

Electronic Supplementary Information for

**Strongly emissive long-lived ^3IL excited state of coumarins in
cyclometalated Ir(III) complexes used as triplet photosensitizers and
application in triplet–triplet annihilation upconversion**

Xiuyu Yi, Caishun Zhang, Song Guo, Jie Ma and Jianzhang Zhao*

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

Phone/Fax: +86 411 8498 6236

E-mail: zhaojzh@dlut.edu.cn

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

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1.0 NMR and HR-MS spectra

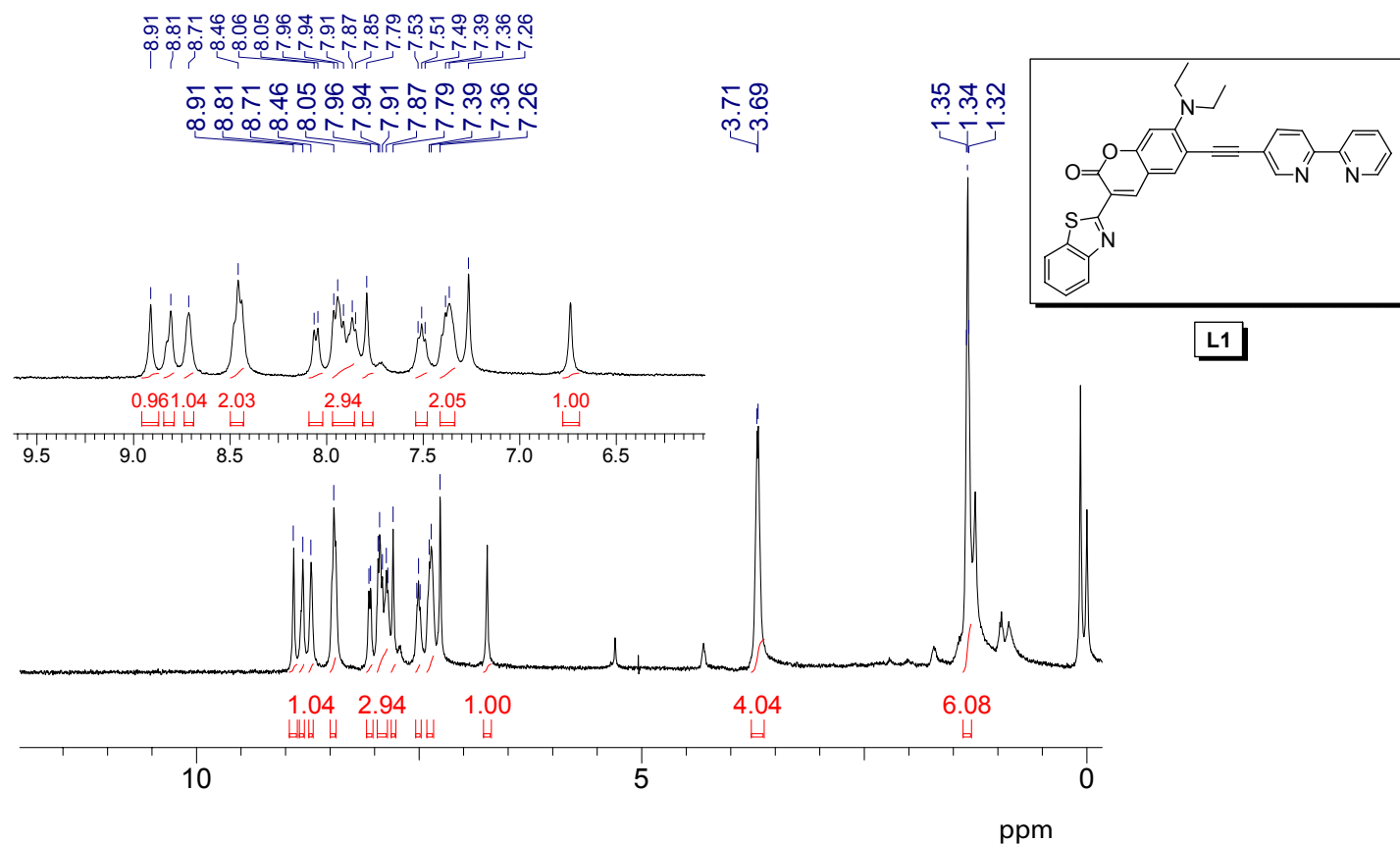


Figure S1. ¹H NMR of **L1** in CDCl₃ (400 MHz), 25°C.

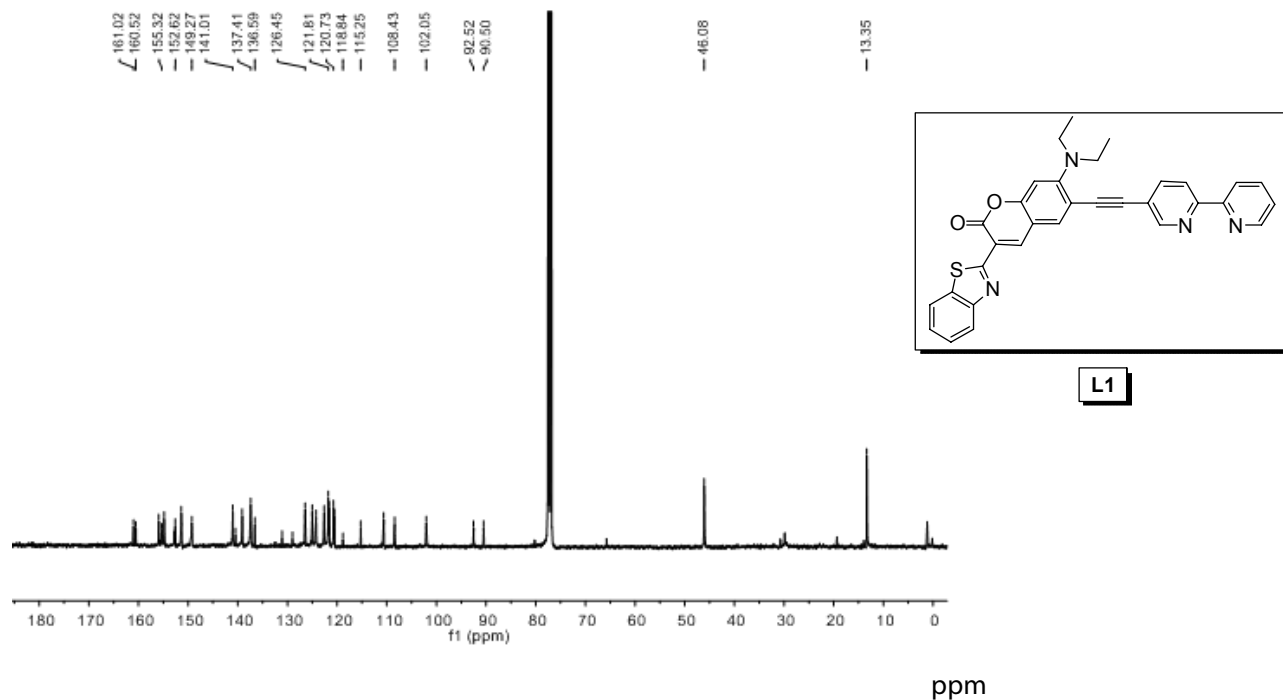


Figure S2. ¹³C NMR of **L1** (CDCl₃, 100 MHz), 25°C.

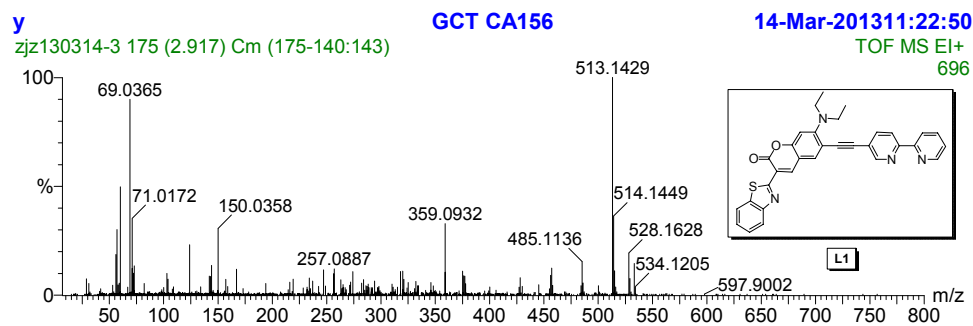


Figure S3. HRMS of **L1**, 25°C.

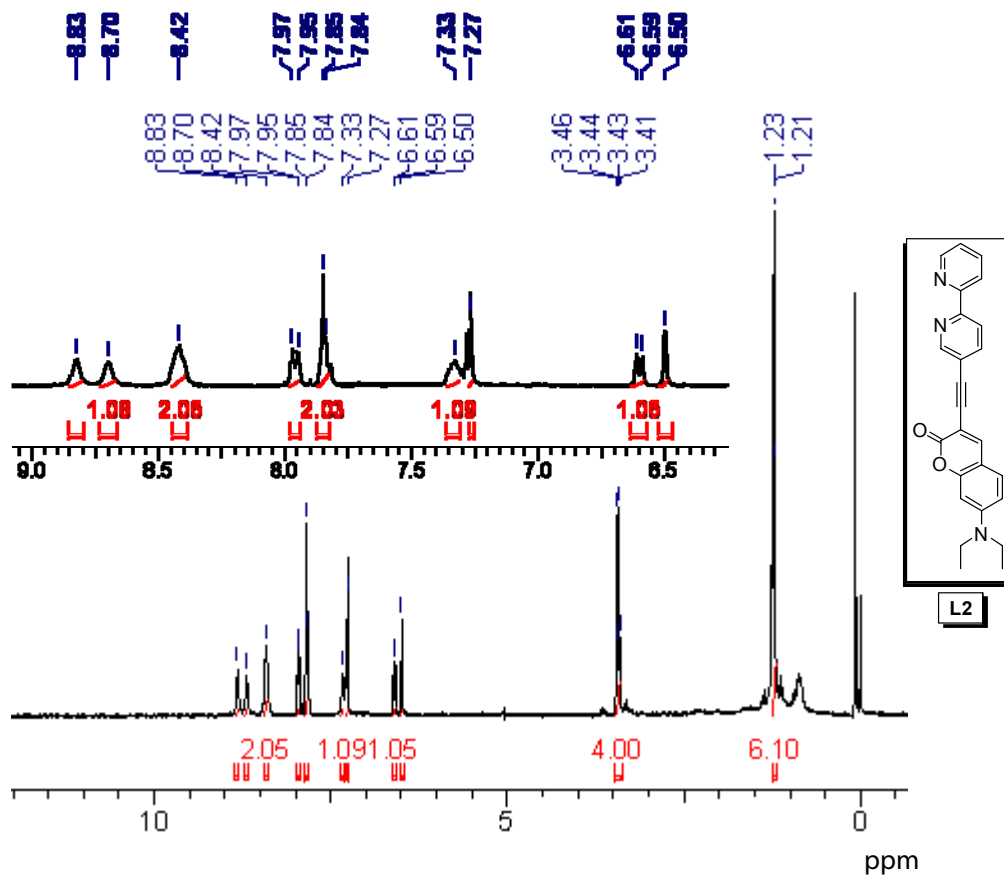


Figure S4. ^1H NMR of **L2** in CDCl_3 (400 MHz), 25°C.

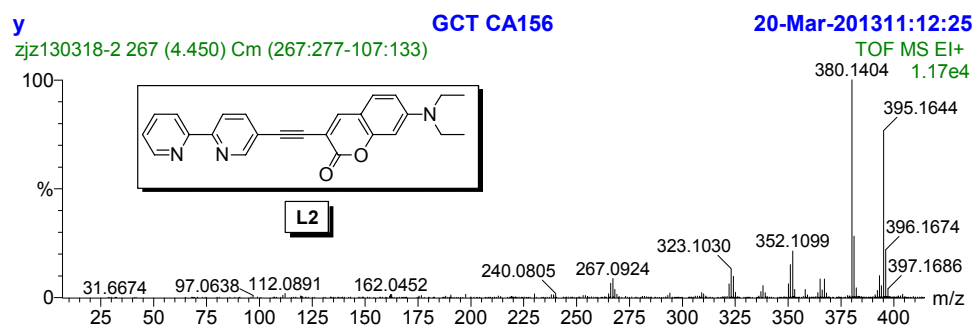


Figure S5. HRMS of **L2**, 25°C.

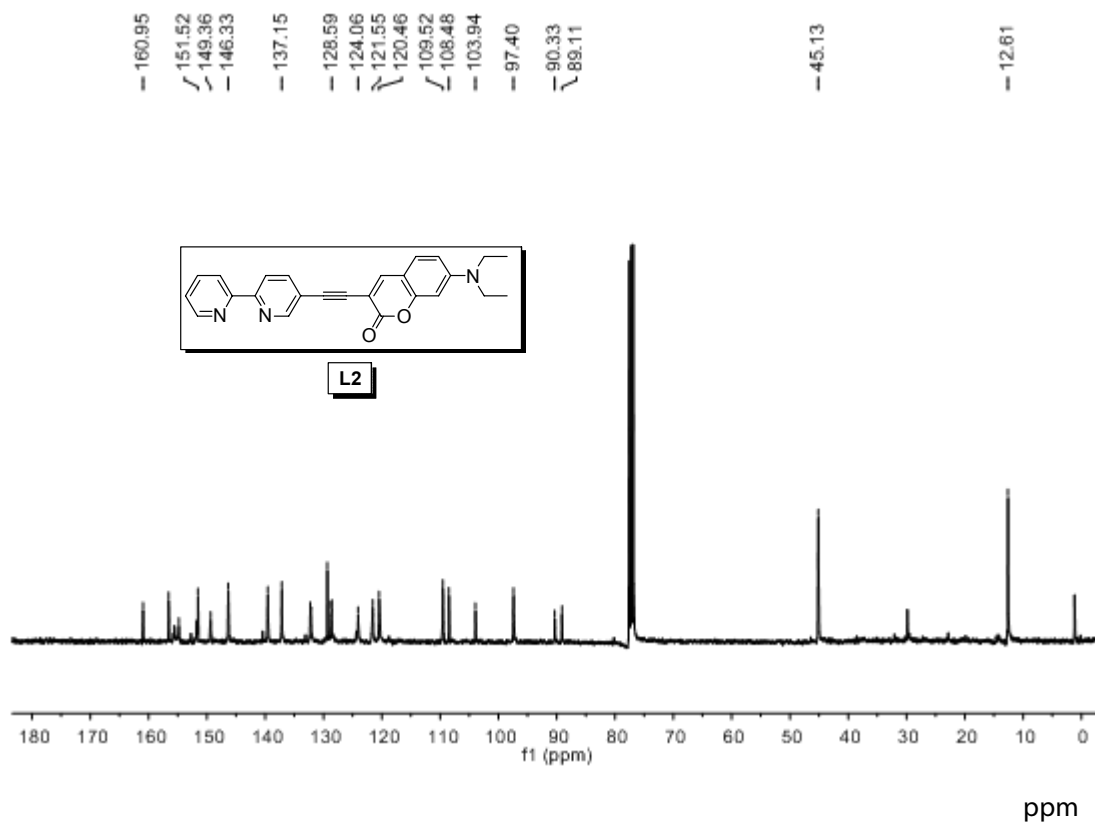
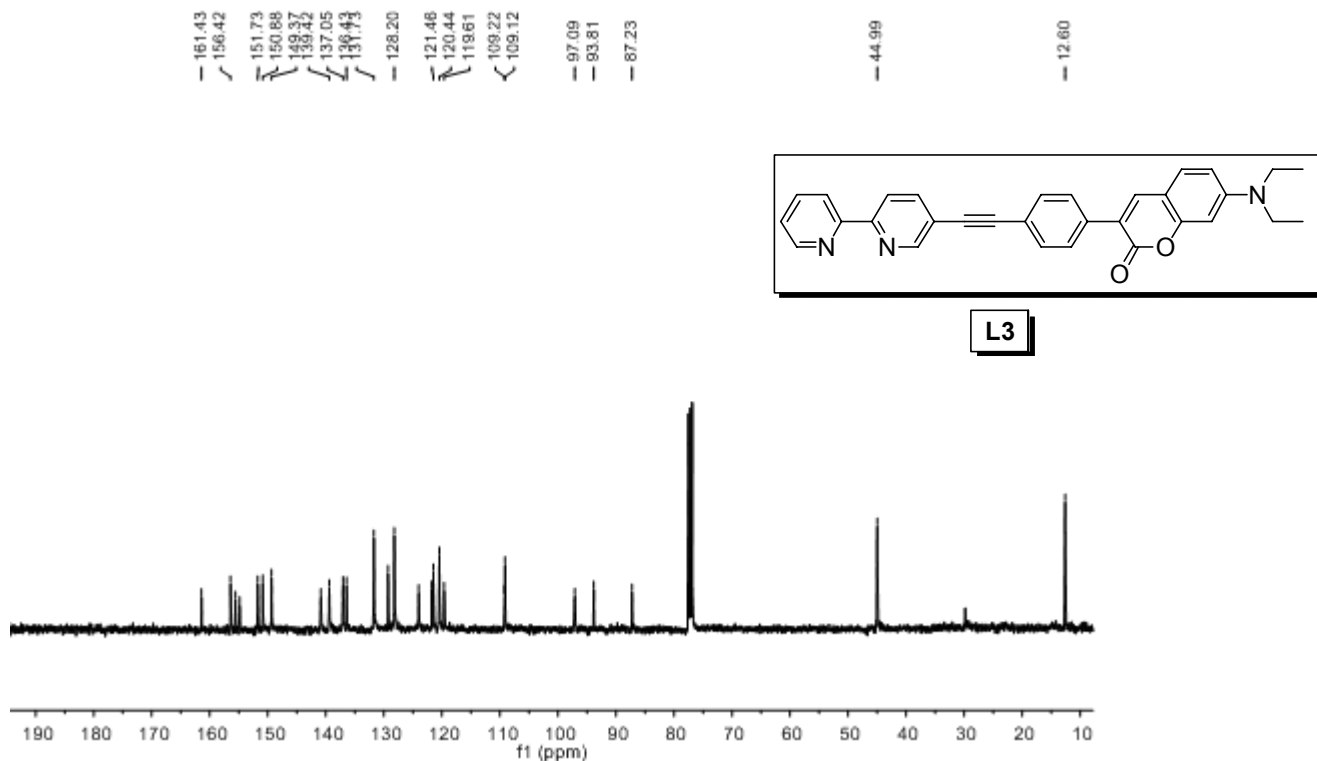
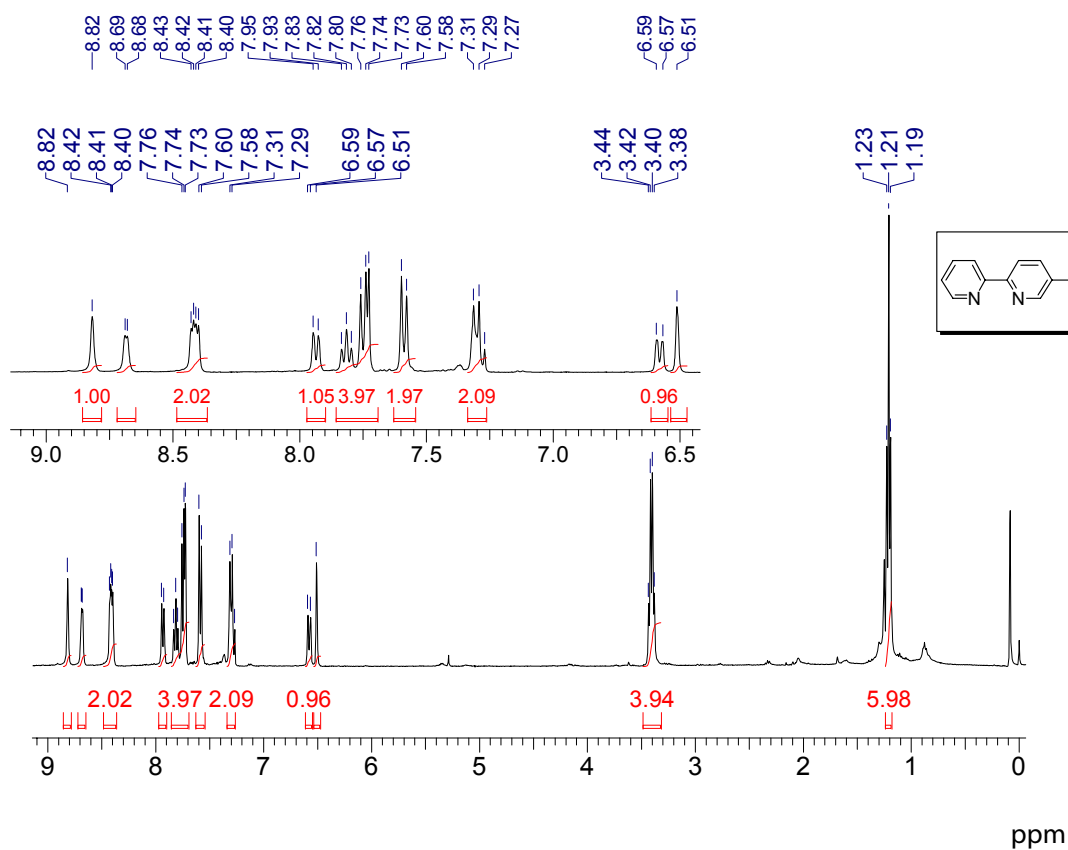


Figure S6. ^{13}C NMR of **L2** (CDCl_3 , 100 MHz), 25°C.



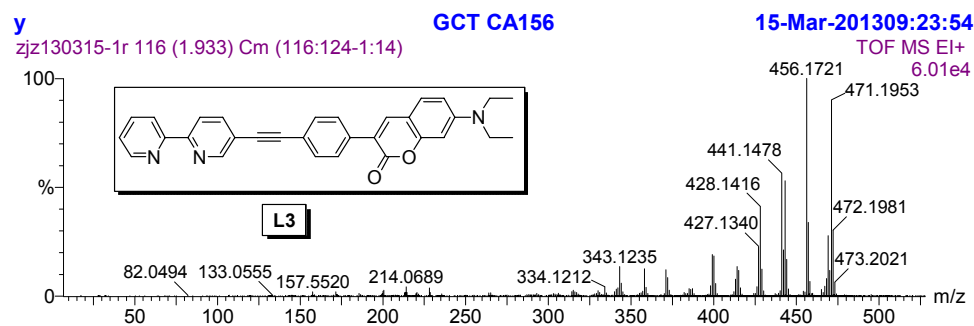


Figure S9. HRMS of **L3**, 25°C.

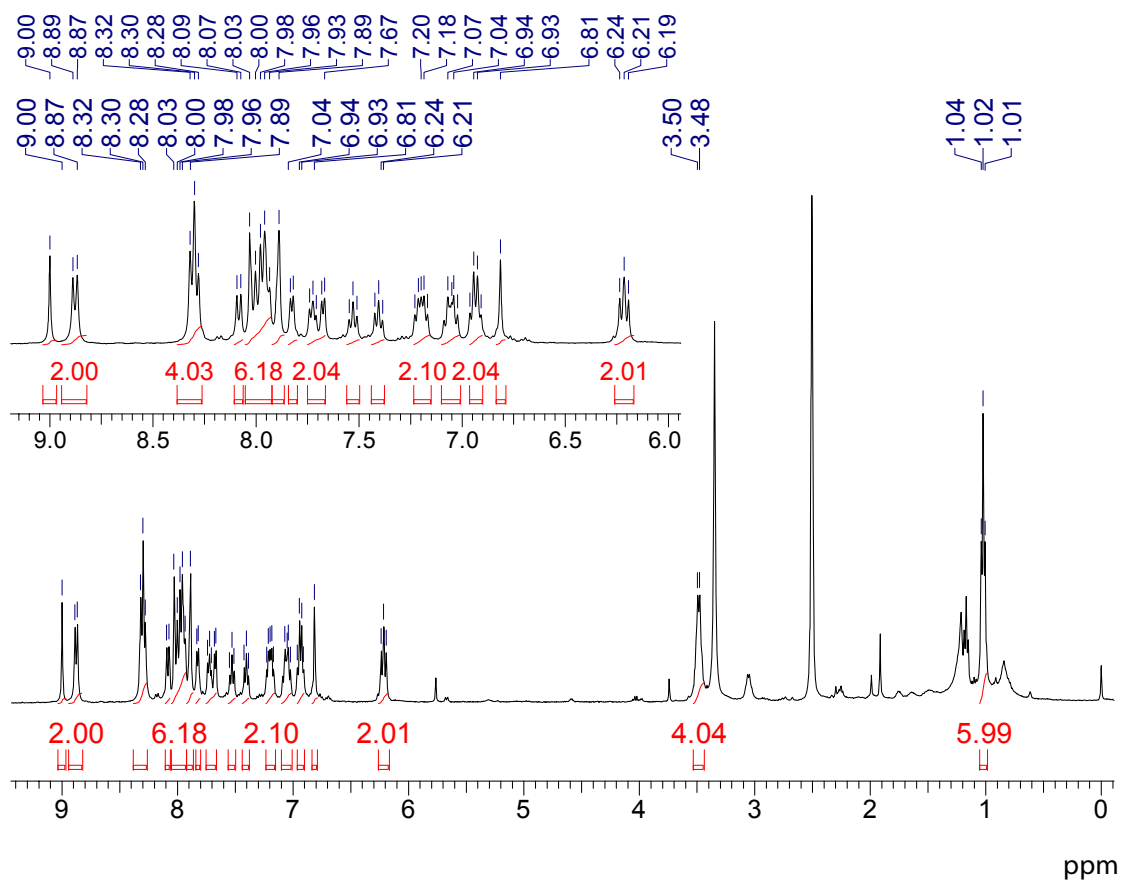


Figure S10. ^1H NMR of **Ir-1** in CDCl_3 (400 MHz), 25°C.

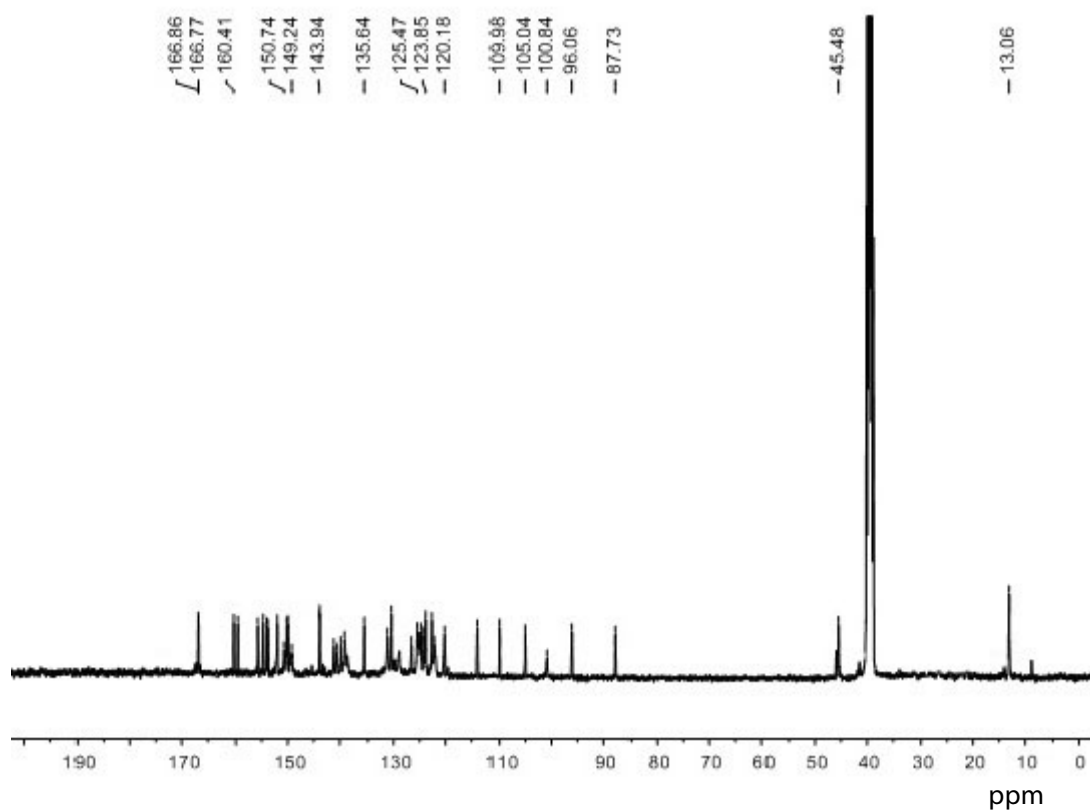


Figure S11. ^{13}C NMR of **Ir-1** ($\text{DMSO-}d_6$, 100 MHz), 25°C.

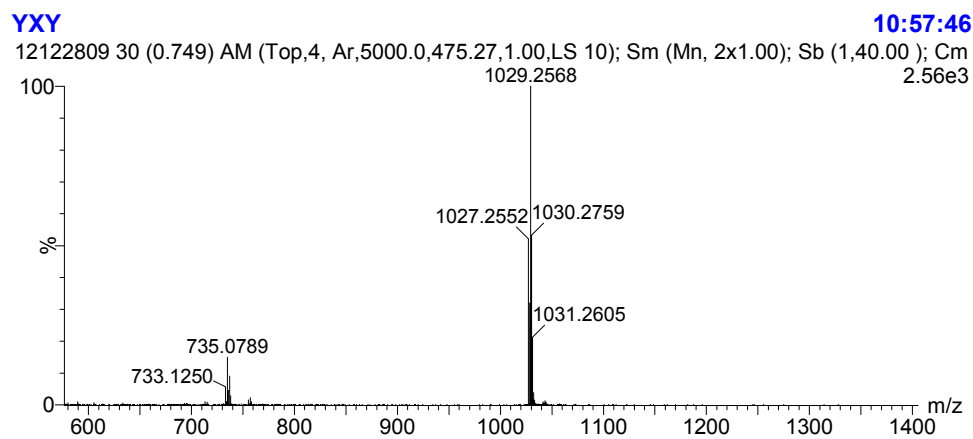


Figure S12. HRMS of **Ir-1**, 25°C.

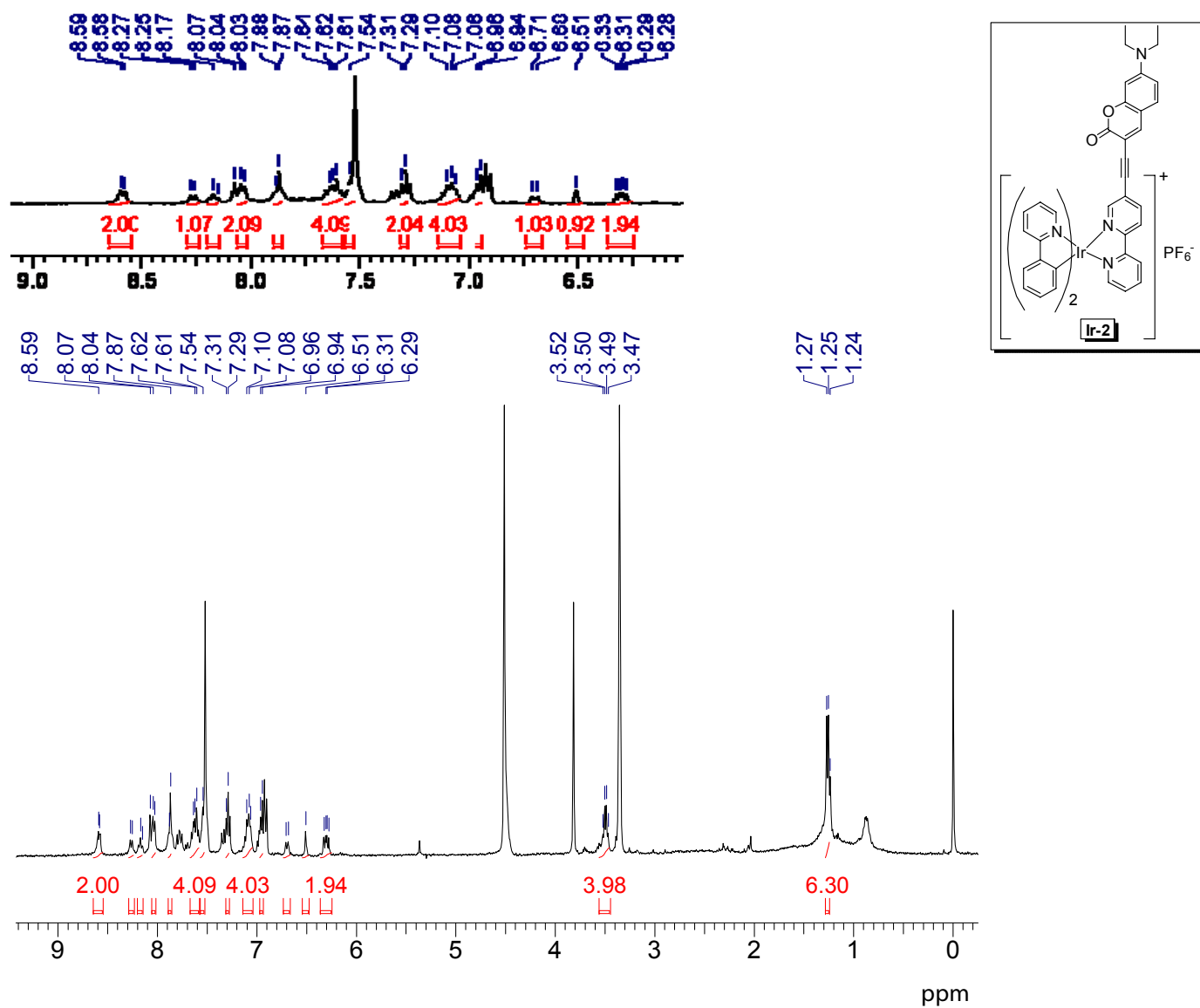


Figure S13. ¹H NMR of Ir-2 in CDCl₃/CD₃OD (400 MHz), 25°C.

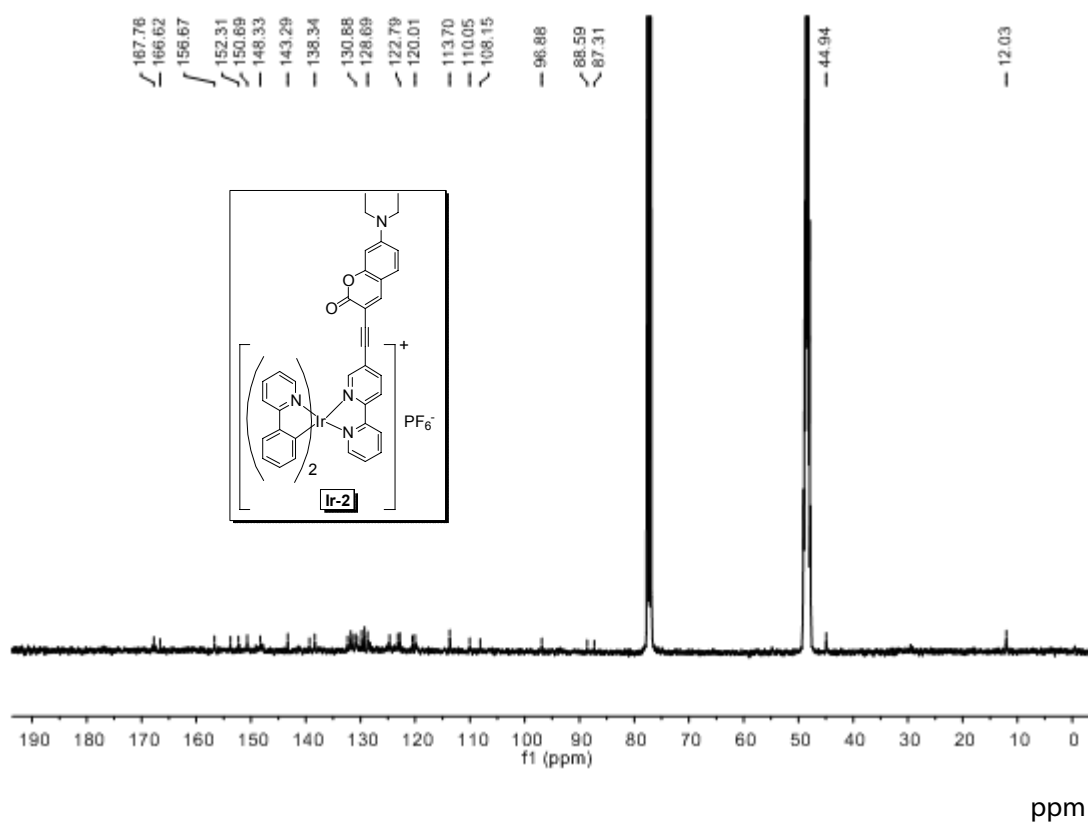


Figure S14. ^{13}C NMR of **Ir-2** ($\text{CDCl}_3/\text{CD}_3\text{OD}$, 100 MHz), 25°C .

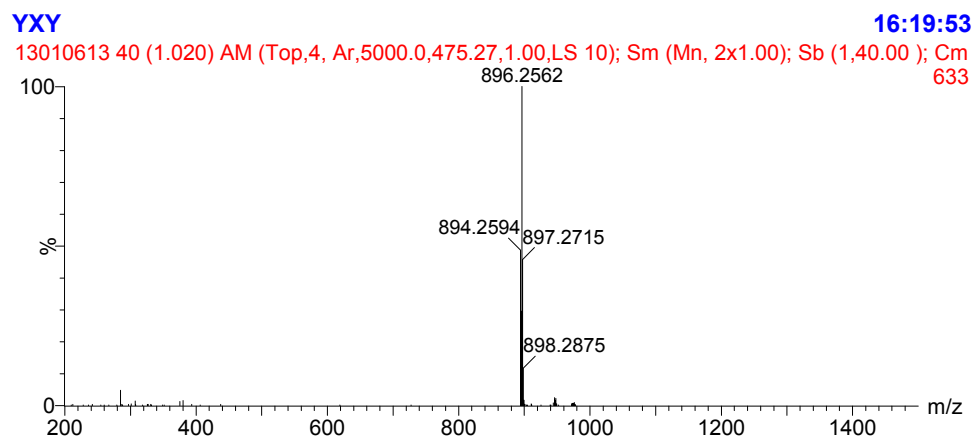


Figure S15. HRMS of **Ir-2**, 25°C .

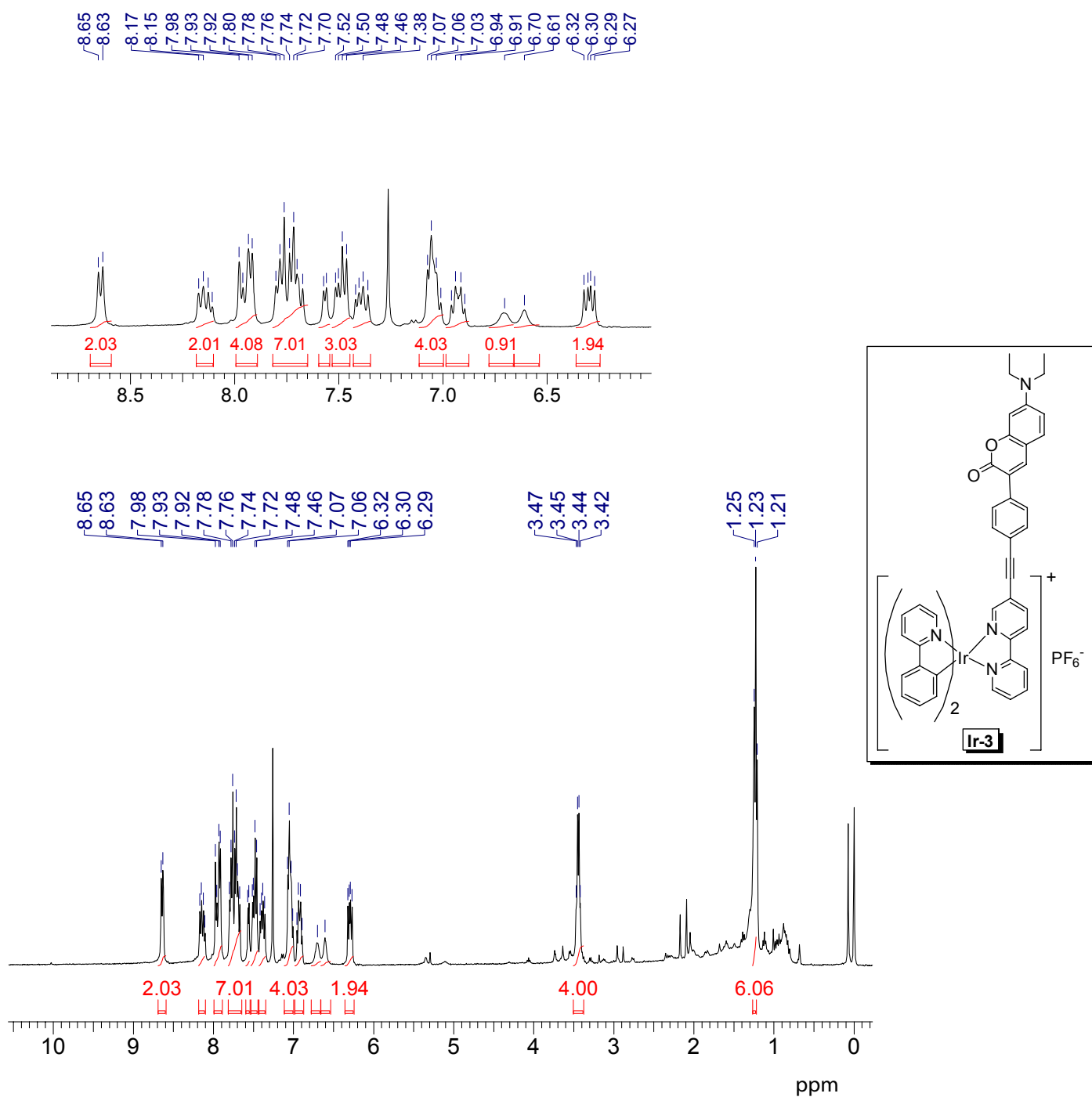


Figure S16. ^1H NMR of Ir-3 in CDCl_3 (400 MHz), 25°C .

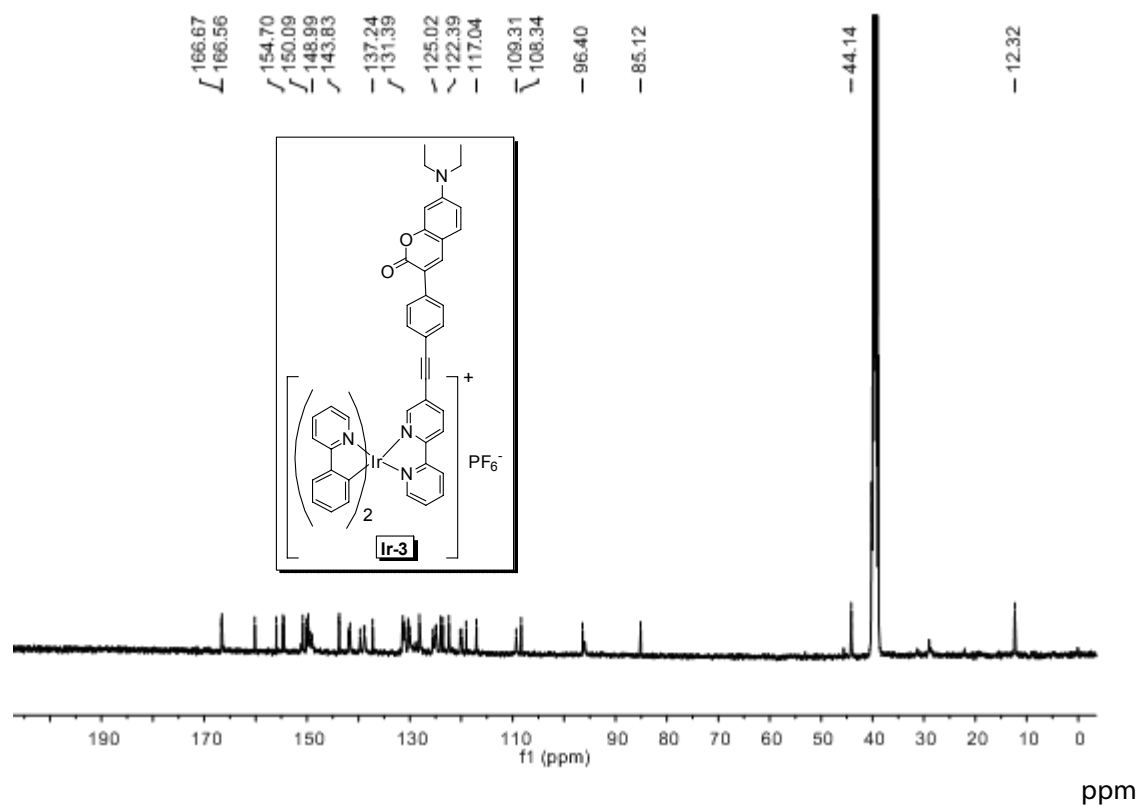


Figure S17. ^{13}C NMR of Ir-3 (DMSO- d_6 , 100 MHz), 25°C.

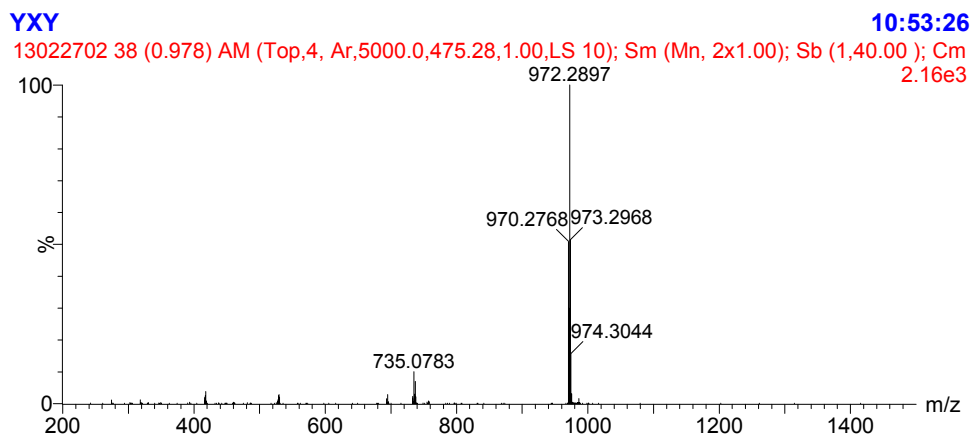


Figure S18. HRMS of Ir-3, 25°C.

2.0 RT and 77 K Spectra data of Ir-3

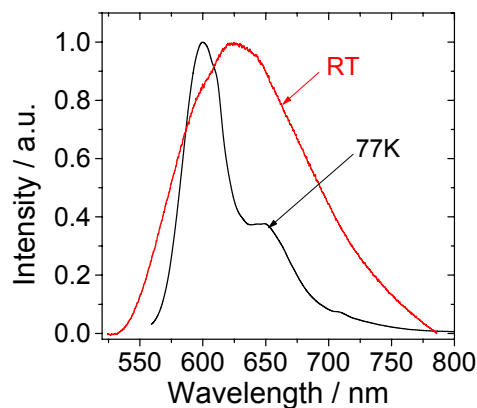


Figure S19. Photoluminescence spectra of the complexes at RT and 77 K. **Ir-3** ($\lambda_{\text{ex}} = 437$ nm). In $\text{C}_2\text{H}_5\text{OH} / \text{CH}_3\text{OH}$ (4:1, v/v), 1.0×10^{-5} M.

3.0 Nanosecond time-resolved transient difference absorption spectrum of Ir-3

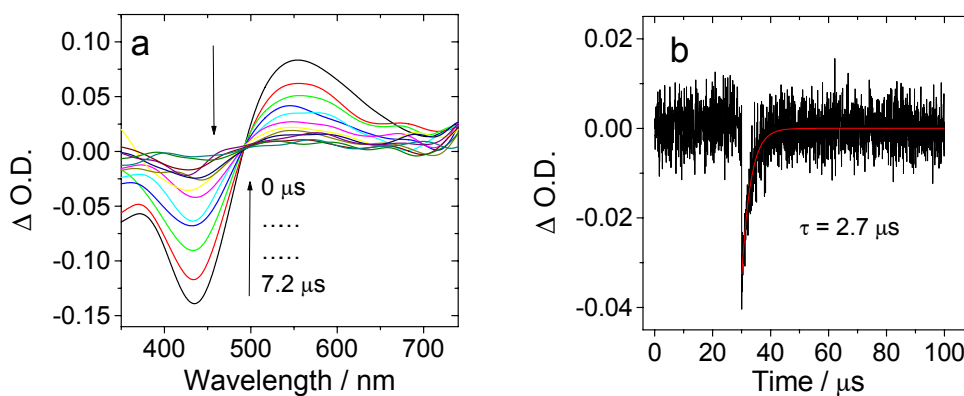


Figure S20. Nanosecond time-resolved transient difference absorption spectra of (a) **Ir-3** in deaerated CH_2Cl_2 at room temperature after pulsed excitation ($\lambda_{\text{ex}} = 532$ nm). Decay trace of (b) **Ir-3** at 450 nm. 1.0×10^{-5} M, 20 °C.

4.0 Delayed fluorescence emission (upconversion) of Ir-3

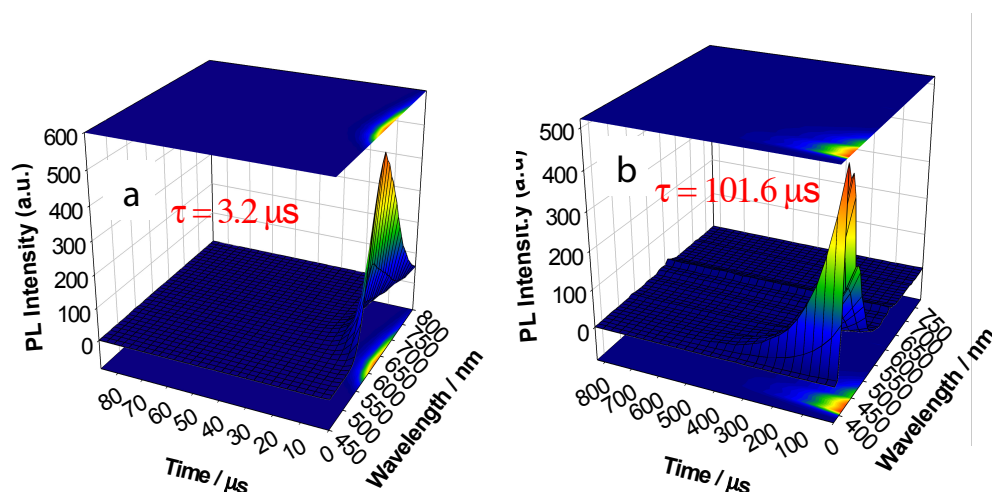


Figure S21. Time-resolved emission spectra (TRES) of Ir(III) complexes alone and the TTA upconversion. With DPA as the triplet acceptor. (e) **Ir-3** alone ($\tau_p = 3.2 \mu\text{s}$). (f) TRES of Ir-3 in the presence of DPA. Upconverted emission in the range of 380 nm –750 nm was observed ($\tau = 101.6 \mu\text{s}$). Note for **Ir-1 –Ir-3** the phosphorescence wavelength are much longer than the upconverted emission wavelength. c [DPA] = $6.0 \times 10^{-5} \text{ M}$; c [sensitizers] = $1.0 \times 10^{-5} \text{ M}$. In deaerated CH_2Cl_2 . Excited with nanosecond pulsed OPO laser synchronized with spectrofluorometer ($\lambda_{\text{ex}} = 473 \text{ nm}$). 20 °C.

5.0 Spin density surfaces of the ligands and DFT calculations on Ir-2 and Ir-3

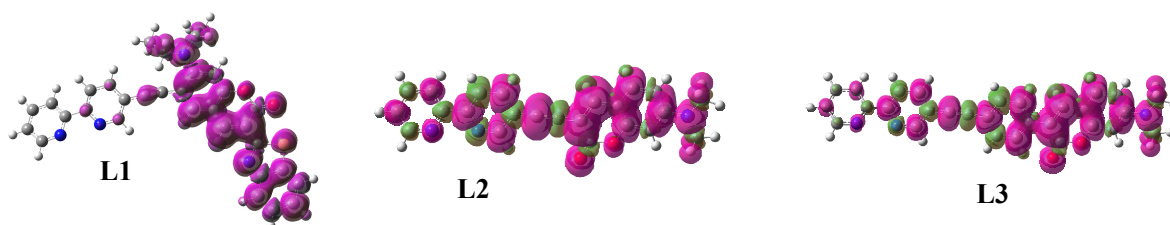


Figure S22. Spin density of the complexes **L1**, **L2** and **L3**. Optimized at B3LYP/6-31G(d) level. CH_2Cl_2 was used as solvent in the calculation.

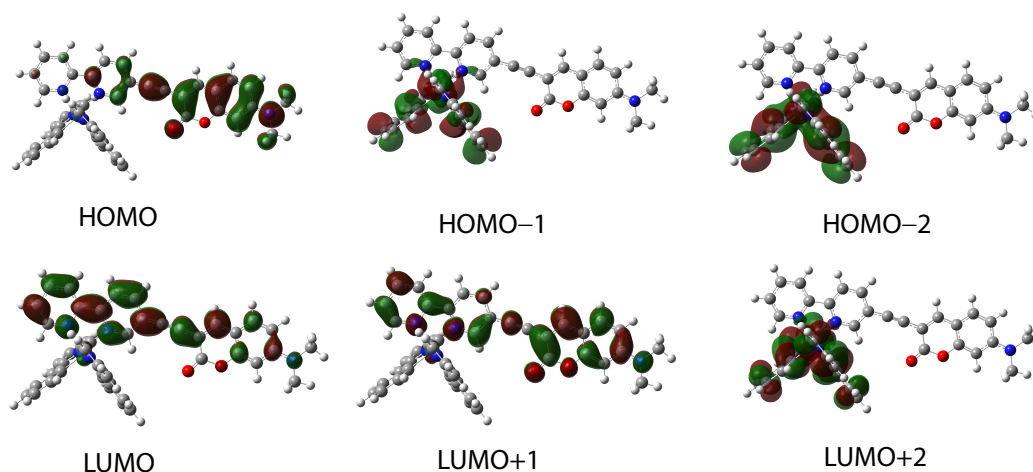


Figure S23. Frontier molecular orbitals of **Ir-2**. CH_2Cl_2 was used as solvent in the calculations. Calculated by DFT at the B3LYP/6-31G/LanL2DZ level using Gaussian 09W.

Table S1. Electronic Excitation Energies (eV) and corresponding Oscillator Strengths (f), main configurations and CI coefficients of the Low-lying Electronically Excited States of complex **Ir-2**. Calculated by TDDFT//B3LYP/6-31G/LanL2DZ, based on the DFT//B3LYP/6-31G/LanL2DZ Optimized Ground State Geometries. CH_2Cl_2 was used as solvent in the calculations.

		TDDFT//B3LYP/6-31G			
	Electronic transition	Energy (eV) ^a	f ^b	Composition ^c	CI ^d
Singlet	$S_0 \rightarrow S_1$	2.95 eV 420 nm	1.9624	H $\rightarrow$ L	0.6113
				H $\rightarrow$ L+1	0.2712
	$S_0 \rightarrow S_3$	3.71 eV 334 nm	0.1727	H-2 $\rightarrow$ L+3	0.2074
				H-1 $\rightarrow$ L+2	0.6473
	$S_0 \rightarrow S_{13}$	4.50 eV 276 nm	0.3060	H-3 $\rightarrow$ L+2	0.4396
				H-2 $\rightarrow$ L+3	0.3608
	$S_0 \rightarrow S_{23}$	4.78 eV 259 nm	0.2484	H-7 $\rightarrow$ L+3	0.3072
				H-5 $\rightarrow$ L+3	0.3907
	$S_0 \rightarrow S_{28}$	5.02 eV 247 nm	0.1310	H-7 $\rightarrow$ L+3	0.2269
Triplet	$T_1 \rightarrow S_0$	1.85 eV 668 nm	0.0000 ^e	H $\rightarrow$ L	0.5145
				H $\rightarrow$ L+1	0.3552
	$T_2 \rightarrow S_0$	2.52 eV 491 nm	0.0000	H-4 $\rightarrow$ L	0.3674
				H $\rightarrow$ L+1	0.4066
	$T_3 \rightarrow S_0$	2.72 eV 455 nm	0.0000	H-3 $\rightarrow$ L+2	0.2648
				H-2 $\rightarrow$ L+3	0.3692
				H-1 $\rightarrow$ L+2	0.3529

^a Only the selected low-lying excited states are presented. ^b oscillator strength. ^c H stands for HOMO and L stands for LUMO. 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.

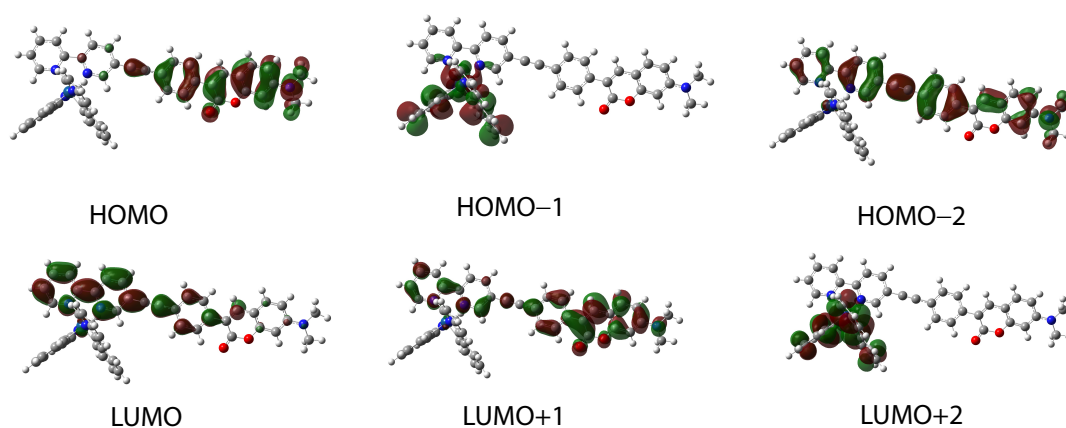


Figure S24. Frontier molecular orbitals of **Ir-3**. Calculated by DFT at the B3LYP/6-31G/LanL2DZ level using Gaussian 09W. CH₂Cl₂ was used as solvent in the calculations.

Table S2. Electronic Excitation Energies (eV) and corresponding Oscillator Strengths (*f*), main configurations and CI coefficients of the Low-lying Electronically Excited States of complex **Ir-3**. Calculated by TDDFT//B3LYP/6-31G/LanL2DZ, based on the DFT//B3LYP/6-31G/LanL2DZ Optimized Ground State Geometries. CH₂Cl₂ was used as solvent in the calculations.

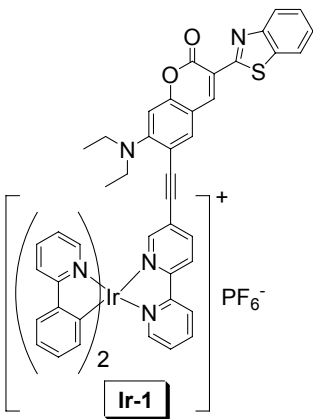
		TDDFT//B3LYP/6-31G			
		Electronic transition	Energy (eV) ^a	<i>f</i> ^b	Composition ^c
					CI ^d
Singlet	$S_0 \rightarrow S_1$	3.08 eV 402 nm	2.4133	H-2→L	0.2674
				H→L	0.4865
				H→L+1	0.3945
	$S_0 \rightarrow S_4$	3.72 eV 333 nm	0.1754	H-3 →L+3	0.2073
				H-1 →L+2	0.6482
	$S_0 \rightarrow S_7$	3.93 eV 316 nm	0.1357	H-8→L	0.3487
				H-5→L	0.3889
				H-3→L	0.3168
	$S_0 \rightarrow S_8$	4.20 eV 295 nm	0.2097	H-2→ L	0.3932
				H→ L	0.4203
Triplet	$S_0 \rightarrow S_{13}$	4.52 eV 274 nm	0.1354	H-3→ L+2	0.2269
				H-8 →L+3	0.2915
				H-5 →L+3	0.4216
				H-1 →L+6	0.1890
				H-2→L	0.3190
				H→L	0.3424
	$T_1 \rightarrow S_0$	1.96 eV 634 nm	0.0000 ^e	H→L+1	0.4262
				H-2→L	0.3891
				H→L+1	0.3925
				H-3→L+3	0.3712
	$T_2 \rightarrow S_0$	2.30 eV 539 nm	0.0000	H-1→L+2	0.3634
	$T_3 \rightarrow S_0$	2.73 eV 455 nm	0.0000		

^a Only the selected low-lying excited states are presented. ^b oscillator strength. ^c H stands for HOMO and L stands for LUMO. 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.

6.0 Optimized geometries of the complexes

Optimized ground state geometry of **Ir-1**

1 1			
C	-1.34402027	1.55906564	-0.03420495
C	-1.54444651	3.94550791	-0.22199212
H	-0.75986741	0.65270198	0.07364955
C	-2.91780127	3.77634711	-0.30643609
H	-1.11207508	4.93873685	-0.26114315
C	-3.47382266	2.49183561	-0.25356512
C	-4.92679730	2.23171532	-0.33835665
C	-5.87145082	3.24236903	-0.55530997
C	-6.62412322	0.62981300	-0.26252209
C	-7.22351324	2.91902870	-0.62242223
C	-7.61043627	1.58809775	-0.47302197
H	-6.86802361	-0.41926441	-0.14099704
H	-7.96084876	3.69705443	-0.79101571
H	-8.65170898	1.28952309	-0.51869591
N	-5.31764899	0.93743082	-0.19391831
C	-0.71261205	2.81753674	-0.08268655
C	-3.24609796	-0.21169673	-2.94736467
C	-4.16715584	-1.60191821	-4.66272279
H	-2.64462349	0.62209813	-2.60863074
C	-4.78371584	-2.35503680	-3.67183788
H	-4.29647133	-1.86474684	-5.70797833
C	-4.61508797	-2.01826696	-2.32129831
H	-5.39525961	-3.20869114	-3.93867992
C	-5.19306127	-2.73058783	-1.17979354
C	-6.02534334	-3.85552240	-1.31260098
C	-5.39180541	-2.86265637	1.22169177
C	-6.53934659	-4.48096851	-0.18087254
H	-6.27581971	-4.24685411	-2.29462873
C	-6.21971226	-3.98070402	1.08664602
H	-5.16201000	-2.50085090	2.21990115
H	-7.18173427	-5.35070326	-0.28363917
H	-6.61669119	-4.46686763	1.97472130
C	-3.37921007	-0.50764516	-4.29604248
H	-2.87579737	0.10658559	-5.03390439
C	-1.31702474	-2.41308621	-0.58595497
C	0.22357653	-3.20472112	1.11771135
C	-2.07373027	-1.71029620	0.36639833
H	-1.60875425	-2.39214308	-1.63218306
C	-0.50680897	-2.52258632	2.08591105
H	1.10217944	-3.77705677	1.40086099
C	-1.64492636	-1.78322978	1.71992550
H	-0.18618428	-2.56947129	3.12281947
C	-2.46351679	-1.04007270	2.68030196
C	-2.24956443	-0.97634989	4.06451883
C	-4.34984755	0.34409537	2.91263283
C	-3.10689463	-0.24029541	4.87189179
H	-1.41256968	-1.50732629	4.50203352
C	-4.18120092	0.43491545	4.28657457
H	-5.16728014	0.84674940	2.41151314
H	-2.94165449	-0.19346682	5.94373632
H	-4.87740229	1.02033311	4.87627584
N	-3.52010690	-0.37033425	2.12593452
C	-0.18561127	-3.14749338	-0.21956124
H	0.37975059	-3.68052873	-0.98041128
Ir	-3.70171227	-0.54947701	0.05733859
N	-2.66877730	1.40326462	-0.11672999
C	-4.86051974	-2.20627473	0.09932410

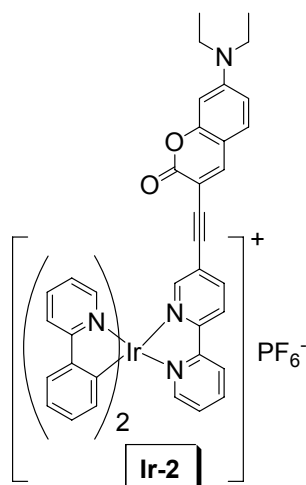


N	-3.84482602	-0.93928654	-1.98349741
H	-5.55964249	4.27190063	-0.67736859
H	-3.55210406	4.64779214	-0.40738980
C	0.69830911	2.90488969	0.01065120
C	1.91268683	2.96377252	0.09800863
C	3.32950308	2.86096761	0.16221217
C	4.24615183	3.98947856	0.13900276
C	5.20588775	1.27493807	0.06262730
C	6.07733474	2.38295499	-0.01662315
C	7.12435400	-0.22224208	-0.06443343
C	8.01232930	0.93308791	-0.13760544
C	5.62555586	3.68776063	0.01601318
H	6.36993700	4.47004077	-0.01755663
C	5.76764280	-0.02819091	0.03182858
H	5.11744344	-0.89602012	0.08590425
C	3.83493565	1.55631199	0.14528075
H	3.13026844	0.73114492	0.16837594
N	3.83892021	5.29698817	0.20213824
C	4.77745797	6.38625487	-0.12599552
H	4.30059219	7.31354354	0.19749462
H	5.69190145	6.29517754	0.47368245
C	5.10571801	6.48647337	-1.61818547
H	5.79654721	7.31965321	-1.78701763
H	5.57708735	5.57494645	-1.99768368
H	4.19682743	6.66794486	-2.20094467
C	1.60785395	6.43347309	-0.01356905
H	0.74024913	6.75518508	0.57401668
H	2.03763285	7.32447126	-0.48390132
H	1.26724971	5.75935197	-0.80512718
C	2.61718178	5.73560266	0.89914974
H	2.92892357	6.42015074	1.69924736
H	2.15889275	4.87764646	1.38779819
O	7.42515417	2.18931344	-0.11022474
O	9.22637187	0.90400827	-0.22206977
C	7.68098369	-1.57466087	-0.09441914
C	7.67757457	-3.79785645	-0.07287945
C	9.07616596	-3.60664109	-0.19285850
C	9.95623096	-4.69156693	-0.25706252
C	9.42045937	-5.97630935	-0.19970788
C	8.03200908	-6.17898726	-0.07986950
C	7.15622068	-5.10223827	-0.01599243
H	11.02738351	-4.54036127	-0.34923145
H	10.08540107	-6.83378886	-0.24810774
H	7.64219119	-7.19190802	-0.03721031
H	6.08409773	-5.24687622	0.07620726
N	6.92870082	-2.63922006	-0.02118579
S	9.42976644	-1.89148124	-0.23711866

Optimized ground state geometry of **Ir-2**

1 1

C	0.18997500	1.15995800	0.04735700
C	0.74925800	3.49993200	0.24438500
H	0.46249500	0.11705100	-0.04612800
C	-0.61131700	3.77949100	0.28756700
H	1.47709600	4.29985000	0.30703900
C	-1.55299500	2.74137100	0.20867100
C	-3.00879000	2.94621400	0.24876100
C	-3.61608000	4.21158000	0.29991300
C	-5.13106000	1.91422400	0.26822100
C	-5.00652600	4.31397500	0.33701400
C	-5.77890900	3.14668400	0.32206500
H	-5.67403900	0.97842800	0.25241000



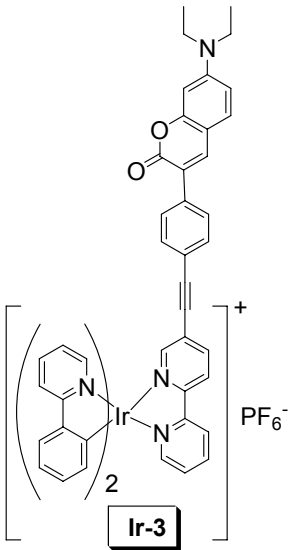
H	-5.47949400	5.28852000	0.37463500
H	-6.86080300	3.18679400	0.34889500
N	-3.77971500	1.81169800	0.23376200
C	1.18769000	2.16099100	0.12158700
C	-2.29862900	0.64920700	-2.88839600
C	-3.66886800	-0.10890600	-4.70847700
H	-1.46001100	1.19769500	-2.48358400
C	-4.44571400	-0.81100600	-3.79206400
H	-3.90778900	-0.14261200	-5.76548100
C	-4.13605800	-0.77581100	-2.42089000
H	-5.29021600	-1.39679000	-4.13074200
C	-4.85182400	-1.47494500	-1.35759300
C	-5.99394500	-2.26864600	-1.58177600
C	-4.96655300	-1.97198100	1.00856100
C	-6.61879000	-2.91003200	-0.51440600
H	-6.39668000	-2.39097800	-2.58258700
C	-6.10129800	-2.76013800	0.78086200
H	-4.58465700	-1.88501000	2.02019500
H	-7.49605600	-3.52418800	-0.68592300
H	-6.58176700	-3.26470100	1.61392500
C	-2.57234500	0.63581000	-4.25034800
H	-1.94008000	1.18908500	-4.93343100
C	-1.02840800	-2.40102200	-1.15806000
C	0.30485500	-3.90991100	0.21109300
C	-1.48344100	-1.71177800	-0.02030500
H	-1.36224200	-2.09943700	-2.14507200
C	-0.13424200	-3.25252600	1.35748000
H	0.99480200	-4.74231400	0.29104800
C	-1.02196700	-2.16382600	1.25029800
H	0.22006600	-3.58622600	2.32775900
C	-1.52850800	-1.42411500	2.40099700
C	-1.24473600	-1.69513100	3.75206400
C	-2.91985700	0.37615700	3.07260800
C	-1.80883600	-0.92039500	4.76016300
H	-0.58663400	-2.51723700	4.00075300
C	-2.66594400	0.13581900	4.41676100
H	-3.57804500	1.17157700	2.75306000
H	-1.59003600	-1.13467600	5.80023800
H	-3.12911600	0.75654100	5.17356600
N	-2.36759500	-0.37548300	2.08600400
C	-0.14563900	-3.48223500	-1.04612200
H	0.19470700	-3.99358800	-1.94139300
Ir	-2.69818600	-0.08263800	0.05482800
N	-1.12522800	1.44144800	0.08763000
C	-4.31477400	-1.30876300	-0.04725700
N	-3.05631900	-0.03252600	-1.99185200
H	-3.01137600	5.10893200	0.30470400
H	-0.93710800	4.80670800	0.38852000
C	5.01507400	0.88226600	-0.04432300
C	6.14662700	1.68011500	-0.00286600
H	6.02921600	2.75614400	0.08475800
O	4.22291800	-1.39395900	-0.20641900
C	5.13947100	-0.57723400	-0.16198000
O	6.46731500	-1.07879600	-0.22982000
C	7.59566300	-0.27009800	-0.18812100
C	8.82646600	-0.89621100	-0.26361900
H	8.84471500	-1.97227600	-0.35085500
C	7.45214000	1.13616000	-0.07222600
C	8.64638300	1.90161800	-0.03540500
H	8.57411000	2.98128800	0.05243100
C	9.88675500	1.30512800	-0.10864100
H	10.77153600	1.92531000	-0.07675800
C	10.01332200	-0.11904400	-0.22529200
N	11.24809200	-0.71387800	-0.29712500
C	11.35817600	-2.17417700	-0.41128100

H	12.41120700	-2.45132000	-0.44664300
H	10.90026500	-2.67729900	0.44924300
H	10.87569000	-2.54138400	-1.32551300
C	12.47381100	0.09505500	-0.26088900
H	12.55564400	0.65999500	0.67577700
H	13.33685700	-0.56598700	-0.33325300
H	12.51472700	0.80088800	-1.09950200
C	3.70596700	1.40263100	0.02058200
C	2.54889500	1.79481100	0.07117500

Optimized ground state geometry of Ir-3

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C	-1.28218900	1.11267500	-0.14158700
C	-0.71839300	3.44982400	-0.33883100
H	-1.01820500	0.06716200	-0.05431900
C	-2.07728200	3.73621100	-0.35280000
H	0.01274400	4.24622100	-0.40644900
C	-3.02179300	2.70121400	-0.26394300
C	-4.47674500	2.91334100	-0.27966300
C	-5.07812300	4.16960700	-0.45941300
C	-6.60427800	1.90506000	-0.11864900
C	-6.46840500	4.28026500	-0.46384800
C	-7.24638200	3.12964800	-0.29061300
H	-7.15248900	0.98222500	0.01683800
H	-6.93680600	5.24767900	-0.60357000
H	-8.32834300	3.17592700	-0.29060500
N	-5.25294600	1.79518000	-0.10937900
C	-0.28127900	2.10755500	-0.23382900
C	-3.75144700	0.07084900	-2.94724100
C	-5.12494500	-0.98895900	-4.60731200
H	-2.90809700	0.67468400	-2.64419300
C	-5.91261400	-1.50548700	-3.58318700
H	-5.36131900	-1.20974500	-5.64212000
C	-5.60682500	-1.22602600	-2.23937200
H	-6.76338500	-2.13285200	-3.81493600
C	-6.33426200	-1.71384900	-1.07118100
C	-7.47993800	-2.52907800	-1.15572900
C	-6.47004000	-1.76716600	1.34478700
C	-8.11715900	-2.96030100	0.00575000
H	-7.87530200	-2.83144100	-2.12055100
C	-7.60871800	-2.57745300	1.25579300
H	-6.09567000	-1.49787000	2.32675000
H	-8.99708900	-3.59103300	-0.05779800
H	-8.09904300	-2.91761200	2.16309400
C	-4.02076700	-0.18621900	-4.28567900
H	-3.38011300	0.22756700	-5.05433100
C	-2.53190400	-2.62415900	-0.66090400
C	-1.26484800	-3.89161100	0.98734500
C	-2.98647600	-1.72763100	0.32299000
H	-2.84575000	-2.50187300	-1.69201700
C	-1.70013600	-3.02231600	1.98518500
H	-0.61013600	-4.72018700	1.23419500
C	-2.55360900	-1.94874300	1.66304100
H	-1.37534500	-3.18491900	3.00825300
C	-3.05649100	-0.99717100	2.64919900
C	-2.79146100	-1.01652700	4.03023900
C	-4.40722200	0.92865800	2.95185400
C	-3.34430700	-0.05310900	4.86791900
H	-2.15656000	-1.79221600	4.43787400
C	-4.17005500	0.93978600	4.32053700
H	-5.04132000	1.66591900	2.48026300
H	-3.14025300	-0.07339100	5.93252000



H	-4.62250700	1.70339400	4.94079200
N	-3.86781200	-0.00901600	2.13148300
C	-1.68325200	-3.68965300	-0.33619200
H	-1.35030500	-4.36883900	-1.11535400
Ir	-4.17940700	-0.09968700	0.07799400
N	-2.59750900	1.39972000	-0.15705800
C	-5.80565000	-1.31309500	0.19082400
N	-4.52079200	-0.42816100	-1.94604100
H	-4.46893800	5.05250800	-0.60135300
H	-2.40001100	4.76660200	-0.42800900
C	7.83519100	0.03074200	-0.25205000
C	8.78774900	0.91884500	0.20483500
H	8.47041400	1.87456700	0.61077500
O	7.56483900	-2.20989400	-1.14232300
C	8.27068600	-1.28324400	-0.73614300
O	9.67315200	-1.52375100	-0.74496700
C	10.61414900	-0.60999600	-0.29620400
C	11.94742800	-0.98179800	-0.35172500
H	12.18769700	-1.95849100	-0.74477000
C	10.18181200	0.64003700	0.20124200
C	11.18480700	1.52747800	0.66227300
H	10.89004900	2.49623300	1.05447300
C	12.52200800	1.18738500	0.61907000
H	13.25617000	1.89511300	0.97833900
C	12.94254900	-0.08285100	0.10667000
N	14.27612600	-0.42109300	0.06298700
C	14.68662200	-1.72512300	-0.46935000
H	15.77332900	-1.79947100	-0.43508200
H	14.26776300	-2.55015100	0.12098400
H	14.36770200	-1.85004500	-1.51181400
C	15.29982900	0.51083000	0.54864600
H	15.15805400	0.74890700	1.61047700
H	16.28122500	0.05087300	0.43421700
H	15.29566300	1.44902600	-0.02081500
C	1.08593000	1.75842100	-0.22321400
C	2.27161600	1.45626300	-0.22256800
C	3.64393700	1.09960800	-0.22919300
C	4.04054000	-0.25554600	-0.15319100
C	4.65041600	2.08858300	-0.33139400
C	5.38448200	-0.60908800	-0.17332100
H	3.28206100	-1.02733300	-0.07977700
C	5.99118500	1.72874600	-0.35191500
H	4.36635700	3.13229200	-0.41157300
C	6.39747400	0.37524400	-0.26296500
H	5.66408800	-1.65203400	-0.13827700
H	6.73605900	2.50717700	-0.47323800