

Electronic Supplementary Information (ESI)

AIE-active Ir(III) Complexes Functionalized with a Cationic Schiff Base Ligand: Synthesis, Photophysical Properties and Their Applications in Photodynamic Therapy

Shengnan Liu,^{‡a} Jiahong Han,^{‡a} Weijin Wang,^a Yulei Chang,^{*b} Runlin Wang,^a Ziwei Wang,^a Guangzhe Li,^{*c} Dongxia Zhu^{*a} and Martin R. Bryce^{*d}

^a *Key Laboratory of Nanobiosensing and Nanobioanalysis at Universities of Jilin Province, Department of Chemistry, Northeast Normal University, 5268 Renmin Street, Changchun, Jilin Province 130024, P. R. China.*

E-mail: zhudx047@nenu.edu.cn

^b *State Key Laboratory of Luminescence and Applications, Changchun Institute of Optics, Fine Mechanics and Physics, Chinese Academy of Sciences, Changchun Jilin Province 130033, China.*

Email: yuleichang@ciomp.ac.cn

^c *Jilin Provincial Science and Technology Innovation Center of Health Food of Chinese Medicine, Changchun University of Chinese Medicine, Changchun, Jilin Province 130117, P. R. China.*

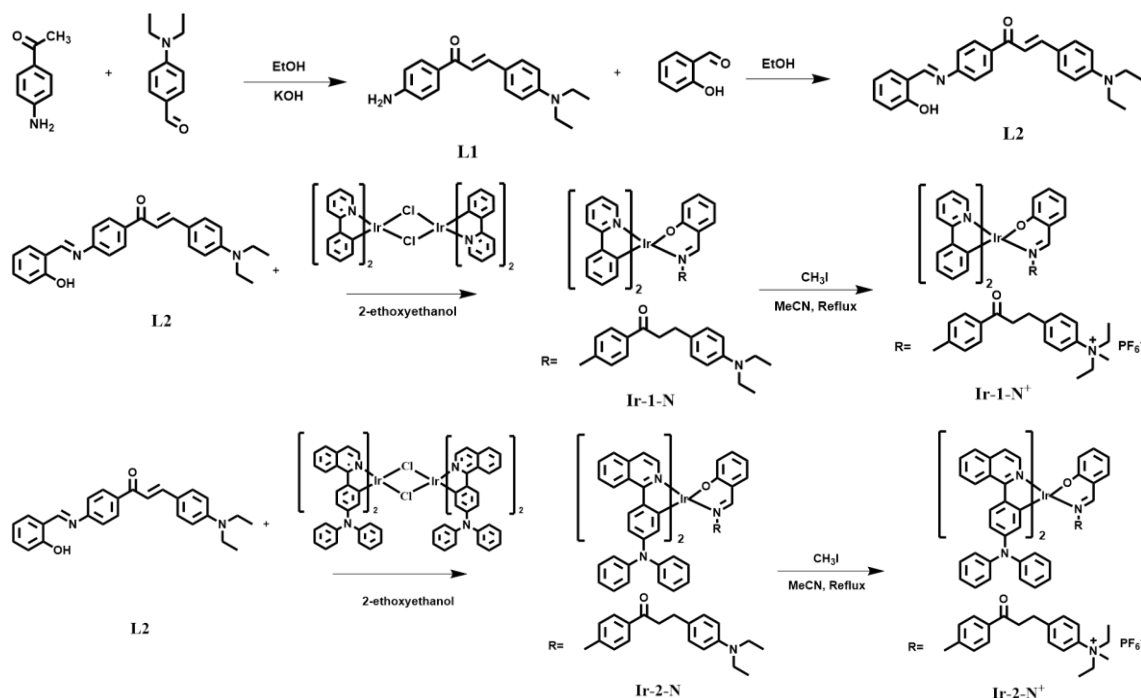
E-mail: 1993008106@qq.com

^d *Department of Chemistry, Durham University, Durham, DH1 3LE, UK.*

E-mail: m.r.bryce@durham.ac.uk

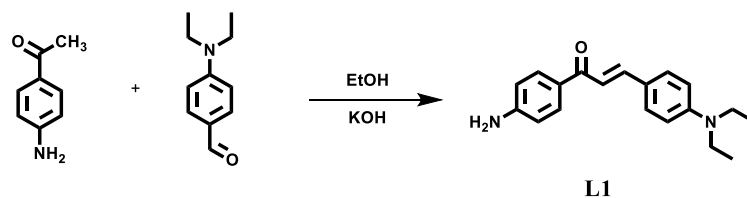
[‡]*The authors contributed equally to the preparation of this work.*

Supplementary Figures and Tables



Scheme S1 Synthetic routes of L1, L2, Ir-1-N⁺, and Ir-2-N⁺.

Synthesis of L1

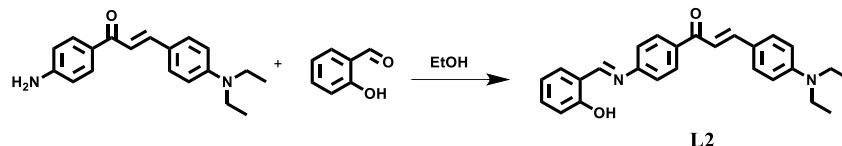


Scheme S1. Synthetic route for L1.

Following the literature procedure,¹ 4-aminoacetophenone (0.540 g, 4 mmol) and *N,N*-diethyl-4-aminobenzaldehyde (0.708 g, 4 mmol) were dissolved in ethanol (40 mL) and 10% KOH solution (20 mL) was added. The reaction was stirred at RT for 24 h. After completion of the reaction, extraction was performed with CH₂Cl₂ to remove KOH, and the organic layer was dried over anhydrous Na₂SO₄. The solvent was removed by a rotary evaporator. Using ethyl acetate (EA) and petroleum ether (PE) as eluents (EA/PE from 1/10 to 1/1, v/v), the crude product was purified by silica gel column chromatography to obtain a yellow solid. Yield: 43%. ¹H NMR (500 MHz, CDCl₃, δ [ppm]): 7.95-7.89 (m, 2H), 7.76 (d, *J* = 15.4 Hz, 1H), 7.52 (d, *J* = 8.8 Hz, 2H), 7.33 (d, *J* = 15.4 Hz, 1H), 6.72-6.63 (m, 4H), 4.10

(s, 2H), 3.41 (q, $J = 7.1$ Hz, 4H), 1.20 (t, $J = 7.1$ Hz, 6H).

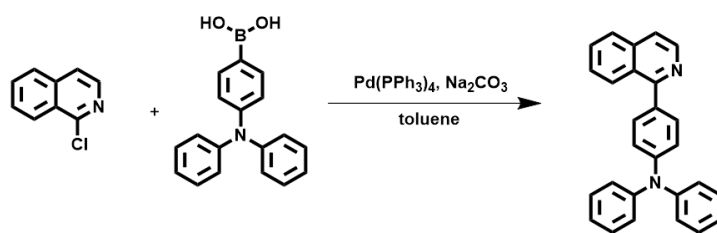
Synthesis of L2



Scheme S2. Synthetic route for L2.

The auxiliary ligand **L2** was synthesized by a Schiff base reaction. A mixture of amino chalcone (0.088 g, 0.3 mmol) and *o*-hydroxybenzaldehyde (0.108 g, 0.9 mmol) in ethanol (30 mL) was refluxed with stirring for 8 h to give an orange precipitate. The reaction mixture was cooled to room temperature. The precipitate was filtered to obtain ligand **L2**. Yield: 90%. ^1H NMR (500 MHz, CDCl_3 , δ [ppm]): 13.03 (s, 1H), 8.67 (s, 1H), 8.13-8.07 (m, 2H), 7.82 (d, $J = 15.3$ Hz, 1H), 7.55 (d, $J = 8.5$ Hz, 2H), 7.46-7.40 (m, 2H), 7.38-7.32 (m, 3H), 7.05 (d, $J = 8.3$ Hz, 1H), 6.97 (t, $J = 7.5$ Hz, 1H), 6.67 (t, $J = 8.5$ Hz, 2H), 3.43 (q, $J = 7.1$ Hz, 4H), 1.21 (t, $J = 7.1$ Hz, 6H).

Synthesis of the Cyclometallating ligand

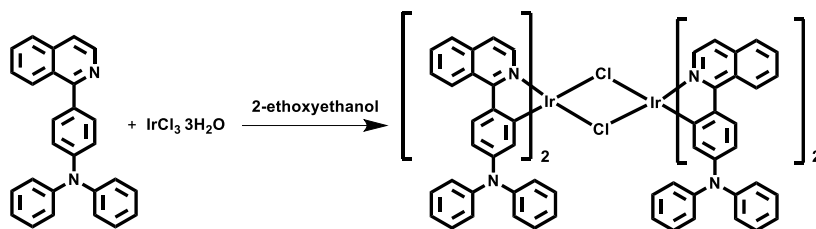


Scheme S3. Synthetic route for the cyclometallating ligand.

1-Chloroisoquinoline (0.496 g, 3.06 mmol) and 4-(triphenylamino)boronic acid (0.972 g, 3.36 mmol) were dissolved in toluene (30 mL) and tetrakis(triphenylphosphine)palladium(0) (0.177 g, 0.15 mmol) was added as a catalyst. Sodium carbonate (20 mL of 2 mol L^{-1} solution) was added and the mixture was refluxed for 48 h under N_2 . The mixture was then left to cool and extracted with dichloromethane. The organic phase was separated, dried over anhydrous MgSO_4 and evaporated. The crude product was purified by silica gel column chromatography (dichloromethane/petroleum ether, 10/3 v/v). A yellow solid was obtained in 74% yield. ^1H

NMR (500 MHz, CDCl₃, δ [ppm]): 8.60 (d, *J* = 5.6 Hz, 1H), 8.24 (d, *J* = 8.5 Hz, 1H), 7.88 (d, *J* = 8.2 Hz, 1H), 7.70 (t, *J* = 8.1 Hz, 1H), 7.64-7.59 (m, 3H), 7.57 (t, *J* = 8.3 Hz, 1H), 7.32-7.27 (m, 4H), 7.25-7.8 (m, 6H), 7.07 (t, *J* = 8.1 Hz, 2H).

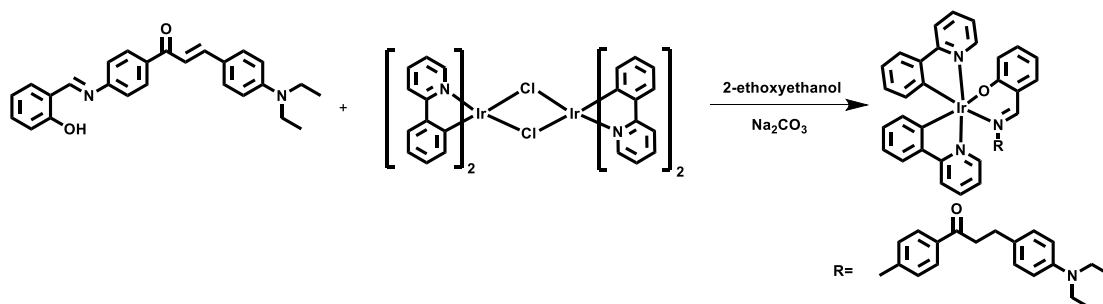
Synthesis of dichloro-bridged diiridium complex



Scheme S4. Synthetic route for the dichloro-bridged diiridium complex.

The cyclometalating ligand (0.930 g, 2.5 mmol) and IrCl₃·3H₂O (0.353 g, 1 mmol) were dissolved in a mixed solution of 2-ethoxyethanol (30 mL) and water (10 mL). The solution was heated to 120 °C and refluxed for 24 h under N₂. The solution was cooled to room temperature and water was added to obtain a precipitate. The mixture was stirred for 5 min and filtered to obtain a red solid which was dried in an oven for 24 h. Yield 80%. ¹H NMR (500 MHz, CDCl₃, δ [ppm]): 8.87 (d, *J* = 6.4 Hz, 1H), 8.76 (d, *J* = 8.4 Hz, 1H), 7.89 (d, *J* = 8.8 Hz, 1H), 7.71-7.61 (m, 2H), 7.58 (d, *J* = 8.0 Hz, 1H), 6.84 (t, *J* = 8.4 Hz, 4H), 6.79-6.74 (m, 4H), 6.70-6.66 (m, 2H), 6.49 (dd, *J* = 8.8, 2.5 Hz, 1H), 6.17 (d, *J* = 6.4 Hz, 1H), 5.53 (d, *J* = 2.4 Hz, 1H).

Synthesis of Ir-1-N

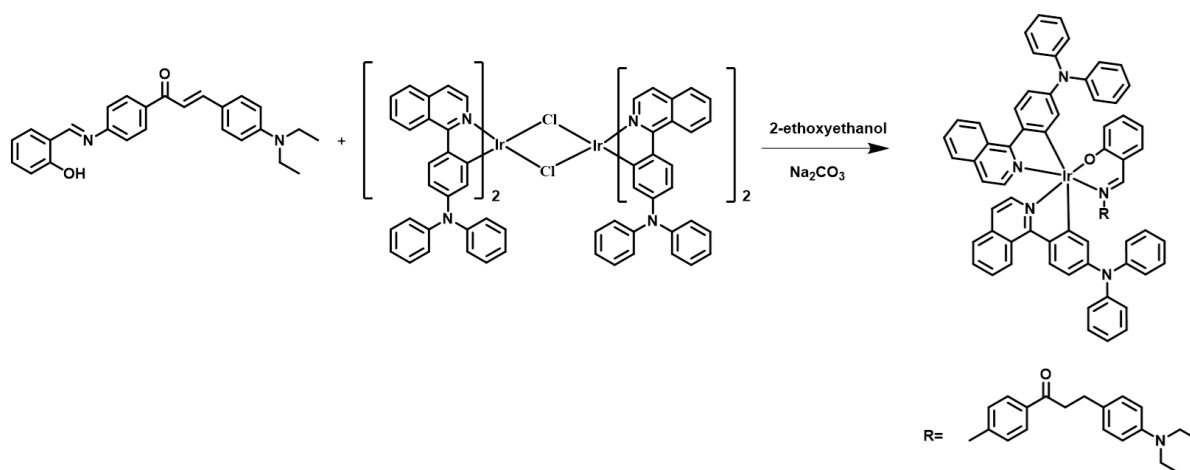


Scheme S5. Synthetic route for **Ir-1-N**. During the reaction the dichloro-bridged complex also acts as a catalyst to reduce the carbon-carbon double bond of the unsaturated ketone in

L2 to a carbon-carbon single bond.²

A mixture of the dichloro-bridged diiridium complex (0.0536 g, 0.05 mmol), Schiff base ligand **L2** (0.0398 g, 0.1 mmol) and Na₂CO₃ (0.1745 g, 1.6 mmol) in 2-ethoxyethanol (25 mL). The was heated to 140 °C under nitrogen atmosphere and refluxed for 8 h. After the reaction was completed, it was cooled to room temperature. Na₂CO₃ was removed by adding ethyl acetate. Using CH₂Cl₂ and petroleum ether as eluents (CH₂Cl₂/petroleum ether from 1/10 to 10/1, v/v), the crude product was purified by silica gel column chromatography. The complex **Ir-1-N** was obtained as an orange solid. Yield: 60%. ¹H NMR (500 MHz, CDCl₃, δ [ppm]): 8.88 (d, *J* = 6.7 Hz, 1H), 8.83 (d, *J* = 5.7 Hz, 1H), 8.08 (s, 1H), 7.88 (d, *J* = 8.1 Hz, 1H), 7.72 (t, *J* = 7.5 Hz, 1H), 7.69-7.64 (m, 1H), 7.58 (d, *J* = 7.7 Hz, 1H), 7.49 (d, *J* = 8.1 Hz, 1H), 7.33 (d, *J* = 3.7 Hz, 1H), 7.31 (d, *J* = 3.7 Hz, 1H), 7.25 (d, *J* = 2.0 Hz, 1H), 7.13 (dd, *J* = 8.0, 6.1 Hz, 2H), 7.09-7.02 (m, 3H), 6.96 (dd, *J* = 5.9, 3.0 Hz, 1H), 6.85 (t, *J* = 7.6 Hz, 1H), 6.74-6.67 (m, 3H), 6.65 (d, *J* = 8.6 Hz, 1H), 6.46-6.51 (m, 2H), 6.40 (t, *J* = 7.4 Hz, 1H), 6.25 (t, *J* = 7.6 Hz, 1H), 6.18 (t, *J* = 8.3 Hz, 2H), 6.16-6.14 (m, 1H), 3.34 (q, *J* = 7.1 Hz, 3H), 3.15 (q, *J* = 7.2 Hz, 1H), 3.03 (q, *J* = 7.1 Hz, 2H), 2.88-2.83 (m, 2H), 1.25 (t, *J* = 7.1 Hz, 2H), 1.15 (t, *J* = 7.0 Hz, 4H). ¹³C{¹H} NMR (151 MHz, CDCl₃) δ 197.89, 167.71, 167.36, 166.03, 160.07, 154.17, 148.82, 148.06, 147.29, 143.47, 143.03, 135.82, 135.76, 134.32, 133.57, 132.18, 132.15, 131.53, 128.35, 128.11, 128.04, 126.66, 123.90, 122.81, 122.49, 121.52, 120.67, 120.36, 120.34, 118.90, 117.98, 116.97, 112.70, 111.16, 43.39, 39.96, 28.42, 11.58. ESI-MS: [m/z] = 901.31 (M⁺ + H) [calcd for C₄₈H₄₃IrN₄O₂ (M⁺) 900.10]. The higher mass peak at 923 in Fig. S7 is from M⁺ + Na. Anal. Calcd. for C₄₈H₄₃IrN₄O₂: C 64.05, H 4.82, N 6.22. Found C 64.02, H 4.80, N 6.24.

Synthesis of Ir-2-N



Scheme S6. Synthetic route for **Ir-2-N**. As in the synthesis of **Ir-1-N**, the dichloro-bridged complex also acts as a catalyst to reduce the carbon-carbon double bond in the unsaturated ketone of **L2** to a carbon-carbon single bond.²

A mixture of the dichloro-bridged diiridium complex (0.0970 g, 0.05 mmol), Schiff base ligand **L2** (0.0398 g, 0.1 mmol) and Na_2CO_3 (0.1745 g, 1.6 mmol) in 2-ethoxyethanol (25 mL) was heated to 140 °C under nitrogen and refluxed for 8 h. After the reaction was completed, it was cooled to room temperature. Na_2CO_3 was removed by adding ethyl acetate. The obtained crude product was purified by column chromatography with ethyl acetate and petroleum ether as eluents (ethyl acetate /petroleum ether from 1/10 to 10/1, v/v), and a red solid of complex **Ir-2-N** was obtained. Yield: 60%. ^1H NMR (500 MHz, CDCl_3 , δ [ppm]): 8.72 (d, $J = 8.4$ Hz, 1H), 8.56 (d, $J = 6.3$ Hz, 1H), 8.45 (d, $J = 6.4$ Hz, 1H), 8.34 (d, $J = 8.6$ Hz, 1H), 8.04 (s, 1H), 7.95 (d, $J = 8.9$ Hz, 1H), 7.73 (d, $J = 8.1$ Hz, 1H), 7.69 (d, $J = 7.9$ Hz, 1H), 7.64-7.52 (m, 4H), 7.49 (d, $J = 8.8$ Hz, 1H), 7.39 (d, $J = 8.2$ Hz, 2H), 7.24-7.20 (m, 1H), 7.10 (t, $J = 7.8$ Hz, 2H), 7.03 (t, $J = 8.0$ Hz, 3H), 6.98-6.93 (m, 4H), 6.89 (dd, $J = 8.5, 7.1$ Hz, 4H), 6.85-6.81 (m, 4H), 6.79-6.75 (m, 4H), 6.75-6.71 (m, 3H), 6.66 (dd, $J = 8.1, 6.7$ Hz, 2H), 6.61 (d, $J = 8.7$ Hz, 2H), 6.58 (dd, $J = 8.8, 2.5$ Hz, 1H), 6.39-6.35 (m, 1H), 6.32 (dd, $J = 8.8, 2.5$ Hz, 1H), 6.22 (d, $J = 8.0$ Hz, 2H), 5.88 (d, $J = 2.5$ Hz, 1H), 5.66 (d, $J = 2.4$ Hz, 1H), 3.32 (q, $J = 7.0$ Hz, 4H), 3.08-3.01 (m, 2H), 2.88 (t, $J = 7.8$ Hz, 2H), 1.14 (t, $J = 7.0$ Hz, 6H). $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) δ 197.59, 167.45, 166.72, 165.83, 159.82, 154.83, 146.44, 145.75, 145.70, 140.18, 139.21, 137.91, 135.74, 135.59, 134.34, 133.43, 132.28, 129.33, 129.02, 128.73, 128.31, 128.15, 127.66, 127.54, 126.82, 126.61, 125.97, 125.21, 124.97, 124.61, 124.43, 124.29, 123.94, 123.73, 122.19, 121.98, 121.88, 120.37, 117.30, 117.25, 112.57, 112.37,

112.24, 111.19, 43.38, 40.01, 28.67, 28.39, 11.59. ESI-MS: $[m/z] = 1335.4860 (M^+ + H)$ [calcd for $C_{80}H_{65}IrN_6O_2 (M^+)$ 1334.63]. Anal. Calcd. for $C_{80}H_{65}IrN_6O_2$: C 71.99, H 4.91, N 6.30. Found C 72.02, H 4.88, N 6.32.

Synthesis of Ir-1-N⁺

The complex **Ir-1-N** (0.0450 g, 0.05 mmol) and acetonitrile were mixed under nitrogen atmosphere. Iodomethane (1 mL) was added dropwise and the mixture was heated for 12 h. After the reaction was completed, it was cooled to room temperature. The mixture was poured into diethyl ether to obtain a yellow precipitate. The precipitate was filtered and dissolved in acetone (10 mL). Saturated KPF_6 (5 mL) was added to the solution with stirring for 2 h. KPF_6 was filtered and the filtrate solution was evaporated to obtain **Ir-1-N⁺** as a yellow solid. Yield: 90%. 1H NMR (500 MHz, $CDCl_3$, δ [ppm]): 8.86 (d, $J = 5.6$ Hz, 1H), 8.81 (d, $J = 5.7$ Hz, 1H), 8.07 (s, 1H), 7.86 (d, $J = 8.1$ Hz, 1H), 7.71 (d, $J = 8.4$ Hz, 1H), 7.68 (d, $J = 8.6$ Hz, 1H), 7.56 (d, $J = 7.7$ Hz, 1H), 7.53 (d, $J = 8.3$ Hz, 1H), 7.43 (d, $J = 8.6$ Hz, 2H), 7.38 (d, $J = 8.6$ Hz, 2H), 7.32 (d, $J = 8.3$ Hz, 2H), 7.23 (d, $J = 7.5$ Hz, 1H), 7.11 (d, $J = 8.1$ Hz, 2H), 7.05 (t, $J = 6.5$ Hz, 1H), 6.99-6.94 (m, 1H), 6.82 (t, $J = 7.4$ Hz, 1H), 6.67 (dd, $J = 8.6, 8.0$ Hz, 2H), 6.48-6.44 (m, 2H), 6.39 (t, $J = 7.3$ Hz, 1H), 6.22 (d, $J = 7.9$ Hz, 2H), 6.19 (d, $J = 8.4$ Hz, 1H), 6.13 (d, $J = 7.3$ Hz, 1H), 5.34 (t, $J = 4.8$ Hz, 1H), 3.85 (q, $J = 7.0$ Hz, 2H), 3.70 (q, $J = 6.9$ Hz, 2H), 3.29 (s, 3H), 3.10 (d, $J = 6.9$ Hz, 2H), 3.03 (d, $J = 7.2$ Hz, 2H), 2.21 (t, $J = 7.5$ Hz, 1H), 2.02 (t, $J = 7.0$ Hz, 4H). $^{13}C\{^1H\}$ NMR (151 MHz, $DMSO-d_6$) δ 196.37, 168.13, 155.87, 154.12, 145.36, 144.80, 144.36, 139.39, 130.84, 130.57, 130.46, 127.89, 124.85, 123.03, 122.32, 122.26, 121.76, 121.50, 121.44, 113.50, 113.00, 63.60, 53.71, 46.25, 38.31, 29.61, 8.68. ESI-MS: $[m/z] = 915.3269 (M^+)$ (calcd: 915.32). Anal. Calcd. for $C_{49}H_{46}IrN_4O_2^+$: C 64.31, H 5.07, N 6.12. Found C 64.32, H 5.05, N 6.14.

Synthesis of Ir-2-N⁺

Following the procedure to obtain **Ir-1-N⁺**, the complex **Ir-2-N** (0.0450 g, 0.05 mmol) and acetonitrile were mixed under nitrogen atmosphere. Iodomethane (1 mL) was added dropwise

and the mixture was heated for 12 h. After the reaction was completed, it was cooled to room temperature. The mixture was poured into diethyl ether to obtain a precipitate. The precipitate was filtered and dissolved in acetone (10 mL). Saturated KPF_6 (5 mL) was added into the solution with stirring for 2 h. KPF_6 was filtered and the filtrate solution was evaporated to obtain **Ir-2-N⁺** as a red solid in 89% yield. ^1H NMR (500 MHz, CDCl_3 , δ [ppm]): 8.69 (d, $J = 8.4$ Hz, 1H), 8.55 (d, $J = 6.3$ Hz, 1H), 8.42 (d, $J = 6.4$ Hz, 1H), 8.55 (d, $J = 6.3$ Hz, 1H), 8.37 (d, $J = 8.7$ Hz, 1H), 8.02 (s, 1H), 7.92 (d, $J = 8.8$ Hz, 1H), 7.72 (d, $J = 8.2$ Hz, 1H), 7.68 (d, $J = 7.9$ Hz, 1H), 7.64 (d, $J = 7.2$ Hz, 1H), 7.61 (d, $J = 9.0$ Hz, 1H), 7.58 (d, $J = 4.8$ Hz, 1H), 7.55 (d, $J = 8.0$ Hz, 1H), 7.49 (d, $J = 8.9$ Hz, 1H), 7.42 (d, $J = 8.8$ Hz, 2H), 7.40-7.34 (m, 4H), 7.22 (t, $J = 8.1$ Hz, 1H), 7.08 (t, $J = 6.5$ Hz, 2H), 7.01 (d, $J = 6.4$ Hz, 1H), 6.95 (t, $J = 7.7$ Hz, 3H), 6.88 (t, $J = 7.7$ Hz, 3H), 6.82 (d, $J = 7.9$ Hz, 4H), 6.77-6.73 (m, 6H), 6.69 (d, $J = 6.8$ Hz, 1H), 6.66 (d, $J = 7.3$ Hz, 2H), 6.56 (d, $J = 8.8$ Hz, 1H), 6.36 (t, $J = 7.4$ Hz, 1H), 6.30 (d, $J = 8.8$ Hz, 1H), 6.30 (d, $J = 8.0$ Hz, 2H), 5.84 (d, $J = 2.4$ Hz, 1H), 5.61 (d, $J = 2.4$ Hz, 1H), 5.35 (t, $J = 4.9$ Hz, 1H), 3.92 (q, $J = 6.3$ Hz, 2H), 3.88 (q, $J = 6.9$ Hz, 2H), 3.38 (s, 3H), 3.11 (q, $J = 6.1$ Hz, 2H), 3.06 (d, $J = 6.6$ Hz, 2H), 2.02 (t, $J = 6.7$ Hz, 6H). $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, $\text{DMSO-}d_6$) δ 196.32, 154.15, 147.17, 146.39, 146.27, 144.39, 143.82, 139.40, 136.90, 130.83, 130.58, 129.39, 127.94, 125.84, 125.22, 124.85, 124.08, 123.78, 122.30, 122.26, 112.99, 63.59, 46.22, 38.30, 29.61, 26.82, 8.69. ESI-MS: $[m/z] = 1349.5000$ (M^+) (calcd: 1349.50). Anal. Calcd. for $\text{C}_{81}\text{H}_{67}\text{IrN}_6\text{O}_2^+$: C 72.14, H 5.01, N 6.23. Found C 72.15, H 5.03, N 6.24.

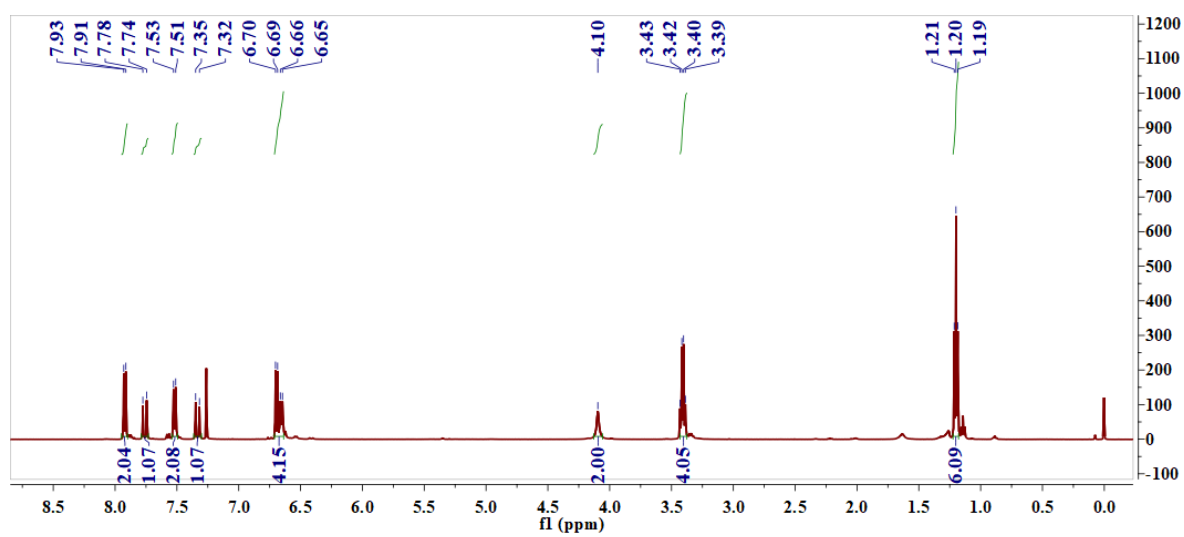


Fig. S1. ^1H NMR spectrum of **L1** in CDCl_3 at room temperature.

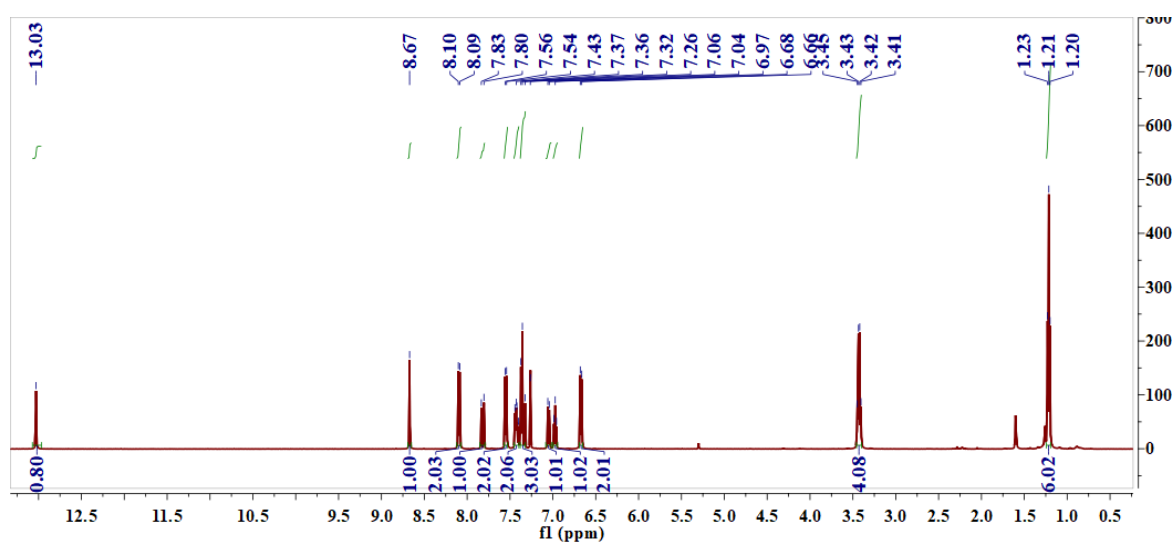


Fig. S2. ^1H NMR spectrum of **L2** in CDCl_3 at room temperature.

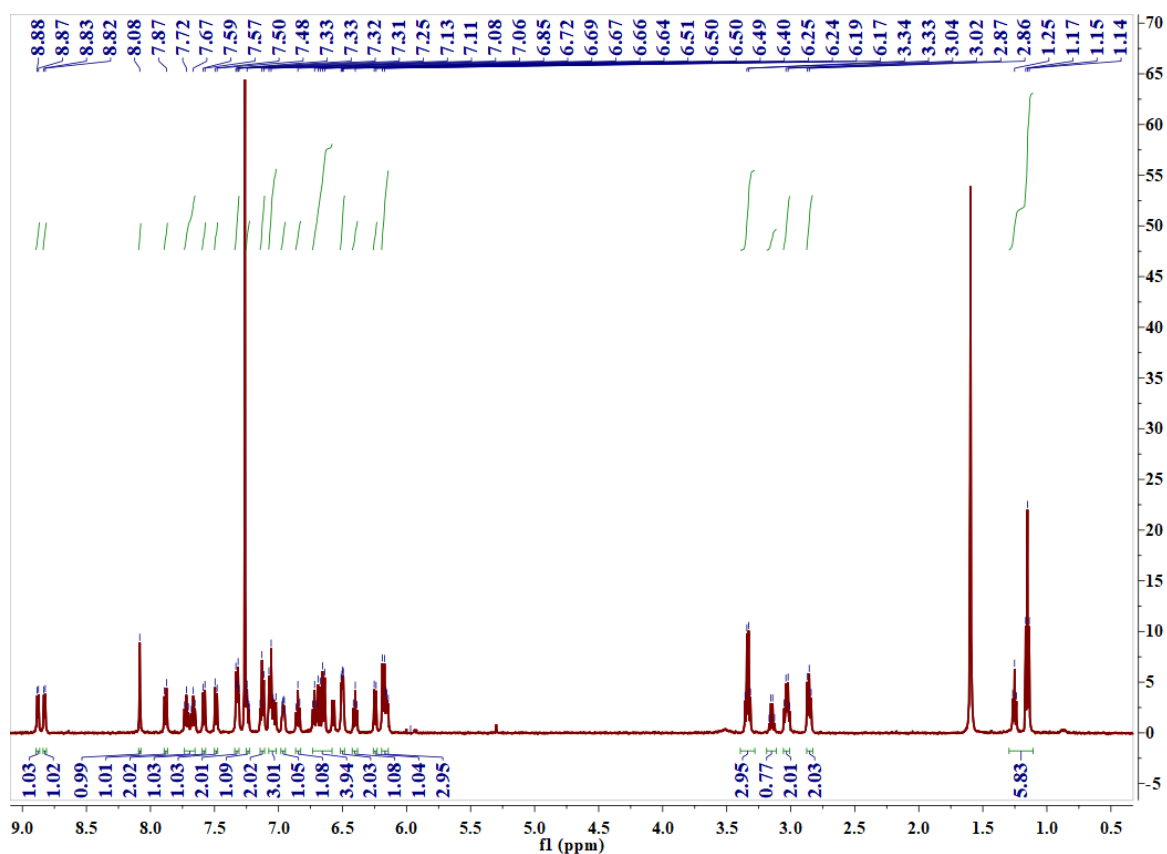


Fig. S3 ^1H NMR spectrum of Ir-1-N in CDCl_3

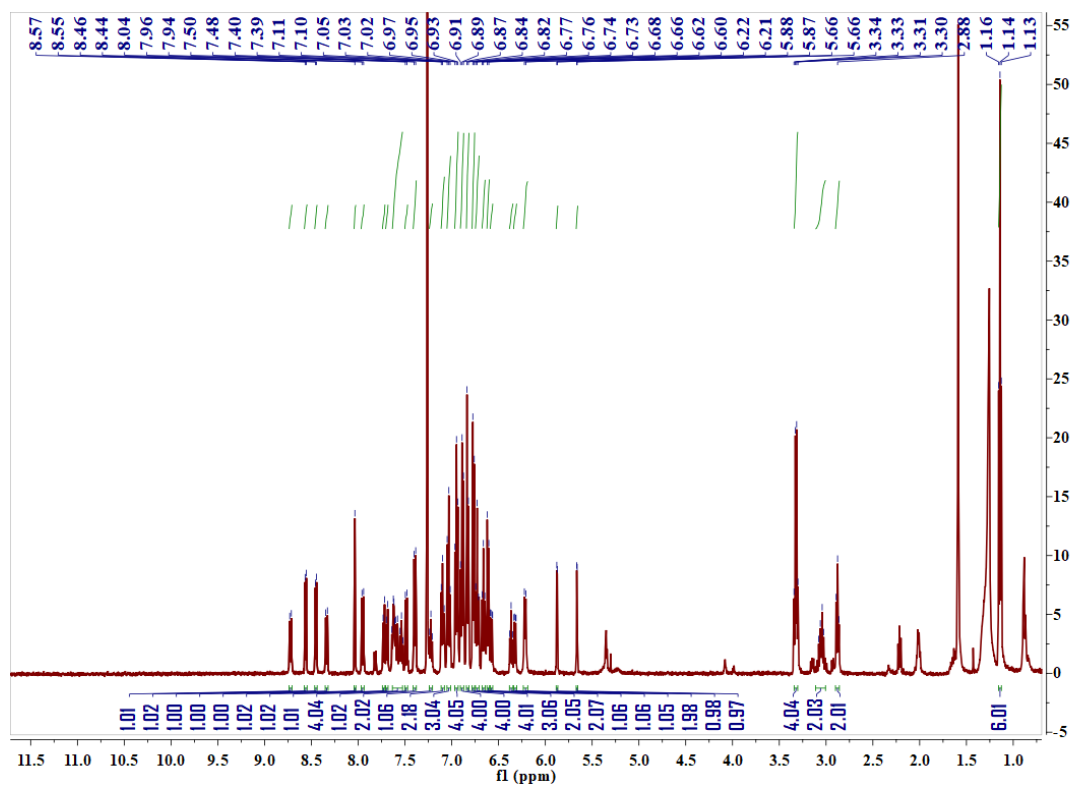


Fig. S4 ^1H NMR spectrum of Ir-2-N in CDCl_3

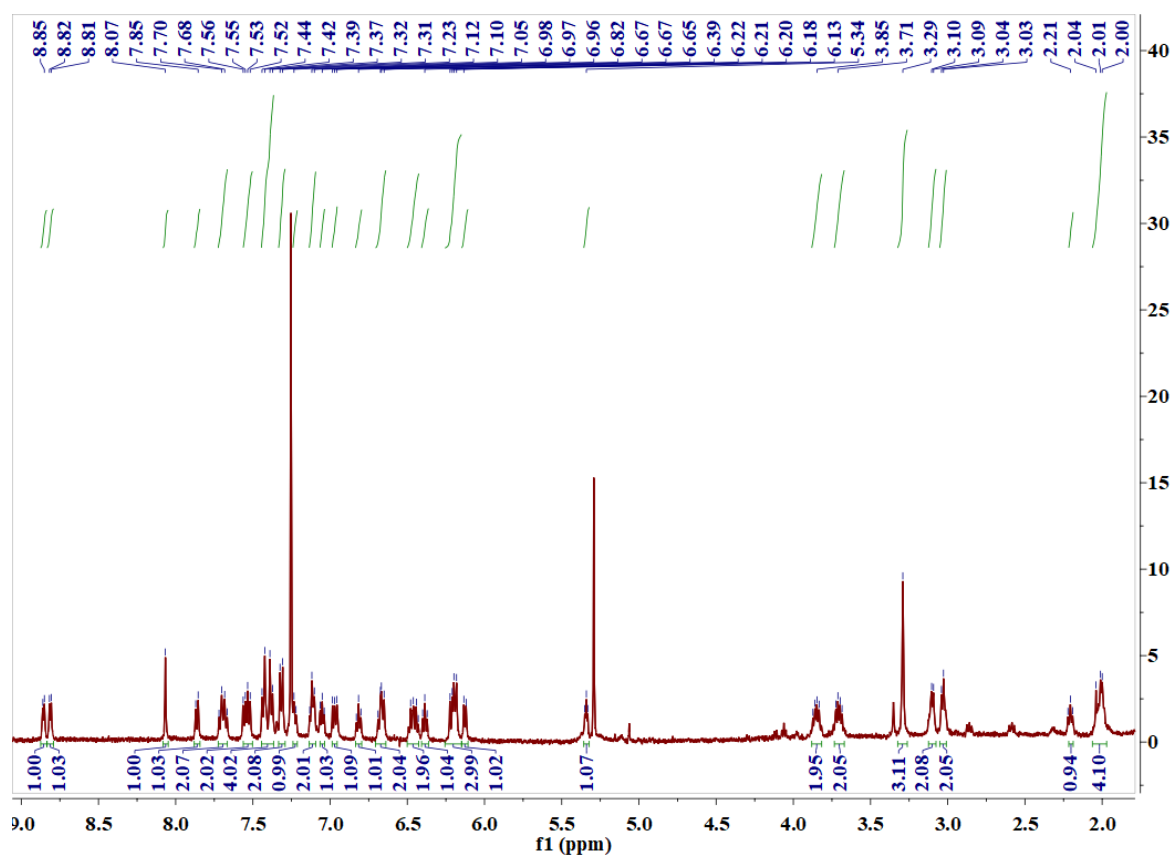


Fig. S5 ^1H NMR spectrum of **Ir-1-N⁺** in CDCl_3 .

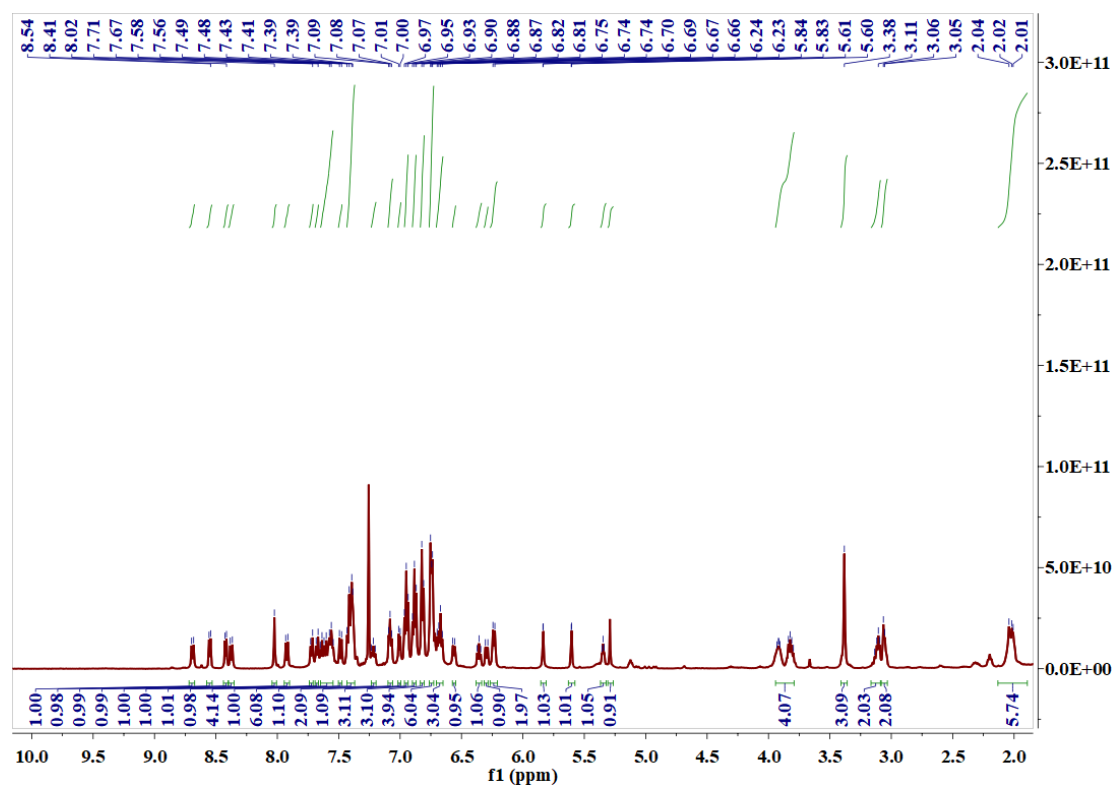


Fig. S6 ^1H NMR spectrum of **Ir-2-N⁺** in CDCl_3 .

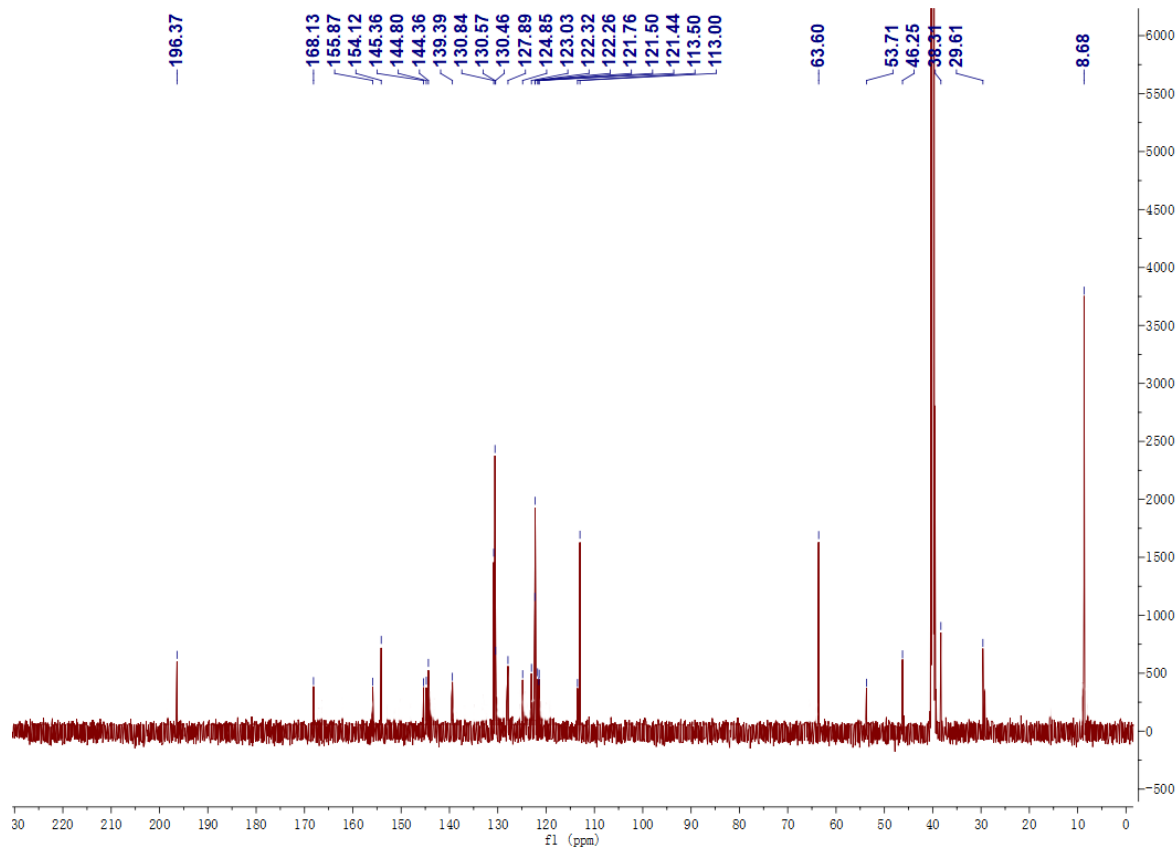


Fig. S7 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **Ir-1-N⁺** in CDCl_3

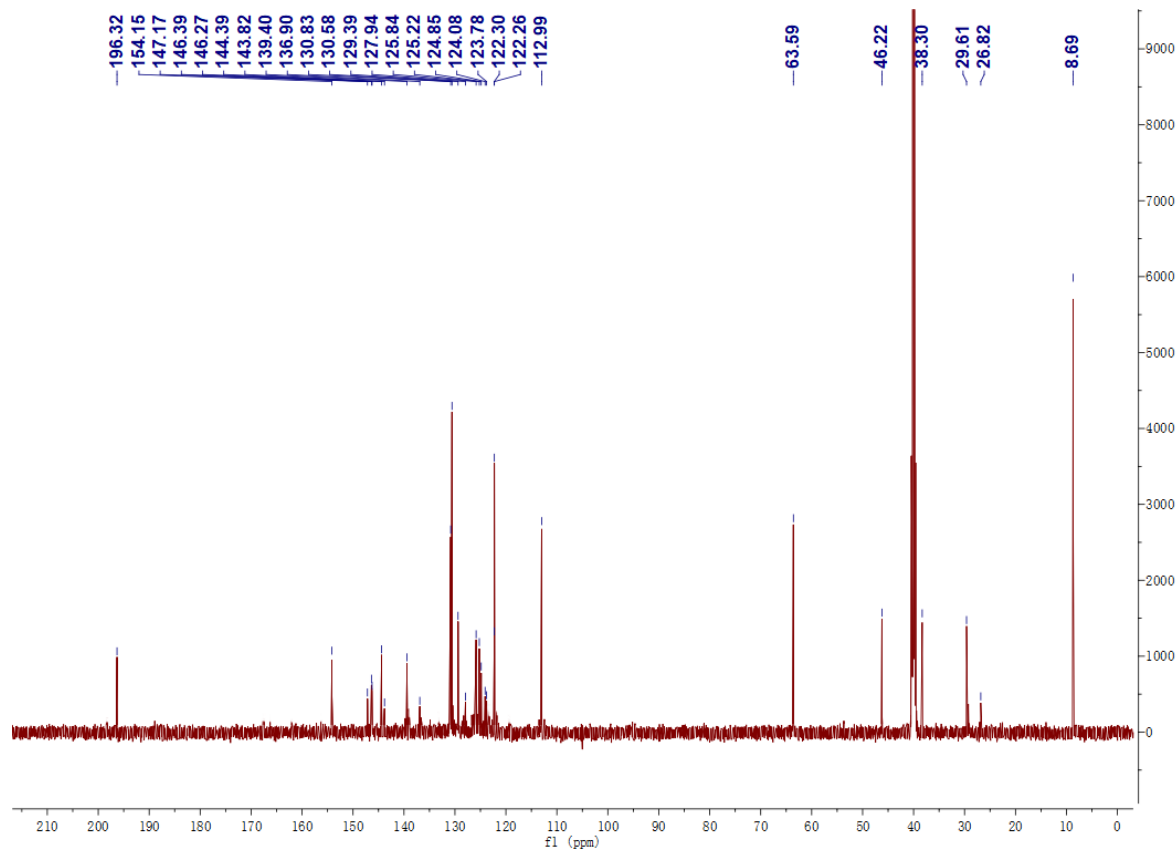


Fig. S8 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **Ir-1-N⁺** in CDCl_3

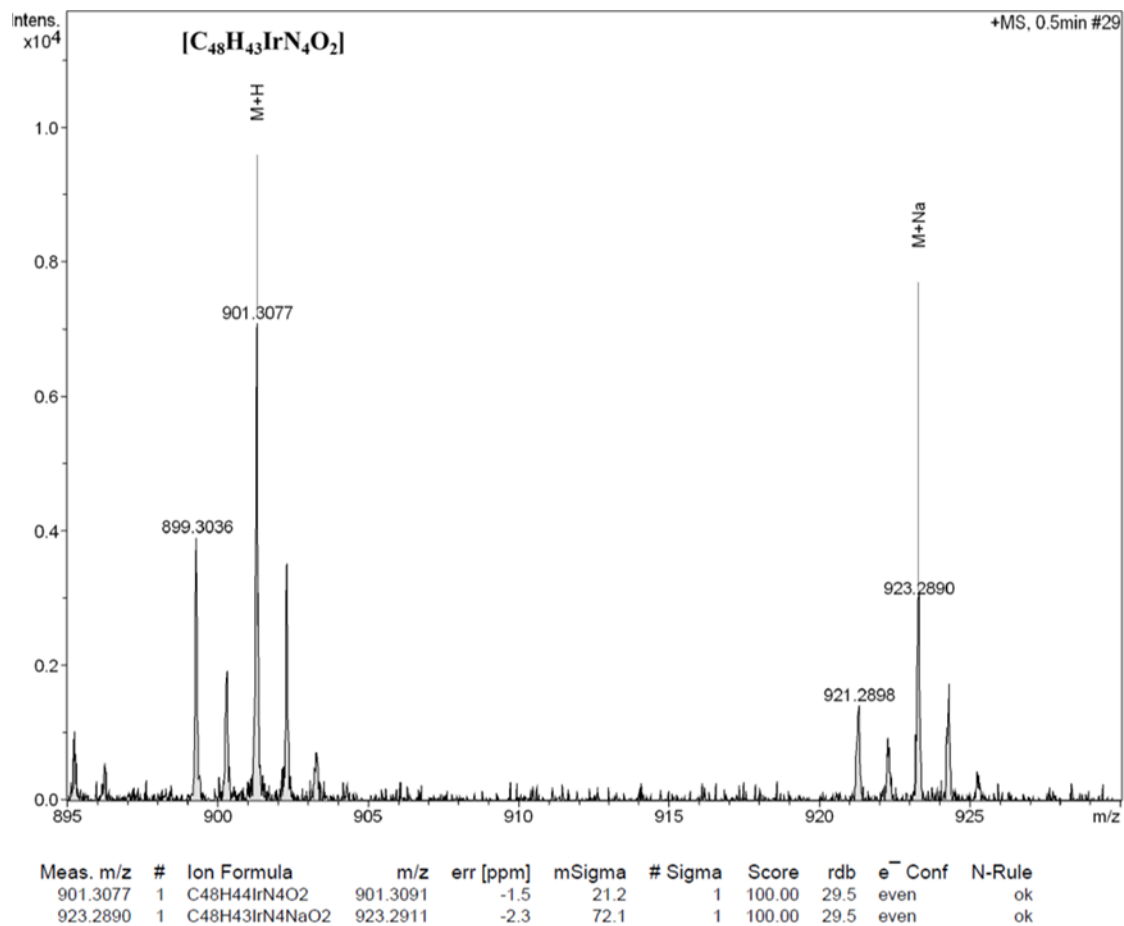


Fig. S9 High Resolution Mass Spectrometry (HRMS) of **Ir-1-N**

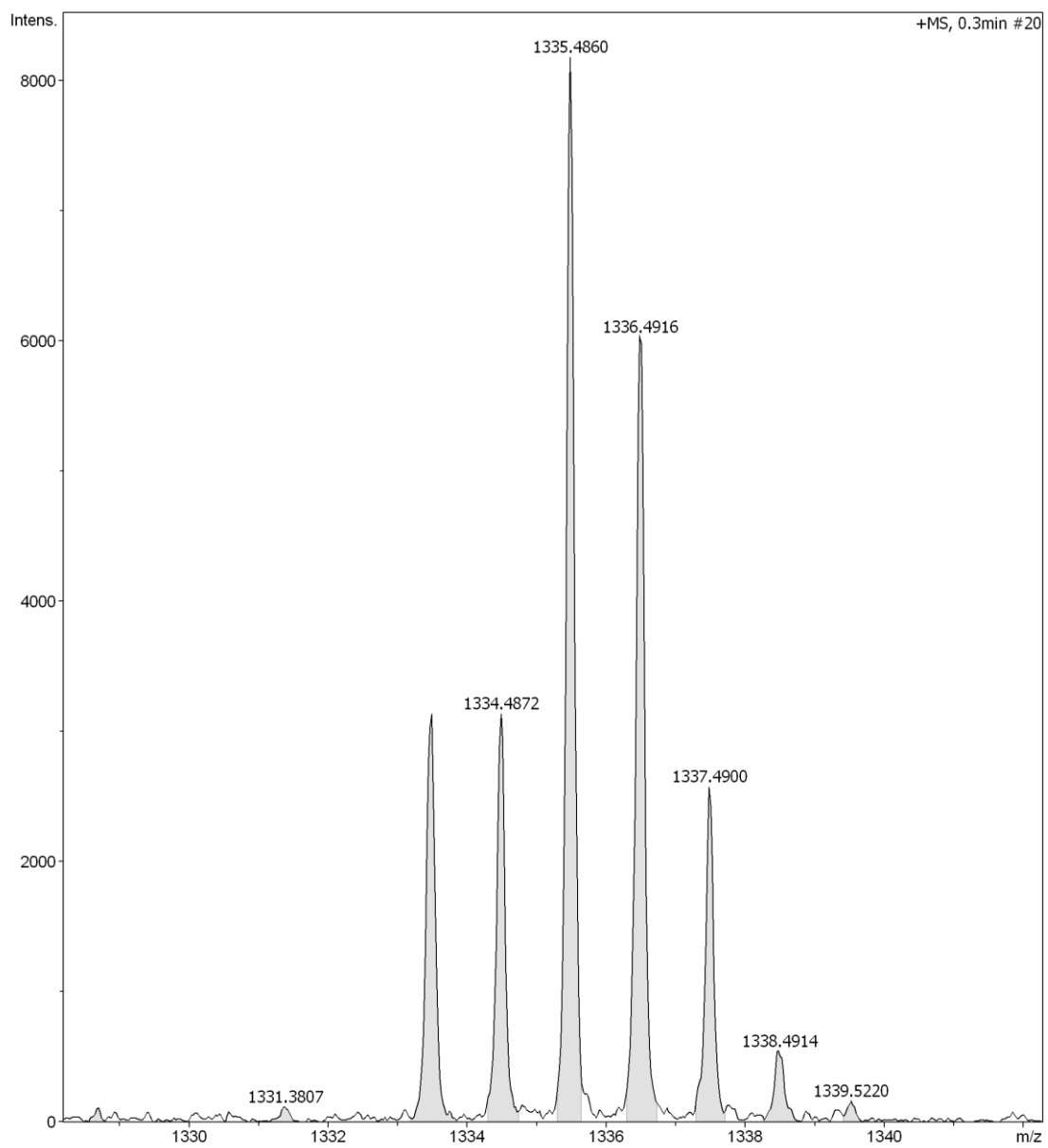


Fig. S10 High Resolution Mass Spectrometry (HRMS) of **Ir-2-N**

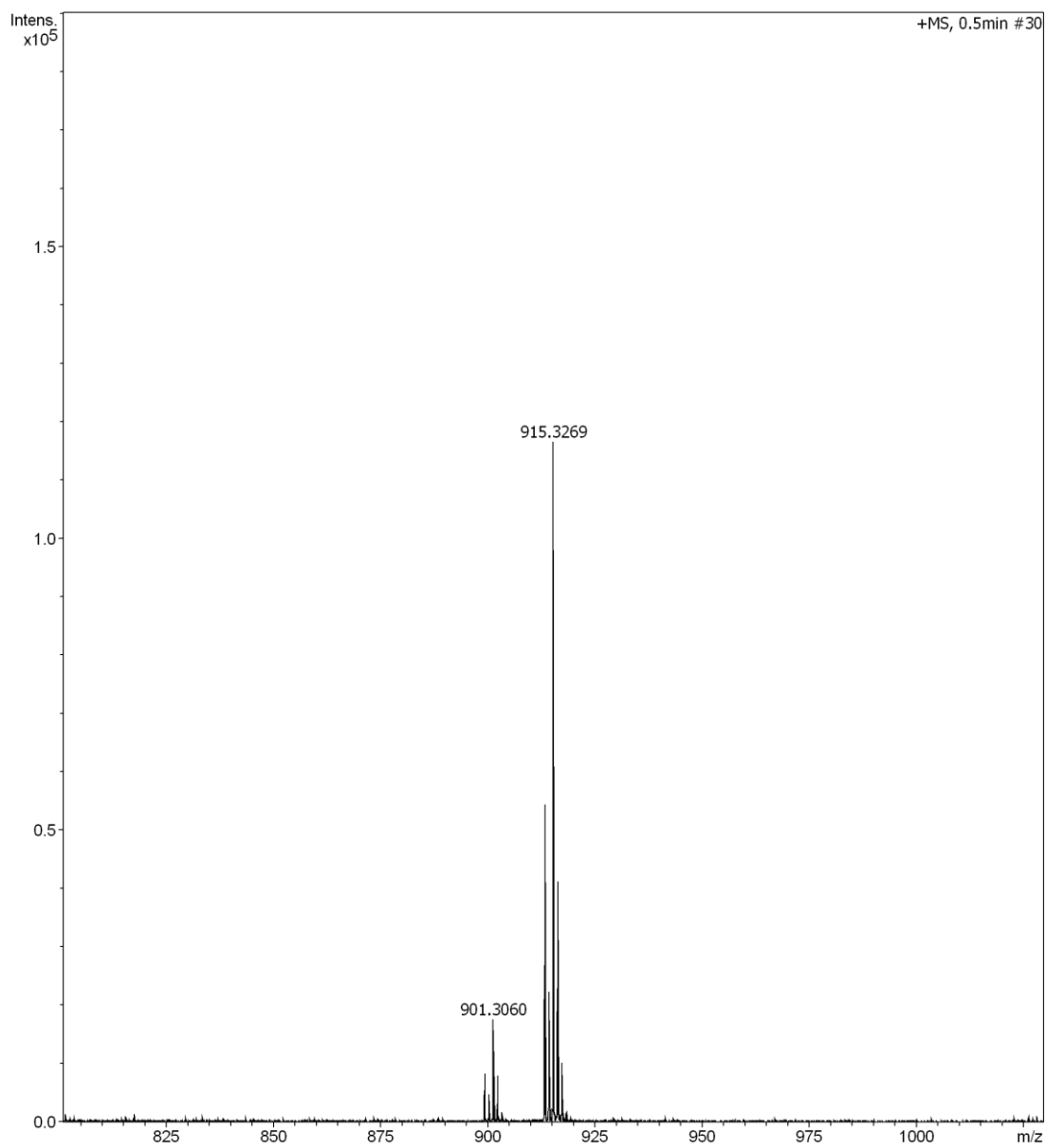


Fig. S11 High Resolution Mass Spectrometry (HRMS) of **Ir-1-N⁺**

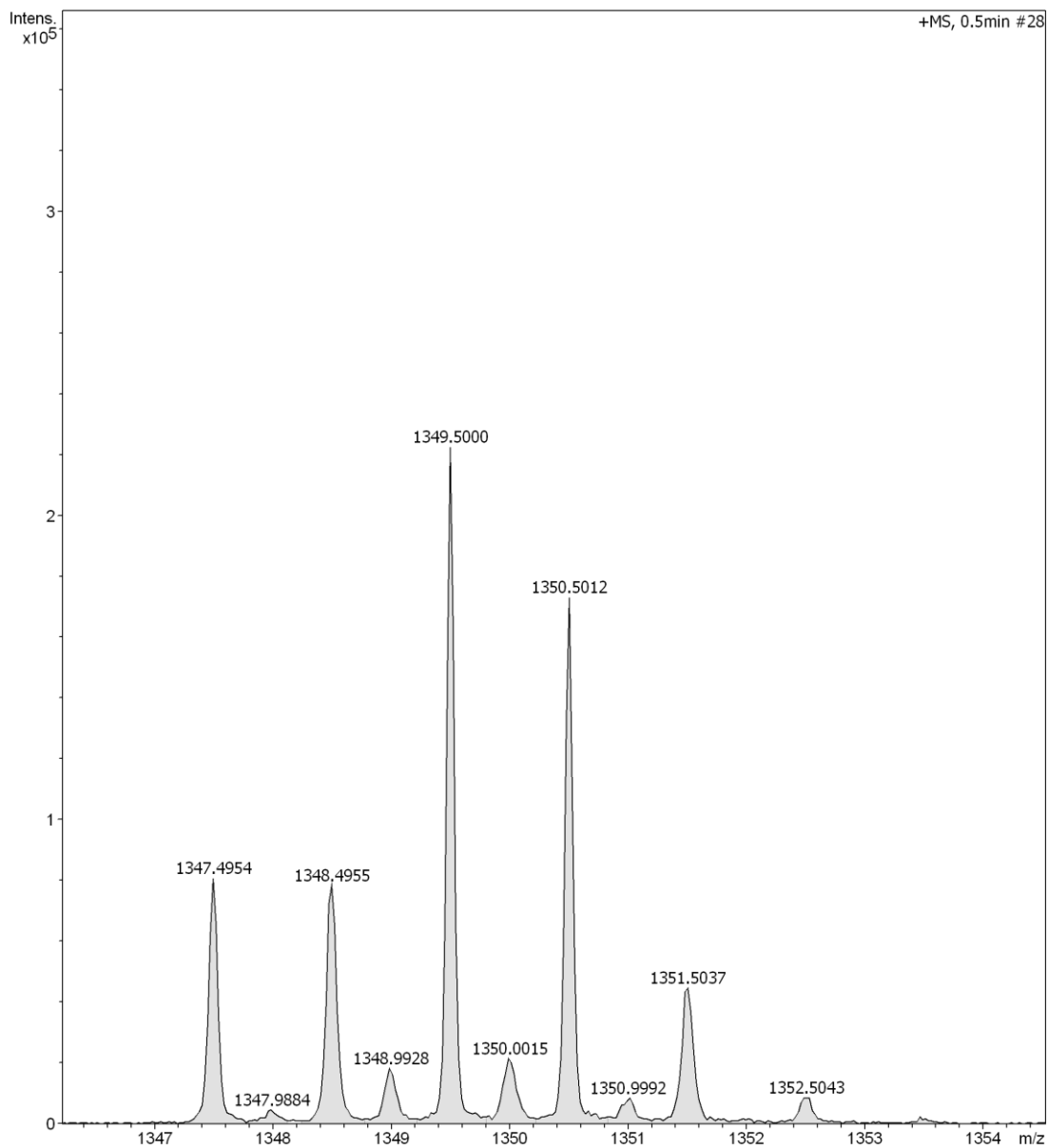


Fig. S12 High Resolution Mass Spectrometry (HRMS) of **Ir-2-N⁺**

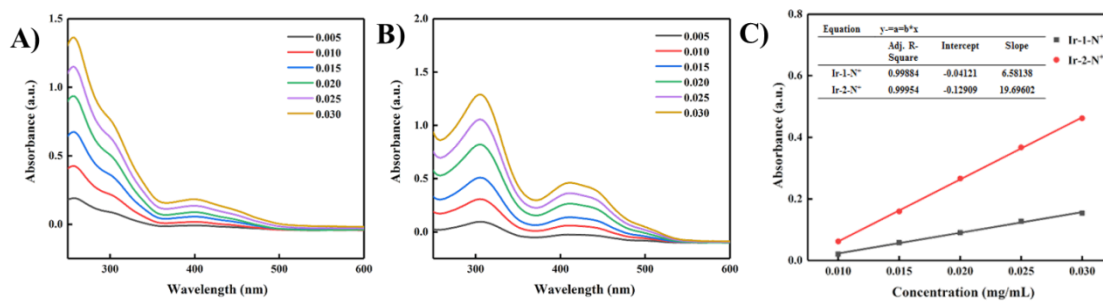


Fig. S13 UV-vis absorption spectra of A) **Ir-1-N⁺** and B) **Ir-2-N⁺** at different concentrations in CH₃CN-water (v/v) =4/1. C) Standard plots of **Ir-1-N⁺** and **Ir-2-N⁺** in CH₃CN-water (v/v) =4/1.

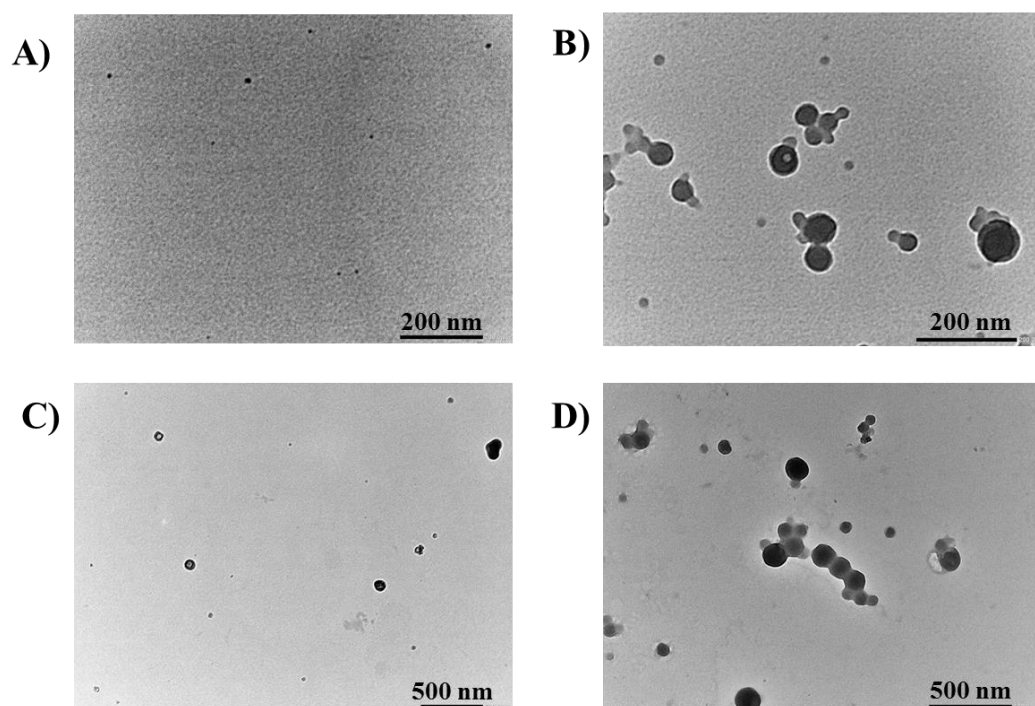


Fig. S14 TEM image of nanoaggregates of **Ir-1-N⁺** formed in CH₃CN-water mixtures with A) 0% and B) 99% water fraction. TEM image of nanoaggregates of **Ir-2-N⁺** formed in CH₃CN-water mixtures with C) 0% and D) 99% water fraction.

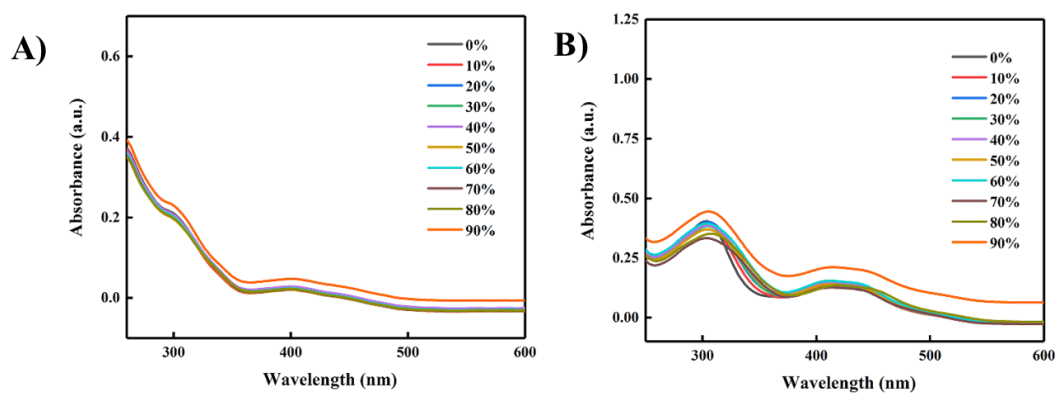


Fig. S15 Absorption spectra of A) **Ir-1-N⁺** and B) **Ir-2-N⁺** in CH₃CN-water mixtures (complex concentration = 1.0×10^{-5} M) with different water fractions (0-99%, v/v).

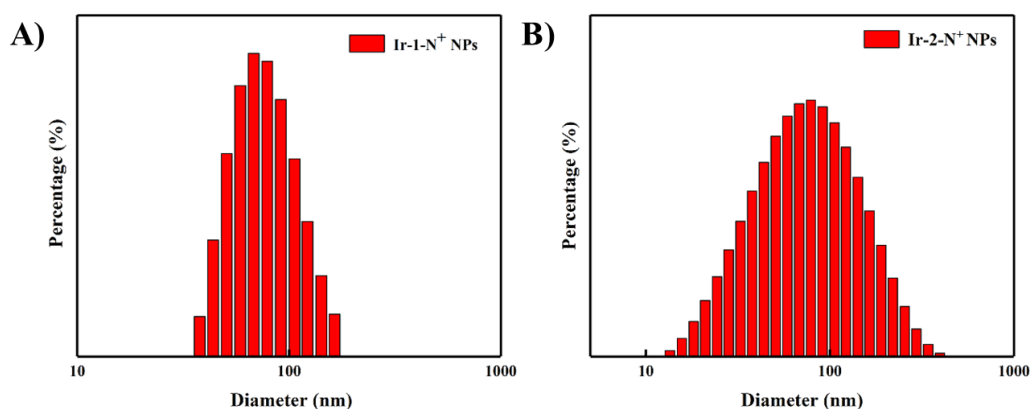


Fig. S16. DLS results of A) **Ir-1-N⁺** and B) **Ir-2-N⁺**.

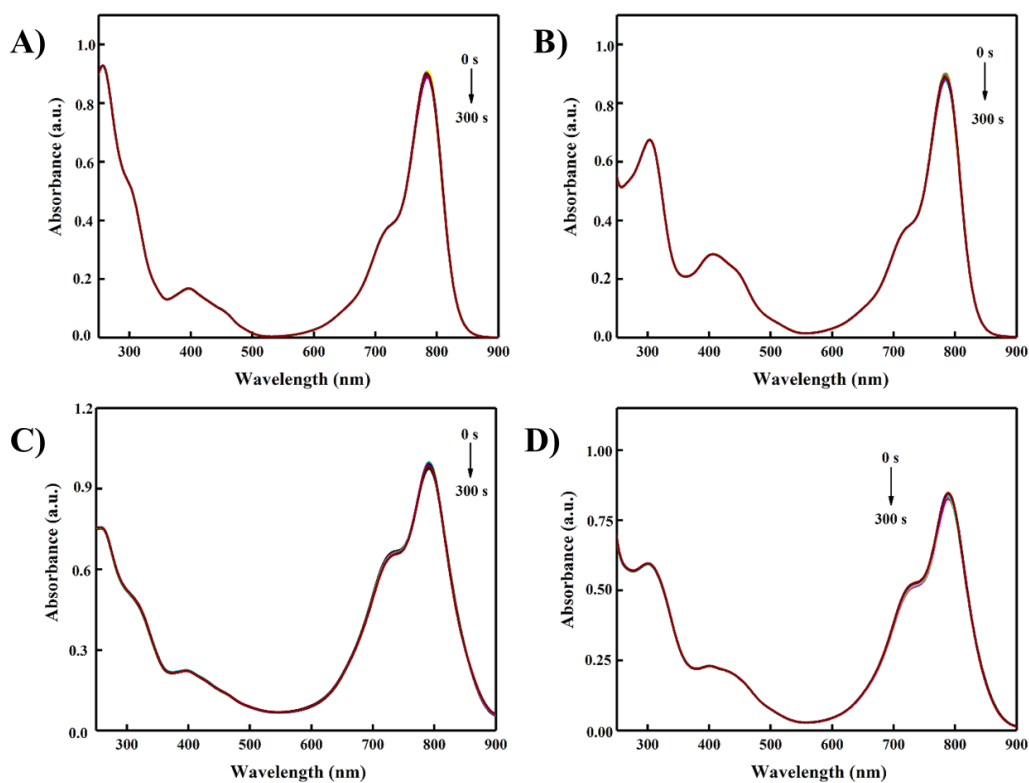


Fig. S17 UV-vis absorption spectra of ICG ($5 \mu\text{g mL}^{-1}$) in the presence of A) **Ir-1-N⁺**, B) **Ir-2-N⁺**, C) **Ir-1-N⁺** NPs and D) **Ir-2-N⁺** NPs ($15 \mu\text{g mL}^{-1}$) at different times under dark conditions. The time interval of spectral recording = 30 s.

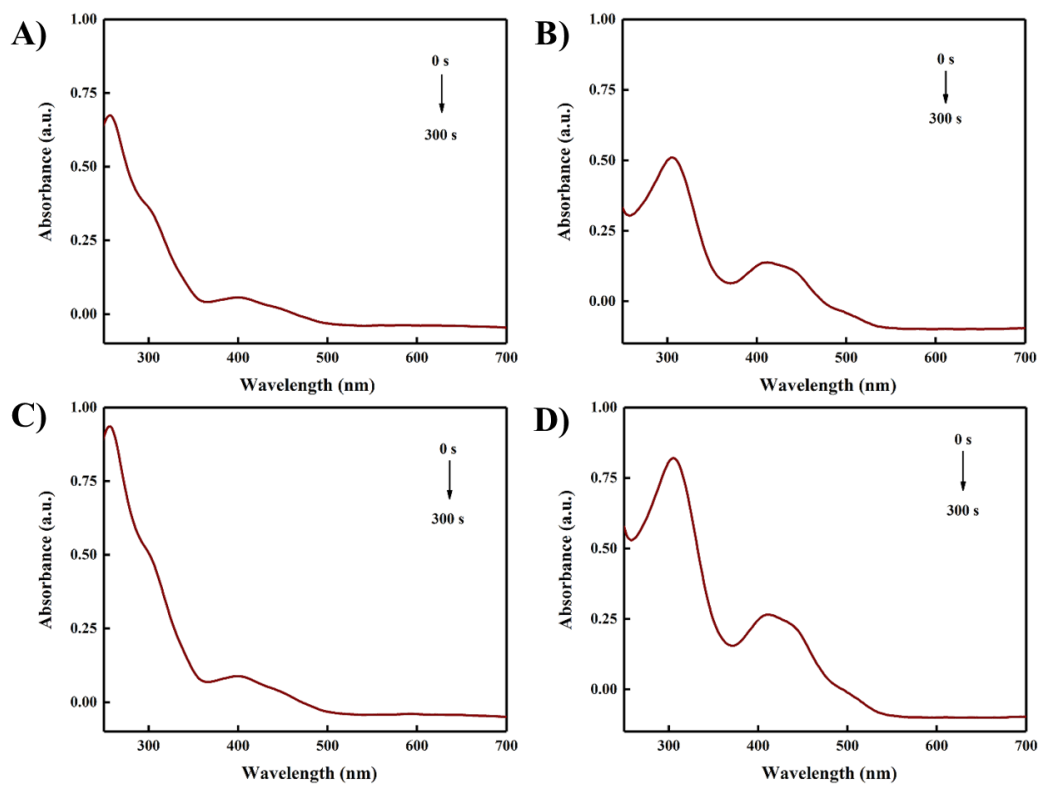
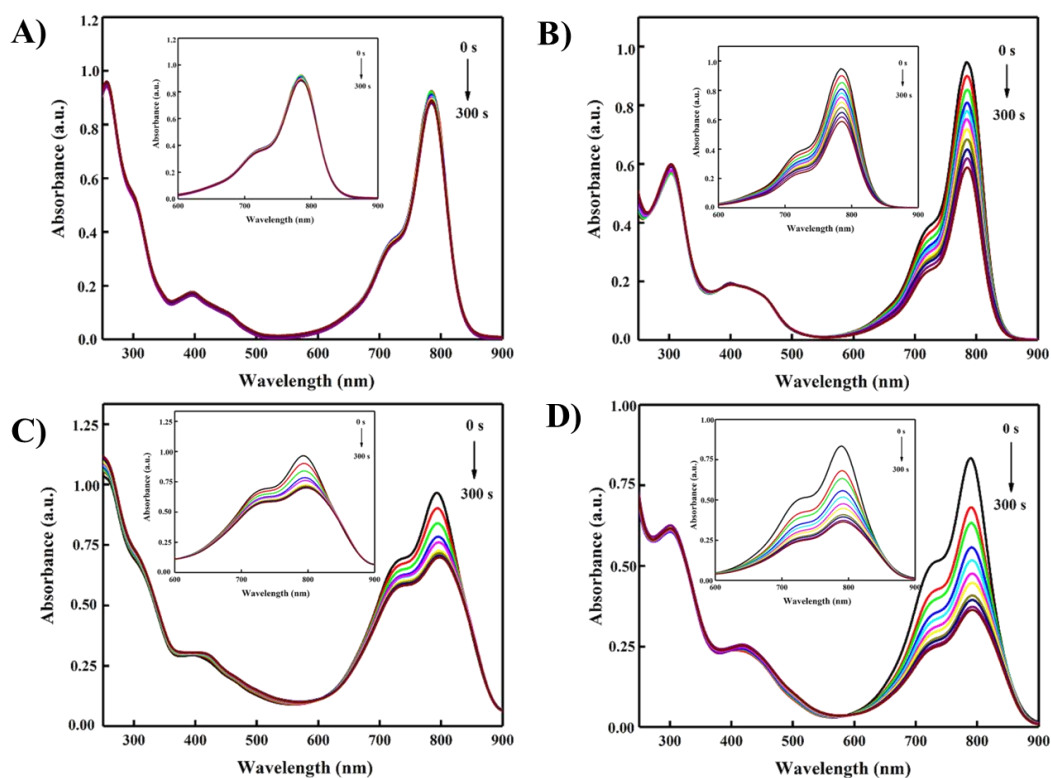


Fig. S18 UV-vis absorption spectra of A) **Ir-1-N⁺**, B) **Ir-2-N⁺**, C) **Ir-1-N⁺ NPs** and D) **Ir-2-N⁺ NPs** ($15 \mu\text{g mL}^{-1}$) at different times upon irradiation of a 425 nm LED at 20 mW cm^{-2} . The time interval of spectral recording = 30 s.



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Fig. S19 UV-vis absorption spectra of ICG ($5 \mu\text{g mL}^{-1}$) in the presence of A) **Ir-1-N⁺**, B) **Ir-2-N⁺**, C) **Ir-1-N⁺** NPs and D) **Ir-2-N⁺** NPs ($15 \mu\text{g mL}^{-1}$) at different times upon irradiation with a 425 nm LED at 20 mW cm^{-2} . The time interval of spectral recording = 30 s.

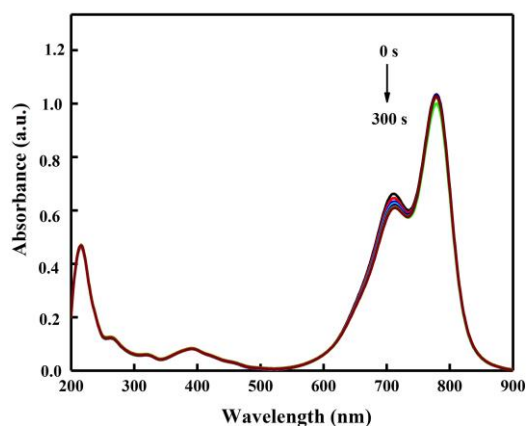


Fig. S20 UV-vis absorption spectra of ICG ($5 \mu\text{g mL}^{-1}$) upon irradiation with a 425 nm LED at 20 mW cm^{-2} . The time interval of spectral recording = 30 s.

Table S1 Photophysical data of **Ir-1-N⁺** and **Ir-2-N⁺**

	λ_{abs} (nm)	λ_{em} (nm)	Φ_{p} (%)	τ_{p} (ns)
Ir-1-N⁺ ^[a]	255; 400	640	17	542.2
Ir-2-N⁺ ^[a]	300; 415	660	19	551.3

^[a] Measured in MeCN/water (v/v = 1/9); concentration: 1.0×10^{-5} M; $\lambda_{\text{ex}} = 425$ nm

Table S2 The equation of time-dependent ¹O₂ generation kinetics in Fig. 4f.

Equation	y=a+b*x		
	Adj. R-Square	Intercept	Slope
Ir-1-N⁺	0.99664	0.01865	0.00043
Ir-2-N⁺	0.99406	0.04084	0.00178
Ir-1-N⁺ NPs	0.98024	0.04794	0.00114
Ir-2-N⁺ NPs	0.98684	0.1019	0.00253

References for SI

1. Y. Liu, N. Song, L. Chen, S. Liu and Z. Xie, *Chem. Asian J.*, 2018, **13**, 989-995.
2. K. Zhang, L. Q. Lu, Y. Jia, Y. Wang, F. D. Lu, F. Pan and W. J. Xiao, *Angew. Chem. Int. Ed.*, 2019, **58**, 13375-13379.