

[(1,2,5,6- η)-Cycloocta-1,5-diene](4-isopropyl-1-methyl-1,2,4-triazol-5-ylidene)(tricyclohexylphosphane- κP)iridium(I) tetrafluoroborate dichloromethane monosolvate

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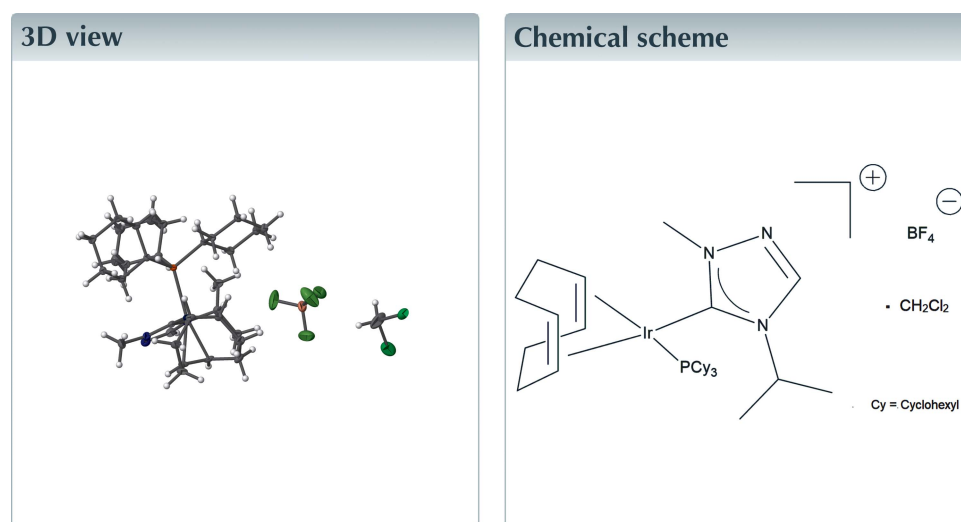
Keywords: crystal structure; iridium; N-heterocyclic carbenes.

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Structural data: full structural data are available from iucrdata.iucr.org

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The title compound, $[\text{Ir}(\text{C}_8\text{H}_{12})(\text{C}_6\text{H}_{11}\text{N}_3)(\text{C}_{18}\text{H}_{33}\text{P})]\text{BF}_4 \cdot \text{CH}_2\text{Cl}_2$, a triazole-based N-heterocyclic carbene iridium(I) cationic complex with a tetrafluoroborate counter-anion, crystallizes with one dichloromethane solvent molecule per formula unit. The Ir^I atom of the cationic complex has a distorted square-planar coordination environment, defined by a bidentate cycloocta-1,5-diene (COD) ligand, an N-heterocyclic carbene, and a tricyclohexylphosphane ligand. The complex crystallizes in a C-centered monoclinic unit cell and has an unusually high number of eight formula units.



Structure description

N-heterocyclic carbenes (NHCs) have emerged as excellent spectator ligands in homogeneous catalysis (Cazin, 2013; de Frémont *et al.*, 2009; Díez-González *et al.*, 2009; Rovis & Nolan, 2013; Ruff *et al.*, 2016; Zuo *et al.*, 2014). Their catalytic activities in the transfer hydrogenation of ketones and imines have also been studied and reported (Albrecht *et al.*, 2002; Gnanamgari *et al.*, 2007). The NHC ligands can be tuned sterically and electronically by having different substituents on the nitrogen atoms (Gusev, 2009). Many imidazole- and triazole-based NHC rhodium and iridium complexes have been synthesized and structurally characterized (Herrmann *et al.*, 2006; Wang & Lin, 1998; Chianese *et al.*, 2004). As part of our ongoing research, we continue to synthesize new imidazole- and triazole-based NHC complexes of rhodium and iridium to study the effect of different substituents on the NHCs and co-ligands coordinating to the transition metal in

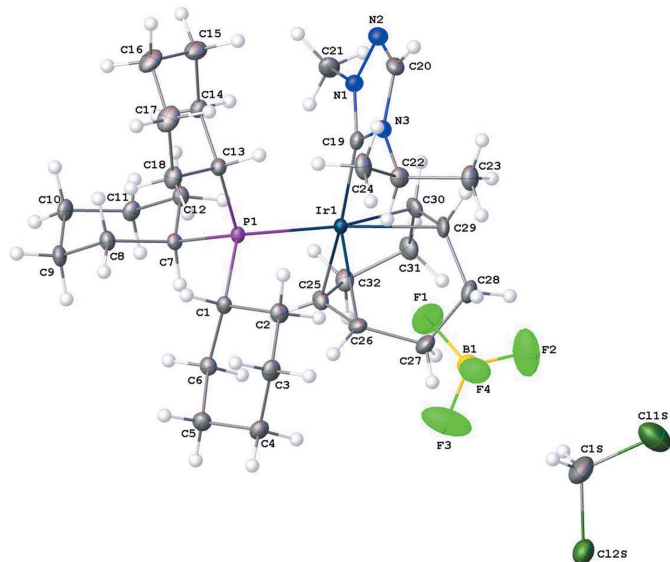


Figure 1
The molecular entities in the crystal structure of the title compound (**4**). Displacement ellipsoids are drawn at the 50% probability level.

transfer hydrogenation reactions (Nichol *et al.*, 2009, 2010, 2011, 2012; Idrees *et al.*, 2017*a,b*; Rood *et al.*, 2021; Rushlow *et al.*, 2021; Newman *et al.*, 2021; Castaldi *et al.*, 2021).

The molecular structure of the title complex, $[\text{Ir}(\text{C}_8\text{H}_{12})(\text{C}_{18}\text{H}_{33}\text{P})(\text{C}_6\text{H}_{11}\text{N}_3)][\text{BF}_4] \cdot \text{CH}_2\text{Cl}_2$ (**4**), comprises an Ir^I cationic complex, a tetrafluoridoborate counter-anion,

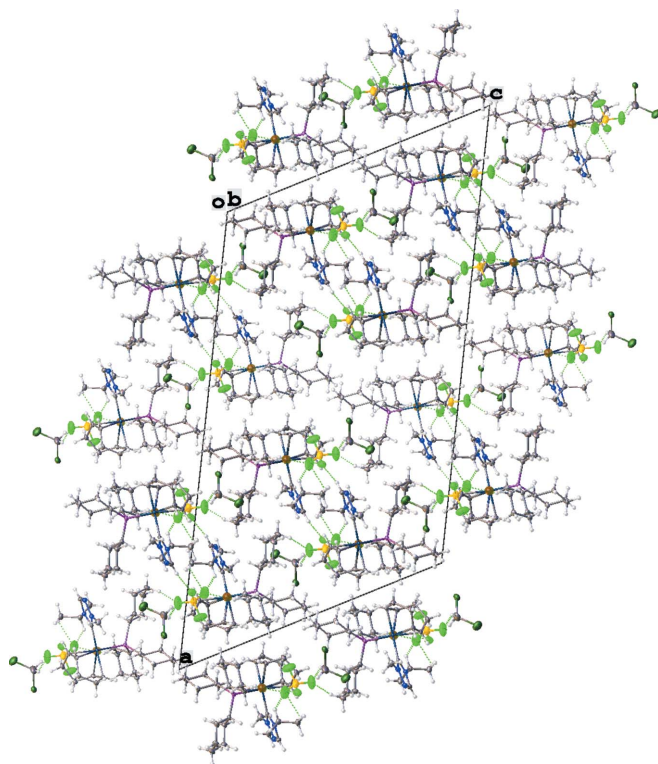


Figure 2
Crystal packing unit-cell diagram of the title compound (**4**) shown along the *b* axis. Non-classical hydrogen-bonding interactions between F and H atoms are shown as dotted green lines.

Table 1
Hydrogen-bond geometry (Å, °).

<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
C2–H2A···F1	0.99	2.54	3.204 (4)	124
C23–H23C···F1	0.98	2.51	3.137 (4)	122
C20–H20···F4 ⁱ	0.95	2.49	3.400 (3)	161
C30–H30···F4 ⁱⁱ	1.00	2.35	3.192 (3)	141
C16–H16B···F2 ⁱⁱⁱ	0.99	2.54	3.404 (4)	146
C22–H22···F1	1.00	2.41	3.094 (4)	125
C31–H31B···F3 ⁱⁱ	0.99	2.35	3.330 (4)	170
C1S–H1SA···F2	0.99	2.50	3.362 (5)	145

Symmetry codes: (i) $-x + \frac{1}{2}, -y + \frac{3}{2}, -z + 1$; (ii) $x, y - 1, z$; (iii) $x, -y + 1, z + \frac{1}{2}$.

and a CH₂Cl₂ solvent molecule, as illustrated in Fig. 1. The coordination sphere around the Ir^I atom, formed by the bidentate (1,2,5,6-η)-cycloocta-1,5-diene (COD), NHC, and tricyclohexylphosphane ligands, results in a distorted square-planar shape. The N1–C19_(NHC)–N3 bond angle in the triazole-based carbene is 102.8 (2)° deviating from the expected 120° for the *sp*²-hybridized carbon atom. Other selected bond lengths and angles in the structure are: Ir1–C19_(NHC) = 2.035 (3) Å, Ir1–P1 = 2.3732 (7) Å, and C19–Ir1–P1 = 94.07 (7)°. The cyclohexyl rings of the tricyclohexylphosphane ligand are all in the expected chair conformation, with the mean planes of the cyclohexyl rings forming dihedral angles of 59.70 (15), 61.77 (14), and 83.20 (15)°. The crystal packing diagram of the title compound is shown in Fig. 2. Several close C–H···F contacts stabilizing the orientation of the [BF₄][−] group with the iridium(I) complex and dichloromethane solvate are reported in Table 1. These non-classical hydrogen-bonds are shown as green dotted lines in Fig. 2.

Synthesis and crystallization

1-Methyl-1,2,4 triazole (1) was purchased from Matrix Scientific. All other compounds used in the syntheses as shown in Fig. 3 were obtained from Sigma-Aldrich and Strem and used as received. All subsequent synthesis procedures were performed under nitrogen using reagent grade solvents, which were used as received without further purification. NMR spectra were recorded at room temperature in CDCl₃ on a 400 MHz Varian spectrometer (operating at 162 MHz for ³¹P) and referenced to the residual solvent peak (δ in ppm).

4-Isopropyl-1-methyl-1,2,4-triazolium bromide (2): 1-methyl-1,2,4-triazole (**1**) (5.01 g, 60.28 mmol) and isopropyl bromide (10.48 g, 85.2 mmol) were added to toluene (20 ml),

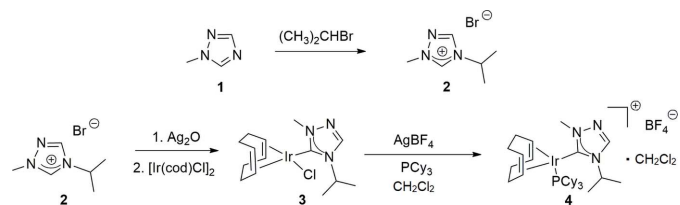


Figure 3
Reaction scheme for the synthesis of the N-heterocyclic carbene (**2**) and subsequent formation of the title compound (**4**).

and the mixture was refluxed for 48 h. Once cooled, the liquid was decanted, the white solid product that had formed was washed with ether, filtered, and dried. Yield: 2.48 g (20%). ^1H NMR: δ 11.79 (s, 1 H, N–C₃H–N), 8.97 (s, 1 H, N–C₃H–N), 5.83 [m, 1 H, CH(CH₃)₂], 4.29 (s, 3 H, N–CH₃), 1.73 [d, 6 H, CH(CH₃)₂]. ^{13}C NMR: δ 143.52 (N–CH–N), 142.65 (N–CH–N), 53.32 [CH(CH₃)₂], 39.62 (N–CH₃), 23.21[CH(CH₃)₂].

[(1,2,5,6- η)-Cycloocta-1,5-diene](4-isopropyl-1-methyl-1,2,4-triazol-5-ylidene) chloroiridium (3): 4-isopropyl-1-methyl-1,2,4-triazolium bromide (2) (0.061 g, 0.300 mmol), Ag₂O (0.035 g, 0.149 mmol), and 10 ml of CH₂Cl₂ were added to an oven-dried flask and stirred under N₂ in the dark for 90 min. The mixture was filtered through Celite into [Ir(COD)Cl]₂ (0.100 g, 0.149 mmol) and stirred in the dark for 90 min. The resulting mixture was filtered through Celite and the solvent was removed under reduced pressure. The red solid product was washed with pentane and allowed to dry overnight under vacuum. Yield: 0.139 g (100%). ^1H NMR: δ 7.91 (s, 1 H, N–C₃H–N), 5.52 [m, 1 H, CH(CH₃)₂], 4.74, 4.76 (m, 4 H, CH of COD), 4.09 (s, 3 H, CH₃–N), 2.96, 2.30, 2.17, 1.86 (m, 8 H, CH₂ of COD), 1.28 [m, 6 H, CH(CH₃)₂]. ^{13}C NMR: δ 181.21 (Ir–C), 138.79 (N–CH–N), 86.59, 85.96 (CH of COD), 51.73 [CH(CH₃)₂], 40.52 (N–CH₃), 33.72, 33.28, 29.65, 29.24 (CH₂ of COD), 24.17, 23.31[CH(CH₃)₂].

[(1,2,5,6- η)-Cycloocta-1,5-diene](4-isopropyl-1-methyl-1,2,4-triazol-5-ylidene)(tricyclohexylphosphane)iridium(I) tetrafluoroborate (4): Tricyclohexylphosphane (0.085 g, 0.308 mmol) and AgBF₄ (0.059 g, 0.308 mmol) were added to an oven-dried flask containing complex 3 (0.140 g, 0.308 mmol) in 10 ml of CH₂Cl₂, and stirred under N₂ in the dark for 90 mins. The mixture was filtered through Celite and the solvent was removed under reduced pressure. The bright-red solid was washed with pentane and dried under vacuum. Yield: 0.214 g (100%). ^1H NMR: δ 8.58 (s, 1 H, N–C₃H–N), 5.29 [m, 1 H, CH(CH₃)₂], 4.38, 3.99 (m, 4 H, CH of COD), 4.05 (s, 3 H, CH₃–N), 2.27–0.86 CH₂ of COD and cyclohexyl, 1.21 [m, 6 H, CH(CH₃)₂]. ^{13}C NMR: δ 178.26 (Ir–C), 142.01 (N–CH–N), 77.30, 77.19, 76.98, 77.66 (CH of COD), 54.23 [CH(CH₃)₂], 40.51 (N–CH₃), 34.94, 34.10, 30.36, 30.14 (CH₂ of COD), 27.79–25.92 (CH₂ of cyclohexyl), 24.50, 22.86 [CH(CH₃)₂]. ^{31}P : δ 39.81.

The title compound (4) was crystallized by slow diffusion of pentane into a CH₂Cl₂ solution.

Refinement

Crystal data, data collection, and structure refinement details are summarized in Table 2.

Acknowledgements

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Table 2

Experimental details.

Crystal data	
Chemical formula	[Ir(C ₈ H ₁₂)(C ₆ H ₁₁ N ₃)(C ₁₈ H ₃₃ P)]-BF ₄ ·CH ₂ Cl ₂
<i>M</i> _r	877.70
Crystal system, space group	Monoclinic, C2/c
Temperature (K)	100
<i>a</i> , <i>b</i> , <i>c</i> (Å)	35.832 (5), 10.2608 (15), 22.034 (3)
β (°)	118.095 (3)
<i>V</i> (Å ³)	7146.7 (17)
<i>Z</i>	8
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	3.98
Crystal size (mm)	0.27 × 0.11 × 0.07
Data collection	
Diffractionmeter	Bruker APEXII CCD
Absorption correction	Multi-scan (SADABS; Krause <i>et al.</i> , 2015)
<i>T</i> _{min} , <i>T</i> _{max}	0.555, 0.746
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	151141, 7958, 7086
<i>R</i> _{int}	0.061
(sin θ / λ) _{max} (Å ⁻¹)	0.643
Refinement	
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.022, 0.052, 1.05
No. of reflections	7958
No. of parameters	409
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ⁻³)	1.83, -0.69

Computer programs: APEX2 and SAINT (Bruker, 2007), olex2.solve (Bourhis *et al.*, 2015), SHELXL (Sheldrick, 2015), OLEX2 (Dolomanov *et al.*, 2009), and publCIF (Westrip, 2010).

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full crystallographic data

IUCrData (2022). 7, x220685 [https://doi.org/10.1107/S241431462200685X]

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(tricyclohexylphosphane- κP)iridium(I) tetrafluoridoborate dichloromethane
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[(1,2,5,6- η)-Cycloocta-1,5-diene](4-isopropyl-1-methyl-1,2,4-triazol-5-ylidene)(tricyclohexylphosphane- κP)iridium(I) tetrafluoridoborate dichloromethane monosolvate

Crystal data

[Ir(C₈H₁₂)(C₆H₁₁N₃)(C₁₈H₃₃P)]BF₄·CH₂Cl₂

$M_r = 877.70$

Monoclinic, *C2/c*

$a = 35.832$ (5) Å

$b = 10.2608$ (15) Å

$c = 22.034$ (3) Å

$\beta = 118.095$ (3)°

$V = 7146.7$ (17) Å³

$Z = 8$

$F(000) = 3552$

$D_x = 1.631$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 9640 reflections

$\theta = 2.5$ – 27.1 °

$\mu = 3.98$ mm⁻¹

$T = 100$ K

Plate, clear light pink

$0.27 \times 0.11 \times 0.07$ mm

Data collection

Bruker APEXII CCD

diffractometer

φ and ω scans

Absorption correction: multi-scan
(SADABS; Krause *et al.*, 2015)

$T_{\min} = 0.555$, $T_{\max} = 0.746$

151141 measured reflections

7958 independent reflections

7086 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.061$

$\theta_{\max} = 27.2$ °, $\theta_{\min} = 1.3$ °

$h = -45 \rightarrow 46$

$k = -13 \rightarrow 13$

$l = -28 \rightarrow 27$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.022$

$wR(F^2) = 0.052$

$S = 1.05$

7958 reflections

409 parameters

1 restraint

Primary atom site location: iterative

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0234P)^2 + 23.3944P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.004$

$\Delta\rho_{\max} = 1.83$ e Å⁻³

$\Delta\rho_{\min} = -0.69$ e Å⁻³

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Ir1	0.37947 (2)	0.36533 (2)	0.66268 (2)	0.01104 (4)
P1	0.39296 (2)	0.44263 (6)	0.77266 (3)	0.01133 (12)
Cl2S	0.40895 (2)	1.15711 (8)	0.42611 (4)	0.02888 (16)
Cl1S	0.32454 (3)	1.06150 (10)	0.33196 (5)	0.0487 (2)
F4	0.33674 (6)	0.95299 (19)	0.51922 (11)	0.0381 (5)
N1	0.29702 (7)	0.2187 (2)	0.62775 (11)	0.0165 (5)
N3	0.28433 (7)	0.4161 (2)	0.59694 (11)	0.0148 (4)
F2	0.34763 (10)	0.7797 (2)	0.46717 (12)	0.0665 (8)
F3	0.40161 (8)	0.8615 (2)	0.56303 (16)	0.0674 (8)
C19	0.31703 (8)	0.3312 (2)	0.63092 (13)	0.0140 (5)
N2	0.25339 (7)	0.2280 (2)	0.59297 (12)	0.0206 (5)
F1	0.34932 (10)	0.7542 (3)	0.56918 (13)	0.0762 (9)
C1	0.41482 (8)	0.6111 (2)	0.79339 (13)	0.0133 (5)
H1	0.409073	0.642915	0.831081	0.016*
C7	0.43280 (8)	0.3465 (2)	0.84639 (13)	0.0124 (5)
H7	0.460500	0.366415	0.847728	0.015*
C13	0.34343 (8)	0.4505 (2)	0.78081 (13)	0.0141 (5)
H13	0.320559	0.472551	0.733675	0.017*
C6	0.46335 (8)	0.6214 (2)	0.82126 (11)	0.0148 (5)
H6A	0.478006	0.573466	0.865319	0.018*
H6B	0.471149	0.580549	0.788106	0.018*
C12	0.42781 (8)	0.1971 (2)	0.83749 (13)	0.0150 (5)
H12A	0.401002	0.169971	0.836486	0.018*
H12B	0.426543	0.171706	0.793210	0.018*
C2	0.38961 (8)	0.7009 (2)	0.73112 (14)	0.0163 (5)
H2A	0.391499	0.666680	0.690660	0.020*
H2B	0.359446	0.700389	0.720122	0.020*
C21	0.31663 (9)	0.0937 (3)	0.65715 (15)	0.0221 (6)
H21A	0.310806	0.031417	0.620001	0.033*
H21B	0.304984	0.060358	0.686421	0.033*
H21C	0.347268	0.105237	0.684765	0.033*
C25	0.44696 (8)	0.3374 (3)	0.69905 (14)	0.0167 (5)
H25	0.465054	0.353427	0.749386	0.020*
C8	0.43839 (8)	0.3886 (3)	0.91742 (13)	0.0158 (5)
H8A	0.443145	0.483866	0.922958	0.019*
H8B	0.412273	0.368539	0.920393	0.019*
C23	0.26856 (9)	0.5766 (3)	0.50488 (14)	0.0224 (6)
H23A	0.237706	0.572301	0.485058	0.034*
H23B	0.278255	0.509140	0.484080	0.034*

H23C	0.276744	0.662600	0.495709	0.034*
C11	0.46487 (9)	0.1279 (2)	0.89647 (13)	0.0158 (5)
H11A	0.460147	0.032577	0.891400	0.019*
H11B	0.491179	0.147151	0.893945	0.019*
C9	0.47579 (9)	0.3179 (3)	0.97497 (13)	0.0172 (5)
H9A	0.478191	0.343834	1.019954	0.021*
H9B	0.502223	0.343751	0.974335	0.021*
C18	0.34015 (9)	0.5541 (3)	0.82801 (14)	0.0193 (6)
H18A	0.346227	0.640997	0.815137	0.023*
H18B	0.361480	0.536406	0.876193	0.023*
C20	0.24711 (8)	0.3498 (3)	0.57501 (14)	0.0185 (6)
H20	0.219940	0.388176	0.549698	0.022*
C26	0.43439 (8)	0.4508 (3)	0.65866 (11)	0.0168 (5)
H26	0.444608	0.531772	0.687085	0.020*
C32	0.45361 (9)	0.2064 (3)	0.67450 (14)	0.0192 (6)
H32A	0.452366	0.137592	0.705011	0.023*
H32B	0.482169	0.203978	0.677949	0.023*
C4	0.45350 (9)	0.8468 (3)	0.76842 (15)	0.0197 (6)
H4A	0.463430	0.938160	0.778773	0.024*
H4B	0.459077	0.815192	0.731018	0.024*
C14	0.33119 (8)	0.3160 (3)	0.79709 (14)	0.0160 (5)
H14A	0.332548	0.250194	0.765315	0.019*
H14B	0.351701	0.290493	0.844618	0.019*
C30	0.37730 (9)	0.2283 (3)	0.58452 (13)	0.0177 (5)
H30	0.355490	0.158421	0.572558	0.021*
C10	0.47030 (9)	0.1703 (3)	0.96657 (14)	0.0179 (5)
H10A	0.495397	0.126619	1.003385	0.022*
H10B	0.445176	0.143510	0.971083	0.022*
C16	0.28327 (10)	0.4211 (3)	0.83670 (16)	0.0258 (6)
H16A	0.253819	0.424430	0.829333	0.031*
H16B	0.301900	0.397242	0.885332	0.031*
C22	0.28870 (9)	0.5548 (3)	0.58210 (14)	0.0174 (5)
H22	0.319547	0.575082	0.602327	0.021*
C15	0.28669 (9)	0.3177 (3)	0.78991 (16)	0.0231 (6)
H15A	0.265871	0.336313	0.741537	0.028*
H15B	0.280048	0.231093	0.802164	0.028*
C29	0.36078 (9)	0.3470 (3)	0.55232 (13)	0.0181 (6)
H29	0.329489	0.346033	0.521651	0.022*
C5	0.47773 (9)	0.7629 (3)	0.83248 (14)	0.0187 (6)
H5A	0.508287	0.766504	0.846153	0.022*
H5B	0.473836	0.799412	0.870709	0.022*
C31	0.42068 (9)	0.1769 (3)	0.60030 (14)	0.0205 (6)
H31A	0.429634	0.217383	0.568440	0.025*
H31B	0.419020	0.081538	0.592699	0.025*
C3	0.40612 (9)	0.8415 (3)	0.74491 (14)	0.0192 (6)
H3A	0.390892	0.893617	0.702391	0.023*
H3B	0.400367	0.880384	0.780789	0.023*
C24	0.26977 (9)	0.6436 (3)	0.61597 (14)	0.0218 (6)

H24A	0.275798	0.734726	0.610367	0.033*
H24B	0.282248	0.622876	0.665071	0.033*
H24C	0.239084	0.630457	0.594223	0.033*
C28	0.38413 (9)	0.4454 (3)	0.53192 (14)	0.0221 (6)
H28A	0.368542	0.529057	0.520982	0.026*
H28B	0.384614	0.414669	0.489710	0.026*
C27	0.42968 (9)	0.4688 (3)	0.58804 (14)	0.0218 (6)
H27A	0.448791	0.407585	0.581380	0.026*
H27B	0.438268	0.558577	0.583636	0.026*
C17	0.29586 (10)	0.5546 (3)	0.82245 (16)	0.0252 (6)
H17A	0.295162	0.618232	0.855678	0.030*
H17B	0.275024	0.582953	0.775659	0.030*
B1	0.35915 (13)	0.8357 (4)	0.53007 (19)	0.0317 (8)
C1S	0.36391 (13)	1.0744 (5)	0.4171 (2)	0.0568 (12)
H1SA	0.372205	0.985789	0.436656	0.068*
H1SB	0.352286	1.120661	0.443906	0.068*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ir1	0.01177 (5)	0.01212 (5)	0.00905 (5)	0.00001 (4)	0.00476 (4)	-0.00061 (4)
P1	0.0132 (3)	0.0105 (3)	0.0100 (3)	0.0009 (2)	0.0053 (3)	0.0001 (2)
Cl2S	0.0298 (4)	0.0360 (4)	0.0242 (4)	0.0020 (3)	0.0155 (3)	0.0033 (3)
Cl1S	0.0400 (5)	0.0429 (5)	0.0466 (5)	-0.0068 (4)	0.0067 (4)	-0.0053 (4)
F4	0.0372 (11)	0.0322 (10)	0.0466 (12)	-0.0052 (9)	0.0210 (10)	-0.0079 (9)
N1	0.0170 (11)	0.0167 (11)	0.0158 (11)	-0.0025 (9)	0.0077 (9)	0.0002 (9)
N3	0.0132 (11)	0.0166 (11)	0.0140 (11)	0.0006 (9)	0.0059 (9)	-0.0001 (9)
F2	0.113 (2)	0.0406 (13)	0.0361 (13)	0.0102 (14)	0.0270 (14)	-0.0078 (10)
F3	0.0350 (13)	0.0366 (13)	0.109 (2)	-0.0045 (10)	0.0166 (14)	-0.0099 (13)
C19	0.0168 (13)	0.0161 (12)	0.0102 (12)	0.0004 (10)	0.0072 (10)	-0.0002 (9)
N2	0.0167 (12)	0.0261 (13)	0.0190 (12)	-0.0035 (10)	0.0083 (10)	-0.0009 (10)
F1	0.091 (2)	0.0757 (19)	0.0468 (15)	-0.0387 (16)	0.0203 (14)	0.0237 (13)
C1	0.0173 (13)	0.0107 (12)	0.0120 (12)	-0.0002 (9)	0.0069 (10)	-0.0010 (9)
C7	0.0117 (12)	0.0128 (12)	0.0112 (12)	0.0013 (9)	0.0040 (10)	0.0013 (9)
C13	0.0140 (12)	0.0164 (12)	0.0126 (12)	0.0004 (10)	0.0068 (10)	-0.0006 (10)
C6	0.0161 (13)	0.0134 (12)	0.0142 (12)	0.0009 (10)	0.0066 (10)	-0.0009 (9)
C12	0.0186 (13)	0.0124 (12)	0.0133 (13)	0.0024 (10)	0.0070 (11)	0.0007 (10)
C2	0.0174 (13)	0.0136 (12)	0.0161 (13)	0.0030 (10)	0.0064 (11)	0.0019 (10)
C21	0.0269 (15)	0.0148 (13)	0.0214 (14)	-0.0034 (11)	0.0086 (12)	0.0014 (11)
C25	0.0150 (13)	0.0224 (14)	0.0135 (13)	0.0005 (10)	0.0073 (11)	-0.0042 (10)
C8	0.0177 (13)	0.0162 (13)	0.0120 (12)	0.0011 (10)	0.0059 (11)	-0.0009 (10)
C23	0.0260 (15)	0.0234 (14)	0.0151 (14)	0.0054 (12)	0.0074 (12)	0.0033 (11)
C11	0.0201 (13)	0.0122 (12)	0.0158 (13)	0.0034 (10)	0.0092 (11)	0.0029 (10)
C9	0.0193 (13)	0.0198 (13)	0.0096 (12)	0.0011 (11)	0.0043 (11)	0.0002 (10)
C18	0.0240 (15)	0.0192 (13)	0.0173 (14)	0.0037 (11)	0.0119 (12)	-0.0006 (10)
C20	0.0116 (12)	0.0263 (15)	0.0156 (13)	-0.0013 (11)	0.0048 (11)	-0.0007 (11)
C26	0.0159 (13)	0.0194 (13)	0.0183 (13)	-0.0043 (10)	0.0107 (11)	-0.0026 (10)
C32	0.0175 (13)	0.0235 (14)	0.0169 (13)	0.0057 (11)	0.0084 (11)	-0.0011 (11)

C4	0.0243 (15)	0.0178 (13)	0.0193 (14)	-0.0028 (11)	0.0120 (12)	0.0014 (11)
C14	0.0172 (13)	0.0171 (12)	0.0151 (13)	0.0002 (10)	0.0086 (11)	0.0004 (10)
C30	0.0187 (14)	0.0202 (13)	0.0131 (13)	-0.0028 (10)	0.0067 (11)	-0.0080 (10)
C10	0.0213 (14)	0.0176 (13)	0.0129 (13)	0.0043 (11)	0.0065 (11)	0.0051 (10)
C16	0.0239 (15)	0.0332 (16)	0.0294 (16)	0.0060 (13)	0.0200 (13)	0.0065 (13)
C22	0.0180 (13)	0.0152 (13)	0.0174 (13)	0.0034 (10)	0.0071 (11)	0.0031 (10)
C15	0.0162 (14)	0.0282 (15)	0.0259 (15)	-0.0001 (11)	0.0108 (12)	0.0041 (12)
C29	0.0189 (13)	0.0272 (15)	0.0085 (12)	-0.0007 (11)	0.0068 (11)	-0.0033 (10)
C5	0.0216 (14)	0.0166 (13)	0.0175 (14)	-0.0031 (11)	0.0089 (12)	-0.0017 (10)
C31	0.0244 (15)	0.0197 (13)	0.0183 (14)	0.0015 (11)	0.0107 (12)	-0.0072 (11)
C3	0.0253 (15)	0.0140 (13)	0.0177 (14)	0.0014 (11)	0.0097 (12)	0.0029 (10)
C24	0.0255 (15)	0.0212 (14)	0.0143 (13)	0.0087 (11)	0.0059 (12)	0.0024 (11)
C28	0.0255 (15)	0.0291 (15)	0.0140 (13)	0.0020 (12)	0.0113 (12)	0.0038 (11)
C27	0.0252 (15)	0.0256 (15)	0.0207 (14)	-0.0042 (12)	0.0160 (13)	0.0000 (11)
C17	0.0277 (16)	0.0267 (15)	0.0283 (16)	0.0113 (12)	0.0190 (14)	0.0037 (12)
B1	0.041 (2)	0.0238 (18)	0.0246 (19)	-0.0130 (15)	0.0110 (17)	0.0005 (14)
C1S	0.048 (2)	0.096 (4)	0.034 (2)	-0.021 (2)	0.0252 (19)	0.004 (2)

Geometric parameters (Å, °)

Ir1—P1	2.3732 (7)	C11—H11B	0.9900
Ir1—C19	2.035 (3)	C11—C10	1.526 (4)
Ir1—C25	2.179 (3)	C9—H9A	0.9900
Ir1—C26	2.194 (3)	C9—H9B	0.9900
Ir1—C30	2.196 (3)	C9—C10	1.528 (4)
Ir1—C29	2.205 (3)	C18—H18A	0.9900
P1—C1	1.863 (3)	C18—H18B	0.9900
P1—C7	1.862 (3)	C18—C17	1.533 (4)
P1—C13	1.868 (3)	C20—H20	0.9500
Cl2S—C1S	1.750 (4)	C26—H26	1.0000
Cl1S—C1S	1.742 (4)	C26—C27	1.496 (3)
F4—B1	1.403 (5)	C32—H32A	0.9900
N1—C19	1.343 (3)	C32—H32B	0.9900
N1—N2	1.383 (3)	C32—C31	1.530 (4)
N1—C21	1.460 (3)	C4—H4A	0.9900
N3—C19	1.366 (3)	C4—H4B	0.9900
N3—C20	1.367 (3)	C4—C5	1.528 (4)
N3—C22	1.484 (3)	C4—C3	1.525 (4)
F2—B1	1.372 (4)	C14—H14A	0.9900
F3—B1	1.368 (5)	C14—H14B	0.9900
N2—C20	1.298 (4)	C14—C15	1.527 (4)
F1—B1	1.361 (4)	C30—H30	1.0000
C1—H1	1.0000	C30—C29	1.394 (4)
C1—C6	1.551 (4)	C30—C31	1.519 (4)
C1—C2	1.543 (3)	C10—H10A	0.9900
C7—H7	1.0000	C10—H10B	0.9900
C7—C12	1.546 (3)	C16—H16A	0.9900
C7—C8	1.543 (3)	C16—H16B	0.9900

C13—H13	1.0000	C16—C15	1.524 (4)
C13—C18	1.530 (4)	C16—C17	1.520 (4)
C13—C14	1.541 (4)	C22—H22	1.0000
C6—H6A	0.9900	C22—C24	1.525 (4)
C6—H6B	0.9900	C15—H15A	0.9900
C6—C5	1.522 (3)	C15—H15B	0.9900
C12—H12A	0.9900	C29—H29	1.0000
C12—H12B	0.9900	C29—C28	1.509 (4)
C12—C11	1.527 (3)	C5—H5A	0.9900
C2—H2A	0.9900	C5—H5B	0.9900
C2—H2B	0.9900	C31—H31A	0.9900
C2—C3	1.534 (4)	C31—H31B	0.9900
C21—H21A	0.9800	C3—H3A	0.9900
C21—H21B	0.9800	C3—H3B	0.9900
C21—H21C	0.9800	C24—H24A	0.9800
C25—H25	1.0000	C24—H24B	0.9800
C25—C26	1.404 (4)	C24—H24C	0.9800
C25—C32	1.510 (4)	C28—H28A	0.9900
C8—H8A	0.9900	C28—H28B	0.9900
C8—H8B	0.9900	C28—C27	1.533 (4)
C8—C9	1.526 (4)	C27—H27A	0.9900
C23—H23A	0.9800	C27—H27B	0.9900
C23—H23B	0.9800	C17—H17A	0.9900
C23—H23C	0.9800	C17—H17B	0.9900
C23—C22	1.520 (4)	C1S—H1SA	0.9900
C11—H11A	0.9900	C1S—H1SB	0.9900
C19—Ir1—P1	94.07 (7)	C25—C26—Ir1	70.68 (15)
C19—Ir1—C25	162.50 (10)	C25—C26—H26	112.2
C19—Ir1—C26	156.41 (10)	C25—C26—C27	127.4 (2)
C19—Ir1—C30	89.60 (10)	C27—C26—Ir1	115.31 (17)
C19—Ir1—C29	83.82 (10)	C27—C26—H26	112.2
C25—Ir1—P1	90.64 (7)	C25—C32—H32A	109.0
C25—Ir1—C26	37.45 (10)	C25—C32—H32B	109.0
C25—Ir1—C30	80.07 (10)	C25—C32—C31	112.7 (2)
C25—Ir1—C29	95.89 (10)	H32A—C32—H32B	107.8
C26—Ir1—P1	98.76 (6)	C31—C32—H32A	109.0
C26—Ir1—C30	85.73 (9)	C31—C32—H32B	109.0
C26—Ir1—C29	78.59 (9)	H4A—C4—H4B	108.1
C30—Ir1—P1	158.38 (7)	C5—C4—H4A	109.5
C30—Ir1—C29	36.92 (10)	C5—C4—H4B	109.5
C29—Ir1—P1	164.70 (7)	C3—C4—H4A	109.5
C1—P1—Ir1	114.85 (8)	C3—C4—H4B	109.5
C1—P1—C13	104.19 (11)	C3—C4—C5	110.6 (2)
C7—P1—Ir1	114.70 (8)	C13—C14—H14A	109.4
C7—P1—C1	102.49 (11)	C13—C14—H14B	109.4
C7—P1—C13	108.17 (12)	H14A—C14—H14B	108.0
C13—P1—Ir1	111.52 (8)	C15—C14—C13	111.3 (2)

C19—N1—N2	113.9 (2)	C15—C14—H14A	109.4
C19—N1—C21	126.8 (2)	C15—C14—H14B	109.4
N2—N1—C21	119.3 (2)	Ir1—C30—H30	113.6
C19—N3—C20	108.6 (2)	C29—C30—Ir1	71.89 (15)
C19—N3—C22	125.4 (2)	C29—C30—H30	113.6
C20—N3—C22	125.9 (2)	C29—C30—C31	124.3 (3)
N1—C19—Ir1	129.73 (19)	C31—C30—Ir1	112.85 (17)
N1—C19—N3	102.8 (2)	C31—C30—H30	113.6
N3—C19—Ir1	126.77 (19)	C11—C10—C9	110.7 (2)
C20—N2—N1	103.0 (2)	C11—C10—H10A	109.5
P1—C1—H1	106.2	C11—C10—H10B	109.5
C6—C1—P1	115.09 (17)	C9—C10—H10A	109.5
C6—C1—H1	106.2	C9—C10—H10B	109.5
C2—C1—P1	109.51 (17)	H10A—C10—H10B	108.1
C2—C1—H1	106.2	H16A—C16—H16B	108.0
C2—C1—C6	112.9 (2)	C15—C16—H16A	109.4
P1—C7—H7	105.1	C15—C16—H16B	109.4
C12—C7—P1	114.79 (17)	C17—C16—H16A	109.4
C12—C7—H7	105.1	C17—C16—H16B	109.4
C8—C7—P1	114.64 (17)	C17—C16—C15	111.2 (2)
C8—C7—H7	105.1	N3—C22—C23	110.1 (2)
C8—C7—C12	111.0 (2)	N3—C22—H22	108.1
P1—C13—H13	105.1	N3—C22—C24	110.4 (2)
C18—C13—P1	118.41 (18)	C23—C22—H22	108.1
C18—C13—H13	105.1	C23—C22—C24	111.9 (2)
C18—C13—C14	110.1 (2)	C24—C22—H22	108.1
C14—C13—P1	111.79 (17)	C14—C15—H15A	109.5
C14—C13—H13	105.1	C14—C15—H15B	109.5
C1—C6—H6A	109.4	C16—C15—C14	110.5 (2)
C1—C6—H6B	109.4	C16—C15—H15A	109.5
H6A—C6—H6B	108.0	C16—C15—H15B	109.5
C5—C6—C1	111.1 (2)	H15A—C15—H15B	108.1
C5—C6—H6A	109.4	Ir1—C29—H29	114.1
C5—C6—H6B	109.4	C30—C29—Ir1	71.19 (15)
C7—C12—H12A	109.5	C30—C29—H29	114.1
C7—C12—H12B	109.5	C30—C29—C28	125.1 (3)
H12A—C12—H12B	108.1	C28—C29—Ir1	110.39 (18)
C11—C12—C7	110.5 (2)	C28—C29—H29	114.1
C11—C12—H12A	109.5	C6—C5—C4	112.7 (2)
C11—C12—H12B	109.5	C6—C5—H5A	109.0
C1—C2—H2A	109.2	C6—C5—H5B	109.0
C1—C2—H2B	109.2	C4—C5—H5A	109.0
H2A—C2—H2B	107.9	C4—C5—H5B	109.0
C3—C2—C1	112.1 (2)	H5A—C5—H5B	107.8
C3—C2—H2A	109.2	C32—C31—H31A	109.3
C3—C2—H2B	109.2	C32—C31—H31B	109.3
N1—C21—H21A	109.5	C30—C31—C32	111.6 (2)
N1—C21—H21B	109.5	C30—C31—H31A	109.3

N1—C21—H21C	109.5	C30—C31—H31B	109.3
H21A—C21—H21B	109.5	H31A—C31—H31B	108.0
H21A—C21—H21C	109.5	C2—C3—H3A	109.3
H21B—C21—H21C	109.5	C2—C3—H3B	109.3
Ir1—C25—H25	114.5	C4—C3—C2	111.4 (2)
C26—C25—Ir1	71.87 (15)	C4—C3—H3A	109.3
C26—C25—H25	114.5	C4—C3—H3B	109.3
C26—C25—C32	124.7 (2)	H3A—C3—H3B	108.0
C32—C25—Ir1	108.68 (18)	C22—C24—H24A	109.5
C32—C25—H25	114.5	C22—C24—H24B	109.5
C7—C8—H8A	109.5	C22—C24—H24C	109.5
C7—C8—H8B	109.5	H24A—C24—H24B	109.5
H8A—C8—H8B	108.1	H24A—C24—H24C	109.5
C9—C8—C7	110.7 (2)	H24B—C24—H24C	109.5
C9—C8—H8A	109.5	C29—C28—H28A	108.9
C9—C8—H8B	109.5	C29—C28—H28B	108.9
H23A—C23—H23B	109.5	C29—C28—C27	113.2 (2)
H23A—C23—H23C	109.5	H28A—C28—H28B	107.8
H23B—C23—H23C	109.5	C27—C28—H28A	108.9
C22—C23—H23A	109.5	C27—C28—H28B	108.9
C22—C23—H23B	109.5	C26—C27—C28	112.0 (2)
C22—C23—H23C	109.5	C26—C27—H27A	109.2
C12—C11—H11A	109.2	C26—C27—H27B	109.2
C12—C11—H11B	109.2	C28—C27—H27A	109.2
H11A—C11—H11B	107.9	C28—C27—H27B	109.2
C10—C11—C12	112.0 (2)	H27A—C27—H27B	107.9
C10—C11—H11A	109.2	C18—C17—H17A	109.2
C10—C11—H11B	109.2	C18—C17—H17B	109.2
C8—C9—H9A	109.4	C16—C17—C18	112.2 (2)
C8—C9—H9B	109.4	C16—C17—H17A	109.2
C8—C9—C10	111.0 (2)	C16—C17—H17B	109.2
H9A—C9—H9B	108.0	H17A—C17—H17B	107.9
C10—C9—H9A	109.4	F2—B1—F4	108.1 (3)
C10—C9—H9B	109.4	F3—B1—F4	109.2 (3)
C13—C18—H18A	109.5	F3—B1—F2	110.3 (4)
C13—C18—H18B	109.5	F1—B1—F4	109.7 (3)
C13—C18—C17	110.8 (2)	F1—B1—F2	109.8 (3)
H18A—C18—H18B	108.1	F1—B1—F3	109.7 (3)
C17—C18—H18A	109.5	Cl2S—C1S—H1SA	108.9
C17—C18—H18B	109.5	Cl2S—C1S—H1SB	108.9
N3—C20—H20	124.1	Cl1S—C1S—Cl2S	113.3 (2)
N2—C20—N3	111.8 (2)	Cl1S—C1S—H1SA	108.9
N2—C20—H20	124.1	Cl1S—C1S—H1SB	108.9
Ir1—C26—H26	112.2	H1SA—C1S—H1SB	107.7
Ir1—P1—C1—C6	-83.03 (17)	C13—P1—C1—C2	-76.91 (19)
Ir1—P1—C1—C2	45.38 (19)	C13—P1—C7—C12	81.0 (2)
Ir1—P1—C7—C12	-44.1 (2)	C13—P1—C7—C8	-49.2 (2)

Ir1—P1—C7—C8	-174.36 (15)	C13—C18—C17—C16	55.1 (3)
Ir1—P1—C13—C18	-149.88 (17)	C13—C14—C15—C16	-57.3 (3)
Ir1—P1—C13—C14	80.59 (18)	C6—C1—C2—C3	-50.3 (3)
Ir1—C25—C26—C27	-107.6 (3)	C12—C7—C8—C9	56.0 (3)
Ir1—C25—C32—C31	41.4 (3)	C12—C11—C10—C9	-56.5 (3)
Ir1—C26—C27—C28	10.0 (3)	C2—C1—C6—C5	49.8 (3)
Ir1—C30—C29—C28	102.2 (3)	C21—N1—C19—Ir1	10.7 (4)
Ir1—C30—C31—C32	13.9 (3)	C21—N1—C19—N3	-178.9 (2)
Ir1—C29—C28—C27	36.2 (3)	C21—N1—N2—C20	179.2 (2)
P1—C1—C6—C5	176.53 (17)	C25—C26—C27—C28	94.3 (3)
P1—C1—C2—C3	-179.95 (18)	C25—C32—C31—C30	-36.9 (3)
P1—C7—C12—C11	173.23 (17)	C8—C7—C12—C11	-54.8 (3)
P1—C7—C8—C9	-171.94 (18)	C8—C9—C10—C11	57.0 (3)
P1—C13—C18—C17	174.26 (19)	C18—C13—C14—C15	57.3 (3)
P1—C13—C14—C15	-168.97 (19)	C20—N3—C19—Ir1	170.16 (19)
N1—N2—C20—N3	-0.2 (3)	C20—N3—C19—N1	-0.7 (3)
C19—N1—N2—C20	-0.2 (3)	C20—N3—C22—C23	-58.8 (3)
C19—N3—C20—N2	0.6 (3)	C20—N3—C22—C24	65.3 (3)
C19—N3—C22—C23	116.4 (3)	C26—C25—C32—C31	-39.0 (4)
C19—N3—C22—C24	-119.5 (3)	C32—C25—C26—Ir1	100.6 (3)
N2—N1—C19—Ir1	-169.89 (18)	C32—C25—C26—C27	-7.0 (4)
N2—N1—C19—N3	0.6 (3)	C14—C13—C18—C17	-55.4 (3)
C1—P1—C7—C12	-169.26 (19)	C30—C29—C28—C27	-44.6 (4)
C1—P1—C7—C8	60.5 (2)	C22—N3—C19—Ir1	-5.8 (4)
C1—P1—C13—C18	-25.4 (2)	C22—N3—C19—N1	-176.6 (2)
C1—P1—C13—C14	-154.96 (18)	C22—N3—C20—N2	176.5 (2)
C1—C6—C5—C4	-53.7 (3)	C15—C16—C17—C18	-55.1 (3)
C1—C2—C3—C4	53.8 (3)	C29—C30—C31—C32	97.0 (3)
C7—P1—C1—C6	42.0 (2)	C29—C28—C27—C26	-30.5 (3)
C7—P1—C1—C2	170.42 (17)	C5—C4—C3—C2	-56.8 (3)
C7—P1—C13—C18	83.1 (2)	C31—C30—C29—Ir1	-105.8 (2)
C7—P1—C13—C14	-46.4 (2)	C31—C30—C29—C28	-3.6 (4)
C7—C12—C11—C10	55.3 (3)	C3—C4—C5—C6	57.6 (3)
C7—C8—C9—C10	-57.1 (3)	C17—C16—C15—C14	55.7 (3)
C13—P1—C1—C6	154.69 (17)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C2—H2 <i>A</i> ...F1	0.99	2.54	3.204 (4)	124
C23—H23 <i>C</i> ...F1	0.98	2.51	3.137 (4)	122
C20—H20...F4 ⁱ	0.95	2.49	3.400 (3)	161
C30—H30...F4 ⁱⁱ	1.00	2.35	3.192 (3)	141
C16—H16 <i>B</i> ...F2 ⁱⁱⁱ	0.99	2.54	3.404 (4)	146
C22—H22...F1	1.00	2.41	3.094 (4)	125

C31—H31B···F3 ⁱⁱ	0.99	2.35	3.330 (4)	170
C1S—H1SA···F2	0.99	2.50	3.362 (5)	145

Symmetry codes: (i) $-x+1/2, -y+3/2, -z+1$; (ii) $x, y-1, z$; (iii) $x, -y+1, z+1/2$.