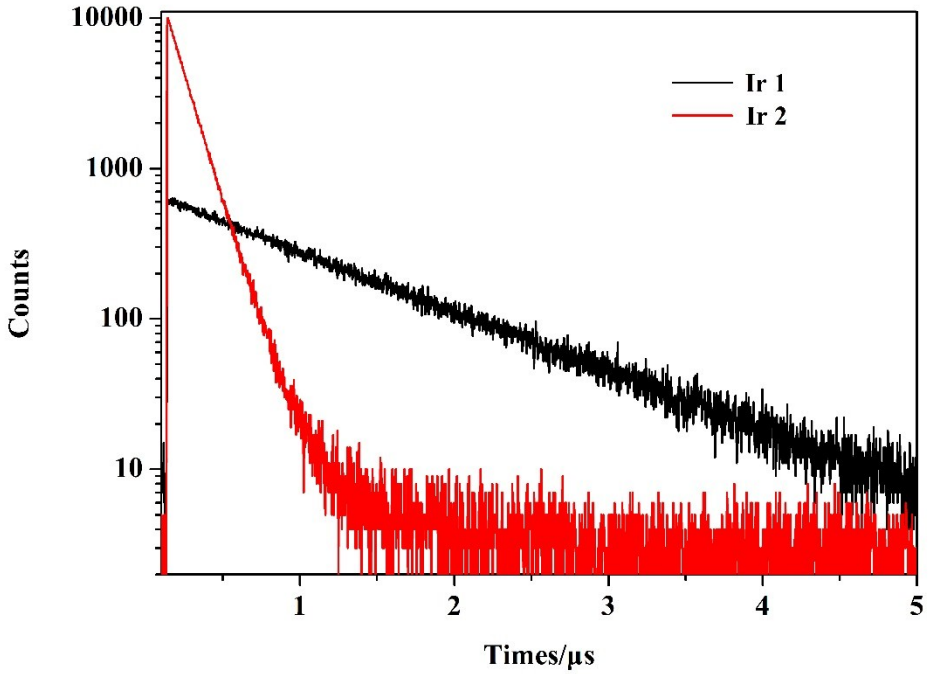


Fig. S2 Phosphorescence decay profiles of **Ir1** and **Ir2** in CH_2Cl_2 at room temperature.

Table S1 The photoluminescence quantum yields (Φ_{PL}) of complexes **Ir1** and **Ir2** in different states

	Photoluminescence quantum yields (Φ_{PL})		
	In CH_3CN	Solid state	CH_3CN/H_2O f_w (70%)
Ir1	3.1%	12.5%	-
Ir2	0.7%	6.1%	12.2%

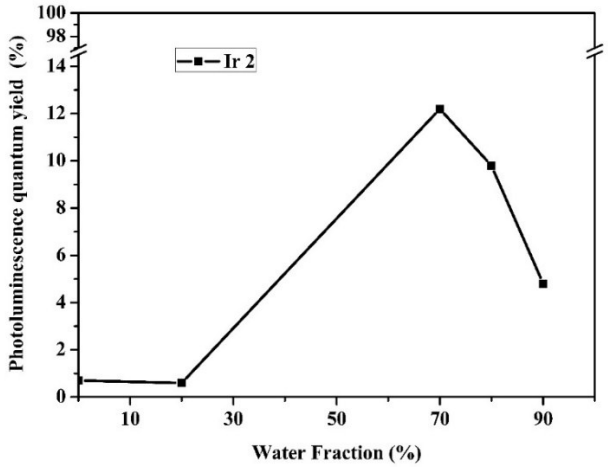


Fig. S3 The photoluminescence quantum yields (Φ_{PL}) of complex **Ir2** (5.0×10^{-5} M) in H_2O/CH_3CN with different water fractions (0-90%) at room temperature.

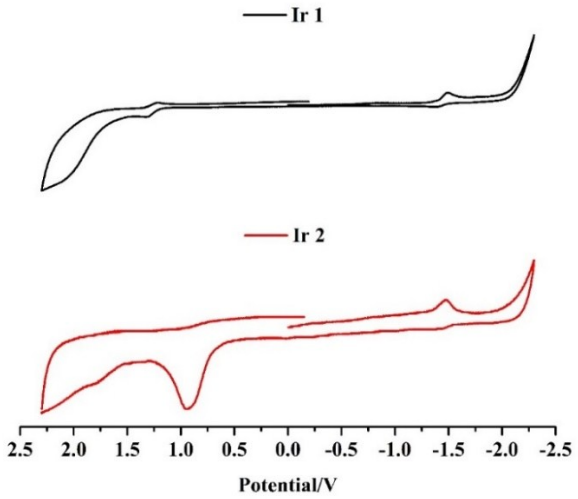


Fig. S4 Cyclic voltammograms of Ir(III) complexes **Ir1** and **Ir2** in CH_2Cl_2 (1.0×10^{-3} M).

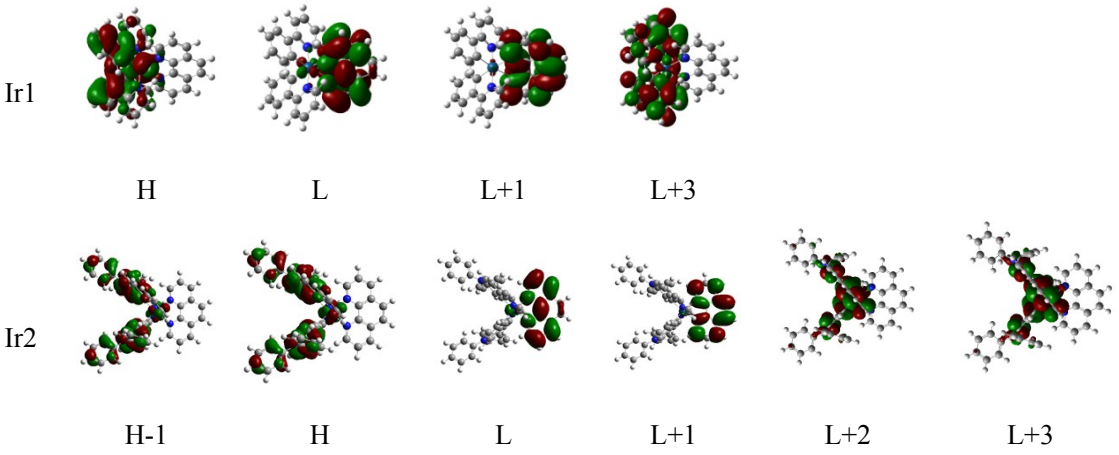


Fig. S5 Electron density maps of **Ir1** and **Ir2** calculated by a TD-DFT approach.

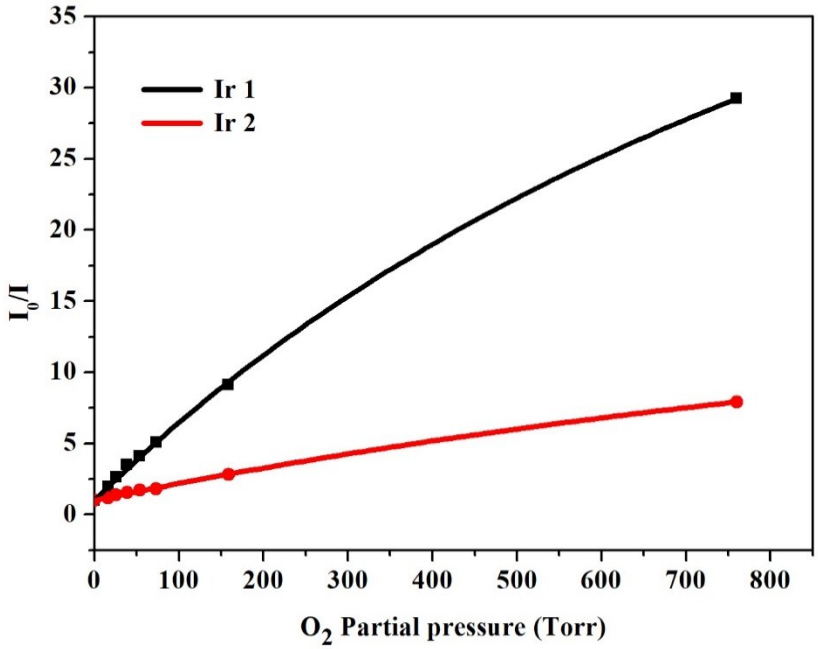


Fig. S6 Stern-Volmer plots (intensity ratios I_0/I versus O_2 partial pressure) of **Ir1** and **Ir2** in CH_2Cl_2 (1.0×10^{-5} M).

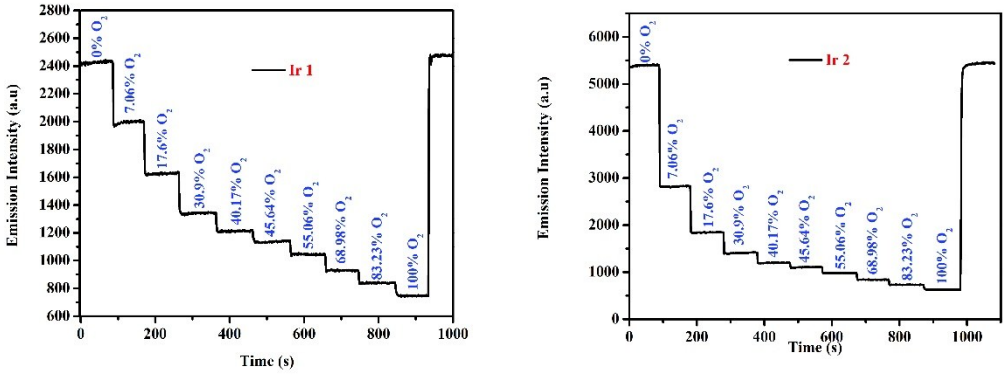


Fig. S7 Variation of the emission intensity of **Ir1** and **Ir2** immobilized in EC films with the oxygen concentrations.

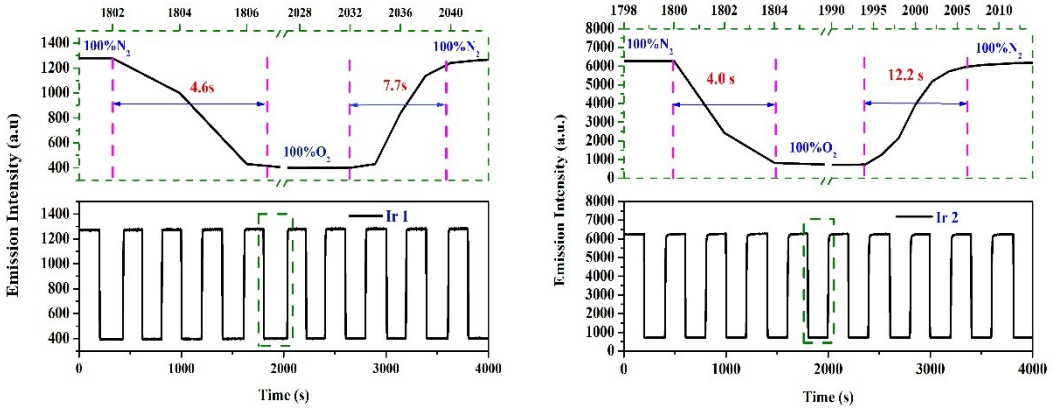


Fig. S8 Response times and relative intensity change for **Ir1** (left) and **Ir2** (right) immobilized in EC films on switching between 100% nitrogen and 100% oxygen for 4000 s.

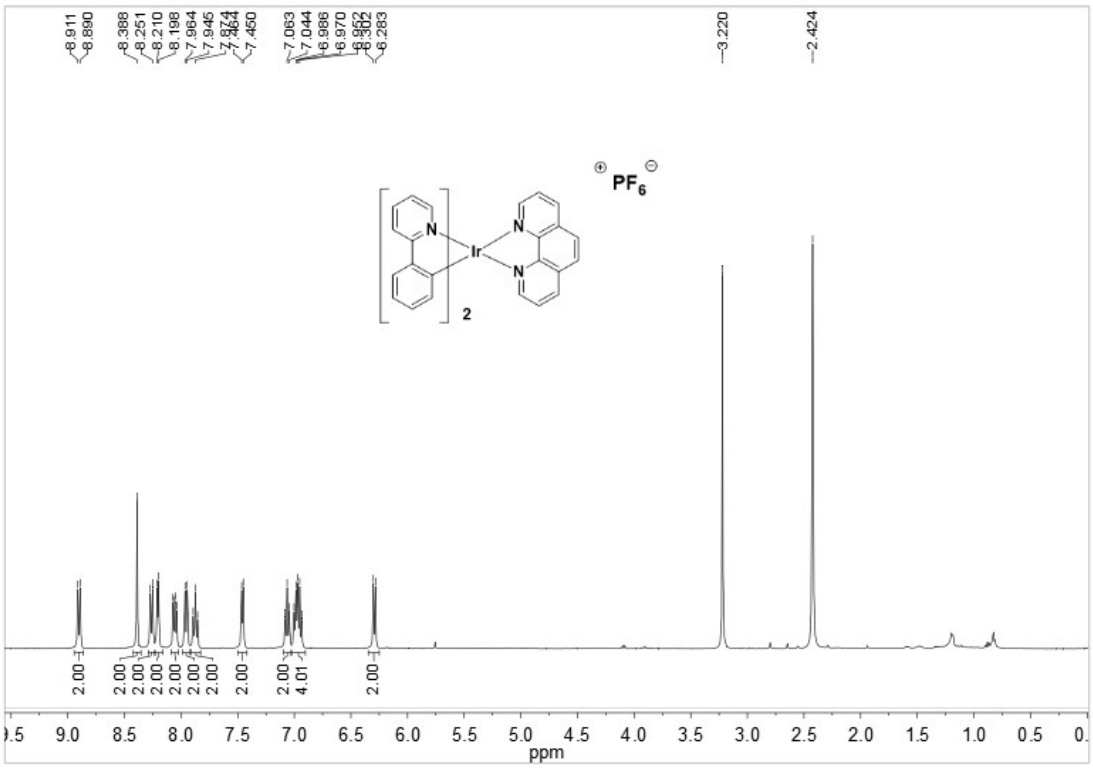


Fig. S9 The ^{1}H NMR spectrum of **Ir1** in DMSO-d_6.

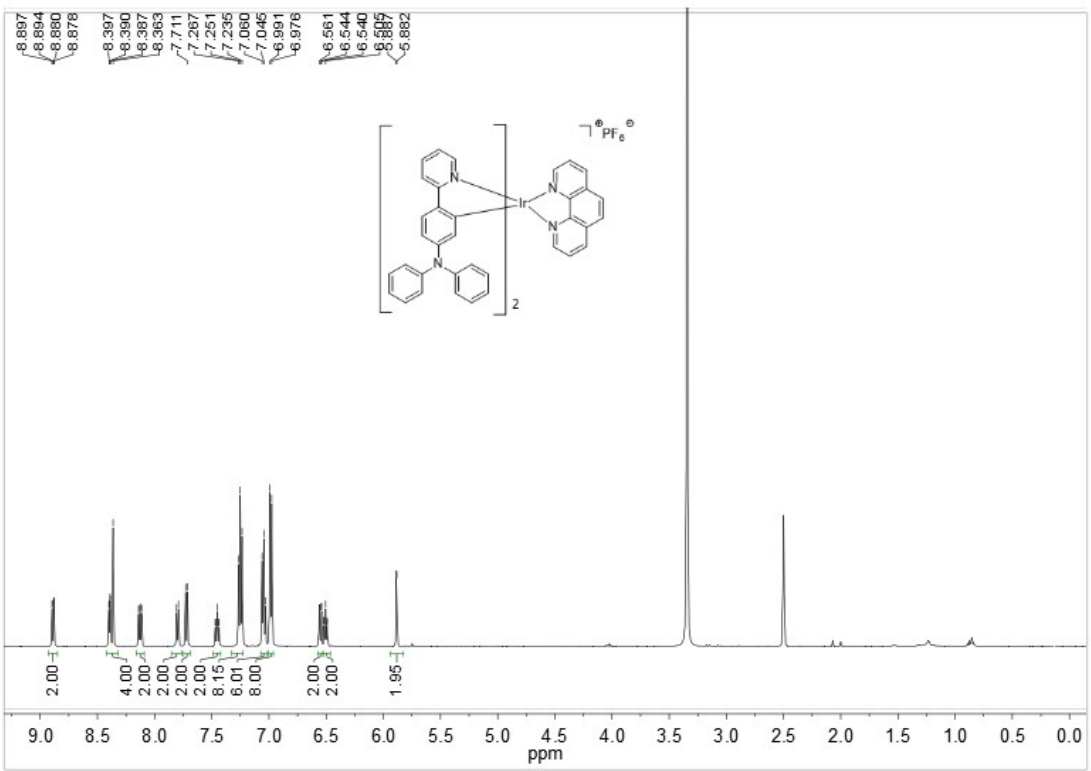


Fig. S10 The ^{1}H NMR spectrum of **Ir2** in DMSO-d_6.

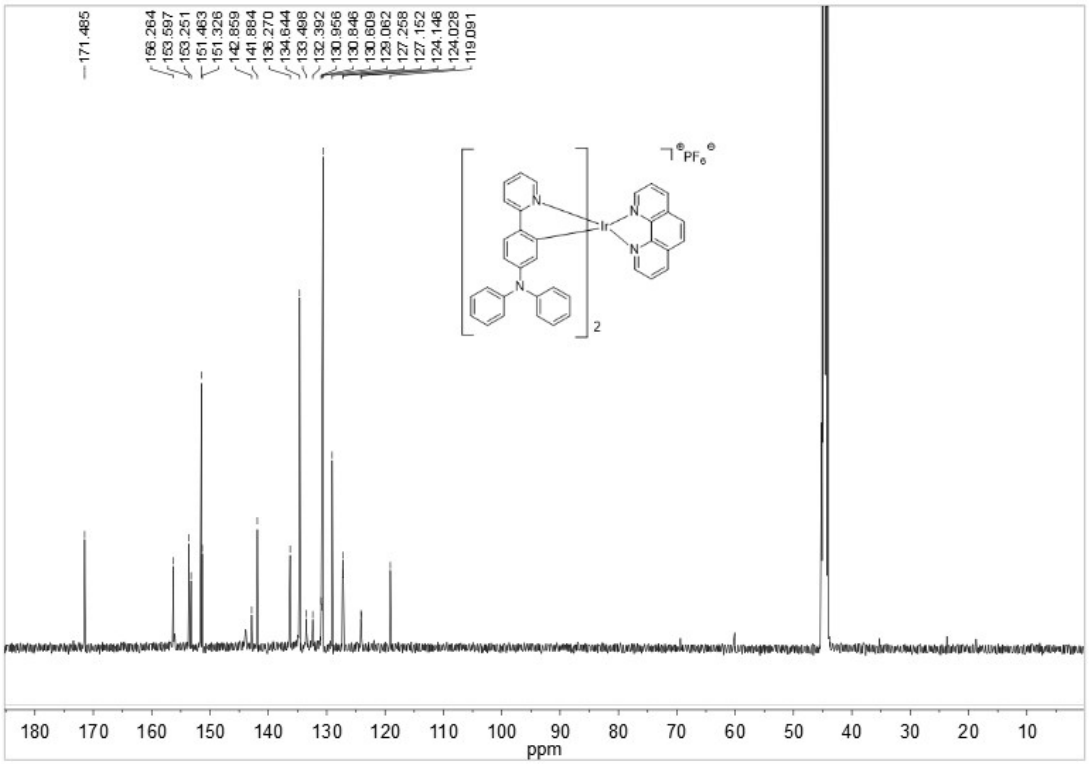


Fig. S11 The ^{13}C NMR spectrum of **Ir2** in DMSO-d_6.

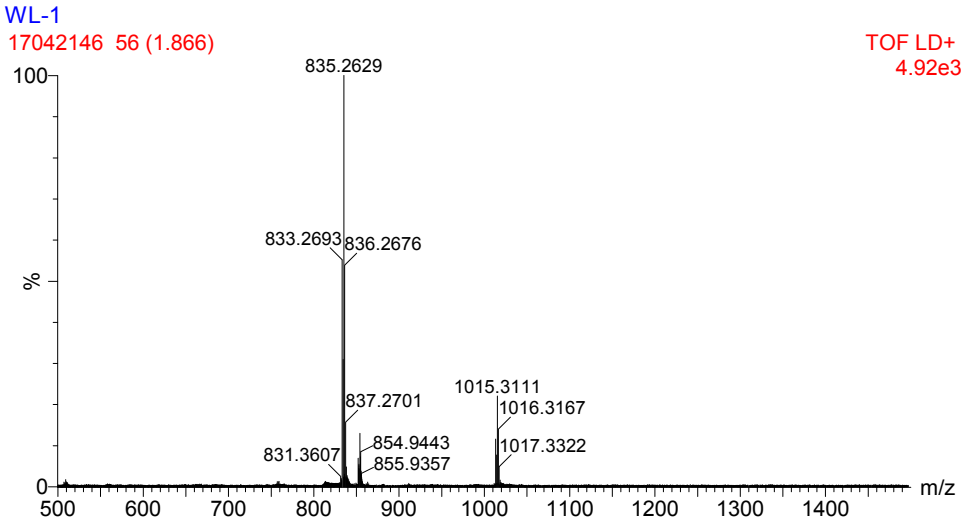


Fig. S12 The HRMS spectrum of cationic portion of **Ir2**.

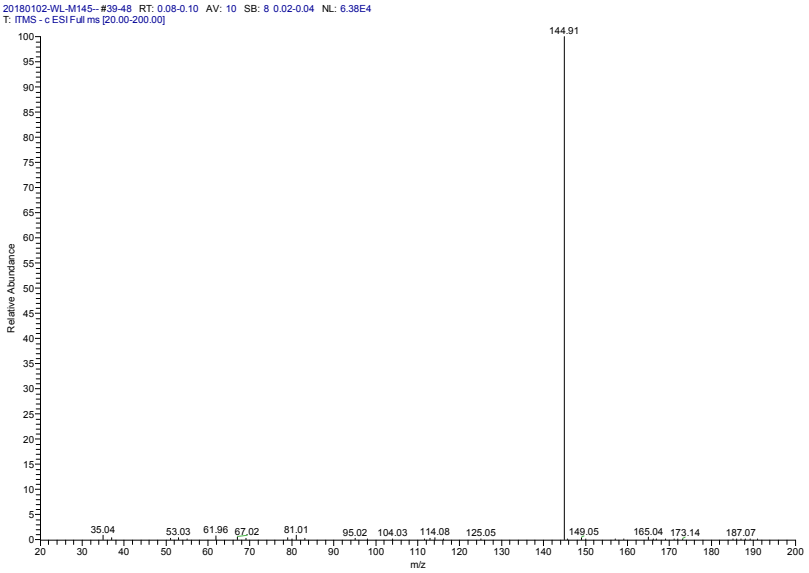


Fig. S13 The MS spectrum of PF_6^-.