

Supporting Information

Efficient bluish green electroluminescence of iridium complexes with good electron mobility

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General information

¹H 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 K α radiation ($\lambda = 0.71073 \text{ \AA}$) at room temperature. Cell parameters were retrieved using SMART software and refined using *SAINTE*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 ω 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 \AA /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 \AA /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.

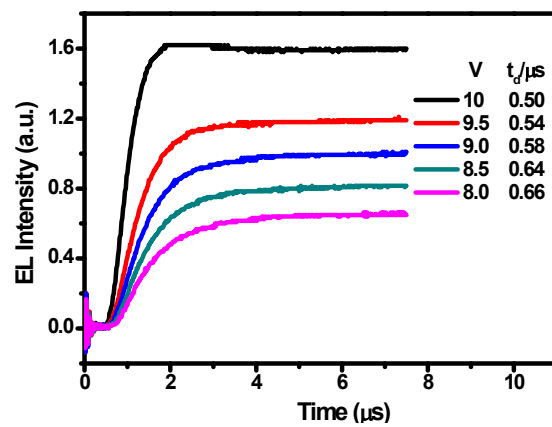


Figure S1 the transient EL signals for the device structure of ITO/TAPC (50nm)/Ir complexes (60nm)/ LiF (1 nm)/ Al (100 nm) under different applied fields of **Ir1**.

Table S1. Crystallographic data of Ir1 and Ir2.

	Ir1	Ir2
Formula	C ₄₂ H ₂₈ F ₆ IrN ₉ O ₂ P ₂	C ₄₂ H ₂₆ F ₈ IrN ₉ O ₂ P ₂
FW	1058.46	1094.88
T (K)	296	296
Wavelength (Å)	0.71073	0.71073
Crystal system	monoclinic	monoclinic
Space group	P 21/c	P 21/c
<i>a</i> (Å)	11.5095(6)	11.479(3)
<i>b</i> (Å)	16.3355(9)	15.111(4)
<i>c</i> (Å)	22.6258(12)	24.778(7)
α (deg)	90	90
β (deg)	99.990(1)	97.796(5)
γ (deg)	90	90
<i>V</i> (Å ³)	4189.5(4)	4258(2)
<i>Z</i>	4	4
ρ_{calcd} (g/cm ³)	1.678	1.708
μ (Mo K α) (mm ⁻¹)	3.339	3.295
<i>F</i> (000)	2079.2	2144.0
Reflns collected	29798	28582
Unique	10356	9712
Data/restraints/params	10356 / 6 / 692	9712 / 1 / 577
GOF on <i>F</i> ²	1.019	1.028
<i>R</i> ₁ ^a , <i>wR</i> ₂ ^b [<i>I</i> > 2 σ (<i>I</i>)]	0.0277, 0.0569	0.0413, 0.0887
<i>R</i> ₁ ^a , <i>wR</i> ₂ ^b (all data)	0.0437, 0.0645	0.0626, 0.0969
CCDC NO	1584485	1584486

$$R_1^a = \frac{\sum ||F_o| - |F_c||}{\sum F_o}. \quad wR_2^b = \left[\frac{\sum w(F_o^2 - F_c^2)^2}{\sum w(F_o^2)} \right]^{1/2}$$

Table S2(a) The selected bond lengths and angles of Ir1.

Selected bonds Å					
Ir1-O1	2.195(2)	N7-C28	1.341(5)	C20-C21	1.408(6)
Ir1-O2	2.207(2)	N8-C30	1.362(4)	C21-C22	1.376(8)
Ir1-N5	2.044(2)	N8-C31	1.334(4)	C22-C23	1.352(8)
Ir1-N8	2.043(2)	N9-C30	1.324(4)	C23-C24	1.361(7)
Ir1-C27	1.959(3)	N9-C32	1.328(5)	C25-C26	1.529(6)
Ir1-C36	1.962(3)	C1-C2	1.374(6)	C25-F4	1.265(19)
P1-O1	1.522(2)	C1-C6	1.391(6)	C25-F6	1.274(9)
P1-N1	1.584(3)	C2-C3	1.410(7)	C25-F4A	1.260(10)
P1-C1	1.794(3)	C3-C4	1.349(10)	C27-C29	1.415(5)
P1-C7	1.817(4)	C4-C5	1.349(10)	C28-C29	1.368(5)
P2-O2	1.514(2)	C5-C6	1.374(7)	C29-C30	1.462(5)
P2-N1	1.579(3)	C7-C8	1.378(5)	C31-C33	1.374(5)
P2-C13	1.795(3)	C7-C12	1.375(5)	C32-C33	1.374(6)
P2-C19	1.803(3)	C8-C9	1.385(6)	C34-C35	1.531(6)
F5-C25	1.275(8)	C9-C10	1.350(7)	C34-F1	1.285(10)
N2-C35	1.305(5)	C10-C11	1.358(6)	C34-F2	1.317(9)
N2-C37	1.350(5)	C11-C12	1.374(6)	C34-F3	1.247(14)
N3-C35	1.337(5)	C13-C14	1.384(5)	C34-F1A	1.200(13)
N3-C36	1.352(4)	C13-C18	1.377(5)	C34-F2A	1.342(17)
N4-C39	1.329(4)	C14-C15	1.377(7)	C34-F3A	1.315(18)
N4-C41	1.338(5)	C15-C16	1.362(8)	C36-C38	1.414(4)
N5-C39	1.353(4)	C16-C17	1.375(8)	C37-C38	1.373(5)
N5-C40	1.341(4)	C17-C18	1.387(6)	C38-C39	1.454(4)
N6-C26	1.333(4)	C19-C20	1.383(5)	C40-C42	1.375(5)
N6-C27	1.344(4)	C19-C24	1.392(5)	C41-C42	1.371(6)
N7-C26	1.316(5)	--	--	--	--
Selected angles°					
O1-Ir1-O2	90.66(8)	C15-C16-C17	121.2(5)		
N5-Ir1-O1	90.08(9)	C16-C17-C18	118.7(5)		
N5-Ir1-O2	93.70(9)	C13-C18-C17	120.9(5)		
N8-Ir1-O1	93.68(9)	C20-C19-P2	121.1(3)		
N8-Ir1-O2	91.15(9)	C20-C19-C24	119.1(4)		
N8-Ir1-N5	173.83(10)	C24-C19-P2	119.8(3)		
C27-Ir1-O1	172.88(11)	C19-C20-C21	118.8(4)		
C27-Ir1-O2	84.56(11)	C22-C21-C20	119.1(5)		
C27-Ir1-N5	95.48(12)	C23-C22-C21	122.5(5)		
C27-Ir1-N8	81.17(12)	C22-C23-C24	118.4(5)		
C27-Ir1-C36	94.80(13)	C23-C24-C19	122.0(5)		
C36-Ir1-O1	90.45(11)	F5-C25-C26	112.2(6)		
C36-Ir1-O2	174.52(10)	F4-C25-F5	133.4(15)		
C36-Ir1-N5	80.93(12)	F4-C25-C26	111.4(9)		
C36-Ir1-N8	94.14(12)	F4-C25-F6	77(2)		
O1-P1-N1	118.75(14)	F6-C25-F5	101.8(5)		
O1-P1-C1	108.21(17)	F6-C25-C26	110.7(6)		

O1-P1-C7	108.69(14)	F4A-C25-F5	96.8(14)
N1-P1-C1	106.98(17)	F4A-C25-C26	114.4(6)
N1-P1-C7	107.25(17)	N6-C26-C25	113.8(4)
C1-P1-C7	106.30(15)	N7-C26-N6	129.9(4)
O2-P2-N1	117.52(14)	N7-C26-C25	116.3(4)
O2-P2-C13	109.00(14)	N6-C27-Ir1	125.8(2)
O2-P2-C19	109.03(15)	N6-C27-C29	119.2(3)
N1-P2-C13	107.71(17)	C29-C27-Ir1	114.6(2)
N1-P2-C19	108.72(17)	N7-C28-C29	122.0(4)
C13-P2-C19	104.01(15)	C27-C29-C30	115.4(3)
P1-O1-Ir1	124.72(12)	C28-C29-C27	118.8(3)
P2-O2-Ir1	123.43(12)	C28-C29-C30	125.7(3)
P2-N1-P1	126.5(2)	N8-C30-C29	113.0(3)
C35-N2-C37	114.4(3)	N9-C30-N8	124.6(3)
C35-N3-C36	115.5(3)	N9-C30-C29	122.3(3)
C39-N4-C41	116.7(3)	N8-C31-C33	120.5(3)
C39-N5-Ir1	115.0(2)	N9-C32-C33	122.5(4)
C40-N5-Ir1	126.8(2)	C31-C33-C32	118.0(4)
C40-N5-C39	118.2(3)	F1-C34-C35	111.3(6)
C26-N6-C27	115.6(3)	F1-C34-F2	106.2(13)
C26-N7-C28	114.4(3)	F2-C34-C35	112.6(5)
C30-N8-Ir1	115.4(2)	F3-C34-C35	111.8(7)
C31-N8-Ir1	126.9(2)	F3-C34-F1	107.4(17)
C31-N8-C30	117.7(3)	F3-C34-F2	107.1(17)
C30-N9-C32	116.7(3)	F1A-C34-C35	116.4(8)
C2-C1-P1	120.7(3)	F1A-C34-F2A	115(3)
C2-C1-C6	119.2(4)	F1A-C34-F3A	105(3)
C6-C1-P1	120.1(3)	F2A-C34-C35	105.8(10)
C1-C2-C3	119.6(6)	F3A-C34-C35	114.8(7)
C4-C3-C2	119.8(7)	F3A-C34-F2A	98(3)
C3-C4-C5	120.6(5)	N2-C35-N3	130.5(4)
C4-C5-C6	121.2(6)	N2-C35-C34	115.9(4)
C5-C6-C1	119.6(5)	N3-C35-C34	113.6(4)
C8-C7-P1	121.0(3)	N3-C36-Ir1	126.7(2)
C12-C7-P1	120.8(3)	N3-C36-C38	118.6(3)
C12-C7-C8	118.1(4)	C38-C36-Ir1	114.6(2)
C7-C8-C9	120.3(5)	N2-C37-C38	121.4(4)
C10-C9-C8	120.7(5)	C36-C38-C39	115.2(3)
C9-C10-C11	119.4(5)	C37-C38-C36	119.5(3)
C10-C11-C12	121.0(5)	C37-C38-C39	125.1(3)
C11-C12-C7	120.5(4)	N4-C39-N5	124.2(3)
C14-C13-P2	120.2(3)	N4-C39-C38	122.1(3)
C18-C13-P2	120.8(3)	N5-C39-C38	113.7(3)
C18-C13-C14	118.9(4)	N5-C40-C42	120.4(3)
C15-C14-C13	120.4(5)	N4-C41-C42	122.7(4)
C16-C15-C14	119.8(5)	C41-C42-C40	117.7(4)

Table S2(b) The selected bond lengths and angles of **Ir2**.

Selected bonds Å					
Ir(1)-C(55)	1.956(5)	C(14)-C(62)	1.376(9)	C(36)-H(36)	0.93
Ir(1)-C(10)	1.965(5)	C(14)-C(23)	1.381(8)	C(37)-C(49)	1.319(12)
Ir(1)-N(7)	2.039(4)	C(15)-C(60)	1.358(7)	C(37)-C(69)	1.329(12)
Ir(1)-N(8)	2.046(4)	C(15)-C(55)	1.417(6)	C(37)-H(37)	0.9300
Ir(1)-O(2)	2.200(3)	C(15)-C(56)	1.455(7)	C(38)-C(66)	1.354(10)
Ir(1)-O(1)	2.212(3)	C(16)-N(9)	1.321(6)	C(43)-H(43)	0.93
P(1)-O(1)	1.529(3)	C(17)-N(1)	1.317(7)	C(46)-H(46)	0.93
P(1)-N(5)	1.593(5)	C(21)-C(63)	1.503(8)	C(47)-C(69)	1.386(11)
P(1)-C(30)	1.796(5)	C(22)-C(28)	1.356(8)	C(47)-H(47)	0.93
P(1)-C(13)	1.799(5)	C(22)-H(22)	0.93	C(48)-H(48)	0.93
P(2)-O(2)	1.523(3)	C(23)-C(46)	1.362(9)	C(49)-H(49)	0.93
P(2)-N(5)	1.583(5)	C(23)-H(23)	0.93	N(7)-C(59)	1.337(7)
P(2)-C(14)	1.798(6)	C(24)-C(67)	1.399(9)	N(7)-C(56)	1.362(6)
P(2)-C(12)	1.801(5)	C(24)-H(24)	0.93	F(8)-C(57)	1.343(7)
N(8)-C(22)	1.334(7)	C(25)-H(25)	0.93	C(57)-C(58)	1.362(10)
N(8)-C(16)	1.353(6)	C(26)-C(27)	1.388(8)	C(57)-C(59)	1.367(8)
N(2)-C(17)	1.331(6)	C(26)-H(26)	0.93	C(58)-H(58)	0.93
N(2)-C(55)	1.344(6)	C(27)-C(33)	1.370(9)	C(59)-H(59)	0.93
F(4)-C(28)	1.343(7)	C(27)-H(27)	0.93	C(60)-H(60)	0.93
C(8)-C(25)	1.369(7)	C(28)-C(43)	1.367(9)	F(7)-C(63)	1.256(8)
C(8)-C(10)	1.414(6)	C(29)-F(2)	1.215(8)	C(62)-C(68)	1.408(12)
C(8)-C(16)	1.454(7)	C(29)-F(1)	1.284(7)	C(62)-H(62)	0.93
N(4)-C(21)	1.319(6)	C(29)-F(3)	1.346(9)	C(63)-F(6)	1.221(8)
N(4)-C(10)	1.342(6)	C(30)-C(41)	1.339(8)	C(63)-F(5)	1.293(8)
N(6)-C(56)	1.323(6)	C(30)-C(47)	1.3798(11)	C(66)-C(67)	1.335(10)
N(6)-C(58)	1.334(8)	N(1)-C(60)	1.347(7)	C(66)-H(66)	0.93
C(12)-C(36)	1.371(8)	C(33)-C(48)	1.343(9)	C(67)-H(67)	0.93
C(12)-C(24)	1.383(8)	C(33)-H(33)	0.93	C(68)-H(68)	0.93
C(13)-C(26)	1.380(7)	C(36)-C(38)	1.394(8)	C(69)-H(69)	0.93
C(13)-C(19)	1.389(7)				
Selected angles°					
C(55)-Ir(1)-C(10)	86.40(19)	F(2)-C(29)-F(3)	104.2(8)		
C(55)-Ir(1)-N(7)	81.12(18)	F(1)-C(29)-F(3)	100.4(6)		
C(10)-Ir(1)-N(7)	90.58(18)	F(2)-C(29)-C(17)	115.7(6)		
C(55)-Ir(1)-N(8)	95.73(17)	F(1)-C(29)-C(17)	115.1(6)		
C(10)-Ir(1)-N(8)	80.99(18)	F(3)-C(29)-C(17)	107.7(6)		
N(7)-Ir(1)-N(8)	171.20(16)	C(41)-C(30)-C(47)	117.4(6)		
C(55)-Ir(1)-O(2)	172.59(16)	C(41)-C(30)-P(1)	122.5(4)		
C(10)-Ir(1)-O(2)	94.18(16)	C(47)-C(30)-P(1)	120.0(5)		
N(7)-Ir(1)-O(2)	91.48(15)	C(17)-N(1)-C(60)	114.2(5)		
N(8)-Ir(1)-O(2)	91.66(14)	C(48)-C(33)-C(27)	120.3(6)		
C(55)-Ir(1)-O(1)	91.40(16)	C(48)-C(33)-H(33)	119.8		
C(10)-Ir(1)-O(1)	171.20(16)	C(27)-C(33)-H(33)	119.8		
N(7)-Ir(1)-O(1)	97.50(14)	C(12)-C(36)-C(38)	120.9(6)		
N(8)-Ir(1)-O(1)	90.77(14)	C(12)-C(36)-H(36)	119.5		
O(2)-Ir(1)-O(1)	89.10(12)	C(38)-C(36)-H(36)	119.5		

O(1)-P(1)-N(5)	116.3(2)	C(49)-C(37)-C(69)	120.0(9)
O(1)-P(1)-C(30)	108.7(2)	C(49)-C(37)-H(37)	120.0
N(5)-P(1)-C(30)	109.5(3)	C(69)-C(37)-H(37)	120.0
O(1)-P(1)-C(13)	108.9(2)	C(66)-C(38)-C(36)	119.9(7)
N(5)-P(1)-C(13)	108.0(3)	C(66)-C(38)-H(38)	120.0
C(30)-P(1)-C(13)	104.9(2)	C(36)-C(38)-H(38)	120.0
O(2)-P(2)-N(5)	117.6(2)	C(30)-C(41)-C(49)	120.7(7)
O(2)-P(2)-C(14)	106.5(2)	C(30)-C(41)-H(41)	119.6
N(5)-P(2)-C(14)	111.6(3)	C(49)-C(41)-H(41)	119.6
O(2)-P(2)-C(12)	107.6(2)	C(46)-C(42)-C(68)	120.4(9)
N(5)-P(2)-C(12)	106.0(3)	C(46)-C(42)-H(42)	119.8
C(14)-P(2)-C(12)	107.1(2)	C(68)-C(42)-H(42)	119.8
C(22)-N(8)-C(16)	118.1(4)	N(9)-C(43)-C(28)	121.7(6)
C(22)-N(8)-Ir(1)	127.1(4)	N(9)-C(43)-H(43)	119.1
C(16)-N(8)-Ir(1)	114.8(3)	C(28)-C(43)-H(43)	119.1
C(17)-N(2)-C(55)	115.8(4)	C(42)-C(46)-C(23)	119.4(8)
C(25)-C(8)-C(10)	118.3(5)	C(42)-C(46)-H(46)	120.3
C(25)-C(8)-C(16)	126.4(5)	C(23)-C(46)-H(46)	120.3
C(10)-C(8)-C(16)	115.2(4)	C(30)-C(47)-C(69)	120.5(7)
C(21)-N(4)-C(10)	116.0(4)	C(30)-C(47)-H(47)	119.7
N(4)-C(10)-C(8)	119.3(4)	C(69)-C(47)-H(47)	119.7
N(4)-C(10)-Ir(1)	125.9(4)	C(33)-C(48)-C(19)	120.7(6)
C(8)-C(10)-Ir(1)	114.4(4)	C(33)-C(48)-H(48)	119.7
C(56)-N(6)-C(58)	117.4(5)	C(19)-C(48)-H(48)	119.7
C(36)-C(12)-C(24)	117.8(5)	C(37)-C(49)-C(41)	120.9(9)
C(36)-C(12)-P(2)	121.7(4)	C(37)-C(49)-H(49)	119.5
C(24)-C(12)-P(2)	120.5(5)	C(41)-C(49)-H(49)	119.5
C(26)-C(13)-C(19)	118.4(5)	P(2)-O(2)-Ir(1)	123.05(19)
C(26)-C(13)-P(1)	119.4(4)	P(1)-O(1)-Ir(1)	121.26(18)
C(19)-C(13)-P(1)	122.1(4)	C(59)-N(7)-C(56)	117.9(5)
C(62)-C(14)-C(23)	116.8(6)	C(59)-N(7)-Ir(1)	126.0(4)
C(62)-C(14)-P(2)	122.2(5)	C(56)-N(7)-Ir(1)	115.2(3)
C(23)-C(14)-P(2)	120.9(5)	P(2)-N(5)-P(1)	123.3(3)
C(60)-C(15)-C(55)	119.0(5)	N(2)-C(55)-C(15)	119.0(4)
C(60)-C(15)-C(56)	125.9(5)	N(2)-C(55)-Ir(1)	126.0(3)
C(55)-C(15)-C(56)	115.1(4)	C(15)-C(55)-Ir(1)	114.9(3)
N(9)-C(16)-N(8)	124.6(5)	N(6)-C(56)-N(7)	124.2(5)
N(9)-C(16)-C(8)	121.3(5)	N(6)-C(56)-C(15)	122.5(5)
N(8)-C(16)-C(8)	114.0(4)	N(7)-C(56)-C(15)	113.3(4)
N(1)-C(17)-N(2)	129.7(5)	F(8)-C(57)-C(58)	121.6(6)
N(1)-C(17)-C(29)	116.0(5)	F(8)-C(57)-C(59)	118.5(6)
N(2)-C(17)-C(29)	114.2(5)	C(58)-C(57)-C(59)	119.9(6)
C(21)-N(3)-C(25)	113.5(5)	N(6)-C(58)-C(57)	121.1(6)
C(48)-C(19)-C(13)	120.3(6)	N(6)-C(58)-H(58)	119.4
C(48)-C(19)-H(19)	119.9	C(57)-C(58)-H(58)	119.4
C(13)-C(19)-H(19)	119.9	N(7)-C(59)-C(57)	119.4(6)
C(43)-N(9)-C(16)	116.7(5)	N(7)-C(59)-H(59)	120.3
N(4)-C(21)-N(3)	130.0(5)	C(57)-C(59)-H(59)	120.3
N(4)-C(21)-C(63)	115.5(5)	N(1)-C(60)-C(15)	122.1(5)

N(3)-C(21)-C(63)	114.4(5)	N(1)-C(60)-H(60)	118.9
N(8)-C(22)-C(28)	119.1(5)	C(15)-C(60)-H(60)	118.9
N(8)-C(22)-H(22)	120.5	C(14)-C(62)-C(68)	118.9(8)
C(28)-C(22)-H(22)	120.5	C(14)-C(62)-H(62)	120.6
C(46)-C(23)-C(14)	123.1(7)	C(68)-C(62)-H(62)	120.6
C(46)-C(23)-H(23)	118.4	F(6)-C(63)-F(7)	108.0(8)
C(14)-C(23)-H(23)	118.4	F(6)-C(63)-F(5)	104.5(7)
C(12)-C(24)-C(67)	120.3(7)	F(7)-C(63)-F(5)	99.5(7)
C(12)-C(24)-H(24)	119.8	F(6)-C(63)-C(21)	113.8(6)
C(67)-C(24)-H(24)	119.8	F(7)-C(63)-C(21)	115.4(6)
N(3)-C(25)-C(8)	122.4(5)	F(5)-C(63)-C(21)	114.3(6)
N(3)-C(25)-H(25)	118.8	C(67)-C(66)-C(38)	120.5(6)
C(8)-C(25)-H(25)	118.8	C(67)-C(66)-H(66)	119.7
C(13)-C(26)-C(27)	120.3(6)	C(38)-C(66)-H(66)	119.7
C(13)-C(26)-H(26)	119.9	C(66)-C(67)-C(24)	120.5(7)
C(27)-C(26)-H(26)	119.9	C(66)-C(67)-H(67)	119.8
C(33)-C(27)-C(26)	120.0(6)	C(24)-C(67)-H(67)	119.8
C(33)-C(27)-H(27)	120.0	C(42)-C(68)-C(62)	121.4(9)
C(26)-C(27)-H(27)	120.0	C(42)-C(68)-H(68)	119.3
F(4)-C(28)-C(22)	119.8(6)	C(62)-C(68)-H(68)	119.3
F(4)-C(28)-C(43)	120.5(5)	C(37)-C(69)-C(47)	120.3(8)
C(22)-C(28)-C(43)	119.7(6)	C(37)-C(69)-H(69)	119.8r
F(2)-C(29)-F(1)	111.8(8)	C(47)-C(69)-H(69)	119.8

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