Electronic Supplementary Material (ESI) for Materials Chemistry Frontiers.

Supporting Information

Highly efficient yellow electroluminescence of iridium complexes with good 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}.

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* [1] 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* [2] 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*.[3] 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^{-1}. The deposition rate for organic compounds is 1-2 Å s^{-1}. The phosphor and host were co-evaporated from two separate sources. The cathode consisting of LiF/Al was deposited by evaporation of LiF with a deposition rate of 0.1 Å s^{-1} and then by evaporation of Al metal with a rate of 3 Å s^{-1}. The effective area of the emitting diode is 0.1 cm^2. The characteristics of the devices were measured with a computer 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 CIE coordinates were calculated using a test program of the spectra scan PR650 spectrophotometer.

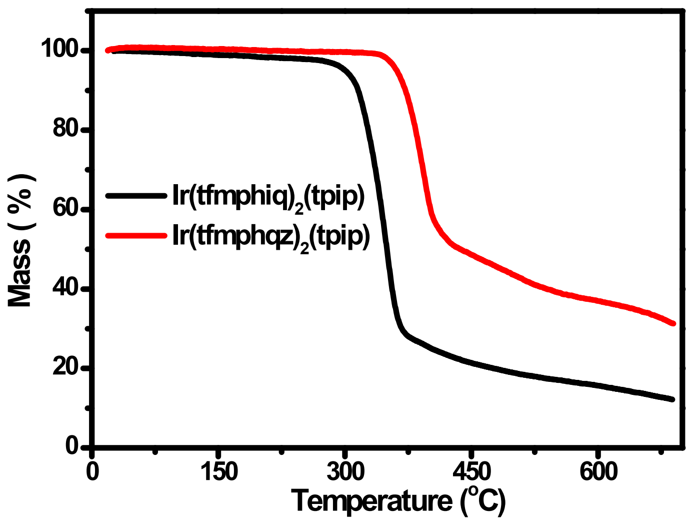
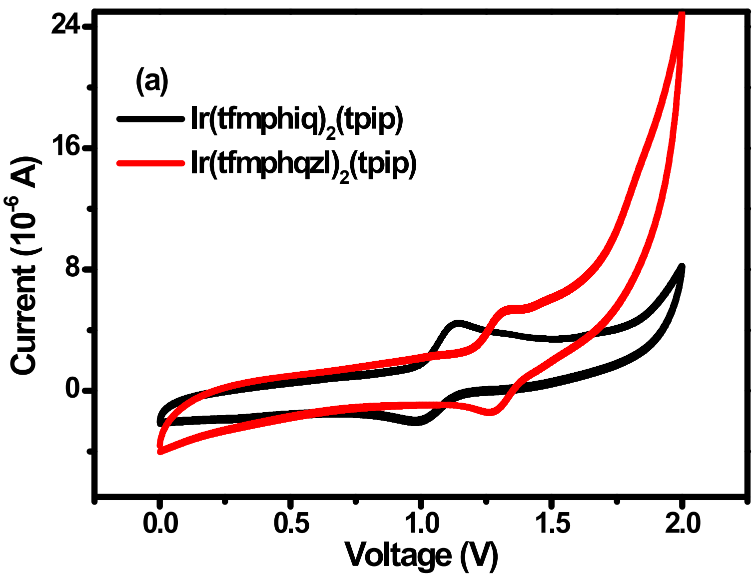


Fig. S1 The TGA curves of **Ir(tfmphiq)$_2$(tpip)** and **Ir(tfmphqz)$_2$(tpip)** complexes.



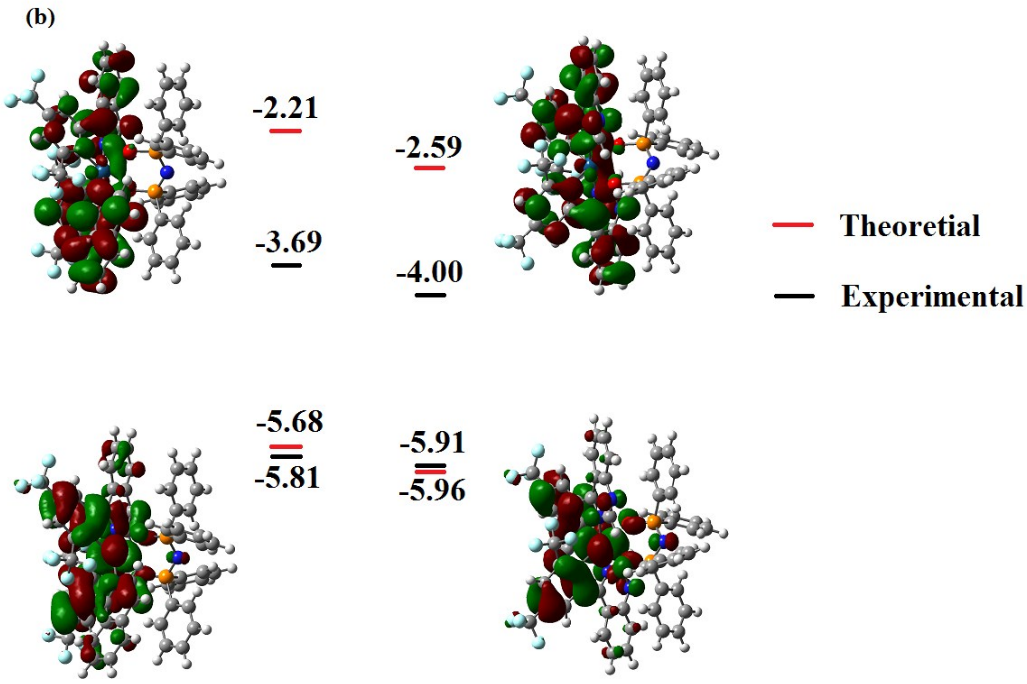


Fig. S2 (a) the cyclic voltammogram curve of **Ir(tfmphiq)$_2$(tpip)** and **Ir(tfmphqz)$_2$(tpip)**; (b) Contour plots of **Ir(tfmphiq)$_2$(tpip)** and **Ir(tfmphqz)$_2$(tpip)**.

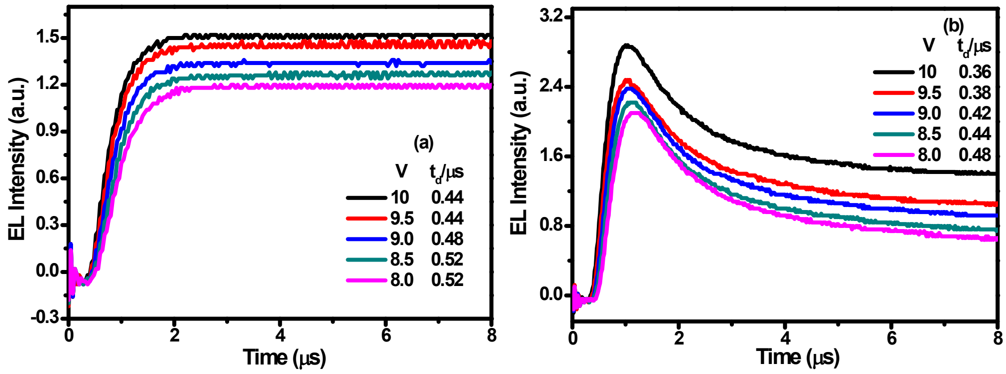


Fig. S3 (a), (b) the transient EL signals for the device structure of ITO/TAPC (50nm)/Ir complexes (60nm) under different applied fields of **Ir(tfmphiq)$_2$(tpip)** and **Ir(tfmphqz)$_2$(tpip)**.

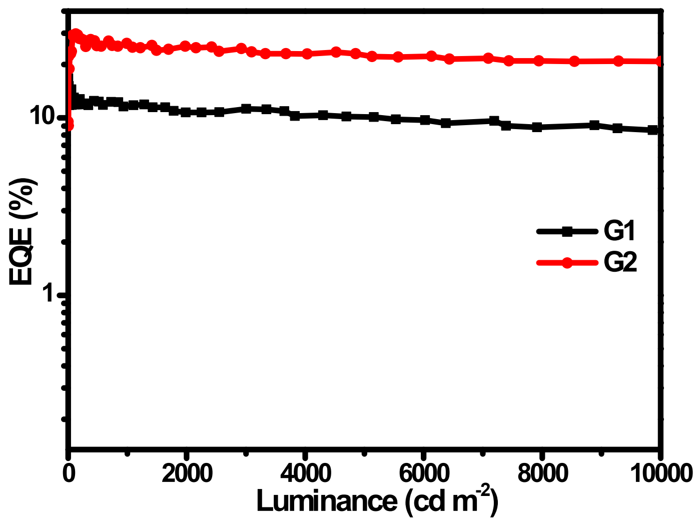


Fig. S4. The external quantum efficiency – luminance (*EQE – L*) curves of **G1 and G2**.

Table S1. Crystallographic data of Ir(tfmphqz)$_2$(tpip).

	Ir(tfmpqz)$_2$(tpip)
Formula	$C_{56}H_{34}F_{12}IrN_5O_2P_2$
FW	1291.04
T (K)	296
Wavelength (Å)	0.71073
Crystal system	orthorhombic
Space group	*P b c n*
a (Å)	22.853(3)
b (Å)	23.830(3)
c (Å)	18.909(2)
α (deg)	90.00
β (deg)	90.00
γ (deg)	90.00
V (Å^3)	10298(2)
Z	8
ρ_{calcd} (mg/cm^3)	1.666
μ (Mo Kα) (mm^{-1})	2.747
F (000)	5088.0
Reflns collected	68219
Unique	11895
Data/restraints/params	11895 / 0 / 703
GOF on F^2	0.989
$R_1{}^a$, $wR_2{}^b$ [$I > 2\sigma(I)$]	0.0389, 0.0665
$R_1{}^a$, $wR_2{}^b$ (all data)	0.1017, 0.0837
CCDC NO	1582727

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

Table S2(a) The selected bond lengths and angels of Ir(tfmphqz)$_2$(tpip).

Selected bonds Å					
C(1)-C(2)	1.393(7)	C(19)-C(20)	1.395(6)	C(39)-H(39)	0.93
C(1)-C(7)	1.424(6)	C(19)-H(19)	0.93	C(40)-C(41)	1.353(9)
C(1)-C(6)	1.451(6)	C(20)-C(21)	1.430(6)	C(40)-H(40)	0.93
C(2)-C(3)	1.378(7)	C(20)-C(22)	1.453(6)	C(41)-H(41)	0.93
C(2)-H(2)	0.93	C(21)-Ir(01)	2.019(5)	C(42)-C(47)	1.381(7)
C(3)-C(55)	1.364(7)	C(22)-N(1)	1.340(5)	C(42)-C(43)	1.381(7)
C(3)-C(4)	1.477(8)	C(22)-C(25)	1.427(6)	C(42)-P(1)	1.807(5)
C(4)-F(7)	1.254(8)	C(23)-N(2)	1.295(6)	C(43)-C(44)	1.379(8)
C(4)-F(8)	1.279(7)	C(23)-N(1)	1.358(6)	C(43)-H(43)	0.93
C(4)-F(9)	1.285(8)	C(23)-H(23)	0.93	C(44)-C(45)	1.359(10)
C(5)-C(55)	1.383(7)	C(24)-N(2)	1.372(6)	C(44)-H(44)	0.93
C(5)-C(7)	1.411(6)	C(24)-C(25)	1.406(7)	C(45)-C(46)	1.365(10)
C(5)-C(56F)	1.507(7)	C(24)-C(29)	1.414(7)	C(45)-H(45)	0.93
C(6)-N(3)	1.333(6)	C(25)-C(26)	1.424(6)	C(46)-C(47)	1.375(8)
C(6)-C(10)	1.429(6)	C(26)-C(27)	1.366(7)	C(46)-H(46)	0.93
C(7)-Ir(01)	2.019(5)	C(26)-H(26)	0.93	C(47)-H(47)	0.93
C(8)-N(4)	1.297(6)	C(27)-C(28)	1.359(8)	C(48)-C(49)	1.371(7)
C(8)-N(3)	1.355(6)	C(27)-H(27)	0.93	C(48)-C(53)	1.374(8)
C(8)-H(8)	0.93	C(28)-C(29)	1.361(8)	C(48)-P(1)	1.799(5)
C(9)-N(4)	1.363(7)	C(28)-H(28)	0.93	C(49)-C(50)	1.388(9)
C(9)-C(14)	1.415(7)	C(29)-H(29)	0.93	C(49)-H(49)	0.93
C(9)-C(10)	1.419(7)	C(30)-C(32)	1.371(7)	C(50)-C(51)	1.352(10)
C(10)-C(11)	1.411(7)	C(30)-C(31)	1.380(7)	C(50)-H(50)	0.93
C(11)-C(12)	1.372(7)	C(30)-P(2)	1.811(5)	C(51)-C(52)	1.345(10)
C(11)-H(11)	0.93	C(31)-C(33)	1.384(8)	C(51)-H(51)	0.93
C(12)-C(13)	1.391(8)	C(31)-H(31)	0.93	C(52)-C(53)	1.387(8)
C(12)-H(12)	0.93	C(32)-C(35)	1.396(7)	C(52)-H(52)	0.93
C(13)-C(14)	1.340(8)	C(32)-H(32)	0.93	C(53)-H(53)	0.93
C(13)-H(13)	0.93	C(33)-C(34)	1.360(9)	C(54)-H(54)	0.93
C(14)-H(14)	0.93	C(33)-H(33)	0.93	C(55)-H(55)	0.93
C(15)-F(6)	1.232(9)	C(34)-C(35)	1.354(9)	C(56F)-F(11)	1.325(6)
C(15)-F(4)	1.257(8)	C(34)-H(34)	0.93	C(56F)-F(12)	1.340(6)
C(15)-F(5)	1.291(9)	C(35)-H(35)	0.93	C(56F)-F(10)	1.342(7)
C(15)-C(18)	1.473(8)	C(36)-C(41)	1.374(8)	Ir(01)-N(3)	2.047(4)
C(16)-F(1)	1.319(6)	C(36)-C(37)	1.379(8)	Ir(01)-N(1)	2.047(4)
C(16)-F(2)	1.347(7)	C(36)-H(36)	0.93	Ir(01)-O(1)	2.155(3)
C(16)-F(3)	1.352(6)	C(37)-C(38)	1.380(7)	Ir(01)-O(2)	2.172(3)
C(16)-C(17)	1.495(7)	C(37)-P(2)	1.804(5)	N(5)-P(1)	1.578(4)
C(17)-C(21)	1.400(6)	C(38)-C(39)	1.385(8)	N(5)-P(2)	1.579(4)
C(17)-C(54)	1.400(7)	C(38)-H(38)	0.93	O(1)-P(1)	1.516(4)
C(18)-C(19)	1.359(7)	C(39)-C(40)	1.372(10)	O(2)-P(2)	1.521(3)
C(18)-C(54)	1.378(7)				

Selected angels°			
C(2)-C(1)-C(7)	122.2(5)	C(35)-C(34)-H(34)	119.5
C(2)-C(1)-C(6)	121.3(4)	C(33)-C(34)-H(34)	119.5
C(7)-C(1)-C(6)	116.0(4)	C(34)-C(35)-C(32)	119.9(7)

C(12)-C(11)-H(11)	119.3	C(46)-C(45)-H(45)	120.1
C(10)-C(11)-H(11)	119.3	C(45)-C(46)-C(47)	121.4(7)
C(11)-C(12)-C(13)	119.8(6)	C(45)-C(46)-H(46)	119.3
C(11)-C(12)-H(12)	120.1	C(47)-C(46)-H(46)	119.3
C(13)-C(12)-H(12)	120.1	C(46)-C(47)-C(42)	119.2(6)
C(14)-C(13)-C(12)	121.3(6)	C(46)-C(47)-H(47)	120.4
C(14)-C(13)-H(13)	119.4	C(42)-C(47)-H(47)	120.4
C(12)-C(13)-H(13)	119.4	C(49)-C(48)-C(53)	118.6(6)
C(13)-C(14)-C(9)	120.5(6)	C(49)-C(48)-P(1)	120.7(5)
C(13)-C(14)-H(14)	119.8	C(53)-C(48)-P(1)	120.7(4)
C(9)-C(14)-H(14)	119.8	C(48)-C(49)-C(50)	120.5(7)
F(6)-C(15)-F(4)	107.8(9)	C(48)-C(49)-H(49)	119.7
F(6)-C(15)-F(5)	101.2(8)	C(50)-C(49)-H(49)	119.7
F(4)-C(15)-F(5)	103.1(8)	C(51)-C(50)-C(49)	120.0(8)
F(6)-C(15)-C(18)	115.9(8)	C(51)-C(50)-H(50)	120
F(4)-C(15)-C(18)	114.9(7)	C(49)-C(50)-H(50)	120
F(5)-C(15)-C(18)	112.4(8)	C(52)-C(51)-C(50)	120.3(7)
F(1)-C(16)-F(2)	106.5(5)	C(52)-C(51)-H(51)	119.8
F(1)-C(16)-F(3)	106.0(5)	C(50)-C(51)-H(51)	119.8
F(2)-C(16)-F(3)	104.4(5)	C(51)-C(52)-C(53)	120.6(8)
F(1)-C(16)-C(17)	114.9(5)	C(51)-C(52)-H(52)	119.7
F(2)-C(16)-C(17)	111.6(5)	C(53)-C(52)-H(52)	119.7
F(3)-C(16)-C(17)	112.6(5)	C(48)-C(53)-C(52)	120.0(6)
C(21)-C(17)-C(54)	121.9(5)	C(48)-C(53)-H(53)	120
C(21)-C(17)-C(16)	123.1(5)	C(52)-C(53)-H(53)	120
C(54)-C(17)-C(16)	115.0(5)	C(18)-C(54)-C(17)	121.3(5)
C(19)-C(18)-C(54)	119.0(5)	C(18)-C(54)-H(54)	119.4
C(19)-C(18)-C(15)	120.1(6)	C(17)-C(54)-H(54)	119.4
C(54)-C(18)-C(15)	120.9(6)	C(3)-C(55)-C(5)	121.4(5)
C(18)-C(19)-C(20)	120.4(5)	C(3)-C(55)-H(55)	119.3
C(18)-C(19)-H(19)	119.8	C(5)-C(55)-H(55)	119.3
C(20)-C(19)-H(19)	119.8	F(11)-C(56F)-F(12)	105.9(5)
C(19)-C(20)-C(21)	122.5(5)	F(11)-C(56F)-F(10)	106.8(5)
C(19)-C(20)-C(22)	120.9(4)	F(12)-C(56F)-F(10)	105.7(5)
C(21)-C(20)-C(22)	116.2(4)	F(11)-C(56F)-C(5)	113.7(5)
C(17)-C(21)-C(20)	114.3(4)	F(12)-C(56F)-C(5)	112.4(5)
C(17)-C(21)-Ir(01)	133.9(3)	F(10)-C(56F)-C(5)	111.7(5)
C(20)-C(21)-Ir(01)	111.7(3)	C(21)-Ir(01)-C(7)	93.76(19)
N(1)-C(22)-C(25)	119.5(5)	C(21)-Ir(01)-N(3)	105.27(17)
N(1)-C(22)-C(20)	112.9(4)	C(7)-Ir(01)-N(3)	80.08(17)
C(25)-C(22)-C(20)	127.5(4)	C(21)-Ir(01)-N(1)	80.67(17)
N(2)-C(23)-N(1)	126.8(4)	C(7)-Ir(01)-N(1)	106.15(17)
N(2)-C(23)-H(23)	116.6	N(3)-Ir(01)-N(1)	171.31(16)
N(1)-C(23)-H(23)	116.6	C(21)-Ir(01)-O(1)	171.27(15)
N(2)-C(24)-C(25)	122.9(4)	C(7)-Ir(01)-O(1)	88.42(16)
N(2)-C(24)-C(29)	117.5(5)	N(3)-Ir(01)-O(1)	83.42(13)
C(25)-C(24)-C(29)	119.5(5)	N(1)-Ir(01)-O(1)	90.61(13)
C(24)-C(25)-C(26)	118.3(5)	C(21)-Ir(01)-O(2)	86.72(16)
C(24)-C(25)-C(22)	115.8(4)	C(7)-Ir(01)-O(2)	171.83(15)

C(26)-C(25)-C(22)	125.8(5)	N(3)-Ir(01)-O(2)	91.92(14)
C(27)-C(26)-C(25)	119.7(5)	N(1)-Ir(01)-O(2)	81.98(13)
C(27)-C(26)-H(26)	120.2	O(1)-Ir(01)-O(2)	92.32(12)
C(25)-C(26)-H(26)	120.2	C(22)-N(1)-C(23)	118.5(4)
C(28)-C(27)-C(26)	120.9(5)	C(22)-N(1)-Ir(01)	114.7(3)
C(28)-C(27)-H(27)	119.5	C(23)-N(1)-Ir(01)	125.5(3)
C(26)-C(27)-H(27)	119.5	C(23)-N(2)-C(24)	115.6(4)
C(27)-C(28)-C(29)	121.9(6)	C(6)-N(3)-C(8)	119.7(4)
C(27)-C(28)-H(28)	119.1	C(6)-N(3)-Ir(01)	115.9(3)
C(29)-C(28)-H(28)	119.1	C(8)-N(3)-Ir(01)	123.3(4)
C(28)-C(29)-C(24)	119.2(6)	C(8)-N(4)-C(9)	116.3(5)
C(28)-C(29)-H(29)	120.4	P(1)-N(5)-P(2)	131.0(3)
C(24)-C(29)-H(29)	120.4	P(1)-O(1)-Ir(01)	127.94(18)
C(32)-C(30)-C(31)	118.9(5)	P(2)-O(2)-Ir(01)	128.59(18)
C(32)-C(30)-P(2)	121.7(4)	O(1)-P(1)-N(5)	118.3(2)
C(31)-C(30)-P(2)	119.4(4)	O(1)-P(1)-C(48)	107.0(2)
C(30)-C(31)-C(33)	120.7(6)	N(5)-P(1)-C(48)	107.6(2)
C(30)-C(31)-H(31)	119.6	O(1)-P(1)-C(42)	107.7(2)
C(33)-C(31)-H(31)	119.6	N(5)-P(1)-C(42)	109.7(2)
C(30)-C(32)-C(35)	120.1(5)	C(48)-P(1)-C(42)	105.8(2)
C(30)-C(32)-H(32)	119.9	O(2)-P(2)-N(5)	117.7(2)
C(35)-C(32)-H(32)	119.9	O(2)-P(2)-C(37)	107.1(2)
C(34)-C(33)-C(31)	119.5(6)	N(5)-P(2)-C(37)	110.0(2)
C(34)-C(33)-H(33)	120.3	O(2)-P(2)-C(30)	109.2(2)
C(31)-C(33)-H(33)	120.3	N(5)-P(2)-C(30)	108.0(2)
C(35)-C(34)-C(33)	120.9(6)	C(37)-P(2)-C(30)	104.0(2)

References

1 *SAINT-Plus, version 6.02*, Bruker Analytical X-ray System, Madison, WI, 1999.

2 G. M. Sheldrick, *SADABS An empirical absorption correction program, Bruker Analytical X-ray Systems*, Madison, WI, 1996.

3 G. M. Sheldrick, *SHELXTL-2014*, Universität of Göttingen, Göttingen, Germany, 2014.