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# Bis{*N*,*N*-bis[(diphenylphosphanyl)-methyl]aniline-$\kappa^2P,P'$}copper(I) tetrafluoridoborate

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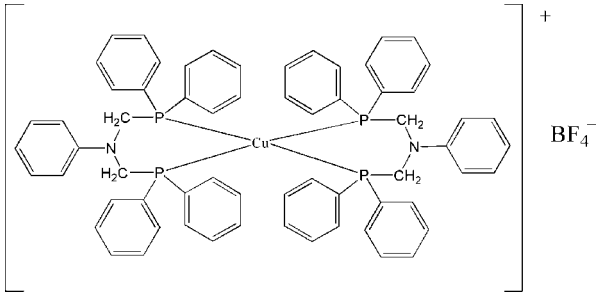
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.009 Å; $R$ factor = 0.059; $wR$ factor = 0.198; data-to-parameter ratio = 14.5.

In the cation of the title compound, $[Cu(C_{32}H_{29}NP_2)_2]BF_4$, the $Cu^I$ atom is four-coordinated in a distorted tetrahedral geometry by four P atoms from two *N*,*N*-bis[(diphenylphosphanyl)methyl]aniline ligands. In the crystal, the cations are linked by C—H$\cdots\pi$ interactions, forming chains along the *a* axis. Intramolecular C—H$\cdots$N and intermolecular C—H$\cdots$F hydrogen bonds are also observed.

## Related literature

For the structures and properties of related copper(I) complexes, see: Saravanabharathi *et al.* (2002); Chen *et al.* (2004); Sivasankar *et al.* (2004); Wang *et al.* (2008); Huang *et al.* (2009).




## Experimental

### Crystal data

$[Cu(C_{32}H_{29}NP_2)_2]BF_4$
$M_r$ = 1129.35
Triclinic, $P\overline{1}$
$a$ = 11.004 (2) Å
$b$ = 12.642 (3) Å
$c$ = 21.725 (4) Å
$\alpha$ = 79.601 (3)°
$\beta$ = 78.593 (3)°
$\gamma$ = 76.110 (3)°
$V$ = 2847.7 (10) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.55 mm$^{-1}$
$T$ = 296 K
0.20 × 0.10 × 0.10 mm

### Data collection

Bruker SMART 1000 CCD diffractometer
15689 measured reflections
9918 independent reflections
6522 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.035

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.198
$S$ = 1.06
9918 reflections
685 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.73 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.47 e Å$^{-3}$

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

*Cg*1 and *Cg*2 are the centroids of the C33–C38 and C1–C6 rings, respectively.

| $D$—H$\cdots A$ | $D$—H | H$\cdots A$ | $D\cdots A$ | $D$—H$\cdots A$ |
|---|---|---|---|---|
| C22—H22$\cdots$N1 | 0.93 | 2.53 | 3.189 (6) | 128 |
| C7—H7$A\cdots$F3$^{i}$ | 0.97 | 2.25 | 3.181 (6) | 161 |
| C18—H18$\cdots Cg1^{i}$ | 0.93 | 2.72 | 3.653 (6) | 177 |
| C42—H42$\cdots Cg2^{ii}$ | 0.93 | 2.88 | 3.678 (5) | 144 |

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2534).

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# supplementary materials

*Acta Cryst.* (2011). E**67**, m96 [ **doi:10.1107/S160053681005186X** ]

# Bis{*N*,*N*-bis[(diphenylphosphanyl)methyl]aniline-$\kappa^2 P,P'$}copper(I) tetrafluoridoborate

**J. Shang, L.-L. Huang, T.-H. Huang, K. Ma and Q.-L. Ni**

## Comment

Copper(I) complexes containing phosphine ligands have received much attention so far due to their special structures, novel reactivity, as well as catalytic and luminescent properties (Saravanabharathi *et al.*, 2002; Chen *et al.*,2004; Sivasankar *et al.*, 2004; Wang *et al.*, 2008; Huang *et al.*, 2009). Herein, we report the synthesis and crystal structure of the new mononuclear copper(I) title complex.

In the cation of the title compound, the copper(I) atom adopts a distorted tetrahedral geometry provided by four P atoms from two phosphine ligands (Fig. 1). The Cu—P bond distances are in the range 2.2972 (12)–2.3153 (14) Å. An intramolecular C—H···N hydrogen bond is present (Table 1). In the crystal structure, intermolecular C—H···π interactions link adjacent cations into chains parallel to the *a* axis (Fig. 2). Intermolecular C—H···F hydrogen bonds involving the tetrafluoridoborate anion are also observed (Table 1).

## Experimental

$[Cu(CH_3CN)_4]BF_4$ (0.0158 g, 0.05 mmol) was added with stirring to a solution of *N*,*N*-bis[(diphenylphosphanyl)methyl]aniline (0.0489 g, 0.10 mmol) in $CH_3CN$ (5 ml). The resulting solution was allowed to stir for 1 h at room temperature. Slow diffusion of diethyl ether into the solution geve colourless block crystals suitable for X-ray analysis after three days.

## Refinement

Anisotropic displacement parameters were applied to all non-hydrogen atoms. All hydrogen atoms were generated geometrically and refined with a riding model, with C–H = 0.93–0.97 Å, and with $U_{iso}$(H) = 1.2 $U_{eq}$(C).

## Figures

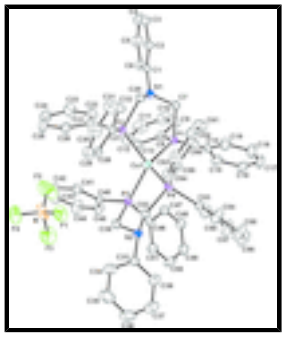

Fig. 1. The structure of the title compound with displacement ellipsoids drawn at the 25% probability level. Hydrogen atoms are omitted for clarity.

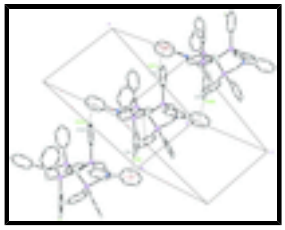

Fig. 2. Partial crystal packing of the title compound showing the chains of cations parallel to the *a* axis. C—H···π interactions are shown as dashed lines.

**Bis{*N*,*N*-bis[(diphenylphosphanyl)methyl]aniline- $\kappa^2$*P*,*P*'}copper(I) tetrafluoridoborate**

*Crystal data*

| | |
|---|---|
| $[Cu(C_{32}H_{29}NP_2)_2]BF_4$ | $Z = 2$ |
| $M_r = 1129.35$ | $F(000) = 1172$ |
| Triclinic, $P\overline{1}$ | $D_x = 1.317$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| $a = 11.004$ (2) Å | Cell parameters from 1884 reflections |
| $b = 12.642$ (3) Å | $\theta = 2.3$–$21.7°$ |
| $c = 21.725$ (4) Å | $\mu = 0.55$ mm$^{-1}$ |
| $\alpha = 79.601$ (3)° | $T = 296$ K |
| $\beta = 78.593$ (3)° | Block, colourless |
| $\gamma = 76.110$ (3)° | 0.20 × 0.10 × 0.10 mm |
| $V = 2847.7$ (10) Å$^3$ | |

*Data collection*

| | |
|---|---|
| Bruker SMART 1000 CCD diffractometer | 6522 reflections with $I > 2\sigma(I)$ |
| Radiation source: fine-focus sealed tube | $R_{int} = 0.035$ |
| graphite | $\theta_{max} = 25.0°$, $\theta_{min} = 1.7°$ |
| φ and ω scans | $h = -13\rightarrow12$ |
| 15689 measured reflections | $k = -14\rightarrow15$ |
| 9918 independent reflections | $l = -25\rightarrow22$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.059$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.198$ | H-atom parameters constrained |
| $S = 1.06$ | $w = 1/[\sigma^2(F_o^2) + (0.114P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 9918 reflections | $(\Delta/\sigma)_{max} < 0.001$ |
| 685 parameters | $\Delta\rho_{max} = 0.73$ e Å$^{-3}$ |
| 0 restraints | $\Delta\rho_{min} = -0.47$ e Å$^{-3}$ |

*Special details*

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

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on $F^2$, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative $F^2$. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on $F^2$ are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.1283 (4) | 0.5357 (4) | 0.15568 (19) | 0.0405 (11) |
| C2 | 0.0669 (5) | 0.4537 (4) | 0.1860 (2) | 0.0449 (12) |
| H2 | 0.0478 | 0.4436 | 0.2300 | 0.054* |
| C3 | 0.0330 (5) | 0.3855 (5) | 0.1521 (2) | 0.0590 (14) |
| H3 | −0.0078 | 0.3297 | 0.1733 | 0.071* |
| C4 | 0.0596 (6) | 0.4004 (5) | 0.0871 (3) | 0.0689 (17) |
| H4 | 0.0375 | 0.3543 | 0.0642 | 0.083* |
| C5 | 0.1186 (6) | 0.4831 (6) | 0.0561 (2) | 0.0688 (17) |
| H5 | 0.1356 | 0.4938 | 0.0120 | 0.083* |
| C6 | 0.1531 (5) | 0.5507 (4) | 0.0896 (2) | 0.0519 (13) |
| H6 | 0.1931 | 0.6068 | 0.0680 | 0.062* |
| C7 | 0.0813 (4) | 0.7133 (4) | 0.19308 (18) | 0.0377 (10) |
| H7A | 0.0273 | 0.7111 | 0.2342 | 0.045* |
| H7B | 0.0275 | 0.7280 | 0.1608 | 0.045* |
| C8 | 0.2195 (5) | 0.8354 (4) | 0.09759 (18) | 0.0450 (12) |
| C9 | 0.1341 (6) | 0.8604 (5) | 0.0548 (2) | 0.0611 (15) |
| H9 | 0.0475 | 0.8787 | 0.0695 | 0.073* |
| C10 | 0.1778 (9) | 0.8581 (5) | −0.0101 (3) | 0.090 (2) |
| H10 | 0.1208 | 0.8760 | −0.0387 | 0.108* |
| C11 | 0.3080 (9) | 0.8288 (7) | −0.0315 (3) | 0.097 (3) |
| H11 | 0.3376 | 0.8259 | −0.0745 | 0.116* |
| C12 | 0.3903 (7) | 0.8051 (6) | 0.0092 (3) | 0.084 (2) |
| H12 | 0.4767 | 0.7863 | −0.0059 | 0.100* |
| C13 | 0.3493 (5) | 0.8078 (5) | 0.0743 (2) | 0.0588 (15) |
| H13 | 0.4081 | 0.7912 | 0.1019 | 0.071* |
| C14 | 0.0359 (4) | 0.9437 (4) | 0.19362 (19) | 0.0396 (11) |
| C15 | 0.0258 (6) | 1.0410 (5) | 0.1515 (3) | 0.0627 (15) |
| H15 | 0.0863 | 1.0475 | 0.1153 | 0.075* |
| C16 | −0.0767 (7) | 1.1301 (5) | 0.1640 (3) | 0.0762 (18) |
| H16 | −0.0862 | 1.1944 | 0.1352 | 0.091* |
| C17 | −0.1633 (6) | 1.1207 (5) | 0.2197 (3) | 0.0793 (19) |
| H17 | −0.2304 | 1.1794 | 0.2285 | 0.095* |
| C18 | −0.1505 (6) | 1.0288 (6) | 0.2601 (3) | 0.087 (2) |

| | | | | |
|---|---|---|---|---|
| H18 | −0.2085 | 1.0237 | 0.2974 | 0.104* |
| C19 | −0.0523 (6) | 0.9399 (5) | 0.2478 (3) | 0.0682 (16) |
| H19 | −0.0459 | 0.8760 | 0.2770 | 0.082* |
| C20 | 0.2100 (4) | 0.5532 (4) | 0.24857 (19) | 0.0406 (11) |
| H20A | 0.2284 | 0.4741 | 0.2492 | 0.049* |
| H20B | 0.1418 | 0.5714 | 0.2833 | 0.049* |
| C21 | 0.4793 (5) | 0.5208 (4) | 0.20502 (19) | 0.0407 (11) |
| C22 | 0.4657 (5) | 0.5370 (5) | 0.1414 (2) | 0.0671 (16) |
| H22 | 0.3926 | 0.5823 | 0.1284 | 0.081* |
| C23 | 0.5597 (7) | 0.4862 (7) | 0.0976 (3) | 0.087 (2) |
| H23 | 0.5467 | 0.4926 | 0.0559 | 0.105* |
| C24 | 0.6731 (7) | 0.4258 (6) | 0.1151 (3) | 0.084 (2) |
| H24 | 0.7386 | 0.3957 | 0.0849 | 0.101* |
| C25 | 0.6878 (6) | 0.4109 (5) | 0.1773 (3) | 0.081 (2) |
| H25 | 0.7634 | 0.3703 | 0.1898 | 0.097* |
| C26 | 0.5890 (5) | 0.4568 (4) | 0.2220 (3) | 0.0594 (14) |
| H26 | 0.5985 | 0.4433 | 0.2645 | 0.071* |
| C27 | 0.3773 (4) | 0.5157 (4) | 0.33799 (19) | 0.0398 (11) |
| C28 | 0.4793 (5) | 0.5274 (4) | 0.3640 (2) | 0.0472 (12) |
| H28 | 0.5315 | 0.5747 | 0.3423 | 0.057* |
| C29 | 0.5021 (5) | 0.4674 (5) | 0.4228 (2) | 0.0590 (15) |
| H29 | 0.5712 | 0.4734 | 0.4396 | 0.071* |
| C30 | 0.4250 (6) | 0.4008 (5) | 0.4553 (2) | 0.0636 (16) |
| H30 | 0.4405 | 0.3626 | 0.4947 | 0.076* |
| C31 | 0.3232 (6) | 0.3890 (5) | 0.4307 (2) | 0.0688 (17) |
| H31 | 0.2706 | 0.3428 | 0.4534 | 0.083* |
| C32 | 0.2998 (5) | 0.4458 (5) | 0.3725 (2) | 0.0582 (14) |
| H32 | 0.2315 | 0.4374 | 0.3560 | 0.070* |
| C33 | 0.5601 (5) | 0.9522 (4) | 0.3714 (2) | 0.0475 (12) |
| C34 | 0.6664 (6) | 0.8906 (6) | 0.3953 (3) | 0.0729 (18) |
| H34 | 0.6973 | 0.8177 | 0.3885 | 0.088* |
| C35 | 0.7264 (7) | 0.9388 (8) | 0.4297 (3) | 0.106 (3) |
| H35 | 0.7970 | 0.8973 | 0.4469 | 0.127* |
| C36 | 0.6832 (9) | 1.0463 (9) | 0.4388 (4) | 0.125 (4) |
| H36 | 0.7266 | 1.0790 | 0.4601 | 0.150* |
| C37 | 0.5780 (10) | 1.1046 (8) | 0.4169 (5) | 0.130 (4) |
| H37 | 0.5466 | 1.1770 | 0.4245 | 0.156* |
| C38 | 0.5155 (7) | 1.0578 (6) | 0.3830 (3) | 0.087 (2) |
| H38 | 0.4425 | 1.0990 | 0.3680 | 0.105* |
| C39 | 0.5760 (4) | 0.8560 (4) | 0.28194 (18) | 0.0431 (11) |
| H39A | 0.6091 | 0.7788 | 0.2955 | 0.052* |
| H39B | 0.6473 | 0.8920 | 0.2682 | 0.052* |
| C40 | 0.6242 (4) | 0.8228 (4) | 0.15314 (18) | 0.0363 (10) |
| C41 | 0.6929 (5) | 0.7163 (4) | 0.1626 (2) | 0.0537 (13) |
| H41 | 0.6694 | 0.6696 | 0.1990 | 0.064* |
| C42 | 0.7968 (5) | 0.6777 (5) | 0.1186 (3) | 0.0600 (14) |
| H42 | 0.8421 | 0.6056 | 0.1257 | 0.072* |
| C43 | 0.8326 (6) | 0.7450 (6) | 0.0652 (3) | 0.0733 (18) |
| H43 | 0.9036 | 0.7199 | 0.0363 | 0.088* |

| | | | | |
|---|---|---|---|---|
| C44 | 0.7635 (7) | 0.8495 (6) | 0.0546 (3) | 0.088 (2) |
| H44 | 0.7864 | 0.8953 | 0.0177 | 0.106* |
| C45 | 0.6589 (6) | 0.8883 (5) | 0.0986 (2) | 0.0667 (16) |
| H45 | 0.6123 | 0.9598 | 0.0906 | 0.080* |
| C46 | 0.4497 (4) | 1.0171 (4) | 0.18874 (19) | 0.0411 (11) |
| C47 | 0.3670 (5) | 1.0561 (4) | 0.1449 (2) | 0.0523 (13) |
| H47 | 0.3365 | 1.0060 | 0.1287 | 0.063* |
| C48 | 0.3294 (6) | 1.1660 (5) | 0.1248 (3) | 0.0652 (15) |
| H48 | 0.2744 | 1.1895 | 0.0953 | 0.078* |
| C49 | 0.3720 (6) | 1.2415 (5) | 0.1480 (3) | 0.0702 (17) |
| H49 | 0.3462 | 1.3163 | 0.1344 | 0.084* |
| C50 | 0.4532 (6) | 1.2058 (5) | 0.1916 (3) | 0.0729 (17) |
| H50 | 0.4823 | 1.2567 | 0.2078 | 0.088* |
| C51 | 0.4924 (5) | 1.0938 (5) | 0.2117 (2) | 0.0593 (14) |
| H51 | 0.5480 | 1.0705 | 0.2409 | 0.071* |
| C52 | 0.4153 (4) | 0.8343 (4) | 0.37680 (18) | 0.0410 (11) |
| H52A | 0.3931 | 0.8574 | 0.4186 | 0.049* |
| H52B | 0.4642 | 0.7593 | 0.3811 | 0.049* |
| C53 | 0.1792 (4) | 0.9775 (4) | 0.35609 (18) | 0.0421 (11) |
| C54 | 0.1717 (5) | 1.0548 (5) | 0.3028 (2) | 0.0643 (16) |
| H54 | 0.2039 | 1.0338 | 0.2629 | 0.077* |
| C55 | 0.1158 (7) | 1.1645 (6) | 0.3087 (3) | 0.089 (2) |
| H55 | 0.1134 | 1.2168 | 0.2726 | 0.106* |
| C56 | 0.0644 (7) | 1.1962 (5) | 0.3667 (3) | 0.091 (2) |
| H56 | 0.0290 | 1.2698 | 0.3704 | 0.109* |
| C57 | 0.0656 (7) | 1.1180 (5) | 0.4196 (3) | 0.092 (2) |
| H57 | 0.0268 | 1.1380 | 0.4591 | 0.111* |
| C58 | 0.1241 (6) | 1.0102 (5) | 0.4143 (2) | 0.0743 (19) |
| H58 | 0.1266 | 0.9584 | 0.4506 | 0.089* |
| C59 | 0.1851 (4) | 0.7525 (4) | 0.41001 (17) | 0.0386 (11) |
| C60 | 0.0745 (5) | 0.7287 (5) | 0.4004 (2) | 0.0557 (14) |
| H60 | 0.0452 | 0.7556 | 0.3621 | 0.067* |
| C61 | 0.0068 (6) | 0.6656 (5) | 0.4471 (2) | 0.0658 (16) |
| H61 | −0.0682 | 0.6513 | 0.4403 | 0.079* |
| C62 | 0.0505 (6) | 0.6241 (4) | 0.5034 (2) | 0.0558 (14) |
| H62 | 0.0047 | 0.5818 | 0.5348 | 0.067* |
| C63 | 0.1599 (5) | 0.6443 (4) | 0.5136 (2) | 0.0544 (14) |
| H63 | 0.1896 | 0.6145 | 0.5515 | 0.065* |
| C64 | 0.2287 (5) | 0.7098 (4) | 0.4672 (2) | 0.0498 (12) |
| H64 | 0.3029 | 0.7246 | 0.4747 | 0.060* |
| Cu1 | 0.32004 (5) | 0.78482 (4) | 0.24698 (2) | 0.03413 (18) |
| N1 | 0.1681 (4) | 0.6071 (3) | 0.18859 (15) | 0.0399 (9) |
| N2 | 0.4930 (3) | 0.9051 (3) | 0.33536 (15) | 0.0393 (9) |
| P2 | 0.35284 (11) | 0.59476 (10) | 0.26073 (5) | 0.0351 (3) |
| P1 | 0.16788 (11) | 0.82563 (10) | 0.18260 (4) | 0.0349 (3) |
| P3 | 0.49074 (11) | 0.86914 (10) | 0.21416 (4) | 0.0348 (3) |
| P4 | 0.26725 (11) | 0.83797 (10) | 0.34647 (4) | 0.0361 (3) |
| B | 0.8319 (7) | 0.5762 (7) | 0.3354 (3) | 0.071 (2) |
| F1 | 0.7468 (3) | 0.5932 (3) | 0.38924 (16) | 0.0918 (12) |

| | | | | |
|---|---|---|---|---|
| F2 | 0.7789 (5) | 0.5524 (6) | 0.2914 (2) | 0.165 (3) |
| F3 | 0.8676 (4) | 0.6782 (4) | 0.3124 (2) | 0.1322 (18) |
| F4 | 0.9401 (4) | 0.5048 (4) | 0.34690 (16) | 0.0974 (13) |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.033 (3) | 0.045 (3) | 0.047 (2) | −0.004 (2) | −0.015 (2) | −0.012 (2) |
| C2 | 0.051 (3) | 0.043 (3) | 0.047 (2) | −0.015 (2) | −0.013 (2) | −0.0075 (19) |
| C3 | 0.064 (4) | 0.049 (3) | 0.074 (3) | −0.016 (3) | −0.026 (3) | −0.012 (2) |
| C4 | 0.081 (5) | 0.065 (4) | 0.070 (3) | −0.004 (4) | −0.030 (3) | −0.031 (3) |
| C5 | 0.075 (4) | 0.088 (5) | 0.049 (3) | −0.013 (4) | −0.022 (3) | −0.016 (3) |
| C6 | 0.060 (4) | 0.056 (3) | 0.043 (2) | −0.014 (3) | −0.019 (2) | −0.002 (2) |
| C7 | 0.035 (3) | 0.042 (3) | 0.037 (2) | −0.005 (2) | −0.0119 (18) | −0.0056 (17) |
| C8 | 0.055 (3) | 0.048 (3) | 0.035 (2) | −0.017 (2) | −0.011 (2) | −0.0022 (18) |
| C9 | 0.071 (4) | 0.073 (4) | 0.042 (2) | −0.019 (3) | −0.018 (2) | −0.001 (2) |
| C10 | 0.156 (8) | 0.082 (5) | 0.041 (3) | −0.031 (5) | −0.043 (4) | 0.004 (3) |
| C11 | 0.145 (8) | 0.117 (6) | 0.034 (3) | −0.056 (6) | 0.006 (4) | −0.010 (3) |
| C12 | 0.085 (5) | 0.109 (6) | 0.057 (3) | −0.040 (4) | 0.020 (3) | −0.022 (3) |
| C13 | 0.062 (4) | 0.070 (4) | 0.052 (3) | −0.032 (3) | 0.002 (3) | −0.015 (2) |
| C14 | 0.038 (3) | 0.040 (3) | 0.042 (2) | −0.009 (2) | −0.0149 (19) | 0.0029 (18) |
| C15 | 0.071 (4) | 0.054 (4) | 0.067 (3) | −0.012 (3) | −0.022 (3) | −0.007 (3) |
| C16 | 0.095 (5) | 0.037 (4) | 0.104 (5) | −0.007 (3) | −0.047 (4) | −0.005 (3) |
| C17 | 0.064 (4) | 0.052 (4) | 0.106 (5) | 0.010 (3) | −0.002 (4) | −0.013 (3) |
| C18 | 0.072 (5) | 0.054 (4) | 0.115 (5) | 0.008 (4) | 0.001 (4) | −0.008 (4) |
| C19 | 0.068 (4) | 0.055 (4) | 0.072 (3) | −0.002 (3) | −0.009 (3) | −0.002 (3) |
| C20 | 0.042 (3) | 0.040 (3) | 0.044 (2) | −0.014 (2) | −0.016 (2) | −0.0008 (18) |
| C21 | 0.040 (3) | 0.035 (3) | 0.048 (2) | −0.007 (2) | −0.008 (2) | −0.0074 (18) |
| C22 | 0.052 (4) | 0.088 (5) | 0.061 (3) | −0.003 (3) | −0.011 (3) | −0.024 (3) |
| C23 | 0.078 (5) | 0.125 (6) | 0.064 (3) | −0.022 (5) | 0.009 (3) | −0.046 (4) |
| C24 | 0.076 (5) | 0.081 (5) | 0.086 (4) | −0.018 (4) | 0.031 (4) | −0.037 (4) |
| C25 | 0.058 (4) | 0.061 (4) | 0.104 (5) | 0.013 (3) | 0.005 (4) | −0.017 (3) |
| C26 | 0.055 (4) | 0.046 (3) | 0.070 (3) | −0.003 (3) | −0.010 (3) | −0.002 (2) |
| C27 | 0.032 (3) | 0.040 (3) | 0.045 (2) | −0.001 (2) | −0.011 (2) | −0.0049 (18) |
| C28 | 0.048 (3) | 0.043 (3) | 0.053 (3) | −0.008 (2) | −0.016 (2) | −0.008 (2) |
| C29 | 0.061 (4) | 0.072 (4) | 0.044 (2) | −0.003 (3) | −0.022 (2) | −0.008 (2) |
| C30 | 0.074 (4) | 0.073 (4) | 0.037 (2) | −0.005 (3) | −0.019 (3) | 0.006 (2) |
| C31 | 0.077 (4) | 0.071 (4) | 0.055 (3) | −0.029 (3) | −0.014 (3) | 0.021 (3) |
| C32 | 0.058 (4) | 0.065 (4) | 0.059 (3) | −0.029 (3) | −0.026 (2) | 0.013 (2) |
| C33 | 0.050 (3) | 0.056 (3) | 0.045 (2) | −0.017 (3) | −0.009 (2) | −0.018 (2) |
| C34 | 0.077 (5) | 0.077 (5) | 0.079 (4) | −0.016 (4) | −0.028 (3) | −0.030 (3) |
| C35 | 0.089 (6) | 0.149 (8) | 0.101 (5) | −0.029 (5) | −0.042 (4) | −0.042 (5) |
| C36 | 0.112 (8) | 0.164 (10) | 0.139 (7) | −0.046 (7) | −0.021 (6) | −0.103 (7) |
| C37 | 0.118 (8) | 0.124 (8) | 0.179 (9) | −0.019 (6) | −0.029 (7) | −0.108 (7) |
| C38 | 0.077 (5) | 0.080 (5) | 0.119 (5) | −0.002 (4) | −0.031 (4) | −0.053 (4) |
| C39 | 0.038 (3) | 0.056 (3) | 0.040 (2) | −0.010 (2) | −0.0091 (19) | −0.015 (2) |
| C40 | 0.033 (3) | 0.039 (3) | 0.036 (2) | −0.008 (2) | −0.0007 (18) | −0.0099 (17) |
| C41 | 0.051 (3) | 0.054 (4) | 0.053 (3) | −0.008 (3) | −0.004 (2) | −0.008 (2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C42 | 0.047 (3) | 0.054 (4) | 0.078 (3) | 0.003 (3) | −0.008 (3) | −0.025 (3) |
| C43 | 0.060 (4) | 0.085 (5) | 0.068 (3) | −0.008 (4) | 0.017 (3) | −0.034 (3) |
| C44 | 0.087 (5) | 0.092 (5) | 0.061 (3) | −0.012 (4) | 0.032 (3) | −0.004 (3) |
| C45 | 0.073 (4) | 0.046 (3) | 0.061 (3) | 0.001 (3) | 0.017 (3) | −0.005 (2) |
| C46 | 0.033 (3) | 0.042 (3) | 0.046 (2) | −0.009 (2) | 0.003 (2) | −0.0103 (19) |
| C47 | 0.056 (3) | 0.044 (3) | 0.059 (3) | −0.006 (3) | −0.017 (2) | −0.007 (2) |
| C48 | 0.059 (4) | 0.050 (4) | 0.083 (4) | −0.008 (3) | −0.016 (3) | 0.000 (3) |
| C49 | 0.068 (4) | 0.038 (3) | 0.095 (4) | −0.009 (3) | 0.000 (3) | 0.001 (3) |
| C50 | 0.088 (5) | 0.041 (4) | 0.095 (4) | −0.021 (3) | −0.010 (4) | −0.020 (3) |
| C51 | 0.063 (4) | 0.054 (4) | 0.065 (3) | −0.016 (3) | −0.015 (3) | −0.007 (2) |
| C52 | 0.041 (3) | 0.048 (3) | 0.037 (2) | −0.012 (2) | −0.0062 (19) | −0.0108 (19) |
| C53 | 0.039 (3) | 0.049 (3) | 0.036 (2) | −0.008 (2) | −0.0015 (19) | −0.0072 (19) |
| C54 | 0.069 (4) | 0.063 (4) | 0.047 (3) | 0.001 (3) | 0.007 (2) | −0.009 (2) |
| C55 | 0.113 (6) | 0.066 (5) | 0.065 (3) | 0.000 (4) | 0.005 (4) | 0.000 (3) |
| C56 | 0.123 (6) | 0.045 (4) | 0.090 (4) | 0.003 (4) | −0.001 (4) | −0.016 (3) |
| C57 | 0.131 (6) | 0.062 (5) | 0.069 (4) | 0.001 (4) | 0.011 (4) | −0.031 (3) |
| C58 | 0.108 (5) | 0.055 (4) | 0.047 (3) | −0.003 (4) | 0.005 (3) | −0.010 (2) |
| C59 | 0.047 (3) | 0.036 (3) | 0.0306 (19) | −0.006 (2) | −0.0043 (18) | −0.0049 (16) |
| C60 | 0.057 (4) | 0.071 (4) | 0.047 (2) | −0.026 (3) | −0.013 (2) | −0.007 (2) |
| C61 | 0.070 (4) | 0.075 (4) | 0.059 (3) | −0.036 (3) | −0.004 (3) | −0.004 (3) |
| C62 | 0.069 (4) | 0.043 (3) | 0.048 (3) | −0.012 (3) | 0.010 (2) | −0.008 (2) |
| C63 | 0.059 (4) | 0.056 (4) | 0.039 (2) | −0.008 (3) | −0.007 (2) | 0.008 (2) |
| C64 | 0.044 (3) | 0.056 (3) | 0.047 (2) | −0.008 (3) | −0.008 (2) | −0.005 (2) |
| Cu1 | 0.0349 (4) | 0.0381 (3) | 0.0309 (3) | −0.0084 (3) | −0.0073 (2) | −0.0056 (2) |
| N1 | 0.042 (2) | 0.036 (2) | 0.0456 (18) | −0.0072 (19) | −0.0185 (17) | −0.0045 (15) |
| N2 | 0.036 (2) | 0.049 (2) | 0.0366 (17) | −0.0130 (19) | −0.0030 (15) | −0.0121 (15) |
| P2 | 0.0338 (7) | 0.0367 (7) | 0.0362 (5) | −0.0069 (5) | −0.0101 (5) | −0.0042 (4) |
| P1 | 0.0369 (7) | 0.0372 (7) | 0.0317 (5) | −0.0084 (5) | −0.0096 (4) | −0.0026 (4) |
| P3 | 0.0336 (7) | 0.0389 (7) | 0.0323 (5) | −0.0091 (5) | −0.0029 (4) | −0.0061 (4) |
| P4 | 0.0360 (7) | 0.0420 (7) | 0.0303 (5) | −0.0078 (6) | −0.0041 (4) | −0.0073 (4) |
| B | 0.049 (4) | 0.115 (7) | 0.040 (3) | −0.018 (4) | −0.010 (3) | 0.019 (3) |
| F1 | 0.074 (3) | 0.105 (3) | 0.085 (2) | −0.030 (2) | 0.0185 (18) | −0.004 (2) |
| F2 | 0.116 (4) | 0.293 (8) | 0.120 (4) | −0.052 (4) | −0.040 (3) | −0.080 (4) |
| F3 | 0.109 (4) | 0.118 (4) | 0.146 (4) | −0.049 (3) | 0.029 (3) | 0.022 (3) |
| F4 | 0.077 (3) | 0.116 (3) | 0.076 (2) | 0.008 (2) | −0.0128 (19) | 0.008 (2) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| C1—C2 | 1.370 (6) | C34—H34 | 0.9300 |
| C1—C6 | 1.394 (6) | C35—C36 | 1.365 (12) |
| C1—N1 | 1.438 (5) | C35—H35 | 0.9300 |
| C2—C3 | 1.384 (6) | C36—C37 | 1.338 (11) |
| C2—H2 | 0.9300 | C36—H36 | 0.9300 |
| C3—C4 | 1.372 (7) | C37—C38 | 1.385 (9) |
| C3—H3 | 0.9300 | C37—H37 | 0.9300 |
| C4—C5 | 1.366 (8) | C38—H38 | 0.9300 |
| C4—H4 | 0.9300 | C39—N2 | 1.461 (5) |
| C5—C6 | 1.376 (7) | C39—P3 | 1.860 (4) |
| C5—H5 | 0.9300 | C39—H39A | 0.9700 |

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|---|---|---|---|
| C6—H6 | 0.9300 | C39—H39B | 0.9700 |
| C7—N1 | 1.456 (5) | C40—C45 | 1.362 (6) |
| C7—P1 | 1.850 (5) | C40—C41 | 1.378 (7) |
| C7—H7A | 0.9700 | C40—P3 | 1.831 (4) |
| C7—H7B | 0.9700 | C41—C42 | 1.387 (7) |
| C8—C9 | 1.395 (7) | C41—H41 | 0.9300 |
| C8—C13 | 1.399 (7) | C42—C43 | 1.359 (8) |
| C8—P1 | 1.812 (4) | C42—H42 | 0.9300 |
| C9—C10 | 1.400 (7) | C43—C44 | 1.361 (9) |
| C9—H9 | 0.9300 | C43—H43 | 0.9300 |
| C10—C11 | 1.396 (10) | C44—C45 | 1.394 (7) |
| C10—H10 | 0.9300 | C44—H44 | 0.9300 |
| C11—C12 | 1.336 (10) | C45—H45 | 0.9300 |
| C11—H11 | 0.9300 | C46—C51 | 1.376 (7) |
| C12—C13 | 1.400 (7) | C46—C47 | 1.392 (7) |
| C12—H12 | 0.9300 | C46—P3 | 1.825 (5) |
| C13—H13 | 0.9300 | C47—C48 | 1.367 (7) |
| C14—C19 | 1.371 (7) | C47—H47 | 0.9300 |
| C14—C15 | 1.390 (7) | C48—C49 | 1.366 (8) |
| C14—P1 | 1.829 (5) | C48—H48 | 0.9300 |
| C15—C16 | 1.411 (8) | C49—C50 | 1.374 (8) |
| C15—H15 | 0.9300 | C49—H49 | 0.9300 |
| C16—C17 | 1.389 (9) | C50—C51 | 1.393 (8) |
| C16—H16 | 0.9300 | C50—H50 | 0.9300 |
| C17—C18 | 1.320 (9) | C51—H51 | 0.9300 |
| C17—H17 | 0.9300 | C52—N2 | 1.454 (5) |
| C18—C19 | 1.384 (8) | C52—P4 | 1.862 (4) |
| C18—H18 | 0.9300 | C52—H52A | 0.9700 |
| C19—H19 | 0.9300 | C52—H52B | 0.9700 |
| C20—N1 | 1.463 (5) | C53—C54 | 1.376 (7) |
| C20—P2 | 1.851 (4) | C53—C58 | 1.380 (6) |
| C20—H20A | 0.9700 | C53—P4 | 1.824 (5) |
| C20—H20B | 0.9700 | C54—C55 | 1.393 (8) |
| C21—C26 | 1.359 (7) | C54—H54 | 0.9300 |
| C21—C22 | 1.392 (6) | C55—C56 | 1.364 (8) |
| C21—P2 | 1.842 (4) | C55—H55 | 0.9300 |
| C22—C23 | 1.380 (8) | C56—C57 | 1.374 (9) |
| C22—H22 | 0.9300 | C56—H56 | 0.9300 |
| C23—C24 | 1.382 (9) | C57—C58 | 1.375 (8) |
| C23—H23 | 0.9300 | C57—H57 | 0.9300 |
| C24—C25 | 1.366 (9) | C58—H58 | 0.9300 |
| C24—H24 | 0.9300 | C59—C60 | 1.383 (7) |
| C25—C26 | 1.395 (8) | C59—C64 | 1.392 (6) |
| C25—H25 | 0.9300 | C59—P4 | 1.824 (4) |
| C26—H26 | 0.9300 | C60—C61 | 1.384 (7) |
| C27—C32 | 1.392 (7) | C60—H60 | 0.9300 |
| C27—C28 | 1.401 (6) | C61—C62 | 1.373 (7) |
| C27—P2 | 1.826 (4) | C61—H61 | 0.9300 |
| C28—C29 | 1.399 (6) | C62—C63 | 1.355 (7) |

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|---|---|---|---|
| C28—H28 | 0.9300 | C62—H62 | 0.9300 |
| C29—C30 | 1.348 (8) | C63—C64 | 1.404 (7) |
| C29—H29 | 0.9300 | C63—H63 | 0.9300 |
| C30—C31 | 1.382 (8) | C64—H64 | 0.9300 |
| C30—H30 | 0.9300 | Cu1—P1 | 2.2972 (12) |
| C31—C32 | 1.376 (7) | Cu1—P4 | 2.3024 (11) |
| C31—H31 | 0.9300 | Cu1—P3 | 2.3087 (13) |
| C32—H32 | 0.9300 | Cu1—P2 | 2.3153 (14) |
| C33—C38 | 1.358 (8) | B—F2 | 1.324 (8) |
| C33—C34 | 1.379 (8) | B—F4 | 1.347 (8) |
| C33—N2 | 1.456 (5) | B—F1 | 1.360 (7) |
| C34—C35 | 1.386 (8) | B—F3 | 1.415 (9) |
| C2—C1—C6 | 118.3 (4) | N2—C39—H39B | 109.3 |
| C2—C1—N1 | 123.3 (4) | P3—C39—H39B | 109.3 |
| C6—C1—N1 | 118.3 (4) | H39A—C39—H39B | 107.9 |
| C1—C2—C3 | 121.0 (4) | C45—C40—C41 | 118.2 (4) |
| C1—C2—H2 | 119.5 | C45—C40—P3 | 123.2 (4) |
| C3—C2—H2 | 119.5 | C41—C40—P3 | 118.6 (3) |
| C4—C3—C2 | 120.0 (5) | C40—C41—C42 | 121.0 (5) |
| C4—C3—H3 | 120.0 | C40—C41—H41 | 119.5 |
| C2—C3—H3 | 120.0 | C42—C41—H41 | 119.5 |
| C5—C4—C3 | 119.7 (5) | C43—C42—C41 | 120.2 (6) |
| C5—C4—H4 | 120.1 | C43—C42—H42 | 119.9 |
| C3—C4—H4 | 120.1 | C41—C42—H42 | 119.9 |
| C4—C5—C6 | 120.5 (5) | C42—C43—C44 | 119.3 (5) |
| C4—C5—H5 | 119.7 | C42—C43—H43 | 120.3 |
| C6—C5—H5 | 119.7 | C44—C43—H43 | 120.3 |
| C5—C6—C1 | 120.4 (5) | C43—C44—C45 | 120.6 (6) |
| C5—C6—H6 | 119.8 | C43—C44—H44 | 119.7 |
| C1—C6—H6 | 119.8 | C45—C44—H44 | 119.7 |
| N1—C7—P1 | 111.5 (3) | C40—C45—C44 | 120.7 (6) |
| N1—C7—H7A | 109.3 | C40—C45—H45 | 119.7 |
| P1—C7—H7A | 109.3 | C44—C45—H45 | 119.7 |
| N1—C7—H7B | 109.3 | C51—C46—C47 | 117.4 (5) |
| P1—C7—H7B | 109.3 | C51—C46—P3 | 124.1 (4) |
| H7A—C7—H7B | 108.0 | C47—C46—P3 | 118.5 (4) |
| C9—C8—C13 | 118.6 (4) | C48—C47—C46 | 121.8 (5) |
| C9—C8—P1 | 122.3 (4) | C48—C47—H47 | 119.1 |
| C13—C8—P1 | 118.9 (4) | C46—C47—H47 | 119.1 |
| C8—C9—C10 | 120.5 (6) | C49—C48—C47 | 120.4 (6) |
| C8—C9—H9 | 119.7 | C49—C48—H48 | 119.8 |
| C10—C9—H9 | 119.7 | C47—C48—H48 | 119.8 |
| C11—C10—C9 | 119.2 (6) | C48—C49—C50 | 119.3 (6) |
| C11—C10—H10 | 120.4 | C48—C49—H49 | 120.3 |
| C9—C10—H10 | 120.4 | C50—C49—H49 | 120.3 |
| C12—C11—C10 | 120.5 (5) | C49—C50—C51 | 120.3 (5) |
| C12—C11—H11 | 119.7 | C49—C50—H50 | 119.8 |
| C10—C11—H11 | 119.7 | C51—C50—H50 | 119.8 |
| C11—C12—C13 | 121.4 (6) | C46—C51—C50 | 120.8 (5) |

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| C11—C12—H12 | 119.3 | C46—C51—H51 | 119.6 |
| C13—C12—H12 | 119.3 | C50—C51—H51 | 119.6 |
| C8—C13—C12 | 119.7 (5) | N2—C52—P4 | 112.5 (3) |
| C8—C13—H13 | 120.1 | N2—C52—H52A | 109.1 |
| C12—C13—H13 | 120.1 | P4—C52—H52A | 109.1 |
| C19—C14—C15 | 118.0 (5) | N2—C52—H52B | 109.1 |
| C19—C14—P1 | 119.1 (4) | P4—C52—H52B | 109.1 |
| C15—C14—P1 | 122.7 (4) | H52A—C52—H52B | 107.8 |
| C14—C15—C16 | 119.7 (5) | C54—C53—C58 | 118.5 (5) |
| C14—C15—H15 | 120.1 | C54—C53—P4 | 118.2 (3) |
| C16—C15—H15 | 120.1 | C58—C53—P4 | 123.2 (4) |
| C17—C16—C15 | 119.4 (6) | C53—C54—C55 | 120.0 (5) |
| C17—C16—H16 | 120.3 | C53—C54—H54 | 120.0 |
| C15—C16—H16 | 120.3 | C55—C54—H54 | 120.0 |
| C18—C17—C16 | 120.2 (6) | C56—C55—C54 | 120.8 (6) |
| C18—C17—H17 | 119.9 | C56—C55—H55 | 119.6 |
| C16—C17—H17 | 119.9 | C54—C55—H55 | 119.6 |
| C17—C18—C19 | 121.1 (6) | C55—C56—C57 | 119.2 (6) |
| C17—C18—H18 | 119.5 | C55—C56—H56 | 120.4 |
| C19—C18—H18 | 119.5 | C57—C56—H56 | 120.4 |
| C14—C19—C18 | 121.6 (6) | C56—C57—C58 | 120.2 (5) |
| C14—C19—H19 | 119.2 | C56—C57—H57 | 119.9 |
| C18—C19—H19 | 119.2 | C58—C57—H57 | 119.9 |
| N1—C20—P2 | 112.4 (3) | C57—C58—C53 | 121.1 (5) |
| N1—C20—H20A | 109.1 | C57—C58—H58 | 119.4 |
| P2—C20—H20A | 109.1 | C53—C58—H58 | 119.4 |
| N1—C20—H20B | 109.1 | C60—C59—C64 | 118.7 (4) |
| P2—C20—H20B | 109.1 | C60—C59—P4 | 118.1 (3) |
| H20A—C20—H20B | 107.9 | C64—C59—P4 | 123.2 (4) |
| C26—C21—C22 | 118.2 (4) | C59—C60—C61 | 121.0 (5) |
| C26—C21—P2 | 123.3 (4) | C59—C60—H60 | 119.5 |
| C22—C21—P2 | 118.4 (4) | C61—C60—H60 | 119.5 |
| C23—C22—C21 | 120.5 (6) | C62—C61—C60 | 119.9 (5) |
| C23—C22—H22 | 119.8 | C62—C61—H61 | 120.1 |
| C21—C22—H22 | 119.8 | C60—C61—H61 | 120.1 |
| C22—C23—C24 | 120.5 (6) | C63—C62—C61 | 120.3 (5) |
| C22—C23—H23 | 119.8 | C63—C62—H62 | 119.8 |
| C24—C23—H23 | 119.8 | C61—C62—H62 | 119.8 |
| C25—C24—C23 | 119.1 (5) | C62—C63—C64 | 120.6 (5) |
| C25—C24—H24 | 120.4 | C62—C63—H63 | 119.7 |
| C23—C24—H24 | 120.4 | C64—C63—H63 | 119.7 |
| C24—C25—C26 | 119.9 (6) | C59—C64—C63 | 119.5 (5) |
| C24—C25—H25 | 120.0 | C59—C64—H64 | 120.2 |
| C26—C25—H25 | 120.0 | C63—C64—H64 | 120.2 |
| C21—C26—C25 | 121.6 (5) | P1—Cu1—P4 | 119.06 (5) |
| C21—C26—H26 | 119.2 | P1—Cu1—P3 | 117.06 (4) |
| C25—C26—H26 | 119.2 | P4—Cu1—P3 | 95.91 (4) |
| C32—C27—C28 | 118.6 (4) | P1—Cu1—P2 | 98.82 (4) |
| C32—C27—P2 | 123.8 (4) | P4—Cu1—P2 | 107.08 (4) |

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|---|---|---|---|
| C28—C27—P2 | 117.6 (4) | P3—Cu1—P2 | 119.86 (5) |
| C29—C28—C27 | 119.4 (5) | C1—N1—C7 | 114.3 (3) |
| C29—C28—H28 | 120.3 | C1—N1—C20 | 113.8 (4) |
| C27—C28—H28 | 120.3 | C7—N1—C20 | 113.7 (3) |
| C30—C29—C28 | 120.7 (5) | C52—N2—C33 | 111.4 (3) |
| C30—C29—H29 | 119.6 | C52—N2—C39 | 114.9 (4) |
| C28—C29—H29 | 119.6 | C33—N2—C39 | 112.7 (3) |
| C29—C30—C31 | 120.7 (5) | C27—P2—C21 | 103.5 (2) |
| C29—C30—H30 | 119.7 | C27—P2—C20 | 101.0 (2) |
| C31—C30—H30 | 119.7 | C21—P2—C20 | 102.5 (2) |
| C32—C31—C30 | 119.8 (5) | C27—P2—Cu1 | 120.01 (15) |
| C32—C31—H31 | 120.1 | C21—P2—Cu1 | 117.57 (15) |
| C30—C31—H31 | 120.1 | C20—P2—Cu1 | 109.81 (15) |
| C31—C32—C27 | 120.9 (5) | C8—P1—C14 | 105.0 (2) |
| C31—C32—H32 | 119.6 | C8—P1—C7 | 98.7 (2) |
| C27—C32—H32 | 119.6 | C14—P1—C7 | 100.9 (2) |
| C38—C33—C34 | 119.4 (5) | C8—P1—Cu1 | 118.19 (17) |
| C38—C33—N2 | 119.5 (5) | C14—P1—Cu1 | 119.29 (14) |
| C34—C33—N2 | 121.2 (5) | C7—P1—Cu1 | 111.60 (14) |
| C33—C34—C35 | 119.0 (6) | C46—P3—C40 | 102.73 (19) |
| C33—C34—H34 | 120.5 | C46—P3—C39 | 104.1 (2) |
| C35—C34—H34 | 120.5 | C40—P3—C39 | 100.2 (2) |
| C36—C35—C34 | 120.8 (7) | C46—P3—Cu1 | 114.98 (15) |
| C36—C35—H35 | 119.6 | C40—P3—Cu1 | 123.12 (15) |
| C34—C35—H35 | 119.6 | C39—P3—Cu1 | 109.32 (15) |
| C37—C36—C35 | 119.7 (7) | C53—P4—C59 | 103.5 (2) |
| C37—C36—H36 | 120.1 | C53—P4—C52 | 101.4 (2) |
| C35—C36—H36 | 120.1 | C59—P4—C52 | 102.6 (2) |
| C36—C37—C38 | 120.5 (8) | C53—P4—Cu1 | 119.58 (13) |
| C36—C37—H37 | 119.8 | C59—P4—Cu1 | 118.25 (14) |
| C38—C37—H37 | 119.8 | C52—P4—Cu1 | 109.04 (13) |
| C33—C38—C37 | 120.6 (7) | F2—B—F4 | 114.2 (7) |
| C33—C38—H38 | 119.7 | F2—B—F1 | 111.4 (6) |
| C37—C38—H38 | 119.7 | F4—B—F1 | 112.6 (5) |
| N2—C39—P3 | 111.7 (3) | F2—B—F3 | 107.4 (6) |
| N2—C39—H39A | 109.3 | F4—B—F3 | 105.1 (5) |
| P3—C39—H39A | 109.3 | F1—B—F3 | 105.3 (6) |
| C6—C1—C2—C3 | 1.6 (7) | C32—C27—P2—C21 | −105.7 (4) |
| N1—C1—C2—C3 | −178.6 (5) | C28—C27—P2—C21 | 75.0 (4) |
| C1—C2—C3—C4 | −0.7 (8) | C32—C27—P2—C20 | 0.1 (5) |
| C2—C3—C4—C5 | −0.5 (9) | C28—C27—P2—C20 | −179.2 (3) |
| C3—C4—C5—C6 | 0.9 (9) | C32—C27—P2—Cu1 | 120.8 (4) |
| C4—C5—C6—C1 | 0.0 (9) | C28—C27—P2—Cu1 | −58.5 (4) |
| C2—C1—C6—C5 | −1.2 (8) | C26—C21—P2—C27 | −24.3 (5) |
| N1—C1—C6—C5 | 178.9 (5) | C22—C21—P2—C27 | 160.1 (4) |
| C13—C8—C9—C10 | −0.2 (8) | C26—C21—P2—C20 | −129.0 (4) |
| P1—C8—C9—C10 | −174.6 (4) | C22—C21—P2—C20 | 55.4 (4) |
| C8—C9—C10—C11 | 1.0 (9) | C26—C21—P2—Cu1 | 110.5 (4) |
| C9—C10—C11—C12 | −1.2 (11) | C22—C21—P2—Cu1 | −65.1 (4) |

| | | | |
|---|---|---|---|
| C10—C11—C12—C13 | 0.5 (11) | N1—C20—P2—C27 | 179.4 (3) |
| C9—C8—C13—C12 | −0.4 (8) | N1—C20—P2—C21 | −73.9 (4) |
| P1—C8—C13—C12 | 174.2 (4) | N1—C20—P2—Cu1 | 51.7 (3) |
| C11—C12—C13—C8 | 0.3 (9) | P1—Cu1—P2—C27 | −140.72 (17) |
| C19—C14—C15—C16 | −3.0 (8) | P4—Cu1—P2—C27 | −16.53 (18) |
| P1—C14—C15—C16 | −178.1 (4) | P3—Cu1—P2—C27 | 90.97 (18) |
| C14—C15—C16—C17 | 2.7 (9) | P1—Cu1—P2—C21 | 92.04 (17) |
| C15—C16—C17—C18 | −0.9 (11) | P4—Cu1—P2—C21 | −143.77 (17) |
| C16—C17—C18—C19 | −0.6 (12) | P3—Cu1—P2—C21 | −36.28 (18) |
| C15—C14—C19—C18 | 1.5 (9) | P1—Cu1—P2—C20 | −24.49 (14) |
| P1—C14—C19—C18 | 176.8 (5) | P4—Cu1—P2—C20 | 99.70 (15) |
| C17—C18—C19—C14 | 0.3 (11) | P3—Cu1—P2—C20 | −152.80 (14) |
| C26—C21—C22—C23 | 2.1 (9) | C9—C8—P1—C14 | −43.7 (5) |
| P2—C21—C22—C23 | 177.9 (5) | C13—C8—P1—C14 | 141.9 (4) |
| C21—C22—C23—C24 | −5.3 (10) | C9—C8—P1—C7 | 60.1 (5) |
| C22—C23—C24—C25 | 4.3 (11) | C13—C8—P1—C7 | −114.3 (4) |
| C23—C24—C25—C26 | −0.2 (10) | C9—C8—P1—Cu1 | −179.6 (4) |
| C22—C21—C26—C25 | 2.0 (8) | C13—C8—P1—Cu1 | 6.0 (5) |
| P2—C21—C26—C25 | −173.6 (5) | C19—C14—P1—C8 | 156.6 (4) |
| C24—C25—C26—C21 | −3.0 (9) | C15—C14—P1—C8 | −28.3 (5) |
| C32—C27—C28—C29 | 1.3 (7) | C19—C14—P1—C7 | 54.4 (5) |
| P2—C27—C28—C29 | −179.3 (4) | C15—C14—P1—C7 | −130.5 (4) |
| C27—C28—C29—C30 | −1.8 (8) | C19—C14—P1—Cu1 | −68.1 (5) |
| C28—C29—C30—C31 | 1.2 (9) | C15—C14—P1—Cu1 | 107.0 (4) |
| C29—C30—C31—C32 | −0.2 (9) | N1—C7—P1—C8 | 74.9 (3) |
| C30—C31—C32—C27 | −0.3 (9) | N1—C7—P1—C14 | −177.9 (3) |
| C28—C27—C32—C31 | −0.3 (8) | N1—C7—P1—Cu1 | −50.2 (3) |
| P2—C27—C32—C31 | −179.6 (4) | P4—Cu1—P1—C8 | 155.58 (18) |
| C38—C33—C34—C35 | −1.2 (10) | P3—Cu1—P1—C8 | 40.99 (19) |
| N2—C33—C34—C35 | −179.5 (6) | P2—Cu1—P1—C8 | −89.18 (18) |
| C33—C34—C35—C36 | −1.4 (12) | P4—Cu1—P1—C14 | 26.00 (18) |
| C34—C35—C36—C37 | 3.3 (15) | P3—Cu1—P1—C14 | −88.59 (17) |
| C35—C36—C37—C38 | −2.5 (16) | P2—Cu1—P1—C14 | 141.24 (17) |
| C34—C33—C38—C37 | 1.9 (11) | P4—Cu1—P1—C7 | −91.03 (15) |
| N2—C33—C38—C37 | −179.8 (7) | P3—Cu1—P1—C7 | 154.38 (14) |
| C36—C37—C38—C33 | −0.1 (15) | P2—Cu1—P1—C7 | 24.21 (15) |
| C45—C40—C41—C42 | 1.7 (8) | C51—C46—P3—C40 | −96.1 (4) |
| P3—C40—C41—C42 | −178.4 (4) | C47—C46—P3—C40 | 86.0 (4) |
| C40—C41—C42—C43 | 0.1 (8) | C51—C46—P3—C39 | 8.0 (4) |
| C41—C42—C43—C44 | −1.7 (10) | C47—C46—P3—C39 | −169.9 (4) |
| C42—C43—C44—C45 | 1.5 (11) | C51—C46—P3—Cu1 | 127.6 (4) |
| C41—C40—C45—C44 | −1.9 (9) | C47—C46—P3—Cu1 | −50.3 (4) |
| P3—C40—C45—C44 | 178.2 (5) | C45—C40—P3—C46 | −10.2 (5) |
| C43—C44—C45—C40 | 0.3 (11) | C41—C40—P3—C46 | 169.9 (4) |
| C51—C46—C47—C48 | 0.2 (7) | C45—C40—P3—C39 | −117.4 (5) |
| P3—C46—C47—C48 | 178.3 (4) | C41—C40—P3—C39 | 62.8 (4) |
| C46—C47—C48—C49 | −0.4 (8) | C45—C40—P3—Cu1 | 121.4 (4) |
| C47—C48—C49—C50 | 0.1 (9) | C41—C40—P3—Cu1 | −58.5 (4) |
| C48—C49—C50—C51 | 0.4 (9) | N2—C39—P3—C46 | 64.9 (4) |

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|---|---|---|---|
| C47—C46—C51—C50 | 0.3 (7) | N2—C39—P3—C40 | 170.9 (3) |
| P3—C46—C51—C50 | −177.7 (4) | N2—C39—P3—Cu1 | −58.5 (4) |
| C49—C50—C51—C46 | −0.6 (9) | P1—Cu1—P3—C46 | 47.73 (15) |
| C58—C53—C54—C55 | 3.6 (9) | P4—Cu1—P3—C46 | −79.23 (15) |
| P4—C53—C54—C55 | −174.0 (5) | P2—Cu1—P3—C46 | 167.20 (15) |
| C53—C54—C55—C56 | −2.1 (11) | P1—Cu1—P3—C40 | −78.72 (18) |
| C54—C55—C56—C57 | −1.5 (12) | P4—Cu1—P3—C40 | 154.32 (18) |
| C55—C56—C57—C58 | 3.5 (12) | P2—Cu1—P3—C40 | 40.75 (18) |
| C56—C57—C58—C53 | −2.0 (12) | P1—Cu1—P3—C39 | 164.39 (16) |
| C54—C53—C58—C57 | −1.7 (9) | P4—Cu1—P3—C39 | 37.42 (16) |
| P4—C53—C58—C57 | 175.8 (5) | P2—Cu1—P3—C39 | −76.15 (16) |
| C64—C59—C60—C61 | 1.2 (8) | C54—C53—P4—C59 | −148.8 (4) |
| P4—C59—C60—C61 | −179.1 (4) | C58—C53—P4—C59 | 33.8 (5) |
| C59—C60—C61—C62 | −1.1 (9) | C54—C53—P4—C52 | 105.2 (4) |
| C60—C61—C62—C63 | −0.2 (9) | C58—C53—P4—C52 | −72.3 (5) |
| C61—C62—C63—C64 | 1.4 (8) | C54—C53—P4—Cu1 | −14.7 (5) |
| C60—C59—C64—C63 | −0.1 (7) | C58—C53—P4—Cu1 | 167.9 (4) |
| P4—C59—C64—C63 | −179.7 (4) | C60—C59—P4—C53 | 80.7 (4) |
| C62—C63—C64—C59 | −1.2 (8) | C64—C59—P4—C53 | −99.7 (4) |
| C2—C1—N1—C7 | −97.9 (5) | C60—C59—P4—C52 | −174.1 (4) |
| C6—C1—N1—C7 | 82.0 (5) | C64—C59—P4—C52 | 5.5 (4) |
| C2—C1—N1—C20 | 35.1 (6) | C60—C59—P4—Cu1 | −54.2 (4) |
| C6—C1—N1—C20 | −145.1 (4) | C64—C59—P4—Cu1 | 125.5 (3) |
| P1—C7—N1—C1 | −141.0 (3) | N2—C52—P4—C53 | −68.8 (3) |
| P1—C7—N1—C20 | 86.0 (4) | N2—C52—P4—C59 | −175.6 (3) |
| P2—C20—N1—C1 | 138.9 (3) | N2—C52—P4—Cu1 | 58.3 (3) |
| P2—C20—N1—C7 | −87.9 (4) | P1—Cu1—P4—C53 | −46.61 (19) |
| P4—C52—N2—C33 | 146.8 (3) | P3—Cu1—P4—C53 | 78.89 (18) |
| P4—C52—N2—C39 | −83.5 (4) | P2—Cu1—P4—C53 | −157.37 (18) |
| C38—C33—N2—C52 | −101.4 (6) | P1—Cu1—P4—C59 | 80.97 (18) |
| C34—C33—N2—C52 | 76.9 (6) | P3—Cu1—P4—C59 | −153.52 (18) |
| C38—C33—N2—C39 | 127.7 (6) | P2—Cu1—P4—C59 | −29.78 (18) |
| C34—C33—N2—C39 | −54.0 (6) | P1—Cu1—P4—C52 | −162.48 (16) |
| P3—C39—N2—C52 | 83.3 (4) | P3—Cu1—P4—C52 | −36.97 (17) |
| P3—C39—N2—C33 | −147.6 (3) | P2—Cu1—P4—C52 | 86.77 (17) |

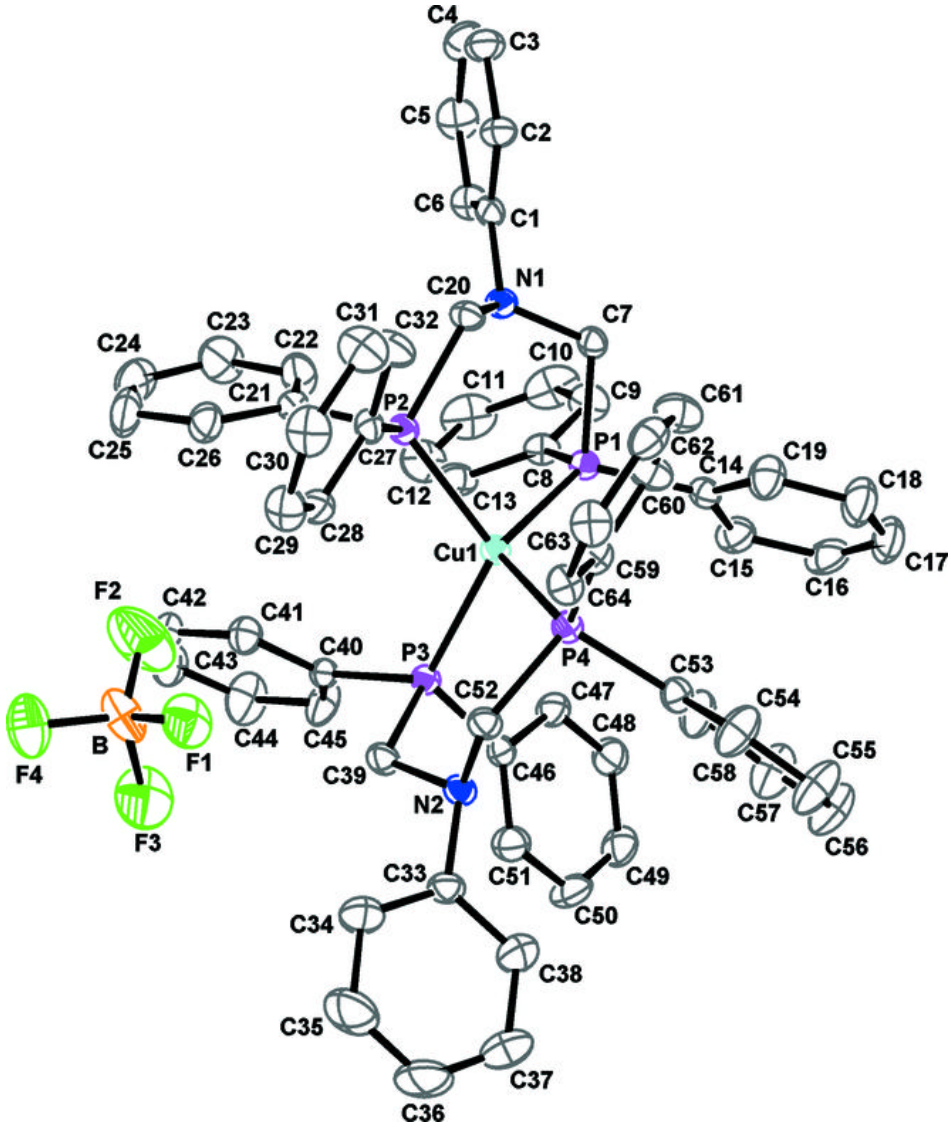
*Hydrogen-bond geometry (Å, °)*

Cg1 and Cg2 are the centroids of the C33–C38 and C1–C6 rings, respectively.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C22—H22···N1 | 0.93 | 2.53 | 3.189 (6) | 128 |
| C7—H7A···F3$^{i}$ | 0.97 | 2.25 | 3.181 (6) | 161 |
| C18—H18···Cg1$^{i}$ | 0.93 | 2.72 | 3.653 (6) | 177 |
| C42—H42···Cg2$^{ii}$ | 0.93 | 2.88 | 3.678 (5) | 144 |

Symmetry codes: (i) *x*−1, *y*, *z*; (ii) *x*+1, *y*, *z*.

**Fig. 1**


C4
C3
C5
C2
C6
C1
N1
C20
C31
C32
C7
C23
C24
C22
C10
C21
C11
C9
C61
P2
P1
C25
C26
C30
C27
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C62
C14
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C42
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C40
P3
P4
C53
C43
C52
C47
C54
B
C44
C45
C48
F4
F1
C39
C46
C58
C55
N2
C57
F3
C56
C33
C51
C49
C50
C34
C38
C35
C37
C36

**Fig. 2**