

Electronic Supplementary Information for:

**Green light-excitable naphthalenediimide acetylide-containing cyclometalated
Ir(III) complex with long-lived triplet excited states as triplet photosensitizer for
triplet-triplet annihilation upconversion**

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1. NMR and HR-MS spectra

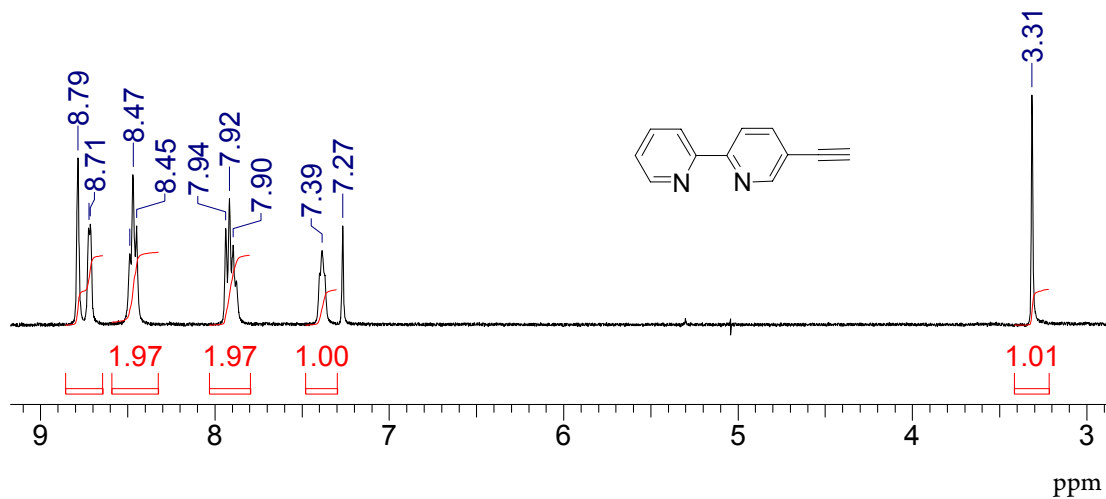


Fig. S1 ^1H NMR of 4 (400 MHz, CDCl_3).

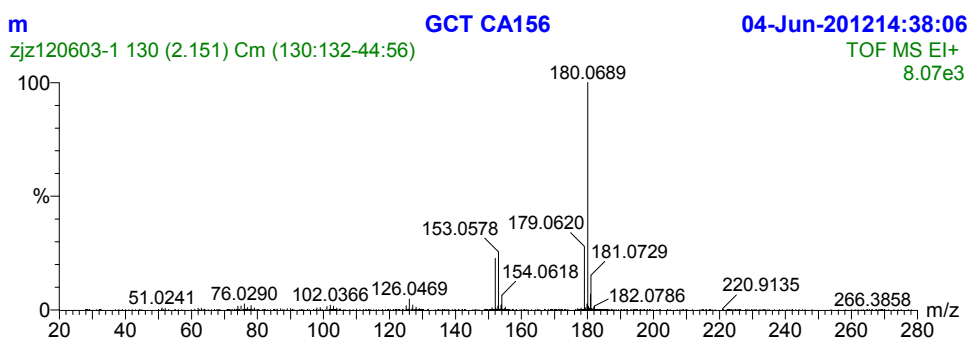


Fig. S2 TOF HRMS ESI of 4.

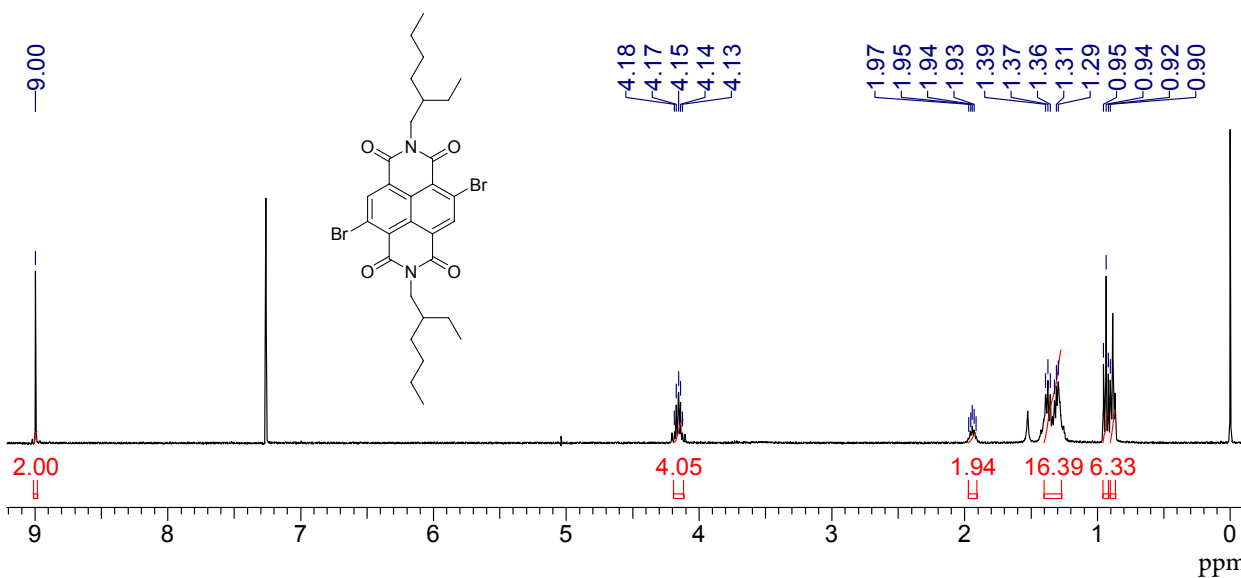


Fig. S3 ^1H NMR of 7 (400 MHz, CDCl_3).

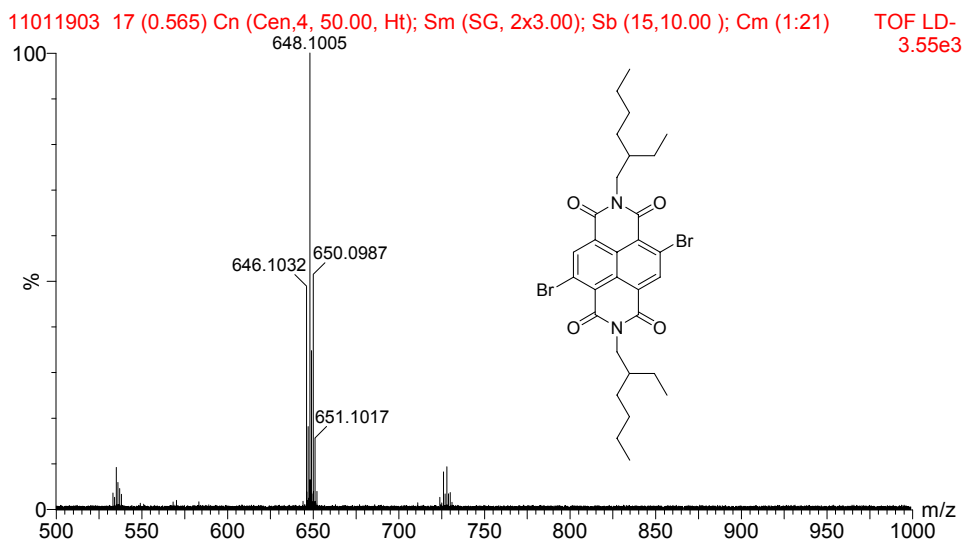


Fig. S4 TOF HRMS ESI of 7.

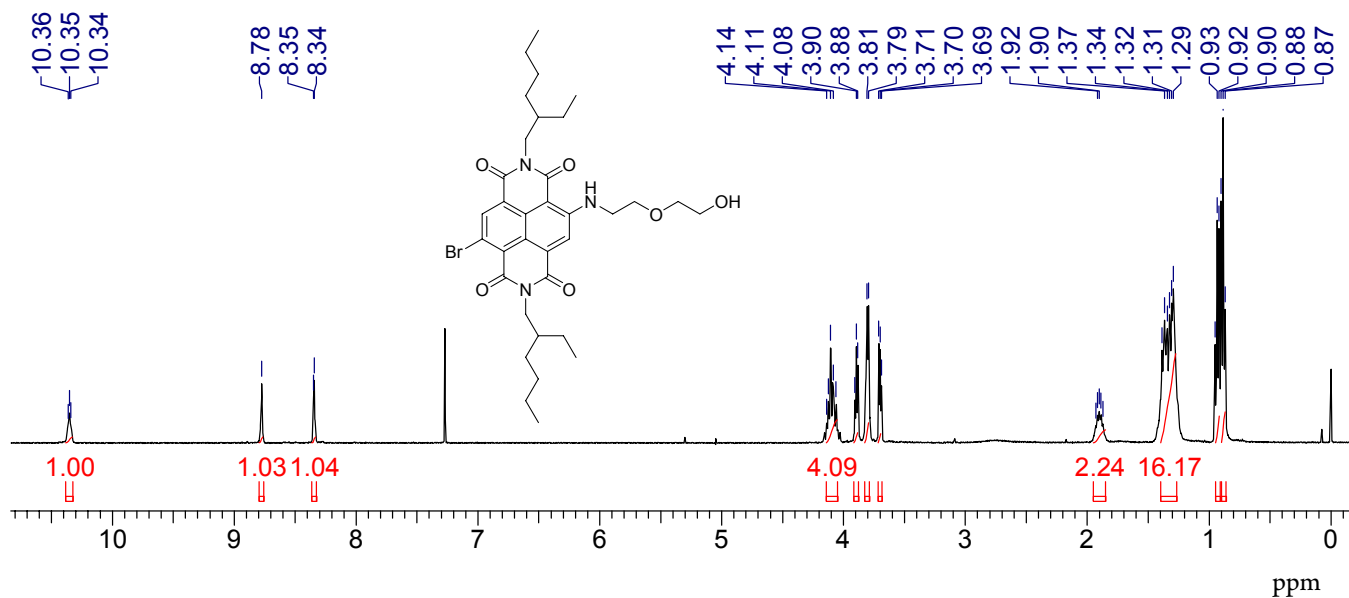


Fig. S5 ^1H NMR of 8 (400 MHz, CDCl_3).

11011706 13 (0.350) AM (Cen,6, 80.00, Ar,5000.0,429.22,0.70,LS 10); Sm (SG, 2x3.00); Sb (1.40, 3.62e4

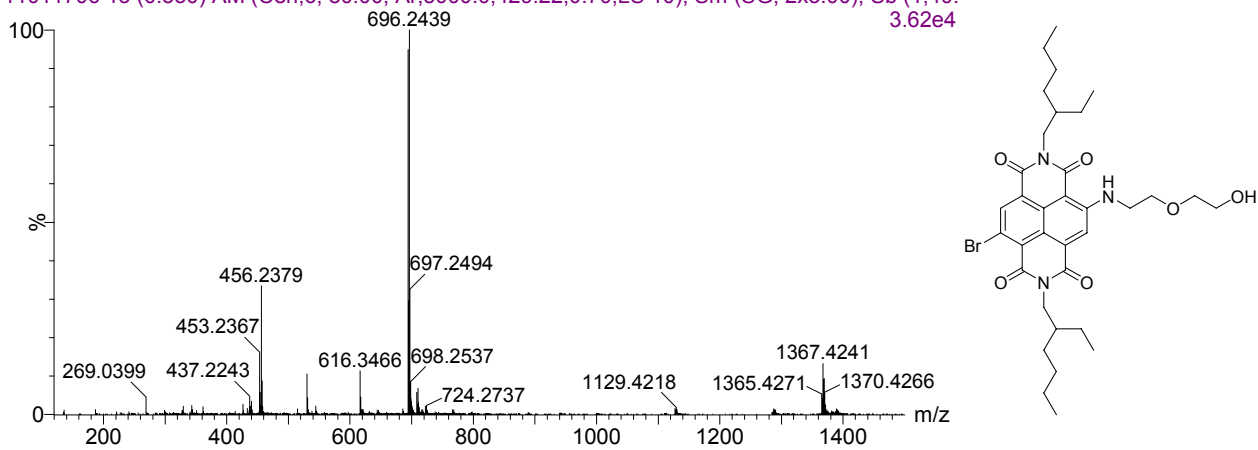


Fig. S6 TOF HRMS ESI of 8.

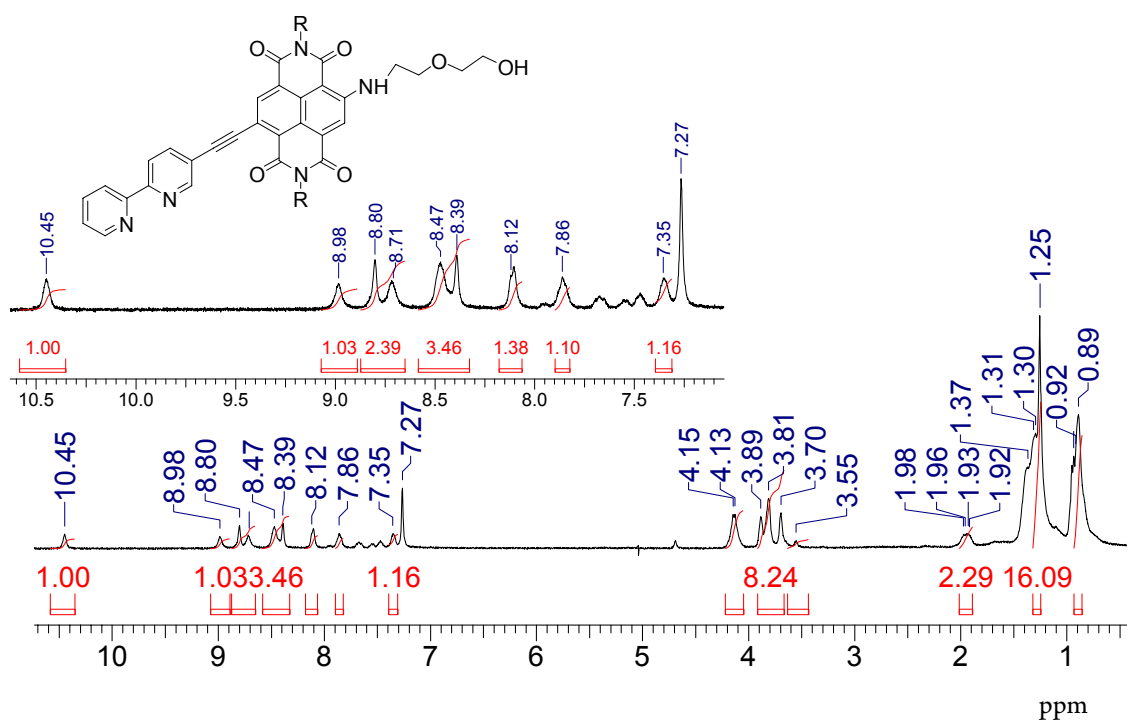


Fig. S7 ¹H NMR of 9 (400 MHz, CDCl₃).

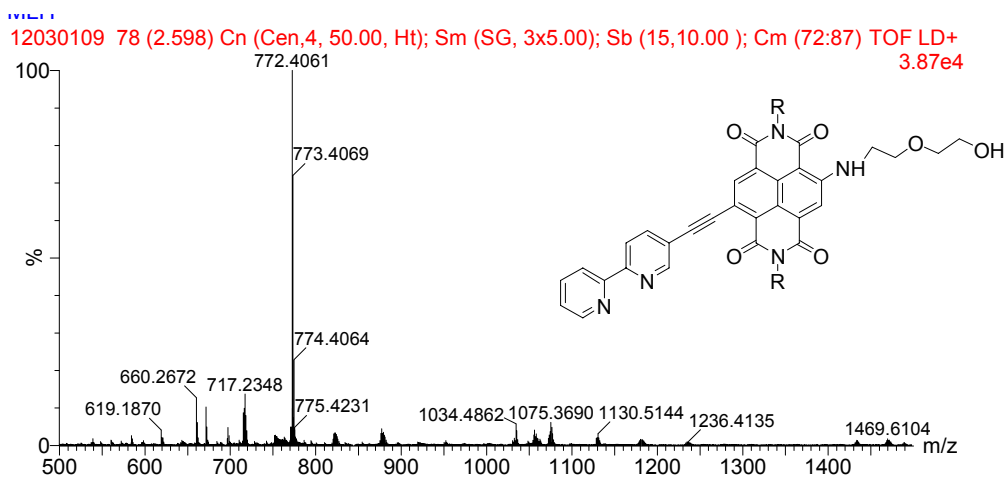


Fig. S8 TOF HRMS ESI of 9.

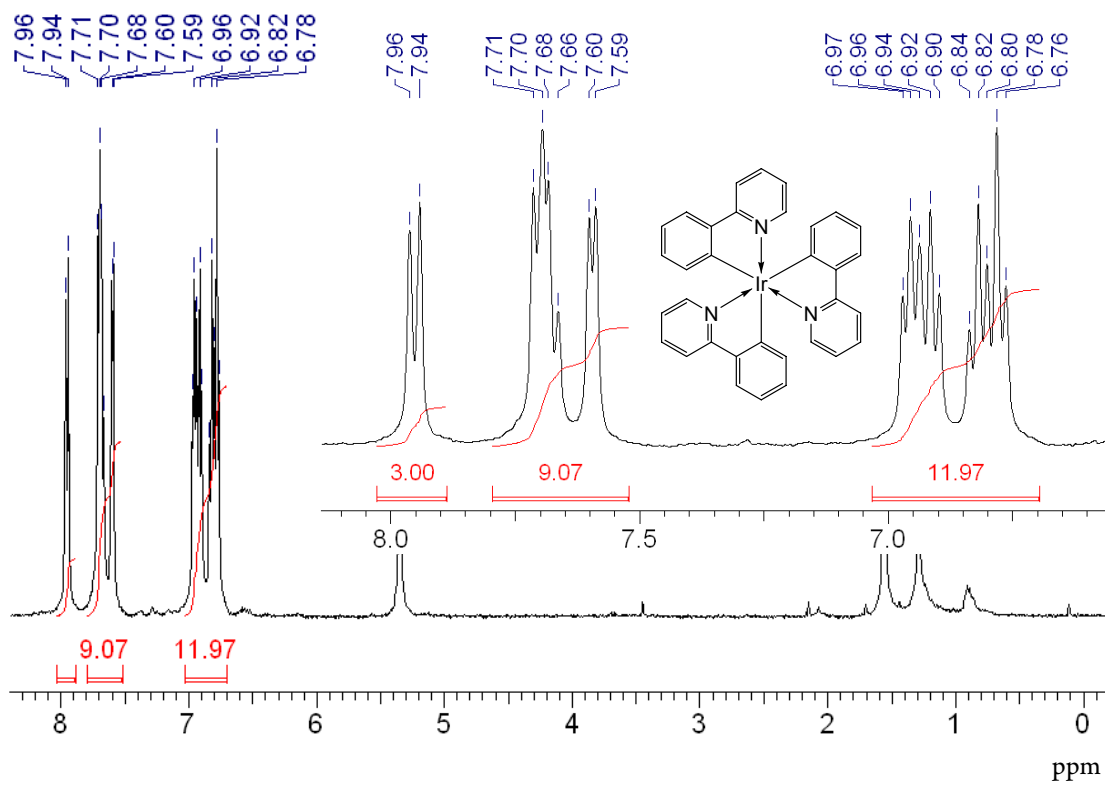


Fig. S9 ^1H NMR of Ir-2 (400 MHz, CDCl_3).

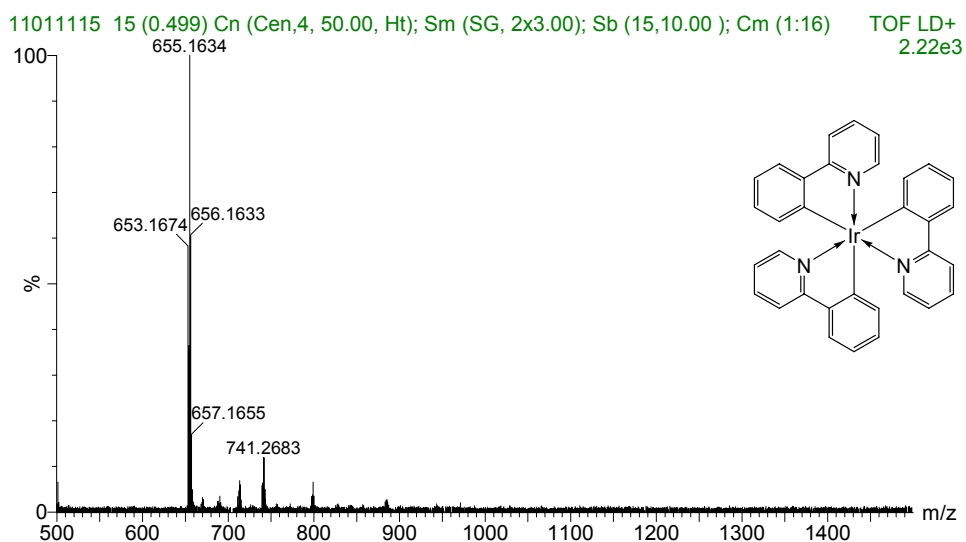


Fig. S10 TOF HRMS ESI of Ir-2.

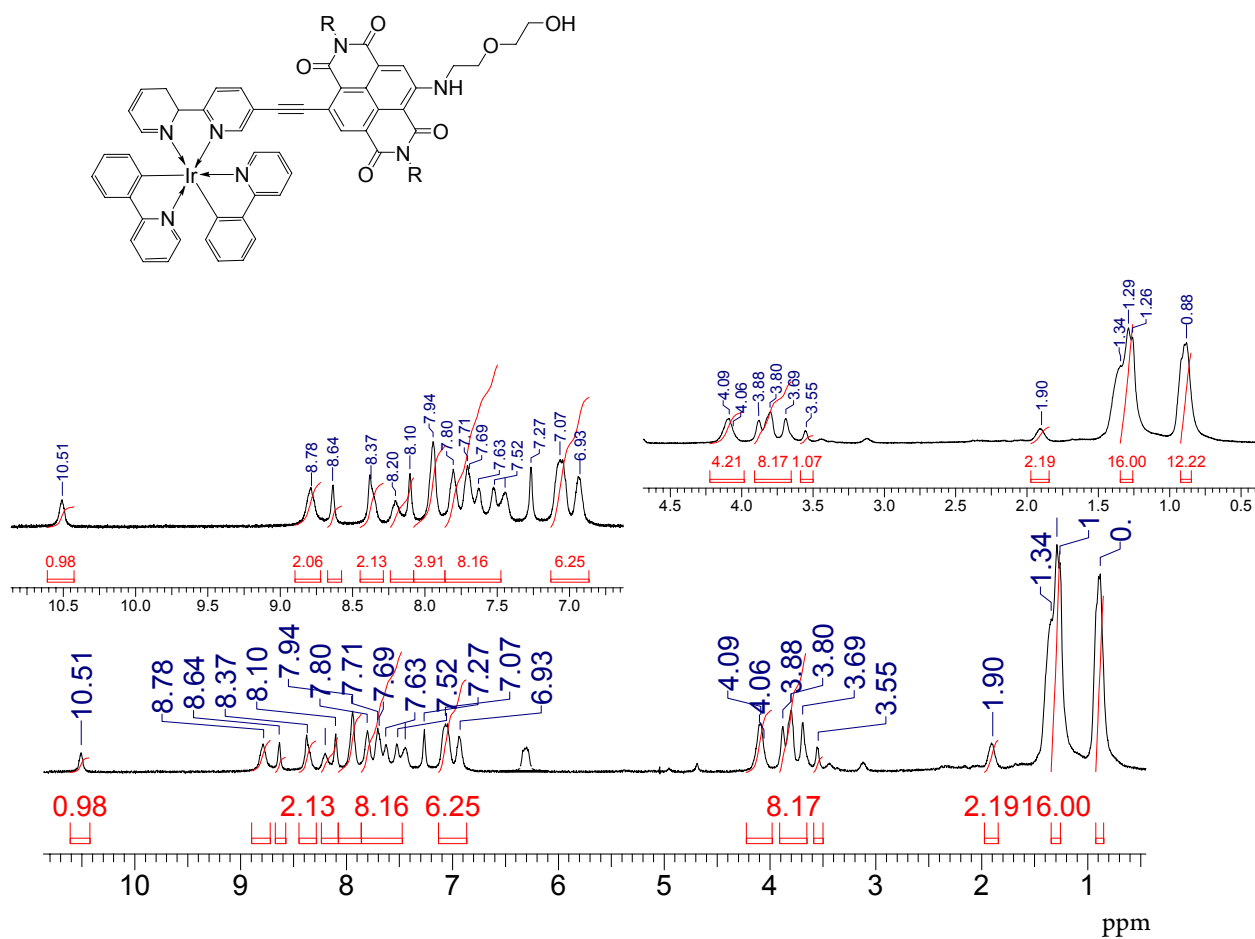


Fig. S11 ^1H NMR of Ir-1 (400 MHz, CDCl_3).

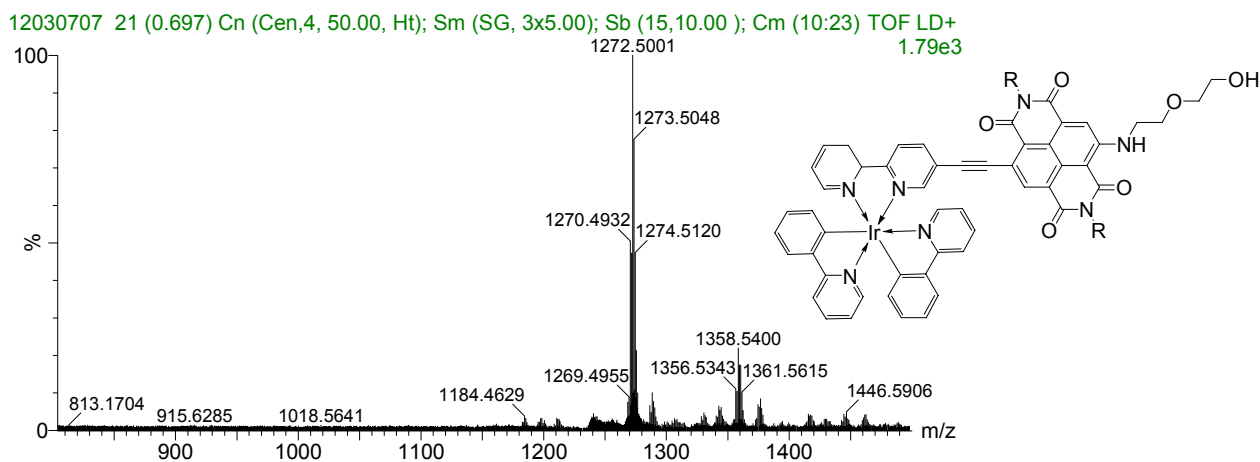


Fig. S12 TOF HRMS ESI of Ir-1.

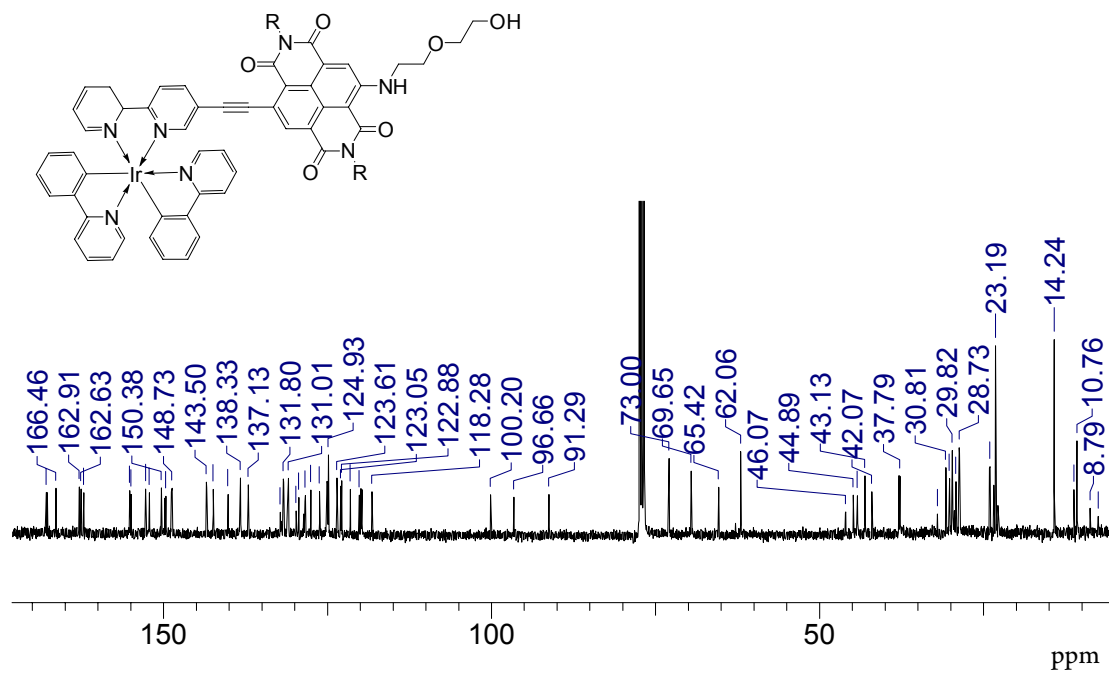


Fig. S13 ^{13}C NMR of Ir-1 (100 MHz, CDCl_3)

2. Calculation details

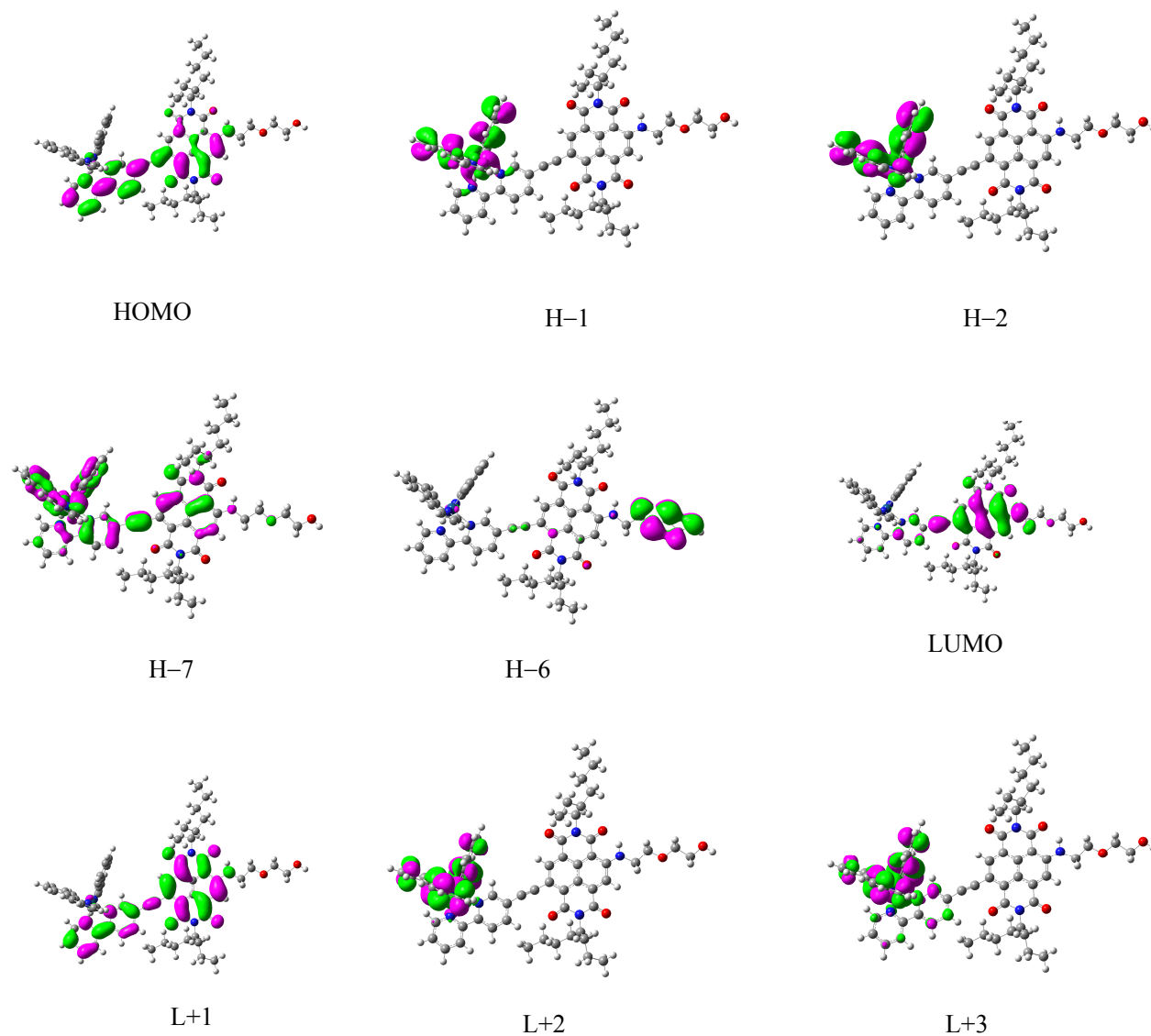


Fig. S14 Frontier molecular orbitals of **Ir-1**. Calculation was performed at B3LYP/6-31G(d)/LanL2DZ level with Gaussian 09W.

Table S1. Selected Electronic Excitation Energies (eV) and corresponding Oscillator Strengths (f), Main Configurations and CI Coefficients of the Low-lying Electronically Excited States of **Ir-1**.^[a]

electronic		TDDFT//B3LYP/6-31G(d)			
transitions		Energy (eV) ^[b]	f ^[c]	composition ^[d]	CI ^[e]
singlet	$S_0 \rightarrow S_1$	2.04 eV (607 nm)	0.0008	H→L	0.6517
				H→L+1	0.2679
	$S_0 \rightarrow S_2$	2.27 eV (545 nm)	0.07364	H-1→L	0.70256
	$S_0 \rightarrow S_4$	2.71 eV (457 nm)	0.2736	H-2→L	0.1011
				H-1→L+1	0.6868
	$S_0 \rightarrow S_{14}$	3.20 eV (387 nm)	0.2000	H-8→L	0.1590
				H-7→L	0.3925
				H-6→L	0.4238
				H-6→L+1	0.1199
				H-5→L+1	0.1115
				H-4→L	0.1096
				H-2→L+1	0.1644
				H→L+2	0.1174
	H→L+3	0.1895			
triplet	$S_0 \rightarrow T_1$	1.56 eV (796 nm)	0.0000	H-1→L	0.6707
				H→L+1	0.1802
	$S_0 \rightarrow T_2$	2.03 eV (611 nm)	0.0000	H→L	0.6408

[a] Calculated by TDDFT//B3LYP/6-31G(d)/LanL2DZ, based on the optimized ground state geometries. [b]

Only the low-lying excited states and some allowed transitions were presented.

[c] Oscillator strength.

[d] Only the main configurations with interaction (CI) coefficients are presented.

[e] CI coefficients are in absolute value.

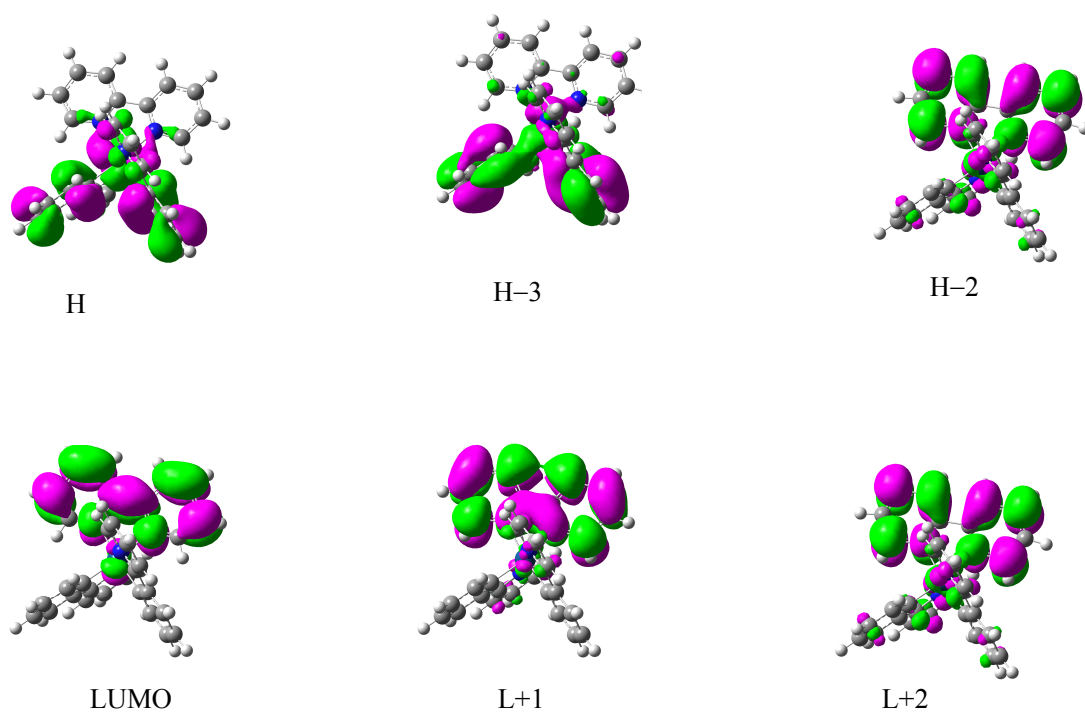


Fig. S15 Frontier molecular orbitals of **Ir-2**. Calculation was performed at B3LYP/6-31G(d)/LanL2DZ level with Gaussian 09W.

Table S2. Selected Electronic Excitation Energies (eV) and corresponding Oscillator Strengths (f), Main Configurations and CI Coefficients of the Low-lying Electronically Excited States of **Ir-2**.^[a]

electronic		TDDFT//B3LYP/6-31G(d)			
transitions		Energy (eV) ^[b]	f ^[c]	composition ^[d]	CI ^[e]
singlet	$S_0 \rightarrow S_1$	2.45eV (505 nm)	0.0002	H→L	0.7026
	$S_0 \rightarrow S_2$	3.11eV (399 nm)	0.0736	H→L+1	0.6956
	$S_0 \rightarrow S_6$	3.40eV (365 nm)	0.0708	H-5→L	0.1777
				H-3→L	0.6509
				H-1→L	0.144273
	$S_0 \rightarrow S_{20}$	4.11eV (302 nm)	0.1034	H-6→L	0.1592
				H-4→L+1	0.1396
				H-4→L+3	0.1484
				H-3→L+2	0.4989
				H-2→L+1	0.1459
H-2→L+2				0.3250	
triplet	$S_0 \rightarrow T_1$	2.42 eV(512 nm)	0.0000	H-1→L+2	0.2015
				H→L	0.6974

[a] Calculated by TDDFT//B3LYP/6-31G(d)/ LanL2DZ, based on the optimized ground stated geometries.

[b] Only the low-lying excited states and some allowed transitions were presented.

[c] Oscillator strength.

[d] Only the main configurations with interaction (CI) coefficients are presented .

[e] CI coefficients are in absolute value.

3. The emission spectra at 77 K

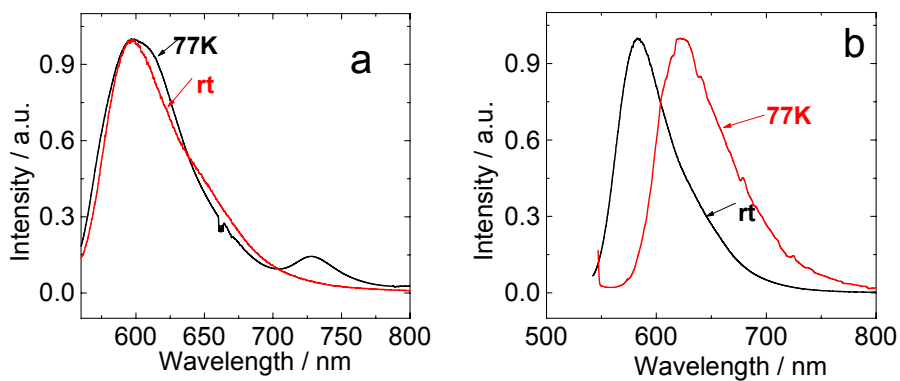


Fig. S16 Photoluminescence spectra of (a) **Ir-1** ($\lambda_{\text{ex}} = 550$ nm) and (b) ligand **9** ($\lambda_{\text{ex}} = 550$ nm) at RT and 77 K (in EtOH–MeOH, 4 : 1, v/v). Please note that due to technical reasons, the solutions were not fully de-aerated. However, this situation does not have any negative impact on the experiments because

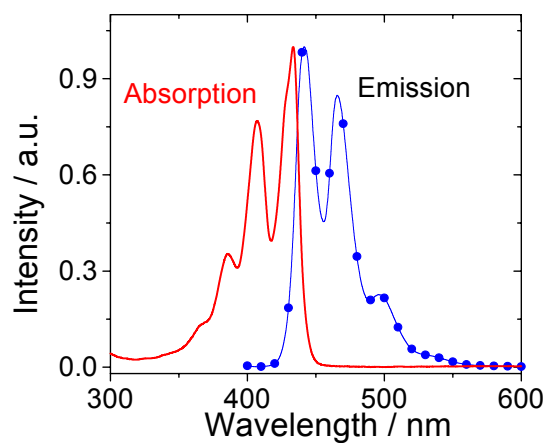


Fig. S17 Absorption and fluorescence spectra of **perylene**, $\lambda_{\text{ex}} = 390$ nm, $c = 1.0 \times 10^{-5}$ M, 20 °C.

4. The excitation spectra and UV-vis absorption spectra

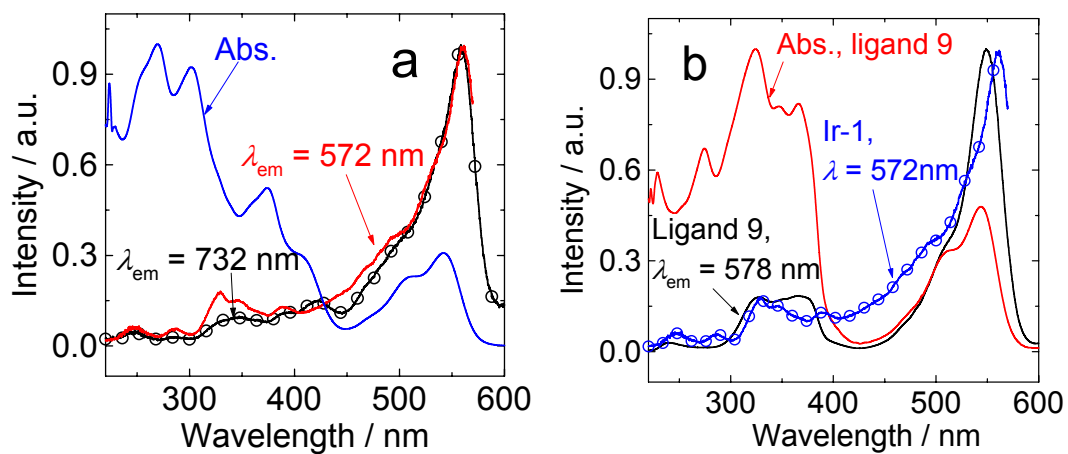


Fig. S18 Normalized UV-Vis absorption and excitation spectra of (a) complex **Ir-1** (with 572 and 732 nm as the emission wavelength, respectively) and (b) ligand **9** and complex **Ir-1** (with 572 nm as the emission wavelength). $c = 1.0 \times 10^{-5}$ M in deaerated CH_2Cl_2 , 20°C.

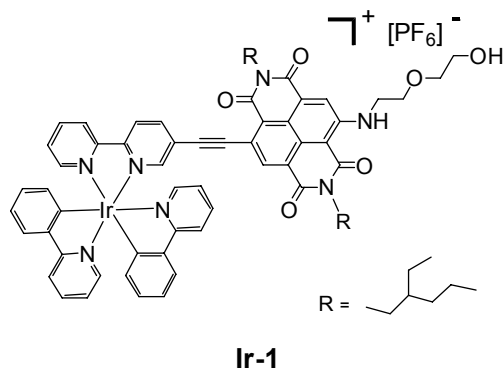
5. Z-matrix

Compound Ir-1. Ground state geometry.

Symbolic Z-matrix:

Charge = 1 Multiplicity = 1

1 1			
C	0.68099224	-1.04947422	-0.38614853
C	-0.52614485	-1.20471232	-0.40403077
C	-2.91973708	-0.63572165	-0.30617058
C	-2.26639595	-2.92537639	-0.64648467
H	-2.69304227	0.41340966	-0.15269765
C	-3.61241219	-3.25334716	-0.69114974
H	-1.49718079	-3.68189888	-0.76217382
C	-4.58682984	-2.25601407	-0.53910485
C	-6.04047596	-2.52549470	-0.58103371
C	-6.57697929	-3.81390536	-0.71012435
C	-8.19184844	-1.61579927	-0.52303820
C	-7.95699879	-3.98725715	-0.74759515
C	-8.78383829	-2.86799445	-0.65364169
H	-8.78244735	-0.70952080	-0.44253094
H	-8.37829071	-4.98286563	-0.84656296
H	-9.86463028	-2.95565305	-0.67745425
N	-6.85908797	-1.44362500	-0.48923800
C	-1.88680441	-1.58105184	-0.45115213
C	-5.42803812	-0.42102234	2.69729118
C	-6.82166773	0.12003023	4.56371433
H	-4.56565452	-0.90010714	2.25017955
C	-7.62596132	0.85430004	3.70381967
H	-7.06466497	0.05853743	5.62023217
C	-7.31234617	0.94015863	2.33845364
H	-8.49900340	1.37195955	4.08313474
C	-8.06465048	1.68531884	1.33087510
C	-9.24394405	2.39578220	1.61538837
C	-8.21133619	2.36062176	-0.98048912
C	-9.90399519	3.08469831	0.60466867
H	-9.65039996	2.41605344	2.62285921
C	-9.38280963	3.06562838	-0.69360194
H	-7.82979595	2.37486304	-1.99726742
H	-10.81334713	3.63585222	0.82430998
H	-9.89118328	3.60899217	-1.48629247
C	-5.69602877	-0.53350305	4.05289508
H	-5.03629376	-1.11469929	4.68749907
C	-4.29346596	2.80058472	1.17873527
C	-3.03618819	4.45679169	-0.07780153
C	-4.72734700	2.17780765	-0.00101479
H	-4.60861659	2.41517853	2.14397340
C	-3.45543811	3.86661880	-1.26414499
H	-2.38726773	5.32688938	-0.10115687
C	-4.29480748	2.73929462	-1.23283309
H	-3.12544182	4.28678262	-2.21018583
C	-4.77839455	2.06403621	-2.43507817
C	-4.51360903	2.44886634	-3.75880055



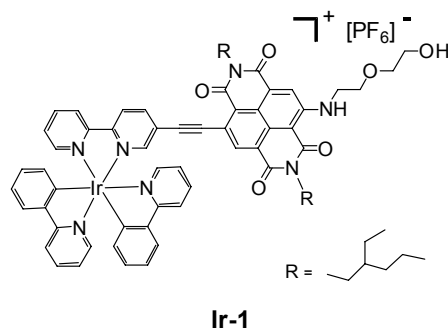
C	-6.07590062	0.26977312	-3.22865145
C	-5.04400322	1.72754224	-4.81859166
H	-3.89528478	3.31861321	-3.94661469
C	-5.84497682	0.61264903	-4.55183604
H	-6.69299310	-0.58025038	-2.96396865
H	-4.84006752	2.02949108	-5.84147684
H	-6.28409043	0.02181209	-5.34799911
N	-5.56134020	0.96710548	-2.19589752
C	-3.45956096	3.92086746	1.14322587
H	-3.13903645	4.38234099	2.07393282
Ir	-5.86398577	0.51521520	-0.18451720
N	-4.21653952	-0.96096801	-0.34456609
C	-7.52545818	1.64992479	0.01618755
N	-6.20723717	0.29064008	1.85837687
H	-5.92554855	-4.67679837	-0.77530675
H	-3.90064760	-4.28552181	-0.85025341
C	6.40845883	2.00443872	-0.14658865
C	6.11971205	0.57073027	-0.25569088
C	4.77433443	0.13672069	-0.28118919
C	3.71336601	1.07355278	-0.20809467
C	3.98708716	2.52716291	-0.10031444
C	7.17361299	-0.38681531	-0.34603200
C	4.44081644	-1.24571638	-0.38859133
C	5.51026771	-2.18332862	-0.46438551
C	6.81708717	-1.77332469	-0.44459686
C	5.22786507	-3.64065988	-0.57211271
C	2.79626176	-3.13225662	-0.55062388
C	3.10120098	-1.67662747	-0.42701120
C	2.06037626	-0.72264489	-0.35456808
C	2.39920036	0.64847461	-0.24425467
H	1.61416647	1.39403634	-0.18814251
H	7.58723031	-2.53256241	-0.50863803
N	5.33419308	2.89711428	-0.02281282
N	3.88107328	-4.02231385	-0.57730550
O	6.11874466	-4.47320693	-0.65314851
O	1.64772404	-3.54988629	-0.62724684
O	7.56069101	2.45993945	-0.15658398
O	3.08595911	3.35684880	-0.06981451
C	3.60362703	-5.47277572	-0.70041737
H	2.58418018	-5.56201955	-1.07387026
H	4.29353046	-5.85075014	-1.45591132
C	3.79239400	-6.26114515	0.61371626
H	4.81187701	-6.05158767	0.96224553
C	2.83279285	-5.82399283	1.74374950
H	3.17598731	-6.30514539	2.67087209
H	2.94616502	-4.74374326	1.91391992
C	1.34207125	-6.14103853	1.54834122
H	1.20233508	-7.22351642	1.42391208
H	0.97998345	-5.66507894	0.62856256
C	0.48134032	-5.66208856	2.72610668
H	0.83736453	-6.13190503	3.65373789
H	0.62146698	-4.57989455	2.85901954
C	-1.01012373	-5.96401291	2.54492778
H	-1.18667216	-7.04065546	2.43097483
H	-1.59711118	-5.62021852	3.40478818
H	-1.40708700	-5.46789437	1.64918109

C	3.71051621	-7.77949670	0.33482130
H	3.63637805	-8.29568874	1.30154050
H	2.77914289	-8.01077611	-0.20097163
C	4.90343007	-8.35767069	-0.43822601
H	4.80946245	-9.44504728	-0.53531654
H	4.98499466	-7.94759875	-1.45097062
H	5.84728768	-8.14778195	0.07823475
C	5.67591152	4.33832255	0.05045739
H	4.75028526	4.87238291	-0.16210565
H	6.38239675	4.52167437	-0.76227914
C	6.30359643	4.79294397	1.39676698
H	6.80038512	3.91983485	1.83795383
C	7.42179850	5.82888242	1.12939778
H	7.92557196	6.04449257	2.08217345
H	8.17524688	5.35539071	0.48501721
C	6.97850492	7.15690046	0.49509868
H	6.25371656	7.66132825	1.14857961
H	6.45372693	6.96739066	-0.45311376
C	8.15326015	8.10885774	0.22796380
H	8.87884805	7.61205746	-0.43164981
H	8.68304670	8.30124388	1.17163193
C	7.72142072	9.43969766	-0.39665005
H	7.02566778	9.97845249	0.25847545
H	8.58168840	10.09384420	-0.57766841
H	7.21542852	9.28138508	-1.35722230
C	5.27667979	5.31518610	2.42425024
H	5.83862267	5.78775265	3.24165906
H	4.67289512	6.11283714	1.97136155
C	4.34253232	4.25597868	3.02260519
H	3.74468469	4.68622995	3.83454919
H	3.64500676	3.86180259	2.27792619
H	4.91252393	3.41700410	3.44255604
N	8.46925014	-0.02267662	-0.33865186
H	8.61946033	0.98526698	-0.27438357
C	9.60800212	-0.92632907	-0.42204746
H	9.60659377	-1.63631151	0.41465232
H	9.57871549	-1.50849262	-1.35186989
C	10.90508271	-0.12112115	-0.38417254
H	10.93124147	0.59461286	-1.22378507
H	10.96108093	0.46267937	0.55070371
O	11.96184983	-1.04418961	-0.47119215
C	13.24368080	-0.43487930	-0.44582996
H	13.35734384	0.27436337	-1.28029224
H	13.39544270	0.12125791	0.49216729
C	14.28606680	-1.53666357	-0.56390559
H	14.12196015	-2.08903194	-1.50187401
H	14.15922148	-2.24441209	0.26974163
O	15.55148168	-0.89569025	-0.53414785
H	16.23757539	-1.57498946	-0.60851296

Compound Ir-1. Triplet state geometry.

Symbolic Z-matrix:

Charge = 1 Multiplicity = 3



13

C	0.72829100	-0.75564300	-0.27865100
C	-0.49124400	-0.87251900	-0.28343900
C	-2.91819500	-0.42803100	-0.22125300
C	-2.11609300	-2.69280400	-0.45039100
H	-2.75966000	0.64033900	-0.12366500
C	-3.43571900	-3.10600600	-0.47570500
H	-1.29500900	-3.39752500	-0.53372000
C	-4.47539400	-2.16587600	-0.36869700
C	-5.90329600	-2.53247800	-0.38616100
C	-6.35275600	-3.86136400	-0.42360400
C	-8.11365000	-1.77070900	-0.37514000
C	-7.71681900	-4.13033100	-0.44022100
C	-8.61916900	-3.06601100	-0.41717500
H	-8.76567300	-0.90422400	-0.35179800
H	-8.06889200	-5.15691500	-0.46765700
H	-9.69143700	-3.22838600	-0.42771100
N	-6.79614400	-1.50484900	-0.36212800
C	-1.82467200	-1.31370500	-0.31652800
C	-5.46117100	-0.15379600	2.74710500
C	-6.89655200	0.44021700	4.56505800
H	-4.56781400	-0.60995700	2.33856000
C	-7.74176200	1.05224300	3.65038900
H	-7.14072200	0.44563200	5.62310500
C	-7.42744900	1.05090600	2.28250400
H	-8.64822300	1.54048800	3.98805000
C	-8.22258600	1.66130100	1.21884900
C	-9.44992500	2.30832500	1.44556800
C	-8.40723800	2.12966200	-1.14052000
C	-10.15237200	2.86318300	0.38230600
H	-9.86172300	2.38208600	2.44838600
C	-9.62657900	2.77164900	-0.91101300
H	-8.02559000	2.08318700	-2.15638800
H	-11.09914600	3.36529200	0.55689600
H	-10.16964500	3.20860500	-1.74542300
C	-5.72901800	-0.17795500	4.10720300
H	-5.03747100	-0.66542700	4.78536600
C	-4.54017500	3.01655200	0.99705200
C	-3.39725000	4.66250000	-0.37628200
C	-4.91965200	2.27768600	-0.13379000
H	-4.83327500	2.68181500	1.98773000
C	-3.76264100	3.95623000	-1.51610000
H	-2.81422600	5.57430800	-0.46323600
C	-4.51814700	2.77613100	-1.40279100
H	-3.45674900	4.32795100	-2.49015600
C	-4.94200600	1.98043100	-2.55292400
C	-4.69269000	2.28359000	-3.90061200
C	-6.10110100	0.04401900	-3.21484300
C	-5.15989400	1.44887700	-4.90552400
H	-4.13587200	3.17887300	-4.15057400
C	-5.88211300	0.30266800	-4.55911400
H	-6.65953000	-0.82495500	-2.88944100
H	-4.96796800	1.68737500	-5.94733500
H	-6.27047800	-0.37592600	-5.31042800
N	-5.64745400	0.85133400	-2.23520000
C	-3.78977100	4.18906000	0.88032200

H	-3.51131000	4.74056500	1.77492500
Ir	-5.93674400	0.53078100	-0.19687100
N	-4.18882600	-0.83713800	-0.24420400
C	-7.67589900	1.55619800	-0.08905000
N	-6.27964400	0.43952700	1.85527400
H	-5.64435000	-4.68058100	-0.43148400
H	-3.65776000	-4.16070700	-0.58552400
C	6.60564500	1.94474000	-0.13789800
C	6.22242400	0.51936800	-0.24234200
C	4.87181700	0.16690800	-0.24213000
C	3.86456700	1.17957600	-0.14465700
C	4.22634700	2.60127400	-0.03434400
C	7.23389100	-0.53577500	-0.35798200
C	4.46010100	-1.21066500	-0.34847900
C	5.47015200	-2.20973900	-0.44990600
C	6.81743200	-1.87418900	-0.45489200
C	5.10060300	-3.62940500	-0.56400400
C	2.70097700	-2.96536300	-0.47542200
C	3.10132800	-1.56022700	-0.36025400
C	2.10412000	-0.50771800	-0.26690700
C	2.52250100	0.83431100	-0.16056200
H	1.78491000	1.62532300	-0.08955900
H	7.53609400	-2.67984700	-0.54029100
N	5.60197800	2.89213100	0.01373900
N	3.73164600	-3.92126200	-0.54546200
O	5.93963800	-4.52131700	-0.67229400
O	1.51887500	-3.31981400	-0.51377900
O	7.78836600	2.31918400	-0.17942500
O	3.38574500	3.49257200	0.02374600
C	3.36310200	-5.34636800	-0.68800100
H	2.33092300	-5.36634400	-1.03621300
H	4.01132000	-5.75086300	-1.46671000
C	3.53647600	-6.17374200	0.60442300
H	4.56906900	-6.01624600	0.94085200
C	2.61365700	-5.72174400	1.75868700
H	2.94990400	-6.23576000	2.67089600
H	2.77237800	-4.65046800	1.94641800
C	1.10859400	-5.97380700	1.57997100
H	0.92279400	-7.04573400	1.42646400
H	0.75432900	-5.45525800	0.68059600
C	0.28692000	-5.49597900	2.78565100
H	0.64008400	-6.00506700	3.69351300
H	0.47134000	-4.42414100	2.94566500
C	-1.21819400	-5.73545700	2.62456700
H	-1.43811000	-6.80086700	2.48300400
H	-1.77651700	-5.39487800	3.50467300
H	-1.61160700	-5.19811300	1.75124700
C	3.38455200	-7.68032500	0.29309900
H	3.28699100	-8.21577300	1.24740800
H	2.44353900	-7.85629000	-0.24710300
C	4.54939800	-8.29421100	-0.49506600
H	4.40262100	-9.37251800	-0.62462000
H	4.65425500	-7.85757900	-1.49435500
H	5.50089700	-8.14543800	0.02842900
C	6.03101700	4.31133000	0.08569700
H	5.13321900	4.89964400	-0.09997600

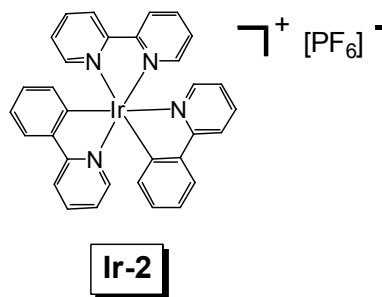
H	6.72557900	4.45713900	-0.74494000
C	6.71892300	4.72021800	1.41632800
H	7.20835200	3.82605100	1.82247700
C	7.85436300	5.73061900	1.12295400
H	8.39673200	5.91856100	2.06006700
H	8.57278400	5.24754200	0.44605700
C	7.42554900	7.07886200	0.52231900
H	6.73864000	7.59344300	1.20778400
H	6.86299300	6.91760400	-0.40927200
C	8.61676200	8.00170700	0.22654800
H	9.30439600	7.49445800	-0.46505000
H	9.18442100	8.16550100	1.15340500
C	8.20056700	9.35272800	-0.36429300
H	7.54318700	9.90049900	0.32211300
H	9.07197400	9.98558300	-0.56610400
H	7.65765100	9.22242900	-1.30871200
C	5.74709400	5.25025800	2.49239000
H	6.35489600	5.68656700	3.29687900
H	5.15277200	6.07634300	2.08028500
C	4.80310400	4.20816900	3.10511200
H	4.25505600	4.63863400	3.95110200
H	4.06071400	3.85660500	2.38302700
H	5.36018500	3.34051300	3.48194400
N	8.54074600	-0.19627600	-0.36690200
H	8.71424900	0.81385700	-0.30365100
C	9.64841200	-1.13087600	-0.47642600
H	9.62082000	-1.84834100	0.35349600
H	9.56795900	-1.70550000	-1.40807700
C	10.97781400	-0.37927900	-0.45535000
H	11.02160900	0.33975500	-1.29153400
H	11.07489700	0.19545600	0.48184600
O	11.98558100	-1.35085900	-0.56495100
C	13.29791200	-0.80582100	-0.56298400
H	13.43197900	-0.10716700	-1.40296700
H	13.49070000	-0.25430100	0.36989500
C	14.28189000	-1.95893900	-0.69167900
H	14.07494500	-2.50751400	-1.62335600
H	14.13451500	-2.65492000	0.14838100
O	15.57632100	-1.37928200	-0.68687500
H	16.22839900	-2.09061400	-0.76797500

Compound Ir-2. Ground state geometry.

Symbolic Z-matrix:

Charge = 1 Multiplicity = 1

1 1			
C	2.19227128	0.18539113	2.20150936
C	4.09064153	-1.32406160	2.32332241
H	1.65528486	1.03475579	2.61235480
C	3.61197005	-1.99619652	1.20671336
H	5.01072268	-1.64597388	2.80358571
C	2.42045096	-1.58339933	0.58054221
C	1.87360146	-2.27660536	-0.58872487
C	2.43089878	-3.41383403	-1.20104384
C	0.12381815	-2.30767290	-2.15043541



C	1.81384322	-3.98897656	-2.30287804
C	0.63101064	-3.42847853	-2.79441139
H	-0.79457136	-1.83294942	-2.47943764
H	2.24582143	-4.86858786	-2.77230823
H	0.11042062	-3.84915103	-3.64817320
N	0.72239745	-1.74148001	-1.08913286
C	3.37147792	-0.22933880	2.81925405
H	3.73572427	0.30284684	3.69577607
C	-0.94309421	-1.99101256	2.20074430
C	-3.20150438	-2.87468099	2.32103865
H	0.06075571	-1.95294549	2.61247812
C	-3.54141640	-2.12412489	1.20350668
H	-3.94233707	-3.50829922	2.80116263
C	-2.58583558	-1.30113908	0.57745004
H	-4.55765346	-2.18106051	0.82125170
C	-2.90903562	-0.48136735	-0.59318923
C	-4.17161619	-0.39203957	-1.20700772
C	-2.05394168	1.04376789	-2.15696927
C	-4.35712042	0.42875236	-2.31043468
H	-5.00287272	-0.96365721	-0.81099106
C	-3.27698471	1.16783979	-2.80249219
H	-1.18115086	1.59786366	-2.48651113
H	-5.33414043	0.49704035	-2.78101363
H	-3.37761280	1.82738985	-3.65791172
C	-1.89420742	-2.80211828	2.81828069
H	-1.61767019	-3.38393387	3.69531763
C	-1.25587985	1.81176531	2.19868718
C	-0.89128894	4.20961254	2.31797069
C	-0.43250522	1.68660277	1.06246062
H	-1.72385578	0.92367730	2.61209784
C	-0.07173154	4.12797501	1.20021005
H	-1.06910476	5.16821726	2.79783840
C	0.16260235	2.88854916	0.57482962
H	0.38794141	5.03593012	0.81761319
C	1.03627496	2.75770968	-0.59421164
C	1.74400518	3.80629947	-1.20924669
C	1.93680852	1.25215467	-2.15133792
C	2.55117751	3.55514421	-2.30977648
H	1.66150515	4.81291786	-0.81618059
C	2.65576037	2.24894584	-2.79755123
H	1.98258960	0.21839297	-2.47773227
H	3.09809849	4.36705819	-2.78131478
H	3.28009004	2.00527474	-3.65061570
N	1.14704111	1.49169659	-1.09112918
C	-1.48217163	3.04147527	2.81574342
H	-2.12366806	3.09320901	3.69323839
Ir	-0.00087185	-0.00062654	0.02591375
N	1.67413837	-0.46820644	1.06609763
C	-1.86701629	0.24436678	-1.09328977
N	-1.24714221	-1.21547317	1.06446130
H	3.31913551	-3.71656457	-0.94127198
H	4.05025228	-2.75218956	0.77720794

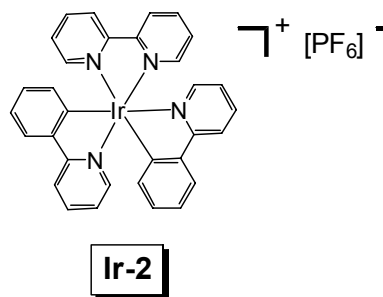
Compound Ir-2. Triplet state geometry.

Symbolic Z-matrix:

Charge = 1 Multiplicity = 3

1 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