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# [$\mu$-1,4-Bis(diphenylphosphanyl)butane-$\kappa^2P$:$P'$]-bis{(4-benzyl-2-neopentyl-1,2,4-triazol-3-ylidene)-[(1,2,5,6-$\eta$)-cycloocta-1,5-diene]iridium(I)} bis(tetrafluoroborate) dichloromethane disolvate

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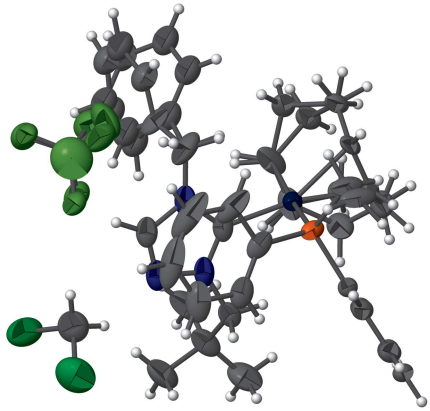
**CCDC reference**: 1563999

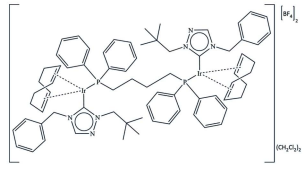
**Structural data**: full structural data are available from iucrdata.iucr.org

The title compound, $[Ir_2(C_{14}H_{19}N_3)_2(C_8H_{12})_2(C_{28}H_{28}P_2)](BF_4)_2\cdot 2CH_2Cl_2$, has triclinic ($P\overline{1}$) symmetry and the dication lies about an inversion center located at the mid-point of the butane chain of the phosphine ligand. The $Ir^I$ ion has a distorted square-planar coordination geometry. The *N*-heterocyclic carbene ligand has an extended S-shaped conformation. The diphosphine ligand acts as a bridge between the two metal centers. This is the first structural report of a complex where the square-planar iridium centers are bridged by a phosphine ligand, and it is of interest with respect to catalysis in transfer hydrogenation reactions. Parts of the triazole and cyclooctadiene ligands and the tetrafluoroborate anion are disordered over two sets of sites.

**3D view**



**Chemical scheme**



## Structure description

*N*-heterocyclic carbene complexes are of interest because of their catalytic properties in transfer hydrogenation reactions. The title compound is the first example of a dimer bridged by a chelating phosphine ligand. Transfer hydrogenation of ketones and imines is an encouraging example of an efficient and benign chemical transformation that exemplifies some of the key aspects of green chemistry. *N*-heterocyclic carbene (NHC) ligands can be tuned sterically and electronically by having different alkyl groups on the nitrogen atoms (Gusev, 2009). Many related NHC rhodium and iridium complexes have been synthesized and structurally characterized (Köcher & Herrmann 1997; Wang & Lin 1998; Chianese *et al.* 2004; Herrmann *et al.* 2006; Nichol *et al.* 2009, 2010, 2011, 2012; Lu *et al.* 2011; Huttenstine *et al.* 2011). Their catalytic activity in transfer hydrogenation reactions

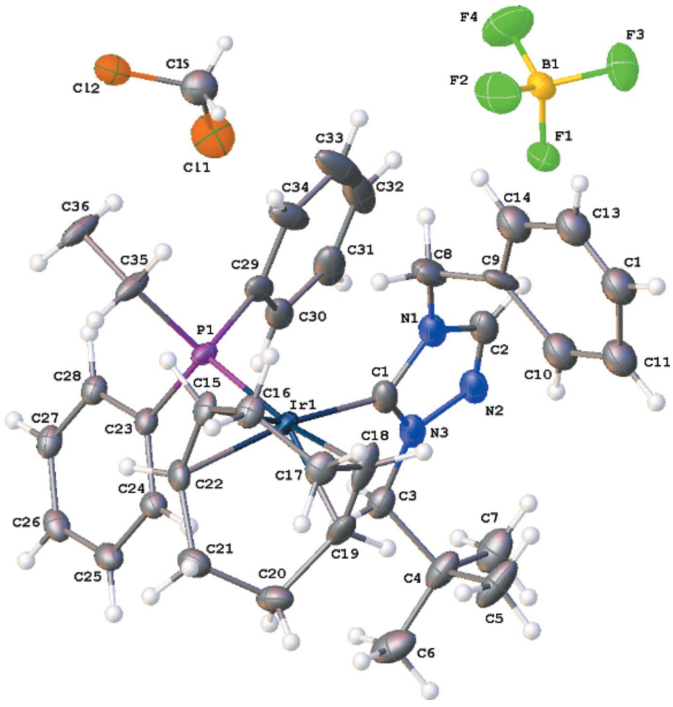



**Figure 1**
The structure of the half molecule of the title complex, showing the atom labelling and 30% probability displacement ellipsoids.

have been studied and reported (Hillier *et al.* 2001; Albrecht *et al.* 2002; Gnanamgari *et al.* 2007).

The title dinuclear ionic complex (Fig. 1) comprises two $Ir^{I}$ cations, two cyclooctadiene ligands, two *N*-heterocyclic carbene ligands, a diphosphine ligand, two tetrafluoroborate counter-anions, and two dichloromethane solvent molecules. As shown in Fig. 2, the two $Ir^{I}$ cations are bridged by the diphosphine ligand and the coordination sphere of each $Ir^{I}$ cation is completed through bonds to cyclooctadiene and the carbene, resulting in a distorted square-planar geometry. Charge balance is achieved by two non-coordinating tetrafluoroborate anions. The carbene atom, C1, deviates from the

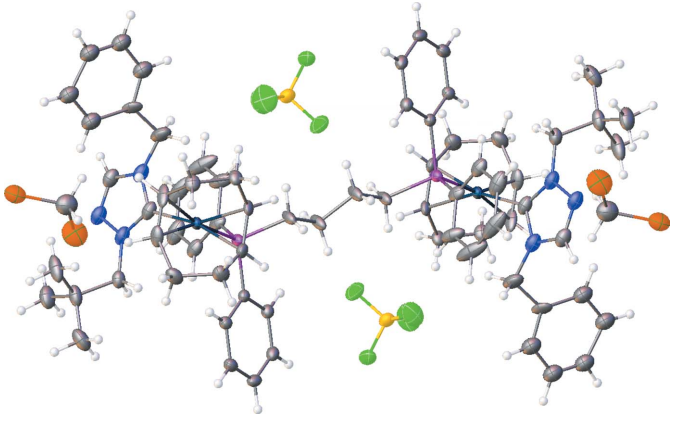


**Figure 2**
The full structure of the title complex with $BF_4^-$ counter-ions and $CH_2Cl_2$ solvent molecules.

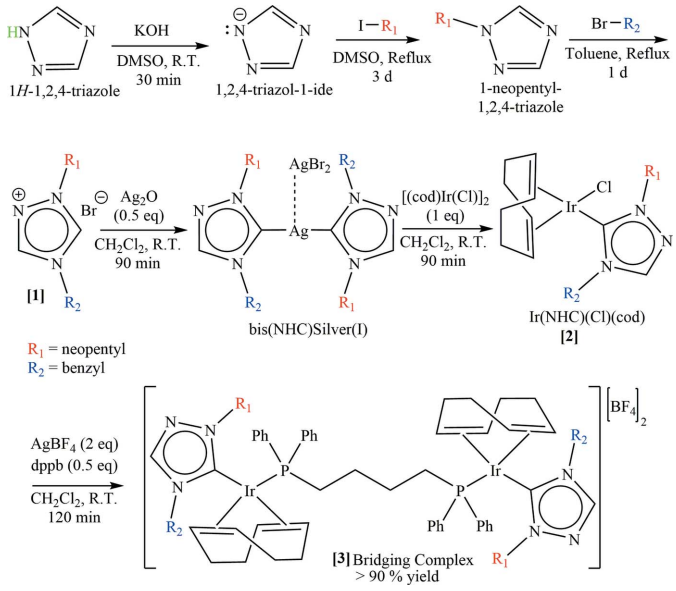



**Figure 3**
Scheme showing the various steps in the synthesis of the title compound.

expected $sp^2$ hybridization in that the N1—C1—N3 bond angle is 103.4 (5)°. Other selected bond lengths [Å] and angles [°] in the structure are: Ir1—P1 2.3257 (13) Å, Ir1—C1 2.041 (6) Å, and C1—Ir1—P1 89.58 (17)°.

## Synthesis and crystallization

Unless otherwise stated, all chemicals were purchased from Sigma–Aldrich and used without further purification, in the dark, and under a nitrogen atmosphere. 1-Neopentyl-1,2,4-triazole (2.2 g, 16 mmol) and benzyl bromide (4.0 g, 23 mmol) were refluxed in toluene (15 ml) for 3 d. After cooling, ether (50 ml) was added and the white solid **[1]** that formed was filtered, washed with ether and air dried (71%). Transmetallation in $CH_2Cl_2$ (10 ml) with **[1]** (0.0923 g, 0.298 mmol), $Ag_2O$ (0.0345 g, 0.149 mmol), and $[Ir(cod)Cl]_2$ (0.100 g, 0.149 mmol), gave a bright-yellow solid **[2]** (82%). In a round-bottom flask, **[2]** (0.168 g, 0.298 mmol), 1,4-bis(diphenylphosphino)butane (0.0635 g, 0.149 mmol), and $AgBF_4$ (0.0580 g, 0.298 mmol) were dissolved in $CH_2Cl_2$ (15 ml) and stirred for 2 h to obtain a bright-red solid **[3]** (99%) (Fig. 3). X-ray quality crystals of **[3]** were grown from $CH_2Cl_2$/pentane by slow diffusion.

## Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. C and H atoms of the benzyl fragment of the triazole ligand are disordered over two sets of sites with occupancy ratios fixed at 0.5766:0.4234 for the C9 atom and the adjacent atoms of the C8 methylene group and refined to 0.523 (7):0.477 (7) for the CH groups. The atoms of the $CH_2$ and CH groups of the cyclooctadiene ligand were similarly disordered with refined occupancies

0.541 (16):0.459 (16) while the F atoms of the tetrafluoroborate anion were also disordered over two sets of sites with occupancies 0.731 (16) and 0.269 (16).


## Funding information

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**Table 1**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $[Ir_2(C_{14}H_{19}N_3)_2(C_8H_{12})_2(C_{28}H_{28}P_2)](BF_4)_2\cdot 2CH_2Cl_2$ |
| $M_r$ | 1829.31 |
| Crystal system, space group | Triclinic, $P\overline{1}$ |
| Temperature (K) | 100 |
| $a, b, c$ (Å) | 10.3518 (5), 11.5088 (5), 17.2483 (8) |
| $\alpha, \beta, \gamma$ (°) | 73.540 (1), 87.276 (1), 72.616 (1) |
| $V$ (Å$^3$) | 1879.13 (15) |
| $Z$ | 1 |
| Radiation type | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 3.79 |
| Crystal size (mm) | 0.3 × 0.15 × 0.08 |
| Data collection | |
| Diffractometer | Bruker APEXII CCD |
| Absorption correction | Multi-scan (*SADABS*; Bruker, 2013) |
| $T_{min}$, $T_{max}$ | 0.565, 0.745 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 37976, 7733, 7082 |
| $R_{int}$ | 0.029 |
| $(\sin\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.627 |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.040, 0.110, 1.06 |
| No. of reflections | 7733 |
| No. of parameters | 520 |
| No. of restraints | 228 |
| H-atom treatment | H-atom parameters constrained |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 2.57, −1.27 |

Computer programs: *APEX2* and *SAINT* (Bruker, 2013), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).


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# full crystallographic data

*IUCrData* (2017). **2**, x171081 [https://doi.org/10.1107/S2414314617010811]

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*Crystal data*

$[Ir_2(C_{14}H_{19}N_3)_2(C_8H_{12})_2(C_{28}H_{28}P_2)](BF_4)_2\cdot 2CH_2Cl_2$
$M_r$ = 1829.31
Triclinic, $P\overline{1}$
$a$ = 10.3518 (5) Å
$b$ = 11.5088 (5) Å
$c$ = 17.2483 (8) Å
$\alpha$ = 73.540 (1)°
$\beta$ = 87.276 (1)°
$\gamma$ = 72.616 (1)°
$V$ = 1879.13 (15) Å$^3$
$Z$ = 1
$F(000)$ = 914
$D_x$ = 1.617 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 9923 reflections
$\theta$ = 2.4–26.4°
$\mu$ = 3.79 mm$^{-1}$
$T$ = 100 K
Block, clear pink
0.3 × 0.15 × 0.08 mm

*Data collection*

Bruker APEXII CCD diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (SADABS; Bruker, 2013)
$T_{min}$ = 0.565, $T_{max}$ = 0.745
37976 measured reflections
7733 independent reflections
7082 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.029
$\theta_{max}$ = 26.5°, $\theta_{min}$ = 2.0°
$h$ = −12→12
$k$ = −14→14
$l$ = −21→21

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.110
$S$ = 1.06
7733 reflections
520 parameters
228 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0717P)^2 + 4.7665P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 2.57 e Å$^{-3}$
$\Delta\rho_{min}$ = −1.27 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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Ir1 | 0.18525 (2) | 0.41927 (2) | 0.29265 (2) | 0.02912 (8) | |
| P1 | 0.37397 (14) | 0.47225 (13) | 0.32136 (8) | 0.0334 (3) | |
| Cl1 | 0.9205 (3) | 0.0758 (3) | 0.0963 (2) | 0.1082 (9) | |
| Cl2 | 0.7401 (3) | −0.0632 (3) | 0.07378 (15) | 0.0934 (7) | |
| F1 | 0.6795 (11) | −0.1208 (10) | 0.3272 (6) | 0.062 (2) | 0.731 (16) |
| N3 | 0.3615 (5) | 0.2971 (5) | 0.1699 (4) | 0.0471 (7) | |
| N1 | 0.3665 (5) | 0.1627 (5) | 0.2837 (4) | 0.0495 (7) | |
| F3 | 0.7015 (12) | −0.3137 (9) | 0.4023 (7) | 0.075 (3) | 0.731 (16) |
| C1 | 0.3074 (6) | 0.2862 (6) | 0.2429 (4) | 0.0467 (7) | |
| N2 | 0.4563 (5) | 0.1863 (5) | 0.1644 (4) | 0.0504 (7) | |
| C3 | 0.3355 (6) | 0.4109 (6) | 0.1036 (4) | 0.0439 (13) | |
| H3A | 0.4192 | 0.4369 | 0.0952 | 0.053* | |
| H3B | 0.2651 | 0.4789 | 0.1195 | 0.053* | |
| C4 | 0.2893 (7) | 0.4028 (8) | 0.0223 (4) | 0.0572 (17) | |
| C15 | 0.0631 (6) | 0.4869 (6) | 0.3879 (3) | 0.0380 (12) | |
| H15 | 0.1186 | 0.4878 | 0.4335 | 0.046* | |
| C16 | −0.0418 (6) | 0.4187 (6) | 0.4151 (3) | 0.0413 (12) | |
| H16A | −0.0001 | 0.3396 | 0.4582 | 0.050* | 0.541 (16) |
| H16B | −0.1162 | 0.4727 | 0.4391 | 0.050* | 0.541 (16) |
| H16C | −0.1327 | 0.4786 | 0.3966 | 0.050* | 0.459 (16) |
| H16D | −0.0390 | 0.3902 | 0.4750 | 0.050* | 0.459 (16) |
| C18 | 0.0132 (7) | 0.3455 (8) | 0.2892 (5) | 0.061 (2) | |
| H18 | 0.0324 | 0.2591 | 0.2816 | 0.073* | 0.541 (16) |
| H18A | 0.0482 | 0.2662 | 0.2719 | 0.073* | 0.459 (16) |
| C19 | 0.0046 (6) | 0.4432 (7) | 0.2237 (4) | 0.0515 (16) | |
| H19 | 0.0321 | 0.4100 | 0.1758 | 0.062* | 0.541 (16) |
| H19A | 0.0145 | 0.4275 | 0.1693 | 0.062* | 0.459 (16) |
| C22 | 0.0510 (6) | 0.5908 (5) | 0.3191 (3) | 0.0400 (12) | |
| H22 | 0.0988 | 0.6516 | 0.3253 | 0.048* | |
| C23 | 0.3886 (3) | 0.6202 (3) | 0.25080 (18) | 0.0337 (10) | |
| C24 | 0.2894 (3) | 0.6885 (3) | 0.1897 (2) | 0.0359 (11) | |
| H24 | 0.2159 | 0.6576 | 0.1842 | 0.043* | |
| C25 | 0.2978 (3) | 0.8021 (3) | 0.13685 (18) | 0.0439 (13) | |
| H25 | 0.2301 | 0.8488 | 0.0951 | 0.053* | |
| C26 | 0.4054 (4) | 0.8473 (3) | 0.1450 (2) | 0.0435 (13) | |
| H26 | 0.4111 | 0.9249 | 0.1089 | 0.052* | |
| C27 | 0.5045 (3) | 0.7789 (3) | 0.2061 (2) | 0.0416 (12) | |
| H27 | 0.5780 | 0.8098 | 0.2116 | 0.050* | |
| C28 | 0.4961 (3) | 0.6654 (3) | 0.25896 (18) | 0.0377 (11) | |

| | | | | | |
|---|---|---|---|---|---|
| H28 | 0.5639 | 0.6187 | 0.3007 | 0.045* | |
| C29 | 0.5353 (3) | 0.3556 (3) | 0.3152 (3) | 0.0454 (14) | |
| C30 | 0.6111 (4) | 0.3689 (4) | 0.2463 (2) | 0.0517 (16) | |
| H30 | 0.5851 | 0.4451 | 0.2031 | 0.062* | |
| C31 | 0.7250 (4) | 0.2708 (5) | 0.2404 (3) | 0.075 (3) | |
| H31 | 0.7768 | 0.2799 | 0.1933 | 0.090* | |
| C32 | 0.7630 (4) | 0.1593 (4) | 0.3035 (4) | 0.101 (4) | |
| H32 | 0.8409 | 0.0923 | 0.2996 | 0.121* | |
| C33 | 0.6872 (5) | 0.1460 (3) | 0.3724 (4) | 0.108 (5) | |
| H33 | 0.7132 | 0.0698 | 0.4155 | 0.129* | |
| C34 | 0.5734 (5) | 0.2441 (4) | 0.3782 (3) | 0.070 (2) | |
| H34 | 0.5215 | 0.2350 | 0.4253 | 0.084* | |
| C35 | 0.3783 (7) | 0.4879 (7) | 0.4234 (3) | 0.0486 (15) | |
| H35A | 0.2989 | 0.5594 | 0.4274 | 0.058* | |
| H35B | 0.3654 | 0.4100 | 0.4614 | 0.058* | |
| C36 | 0.5029 (8) | 0.5092 (8) | 0.4540 (3) | 0.0576 (19) | |
| H36A | 0.5061 | 0.5962 | 0.4261 | 0.069* | |
| H36B | 0.5860 | 0.4483 | 0.4419 | 0.069* | |
| F2 | 0.6024 (10) | −0.1457 (9) | 0.4512 (5) | 0.097 (3) | 0.731 (16) |
| C21 | −0.0693 (7) | 0.6506 (6) | 0.2601 (4) | 0.0536 (16) | |
| H21A | −0.0741 | 0.7406 | 0.2351 | 0.064* | 0.541 (16) |
| H21B | −0.1522 | 0.6494 | 0.2910 | 0.064* | 0.541 (16) |
| H21C | −0.1458 | 0.7001 | 0.2854 | 0.064* | 0.459 (16) |
| H21D | −0.0459 | 0.7098 | 0.2116 | 0.064* | 0.459 (16) |
| C2 | 0.4564 (6) | 0.1088 (6) | 0.2333 (5) | 0.0513 (7) | |
| H2 | 0.5124 | 0.0232 | 0.2485 | 0.062* | |
| F4 | 0.8182 (10) | −0.2001 (11) | 0.4370 (7) | 0.112 (3) | 0.731 (16) |
| B1 | 0.6976 (7) | −0.1936 (6) | 0.4059 (4) | 0.0453 (13) | |
| C6 | 0.2319 (9) | 0.5392 (9) | −0.0307 (5) | 0.075 (2) | |
| H6A | 0.1531 | 0.5836 | −0.0054 | 0.112* | |
| H6B | 0.2045 | 0.5386 | −0.0841 | 0.112* | |
| H6C | 0.3014 | 0.5829 | −0.0365 | 0.112* | |
| C8 | 0.3409 (8) | 0.0996 (6) | 0.3659 (5) | 0.069 (2) | |
| H8BC | 0.3172 | 0.1617 | 0.3978 | 0.082* | 0.4234 |
| H8BD | 0.4244 | 0.0323 | 0.3910 | 0.082* | 0.4234 |
| H8AA | 0.2870 | 0.1635 | 0.3923 | 0.082* | 0.5766 |
| H8AB | 0.4280 | 0.0546 | 0.3970 | 0.082* | 0.5766 |
| C7 | 0.4088 (9) | 0.3341 (10) | −0.0205 (5) | 0.072 (2) | |
| H7A | 0.4807 | 0.3748 | −0.0255 | 0.108* | |
| H7B | 0.3781 | 0.3386 | −0.0744 | 0.108* | |
| H7C | 0.4437 | 0.2450 | 0.0112 | 0.108* | |
| C5 | 0.1801 (8) | 0.3342 (11) | 0.0362 (5) | 0.081 (3) | |
| H5A | 0.2201 | 0.2454 | 0.0672 | 0.122* | |
| H5B | 0.1437 | 0.3378 | −0.0161 | 0.122* | |
| H5C | 0.1069 | 0.3757 | 0.0664 | 0.122* | |
| C9A | 0.2192 (12) | 0.0373 (11) | 0.3687 (8) | 0.0662 (12) | 0.4234 |
| C10A | 0.2247 (12) | −0.0325 (12) | 0.3140 (7) | 0.0661 (12) | 0.477 (7) |
| H10A | 0.2875 | −0.0294 | 0.2721 | 0.079* | 0.477 (7) |

| | | | | | |
|---|---|---|---|---|---|
| C11A | 0.1383 (13) | −0.1066 (10) | 0.3208 (6) | 0.0661 (12) | 0.477 (7) |
| H11A | 0.1421 | −0.1543 | 0.2835 | 0.079* | 0.477 (7) |
| C12A | 0.0464 (12) | −0.1111 (10) | 0.3822 (7) | 0.0662 (12) | 0.477 (7) |
| H12A | −0.0126 | −0.1618 | 0.3869 | 0.079* | 0.477 (7) |
| C13A | 0.0409 (11) | −0.0413 (10) | 0.4368 (6) | 0.0662 (12) | 0.477 (7) |
| H13A | −0.0219 | −0.0443 | 0.4788 | 0.079* | 0.477 (7) |
| C14A | 0.1273 (12) | 0.0329 (10) | 0.4301 (7) | 0.0661 (13) | 0.477 (7) |
| H14A | 0.1235 | 0.0806 | 0.4674 | 0.079* | 0.477 (7) |
| C1S | 0.7754 (10) | 0.0288 (10) | 0.1289 (7) | 0.083 (3) | |
| H1SA | 0.7892 | −0.0201 | 0.1868 | 0.099* | |
| H1SB | 0.6968 | 0.1053 | 0.1238 | 0.099* | |
| C11 | 0.1129 (18) | −0.0748 (14) | 0.3012 (11) | 0.0661 (12) | 0.523 (7) |
| H11 | 0.0619 | −0.0790 | 0.2582 | 0.079* | 0.523 (7) |
| C10 | 0.1955 (17) | 0.0033 (15) | 0.2921 (11) | 0.0661 (12) | 0.523 (7) |
| H10 | 0.2075 | 0.0537 | 0.2398 | 0.079* | 0.523 (7) |
| C12 | 0.1145 (17) | −0.1523 (14) | 0.3881 (10) | 0.0660 (12) | 0.523 (7) |
| H12 | 0.0587 | −0.2070 | 0.4000 | 0.079* | 0.523 (7) |
| C14 | 0.2577 (16) | −0.0702 (13) | 0.4341 (10) | 0.0663 (13) | 0.523 (7) |
| H14 | 0.3070 | −0.0722 | 0.4798 | 0.080* | 0.523 (7) |
| C13 | 0.1813 (16) | −0.1512 (14) | 0.4447 (11) | 0.0663 (12) | 0.523 (7) |
| H13 | 0.1796 | −0.2077 | 0.4968 | 0.080* | 0.523 (7) |
| C17 | −0.1010 (11) | 0.3856 (12) | 0.3496 (7) | 0.045 (3) | 0.541 (16) |
| H17A | −0.1752 | 0.4596 | 0.3196 | 0.054* | 0.541 (16) |
| H17B | −0.1392 | 0.3147 | 0.3738 | 0.054* | 0.541 (16) |
| C20 | −0.0713 (15) | 0.5901 (13) | 0.1928 (9) | 0.055 (4) | 0.541 (16) |
| H20A | −0.0261 | 0.6299 | 0.1452 | 0.066* | 0.541 (16) |
| H20B | −0.1661 | 0.6036 | 0.1761 | 0.066* | 0.541 (16) |
| C20A | −0.1114 (12) | 0.5542 (14) | 0.2355 (10) | 0.042 (4) | 0.459 (16) |
| H20C | −0.1662 | 0.5960 | 0.1841 | 0.050* | 0.459 (16) |
| H20D | −0.1704 | 0.5204 | 0.2770 | 0.050* | 0.459 (16) |
| C17A | −0.0199 (13) | 0.3041 (13) | 0.3827 (9) | 0.042 (4) | 0.459 (16) |
| H17C | −0.1023 | 0.2761 | 0.3889 | 0.051* | 0.459 (16) |
| H17D | 0.0564 | 0.2328 | 0.4131 | 0.051* | 0.459 (16) |
| F1A | 0.733 (3) | −0.123 (3) | 0.3307 (15) | 0.054 (5) | 0.269 (16) |
| F4A | 0.740 (3) | −0.1544 (18) | 0.4651 (11) | 0.079 (6) | 0.269 (16) |
| F3A | 0.749 (2) | −0.3176 (18) | 0.4242 (15) | 0.056 (5) | 0.269 (16) |
| F2A | 0.5535 (19) | −0.1685 (19) | 0.4151 (16) | 0.076 (6) | 0.269 (16) |
| C9 | 0.2672 (11) | 0.0085 (9) | 0.3663 (8) | 0.052 (3) | 0.5766 |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Ir1 | 0.03192 (12) | 0.03271 (12) | 0.02558 (12) | −0.01251 (8) | −0.00290 (7) | −0.00892 (8) |
| P1 | 0.0385 (7) | 0.0366 (7) | 0.0277 (6) | −0.0193 (5) | −0.0084 (5) | −0.0029 (5) |
| Cl1 | 0.0738 (15) | 0.137 (2) | 0.116 (2) | −0.0331 (16) | 0.0187 (14) | −0.0393 (19) |
| Cl2 | 0.127 (2) | 0.0869 (15) | 0.0653 (13) | −0.0450 (15) | 0.0017 (13) | −0.0063 (11) |
| F1 | 0.081 (6) | 0.042 (3) | 0.053 (3) | −0.012 (5) | −0.013 (4) | −0.004 (2) |
| N3 | 0.0329 (13) | 0.0434 (14) | 0.0710 (18) | −0.0071 (11) | −0.0022 (12) | −0.0292 (13) |

| | | | | | | |
|---|---|---|---|---|---|---|
| N1 | 0.0349 (13) | 0.0440 (14) | 0.0730 (18) | −0.0065 (11) | −0.0044 (13) | −0.0263 (13) |
| F3 | 0.100 (7) | 0.059 (4) | 0.084 (7) | −0.046 (4) | 0.030 (5) | −0.029 (4) |
| C1 | 0.0324 (13) | 0.0432 (14) | 0.0705 (18) | −0.0078 (11) | −0.0037 (13) | −0.0282 (13) |
| N2 | 0.0350 (13) | 0.0453 (14) | 0.0741 (18) | −0.0056 (11) | −0.0019 (13) | −0.0278 (13) |
| C3 | 0.039 (3) | 0.054 (3) | 0.047 (3) | −0.016 (3) | 0.004 (2) | −0.025 (3) |
| C4 | 0.048 (3) | 0.092 (5) | 0.051 (4) | −0.030 (3) | 0.007 (3) | −0.041 (4) |
| C15 | 0.050 (3) | 0.047 (3) | 0.030 (3) | −0.024 (3) | 0.015 (2) | −0.024 (2) |
| C16 | 0.044 (3) | 0.053 (3) | 0.037 (3) | −0.025 (3) | 0.014 (2) | −0.019 (2) |
| C18 | 0.055 (4) | 0.102 (6) | 0.074 (5) | −0.061 (4) | 0.031 (3) | −0.063 (5) |
| C19 | 0.031 (3) | 0.069 (4) | 0.062 (4) | −0.005 (3) | −0.016 (3) | −0.038 (4) |
| C22 | 0.051 (3) | 0.033 (3) | 0.041 (3) | −0.012 (2) | 0.008 (2) | −0.021 (2) |
| C23 | 0.044 (3) | 0.032 (2) | 0.029 (2) | −0.015 (2) | 0.003 (2) | −0.010 (2) |
| C24 | 0.041 (3) | 0.035 (3) | 0.031 (3) | −0.011 (2) | 0.004 (2) | −0.009 (2) |
| C25 | 0.058 (3) | 0.037 (3) | 0.031 (3) | −0.008 (3) | 0.001 (2) | −0.007 (2) |
| C26 | 0.062 (4) | 0.032 (3) | 0.037 (3) | −0.018 (3) | 0.016 (3) | −0.008 (2) |
| C27 | 0.053 (3) | 0.044 (3) | 0.038 (3) | −0.026 (3) | 0.011 (2) | −0.017 (2) |
| C28 | 0.043 (3) | 0.041 (3) | 0.035 (3) | −0.019 (2) | 0.005 (2) | −0.014 (2) |
| C29 | 0.038 (3) | 0.039 (3) | 0.061 (4) | −0.019 (2) | −0.020 (3) | −0.006 (3) |
| C30 | 0.039 (3) | 0.045 (3) | 0.076 (5) | −0.011 (2) | −0.016 (3) | −0.022 (3) |
| C31 | 0.039 (3) | 0.072 (5) | 0.126 (8) | −0.005 (3) | −0.021 (4) | −0.052 (5) |
| C32 | 0.045 (4) | 0.052 (5) | 0.209 (13) | 0.008 (4) | −0.062 (6) | −0.052 (6) |
| C33 | 0.056 (5) | 0.041 (4) | 0.205 (13) | −0.017 (4) | −0.066 (7) | 0.014 (6) |
| C34 | 0.052 (4) | 0.042 (3) | 0.103 (6) | −0.021 (3) | −0.036 (4) | 0.014 (4) |
| C35 | 0.068 (4) | 0.068 (4) | 0.024 (3) | −0.049 (3) | −0.008 (2) | −0.002 (2) |
| C36 | 0.078 (5) | 0.088 (5) | 0.026 (3) | −0.065 (4) | −0.010 (3) | −0.002 (3) |
| F2 | 0.089 (6) | 0.097 (6) | 0.081 (5) | 0.020 (4) | 0.011 (4) | −0.038 (4) |
| C21 | 0.053 (4) | 0.044 (3) | 0.052 (4) | 0.002 (3) | −0.004 (3) | −0.011 (3) |
| C2 | 0.0359 (13) | 0.0451 (14) | 0.0750 (18) | −0.0055 (12) | −0.0033 (13) | −0.0265 (13) |
| F4 | 0.072 (5) | 0.148 (8) | 0.118 (7) | −0.031 (5) | −0.033 (4) | −0.038 (6) |
| B1 | 0.049 (3) | 0.032 (3) | 0.050 (3) | −0.006 (2) | −0.005 (2) | −0.008 (2) |
| C6 | 0.066 (5) | 0.112 (7) | 0.043 (4) | −0.020 (5) | −0.003 (3) | −0.025 (4) |
| C8 | 0.079 (5) | 0.035 (3) | 0.080 (5) | −0.015 (3) | −0.032 (4) | 0.006 (3) |
| C7 | 0.069 (5) | 0.106 (7) | 0.064 (5) | −0.038 (5) | 0.022 (4) | −0.050 (5) |
| C5 | 0.065 (5) | 0.156 (9) | 0.066 (5) | −0.064 (5) | 0.019 (4) | −0.068 (6) |
| C9A | 0.070 (3) | 0.049 (3) | 0.077 (3) | −0.017 (2) | 0.002 (2) | −0.014 (2) |
| C10A | 0.070 (3) | 0.049 (3) | 0.077 (3) | −0.017 (2) | 0.002 (2) | −0.014 (2) |
| C11A | 0.070 (3) | 0.049 (3) | 0.077 (3) | −0.017 (2) | 0.002 (2) | −0.014 (2) |
| C12A | 0.070 (3) | 0.049 (3) | 0.077 (3) | −0.018 (2) | 0.002 (2) | −0.014 (2) |
| C13A | 0.070 (3) | 0.049 (3) | 0.077 (3) | −0.017 (2) | 0.002 (2) | −0.014 (2) |
| C14A | 0.070 (3) | 0.049 (3) | 0.077 (3) | −0.017 (2) | 0.002 (2) | −0.014 (2) |
| C1S | 0.075 (6) | 0.079 (6) | 0.087 (7) | −0.015 (5) | 0.011 (5) | −0.022 (5) |
| C11 | 0.070 (3) | 0.049 (3) | 0.077 (3) | −0.017 (2) | 0.002 (2) | −0.014 (2) |
| C10 | 0.070 (3) | 0.049 (3) | 0.077 (3) | −0.017 (2) | 0.002 (2) | −0.014 (2) |
| C12 | 0.070 (3) | 0.049 (3) | 0.077 (3) | −0.018 (2) | 0.002 (2) | −0.014 (2) |
| C14 | 0.070 (3) | 0.049 (3) | 0.077 (3) | −0.018 (2) | 0.002 (2) | −0.014 (2) |
| C13 | 0.070 (3) | 0.049 (3) | 0.077 (3) | −0.018 (2) | 0.002 (2) | −0.013 (2) |
| C17 | 0.034 (6) | 0.059 (8) | 0.050 (7) | −0.021 (6) | 0.011 (5) | −0.021 (6) |
| C20 | 0.050 (7) | 0.058 (8) | 0.042 (8) | 0.000 (6) | −0.008 (6) | −0.007 (6) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C20A | 0.021 (5) | 0.055 (8) | 0.040 (8) | 0.003 (5) | −0.008 (5) | −0.012 (7) |
| C17A | 0.033 (7) | 0.049 (8) | 0.058 (8) | −0.025 (6) | 0.012 (6) | −0.022 (6) |
| F1A | 0.062 (12) | 0.035 (7) | 0.051 (6) | −0.005 (9) | 0.001 (7) | −0.001 (5) |
| F4A | 0.125 (14) | 0.057 (9) | 0.055 (7) | −0.040 (9) | −0.010 (7) | −0.001 (6) |
| F3A | 0.066 (11) | 0.030 (5) | 0.051 (10) | 0.001 (5) | 0.016 (7) | 0.001 (4) |
| F2A | 0.059 (6) | 0.064 (9) | 0.089 (13) | −0.010 (5) | 0.004 (6) | −0.008 (8) |
| C9 | 0.043 (5) | 0.028 (5) | 0.065 (7) | −0.005 (4) | −0.024 (5) | 0.016 (5) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Ir1—P1 | 2.3257 (13) | C34—H34 | 0.9500 |
| Ir1—C1 | 2.041 (6) | C35—H35A | 0.9900 |
| Ir1—C15 | 2.200 (5) | C35—H35B | 0.9900 |
| Ir1—C18 | 2.200 (5) | C35—C36 | 1.526 (8) |
| Ir1—C19 | 2.169 (5) | C36—C36$^{i}$ | 1.541 (11) |
| Ir1—C22 | 2.202 (5) | C36—H36A | 0.9900 |
| P1—C23 | 1.834 (3) | C36—H36B | 0.9900 |
| P1—C29 | 1.824 (3) | F2—B1 | 1.317 (10) |
| P1—C35 | 1.824 (6) | C21—H21A | 0.9900 |
| Cl1—C1S | 1.760 (10) | C21—H21B | 0.9900 |
| Cl2—C1S | 1.731 (11) | C21—H21C | 0.9900 |
| F1—B1 | 1.366 (11) | C21—H21D | 0.9900 |
| N3—C1 | 1.342 (9) | C21—C20 | 1.518 (15) |
| N3—N2 | 1.383 (7) | C21—C20A | 1.475 (16) |
| N3—C3 | 1.437 (8) | C2—H2 | 0.9500 |
| N1—C1 | 1.357 (8) | F4—B1 | 1.355 (10) |
| N1—C2 | 1.375 (8) | B1—F1A | 1.42 (2) |
| N1—C8 | 1.451 (10) | B1—F4A | 1.36 (2) |
| F3—B1 | 1.390 (10) | B1—F3A | 1.31 (2) |
| N2—C2 | 1.268 (9) | B1—F2A | 1.44 (2) |
| C3—H3A | 0.9900 | C6—H6A | 0.9800 |
| C3—H3B | 0.9900 | C6—H6B | 0.9800 |
| C3—C4 | 1.538 (8) | C6—H6C | 0.9800 |
| C4—C6 | 1.528 (12) | C8—H8BC | 0.9900 |
| C4—C7 | 1.536 (10) | C8—H8BD | 0.9900 |
| C4—C5 | 1.536 (10) | C8—H8AA | 0.9900 |
| C15—H15 | 1.0000 | C8—H8AB | 0.9900 |
| C15—C16 | 1.505 (7) | C8—C9A | 1.618 (11) |
| C15—C22 | 1.404 (8) | C8—C9 | 1.467 (13) |
| C16—H16A | 0.9900 | C7—H7A | 0.9800 |
| C16—H16B | 0.9900 | C7—H7B | 0.9800 |
| C16—H16C | 0.9900 | C7—H7C | 0.9800 |
| C16—H16D | 0.9900 | C5—H5A | 0.9800 |
| C16—C17 | 1.499 (13) | C5—H5B | 0.9800 |
| C16—C17A | 1.527 (14) | C5—H5C | 0.9800 |
| C18—H18 | 1.0000 | C9A—C10A | 1.3900 |
| C18—H18A | 1.0000 | C9A—C14A | 1.3900 |
| C18—C19 | 1.334 (11) | C10A—H10A | 0.9500 |

| | | | |
|---|---|---|---|
| C18—C17 | 1.589 (12) | C10A—C11A | 1.3900 |
| C18—C17A | 1.597 (15) | C11A—H11A | 0.9500 |
| C19—H19 | 1.0000 | C11A—C12A | 1.3900 |
| C19—H19A | 1.0000 | C12A—H12A | 0.9500 |
| C19—C20 | 1.579 (14) | C12A—C13A | 1.3900 |
| C19—C20A | 1.523 (13) | C13A—H13A | 0.9500 |
| C22—H22 | 1.0000 | C13A—C14A | 1.3900 |
| C22—C21 | 1.507 (9) | C14A—H14A | 0.9500 |
| C23—C24 | 1.3900 | C1S—H1SA | 0.9900 |
| C23—C28 | 1.3900 | C1S—H1SB | 0.9900 |
| C24—H24 | 0.9500 | C11—H11 | 0.9500 |
| C24—C25 | 1.3900 | C11—C10 | 1.39 (2) |
| C25—H25 | 0.9500 | C11—C12 | 1.51 (2) |
| C25—C26 | 1.3900 | C10—H10 | 0.9500 |
| C26—H26 | 0.9500 | C10—C9 | 1.53 (2) |
| C26—C27 | 1.3900 | C12—H12 | 0.9500 |
| C27—H27 | 0.9500 | C12—C13 | 1.23 (2) |
| C27—C28 | 1.3900 | C14—H14 | 0.9500 |
| C28—H28 | 0.9500 | C14—C13 | 1.36 (2) |
| C29—C30 | 1.3900 | C14—C9 | 1.281 (19) |
| C29—C34 | 1.3900 | C13—H13 | 0.9500 |
| C30—H30 | 0.9500 | C17—H17A | 0.9900 |
| C30—C31 | 1.3900 | C17—H17B | 0.9900 |
| C31—H31 | 0.9500 | C20—H20A | 0.9900 |
| C31—C32 | 1.3900 | C20—H20B | 0.9900 |
| C32—H32 | 0.9500 | C20A—H20C | 0.9900 |
| C32—C33 | 1.3900 | C20A—H20D | 0.9900 |
| C33—H33 | 0.9500 | C17A—H17C | 0.9900 |
| C33—C34 | 1.3900 | C17A—H17D | 0.9900 |

| | | | |
|---|---|---|---|
| C1—Ir1—P1 | 89.58 (17) | C36—C35—H35B | 107.5 |
| C1—Ir1—C15 | 155.3 (3) | C35—C36—C36$^{i}$ | 109.7 (6) |
| C1—Ir1—C18 | 91.4 (2) | C35—C36—H36A | 109.7 |
| C1—Ir1—C19 | 94.6 (2) | C35—C36—H36B | 109.7 |
| C1—Ir1—C22 | 167.4 (3) | C36$^{i}$—C36—H36A | 109.7 |
| C15—Ir1—P1 | 94.96 (16) | C36$^{i}$—C36—H36B | 109.7 |
| C15—Ir1—C22 | 37.2 (2) | H36A—C36—H36B | 108.2 |
| C18—Ir1—P1 | 169.1 (2) | C22—C21—H21A | 108.1 |
| C18—Ir1—C15 | 79.8 (2) | C22—C21—H21B | 108.1 |
| C18—Ir1—C22 | 91.2 (3) | C22—C21—H21C | 109.3 |
| C19—Ir1—P1 | 155.1 (2) | C22—C21—H21D | 109.3 |
| C19—Ir1—C15 | 91.5 (2) | C22—C21—C20 | 116.7 (6) |
| C19—Ir1—C18 | 35.6 (3) | H21A—C21—H21B | 107.3 |
| C19—Ir1—C22 | 80.5 (2) | H21C—C21—H21D | 108.0 |
| C22—Ir1—P1 | 90.23 (16) | C20—C21—H21A | 108.1 |
| C23—P1—Ir1 | 113.07 (11) | C20—C21—H21B | 108.1 |
| C29—P1—Ir1 | 114.12 (14) | C20A—C21—C22 | 111.6 (7) |
| C29—P1—C23 | 103.84 (18) | C20A—C21—H21C | 109.3 |

| | | | |
|---|---|---|---|
| C35—P1—Ir1 | 113.3 (2) | C20A—C21—H21D | 109.3 |
| C35—P1—C23 | 107.4 (2) | N1—C2—H2 | 123.8 |
| C35—P1—C29 | 104.2 (3) | N2—C2—N1 | 112.4 (6) |
| C1—N3—N2 | 112.9 (5) | N2—C2—H2 | 123.8 |
| C1—N3—C3 | 126.3 (5) | F1—B1—F3 | 104.7 (9) |
| N2—N3—C3 | 120.6 (5) | F2—B1—F1 | 111.6 (8) |
| C1—N1—C2 | 107.6 (6) | F2—B1—F3 | 114.1 (9) |
| C1—N1—C8 | 126.2 (6) | F2—B1—F4 | 107.4 (8) |
| C2—N1—C8 | 126.2 (6) | F4—B1—F1 | 110.2 (8) |
| N3—C1—Ir1 | 131.2 (5) | F4—B1—F3 | 108.8 (8) |
| N3—C1—N1 | 103.4 (5) | F1A—B1—F2A | 113.7 (13) |
| N1—C1—Ir1 | 124.9 (5) | F4A—B1—F1A | 107.3 (15) |
| C2—N2—N3 | 103.6 (5) | F4A—B1—F2A | 104.4 (16) |
| N3—C3—H3A | 108.2 | F3A—B1—F1A | 116.6 (17) |
| N3—C3—H3B | 108.2 | F3A—B1—F4A | 107.5 (14) |
| N3—C3—C4 | 116.5 (5) | F3A—B1—F2A | 106.4 (14) |
| H3A—C3—H3B | 107.3 | C4—C6—H6A | 109.5 |
| C4—C3—H3A | 108.2 | C4—C6—H6B | 109.5 |
| C4—C3—H3B | 108.2 | C4—C6—H6C | 109.5 |
| C6—C4—C3 | 106.7 (6) | H6A—C6—H6B | 109.5 |
| C6—C4—C7 | 108.3 (7) | H6A—C6—H6C | 109.5 |
| C6—C4—C5 | 110.5 (7) | H6B—C6—H6C | 109.5 |
| C7—C4—C3 | 111.5 (6) | N1—C8—H8BC | 109.3 |
| C5—C4—C3 | 109.8 (6) | N1—C8—H8BD | 109.3 |
| C5—C4—C7 | 110.0 (7) | N1—C8—H8AA | 109.5 |
| Ir1—C15—H15 | 113.5 | N1—C8—H8AB | 109.5 |
| C16—C15—Ir1 | 111.3 (3) | N1—C8—C9A | 111.7 (7) |
| C16—C15—H15 | 113.5 | N1—C8—C9 | 110.6 (8) |
| C22—C15—Ir1 | 71.5 (3) | H8BC—C8—H8BD | 107.9 |
| C22—C15—H15 | 113.5 | H8AA—C8—H8AB | 108.1 |
| C22—C15—C16 | 125.8 (6) | C9A—C8—H8BC | 109.3 |
| C15—C16—H16A | 108.6 | C9A—C8—H8BD | 109.3 |
| C15—C16—H16B | 108.6 | C9—C8—H8AA | 109.5 |
| C15—C16—H16C | 109.1 | C9—C8—H8AB | 109.5 |
| C15—C16—H16D | 109.1 | C4—C7—H7A | 109.5 |
| C15—C16—C17A | 112.6 (6) | C4—C7—H7B | 109.5 |
| H16A—C16—H16B | 107.5 | C4—C7—H7C | 109.5 |
| H16C—C16—H16D | 107.8 | H7A—C7—H7B | 109.5 |
| C17—C16—C15 | 114.8 (6) | H7A—C7—H7C | 109.5 |
| C17—C16—H16A | 108.6 | H7B—C7—H7C | 109.5 |
| C17—C16—H16B | 108.6 | C4—C5—H5A | 109.5 |
| C17A—C16—H16C | 109.1 | C4—C5—H5B | 109.5 |
| C17A—C16—H16D | 109.1 | C4—C5—H5C | 109.5 |
| Ir1—C18—H18 | 118.1 | H5A—C5—H5B | 109.5 |
| Ir1—C18—H18A | 107.2 | H5A—C5—H5C | 109.5 |
| C19—C18—Ir1 | 71.0 (3) | H5B—C5—H5C | 109.5 |
| C19—C18—H18 | 118.1 | C10A—C9A—C8 | 116.0 (8) |
| C19—C18—H18A | 107.2 | C10A—C9A—C14A | 120.0 |

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| C19—C18—C17 | 109.8 (8) | C14A—C9A—C8 | 123.1 (8) |
| C19—C18—C17A | 145.3 (8) | C9A—C10A—H10A | 120.0 |
| C17—C18—Ir1 | 112.9 (5) | C9A—C10A—C11A | 120.0 |
| C17—C18—H18 | 118.1 | C11A—C10A—H10A | 120.0 |
| C17A—C18—Ir1 | 102.2 (5) | C10A—C11A—H11A | 120.0 |
| C17A—C18—H18A | 107.2 | C12A—C11A—C10A | 120.0 |
| Ir1—C19—H19 | 108.9 | C12A—C11A—H11A | 120.0 |
| Ir1—C19—H19A | 118.9 | C11A—C12A—H12A | 120.0 |
| C18—C19—Ir1 | 73.5 (4) | C11A—C12A—C13A | 120.0 |
| C18—C19—H19 | 108.9 | C13A—C12A—H12A | 120.0 |
| C18—C19—H19A | 118.9 | C12A—C13A—H13A | 120.0 |
| C18—C19—C20 | 139.3 (9) | C12A—C13A—C14A | 120.0 |
| C18—C19—C20A | 107.0 (9) | C14A—C13A—H13A | 120.0 |
| C20—C19—Ir1 | 107.7 (6) | C9A—C14A—H14A | 120.0 |
| C20—C19—H19 | 108.9 | C13A—C14A—C9A | 120.0 |
| C20A—C19—Ir1 | 110.9 (6) | C13A—C14A—H14A | 120.0 |
| C20A—C19—H19A | 118.9 | Cl1—C1S—H1SA | 109.1 |
| Ir1—C22—H22 | 114.0 | Cl1—C1S—H1SB | 109.1 |
| C15—C22—Ir1 | 71.3 (3) | Cl2—C1S—Cl1 | 112.4 (6) |
| C15—C22—H22 | 114.0 | Cl2—C1S—H1SA | 109.1 |
| C15—C22—C21 | 125.0 (6) | Cl2—C1S—H1SB | 109.1 |
| C21—C22—Ir1 | 110.5 (4) | H1SA—C1S—H1SB | 107.9 |
| C21—C22—H22 | 114.0 | C10—C11—H11 | 124.3 |
| C24—C23—P1 | 119.40 (18) | C10—C11—C12 | 111.3 (15) |
| C24—C23—C28 | 120.0 | C12—C11—H11 | 124.3 |
| C28—C23—P1 | 120.59 (18) | C11—C10—H10 | 119.9 |
| C23—C24—H24 | 120.0 | C11—C10—C9 | 120.3 (14) |
| C25—C24—C23 | 120.0 | C9—C10—H10 | 119.9 |
| C25—C24—H24 | 120.0 | C11—C12—H12 | 117.0 |
| C24—C25—H25 | 120.0 | C13—C12—C11 | 125.9 (16) |
| C26—C25—C24 | 120.0 | C13—C12—H12 | 117.0 |
| C26—C25—H25 | 120.0 | C13—C14—H14 | 118.0 |
| C25—C26—H26 | 120.0 | C9—C14—H14 | 118.0 |
| C25—C26—C27 | 120.0 | C9—C14—C13 | 124.0 (16) |
| C27—C26—H26 | 120.0 | C12—C13—C14 | 121.1 (17) |
| C26—C27—H27 | 120.0 | C12—C13—H13 | 119.5 |
| C28—C27—C26 | 120.0 | C14—C13—H13 | 119.5 |
| C28—C27—H27 | 120.0 | C16—C17—C18 | 109.8 (7) |
| C23—C28—H28 | 120.0 | C16—C17—H17A | 109.7 |
| C27—C28—C23 | 120.0 | C16—C17—H17B | 109.7 |
| C27—C28—H28 | 120.0 | C18—C17—H17A | 109.7 |
| C30—C29—P1 | 122.0 (2) | C18—C17—H17B | 109.7 |
| C30—C29—C34 | 120.0 | H17A—C17—H17B | 108.2 |
| C34—C29—P1 | 117.6 (2) | C19—C20—H20A | 109.8 |
| C29—C30—H30 | 120.0 | C19—C20—H20B | 109.8 |
| C31—C30—C29 | 120.0 | C21—C20—C19 | 109.4 (9) |
| C31—C30—H30 | 120.0 | C21—C20—H20A | 109.8 |
| C30—C31—H31 | 120.0 | C21—C20—H20B | 109.8 |

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| C30—C31—C32 | 120.0 | H20A—C20—H20B | 108.2 |
| C32—C31—H31 | 120.0 | C19—C20A—H20C | 108.5 |
| C31—C32—H32 | 120.0 | C19—C20A—H20D | 108.5 |
| C33—C32—C31 | 120.0 | C21—C20A—C19 | 114.9 (9) |
| C33—C32—H32 | 120.0 | C21—C20A—H20C | 108.5 |
| C32—C33—H33 | 120.0 | C21—C20A—H20D | 108.5 |
| C32—C33—C34 | 120.0 | H20C—C20A—H20D | 107.5 |
| C34—C33—H33 | 120.0 | C16—C17A—C18 | 107.9 (9) |
| C29—C34—H34 | 120.0 | C16—C17A—H17C | 110.1 |
| C33—C34—C29 | 120.0 | C16—C17A—H17D | 110.1 |
| C33—C34—H34 | 120.0 | C18—C17A—H17C | 110.1 |
| P1—C35—H35A | 107.5 | C18—C17A—H17D | 110.1 |
| P1—C35—H35B | 107.5 | H17C—C17A—H17D | 108.4 |
| H35A—C35—H35B | 107.0 | C8—C9—C10 | 125.0 (10) |
| C36—C35—P1 | 119.3 (5) | C14—C9—C8 | 117.9 (12) |
| C36—C35—H35A | 107.5 | C14—C9—C10 | 117.1 (13) |

Symmetry code: (i) $-x+1, -y+1, -z+1$.