# Supporting Information

## Efficient green electroluminescence of iridium complexes with high electron mobility

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### General information

$^1$H NMR spectra were measured on a Bruker AM 500 spectrometer. Electrospray ionization mass spectra (ESI-MS) were obtained with ESI-MS (LCQ Fleet, Thermo Fisher Scientific). Elemental analyses for C, H and N were performed on an Elementar Vario MICRO analyzer. TG-DSC measurements were carried out on a DSC 823e analyzer (METTLER). UV-vis absorption and photoluminescence spectra were measured on a Shimadzu UV-3100 and a Hitachi F-4600 spectrophotometer at room temperature, respectively. Cyclic voltammetry measurements were conducted on a MPI-A multifunctional electrochemical and chemiluminescent system at room temperature using $Fc^+/Fc$ as the internal standard and scan rate of 0.05 V $s^{-1}$. The luminescence quantum efficiencies were calculated by comparison of the emission intensities (integrated areas) of a standard sample (*fac*-$Ir(ppy)_3$) and the unknown sample.[1]

### X-ray crystallography

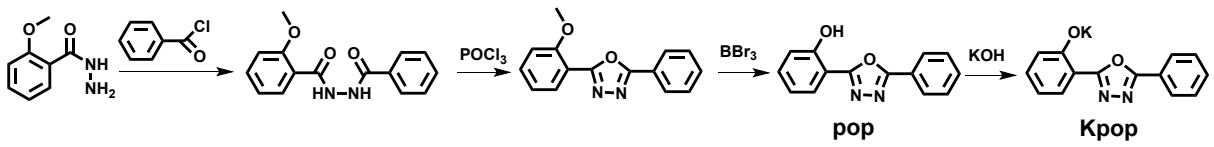
X-ray crystallographic measurements of the single crystals were carried out on a Bruker SMART CCD diffractometer (Bruker Daltonic Inc.) using monochromated Mo Kα radiation (λ = 0.71073 Å) at room temperature. Cell parameters were retrieved using SMART software and refined using *SAINT* [2] program in order to reduce the highly redundant data sets. Data were collected using a narrow-frame method with scan width of 0.30° in $\omega$ and an exposure time of 5 s per frame. Absorption corrections were applied using *SADABS* [3] supplied by Bruker. The structures were solved by Patterson methods and refined by full-matrix least-squares on $F^2$ using the program *SHELXS-2014*.[4] The positions of metal atoms and their first coordination spheres were located from direct-methods E-maps, other non-hydrogen atoms were found in alternating difference Fourier syntheses and least-squares refinement cycles and

during the final cycles refined anisotropically. Hydrogen atoms were placed in calculated position and refined as riding atoms with a uniform value of $U_{iso}$.

**OLEDs fabrication and measurement**

All OLEDs were fabricated on the pre-patterned ITO-coated glass substrate with a sheet resistance of 15 Ω / sq. The deposition rate for organic compounds (TAPC (1,1-*bis*(4-(di-p-tolylamino)phenyl)cyclohexane, mCP (1,3-bis(9H-carbazol-9-yl)benzene, PPO21 3-(diphenylphosphoryl)-9-(4-(diphenyl-phosphoryl)phenyl)-9H-carbazole, TmPyPB (1,3,5-*tri*(m-pyrid-3-yl-phenyl) benzene)) is 1 Å/s. The phosphors and the host PPO21 was co-evaporated to form emitting layer from two separate sources. The cathode of LiF and Al were deposited with deposition rates of 0.1 and 3 Å/s, respectively. The characteristic curves of the devices were measured with a computer which controlled KEITHLEY 2400 source meter with a calibrated silicon diode in air without device encapsulation. On the basis of the uncorrected PL and EL spectra, the Commission Internationale de l'Eclairage (CIE) coordinates were calculated using a test program of the Spectra scan PR650 spectrophotometer.

**Synthesis of pop and Kpop.**




**Scheme S1.** The synthetic routes of the ancillary ligand.

Benzoyl chloride (1.40 g, 10 mmol) was added dropwise to a solution of 2-methoxybenzohydrazine (1.66 g, 10 mmol) and triethylamine (1.01 g, 10 mmol) in chloroform (20 mL) at room temperature (RT). The resulting mixture was stirred for 2 h and then filtered. The collected solid was washed with water and ethanol to give N′-benzoyl-2-methoxybenzohydrazine (2.57 g, 95% yield). A mixture of N′-benzoyl-2-methoxybenzohydrazine and $POCl_3$ (20 mL) in a 50 mL flask was refluxed under nitrogen for 5 h. The excess $POCl_3$ was then distilled out, and the residue was poured into water. The crude solid product was collected by filtration and purified by recrystallization from chloroform/hexane to give 2-(2-methoxyphenyl)-5-phenyl-1,3,4-oxadiazole (1.91 g, 80% yield). Then, to a mixture of 2-(2-methoxyphenyl)-5-phenyl-1,3,4- oxadiazole (1.91 g) in 50 mL $CH_2Cl_2$ cooled to 78 $^oC$ was added $BBr_3$ (12.5 g, 50 mmol in 20 mL $CH_2Cl_2$) dropwise. The mixture was stirred for 24 h at 78 $^oC$ and the resulting solution was poured into water,

extracted with $CH_2Cl_2$ (50 mL, 3 times) and then dried over anhydrous sodium sulfate. The solvent was removed under reduced pressure and recrystallization of the residue from ethanol gave colorless crystals.

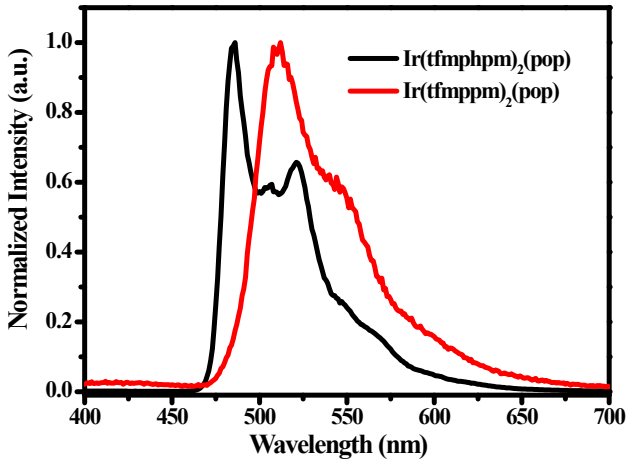



**Fig. S1.** Emission spectra of $Ir(tfmphpm)_2(pop)$ and $Ir(tfmppm)_2(pop)$ complexes in degassed $CH_2Cl_2$ solutions ($5.0 \times 10^{-5}$ mol $L^{-1}$) at 77 K.

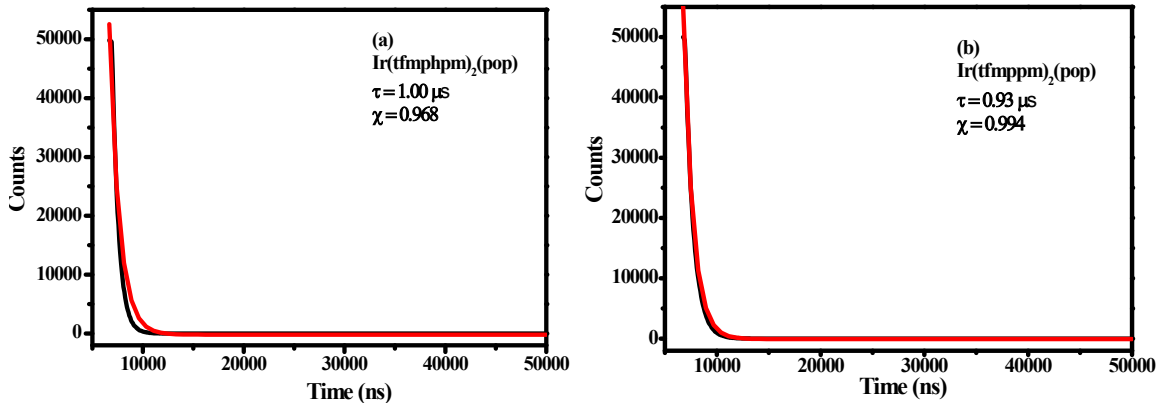



**Fig. S2**. The lifetime curves of $Ir(tfmphpm)_2(pop)$ and $Ir(tfmppm)_2(pop)$ complexes.

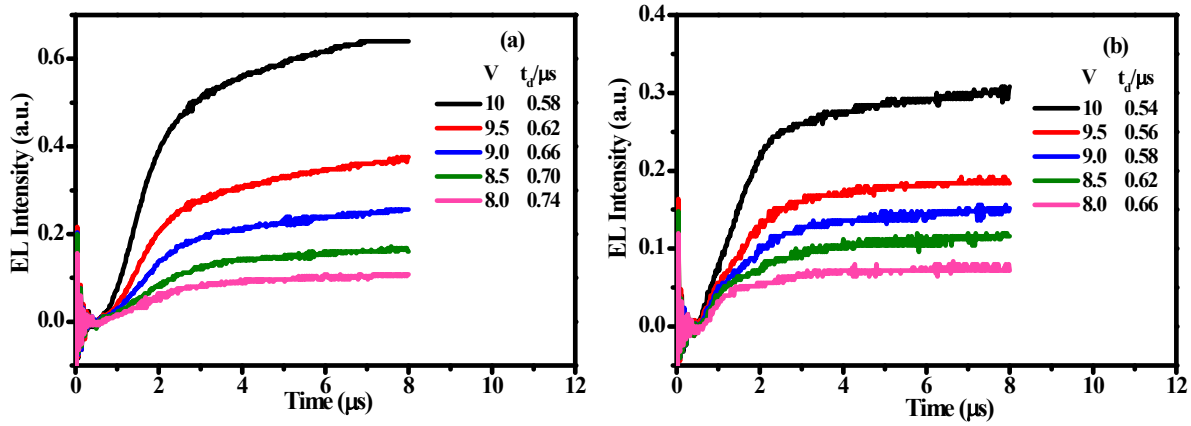
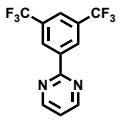
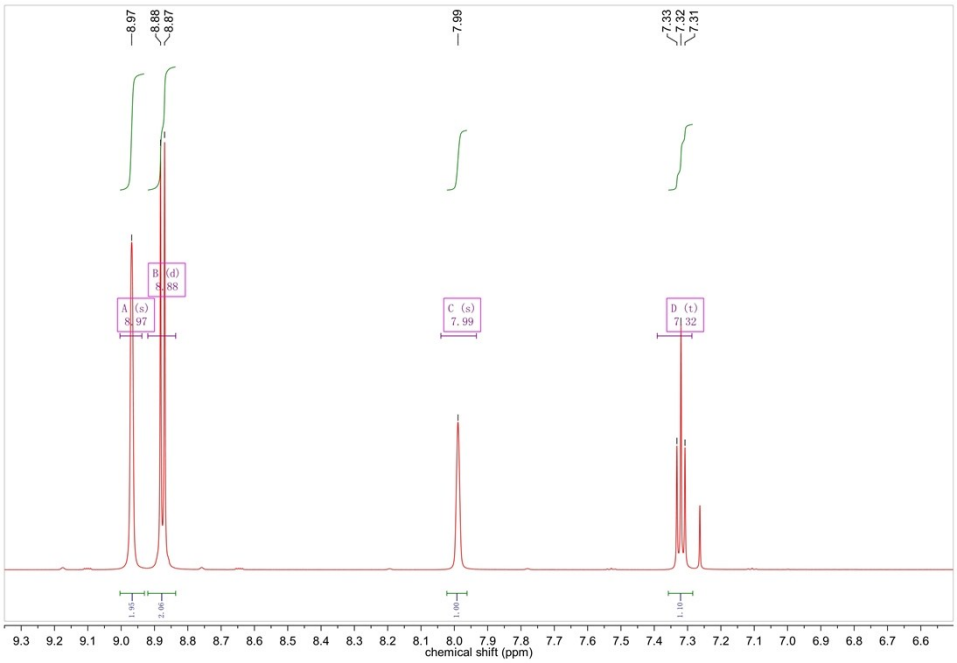
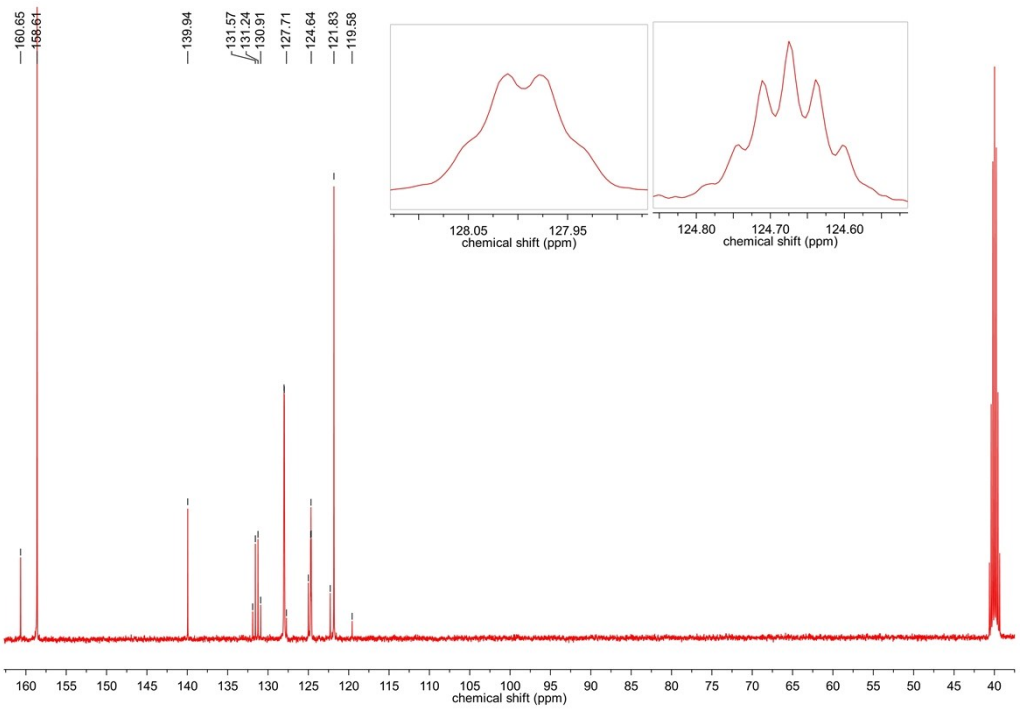


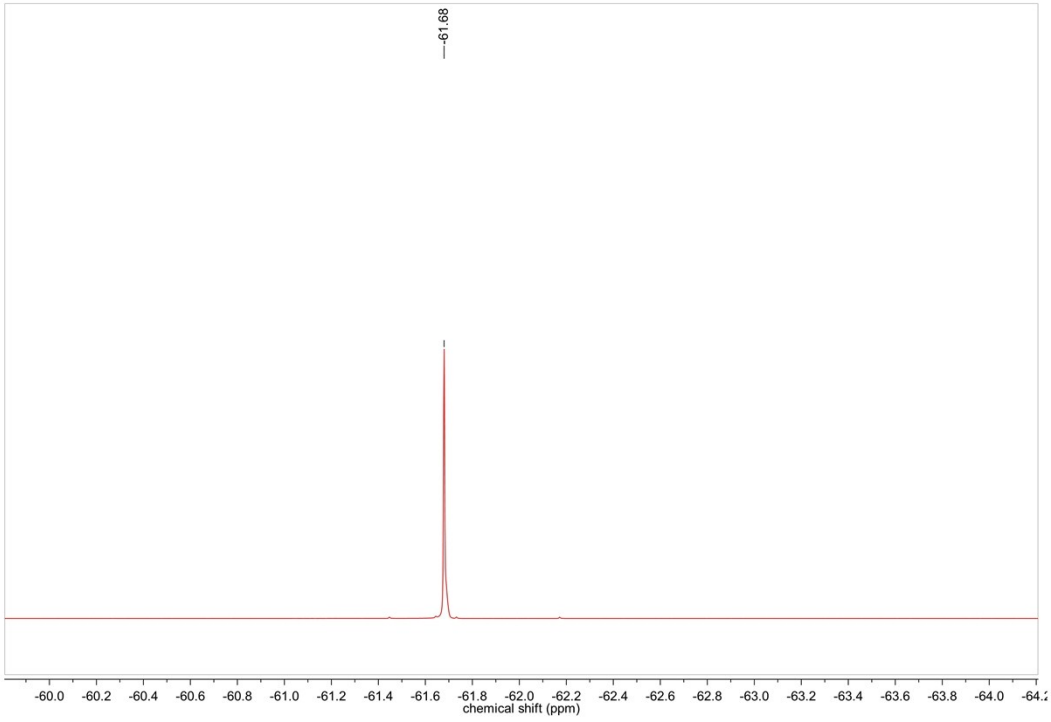

**Fig. S3** the transient EL signals for the device structure of ITO/TAPC (50nm)/Ir complexes (60nm)/ LiF (1 nm)/ Al (100 nm) under different applied fields of $Ir(tfmphpm)_2(pop)$ and $Ir(tfmppm)_2(pop)$.

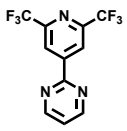



tfmphpm

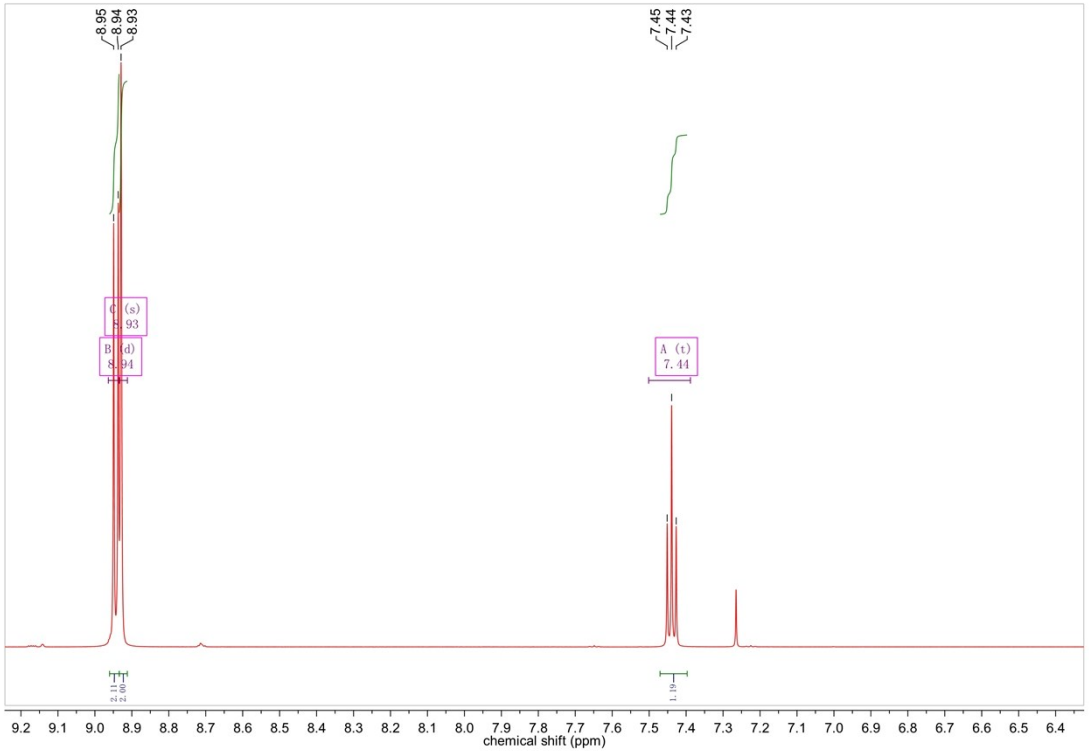


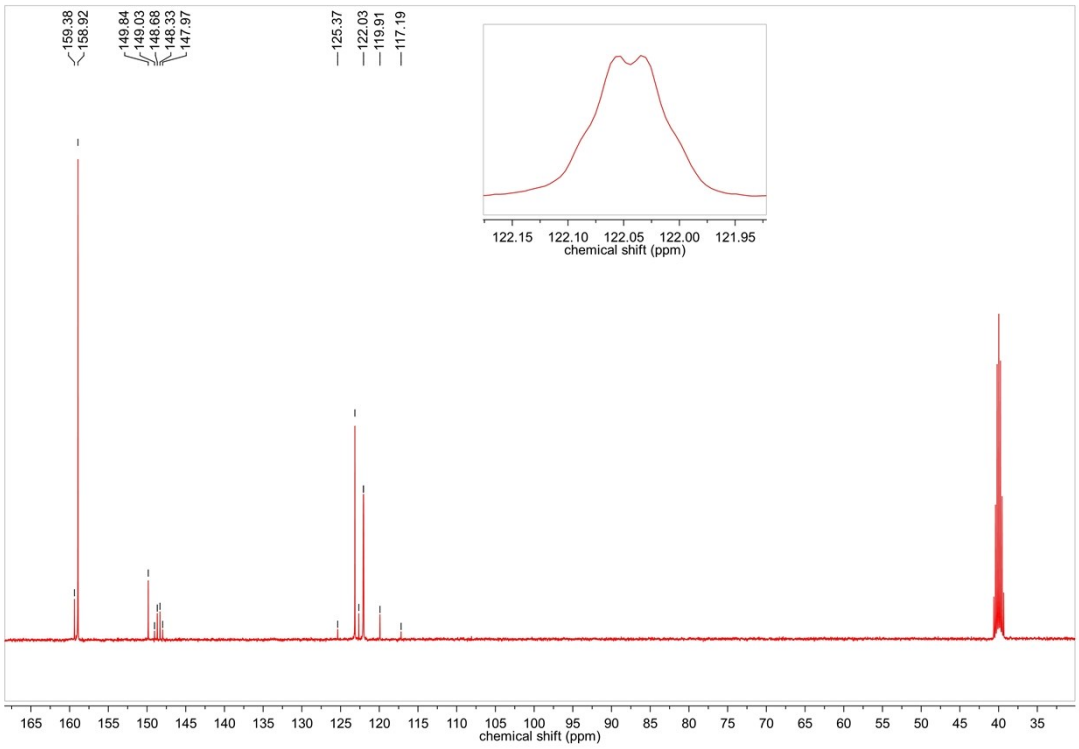

160.65
158.61
139.94
131.57
131.24
130.91
127.71
124.64
121.83
119.58
128.05
127.95
chemical shift (ppm)
124.80
124.70
124.60
chemical shift (ppm)
160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40
chemical shift (ppm)

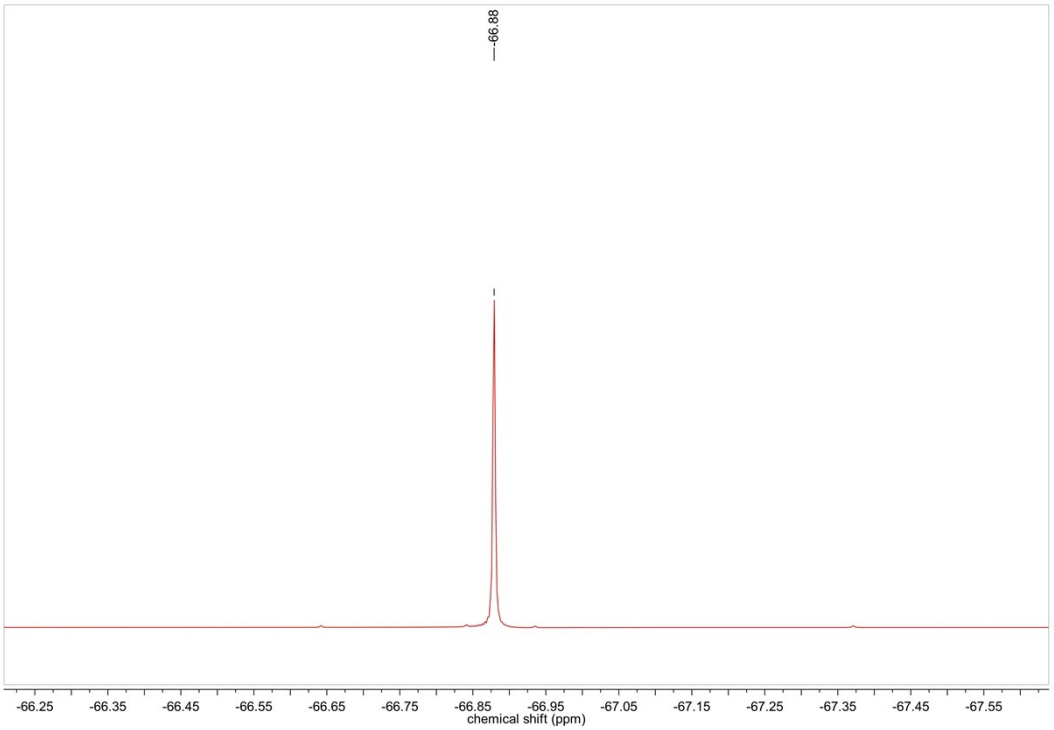

-61.68
-60.0 -60.2 -60.4 -60.6 -60.8 -61.0 -61.2 -61.4 -61.6 -61.8 -62.0 -62.2 -62.4 -62.6 -62.8 -63.0 -63.2 -63.4 -63.6 -63.8 -64.0
chemical shift (ppm)

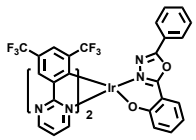

F3C
N
CF3
N
N

**tfmppm**

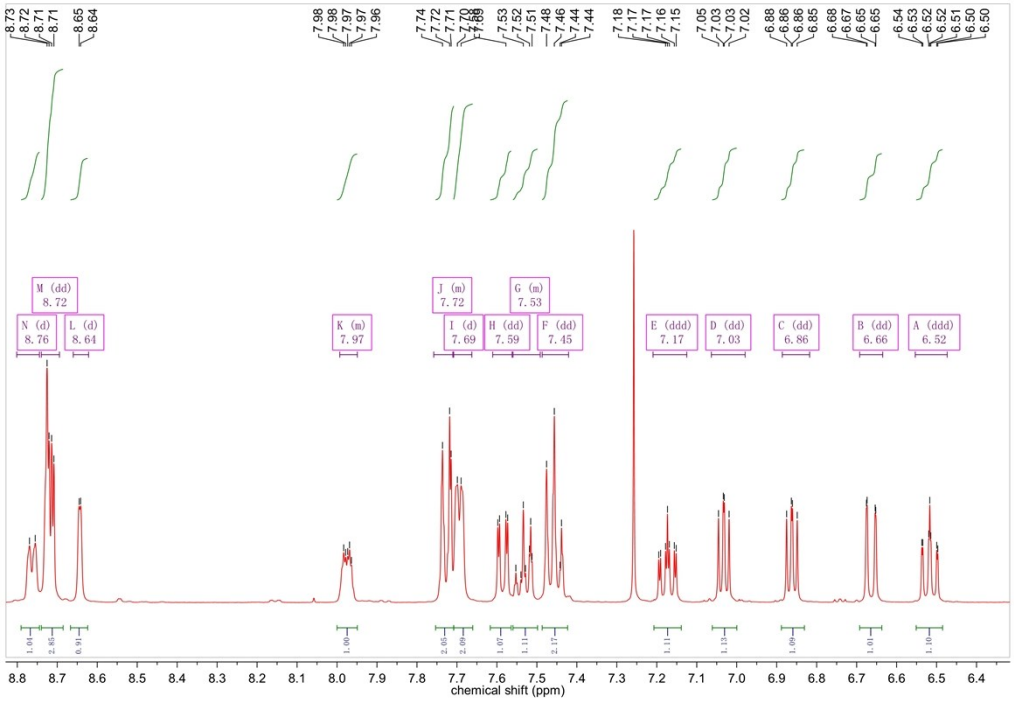

8.95
8.94
8.93
7.45
7.44
7.43
C (s)
7.93
B (d)
8.94
A (t)
7.44
2.11
2.00
1.19
9.2 9.1 9.0 8.9 8.8 8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5 6.4
chemical shift (ppm)

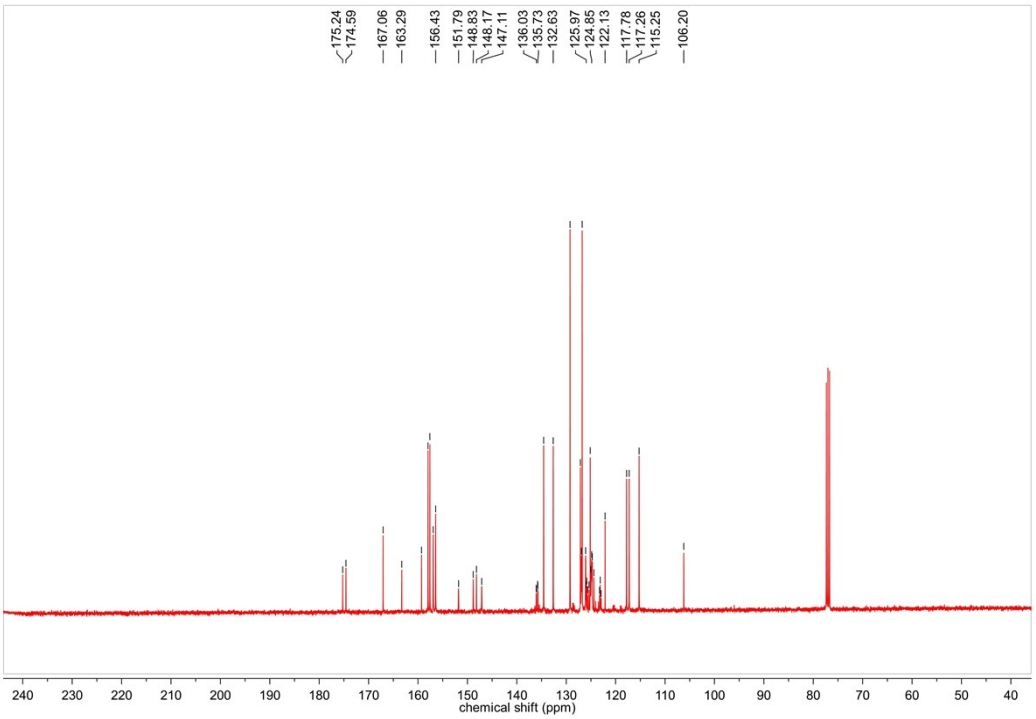

159.38
158.92
149.84
149.03
148.68
148.33
147.97
125.37
122.03
119.91
117.19
122.15 122.10 122.05 122.00 121.95
chemical shift (ppm)
165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35
chemical shift (ppm)

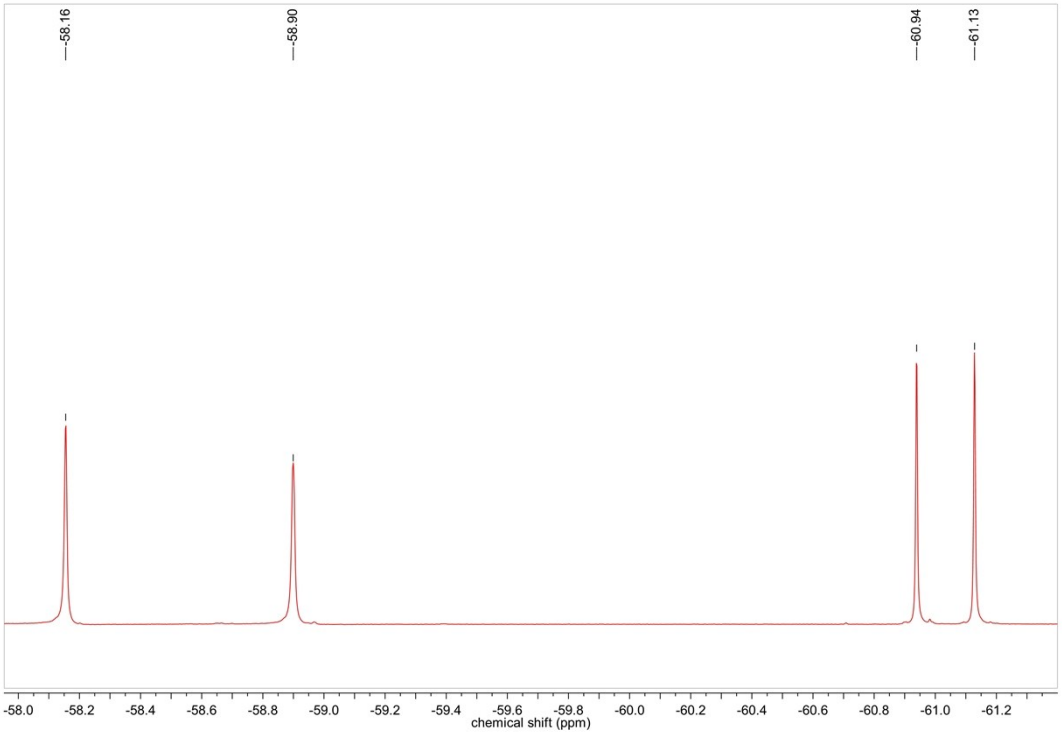


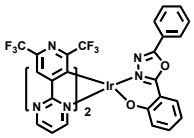




**Ir(tfmphphm)$_2$(pop)**

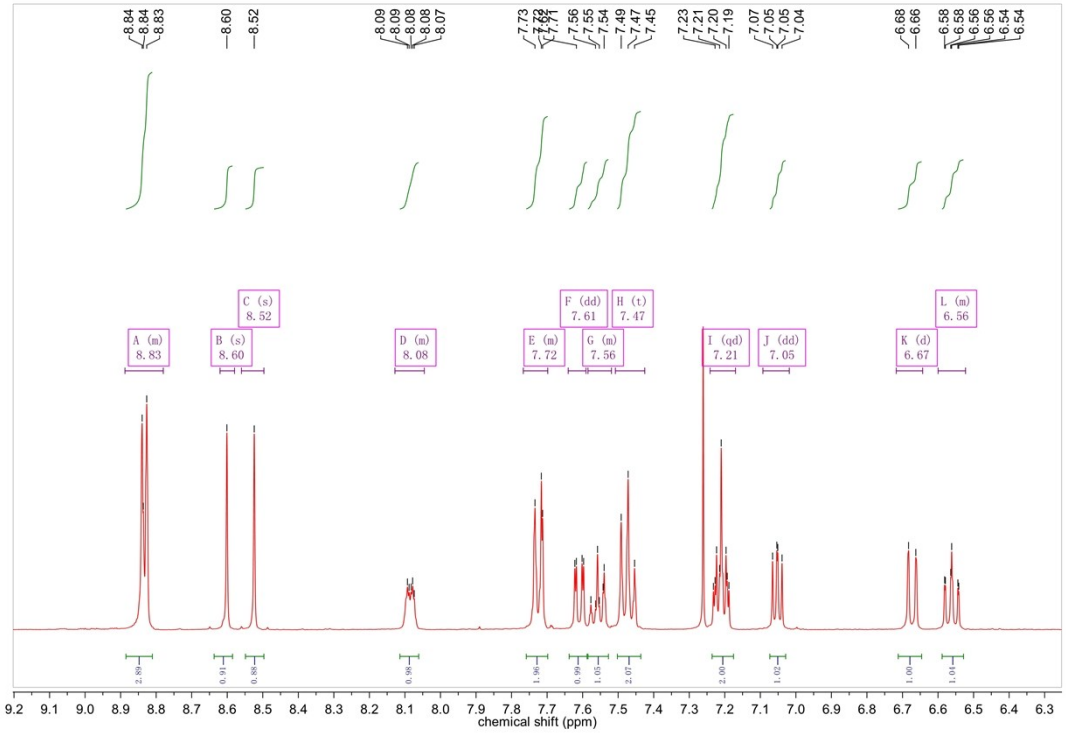


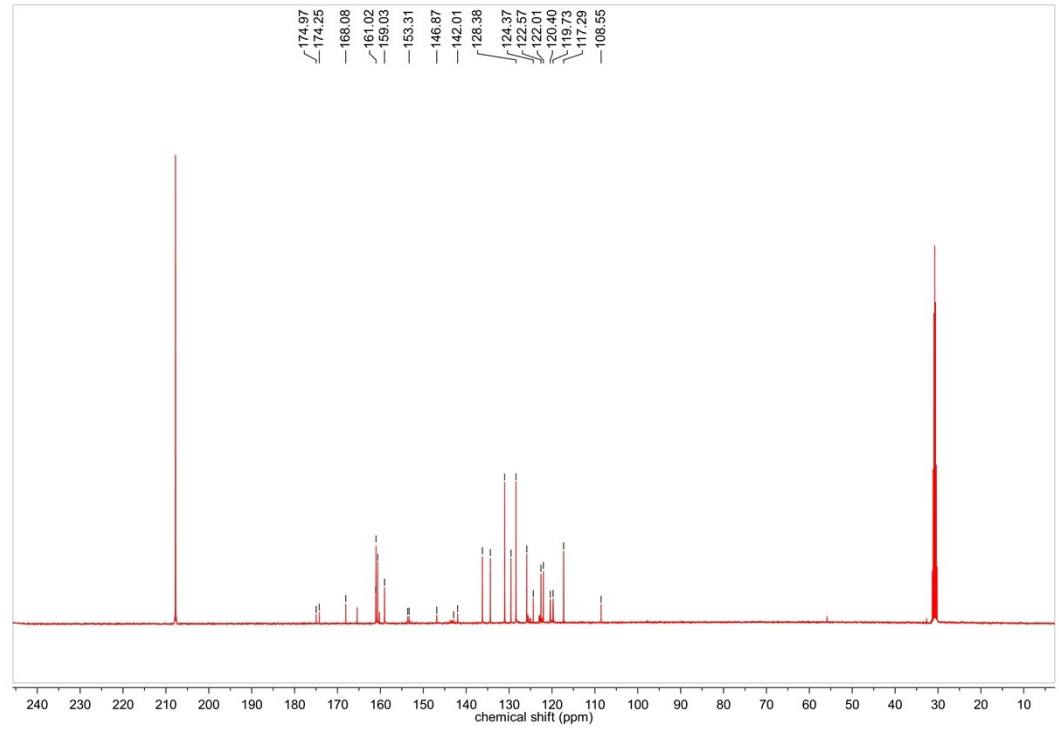

175.24
174.59
167.06
163.29
156.43
151.79
148.83
148.17
147.11
136.03
135.73
132.63
125.97
124.85
122.13
117.78
117.26
115.25
106.20
240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40
chemical shift (ppm)


-58.16
-58.90
-60.94
-61.13
-58.0 -58.2 -58.4 -58.6 -58.8 -59.0 -59.2 -59.4 -59.6 -59.8 -60.0 -60.2 -60.4 -60.6 -60.8 -61.0 -61.2
chemical shift (ppm)



**Ir(tfmppm)$_2$(pop)**



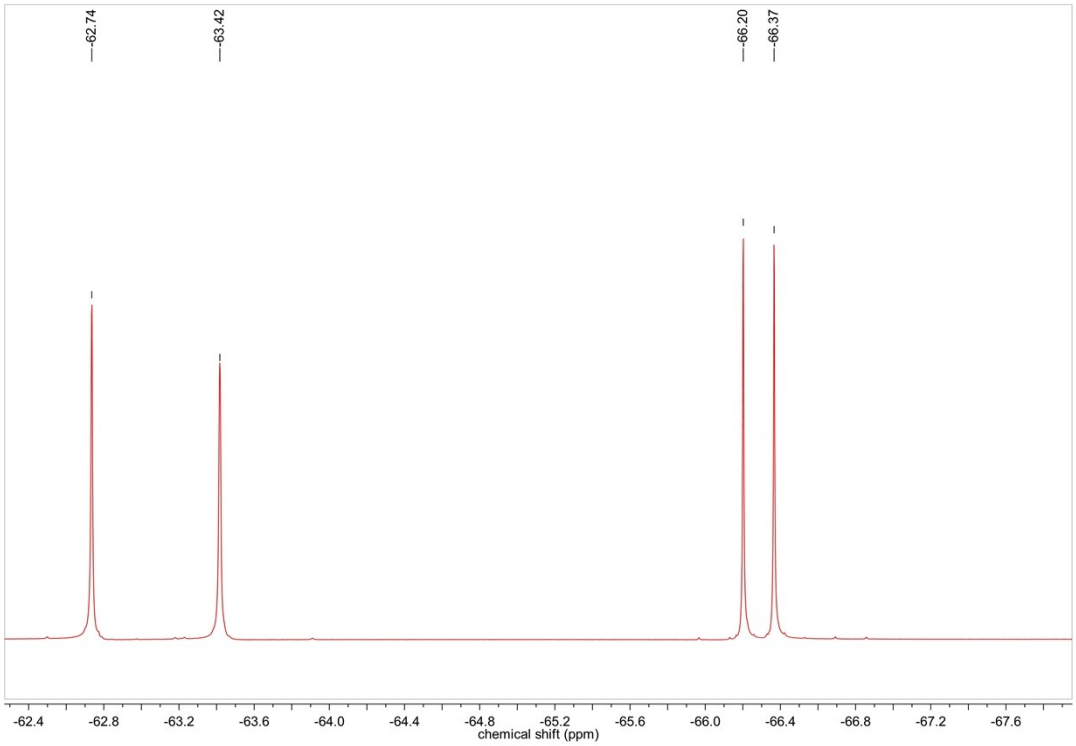



**Fig. S4** the $^{1}H$ NMR, $^{13}C$ NMR and $^{19}F$ NMR spectra of tfmphpm, tfmppm, Ir(tfmphpm)$_2$(pop) and Ir(tfmppm)$_2$(pop).

**Table S1**. Crystallographic data of **Ir(tfmphpm)$_2$(pop)** and **Ir(tfmppm)$_2$(pop)**.

| | **Ir(tfmppm)$_2$(pop)** | **Ir(tfmppm)$_2$(pop)** |
|---|---|---|
| Formula | $C_{38}H_{19}F_{12}IrN_6O_2$ | $C_{36}H_{17}F_{12}IrN_8O_2$ |
| FW | 1011.81 | 1013.78 |
| T (K) | 296(2) | 296(2) |
| Wavelength (Å) | 0.71073 | 0.71073 |
| Crystal system | Triclinic | triclinic |
| Space group | P -1 | P -1 |
| *a* (Å) | 11.3342(4) | 10.1801(5) |
| *b* (Å) | 15.8645(6) | 10.4639(5) |
| *c* (Å) | 21.0886(8) | 19.0893(9) |
| *α* (deg) | 77.2170(10) | 77.9680(10) |
| *β* (deg) | 76.3170(10) | 81.7620(10) |
| *γ* (deg) | 81.2300(10) | 65.3410(10) |
| *V* (Å$^3$) | 3572.9(2) | 1803.79(15) |
| *Z* | 4 | 2 |

| | | |
|---|---|---|
| $\rho_{calcd}$ (mg/cm$^3$) | 1960.0 | 1.867 |
| $\mu$ (Mo Kα) (mm$^{-1}$) | 3.846 | 3.810 |
| $F$ (000) | 1960.0 | 980 |
| Reflns collected | 33189 | 12443 |
| Unique | 8290 | 8290 |
| Data/restraints/params | 16806 / 6 / 1063 | 8290 / 6 / 532 |
| GOF on $F^2$ | 1.026 | 0.978 |
| $R_1{}^a$, $wR_2{}^b$ [$I > 2\sigma(I)$] | 0.0350, 0.0698 | 0.0381, 0.1085 |
| $R_1{}^a$, $wR_2{}^b$ (all data) | 0.0552, 0.0759 | 0.0481, 0.1358 |
| CCDC NO | 1830696 | 1830699 |

$R_1{}^a = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. $wR_2{}^b = [\Sigma w(F_o{}^2 - F_c{}^2)^2/\Sigma w(F_o{}^2)]^{1/2}$

**Table S2a** The selected bond lengths and angles of **Ir(tfmphpm)$_2$(pop)**.

| **Selected bonds Å** | | | | | |
|---|---|---|---|---|---|
| Ir(01)-N(9) | 2.029(3) | N(10)-C(02) | 1.332(5) | C(36)-H(36) | 0.93 |
| Ir(01)-N(8) | 2.039(3) | C(3)-C(24) | 1.414(5) | C(37)-C(40) | 1.398(6) |
| Ir(01)-C(3) | 2.044(4) | C(3)-C(4) | 1.426(5) | C(37)-C(61) | 1.491(6) |
| Ir(01)-C(0) | 2.064(4) | C(4)-C(7) | 1.393(5) | C(38)-C(55) | 1.374(7) |
| Ir(01)-N(11) | 2.080(3) | C(4)-C(11) | 1.466(5) | C(38)-H(38) | 0.93 |
| Ir(01)-O(4) | 2.117(3) | C(5)-C(23) | 1.378(6) | C(39)-H(39) | 0.93 |
| Ir(02)-N(3) | 2.026(4) | C(5)-H(5) | 0.93 | C(40)-C(55) | 1.372(6) |
| Ir(02)-N(1) | 2.031(4) | C(6)-C(37) | 1.405(6) | C(40)-H(40) | 0.93 |
| Ir(02)-C(6) | 2.034(4) | C(6)-C(13) | 1.427(6) | C(41)-C(63) | 1.364(6) |
| Ir(02)-C(8) | 2.038(4) | N(2)-C(51) | 1.322(6) | C(41)-H(41) | 0.93 |
| Ir(02)-N(5) | 2.107(3) | N(2)-C(25) | 1.327(6) | F(22)-C(68) | 1.306(7) |
| Ir(02)-O(2) | 2.116(3) | C(7)-C(31) | 1.377(6) | C(42)-C(54) | 1.382(6) |
| F(1)-C(20) | 1.352(5) | C(7)-H(7) | 0.93 | C(42)-H(42) | 0.93 |
| F(2)-C(20) | 1.347(6) | C(8)-C(10) | 1.421(6) | C(43)-C(50) | 1.468(6) |
| F(3)-C(22) | 1.345(4) | C(8)-C(19) | 1.424(5) | C(44)-H(44) | 0.93 |
| O(2)-C(18) | 1.309(5) | C(9)-C(12) | 1.373(6) | C(45)-C(59) | 1.392(7) |
| F(4)-C(46) | 1.347(5) | C(9)-C(17) | 1.376(6) | C(45)-H(45) | 0.93 |
| F(5)-C(22) | 1.338(5) | C(9)-H(9) | 0.93 | C(47)-C(02) | 1.392(6) |
| O(4)-C(32) | 1.303(5) | C(10)-C(26) | 1.382(6) | C(47)-H(47) | 0.93 |
| F(6)-C(22) | 1.347(5) | C(10)-C(21) | 1.463(6) | F(23)-C(68) | 1.272(7) |
| F(7)-C(15) | 1.346(4) | C(12)-H(12) | 0.93 | C(49)-C(62) | 1.371(6) |
| F(8)-C(15) | 1.347(6) | C(13)-C(38) | 1.377(6) | C(49)-C(63) | 1.392(7) |
| F(9)-C(15) | 1.340(5) | C(13)-C(25) | 1.456(6) | C(49)-H(49) | 0.93 |
| F(10)-C(20) | 1.343(5) | F(20)-C(66) | 1.309(5) | C(50)-C(70) | 1.385(8) |
| F(11)-C(46) | 1.344(5) | C(14)-C(31) | 1.380(6) | C(50)-C(53) | 1.392(8) |
| N(8)-C(17) | 1.338(5) | C(14)-C(24) | 1.392(6) | C(51)-H(51) | 0.93 |
| N(8)-C(2) | 1.357(5) | C(14)-H(14) | 0.93 | C(52)-C(56) | 1.377(7) |
| F(12)-C(61) | 1.342(5) | F(21)-C(64) | 1.336(6) | C(52)-H(52) | 0.93 |

| | | | | | |
|---|---|---|---|---|---|
| O(1I)-C(16) | 1.364(5) | C(15)-C(19) | 1.500(6) | C(53)-C(71) | 1.422(7) |
| O(1I)-C(27) | 1.367(5) | C(16)-C(33) | 1.428(6) | C(53)-H(53) | 0.93 |
| F(13)-C(61) | 1.349(5) | C(17)-H(17) | 0.93 | C(54)-C(66) | 1.482(6) |
| F(14)-C(61) | 1.355(5) | C(18)-C(41) | 1.426(6) | F(24)-C(68) | 1.281(7) |
| N(11)-C(48) | 1.305(5) | C(18)-C(33) | 1.427(5) | C(02)-H(02) | 0.93 |
| N(11)-N(12) | 1.410(4) | N(4)-C(21) | 1.321(6) | C(55)-C(68) | 1.487(6) |
| F(15)-C(46) | 1.337(6) | N(4)-C(52) | 1.343(6) | C(56)-H(56) | 0.93 |
| O(3N)-C(43) | 1.365(5) | C(19)-C(42) | 1.391(6) | C(57)-C(65) | 1.385(7) |
| O(3N)-C(48) | 1.366(5) | C(20)-C(28) | 1.498(6) | C(57)-C(58) | 1.387(7) |
| N(9)-C(35) | 1.341(5) | C(22)-C(24) | 1.503(5) | C(57)-H(57) | 0.93 |
| N(9)-C(11) | 1.355(5) | C(23)-C(44) | 1.375(6) | C(58)-C(67) | 1.374(7) |
| N(1)-C(39) | 1.337(6) | C(23)-C(64) | 1.494(6) | C(59)-C(60) | 1.378(7) |
| N(1)-C(25) | 1.369(5) | C(26)-C(54) | 1.388(6) | C(59)-H(59) | 0.93 |
| N(5)-C(16) | 1.302(5) | C(26)-H(26) | 0.93 | C(60)-H(60) | 0.93 |
| N(5)-N(6) | 1.406(4) | C(27)-C(58) | 1.471(6) | C(62)-H(62) | 0.93 |
| F(16)-C(64) | 1.323(6) | C(28)-C(44) | 1.390(6) | C(63)-H(63) | 0.93 |
| C(0)-C(28) | 1.416(5) | C(29)-C(60) | 1.409(6) | C(65)-C(69) | 1.361(9) |
| C(0)-C(1) | 1.422(5) | C(29)-C(32) | 1.425(6) | C(65)-H(65) | 0.93 |
| F(17)-C(66) | 1.336(6) | C(29)-C(48) | 1.436(6) | C(67)-C(72) | 1.416(7) |
| N(3)-C(30) | 1.343(5) | C(30)-C(56) | 1.376(6) | C(67)-H(67) | 0.93 |
| N(3)-C(21) | 1.366(5) | C(30)-H(30) | 0.93 | C(69)-C(72) | 1.358(9) |
| F(18)-C(66) | 1.344(6) | C(31)-C(46) | 1.496(6) | C(69)-H(69) | 0.93 |
| N(7)-C(12) | 1.328(5) | C(32)-C(36) | 1.415(6) | C(70)-C(74) | 1.384(7) |
| N(7)-C(2) | 1.332(5) | C(33)-C(62) | 1.405(6) | C(70)-H(70) | 0.93 |
| N(6)-C(27) | 1.278(5) | C(34)-C(39) | 1.369(6) | C(71)-C(73) | 1.370(10) |
| C(1)-C(5) | 1.391(6) | C(34)-C(51) | 1.387(6) | C(71)-H(71) | 0.93 |
| C(1)-C(2) | 1.460(5) | C(34)-H(34) | 0.93 | C(72)-H(72) | 0.93 |
| F(19)-C(64) | 1.319(6) | C(35)-C(47) | 1.364(6) | C(73)-C(74) | 1.361(10) |
| N(12)-C(43) | 1.283(6) | C(35)-H(35) | 0.93 | C(73)-H(73) | 0.93 |
| N(10)-C(11) | 1.325(5) | C(36)-C(45) | 1.369(6) | C(74)-H(74) | 0.93 |

| **Selected angles°** | | | |
|---|---|---|---|
| N(9)-Ir(01)-N(8) | 173.67(14) | C(60)-C(29)-C(48) | 118.8(4) |
| N(9)-Ir(01)-C(3) | 81.23(14) | C(32)-C(29)-C(48) | 120.5(4) |
| N(8)-Ir(01)-C(3) | 104.42(14) | N(3)-C(30)-C(56) | 121.5(4) |
| N(9)-Ir(01)-C(0) | 101.17(14) | N(3)-C(30)-H(30) | 119.2 |
| N(8)-Ir(01)-C(0) | 81.38(14) | C(56)-C(30)-H(30) | 119.2 |
| C(3)-Ir(01)-C(0) | 94.87(15) | C(7)-C(31)-C(14) | 119.9(4) |
| N(9)-Ir(01)-N(11) | 84.32(13) | C(7)-C(31)-C(46) | 121.1(4) |
| N(8)-Ir(01)-N(11) | 92.74(13) | C(14)-C(31)-C(46) | 119.0(4) |
| C(3)-Ir(01)-N(11) | 90.12(14) | O(4)-C(32)-C(36) | 117.1(4) |
| C(0)-Ir(01)-N(11) | 173.07(14) | O(4)-C(32)-C(29) | 126.9(4) |
| N(9)-Ir(01)-O(4) | 91.10(12) | C(36)-C(32)-C(29) | 116.0(4) |
| N(8)-Ir(01)-O(4) | 83.13(12) | C(62)-C(33)-C(18) | 120.3(4) |
| C(3)-Ir(01)-O(4) | 171.98(13) | C(62)-C(33)-C(16) | 119.1(4) |
| C(0)-Ir(01)-O(4) | 88.88(13) | C(18)-C(33)-C(16) | 120.5(4) |
| N(11)-Ir(01)-O(4) | 86.78(12) | C(39)-C(34)-C(51) | 117.5(4) |
| N(3)-Ir(02)-N(1) | 173.62(13) | C(39)-C(34)-H(34) | 121.2 |
| N(3)-Ir(02)-C(6) | 104.15(16) | C(51)-C(34)-H(34) | 121.2 |
| N(1)-Ir(02)-C(6) | 81.20(16) | N(9)-C(35)-C(47) | 120.9(4) |

| | | | |
|---|---|---|---|
| N(3)-Ir(02)-C(8) | 81.10(15) | N(9)-C(35)-H(35) | 119.6 |
| N(1)-Ir(02)-C(8) | 101.78(15) | C(47)-C(35)-H(35) | 119.6 |
| C(6)-Ir(02)-C(8) | 97.98(16) | C(45)-C(36)-C(32) | 122.4(4) |
| N(3)-Ir(02)-N(5) | 94.24(14) | C(45)-C(36)-H(36) | 118.8 |
| N(1)-Ir(02)-N(5) | 82.24(13) | C(32)-C(36)-H(36) | 118.8 |
| C(6)-Ir(02)-N(5) | 89.38(14) | C(40)-C(37)-C(6) | 122.2(4) |
| C(8)-Ir(02)-N(5) | 172.05(14) | C(40)-C(37)-C(61) | 115.2(4) |
| N(3)-Ir(02)-O(2) | 81.53(13) | C(6)-C(37)-C(61) | 122.5(4) |
| N(1)-Ir(02)-O(2) | 92.92(13) | C(55)-C(38)-C(13) | 119.2(4) |
| C(6)-Ir(02)-O(2) | 173.33(15) | C(55)-C(38)-H(38) | 120.4 |
| C(8)-Ir(02)-O(2) | 86.27(13) | C(13)-C(38)-H(38) | 120.4 |
| N(5)-Ir(02)-O(2) | 86.68(11) | N(1)-C(39)-C(34) | 120.8(4) |
| C(18)-O(2)-Ir(02) | 128.3(2) | N(1)-C(39)-H(39) | 119.6 |
| C(32)-O(4)-Ir(01) | 128.2(2) | C(34)-C(39)-H(39) | 119.6 |
| C(17)-N(8)-C(2) | 117.5(3) | C(55)-C(40)-C(37) | 120.8(4) |
| C(17)-N(8)-Ir(01) | 126.9(3) | C(55)-C(40)-H(40) | 119.6 |
| C(2)-N(8)-Ir(01) | 115.3(3) | C(37)-C(40)-H(40) | 119.6 |
| C(16)-O(1I)-C(27) | 103.5(3) | C(63)-C(41)-C(18) | 121.8(4) |
| C(48)-N(11)-N(12) | 108.0(3) | C(63)-C(41)-H(41) | 119.1 |
| C(48)-N(11)-Ir(01) | 126.7(3) | C(18)-C(41)-H(41) | 119.1 |
| N(12)-N(11)-Ir(01) | 124.7(3) | C(54)-C(42)-C(19) | 121.4(4) |
| C(43)-O(3N)-C(48) | 103.4(3) | C(54)-C(42)-H(42) | 119.3 |
| C(35)-N(9)-C(11) | 117.9(3) | C(19)-C(42)-H(42) | 119.3 |
| C(35)-N(9)-Ir(01) | 125.4(3) | N(12)-C(43)-O(3N) | 113.4(4) |
| C(11)-N(9)-Ir(01) | 116.4(3) | N(12)-C(43)-C(50) | 125.3(4) |
| C(39)-N(1)-C(25) | 117.6(4) | O(3N)-C(43)-C(50) | 121.3(4) |
| C(39)-N(1)-Ir(02) | 126.8(3) | C(23)-C(44)-C(28) | 121.5(4) |
| C(25)-N(1)-Ir(02) | 115.1(3) | C(23)-C(44)-H(44) | 119.2 |
| C(16)-N(5)-N(6) | 108.1(3) | C(28)-C(44)-H(44) | 119.2 |
| C(16)-N(5)-Ir(02) | 125.2(3) | C(36)-C(45)-C(59) | 121.1(5) |
| N(6)-N(5)-Ir(02) | 125.1(2) | C(36)-C(45)-H(45) | 119.4 |
| C(28)-C(0)-C(1) | 113.1(3) | C(59)-C(45)-H(45) | 119.4 |
| C(28)-C(0)-Ir(01) | 135.9(3) | F(15)-C(46)-F(11) | 106.7(4) |
| C(1)-C(0)-Ir(01) | 110.9(3) | F(15)-C(46)-F(4) | 105.5(4) |
| C(30)-N(3)-C(21) | 117.1(4) | F(11)-C(46)-F(4) | 105.8(4) |
| C(30)-N(3)-Ir(02) | 126.9(3) | F(15)-C(46)-C(31) | 113.6(4) |
| C(21)-N(3)-Ir(02) | 115.3(3) | F(11)-C(46)-C(31) | 111.8(4) |
| C(12)-N(7)-C(2) | 117.1(4) | F(4)-C(46)-C(31) | 112.7(4) |
| C(27)-N(6)-N(5) | 105.2(3) | C(35)-C(47)-C(02) | 117.3(4) |
| C(5)-C(1)-C(0) | 124.5(4) | C(35)-C(47)-H(47) | 121.3 |
| C(5)-C(1)-C(2) | 118.4(4) | C(02)-C(47)-H(47) | 121.3 |
| C(0)-C(1)-C(2) | 116.9(3) | N(11)-C(48)-O(3N) | 110.3(4) |
| C(43)-N(12)-N(11) | 105.0(4) | N(11)-C(48)-C(29) | 129.4(4) |
| C(11)-N(10)-C(02) | 116.6(4) | O(3N)-C(48)-C(29) | 120.2(4) |
| N(7)-C(2)-N(8) | 124.2(4) | C(62)-C(49)-C(63) | 118.9(4) |
| N(7)-C(2)-C(1) | 121.0(4) | C(62)-C(49)-H(49) | 120.6 |
| N(8)-C(2)-C(1) | 114.8(3) | C(63)-C(49)-H(49) | 120.6 |
| C(24)-C(3)-C(4) | 113.5(3) | C(70)-C(50)-C(53) | 121.0(5) |
| C(24)-C(3)-Ir(01) | 135.0(3) | C(70)-C(50)-C(43) | 118.3(5) |

| | | | |
|---|---|---|---|
| C(4)-C(3)-Ir(01) | 111.5(3) | C(53)-C(50)-C(43) | 120.5(5) |
| C(7)-C(4)-C(3) | 124.5(4) | N(2)-C(51)-C(34) | 122.9(5) |
| C(7)-C(4)-C(11) | 118.7(4) | N(2)-C(51)-H(51) | 118.5 |
| C(3)-C(4)-C(11) | 116.8(3) | C(34)-C(51)-H(51) | 118.5 |
| C(23)-C(5)-C(1) | 119.2(4) | N(4)-C(52)-C(56) | 123.2(5) |
| C(23)-C(5)-H(5) | 120.4 | N(4)-C(52)-H(52) | 118.4 |
| C(1)-C(5)-H(5) | 120.4 | C(56)-C(52)-H(52) | 118.4 |
| C(37)-C(6)-C(13) | 113.6(4) | C(50)-C(53)-C(71) | 117.2(6) |
| C(37)-C(6)-Ir(02) | 134.8(3) | C(50)-C(53)-H(53) | 121.4 |
| C(13)-C(6)-Ir(02) | 111.2(3) | C(71)-C(53)-H(53) | 121.4 |
| C(51)-N(2)-C(25) | 116.7(4) | C(42)-C(54)-C(26) | 119.3(4) |
| C(31)-C(7)-C(4) | 118.7(4) | C(42)-C(54)-C(66) | 119.5(4) |
| C(31)-C(7)-H(7) | 120.6 | C(26)-C(54)-C(66) | 121.2(4) |
| C(4)-C(7)-H(7) | 120.6 | N(10)-C(02)-C(47) | 122.7(4) |
| C(10)-C(8)-C(19) | 113.5(4) | N(10)-C(02)-H(02) | 118.7 |
| C(10)-C(8)-Ir(02) | 111.5(3) | C(47)-C(02)-H(02) | 118.7 |
| C(19)-C(8)-Ir(02) | 134.9(3) | C(40)-C(55)-C(38) | 119.7(4) |
| C(12)-C(9)-C(17) | 117.4(4) | C(40)-C(55)-C(68) | 121.8(5) |
| C(12)-C(9)-H(9) | 121.3 | C(38)-C(55)-C(68) | 118.4(5) |
| C(17)-C(9)-H(9) | 121.3 | C(30)-C(56)-C(52) | 116.9(4) |
| C(26)-C(10)-C(8) | 124.8(4) | C(30)-C(56)-H(56) | 121.5 |
| C(26)-C(10)-C(21) | 118.9(4) | C(52)-C(56)-H(56) | 121.5 |
| C(8)-C(10)-C(21) | 116.3(4) | C(65)-C(57)-C(58) | 119.1(6) |
| N(10)-C(11)-N(9) | 124.6(4) | C(65)-C(57)-H(57) | 120.4 |
| N(10)-C(11)-C(4) | 121.8(4) | C(58)-C(57)-H(57) | 120.4 |
| N(9)-C(11)-C(4) | 113.6(3) | C(67)-C(58)-C(57) | 121.8(5) |
| N(7)-C(12)-C(9) | 122.7(4) | C(67)-C(58)-C(27) | 118.0(5) |
| N(7)-C(12)-H(12) | 118.7 | C(57)-C(58)-C(27) | 120.2(5) |
| C(9)-C(12)-H(12) | 118.7 | C(60)-C(59)-C(45) | 118.8(5) |
| C(38)-C(13)-C(6) | 124.2(4) | C(60)-C(59)-H(59) | 120.6 |
| C(38)-C(13)-C(25) | 119.3(4) | C(45)-C(59)-H(59) | 120.6 |
| C(6)-C(13)-C(25) | 116.5(4) | C(59)-C(60)-C(29) | 121.1(4) |
| C(31)-C(14)-C(24) | 120.9(4) | C(59)-C(60)-H(60) | 119.4 |
| C(31)-C(14)-H(14) | 119.5 | C(29)-C(60)-H(60) | 119.4 |
| C(24)-C(14)-H(14) | 119.5 | F(12)-C(61)-F(13) | 106.5(4) |
| F(9)-C(15)-F(7) | 106.0(3) | F(12)-C(61)-F(14) | 104.5(4) |
| F(9)-C(15)-F(8) | 106.5(4) | F(13)-C(61)-F(14) | 105.2(4) |
| F(7)-C(15)-F(8) | 105.1(4) | F(12)-C(61)-C(37) | 113.7(4) |
| F(9)-C(15)-C(19) | 112.3(4) | F(13)-C(61)-C(37) | 113.4(4) |
| F(7)-C(15)-C(19) | 113.0(4) | F(14)-C(61)-C(37) | 112.8(4) |
| F(8)-C(15)-C(19) | 113.3(4) | C(49)-C(62)-C(33) | 121.3(4) |
| N(5)-C(16)-O(1I) | 110.1(3) | C(49)-C(62)-H(62) | 119.3 |
| N(5)-C(16)-C(33) | 130.5(4) | C(33)-C(62)-H(62) | 119.3 |
| O(1I)-C(16)-C(33) | 119.4(4) | C(41)-C(63)-C(49) | 121.4(4) |
| N(8)-C(17)-C(9) | 121.1(4) | C(41)-C(63)-H(63) | 119.3 |
| N(8)-C(17)-H(17) | 119.4 | C(49)-C(63)-H(63) | 119.3 |
| C(9)-C(17)-H(17) | 119.4 | F(19)-C(64)-F(16) | 107.8(4) |
| O(2)-C(18)-C(41) | 117.8(4) | F(19)-C(64)-F(21) | 104.8(5) |
| O(2)-C(18)-C(33) | 126.1(4) | F(16)-C(64)-F(21) | 105.0(5) |

| | | | |
|---|---|---|---|
| C(41)-C(18)-C(33) | 116.0(4) | F(19)-C(64)-C(23) | 113.4(4) |
| C(21)-N(4)-C(52) | 116.4(4) | F(16)-C(64)-C(23) | 113.2(5) |
| C(42)-C(19)-C(8) | 121.9(4) | F(21)-C(64)-C(23) | 111.9(4) |
| C(42)-C(19)-C(15) | 115.4(4) | C(69)-C(65)-C(57) | 119.6(6) |
| C(8)-C(19)-C(15) | 122.6(4) | C(69)-C(65)-H(65) | 120.2 |
| F(10)-C(20)-F(2) | 105.4(3) | C(57)-C(65)-H(65) | 120.2 |
| F(10)-C(20)-F(1) | 105.7(4) | F(20)-C(66)-F(17) | 107.1(4) |
| F(2)-C(20)-F(1) | 105.9(4) | F(20)-C(66)-F(18) | 105.2(5) |
| F(10)-C(20)-C(28) | 113.5(4) | F(17)-C(66)-F(18) | 104.0(4) |
| F(2)-C(20)-C(28) | 114.0(4) | F(20)-C(66)-C(54) | 114.3(4) |
| F(1)-C(20)-C(28) | 111.7(3) | F(17)-C(66)-C(54) | 112.9(5) |
| N(4)-C(21)-N(3) | 124.9(4) | F(18)-C(66)-C(54) | 112.6(4) |
| N(4)-C(21)-C(10) | 121.3(4) | C(58)-C(67)-C(72) | 117.6(6) |
| N(3)-C(21)-C(10) | 113.7(4) | C(58)-C(67)-H(67) | 121.2 |
| F(5)-C(22)-F(3) | 106.5(3) | C(72)-C(67)-H(67) | 121.2 |
| F(5)-C(22)-F(6) | 106.2(3) | F(23)-C(68)-F(24) | 106.1(5) |
| F(3)-C(22)-F(6) | 105.0(3) | F(23)-C(68)-F(22) | 102.3(6) |
| F(5)-C(22)-C(24) | 112.2(4) | F(24)-C(68)-F(22) | 105.0(6) |
| F(3)-C(22)-C(24) | 113.6(3) | F(23)-C(68)-C(55) | 115.0(5) |
| F(6)-C(22)-C(24) | 112.7(4) | F(24)-C(68)-C(55) | 115.0(5) |
| C(44)-C(23)-C(5) | 119.0(4) | F(22)-C(68)-C(55) | 112.2(5) |
| C(44)-C(23)-C(64) | 120.2(4) | C(72)-C(69)-C(65) | 121.9(6) |
| C(5)-C(23)-C(64) | 120.7(4) | C(72)-C(69)-H(69) | 119.1 |
| C(14)-C(24)-C(3) | 122.5(4) | C(65)-C(69)-H(69) | 119.1 |
| C(14)-C(24)-C(22) | 115.3(4) | C(74)-C(70)-C(50) | 120.4(6) |
| C(3)-C(24)-C(22) | 122.1(4) | C(74)-C(70)-H(70) | 119.8 |
| N(2)-C(25)-N(1) | 124.4(4) | C(50)-C(70)-H(70) | 119.8 |
| N(2)-C(25)-C(13) | 121.7(4) | C(73)-C(71)-C(53) | 120.4(6) |
| N(1)-C(25)-C(13) | 113.8(4) | C(73)-C(71)-H(71) | 119.8 |
| C(10)-C(26)-C(54) | 118.9(4) | C(53)-C(71)-H(71) | 119.8 |
| C(10)-C(26)-H(26) | 120.6 | C(69)-C(72)-C(67) | 120.0(6) |
| C(54)-C(26)-H(26) | 120.6 | C(69)-C(72)-H(72) | 120 |
| N(6)-C(27)-O(1I) | 113.1(4) | C(67)-C(72)-H(72) | 120 |
| N(6)-C(27)-C(58) | 128.5(4) | C(74)-C(73)-C(71) | 121.6(6) |
| O(1I)-C(27)-C(58) | 118.4(4) | C(74)-C(73)-H(73) | 119.2 |
| C(44)-C(28)-C(0) | 122.5(4) | C(71)-C(73)-H(73) | 119.2 |
| C(44)-C(28)-C(20) | 114.5(4) | C(73)-C(74)-C(70) | 119.3(7) |
| C(0)-C(28)-C(20) | 122.8(4) | C(73)-C(74)-H(74) | 120.3 |
| C(60)-C(29)-C(32) | 120.6(4) | C(70)-C(74)-H(74) | 120.3 |

**Table S2b** The selected bond lengths and angles of **Ir(tfmppm)$_2$(pop)**.

| **Selected bonds Å** | | | | | |
|---|---|---|---|---|---|
| Ir(1)-N(3) | 2.030(6) | N(5)-C(110) | 1.334(9) | C(62)-C(107) | 1.372(10) |
| Ir(1)-C(4) | 2.034(6) | N(5)-C(40) | 1.357(8) | C(62)-C(115) | 1.478(8) |
| Ir(1)-C(5) | 2.041(6) | N(6)-C(40) | 1.321(8) | C(83)-C(103) | 1.405(14) |
| Ir(1)-N(5) | 2.047(5) | N(6)-C(144) | 1.339(9) | C(83)-H(83) | 0.93 |
| Ir(1)-N(7) | 2.084(5) | N(7)-C(111) | 1.310(8) | C(103)-H(103) | 0.93 |
| Ir(1)-O(2) | 2.105(5) | N(7)-N(8) | 1.423(8) | C(104)-C(116) | 1.457(10) |
| F(1)-C(113) | 1.324(10) | N(8)-C(104) | 1.294(9) | C(107)-C(114) | 1.385(10) |

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|---|---|---|---|---|---|
| F(2)-C(113) | 1.373(10) | C(4)-C(24) | 1.408(8) | C(107)-H(107) | 0.93 |
| F(3)-C(113) | 1.325(9) | C(4)-C(108) | 1.434(8) | C(108)-C(113) | 1.479(9) |
| F(4)-C(71) | 1.312(10) | C(5)-C(62) | 1.417(9) | C(110)-H(110) | 0.93 |
| F(5)-C(71) | 1.313(10) | C(5)-C(38) | 1.441(8) | C(114)-C(124) | 1.481(11) |
| F(6)-C(71) | 1.325(10) | C(17)-C(39) | 1.363(9) | C(116)-C(128) | 1.378(12) |
| F(7)-C(143) | 1.318(8) | C(17)-C(71) | 1.499(10) | C(116)-C(135) | 1.410(13) |
| F(8)-C(143) | 1.334(8) | C(24)-C(39) | 1.395(9) | C(125)-C(130) | 1.339(17) |
| F(9)-C(143) | 1.341(7) | C(24)-C(40) | 1.464(8) | C(125)-C(135) | 1.391(14) |
| F(10)-C(124) | 1.364(14) | C(29)-C(144) | 1.375(11) | C(125)-H(125) | 0.93 |
| F(12)-C(124) | 1.310(13) | C(29)-C(110) | 1.405(10) | C(128)-C(132) | 1.384(13) |
| F(24)-C(124) | 1.242(10) | C(29)-H(29) | 0.93 | C(128)-H(128) | 0.93 |
| O(1)-C(111) | 1.363(8) | C(32)-C(57) | 1.404(10) | C(130)-C(132) | 1.375(16) |
| O(1)-C(104) | 1.380(8) | C(32)-C(43) | 1.419(10) | C(130)-H(130) | 0.93 |
| O(2)-C(32) | 1.314(8) | C(38)-C(143) | 1.520(8) | C(132)-H(132) | 0.93 |
| N(1)-C(108) | 1.333(9) | C(39)-H(39) | 0.93 | C(133)-C(137) | 1.347(12) |
| N(1)-C(17) | 1.346(9) | C(43)-C(111) | 1.418(10) | C(133)-H(133) | 0.93 |
| N(2)-C(114) | 1.321(9) | C(43)-C(54) | 1.419(10) | C(135)-H(135) | 0.93 |
| N(2)-C(38) | 1.336(8) | C(54)-C(103) | 1.345(13) | C(137)-C(142) | 1.354(11) |
| N(3)-C(115) | 1.329(9) | C(54)-H(54) | 0.93 | C(137)-H(137) | 0.93 |
| N(3)-C(142) | 1.386(8) | C(57)-C(83) | 1.385(11) | C(142)-H(142) | 0.93 |
| N(4)-C(115) | 1.320(8) | C(57)-H(57) | 0.93 | C(144)-H(144) | 0.93 |
| N(4)-C(133) | 1.388(9) | | | | |

**Selected angles°**

| | | | |
|---|---|---|---|
| N(3)-Ir(1)-C(4) | 104.8(2) | C(57)-C(83)-C(103) | 120.7(8) |
| N(3)-Ir(1)-C(5) | 80.2(2) | C(57)-C(83)-H(83) | 119.7 |
| C(4)-Ir(1)-C(5) | 95.2(2) | C(103)-C(83)-H(83) | 119.7 |
| N(3)-Ir(1)-N(5) | 173.1(2) | C(54)-C(103)-C(83) | 118.8(8) |
| C(4)-Ir(1)-N(5) | 81.2(2) | C(54)-C(103)-H(103) | 120.6 |
| C(5)-Ir(1)-N(5) | 102.9(2) | C(83)-C(103)-H(103) | 120.6 |
| N(3)-Ir(1)-N(7) | 91.9(2) | N(8)-C(104)-O(1) | 112.5(6) |
| C(4)-Ir(1)-N(7) | 89.3(2) | N(8)-C(104)-C(116) | 127.6(7) |
| C(5)-Ir(1)-N(7) | 171.6(2) | O(1)-C(104)-C(116) | 119.9(6) |
| N(5)-Ir(1)-N(7) | 84.7(2) | C(62)-C(107)-C(114) | 116.9(6) |
| N(3)-Ir(1)-O(2) | 84.2(2) | C(62)-C(107)-H(107) | 121.5 |
| C(4)-Ir(1)-O(2) | 169.92(19) | C(114)-C(107)-H(107) | 121.5 |
| C(5)-Ir(1)-O(2) | 90.7(2) | N(1)-C(108)-C(4) | 124.6(6) |
| N(5)-Ir(1)-O(2) | 89.5(2) | N(1)-C(108)-C(113) | 112.0(6) |
| N(7)-Ir(1)-O(2) | 85.8(2) | C(4)-C(108)-C(113) | 123.4(6) |
| C(111)-O(1)-C(104) | 104.4(5) | N(5)-C(110)-C(29) | 119.2(7) |
| C(32)-O(2)-Ir(1) | 127.2(4) | N(5)-C(110)-H(110) | 120.4 |
| C(108)-N(1)-C(17) | 119.4(6) | C(29)-C(110)-H(110) | 120.4 |
| C(114)-N(2)-C(38) | 118.8(6) | N(7)-C(111)-O(1) | 109.7(6) |
| C(115)-N(3)-C(142) | 116.0(6) | N(7)-C(111)-C(43) | 128.5(6) |
| C(115)-N(3)-Ir(1) | 116.6(4) | O(1)-C(111)-C(43) | 121.7(6) |
| C(142)-N(3)-Ir(1) | 126.5(5) | F(3)-C(113)-F(1) | 107.6(7) |
| C(115)-N(4)-C(133) | 115.4(7) | F(3)-C(113)-F(2) | 105.5(7) |
| C(110)-N(5)-C(40) | 119.0(6) | F(1)-C(113)-F(2) | 105.0(7) |
| C(110)-N(5)-Ir(1) | 126.2(5) | F(3)-C(113)-C(108) | 114.2(7) |
| C(40)-N(5)-Ir(1) | 114.5(4) | F(1)-C(113)-C(108) | 114.2(7) |

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|---|---|---|---|
| C(40)-N(6)-C(144) | 116.3(6) | F(2)-C(113)-C(108) | 109.5(7) |
| C(111)-N(7)-N(8) | 108.5(5) | N(2)-C(114)-C(107) | 123.2(6) |
| C(111)-N(7)-Ir(1) | 127.1(5) | N(2)-C(114)-C(124) | 116.8(6) |
| N(8)-N(7)-Ir(1) | 124.3(4) | C(107)-C(114)-C(124) | 120.0(7) |
| C(104)-N(8)-N(7) | 104.7(5) | N(4)-C(115)-N(3) | 127.3(6) |
| C(24)-C(4)-C(108) | 112.6(5) | N(4)-C(115)-C(62) | 118.1(6) |
| C(24)-C(4)-Ir(1) | 111.3(4) | N(3)-C(115)-C(62) | 114.5(5) |
| C(108)-C(4)-Ir(1) | 135.9(4) | C(128)-C(116)-C(135) | 121.1(8) |
| C(62)-C(5)-C(38) | 111.0(5) | C(128)-C(116)-C(104) | 121.6(8) |
| C(62)-C(5)-Ir(1) | 113.1(4) | C(135)-C(116)-C(104) | 117.3(7) |
| C(38)-C(5)-Ir(1) | 136.0(5) | F(24)-C(124)-F(12) | 110.3(10) |
| N(1)-C(17)-C(39) | 122.1(6) | F(24)-C(124)-F(10) | 105.1(11) |
| N(1)-C(17)-C(71) | 116.0(6) | F(12)-C(124)-F(10) | 96.3(8) |
| C(39)-C(17)-C(71) | 121.8(7) | F(24)-C(124)-C(114) | 117.2(8) |
| C(39)-C(24)-C(4) | 123.1(5) | F(12)-C(124)-C(114) | 114.8(9) |
| C(39)-C(24)-C(40) | 119.5(5) | F(10)-C(124)-C(114) | 110.7(10) |
| C(4)-C(24)-C(40) | 117.3(5) | C(130)-C(125)-C(135) | 122.1(11) |
| C(144)-C(29)-C(110) | 117.5(6) | C(130)-C(125)-H(125) | 118.9 |
| C(144)-C(29)-H(29) | 121.3 | C(135)-C(125)-H(125) | 118.9 |
| C(110)-C(29)-H(29) | 121.3 | C(116)-C(128)-C(132) | 119.3(10) |
| O(2)-C(32)-C(57) | 117.0(6) | C(116)-C(128)-H(128) | 120.4 |
| O(2)-C(32)-C(43) | 125.7(6) | C(132)-C(128)-H(128) | 120.4 |
| C(57)-C(32)-C(43) | 117.2(7) | C(125)-C(130)-C(132) | 120.8(9) |
| N(2)-C(38)-C(5) | 125.4(6) | C(125)-C(130)-H(130) | 119.6 |
| N(2)-C(38)-C(143) | 112.1(5) | C(132)-C(130)-H(130) | 119.6 |
| C(5)-C(38)-C(143) | 122.5(6) | C(130)-C(132)-C(128) | 119.7(10) |
| C(17)-C(39)-C(24) | 118.2(6) | C(130)-C(132)-H(132) | 120.1 |
| C(17)-C(39)-H(39) | 120.9 | C(128)-C(132)-H(132) | 120.1 |
| C(24)-C(39)-H(39) | 120.9 | C(137)-C(133)-N(4) | 120.7(7) |
| N(6)-C(40)-N(5) | 124.8(5) | C(137)-C(133)-H(133) | 119.7 |
| N(6)-C(40)-C(24) | 121.4(6) | N(4)-C(133)-H(133) | 119.7 |
| N(5)-C(40)-C(24) | 113.8(5) | C(125)-C(135)-C(116) | 116.7(10) |
| C(32)-C(43)-C(111) | 121.5(6) | C(125)-C(135)-H(135) | 121.6 |
| C(32)-C(43)-C(54) | 119.6(7) | C(116)-C(135)-H(135) | 121.6 |
| C(111)-C(43)-C(54) | 118.9(7) | C(133)-C(137)-C(142) | 120.6(7) |
| C(103)-C(54)-C(43) | 122.1(9) | C(133)-C(137)-H(137) | 119.7 |
| C(103)-C(54)-H(54) | 119 | C(142)-C(137)-H(137) | 119.7 |
| C(43)-C(54)-H(54) | 119 | C(137)-C(142)-N(3) | 119.9(7) |
| C(83)-C(57)-C(32) | 121.3(8) | C(137)-C(142)-H(142) | 120.1 |
| C(83)-C(57)-H(57) | 119.3 | N(3)-C(142)-H(142) | 120.1 |
| C(32)-C(57)-H(57) | 119.3 | F(7)-C(143)-F(8) | 108.0(5) |
| C(107)-C(62)-C(5) | 124.7(6) | F(7)-C(143)-F(9) | 106.2(6) |
| C(107)-C(62)-C(115) | 120.7(6) | F(8)-C(143)-F(9) | 106.6(6) |
| C(5)-C(62)-C(115) | 114.6(6) | F(7)-C(143)-C(38) | 112.5(5) |
| F(4)-C(71)-F(5) | 108.1(7) | F(8)-C(143)-C(38) | 110.8(6) |
| F(4)-C(71)-F(6) | 105.4(8) | F(9)-C(143)-C(38) | 112.3(5) |
| F(5)-C(71)-F(6) | 104.8(7) | N(6)-C(144)-C(29) | 123.2(6) |
| F(4)-C(71)-C(17) | 113.1(7) | N(6)-C(144)-H(144) | 118.4 |
| F(5)-C(71)-C(17) | 113.4(7) | C(29)-C(144)-H(144) | 118.4 |

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|---|---|---|---|
| F(6)-C(71)-C(17) | 111.5(6) | | |

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