Electronic Supplementary Information (ESI)

A cationic iridium(III) complex showing aggregation-induced phosphorescent emission (AIPE) in the solid state: synthesis, characterization and properties

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NOTE [a] The peaks of tert-butyl groups are not marked in the ^{1}H NMR spectra.

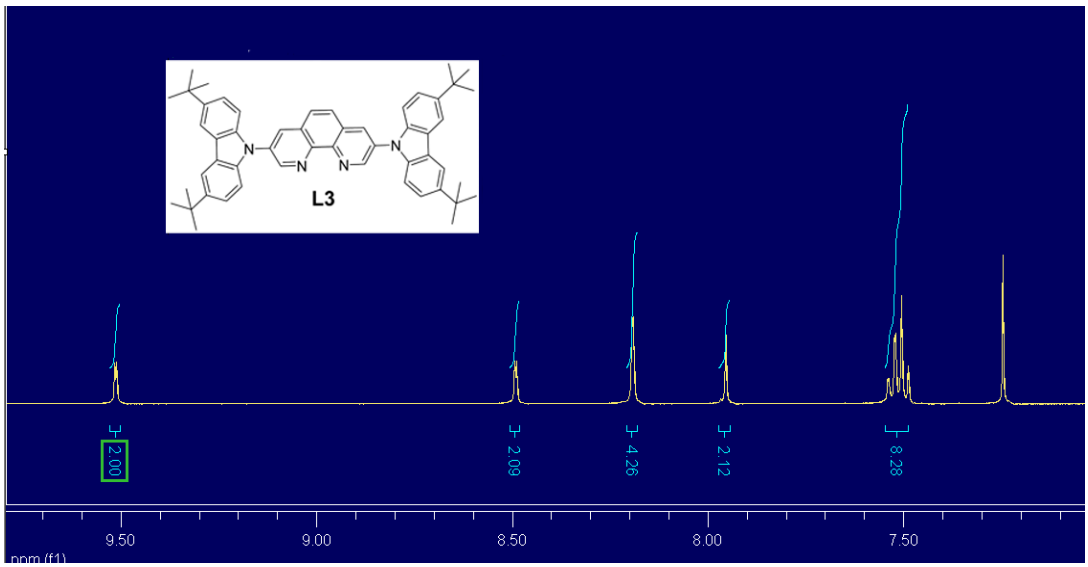


Fig. S1 ^{1}H NMR spectrum of **L3** in $CDCl_3$.[a]

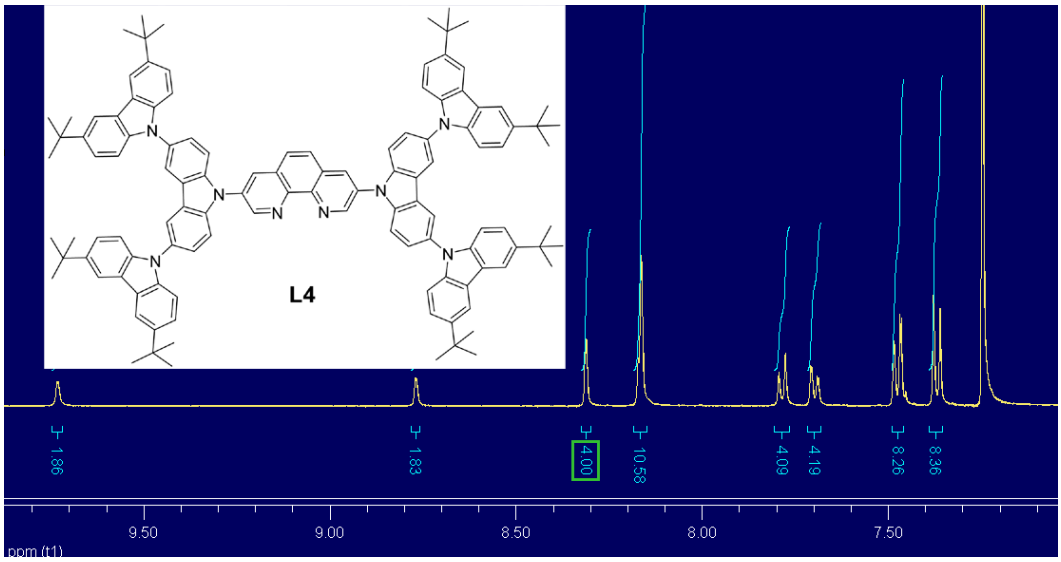


Fig. S2 ^{1}H NMR spectrum of **L4** in $CDCl_3$.[a]

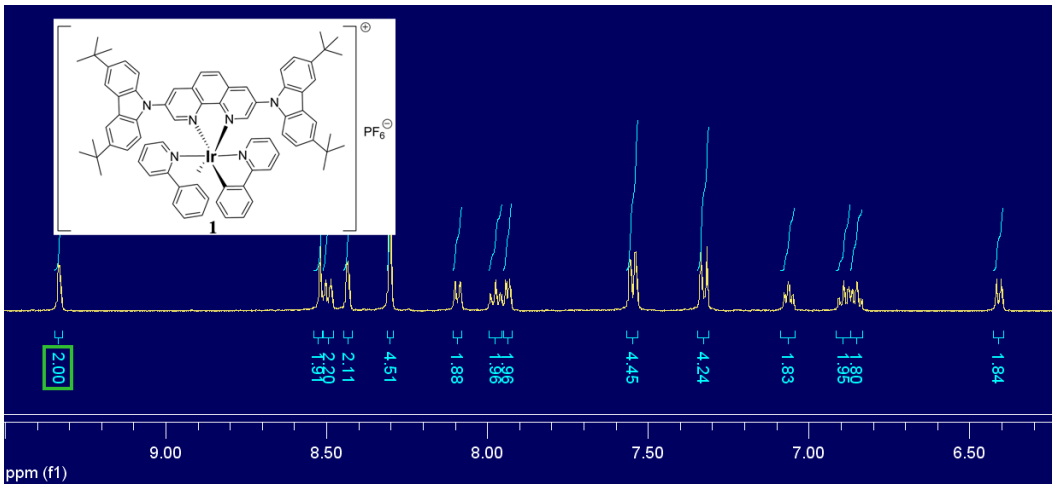


Fig. S3 ^{1}H NMR spectrum of **1** in d_6-DMSO.[a]

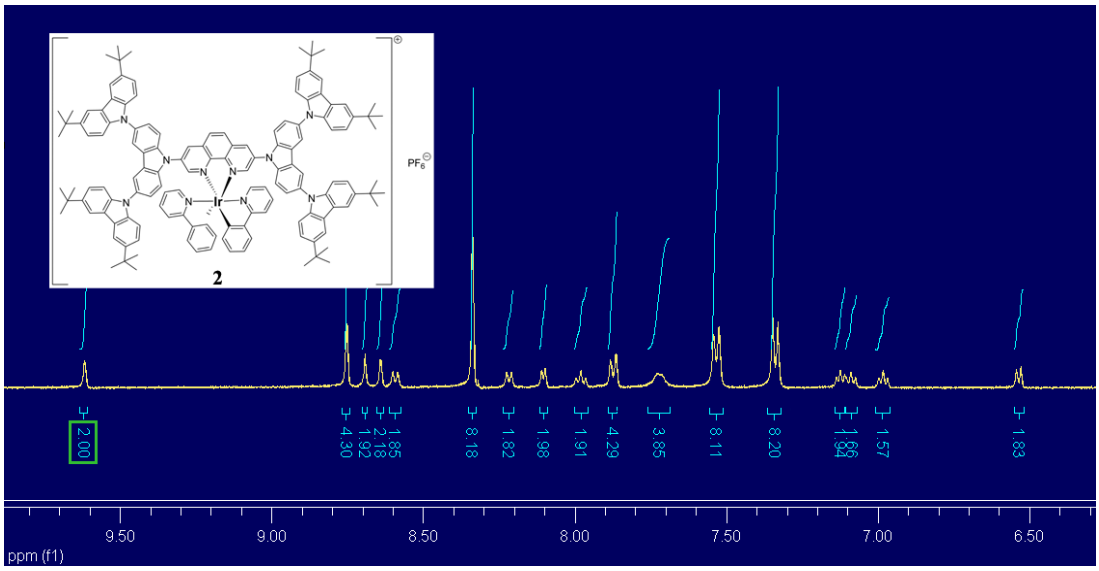


Fig. S4 ^{1}H NMR spectrum of **2** in d_6-DMSO.[a]

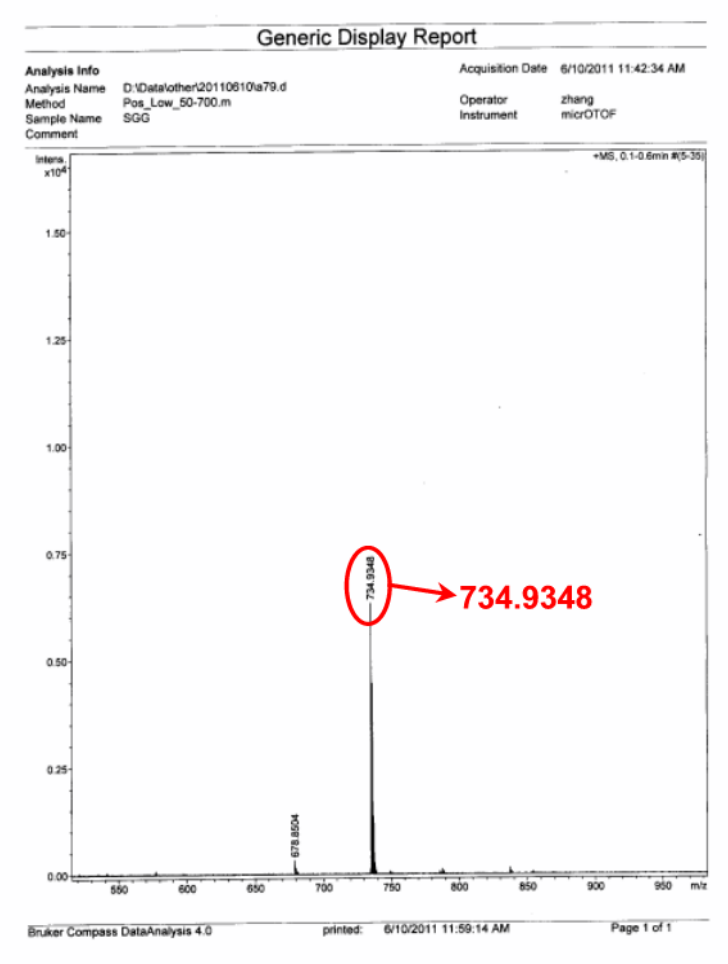


Fig. S5 Copy of High resolution mass spectrum for **L3**.

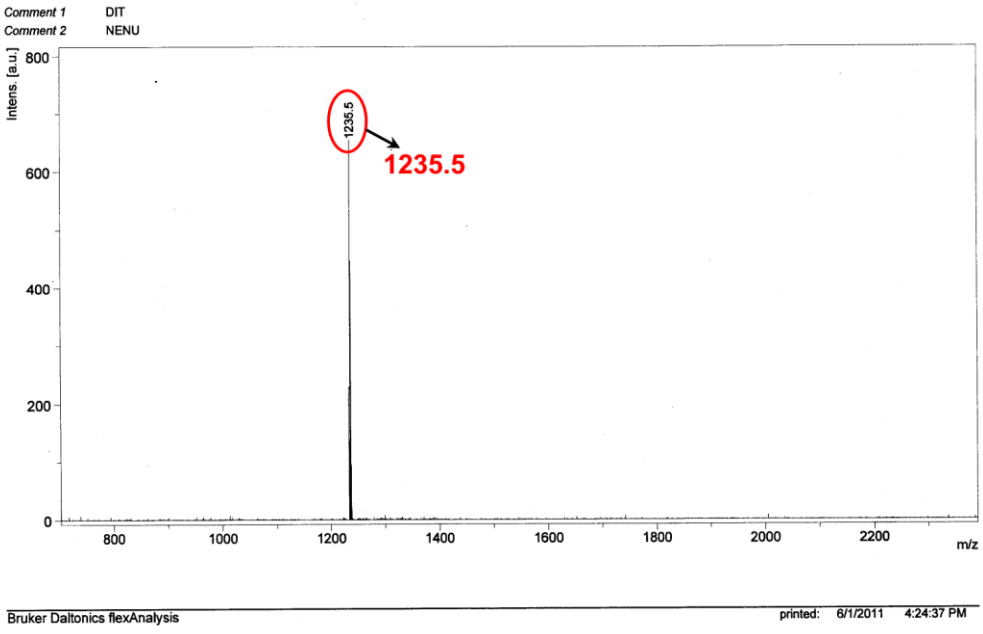


Fig. S6 Copy of the MALDI-TOF MS spectrum for **1** (positive mode).

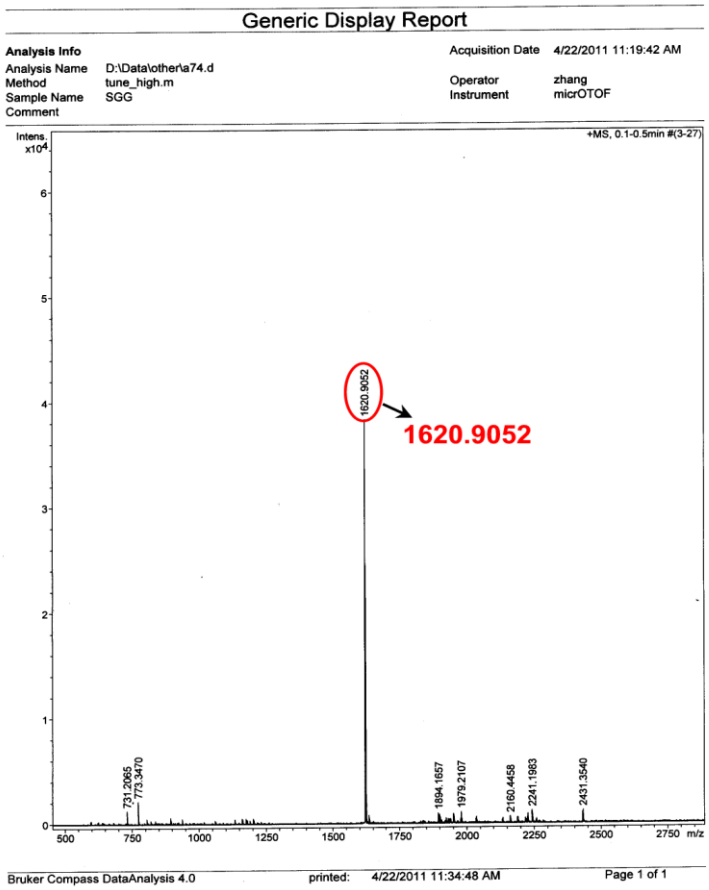


Fig. S7 Copy of High resolution mass spectrum for **L4**.

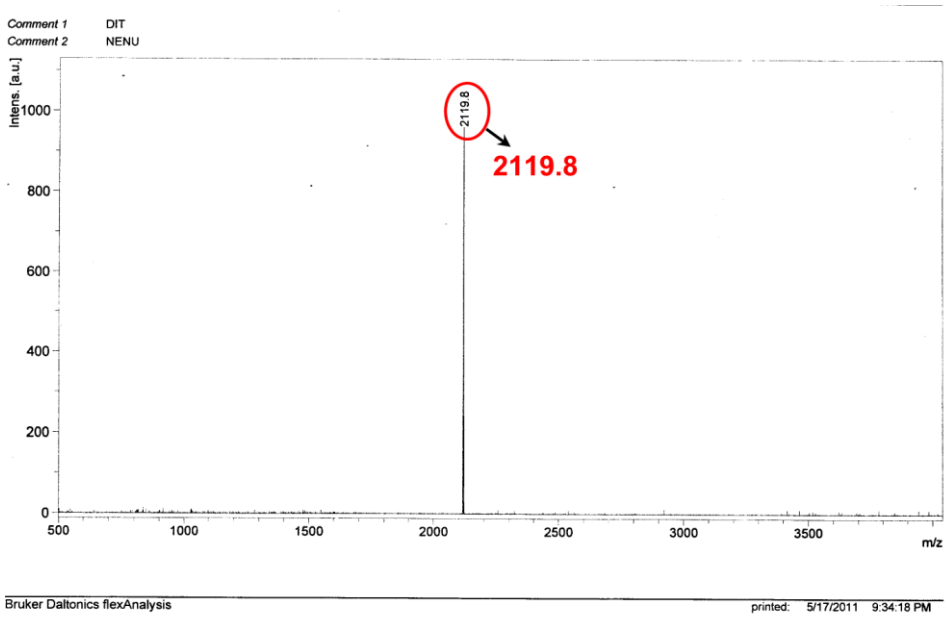


Fig. S8 Copy of the MALDI-TOF MS spectrum for **2** (positive mode)

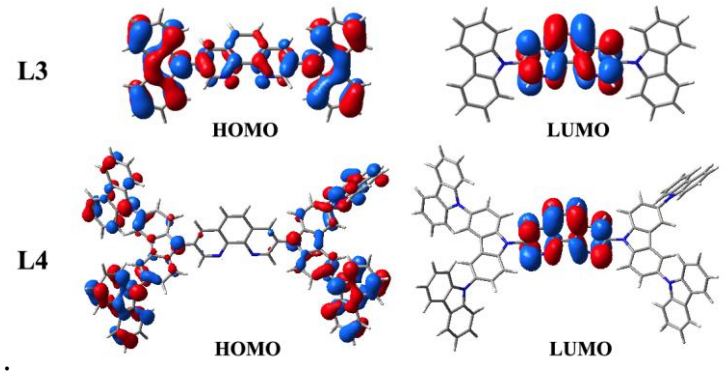


Fig. S9 HOMOs and LUMOs orbitals of **L3** and **L4** ligands.

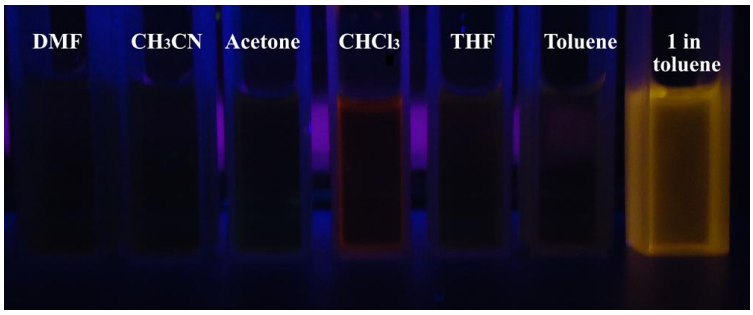


Fig. S10 Luminescent photographs of **2** in various solvents and **1** in toluene solvent at a concentration of 1×10^{-5} mol/L.

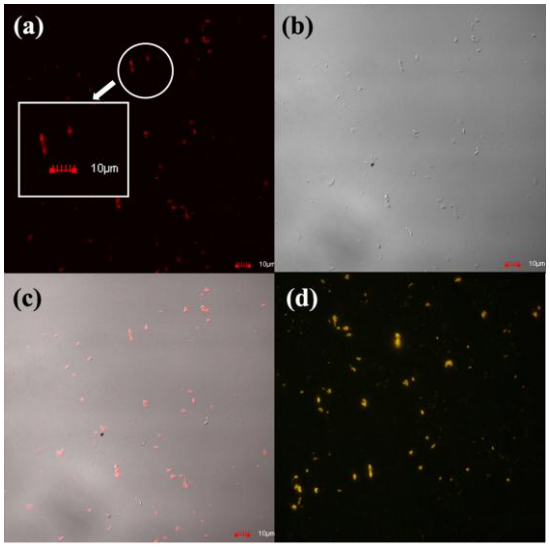


Fig. S11 (a) Confocal luminescence and (b) brightfield images of complex **2** in water–DMSO mixtures with water content of 90% at a concentration of 2×10^{-5} at 298 K. (c) The overlay image of (a) and (b). (d) The CCD images of micro-aggregates. The length of scale bar corresponds to 10 μm.

Table S1 The calculated energy levels of the lower-lying transitions of complexes **1** and **2**.

Complex	States	Assignment	eV	f	Nature
1	T_1	H→L (34%) H-1→L (51%)	1.99	0	MLCT/LLCT MLCT/LLCT/ILCT
2	T_1	H→L (60%) H-9→L (25%)	1.90	0	ILCT MLCT/ILCT

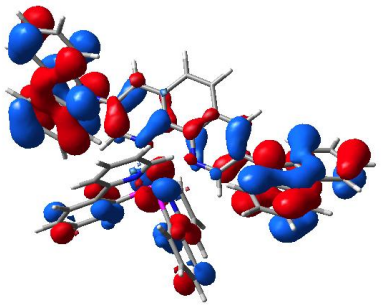
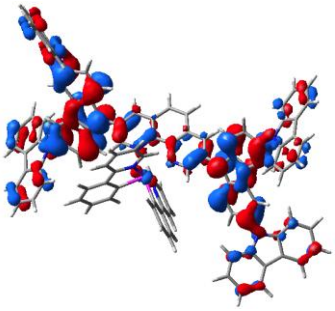
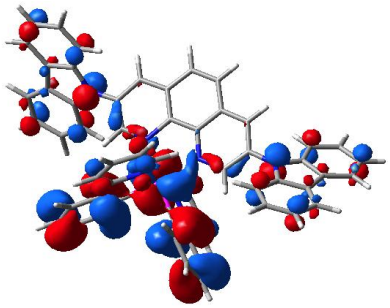
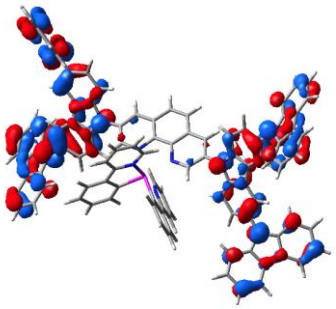
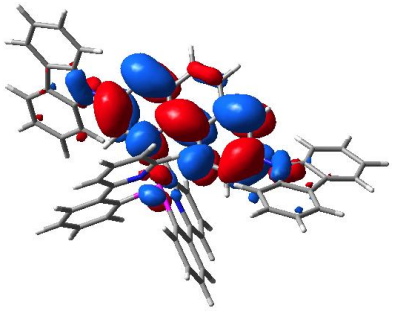
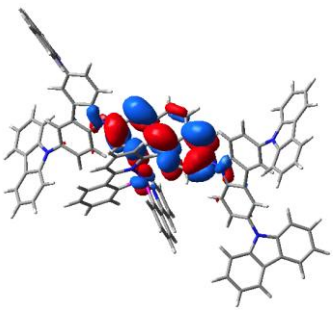
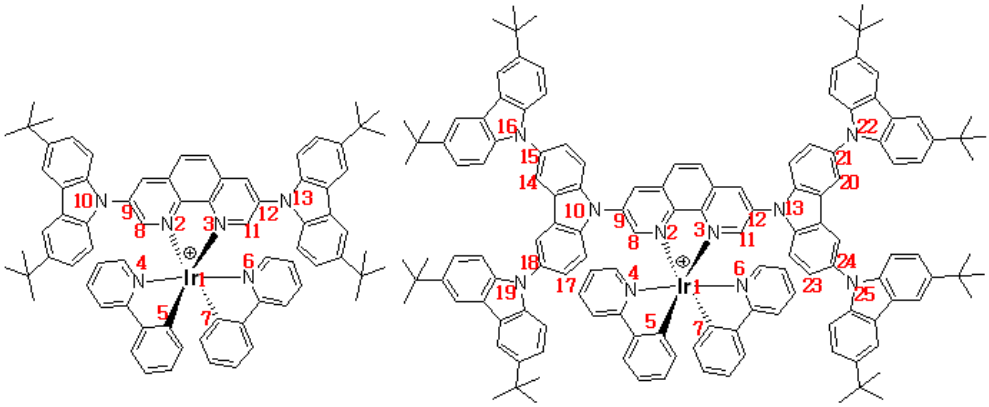
complex **1**	complex **2**
HOMO-1	HOMO-9
	
HOMO	HOMO
	
LUMO	LUMO
	

Fig. S12 Selected frontier orbitals of complexes **1** and **2**.



1 **2**

Table S2 Bond angle (°) and bond length (Å) modifications from S_0 to T_1 as calculated by DFT approach for complexes **1** and **2**.

complex **1**			complex **2**		
Bond length	S_0	T_1	Bond length	S_0	T_1
Ir1-N2	2.2350	2.2117	Ir1-N2	2.2317	2.2057
Ir1-N3	2.2292	2.1103	Ir1-N3	2.2276	2.2073
Ir1-N4	2.0844	2.0818	Ir1-N4	2.0831	2.0749
Ir1-C5	2.0209	2.0162	Ir1-C5	2.0216	2.0238
Ir1-N6	2.0835	2.0814	Ir1-N6	2.0845	2.0804
Ir1-C7	2.0206	2.0162	Ir1-C7	2.0210	2.0239
C9-N10	1.3990	1.4104	C9-N10	1.3995	1.4210
C12-N13	1.3987	1.4103	C12-N13	1.3997	1.4203
			C15-N16	1.4155	1.4152
			C18-N19	1.4159	1.4153
			C21-N22	1.4156	1.4152
			C24-N25	1.4160	1.4150
Bond angle			Bond angle		
N2-Ir1-N3	75.7	76.1	N2-Ir1-N3	75.6	76.4
N4-Ir1-C5	80.0	80.2	N4-Ir1-C5	80.1	80.1
N6-Ir1-N7	80.0	80.2	N6-Ir1-N7	80.0	80.0
C8-C9-N10	119.9	120.1	C8-C9-N10	119.8	120.1
C11-C12-N13	119.9	120.1	C11-C12-N13	119.5	119.8
			C14-C15-N16	120.2	119.9
			C17-C18-N19	119.6	119.6
			C20-C21-N22	120.3	120.0
			C23-C24-N25	119.5	119.5

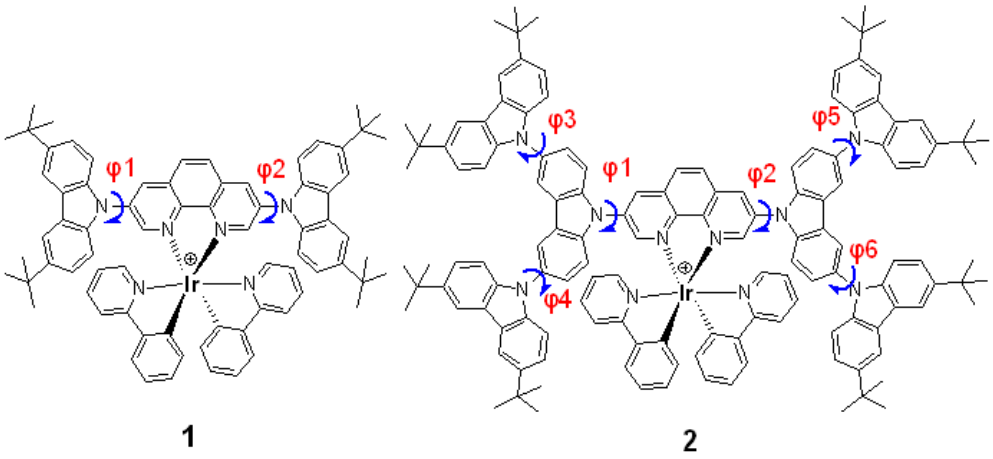


Table S3 Dihedral angle (°) modifications from S_0 to T_1 as calculated by DFT approach for complexes **1** and **2**.

complex **1**			complex **2**		
Dihedral angles	S_0	T_1	Dihedral angles	S_0	T_1
φ_1	47.2	52.0	φ_1	46.7	55.7
φ_2	46.9	51.7	φ_2	45.4	53.2
			φ_3	55.1	51.5
			φ_4	54.7	52.0
			φ_5	54.1	51.5
			φ_6	54.5	51.7

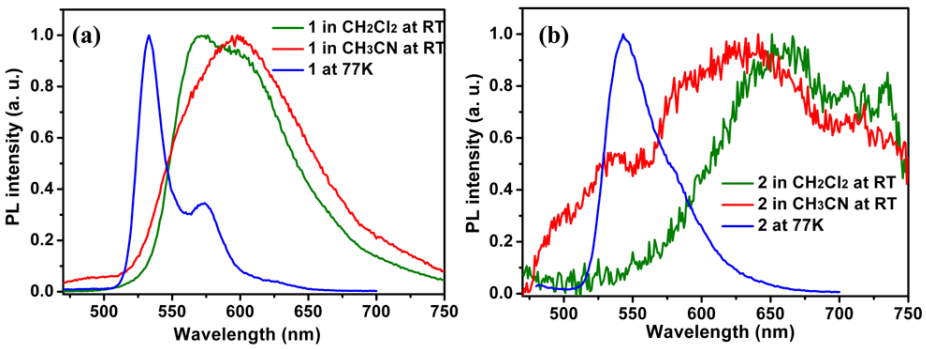


Fig. S13 The emission spectra of **1** and **2** in different medium and temperature.

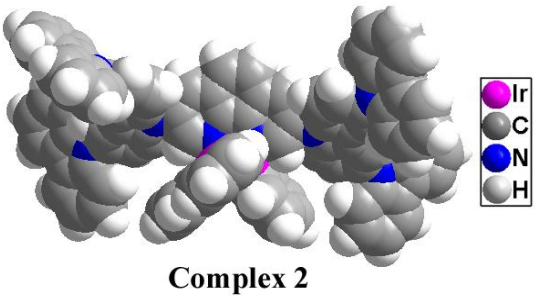


Fig. S14 The space-filling models of complex **2**.

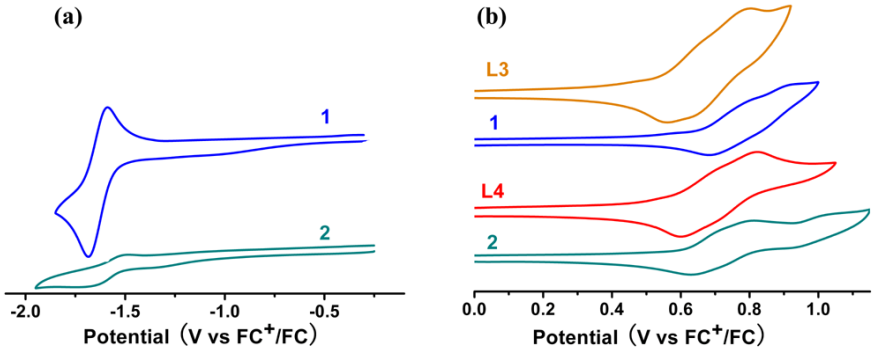


Fig. S15 The CV traces of liangds (**L3** and **L4**) and complexes (**1** and **2**).

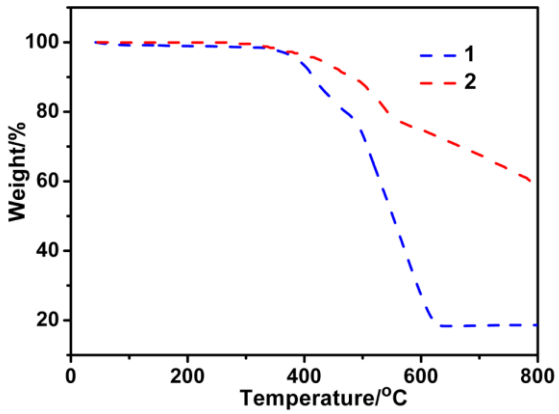


Fig. S16 The TGA curves of complexes **1** and **2**.

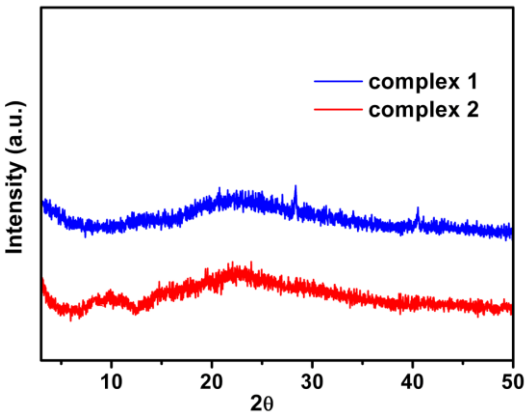


Fig. S17 The XRD curves of complexes **1** and **2**.

The optimized geometry of **1** in ground state at B3LYP/LANL2DZ/6-31G* level

Ir	-0.00408500	-0.00673400	-0.00448700
C	0.00278800	-0.02028700	2.01631600
C	2.01636900	-0.02998100	-0.00476600
C	-3.97708200	0.02149700	-1.95402300
N	-2.21661000	-0.06098100	-0.28183500
C	-4.52985500	-0.10978400	0.40195200
C	-4.93741800	-0.05232600	-0.92792100
C	-0.93812200	0.20536000	-4.93022600
N	-0.28585800	0.09900900	-2.21325000
N	-0.18365600	2.03571800	0.37076100
C	-3.36022000	0.13020100	-4.31191400
H	-3.63525800	0.17302700	-5.36178000
C	-1.96371800	0.13134800	-3.96947700
C	-0.23092100	2.38338100	1.69379200
C	-0.14318200	1.25733100	2.62079500
C	0.39422500	0.20277600	-4.52612700
C	1.64882800	-2.42298200	-0.27760100
C	1.97845300	-3.77996200	-0.41969600
H	3.02073800	-4.07324800	-0.46070000
N	0.33274900	-2.05137000	-0.22072200
C	-4.32248400	0.08079600	-3.34851900
H	-5.37383700	0.08251600	-3.62120400
C	0.05025200	-0.98427100	4.25738000
H	0.13288800	-1.86188200	4.89373100
C	0.66904000	0.13923000	-3.13673300
H	1.69100600	0.11136100	-2.77647100
C	3.99135900	-1.48238200	-0.23454900
H	4.42745600	-2.46857400	-0.36762400
C	2.59682700	-1.31586200	-0.17380800
C	-3.13870600	-0.10438200	0.67422400
H	-2.77583800	-0.12466900	1.69558900
C	-1.59448100	0.08191400	-2.60180600
C	0.10266800	-1.12988100	2.86892900
H	0.23091500	-2.12502400	2.45304200
C	-2.60767400	0.01242500	-1.58783400
C	-0.63431300	-2.98690600	-0.30266800
H	-1.65195700	-2.61982300	-0.24805300
C	4.27465700	0.89214100	0.05062000
H	4.92730500	1.75645900	0.14537800
C	-0.19708700	1.39924100	4.01835900
H	-0.31306000	2.37926900	4.47281700

C	-0.41554000	4.71592000	1.06912600
H	-0.50338400	5.76182600	1.34729900
C	-0.36611200	4.33899800	-0.27664200
H	-0.41332200	5.07002100	-1.07613600
C	2.88923300	1.06227900	0.10973200
H	2.49144400	2.06253100	0.25479800
C	-0.10145300	0.27999200	4.83671800
H	-0.14106700	0.38904300	5.91621000
C	-0.35851500	-4.33834700	-0.44177300
H	-1.17179400	-5.05319500	-0.50007600
C	-0.34894000	3.73613700	2.04925500
H	-0.38276700	4.01032200	3.09697600
C	4.83029200	-0.37991900	-0.12316600
H	5.90749100	-0.50804100	-0.16777300
C	-0.25143500	2.99074300	-0.57818100
H	-0.20558800	2.64210400	-1.60266200
C	0.97977900	-4.73976100	-0.50104200
H	1.23783400	-5.78904200	-0.60792600
H	-5.99360400	-0.07780100	-1.17516000
H	-1.18753500	0.27881400	-5.98354100
C	-8.91841900	1.98828200	2.31671800
C	-8.21979600	2.35344000	1.15519900
C	-7.05129700	1.69384100	0.77306000
C	-6.60066200	0.64899100	1.58233600
C	-7.28061600	0.28369800	2.76757400
C	-8.45064100	0.95954500	3.13025500
H	-9.82692800	2.51853100	2.58530800
H	-8.59145100	3.16763700	0.53992400
H	-6.51426300	2.00369700	-0.11720400
H	-8.98244900	0.68869700	4.03788500
C	-5.39937200	-1.03659900	2.56201000
C	-4.48955900	-2.05411100	2.85651100
C	-4.70437300	-2.80267200	4.01411300
C	-5.80194000	-2.55335000	4.85258900
C	-6.71750700	-1.55149100	4.54080700
C	-6.52243600	-0.78700800	3.38575500
H	-3.64395500	-2.27483200	2.21358200
H	-4.00719300	-3.59655600	4.26570900
H	-5.94118000	-3.15318400	5.74674800
H	-7.57630500	-1.37038600	5.18083600
N	-5.44603200	-0.15591200	1.45821700
C	4.93260100	2.52814200	-5.71074000
C	4.11225600	2.75463000	-4.59480500

C	2.92756900	2.04202100	-4.4069000
C	2.58642500	1.08323400	-5.36318200
C	3.39204700	0.85866700	-6.50443800
C	4.57489900	1.58624500	-6.67193500
H	5.84880900	3.09868700	-5.82799400
H	4.39985100	3.50183800	-3.86093400
H	2.30138000	2.24538500	-3.54472000
H	5.20116100	1.42301000	-7.54435300
C	1.53496100	-0.50302400	-6.63772900
C	0.68505800	-1.49468300	-7.13206200
C	1.03474200	-2.10936100	-8.33472300
C	2.20375800	-1.75242600	-9.02494900
C	3.05777400	-0.77844200	-8.51417500
C	2.72828400	-0.14875900	-7.30917500
H	-0.21186100	-1.79905900	-6.60313600
H	0.38756700	-2.88159200	-8.74021100
H	2.44629600	-2.24647300	-9.96077800
H	3.97111800	-0.51486800	-9.03980800
N	1.44905800	0.24789300	-5.44352500

The optimized geometry of **1** in excited-state UB3LYP/LANL2DZ/6-31G* level

Ir	0.01142200	0.00157800	0.01121600
C	-0.01718100	0.03652400	2.02686600
C	2.02689200	-0.04553300	-0.01155900
C	-3.97083000	-0.04723000	-1.95618400
N	-2.18212700	-0.07417200	-0.26147000
C	-4.49300200	-0.18696300	0.40393000
C	-4.92071200	-0.13229200	-0.95025100
C	-0.93119700	0.19107000	-4.92221100
N	-0.25290800	0.09425600	-2.18199800
N	-0.16505000	2.05146800	0.32848100
C	-3.34345900	0.07525000	-4.31661900
H	-3.61763500	0.11355600	-5.36744400
C	-1.94123700	0.10434100	-3.97686500
C	-0.22116000	2.43666100	1.63973000
C	-0.14648200	1.33431200	2.59824100
C	0.42208600	0.22759800	-4.48906400
C	1.62547900	-2.44196300	-0.23085400
C	1.93489500	-3.80396300	-0.35920600
H	2.97237300	-4.11450200	-0.39749700
N	0.31654700	-2.04884000	-0.17609100
C	-4.30516700	-0.00028500	-3.35916800
H	-5.35532600	-0.02458000	-3.63748300

C	-0.00033500	-0.87057000	4.29446000
H	0.06262600	-1.73101800	4.95597400
C	0.69857800	0.17222600	-3.11818500
H	1.72385200	0.16976800	-2.76328900
C	3.98085300	-1.53399700	-0.19737500
H	4.40427000	-2.52931700	-0.29964700
C	2.59060600	-1.34604400	-0.14685100
C	-3.12247100	-0.15084100	0.68582300
H	-2.77144800	-0.16277400	1.71240100
C	-1.58951900	0.05531100	-2.58343900
C	0.05116700	-1.05352100	2.91210500
H	0.15762900	-2.06113100	2.52026300
C	-2.57821500	-0.01739100	-1.59905500
C	-0.66610600	-2.96610600	-0.25753900
H	-1.67586800	-2.57702600	-0.21684200
C	4.29992400	0.84740600	0.01717700
H	4.96656300	1.70335400	0.08702900
C	-0.20016400	1.51395000	3.98948800
H	-0.29804600	2.50719000	4.41878000
C	-0.40945400	4.74873000	0.94831700
H	-0.50128600	5.80201500	1.19581500
C	-0.35955200	4.33219600	-0.38473900
H	-0.41419700	5.03905400	-1.20530600
C	2.91855500	1.03864600	0.06553800
H	2.53245200	2.04800000	0.17642300
C	-0.12693600	0.41361500	4.83780800
H	-0.16632700	0.55288400	5.91394700
C	-0.41049800	-4.32378200	-0.38613600
H	-1.23534700	-5.02511100	-0.44723300
C	-0.34216500	3.79744200	1.95737400
H	-0.38151300	4.10167000	2.99667900
C	4.83571900	-0.43936700	-0.11511700
H	5.91109300	-0.58507600	-0.15199300
C	-0.23850000	2.97538300	-0.64855000
H	-0.19771900	2.59241700	-1.66062400
C	0.92003900	-4.74842900	-0.43509000
H	1.16111400	-5.80267800	-0.53275500
H	-5.97741800	-0.18590000	-1.19049200
H	-1.16722600	0.26034300	-5.97891700
C	-8.78194900	2.02163300	2.38239000
C	-8.05092400	2.40459000	1.24710800
C	-6.91039500	1.70577500	0.85149500
C	-6.52985300	0.60079300	1.61944600

C	-7.24562500	0.21380400	2.78025100
C	-8.38060000	0.93057000	3.15850000
H	-9.66521900	2.58558100	2.66605400
H	-8.37324100	3.26445900	0.66766100
H	-6.33778600	2.01830300	-0.01481000
H	-8.94182700	0.65129300	4.04550400
C	-5.43062000	-1.18346100	2.50716200
C	-4.55989800	-2.25097100	2.74663600
C	-4.80456000	-3.04722600	3.86534300
C	-5.89169500	-2.79347500	4.71570400
C	-6.76943200	-1.73634800	4.45910000
C	-6.54305600	-0.92450000	3.34817300
H	-3.72697600	-2.46226500	2.08512500
H	-4.14261100	-3.88153600	4.07713400
H	-6.05722200	-3.43113300	5.57863200
H	-7.61838300	-1.55655300	5.11235600
N	-5.42949900	-0.25425000	1.45635600
C	4.76605900	2.81011400	-5.83149500
C	3.91503000	3.05497500	-4.74288900
C	2.78720500	2.26673600	-4.51463400
C	2.53911600	1.21620300	-5.40343900
C	3.38069200	0.96690700	-6.51762800
C	4.50088800	1.77043800	-6.72735200
H	5.63624400	3.44114100	-5.98393300
H	4.13359100	3.87596300	-4.06664000
H	2.12560000	2.47154200	-3.68020900
H	5.15470300	1.59768200	-7.57733100
C	1.63572900	-0.53980400	-6.53508200
C	0.85717900	-1.62981100	-6.93686700
C	1.24849100	-2.31282400	-8.08839900
C	2.38987400	-1.92949600	-8.80964000
C	3.17657900	-0.85412300	-8.38714400
C	2.80271600	-0.15316300	-7.24093200
H	-0.01395200	-1.94325400	-6.37216100
H	0.66074900	-3.16064600	-8.42717600
H	2.66994400	-2.48096900	-9.70188600
H	4.06818700	-0.57469200	-8.94095100
N	1.47843800	0.29820000	-5.42080300

The optimized geometry of **2** in ground state at B3LYP/LANL2DZ/6-31G* level

Ir	-0.20944100	-0.53692600	-0.18626000
C	-0.30375800	-0.97235100	1.78562600
C	1.78478100	-0.86447500	-0.17423500
C	-4.05271200	0.43706000	-2.15793000
N	-2.39306700	-0.20046300	-0.50108700
C	-4.71729500	-0.04108800	0.12293400
C	-6.71263700	0.77809000	1.39108700
C	-5.05741100	0.31326200	-1.17999100
C	2.58667400	-0.30705500	-5.49688300
C	-0.88562200	0.75077400	-4.98864700
N	-0.37595300	0.05934500	-2.32607400
N	-0.09799400	1.38439000	0.61096200
C	-3.32263300	0.89858400	-4.44013200
H	-3.54421700	1.16979900	-5.46824300
C	-7.48004300	0.31153200	2.48356000
C	-1.95299700	0.65739800	-4.07506300
C	-0.15960600	1.45333500	1.97644900
C	-0.29048400	0.15989800	2.64439700
C	0.41638500	0.51011000	-4.55901600
C	1.08253200	-3.07134500	-0.93218600
C	-5.78639800	-1.19788400	2.07160300
C	1.21669600	-4.40756200	-1.34182400
H	2.20558400	-4.84315400	-1.42285500
C	-6.89423000	-0.94408100	2.91329500
N	-0.16655400	-2.52244500	-0.81949200
C	2.76453400	-1.53291900	-4.85274300
H	2.03082900	-1.93427000	-4.16192400
C	-4.32554900	0.79750500	-3.52292700
H	-5.35502200	0.98853800	-3.81160700
C	-0.52239300	-2.37347700	3.77176700
H	-0.60474200	-3.36570200	4.20854300
C	0.61980400	0.17339100	-3.19724500
H	1.61974100	0.00805900	-2.81184600
C	3.53370900	-2.52386700	-0.67876600
H	3.82565600	-3.51942700	-1.00144800
C	2.17712900	-2.16354200	-0.59578900
C	-3.35180800	-0.28540500	0.41460400
H	-3.03793100	-0.54442200	1.41960200
C	-1.65698700	0.29050000	-2.73797800
C	1.77865300	1.66858600	-6.31389500
C	1.57046800	3.74574200	-7.47967000
H	1.04058800	4.67214800	-7.67424400

C	3.52557800	0.16829800	-6.44148800
C	3.01494800	1.42488500	-6.95642500
C	-0.41645900	-2.23554300	2.38526900
H	-0.41440000	-3.13131000	1.77120300
C	-2.71400400	0.16965800	-1.77596200
C	-1.25478200	-3.26538400	-1.10523700
H	-2.21008200	-2.76713400	-0.99266300
C	3.50936000	2.33723000	-7.89168400
H	4.44175900	2.15199300	-8.41496500
C	4.68475300	-0.56547100	-6.70588600
H	5.43136600	-0.20037700	-7.40361200
C	4.15083700	-0.32154300	0.07645700
H	4.91875000	0.39952100	0.34502900
C	1.05181500	2.83401500	-6.56379900
H	0.12364200	3.05545200	-6.04799500
C	-8.55009600	1.07102400	2.96226000
H	-9.13177400	0.74152500	3.81706500
C	-0.39854300	0.01686500	4.03861700
H	-0.39077400	0.88755800	4.68836700
C	0.04749100	3.86314100	1.85875300
H	0.10704400	4.82898300	2.35128100
C	4.88125400	-1.78434000	-6.05049200
C	-5.03408500	-2.36709300	2.20081000
H	-4.20666600	-2.59829000	1.53870400
C	0.11013900	3.76998000	0.46491100
H	0.22014300	4.64839600	-0.16122600
C	-6.99088600	2.00393000	0.78336900
H	-6.39409100	2.38853600	-0.03669400
C	2.80391400	0.03988100	0.16121500
H	2.55337500	1.04119400	0.49928300
C	-8.85632300	2.28432000	2.33928900
C	-7.22541100	-1.84707600	3.92656600
H	-8.05423300	-1.65353600	4.59973300
C	3.91313900	-2.26269100	-5.14419800
H	4.06975400	-3.22873300	-4.67650400
C	-5.39007700	-3.26775000	3.20082100
H	-4.83750600	-4.19462100	3.31123400
C	-0.51570000	-1.24816700	4.60271900
H	-0.59552600	-1.35886300	5.67984200
C	2.78439400	3.50305200	-8.15484100
C	-1.17307700	-4.58789400	-1.51310400
H	-2.07832900	-5.14462500	-1.72847700
C	-6.46894700	-3.01334100	4.07191800

C	-8.07381700	2.73943000	1.25799400
H	-8.33260800	3.68117400	0.78584200
C	-0.08799500	2.70393600	2.60935400
H	-0.13278000	2.75710000	3.69064300
C	4.52044600	-1.60411300	-0.34318400
H	5.56824500	-1.88307500	-0.40081800
C	0.03304800	2.51297600	-0.11467800
H	0.08326500	2.38045800	-1.18854000
C	0.09335100	-5.16887300	-1.63169700
H	0.19994300	-6.20311100	-1.94466400
C	2.56266900	4.95096100	-10.19188400
C	4.53769200	5.05255200	-9.06448600
C	1.28267200	4.62690600	-10.64951200
C	3.38443400	5.87885500	-10.87968000
C	5.57743600	4.90098400	-8.14330700
C	4.64088100	5.94466900	-10.16110100
C	0.82453400	5.26470400	-11.80159300
H	0.66572200	3.89699500	-10.13536300
C	2.90042400	6.50550300	-12.03400300
C	6.73902400	5.64428400	-8.34826100
H	5.48710000	4.23468800	-7.29159200
C	5.81842100	6.67912700	-10.34448000
C	1.62028700	6.19810900	-12.48712600
H	-0.16743700	5.02945800	-12.17743500
H	3.51891400	7.21864800	-12.57222100
C	6.86381200	6.52193100	-9.43854600
H	7.56261300	5.54199900	-7.64704900
H	5.91279500	7.36585400	-11.18133100
H	1.23402100	6.67846200	-13.38122800
H	7.78313400	7.08449900	-9.57167400
N	3.26935800	4.45110900	-9.08747800
H	9.76982500	-4.55923400	-3.19191600
C	8.97984900	-4.13042300	-3.80140200
C	7.95669800	-3.38645700	-3.18977200
C	8.99286000	-4.31417100	-5.18160000
C	6.92378800	-2.81953700	-3.93552900
H	7.97277900	-3.24370700	-2.11235000
C	7.96843400	-3.75512500	-5.95435100
H	9.79139500	-4.87945000	-5.65440600
C	6.93572100	-3.02003900	-5.31897500
H	6.14529200	-2.23570900	-3.45439900
C	7.68966500	-3.73273400	-7.37604500
C	6.49960600	-2.98339600	-7.55246200

C	8.32915300	-4.28482300	-8.49239800
C	5.93151000	-2.79682000	-8.81534900
C	7.77616800	-4.09088700	-9.75513500
H	9.24309000	-4.86053600	-8.37352900
C	6.58730000	-3.35769600	-9.91023400
H	5.00783300	-2.24223100	-8.94459400
H	8.26408300	-4.51229300	-10.62899600
H	6.16654500	-3.22499900	-10.90305500
N	6.04502000	-2.55253100	-6.29622000
H	-13.65533300	0.24990900	2.59001400
C	-13.19999500	1.20991000	2.81704600
C	-14.00077900	2.25750900	3.30283100
C	-11.83029500	1.37536600	2.61632000
C	-13.44308100	3.50024600	3.59054200
H	-15.06434800	2.09539700	3.45067600
C	-11.27484500	2.62113400	2.91954300
H	-11.22282000	0.56307200	2.23055100
C	-12.07015700	3.69296200	3.39672600
H	-14.06558300	4.31225400	3.95645900
C	-11.18838000	4.82985000	3.56879400
C	-9.89007700	4.40780000	3.18687900
C	-11.38306600	6.14139800	4.01739900
C	-8.78857800	5.26399800	3.26704100
C	-10.29243100	7.00426600	4.08544500
H	-12.37238200	6.47958500	4.31344200
C	-9.00951600	6.56492700	3.71736000
H	-7.79151000	4.92985400	2.99884000
H	-10.43151600	8.02430000	4.43124400
H	-8.16910100	7.25003300	3.78824400
N	-9.94847200	3.06261200	2.79223800
H	-11.13877300	-6.60186700	6.34098200
C	-10.25846100	-6.03604900	6.05081500
C	-10.32588400	-5.16254800	4.95205800
C	-9.07303200	-6.18478400	6.76540200
C	-9.22019200	-4.41509200	4.54917200
H	-11.25762000	-5.06672800	4.40149600
C	-7.94766600	-5.44623900	6.38087100
H	-9.02009900	-6.86810900	7.60862100
C	-8.03752600	-4.55880200	5.27930200
H	-9.27982800	-3.75181300	3.69239600
C	-6.58701400	-5.37228600	6.87350600
C	-5.89961700	-4.44386400	6.05148700
C	-5.90876000	-5.99324800	7.92877000

C	-4.56100300	-4.11350200	6.28051600
C	-4.57086700	-5.67982500	8.15360000
H	-6.42198700	-6.70695900	8.56750800
C	-3.90915200	-4.74590000	7.33853500
H	-4.04506800	-3.38349700	5.66485400
H	-4.03441300	-6.15548300	8.96931000
H	-2.86821400	-4.50610500	7.53829700
N	-6.78709100	-3.95190600	5.08318300
N	1.51835500	0.61074000	-5.41611200
N	-5.67437700	-0.14458300	1.13879700
H	-6.09592200	0.48009900	-1.44638800
H	-1.08178100	0.99396800	-6.02777000

The optimized geometry of **2** in excited state at UB3LYP/LANL2DZ/6-31G* level

Ir	0.01812400	0.08826400	0.04637300
C	0.00585900	0.15035000	2.06916200
C	2.04199500	0.10299200	0.05316800
C	-3.92110900	-0.36816900	-1.92555600
N	-2.16399900	-0.08141700	-0.22670600
C	-4.47007600	-0.27309400	0.42966100
C	-6.54464500	0.53086900	1.57712900
C	-4.87780300	-0.42569000	-0.91910200
C	2.71647300	-0.54119300	-5.35252100
C	-0.86742400	-0.13488400	-4.88511900
N	-0.23292500	0.11009300	-2.14645300
N	-0.21751900	2.12868600	0.34051300
C	-3.26789600	-0.43459600	-4.28183700
H	-3.52759000	-0.53932500	-5.33208500
C	-7.26652900	0.20582700	2.75544400
C	-1.88384400	-0.21677900	-3.94057500
C	-0.28272100	2.53235600	1.64674900
C	-0.17249800	1.44851600	2.62203400
C	0.46236500	0.08769100	-4.44927900
C	1.71726700	-2.30431700	-0.14226700
C	-5.40669700	-1.14055400	2.59266100
C	2.06910200	-3.65975600	-0.24265500
H	3.11633100	-3.93852600	-0.26044000
C	-6.53413100	-0.86166400	3.40941400
N	0.39502100	-1.95190500	-0.10735500
C	3.11875600	-1.54943200	-4.47029100
H	2.47771300	-1.88410400	-3.66236400
C	-4.23411400	-0.50358100	-3.32677700

H	-5.27194300	-0.66235200	-3.60804600
C	0.06276800	-0.71552800	4.35356700
H	0.16454600	-1.56344100	5.02736800
C	0.71796600	0.20660300	-3.08156400
H	1.72574100	0.38825500	-2.72093600
C	4.04468600	-1.32798700	-0.11032900
H	4.49557500	-2.31328900	-0.19731900
C	2.64709200	-1.17881100	-0.06653200
C	-3.11422000	-0.10087100	0.71499000
H	-2.77541100	0.02090300	1.73928400
C	-1.55083300	-0.09448100	-2.54941400
C	1.58192400	1.07110700	-6.46345000
C	0.94834600	2.78480700	-8.00550400
H	0.25555900	3.54982100	-8.33951800
C	3.54288000	-0.13352700	-6.43250600
C	2.81429000	0.89724500	-7.14653000
C	0.12379300	-0.91803200	2.97328700
H	0.27359100	-1.92725300	2.59907600
C	-2.54482500	-0.17759000	-1.56437700
C	-0.55616900	-2.90308200	-0.17940700
H	-1.57753700	-2.54458900	-0.15303500
C	3.09798800	1.66091900	-8.27779700
H	4.01954300	1.52141500	-8.83357600
C	4.79779600	-0.71487400	-6.60886700
H	5.45980800	-0.39151300	-7.40556900
C	4.29125600	1.05989300	0.08462800
H	4.93064400	1.93719400	0.14980900
C	0.64692700	2.02378100	-6.88262300
H	-0.27885300	2.18202800	-6.34046600
C	-8.42566800	0.90904500	3.07852300
H	-8.97413200	0.69979800	3.99126600
C	-0.23610400	1.64947100	4.01187700
H	-0.37406200	2.64598000	4.42326300
C	-0.52986500	4.82874900	0.91897200
H	-0.64741700	5.88335000	1.15020800
C	5.21333200	-1.71225600	-5.71727500
C	-4.49503700	-2.14524500	2.93300300
H	-3.64789300	-2.37744500	2.29726000
C	-0.46619500	4.39328700	-0.40792000
H	-0.53313600	5.08623100	-1.23946800
C	-6.96508600	1.56001500	0.72791100
H	-6.40993900	1.81364800	-0.16838200
C	2.90399600	1.20996600	0.13031400

H	2.49049700	2.20960300	0.23274000
C	-8.86339900	1.92706100	2.22089600
C	-6.73470700	-1.57638400	4.58937700
H	-7.57131300	-1.35692100	5.24484000
C	4.36621200	-2.12762200	-4.66636600
H	4.69664200	-2.92826900	-4.01370100
C	-4.71310000	-2.85596900	4.10654200
H	-4.03690100	-3.65721100	4.38464100
C	-0.11919900	0.56917000	4.87868100
H	-0.16300700	0.72460700	5.95272200
C	2.15855800	2.60562500	-8.71150600
C	-0.25785600	-4.25406100	-0.28064900
H	-1.05992100	-4.98196200	-0.33491200
C	-5.81733200	-2.57512200	4.94090700
C	-8.13007100	2.24320000	1.05601500
H	-8.49887100	3.02414800	0.39967900
C	-0.43948700	3.89532000	1.94209800
H	-0.48472600	4.21428100	2.97684900
C	4.86766800	-0.21035300	-0.03581100
H	5.94773200	-0.32397200	-0.06065500
C	-0.31117300	3.03648200	-0.65050500
H	-0.25407700	2.63816000	-1.65600700
C	1.08606500	-4.63721600	-0.31028000
H	1.36136200	-5.68514300	-0.38472400
C	1.56447200	3.53887900	-10.96224500
C	3.58331900	4.13678900	-10.09812300
C	0.31888600	2.95216800	-11.20472400
C	2.18399200	4.38960000	-11.91230700
C	4.69595700	4.33336600	-9.27447200
C	3.47062300	4.77156400	-11.36106600
C	-0.31582600	3.25397900	-12.40901400
H	-0.13779900	2.27725500	-10.48901800
C	1.52800000	4.67601600	-13.11232500
C	5.71600700	5.15680700	-9.74960800
H	4.76315800	3.87360600	-8.29440800
C	4.50561900	5.59345400	-11.81407900
C	0.27593700	4.10993500	-13.35208900
H	-1.28536000	2.81260200	-12.62116900
H	1.98928900	5.32486500	-13.85158000
C	5.62816900	5.77695700	-11.00659300
H	6.59242300	5.32413600	-9.13023700
H	4.43510400	6.08798900	-12.77885300
H	-0.24404500	4.32628200	-14.28046700

H	6.43962100	6.41212700	-11.34886900
N	2.42080400	3.38831500	-9.86099500
H	10.52822800	-3.03206200	-2.59433400
C	9.67052200	-2.86645100	-3.23934300
C	8.53344200	-2.21896600	-2.72938100
C	9.71212100	-3.28878600	-4.56790700
C	7.41116000	-1.98719900	-3.52407000
H	8.52762700	-1.88513000	-1.69556300
C	8.60024500	-3.06930500	-5.38518700
H	10.59949500	-3.77528000	-4.96317400
C	7.45291200	-2.43081100	-4.84972900
H	6.54434100	-1.47161900	-3.12425000
C	8.31722400	-3.34529500	-6.78113100
C	7.00966300	-2.86218400	-7.04019500
C	9.03962400	-3.96267200	-7.80545200
C	6.40703100	-3.01156300	-8.29297700
C	8.45237300	-4.09610900	-9.06359700
H	10.04252500	-4.33881500	-7.62357600
C	7.14884900	-3.62944100	-9.29901700
H	5.39377100	-2.67175600	-8.47826100
H	9.00470900	-4.57258200	-9.86791900
H	6.70440900	-3.75591000	-10.28197300
N	6.48902200	-2.30722800	-5.86193200
H	-13.33173800	-0.57862000	3.19474600
C	-13.00488700	0.45697100	3.17160200
C	-13.92525700	1.47943600	3.45403200
C	-11.67781900	0.74327400	2.85357100
C	-13.53614000	2.81836200	3.41287500
H	-14.95190700	1.22426900	3.69881500
C	-11.28949200	2.08640100	2.83470400
H	-10.97813300	-0.05141600	2.61820300
C	-12.21129200	3.13100100	3.09832300
H	-14.25536900	3.60676600	3.61640300
C	-11.48895100	4.37978800	2.94479500
C	-10.15700500	4.04544600	2.59208000
C	-11.84754000	5.72224000	3.09114800
C	-9.17790700	5.02683400	2.41086600
C	-10.88039800	6.70741700	2.89254100
H	-12.86362200	5.99501800	3.36222300
C	-9.56080200	6.35916400	2.56152300
H	-8.15265000	4.76623700	2.17130200
H	-11.14749400	7.75421500	3.00185000
H	-8.81958900	7.14117100	2.42389200

N	-10.04180300	2.64856000	2.52694600
H	-9.99737100	-6.01504800	8.17458900
C	-9.19216000	-5.44483200	7.72125600
C	-9.38355700	-4.85605400	6.46066200
C	-7.97565100	-5.31288900	8.39102100
C	-8.37474500	-4.11585100	5.84533400
H	-10.33358000	-4.98273800	5.94957500
C	-6.94954700	-4.57463500	7.79599400
H	-7.82700000	-5.78302500	9.35910500
C	-7.16528800	-3.97035800	6.53153900
H	-8.52387600	-3.67995100	4.86333100
C	-5.58738000	-4.26199000	8.18595500
C	-5.02838800	-3.48141700	7.14246800
C	-4.81839900	-4.55576400	9.31486500
C	-3.72914400	-2.97090400	7.22233400
C	-3.51478500	-4.06580000	9.39289000
H	-5.23175500	-5.15137400	10.12400000
C	-2.98225200	-3.27856400	8.35896300
H	-3.31539100	-2.34893300	6.43577700
H	-2.90717000	-4.28823800	10.26492300
H	-1.96936900	-2.89588000	8.44589500
N	-5.99344300	-3.30735900	6.13924700
N	1.53065100	0.19438800	-5.37909900
N	-5.42240100	-0.29322500	1.48409000
H	-5.92252400	-0.59666800	-1.15945100
H	-1.08508300	-0.25773800	-5.94141800