

Electronic Supplementary Information for:

Observation of the long-lived triplet excited state of perylenebisimide (PBI) in $C^{\wedge}N$ cyclometalated Ir(III) complexes and application in photocatalytic oxidation

Jifu Sun, Fangfang Zhong and Jianzhang Zhao*

*State Key Laboratory of Fine Chemicals, School of Chemical Engineering, Dalian University of Technology,
E-208 West Campus, 2 Ling Gong Rd., Dalian 116024, P. R. China*

E-mail: zhaojzh@dlut.edu.cn

<http://finechem.dlut.edu.cn/photochem>



QR code of the author address

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NMR and HR MS spectra

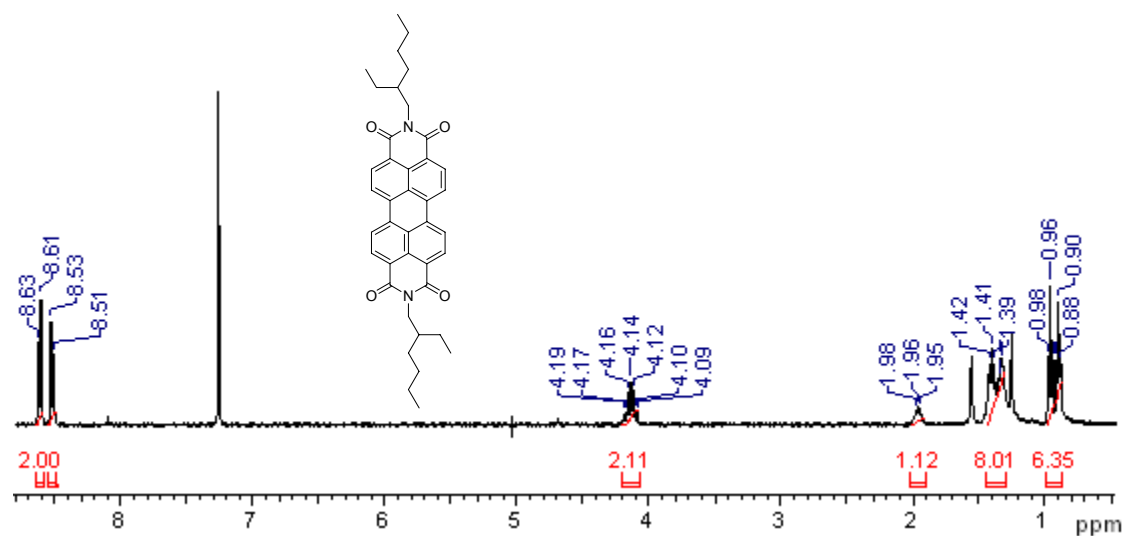


Fig. S1 ¹H NMR spectrum of **2** (CDCl₃, 400 MHz).

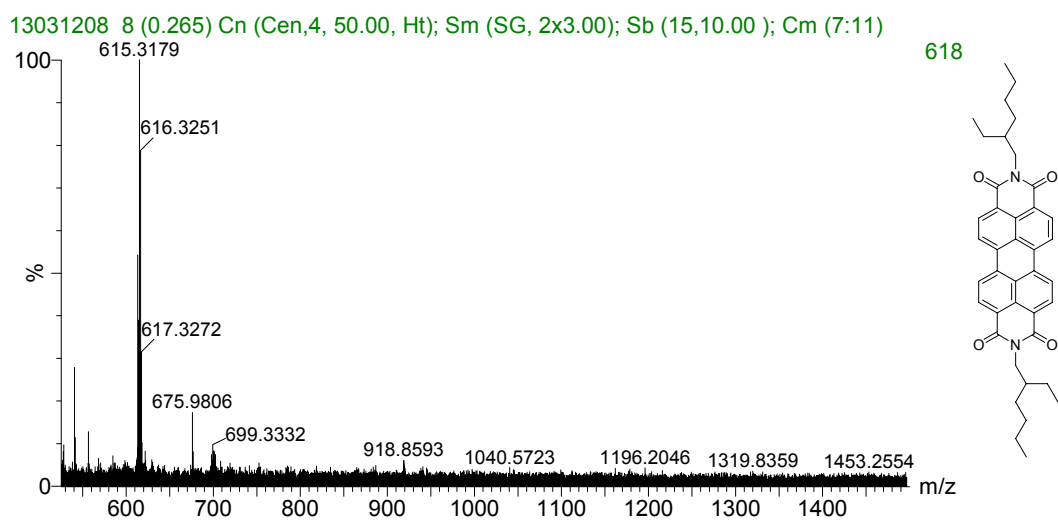


Fig. S2 TOF MALDI HRMS of **2**.

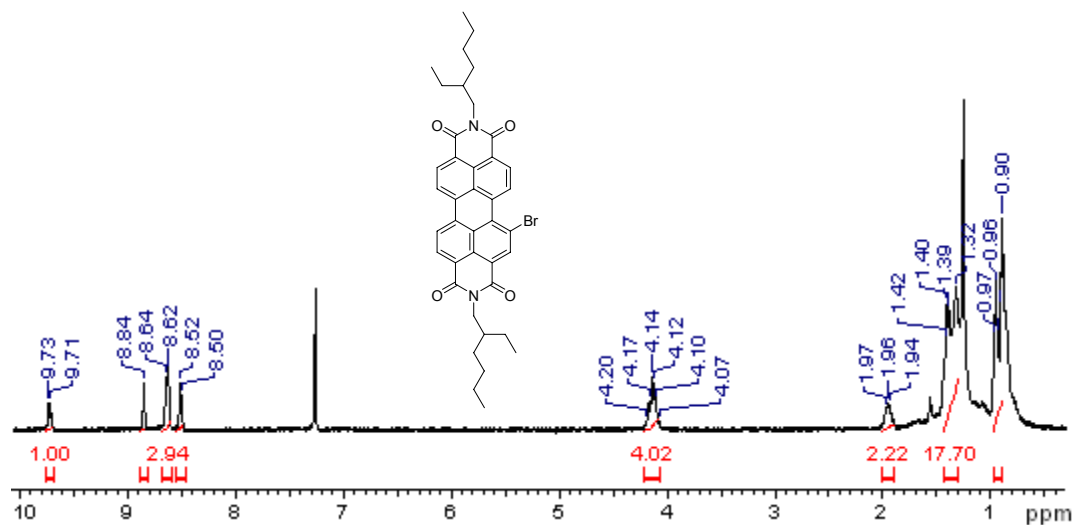


Fig. S3 ^1H NMR spectrum of **3** (CDCl_3 , 400 MHz).

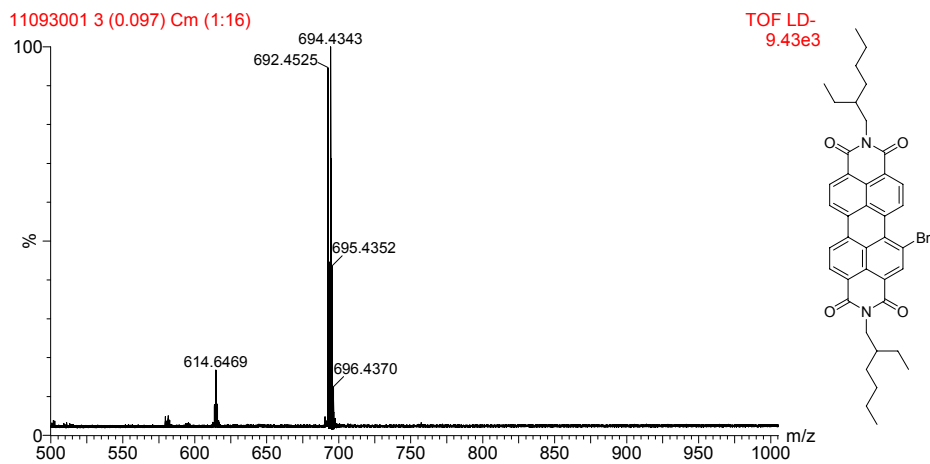


Fig. S4 TOF MALDI HRMS of **3**.

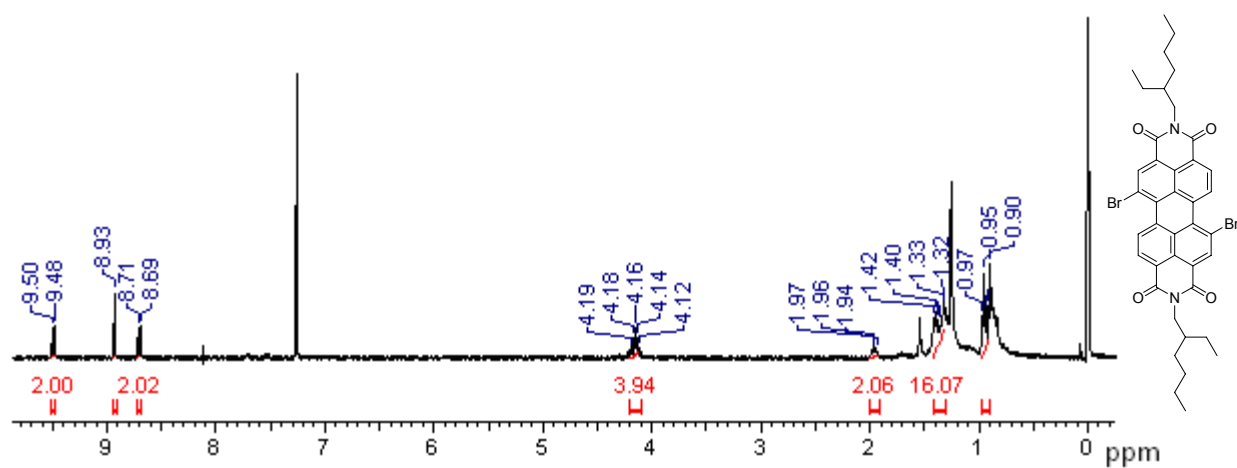


Fig. S5 ¹H NMR spectrum of **4** (CDCl₃, 400 MHz).

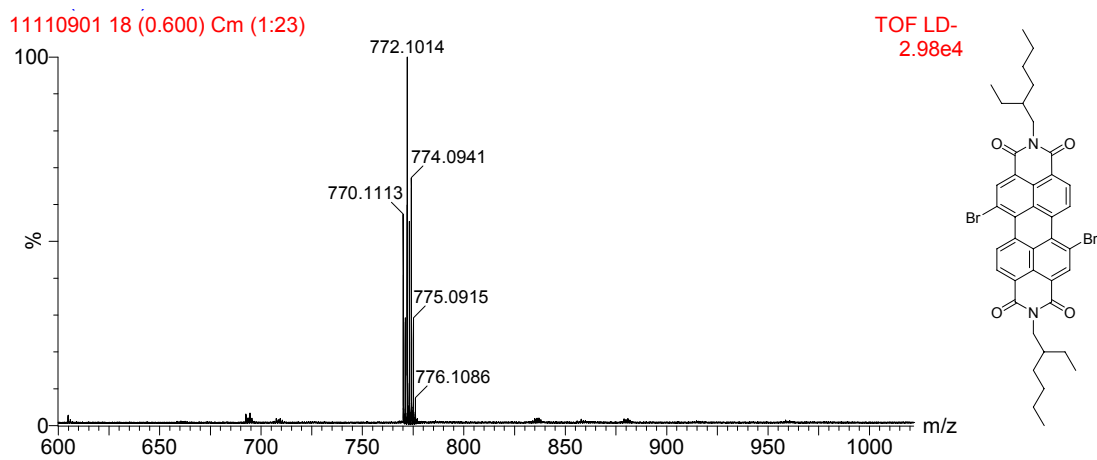


Fig. S6 TOF MALDI HRMS of **4**.

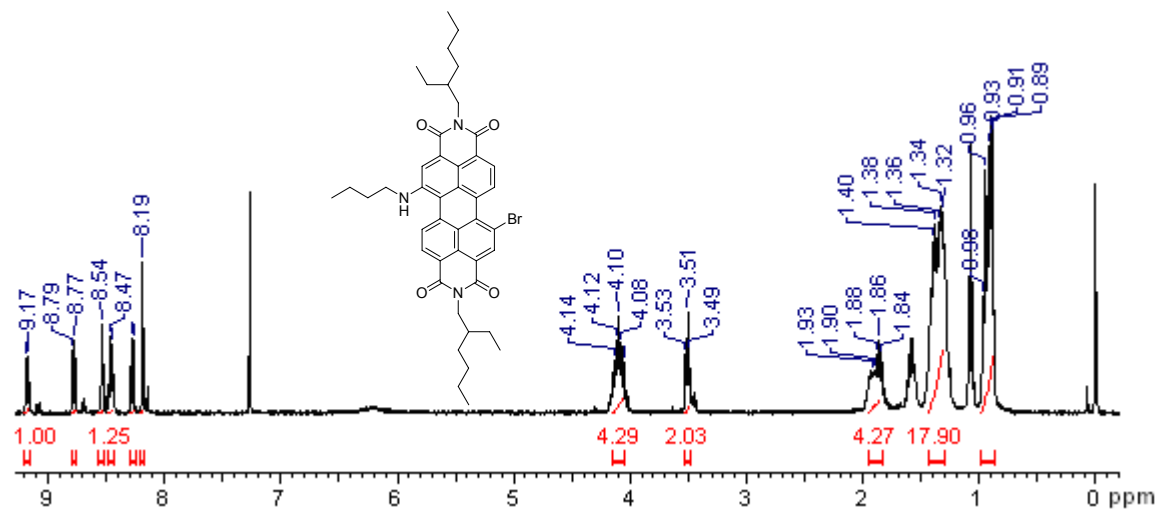


Fig. S7 ^1H NMR spectrum of **5** (CDCl_3 , 400 MHz).

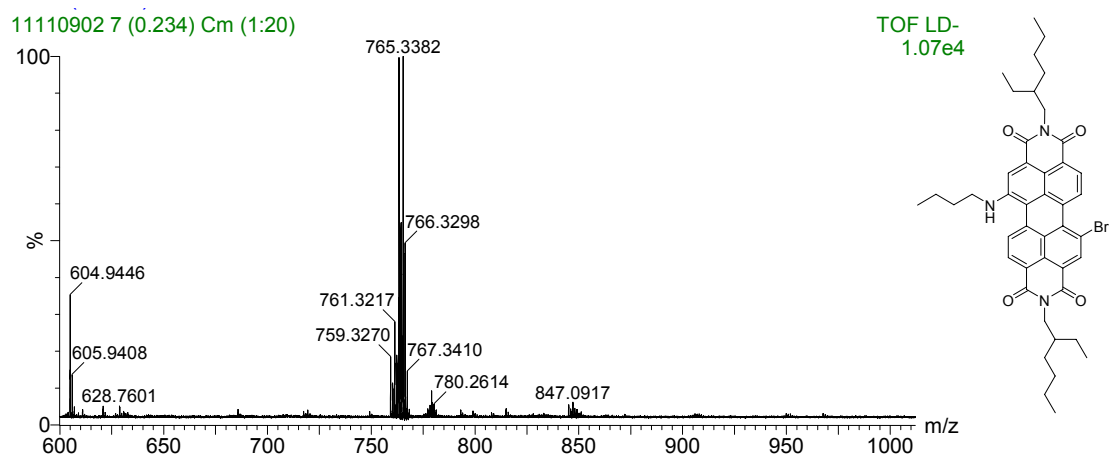


Fig. S8 TOF MALDI HRMS of **5**.

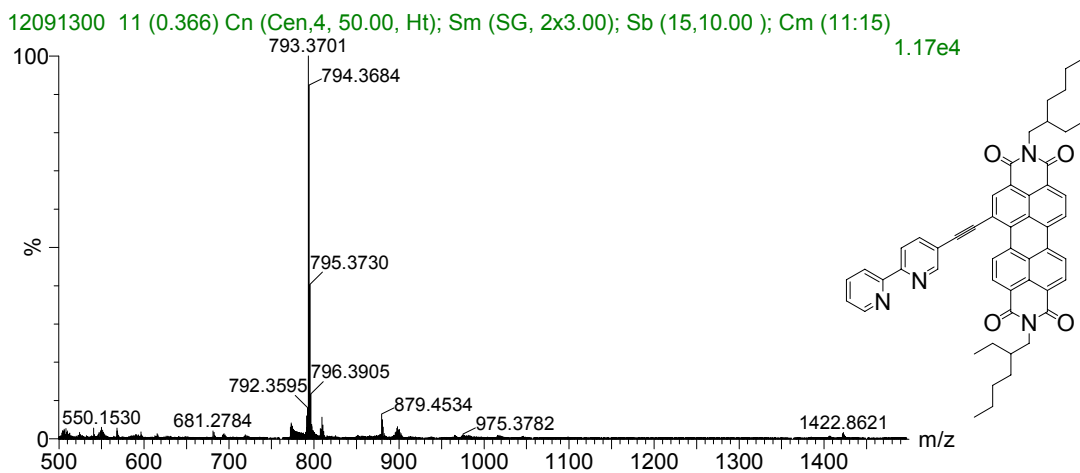


Fig. S9 TOF MALDI HR MS of **L2**.

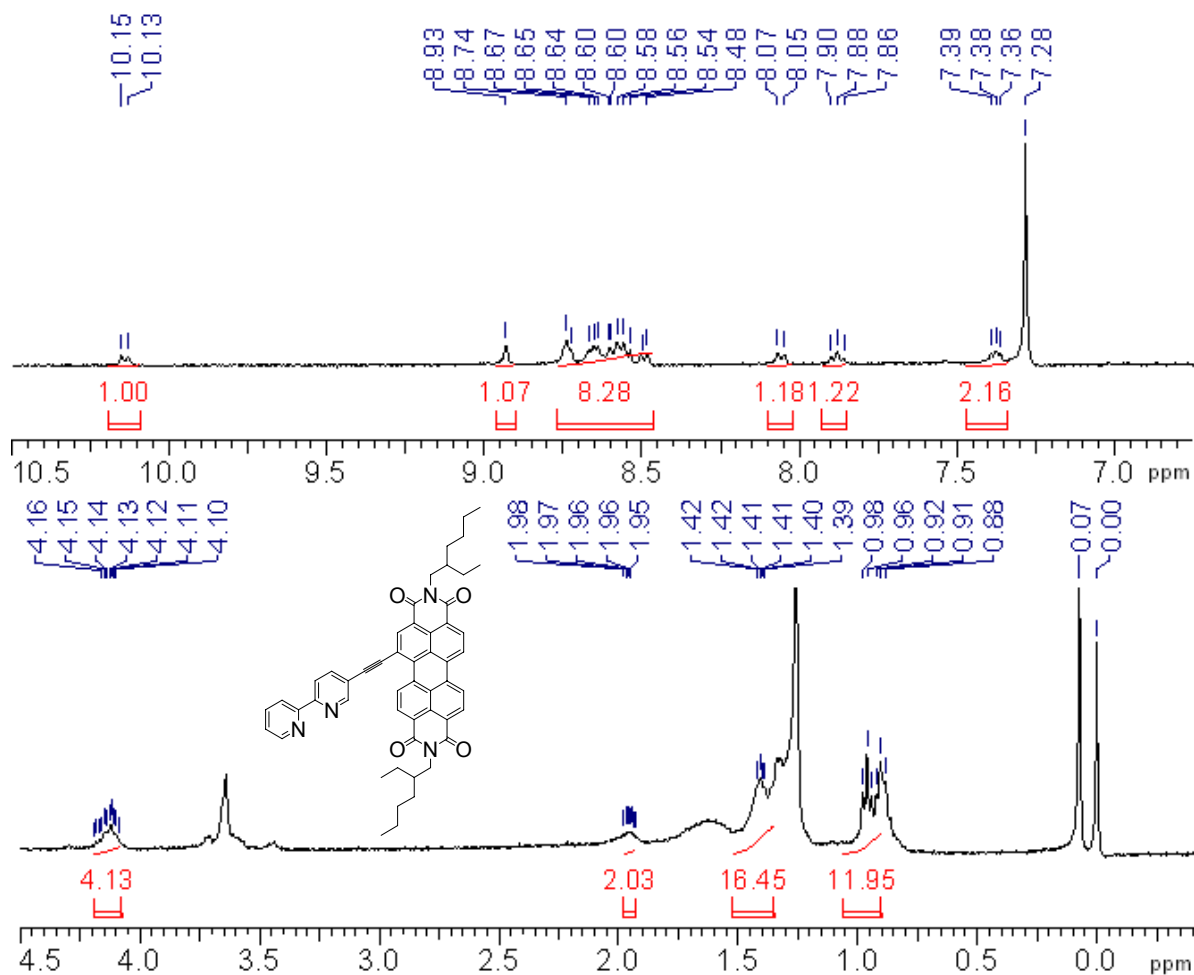


Fig. S10 ^1H NMR spectra of **L2** (CDCl_3 , 400 MHz).

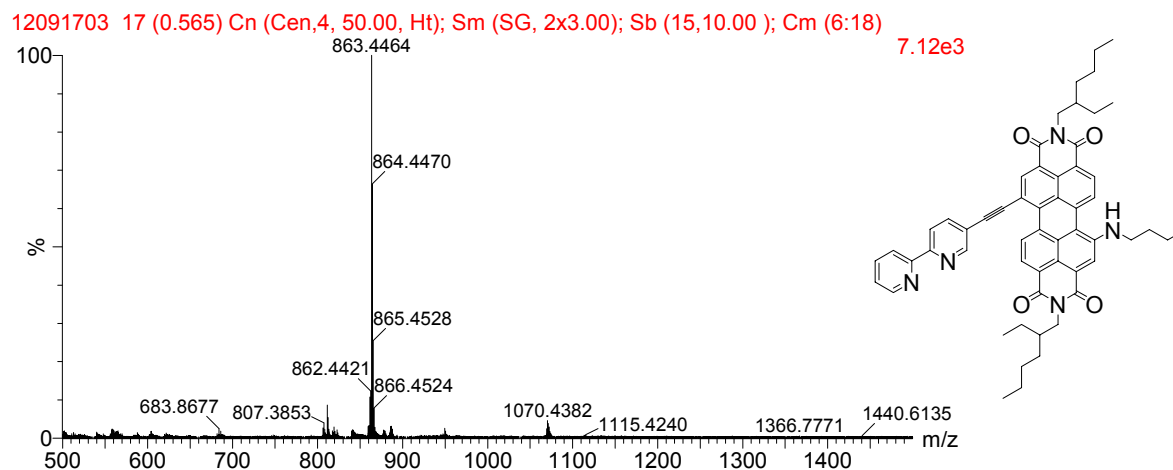


Fig. S11 TOF MALDI HRMS of **L3**.

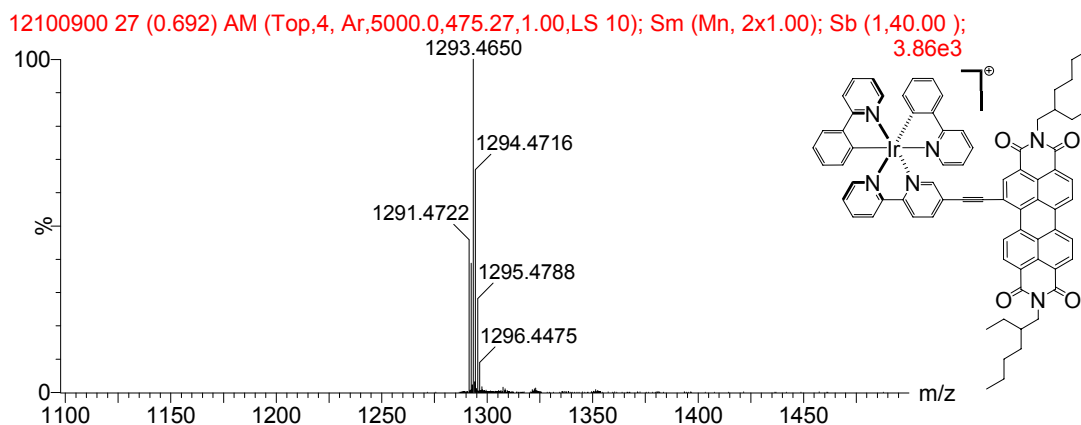


Fig. S12 TOF ESI HRMS of **Ir-2**.

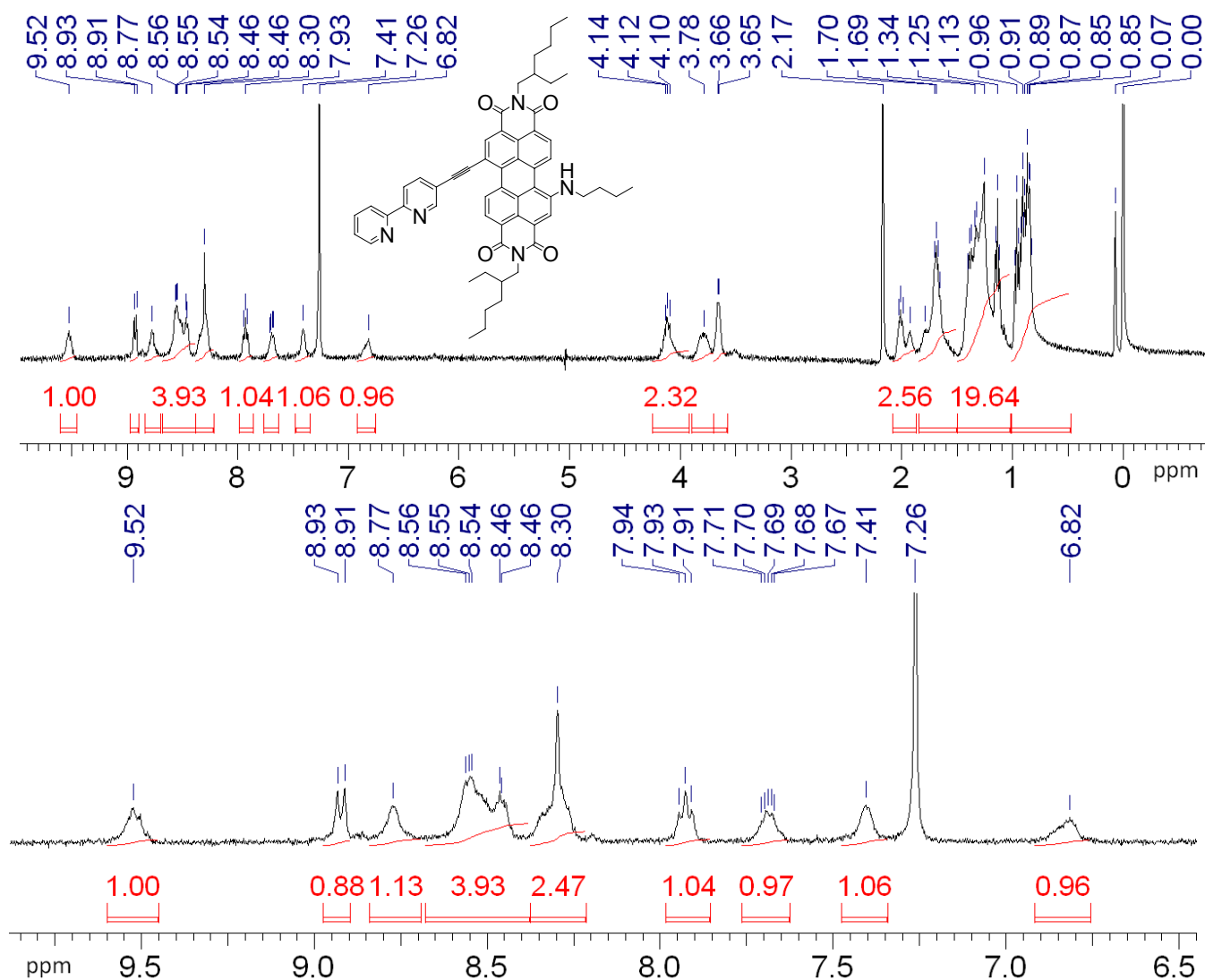


Fig. S13 ^1H NMR spectra of **L3** (CDCl_3 , 400 MHz).

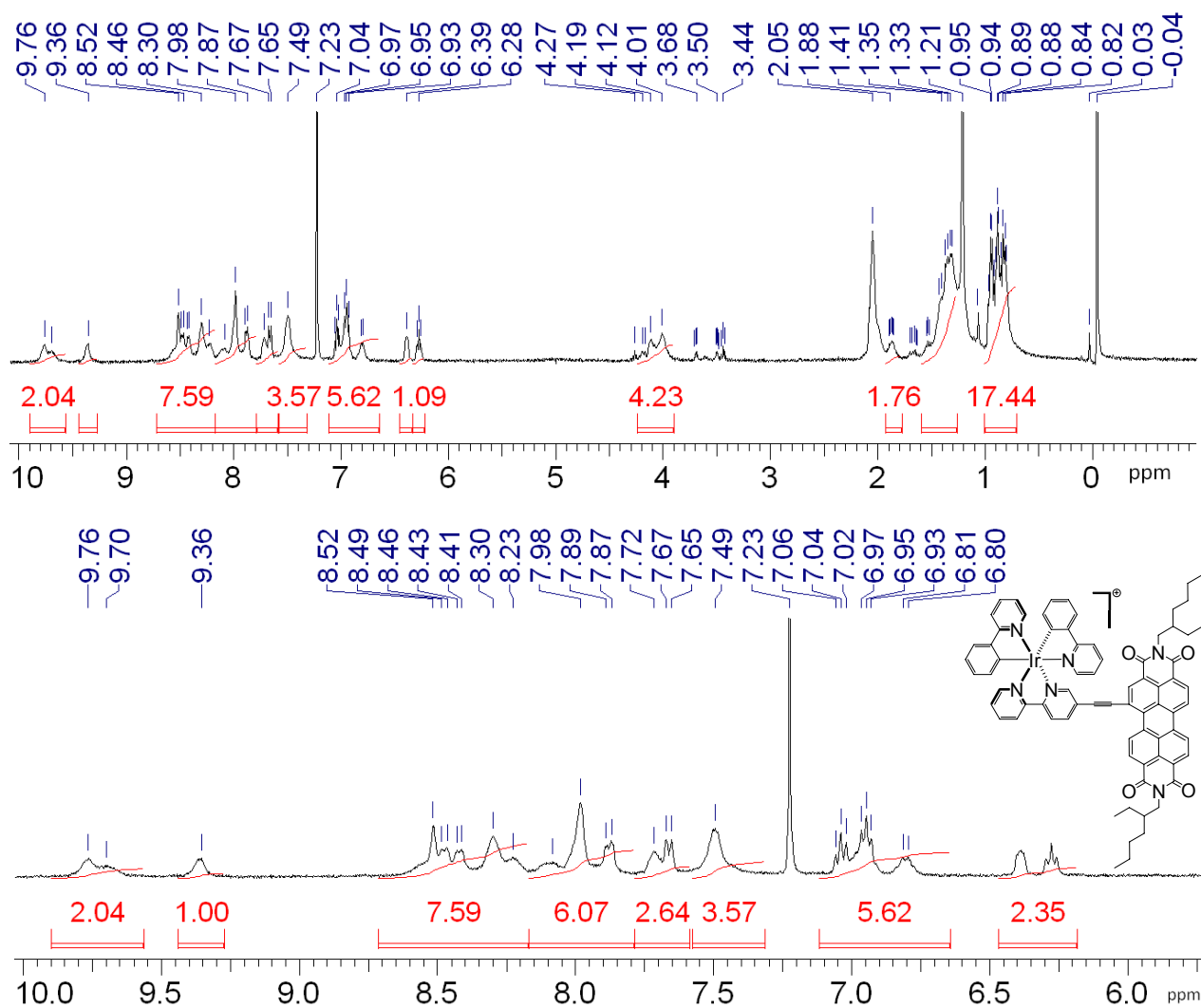


Fig. S14 ^1H NMR spectra of **Ir-2** (CDCl_3 , 400 MHz).

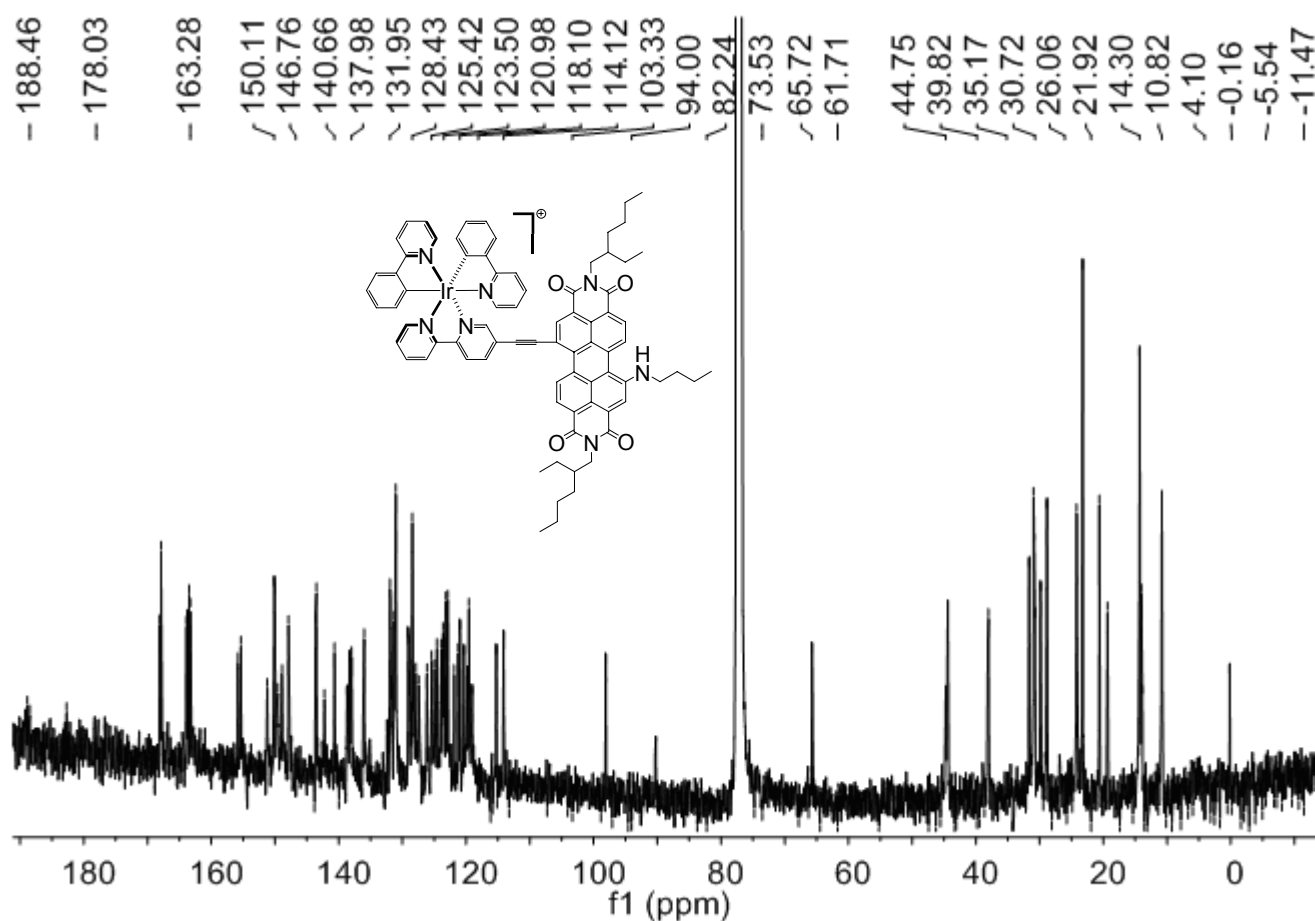


Fig. S15 ^{13}C NMR spectrum of **Ir-3** (CDCl_3 , 100 MHz).

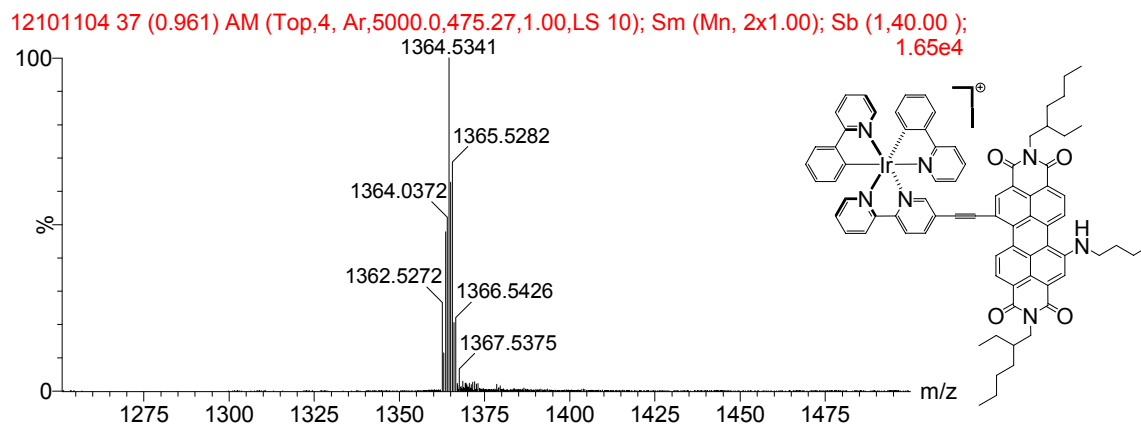


Fig. S16 TOF ESI HRMS of **Ir-3**.

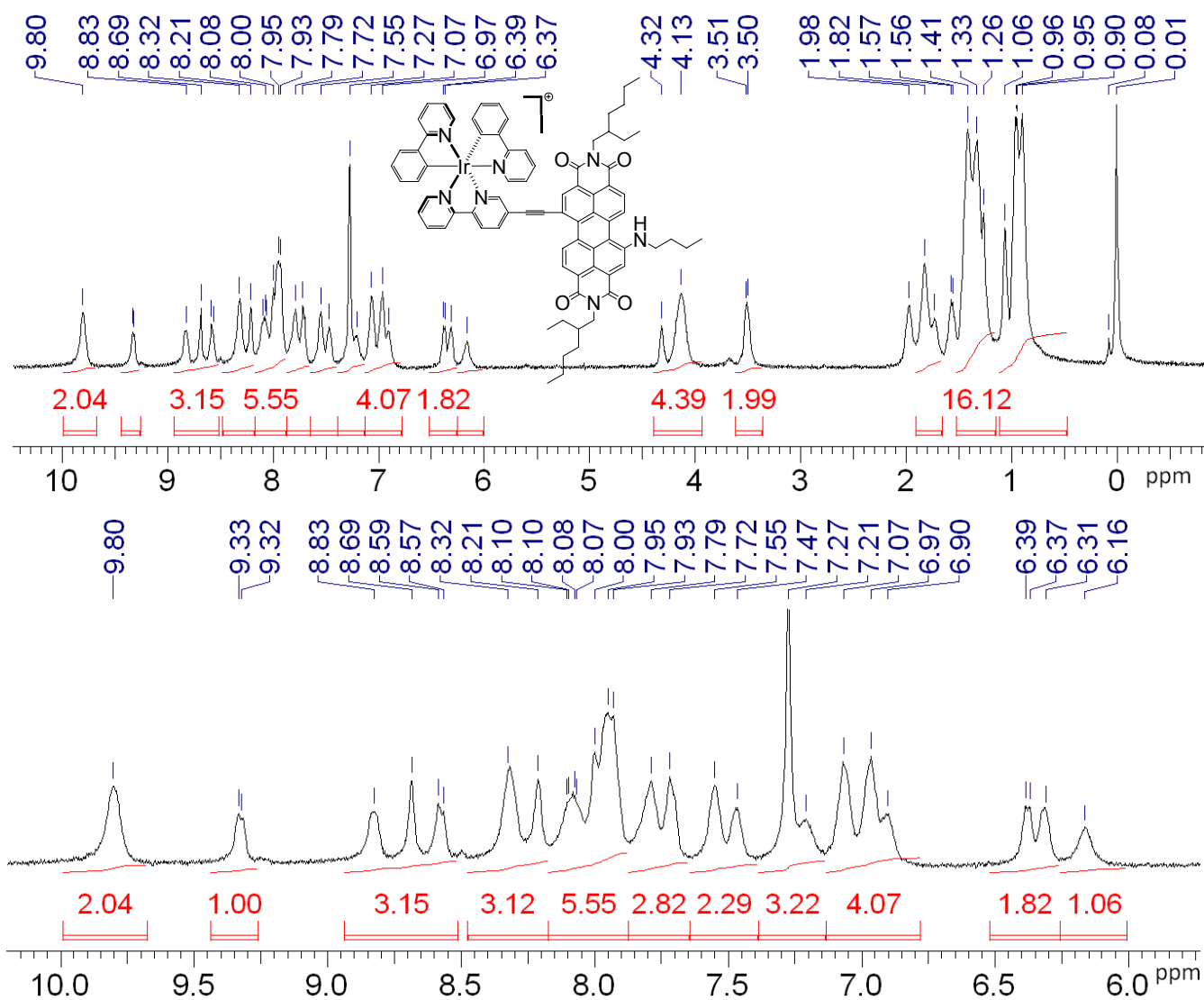


Fig. S17 ^1H NMR spectra of **Ir-3** (CDCl_3 , 400 MHz).

Nanosecond time-resolved transient difference absorption of the Ir(III) complexes

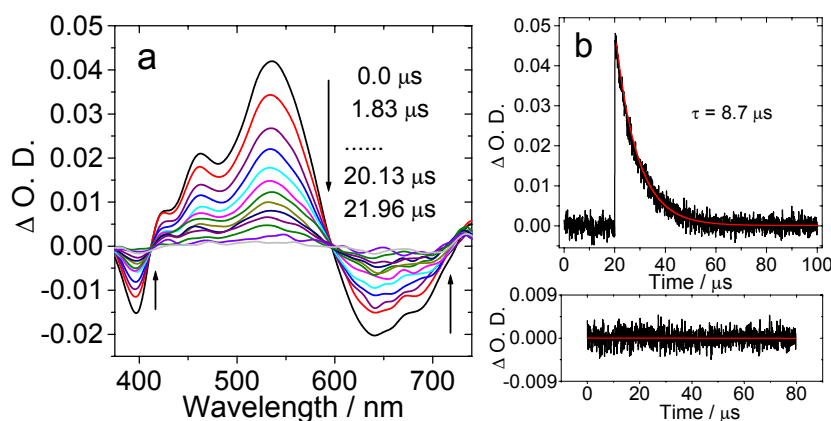


Fig. S18 Nanosecond time-resolved transient difference absorption spectra. (a) **Ir-3** ($\lambda_{\text{ex}} = 355$ nm).

(b) Decay trace of **Ir-3** at 530 nm. $c = 1.0 \times 10^{-5}$ M in deoxygenated CH_3CN at 25 °C.

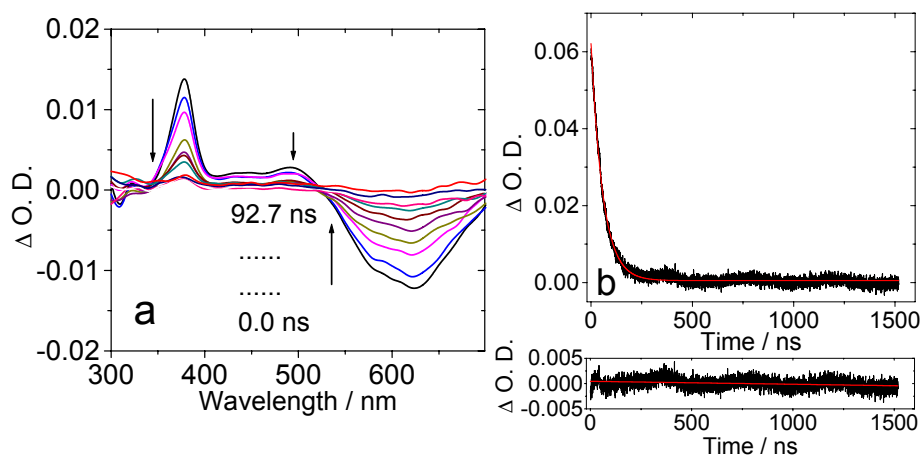


Fig. S19 Nanosecond time-resolved transient difference absorption spectra. (a) **Ir-1** ($\lambda_{\text{ex}} = 355$ nm).

(b) Decay trace of **Ir-1** at 610 nm. $c = 1.0 \times 10^{-5}$ M in air-saturated CH_3CN at 25 °C.

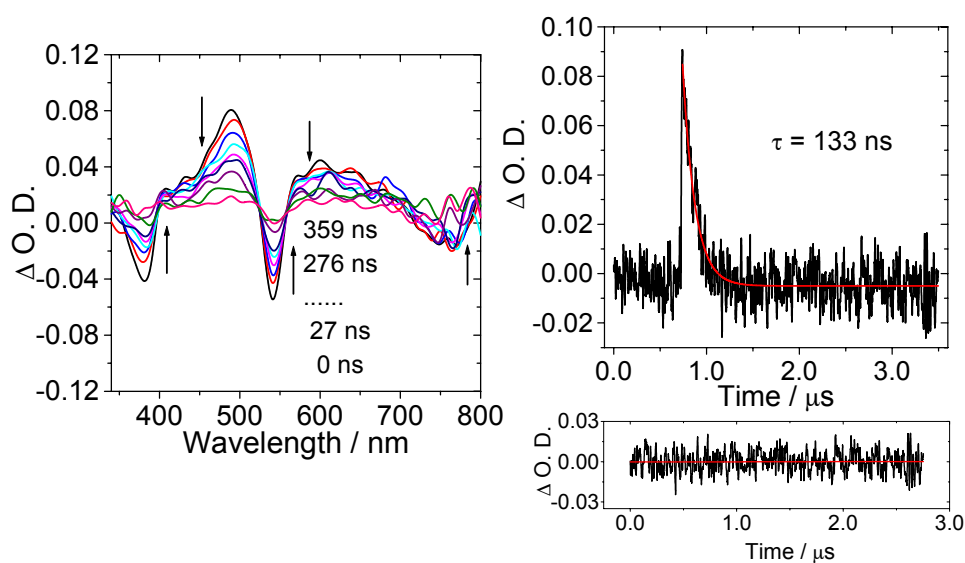


Fig. S20 Nanosecond time-resolved transient difference absorption spectra. (a) **Ir-2** ($\lambda_{\text{ex}} = 532$ nm).
(b) Decay trace of **Ir-2** at 540 nm. $c = 1.0 \times 10^{-5}$ M in air-saturated CH_3CN at 25 °C.

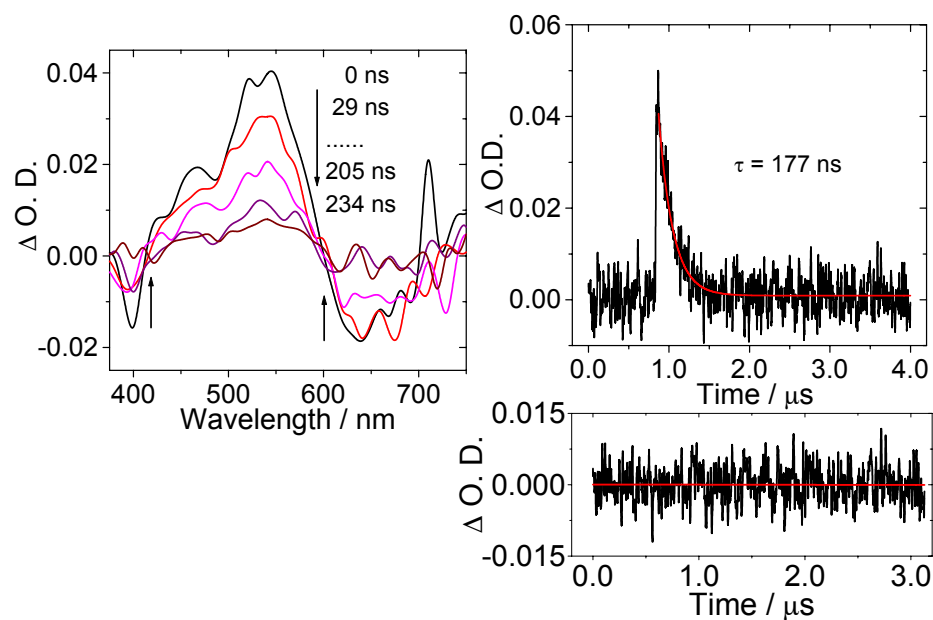


Fig. S21 Nanosecond time-resolved transient difference absorption spectra. (a) **Ir-3** ($\lambda_{\text{ex}} = 355$ nm).
(b) Decay trace of **Ir-1** at 530 nm. $c = 1.0 \times 10^{-5}$ M in air-saturated CH_3CN at 25 °C.

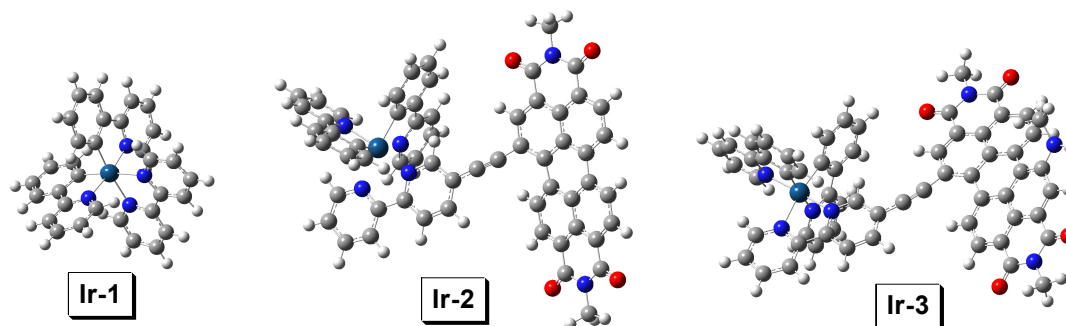


Fig. S22 Optimized structures of the complexes of **Ir-1**, **Ir-2** and **Ir-3**. Calculated at B3LYP/6-31G (d) level with Gaussian 09.

Table S1 Electronic Excitation Energies (eV) and corresponding Oscillator Strengths (f), main Configurations and CI coefficients of the Low-lying Electronic Excited States of the complex **Ir-1** calculated by TDDFT//B3LYP/6-31G(d) based on the TDDFT//B3LYP/6-31G(d) Optimized Ground State Geometries.

	Electronic transition	TDDFT//B3LYP/6-31G(d)				
		Energy ^a	f ^b	Composition ^c	CI ^d	Character
Singlet	$S_0 \rightarrow S_4$	2.89 eV / 429 nm	0.0384	H – 5 $\rightarrow$ L	0.1499	LLCT / MLCT
				H – 3 $\rightarrow$ L	0.6756	LLCT / MLCT
	$S_0 \rightarrow S_8$	3.12 eV / 396 nm	0.0354	H – 5 $\rightarrow$ L	0.6577	LLCT / MLCT
				H – 3 $\rightarrow$ L	0.1652	LLCT / MLCT
	$S_0 \rightarrow S_{10}$	3.36 eV / 369 nm	0.0388	H $\rightarrow$ L + 4	0.6885	LLCT / MLCT
	$S_0 \rightarrow S_{18}$	3.85 eV / 322 nm	0.0597	H – 3 $\rightarrow$ L + 1	0.5106	LLCT / MLCT
				H – 2 $\rightarrow$ L + 1	0.2163	LLCT / MLCT
Triplet	$S_0 \rightarrow T_1$	1.94eV / 637 nm	0.0000 ^e	H $\rightarrow$ L	0.6999	LLCT / MLCT

^a Only the selected low-lying excited states are presented. ^b Oscillator strengths. ^c Only the main configurations are presented. ^d The CI coefficients are in absolute values. ^e No spin-orbital coupling effect was considered, thus the f values are zero.

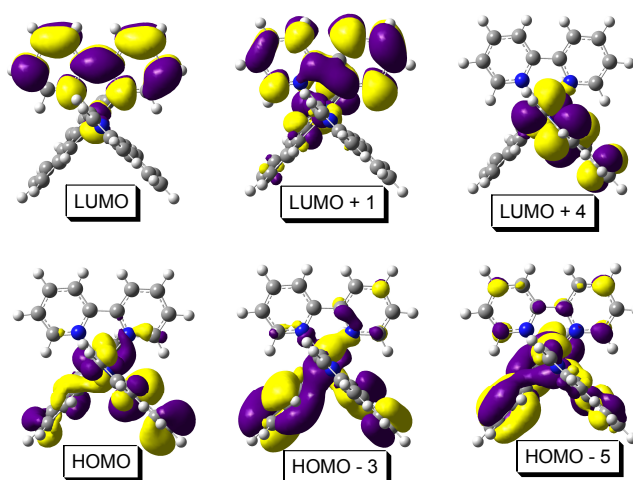


Fig. S23 Electron density maps of the frontier molecular orbital of the complex **Ir-1**. Based on ground state optimized geometry by the TDDFT calculations at the B3LYP/6-31g(d) level with Gaussian 09W.

Table S2 Electronic Excitation Energies (eV) and corresponding Oscillator Strengths (f), main Configurations and CI coefficients of the Low-lying Electronic Excited States of the complex **Ir-3** calculated by TDDFT//B3LYP/6-31G(d) based on the TDDFT//B3LYP/6-31G(d) Optimized Ground State Geometries.

Electronic		TDDFT//B3LYP/6-31G(d)				
transition		Energy ^a	f^b	Composition ^c	CI ^d	Character
Singlet	$S_0 \rightarrow S_1$	1.79 eV / 691 nm	0.4512	H $\rightarrow$ L	0.7028	ILCT
	$S_0 \rightarrow S_3$	2.25 eV / 550 nm	0.1655	H - 2 $\rightarrow$ L	0.3322	ILCT/LLCT
				H $\rightarrow$ L + 1	0.6067	ILCT
				H - 6 $\rightarrow$ L	0.4650	LLCT/MLCT
	$S_0 \rightarrow S_{11}$	2.99 eV / 415 nm	0.3770	H - 5 $\rightarrow$ L	0.4061	LLCT/MLCT
Triplet	$S_0 \rightarrow S_{17}$	3.13 eV / 395 nm	0.1483	H - 3 $\rightarrow$ L + 1	0.6553	ILCT
	$S_0 \rightarrow T_1$	1.14 eV / 1090 nm	0.0000 ^e	H $\rightarrow$ L	0.5865	ILCT
				H $\rightarrow$ L + 1	0.3806	ILCT

^a Only the selected low-lying excited states are presented. ^b Oscillator strengths. ^c Only the main configurations are presented. ^d The CI coefficients are in absolute values. ^e No spin-orbital coupling effect was considered, thus the f values are zero.

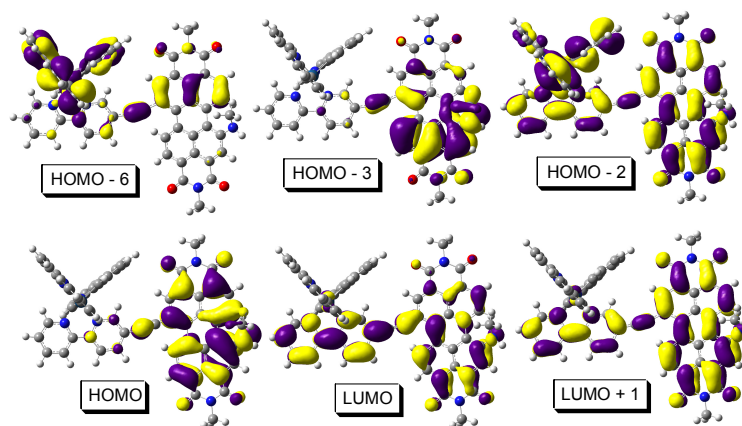


Fig. S24 Electron density maps of the frontier molecular orbital of the complex **Ir-3**. Based on ground state optimized geometry by the TDDFT calculations at the B3LYP/6-31g(d) level with Gaussian 09W.

Photooxidation

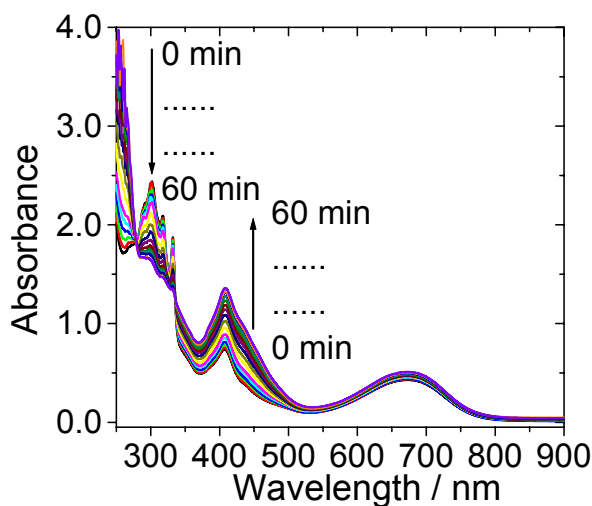


Fig. S25 The changes of UV-Vis absorption spectra by using **Ir-3** as the sensitizer. Irradiated with 35 W xenon lamp (20 mW cm^{-2} at the photoreactor). c [photosensitizer] = $2.0 \times 10^{-5} \text{ M}$ in $\text{CH}_2\text{Cl}_2/\text{CH}_3\text{OH}$ (9:1, v/v) at 20°C .

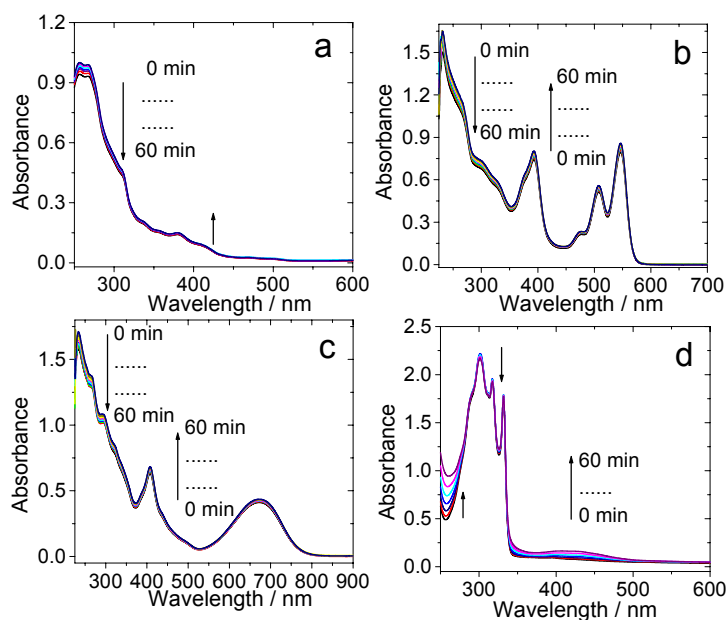


Fig. S26 UV-Vis absorption spectral change of complexes (a) **Ir-1**, (b) **Ir-2**, (c) **Ir-3** (2.0×10^{-5} M) and (d) the substrate **DHN** (2.0×10^{-4} M) upon irradiation ($\lambda > 385$ nm) in $\text{CH}_2\text{Cl}_2/\text{CH}_3\text{OH}$ (9:1, v/v) mixed solvent, 25°C. Irradiated with 35 W xenon lamp (with an intensity in the photo-reactor of 20 mW cm^{-2} . The UV light with wavelength shorter than 385 nm was blocked by 0.72 M NaNO_2 solution).

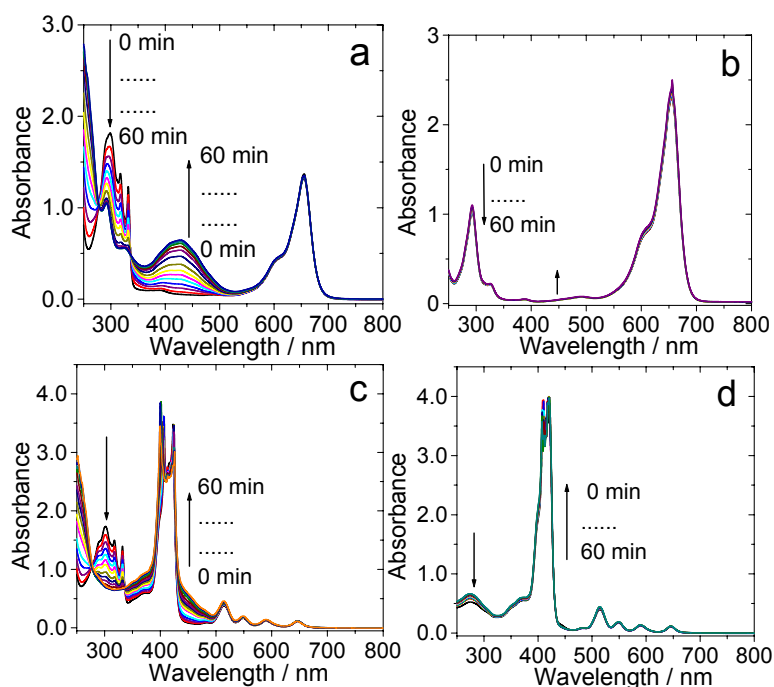


Fig. S27 Photooxidation of DHN (2.0×10^{-4} M) using **MB** and **TPP** as sensitizers, in $\text{CH}_2\text{Cl}_2/\text{CH}_3\text{OH}$ (9:1, v/v), 2.0×10^{-5} M, 25°C. Irradiated with 35 W xenon lamp (20 mW cm^{-2} in the photoreactor. The UV light with wavelength shorter than 385 nm was blocked by 0.72 M NaNO_2 solution). (a) UV-Vis absorption spectral change for DHN using **MB** as a sensitizer, (b) UV-Vis absorption spectral change of **MB** upon irradiation, (c) UV-vis absorption spectral change for DHN using **TPP** as a sensitizer, (d) UV-vis absorption spectral change of **TPP** upon irradiation.

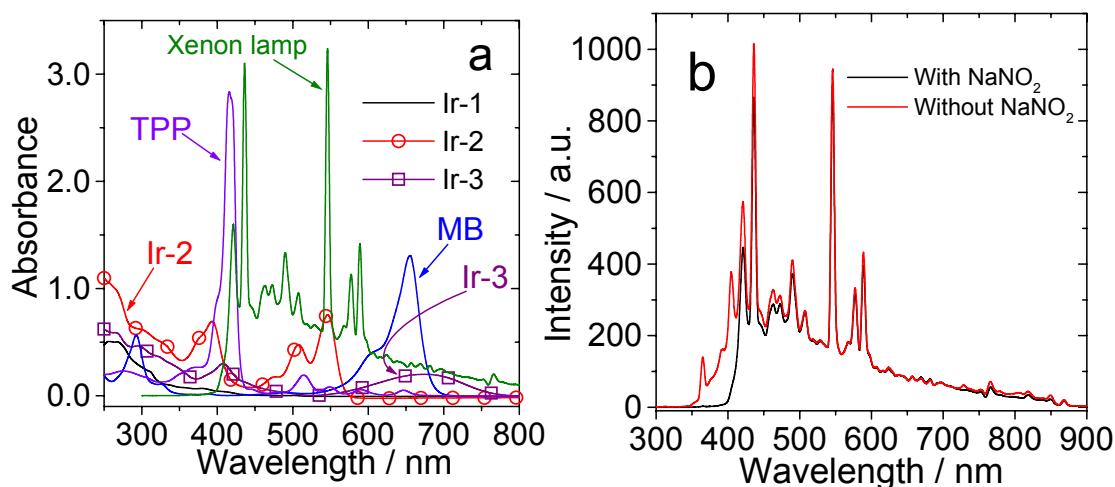


Fig. S28 (a) comparison of the UV-Vis absorption spectra of complexes **Ir-1**, **Ir-2**, **Ir-3**, **MB**, **TPP** and the emission spectra of the 35 W xenon lamp (measured with spectrofluorometer). In CH₂Cl₂/CH₃OH (9:1, v/v), 1.0×10^{-5} M, 20°C. The excitation of xenon lamp with wavelength shorter than 387 nm was blocked by 0.72 M NaNO₂ solution. (b) The emission spectrum of the 35 W xenon lamp with and without the NaNO₂ solution filter.

UV-vis absorption and emission spectra

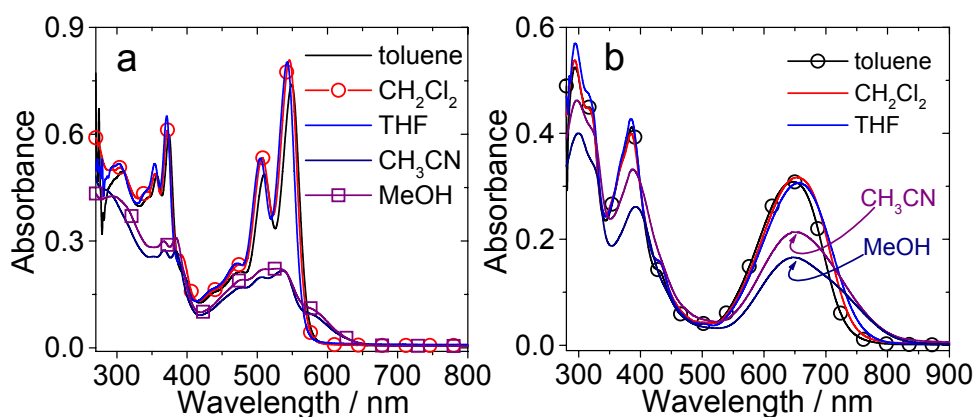


Fig. S29 Solvents polarity-dependency of the UV-Vis absorption of the ligands. (a) **L2**; (b) **L3**. $c = 1.0 \times 10^{-5}$ M, 20 °C.

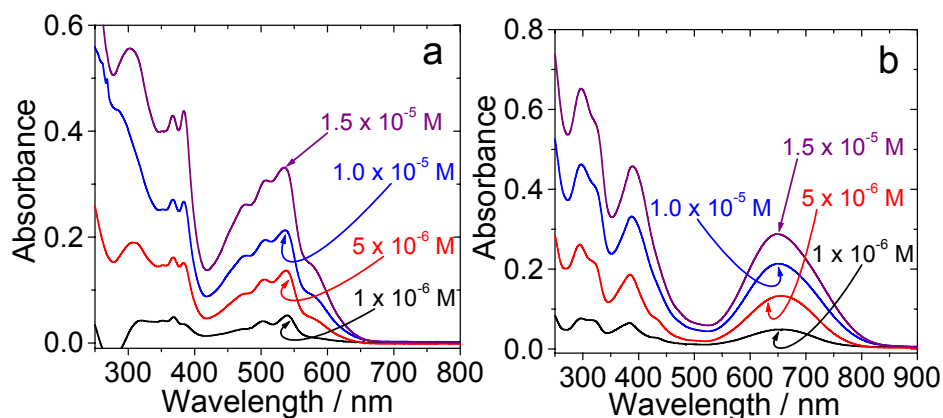


Fig. S30 UV-Vis absorption spectra of the ligands **L2** (a) and **L3** (b) at the different concentration in CH_3CN at 20 °C.

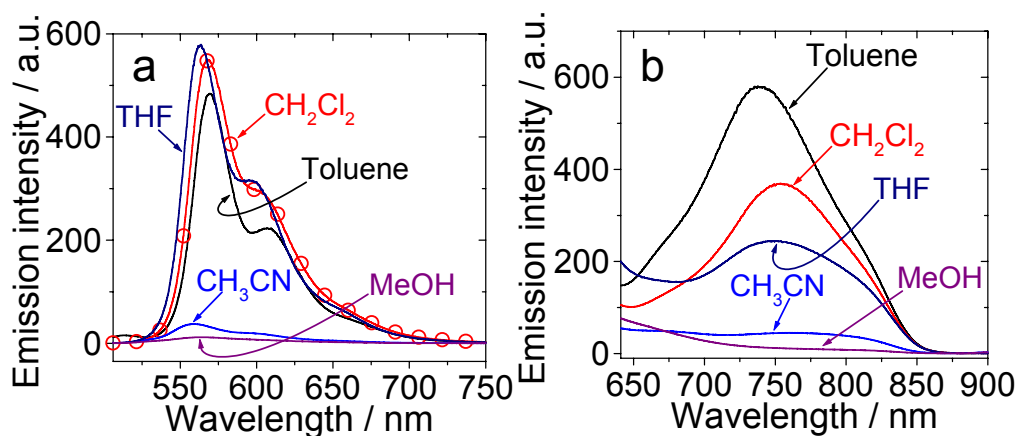


Fig. S31 Solvents polarity-dependency of the emission of ligands under the same conditions. (a) **L2**,

$\lambda_{\text{ex}} = 500$ nm; (b) **L3**, $\lambda_{\text{ex}} = 600$ nm. $c = 1.0 \times 10^{-5}$ M, 20 °C.

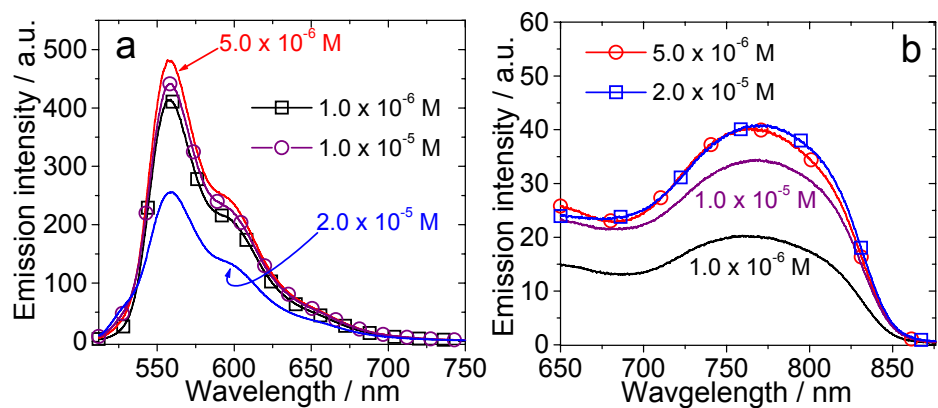


Fig. S32 Fluorescence emission spectra of the ligands **L2** (a) and **L3** (b) at different concentration in CH_3CN at 20 °C.

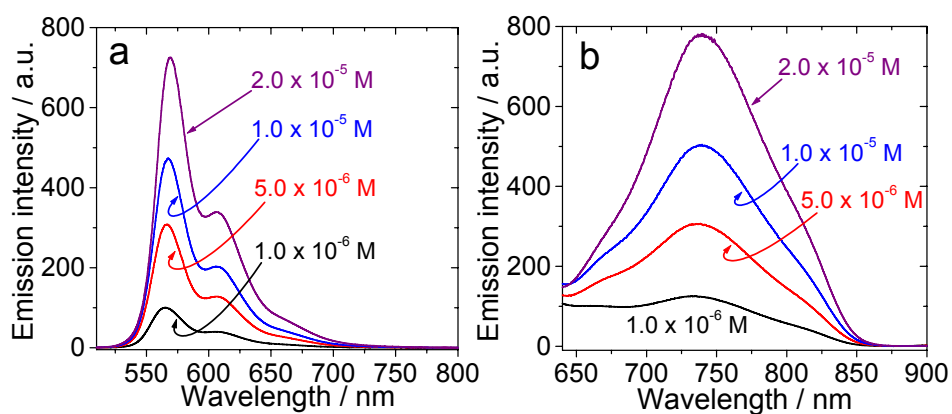


Fig. S33 Fluorescence emission spectra of the ligands **L2** (a) and **L3** (b) at different concentration in toluene. 20 °C.

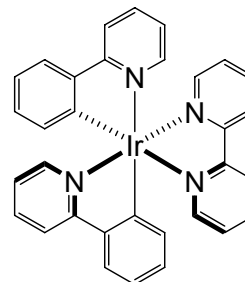
DFT/TDDFT calculations

Z-matrix, number of imaginary frequencies and total energy of the compounds (there are no imaginary frequencies for all the structures).

Ir-1 ground state configuration (B3LYP/6-31G/LANL2DZ)

Symbolic Z-matrix:

Charge = 1 Multiplicity = 1



C	-1.68151700	1.66936200	-2.04457600
C	-4.08275800	1.75655000	-2.14431600
H	-0.69360500	1.96541800	-2.37142100
C	-4.12705700	0.82860100	-1.10218000
H	-5.00206900	2.14087900	-2.57056700
C	-2.93306200	0.33847300	-0.55427900
C	-2.88157700	-0.64102800	0.55002400
C	-4.01801400	-1.24928100	1.10186000
C	-1.49814000	-1.82852500	2.04473500
C	-3.87740100	-2.16246900	2.14850900
C	-2.59717600	-2.45628400	2.62917700
H	-0.48486400	-2.01829200	2.37301400
H	-4.75181600	-2.63706200	2.57825600
H	-2.44779700	-3.15939900	3.43925200
N	-1.63318500	-0.94051600	1.02941200
C	-2.84036400	2.18352100	-2.62451500
H	-2.76574600	2.90304000	-3.43050300
C	-0.44673300	-2.04136400	-2.22445600
C	0.71455700	-4.12705600	-2.48065600
H	-1.17287800	-1.30436800	-2.53659500
C	1.45045300	-3.82324200	-1.33965900
H	0.89157700	-5.05433200	-3.01371100

C	1.22769400	-2.61950100	-0.64745300
H	2.20539600	-4.51044900	-0.98077200
C	1.93244400	-2.17219700	0.55014500
C	2.93331800	-2.92971100	1.18969100
C	2.19936800	-0.42026700	2.19885200
C	3.56324900	-2.43349600	2.32899000
H	3.22516200	-3.90134000	0.80341400
C	3.19376500	-1.17715000	2.83132800
H	1.94428700	0.55163300	2.60743700
H	4.33652200	-3.01384400	2.82012000
H	3.68755100	-0.78482900	3.71527700
C	-0.25328500	-3.21912700	-2.93494600
H	-0.84170100	-3.41765800	-3.82198700
C	2.15194800	0.64041500	-2.19377900
C	3.29824300	2.78472300	-2.32630400
C	1.44729300	1.04583700	-1.04597500
H	2.00115500	-0.35385100	-2.60016800
C	2.61866200	3.21422400	-1.18851000
H	4.00697700	3.44191000	-2.81799400
C	1.70118100	2.35757500	-0.54887700
H	2.80719700	4.21175100	-0.80401500
C	0.95243300	2.73116200	0.64736400
C	1.05333900	3.95030500	1.34113300
C	-0.65996500	1.98856300	2.22016600
C	0.28892900	4.17850600	2.48100000
H	1.73776300	4.70899000	0.98486800
C	-0.58579200	3.17907700	2.93199500
H	-1.31068000	1.18343500	2.53046000
H	0.37310400	5.11786400	3.01565400
H	-1.19292900	3.31756900	3.81780900
N	0.08371800	1.76309100	1.10664200

C	3.06288800	1.49559100	-2.82640200
H	3.59602800	1.15522000	-3.70903400
Ir	0.05023500	0.00223300	-0.00102700
N	-1.72303300	0.76677600	-1.03421900
C	1.54359900	-0.89440900	1.04853800
N	0.26784900	-1.74306300	-1.10889500
H	-5.00379400	-1.02162300	0.71818400
H	-5.08354200	0.49912700	-0.71825000

1 3 1.0 16 1.5 57 1.5

2 4 1.5 5 1.0 16 1.5

3

4 6 1.5 61 1.0

5

6 7 1.0 57 1.5

7 8 1.5 15 1.5

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11 14 1.0

12

13

14

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60

61

SCF Done: E(RB3LYP) = -1557.17236452 a.u.

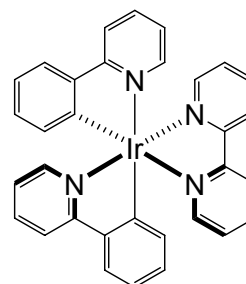
Number of Imaginary frequencies: 0

Ir-1 lowest-lying triplet state configuration (B3LYP/6-31G/LANL2DZ)

Symbolic Z-matrix:

Charge = 1 Multiplicity = 3

C	-1.68151700	1.66936200	-2.04457600
C	-4.08275800	1.75655000	-2.14431600
H	-0.69360500	1.96541800	-2.37142100
C	-4.12705700	0.82860100	-1.10218000
H	-5.00206900	2.14087900	-2.57056700
C	-2.93306200	0.33847300	-0.55427900
C	-2.88157700	-0.64102800	0.55002400
C	-4.01801400	-1.24928100	1.10186000
C	-1.49814000	-1.82852500	2.04473500
C	-3.87740100	-2.16246900	2.14850900
C	-2.59717600	-2.45628400	2.62917700
H	-0.48486400	-2.01829200	2.37301400
H	-4.75181600	-2.63706200	2.57825600
H	-2.44779700	-3.15939900	3.43925200



N	-1.63318500	-0.94051600	1.02941200
C	-2.84036400	2.18352100	-2.62451500
H	-2.76574600	2.90304000	-3.43050300
C	-0.44673300	-2.04136400	-2.22445600
C	0.71455700	-4.12705600	-2.48065600
H	-1.17287800	-1.30436800	-2.53659500
C	1.45045300	-3.82324200	-1.33965900
H	0.89157700	-5.05433200	-3.01371100
C	1.22769400	-2.61950100	-0.64745300
H	2.20539600	-4.51044900	-0.98077200
C	1.93244400	-2.17219700	0.55014500
C	2.93331800	-2.92971100	1.18969100
C	2.19936800	-0.42026700	2.19885200
C	3.56324900	-2.43349600	2.32899000
H	3.22516200	-3.90134000	0.80341400
C	3.19376500	-1.17715000	2.83132800
H	1.94428700	0.55163300	2.60743700
H	4.33652200	-3.01384400	2.82012000
H	3.68755100	-0.78482900	3.71527700
C	-0.25328500	-3.21912700	-2.93494600
H	-0.84170100	-3.41765800	-3.82198700
C	2.15194800	0.64041500	-2.19377900
C	3.29824300	2.78472300	-2.32630400
C	1.44729300	1.04583700	-1.04597500
H	2.00115500	-0.35385100	-2.60016800
C	2.61866200	3.21422400	-1.18851000
H	4.00697700	3.44191000	-2.81799400
C	1.70118100	2.35757500	-0.54887700
H	2.80719700	4.21175100	-0.80401500
C	0.95243300	2.73116200	0.64736400
C	1.05333900	3.95030500	1.34113300

C	-0.65996500	1.98856300	2.22016600
C	0.28892900	4.17850600	2.48100000
H	1.73776300	4.70899000	0.98486800
C	-0.58579200	3.17907700	2.93199500
H	-1.31068000	1.18343500	2.53046000
H	0.37310400	5.11786400	3.01565400
H	-1.19292900	3.31756900	3.81780900
N	0.08371800	1.76309100	1.10664200
C	3.06288800	1.49559100	-2.82640200
H	3.59602800	1.15522000	-3.70903400
Ir	0.05023500	0.00223300	-0.00102700
N	-1.72303300	0.76677600	-1.03421900
C	1.54359900	-0.89440900	1.04853800
N	0.26784900	-1.74306300	-1.10889500
H	-5.00379400	-1.02162300	0.71818400
H	-5.08354200	0.49912700	-0.71825000

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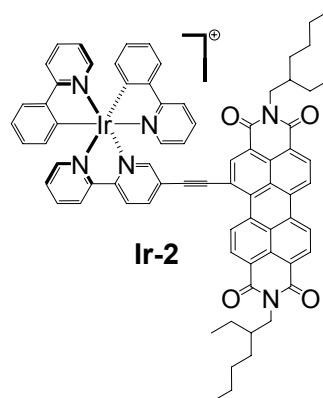
Number of Imaginary frequencies: 0

Ir-2 ground state configuration (B3LYP/6-31G/LANL2DZ)

Symbolic Z-matrix:

Charge = 1 Multiplicity = 1

C	1.20601300	-0.52623700	-0.01267300
C	-0.07726500	-2.55365000	-0.18902900
H	1.28798000	0.54966300	0.06735400
C	1.12020500	-3.24848000	-0.24107200
H	-1.02473100	-3.07886300	-0.24344700



C	2.34149600	-2.56709900	-0.17672800
H	1.10398600	-4.32770000	-0.33227100
C	3.65237200	-3.23771200	-0.22805300
C	3.81569300	-4.62060400	-0.37997800
C	5.96689600	-2.94374000	-0.17109600
C	5.09753600	-5.15996100	-0.42496000
H	2.95463600	-5.27183600	-0.46950400
C	6.19705500	-4.30758600	-0.31893600
H	6.78356000	-2.23432100	-0.09289700
H	5.23440700	-6.22995800	-0.54551200
H	7.21322500	-4.68485800	-0.35489100
N	4.73181600	-2.42035000	-0.12117200
C	-0.05452200	-1.15017000	-0.06564400
C	3.55320300	-0.51130300	-3.00472200
C	5.13140400	0.09329800	-4.74890400
C	4.46996100	-0.16905200	-1.99953000
H	2.56366600	-0.87468000	-2.73963900
C	6.06165800	0.44232400	-3.77681800
H	5.37921700	0.19233200	-5.80134100
C	5.73880500	0.31570800	-2.41461600
H	7.03429300	0.81588900	-4.08498600
C	6.65399500	0.67850900	-1.33469100
C	7.94634400	1.20274300	-1.49047400
C	6.90372200	0.79100300	1.00367800
C	8.71483900	1.51855800	-0.37902300
H	8.33731900	1.36555300	-2.48778600
C	8.18468600	1.31021400	0.89776900
H	6.43908600	0.61868100	1.96607300

H	9.71297700	1.92757700	-0.50317400
H	8.74494100	1.55031200	1.79452300
N	6.15821100	0.47335800	-0.07456000
C	3.87538900	-0.38281000	-4.35821600
H	3.14219100	-0.65232300	-5.11444000
C	3.28801300	2.55619400	-0.73592000
C	2.54501200	4.19534600	0.89251800
C	3.54850300	1.61069700	0.26850900
H	3.46783500	2.29666300	-1.77424900
C	2.79716600	3.28400800	1.91073600
H	2.15669200	5.18162000	1.12738000
C	3.29365000	2.00075300	1.61438600
H	2.60111400	3.57813000	2.93781200
C	3.55530300	1.00320400	2.65994500
C	3.35476600	1.19571700	4.03811600
C	4.29607000	-1.18365200	3.08379400
C	3.63522500	0.17326700	4.93426000
H	2.97967000	2.14498000	4.40114800
C	4.11705800	-1.04830300	4.45320500
H	4.66907900	-2.10688500	2.65183900
H	3.48023000	0.32444400	5.99849000
H	4.34807800	-1.87283200	5.11872200
N	4.02912100	-0.19449600	2.21189000
C	2.79240900	3.82705800	-0.43323000
H	2.59662700	4.53367100	-1.23571600
Ir	4.23028100	-0.29140600	0.01147400
C	-1.23260900	-0.37122600	0.00675500
N	2.36142600	-1.20398000	-0.06517700

C	-2.26667600	0.26993500	0.08164200
C	-4.73933200	0.77953400	0.10506500
C	-5.20975300	-0.60068600	0.28790200
C	-5.72012700	1.80696400	-0.09504600
C	-6.56790100	-0.92134500	-0.03867800
C	-7.51493100	0.08811000	-0.38601200
C	-7.10436500	1.49300900	-0.30131700
C	-9.19796400	-1.64242100	-0.76784100
C	-8.31483300	-2.63173300	-0.36876600
C	-6.99600000	-2.28320200	0.00924100
C	-6.10950200	-3.29295700	0.45392700
C	-4.83861700	-2.94809300	0.87565500
H	-4.19137900	-3.72705900	1.26495600
H	-10.20161900	-1.92656500	-1.06521900
C	-3.00904500	2.53646900	0.07828400
C	-3.95579200	3.52835700	0.00042400
C	-5.32538500	3.18132200	-0.11259600
H	-1.96186600	2.81496700	0.11189700
C	-6.28709400	4.20636100	-0.25003500
C	-7.62589800	3.87920000	-0.39247300
H	-8.35229900	4.67938300	-0.48658600
C	-3.37108800	1.16332400	0.11275000
C	-8.80287800	-0.29958600	-0.76434900
H	-9.52871100	0.44487800	-1.06964800
C	-6.53509000	-4.71511900	0.50220300
C	-8.77274000	-4.04536500	-0.34239700
O	-9.90090700	-4.36634300	-0.68471300
O	-5.78574900	-5.60919500	0.87361000

C	-3.51034500	4.94803100	-0.00143900
C	-5.88425700	5.63434300	-0.24373700
N	-4.51490800	5.91372600	-0.11847200
O	-6.69192600	6.54596900	-0.34218900
O	-2.32893300	5.25317200	0.09546600
C	-4.13742400	7.33313500	-0.11857500
H	-3.05482600	7.38820200	-0.03179500
H	-4.47463200	7.80314000	-1.04511200
H	-4.61745900	7.84224100	0.72046500
N	-7.84109200	-5.00131200	0.09782800
C	-8.24816800	-6.41156200	0.14693600
H	-7.60311300	-7.00491900	-0.50548200
H	-8.14779300	-6.78784900	1.16754800
H	-9.28272200	-6.46964100	-0.18316600
C	-8.02178900	2.53922500	-0.42718000
H	-9.07653600	2.32281100	-0.54718000
C	-4.39845400	-1.62110000	0.79447400
H	-3.40429900	-1.39105200	1.14806400

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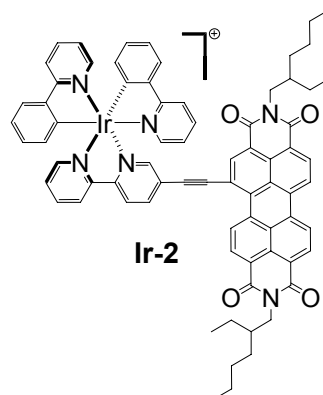
Number of Imaginary frequencies: 0

Ir-2 triplet state configuration (B3LYP/6-31G/LANL2DZ)

Symbolic Z-matrix:

Charge = 1 Multiplicity = 3

C	1.22220800	-0.48079100	-0.15452900
C	-0.07262500	-2.46895900	-0.57505800
H	1.30754000	0.57812300	0.05114100
C	1.12023700	-3.16027800	-0.69162600



H	-1.02281900	-2.97772600	-0.69692500
C	2.34674400	-2.50041800	-0.53172200
H	1.09948500	-4.22197100	-0.90556800
C	3.65161600	-3.16853000	-0.64450200
C	3.80962400	-4.52135700	-0.97638900
C	5.96772400	-2.90585500	-0.51182200
C	5.08779100	-5.06097700	-1.07145300
H	2.94607600	-5.14674800	-1.16807200
C	6.19146600	-4.23964300	-0.83632800
H	6.78855400	-2.22144300	-0.32786200
H	5.21971800	-6.10660700	-1.33120900
H	7.20560300	-4.61737400	-0.90698100
N	4.73569300	-2.38219100	-0.41065600
C	-0.04393000	-1.08443700	-0.29798800
C	3.69590100	-0.06638700	-3.03398000
C	5.34419000	0.77963800	-4.60418800
C	4.56995600	0.12023500	-1.95301000
H	2.69824400	-0.46259000	-2.86468200
C	6.23398900	0.97601900	-3.55451700
H	5.63495300	1.03098900	-5.61966400
C	5.85549100	0.65245300	-2.23995100
H	7.21875500	1.38421800	-3.76470100
C	6.72588500	0.84493400	-1.08207100
C	8.02279900	1.38028600	-1.10522600
C	6.88172300	0.60120800	1.25463000
C	8.74582800	1.52014600	0.07087100
H	8.45353500	1.69034200	-2.04989500
C	8.16579500	1.12300000	1.27934900
H	6.37868200	0.28700100	2.16027200
H	9.74782300	1.93798100	0.04971800
H	8.69018400	1.22042500	2.22338600
N	6.17983000	0.45569800	0.11208700
C	4.07327800	0.25803100	-4.33944200
H	3.37241500	0.10592600	-5.15661700
C	3.37587000	2.65493900	-0.35340800
C	2.59501800	4.05575900	1.46831800
C	3.57679900	1.56653700	0.51028300
H	3.59784300	2.54738600	-1.41029900
C	2.78810300	2.99976500	2.35064900
H	2.21688000	5.00685000	1.83067100
C	3.27346100	1.76223800	1.88817000
H	2.55566500	3.14555600	3.40165700
C	3.47625300	0.61759600	2.78590800
C	3.21886200	0.61119300	4.16797800
C	4.16742800	-1.62213300	2.91524500
C	3.44584800	-0.53618300	4.91580000
H	2.84109900	1.50459700	4.65039000
C	3.93057300	-1.68420400	4.28126200
H	4.54568700	-2.48050300	2.36906500
H	3.24689000	-0.53830000	5.98345600
H	4.12069900	-2.60148700	4.82768600
N	3.95316800	-0.51126500	2.18719200
C	2.89076500	3.87926100	0.11335300
H	2.74235600	4.70034700	-0.58341500
Ir	4.24634100	-0.29145200	0.00717400
C	-1.21447600	-0.31274500	-0.15827200

N	2.37230800	-1.15802200	-0.25917600
C	-2.25216900	0.32229500	-0.03086600
C	-4.76448800	0.76631900	0.04536300
C	-5.20020000	-0.58451000	0.20426500
C	-5.75226800	1.78639500	-0.14672000
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C	-8.33034600	-2.63439000	-0.27232900
C	-6.99382300	-2.28336400	0.02023100
C	-6.07966900	-3.29466400	0.39059900
C	-4.76086600	-2.94725600	0.73384100
H	-4.09905500	-3.73470500	1.07828400
H	-10.27543100	-1.93770400	-0.84994700
C	-3.03716300	2.55121700	0.09604600
C	-4.01114700	3.53522600	0.01222400
C	-5.37389100	3.16971800	-0.14689600
H	-1.99873700	2.85867500	0.14562000
C	-6.33826500	4.18094800	-0.29544900
C	-7.69508200	3.84752100	-0.46533100
H	-8.41588100	4.65031400	-0.57191900
C	-3.36049000	1.18600000	0.07291200
C	-8.87820500	-0.31520100	-0.65313300
H	-9.61669200	0.42783100	-0.92601700
C	-6.49274700	-4.70987500	0.45715800
C	-8.78197600	-4.04349100	-0.22269000
O	-9.93590500	-4.35901700	-0.48748000
O	-5.71343300	-5.60579000	0.76823900
C	-3.58507900	4.95511000	0.03957700
C	-5.95358200	5.61130600	-0.27084100
N	-4.59604400	5.91027800	-0.10216100
O	-6.77605800	6.50972700	-0.39113900
O	-2.40921600	5.27259800	0.17970500
C	-4.23728200	7.33453200	-0.08093400
H	-3.15852200	7.40266300	0.03853600
H	-4.55288500	7.80678600	-1.01387600
H	-4.74827800	7.83101900	0.74730600
N	-7.82375600	-4.99948900	0.14435100
C	-8.22343800	-6.41079300	0.21326000
H	-7.63084200	-6.99744300	-0.49284500
H	-8.04215800	-6.79489900	1.21962000
H	-9.28067600	-6.46851900	-0.03511200
C	-8.07672600	2.52746800	-0.48921100
H	-9.12752300	2.29685200	-0.60948300
C	-4.33521900	-1.64257000	0.64812500
H	-3.32904800	-1.40442200	0.95712200

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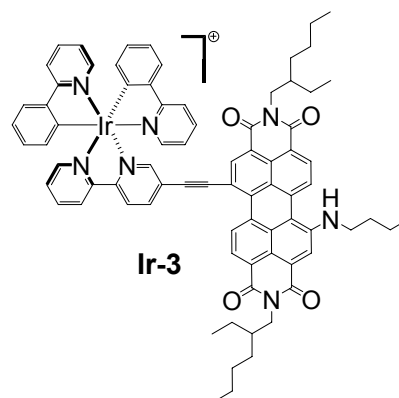
Number of Imaginary frequencies: 0

Ir-3 ground state configuration (B3LYP/6-31G/LANL2DZ)

Symbolic Z-matrix:

Charge = 1 Multiplicity = 1

C	-1.47549200	-0.87850400	-0.11738200
C	-0.39939800	-3.02226700	-0.27606000
H	-1.44192500	0.19998600	-0.05072100
C	-1.66246400	-3.59589300	-0.25219400
H	0.48780200	-3.64252700	-0.34414600
C	-2.81006300	-2.79743100	-0.16690600
H	-1.75530800	-4.67404700	-0.30389900
C	-4.18350000	-3.32876300	-0.14239000
C	-4.49074100	-4.69538300	-0.16889800
C	-6.45320900	-2.79418500	-0.04172000
C	-5.82072200	-5.10148100	-0.13150400
H	-3.70177100	-5.43666500	-0.21100800
C	-6.82441800	-4.13448200	-0.06500000
H	-7.19147900	-2.00190200	0.01936600
H	-6.06857400	-6.15813900	-0.14864900
H	-7.87346000	-4.40701000	-0.02641900
N	-5.17160100	-2.39699300	-0.08626000
C	-0.28257200	-1.62037500	-0.21564100
C	-3.71973500	-1.03743200	2.96288300
C	-5.15677700	-0.48175800	4.84024100
C	-4.61178500	-0.44949700	2.05349500
H	-2.79466900	-1.48385500	2.60725900
C	-6.06083000	0.10906300	3.96515900
H	-5.36002900	-0.49579300	5.90674800
C	-5.79559900	0.12829200	2.58483800
H	-6.96793500	0.55579900	4.36291600
C	-6.68723200	0.74137300	1.60274200
C	-7.89701000	1.39517100	1.88231000
C	-6.98883100	1.18900200	-0.68866900
C	-8.65135700	1.94536700	0.85579800
H	-8.23463700	1.47249400	2.90900900
C	-8.18993100	1.84217900	-0.45986500
H	-6.57794800	1.08775300	-1.68503500
H	-9.58520500	2.45382700	1.07583100
H	-8.74142600	2.26393400	-1.29275000
N	-6.25785300	0.64481500	0.30579000
C	-3.98494100	-1.05466000	4.33441400
H	-3.27281600	-1.51462500	5.01523700
C	-3.08275000	2.23122700	1.10702600
C	-1.94922900	3.83805700	-0.32025000
C	-3.50979200	1.48113600	0.00006500
H	-3.33045700	1.89523800	2.10871700
C	-2.39234900	3.13885600	-1.43726500
H	-1.31300900	4.70897000	-0.43801800
C	-3.17056600	1.97469800	-1.29224500



H	-2.10966400	3.49617100	-2.42328100
C	-3.62767300	1.19168500	-2.44736800
C	-3.43422800	1.54151600	-3.79531700
C	-4.74925900	-0.75617100	-3.12415900
C	-3.91121000	0.71791800	-4.80573300
H	-2.91448100	2.45879200	-4.04459500
C	-4.58474800	-0.46099400	-4.47007300
H	-5.26547100	-1.65506500	-2.80242700
H	-3.76191600	0.99061800	-5.84633200
H	-4.97333200	-1.13215000	-5.22816600
N	-4.29175600	0.04044300	-2.14132900
C	-2.31173100	3.38664200	0.95293400
H	-1.97840000	3.93140600	1.83270000
Ir	-4.44507100	-0.32707400	0.03543600
C	0.93614700	-0.90623400	-0.25696400
N	-2.69104500	-1.43686400	-0.09453900
C	1.91937600	-0.18547800	-0.29616200
C	4.32529000	0.58898400	-0.24175800
C	4.96382000	-0.71814500	-0.41078900
C	5.18015400	1.71937800	-0.04751500
C	6.32526300	-0.88556600	0.00392200
C	7.09673000	0.21497800	0.49943100
C	6.57685100	1.55696900	0.24764200
C	8.24522800	-2.37887500	0.34846500
C	6.91464000	-2.17904800	-0.10354800
C	6.20422800	-3.25349800	-0.67434400
C	4.91309200	-3.05489600	-1.14085600
H	4.39305600	-3.88304100	-1.60986100
C	2.41874300	2.14467900	-0.34523000
C	3.25546000	3.23562300	-0.31850700
C	4.65191200	3.04350300	-0.16101500
H	1.34913900	2.30874400	-0.41428800
C	5.51004900	4.16332400	-0.13071900
C	6.87849600	3.97283700	0.00645200
H	7.53031700	4.83975700	-0.02567400
C	2.92358300	0.81773800	-0.31022100
C	8.34584900	-0.06436200	1.11621400
C	6.82996800	-4.59425400	-0.80500700
C	8.90584500	-3.70813000	0.23201100
O	10.04854500	-3.89748200	0.62297800
O	6.23909200	-5.54904500	-1.29018900
C	2.67188700	4.59711500	-0.43117800
C	4.97065600	5.53367300	-0.26635900
N	3.57681200	5.66252600	-0.40420300
O	5.67908800	6.53042300	-0.26075900
O	1.46426100	4.77988900	-0.54480500
C	3.06286800	7.03222700	-0.52633800
H	1.98095800	6.97356600	-0.61828400
H	3.34362000	7.61173200	0.35617900
H	3.49901500	7.51275400	-1.40524500
N	8.14590800	-4.73422900	-0.34630500
C	8.74941700	-6.06611900	-0.48579200
H	8.15653100	-6.79928200	0.06602200
H	8.76354600	-6.35534700	-1.53914100
H	9.76059300	-6.01505000	-0.08895500
C	7.39863900	2.69317500	0.21143000

H	8.46862800	2.57135800	0.32898300
C	4.30688100	-1.80505100	-1.00487000
H	3.30508000	-1.67593700	-1.38961200
N	9.05132600	0.84008300	1.88765700
C	8.43019400	1.72352200	2.87464900
H	7.44061200	1.35021500	3.15978200
H	9.06454400	1.74852500	3.76437100
H	8.31119600	2.74824200	2.50659000
C	8.92290100	-1.35403900	0.95858000
H	9.91415400	-1.55725700	1.35528000
H	9.95104800	0.48214300	2.18015000

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SCF Done: E(RB3LYP) = -3136.82251039 a.u.

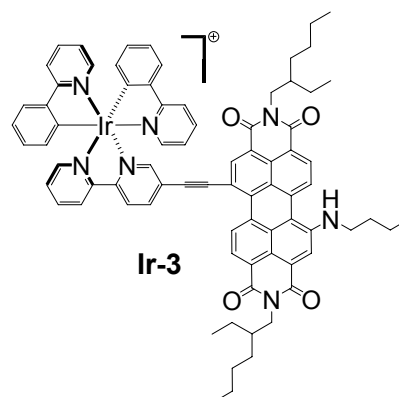
Number of Imaginary frequencies: 0

Ir-3 ground state configuration (B3LYP/6-31G/LANL2DZ)

Symbolic Z-matrix:

Charge = 1 Multiplicity = 3

C	-1.49376282	-0.85374818	-0.01862200
C	-0.39401514	-2.99502534	0.01293139
H	-1.47178283	0.22704880	-0.03669915
C	-1.65055903	-3.57709987	0.05689397
H	0.50032474	-3.60872692	0.01103850
C	-2.80911597	-2.78671169	0.05521100
H	-1.73286896	-4.65697193	0.08660750
C	-4.17508187	-3.32837608	0.08236546
C	-4.47021480	-4.69710181	0.15629516
C	-6.45289125	-2.81523596	0.05920112
C	-5.79634686	-5.11435660	0.17956785
H	-3.67357878	-5.42988833	0.20234949
C	-6.81125575	-4.15715577	0.13013528
H	-7.20019034	-2.02979763	0.02768158
H	-6.03379896	-6.17184331	0.23981313
H	-7.85849186	-4.43822246	0.15144699
N	-5.17447461	-2.40678622	0.03037008
C	-0.29046016	-1.58858224	-0.03587070
C	-3.83376952	-0.81856511	3.01687398
C	-5.33847466	-0.15352549	4.80356295
C	-4.70321502	-0.31048335	2.03996185
H	-2.89241536	-1.27571709	2.72336765
C	-6.22142844	0.35904424	3.86040277
H	-5.57629988	-0.09532236	5.86140656
C	-5.91144662	0.28483812	2.49132174
H	-7.14715783	0.81800684	4.19653551
C	-6.77860207	0.81382143	1.44091454
C	-8.00515598	1.46710594	1.63593108
C	-7.01110118	1.09744883	-0.88421814



C	-8.73254170	1.93410509	0.55043230
H	-8.37745287	1.60950846	2.64349947
C	-8.22703164	1.74725298	-0.73959476
H	-6.56749332	0.93347095	-1.85804906
H	-9.67948978	2.44247227	0.70497932
H	-8.75629700	2.10202558	-1.61693838
N	-6.30586401	0.63425236	0.16819010
C	-4.14311221	-0.74226432	4.37710157
H	-3.44754887	-1.14182718	5.11112212
C	-3.17331181	2.31705961	0.95655416
C	-2.04444756	3.85435126	-0.54794418
C	-3.56099676	1.48832629	-0.10829914
H	-3.43685231	2.04077650	1.97240191
C	-2.44527982	3.07402649	-1.62639599
H	-1.42941714	4.73397705	-0.70818375
C	-3.20076724	1.90372600	-1.42229217
H	-2.14878562	3.37376115	-2.62749856
C	-3.61035676	1.03454441	-2.53299629
C	-3.38990454	1.29829181	-3.89619332
C	-4.66266217	-0.98452410	-3.10390544
C	-3.81804848	0.39584542	-4.86019346
H	-2.88752908	2.21069301	-4.19416632
C	-4.46846561	-0.77652305	-4.46223150
H	-5.16245005	-1.87462919	-2.73512599
H	-3.64802355	0.60218710	-5.91282629
H	-4.81715804	-1.50859193	-5.18239972
N	-4.25465717	-0.11022295	-2.16638153
C	-2.42391891	3.47725610	0.74431326
H	-2.12219593	4.08531486	1.59349411
Ir	-4.47282057	-0.32764254	0.02454496
C	0.92014489	-0.87215939	-0.11083005
N	-2.70267716	-1.42110925	0.02409009
C	1.91170171	-0.16045736	-0.18725230
C	4.35541265	0.57348903	-0.18347138
C	4.96255583	-0.71767333	-0.31801969
C	5.21376323	1.70236589	-0.01535045
C	6.34571894	-0.87972645	0.03212074
C	7.13667208	0.22818427	0.46616217
C	6.61294472	1.54475084	0.25717438
C	8.31779131	-2.34975533	0.24079426
C	6.95012048	-2.17275121	-0.10043665
C	6.21453945	-3.26088987	-0.59476174
C	4.86953305	-3.07994651	-0.96909841
H	4.33648529	-3.92949882	-1.38245284
C	2.44102157	2.13939090	-0.33107718
C	3.29421881	3.23104360	-0.30386610
C	4.68827547	3.03171515	-0.12793726
H	1.37449538	2.32046567	-0.40327765
C	5.54059523	4.15020289	-0.07870247
C	6.92653410	3.97479073	0.07660051
H	7.56519992	4.85079023	0.05631731
C	2.92262470	0.82034726	-0.25898652
C	8.45967077	-0.05227132	1.01694994
C	6.83493246	-4.58892945	-0.75595111
C	8.97885535	-3.66638782	0.09183834
O	10.15588689	-3.83621640	0.39101380

O	6.21431793	-5.56067073	-1.17575519
C	2.71378179	4.58930685	-0.42548759
C	5.00219104	5.52185960	-0.21656301
N	3.61637004	5.65643975	-0.37805874
O	5.72018788	6.51316729	-0.18871850
O	1.50783419	4.77015493	-0.56532676
C	3.10518692	7.02713149	-0.50435629
H	2.02543506	6.96862422	-0.61908990
H	3.36723671	7.60197774	0.38689439
H	3.55925433	7.51130539	-1.37204829
N	8.18647518	-4.70850995	-0.40655030
C	8.79144649	-6.03533902	-0.57604761
H	8.26665876	-6.76344733	0.04722433
H	8.70432539	-6.34845765	-1.61896121
H	9.83609032	-5.96315189	-0.28234024
C	7.44585960	2.71066949	0.24242388
H	8.51532518	2.58200154	0.34693375
C	4.26384597	-1.85313146	-0.83430050
H	3.24362648	-1.73660754	-1.16794194
N	9.17869443	0.89115635	1.73863826
C	8.61978112	1.57410375	2.91424316
H	7.60989111	1.92454386	2.70855963
H	8.58927458	0.90504493	3.78544084
H	9.24337290	2.43975723	3.15249457
C	9.03685984	-1.30726810	0.80722793
H	10.04579993	-1.51465651	1.15301542
H	10.12576067	0.57147795	1.91810047

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SCF Done: E(RB3LYP) = -3136.78181735 a.u.

Number of Imaginary frequencies: 0