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# {Dimethyl [(phenylsulfonyl)amido]-phosphato-$\kappa^2O,O'$}bis(triphenylphosphane-$\kappa P$)copper(I)

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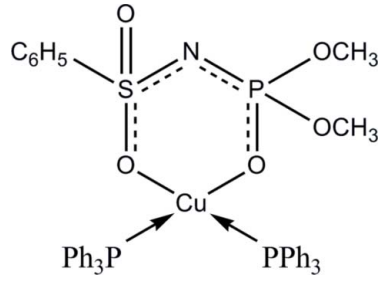
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.008 Å; $R$ factor = 0.086; $wR$ factor = 0.120; data-to-parameter ratio = 21.2.

In the title complex, $[Cu(C_8H_{11}NO_5PS)(C_{18}H_{15}P)_2]$, the $Cu^I$ ion is coordinated by two triphenylphosphane molecules and two O atoms of the chelating dimethyl(phenylsulfonyl)amidophosphate anion, generating a squashed $CuO_2P_2$ tetrahedron. In the six-membered chelate ring, the Cu, P and O atoms are almost coplanar (r.m.s. deviation = 0.024 Å), with the N and S atoms displaced in the same direction, by 0.708 (5) and 0.429 (2) Å, respectively.

## Related literature

For the synthesis of sulfonylamide derivatives, see: Kirsanov (1965); Moroz *et al.* (2012). For details of the pharmacological and biological properties of sulfonylamide derivatives, see: Kishino & Saito (1979); Xu & Angell (2000). For $Cu^I$-containing complexes with triphenylphosphane, see: Barron *et al.* (1987); Yang *et al.* (2001); Zabirov *et al.* (2003). For details of potential applications of $Cu^I$-containing complexes, see: Nagashima *et al.* (1993); Nondek *et al.* (1987); Tarkhanova *et al.* (2001); Zazybin *et al.* (2006); Verat *et al.* (2006). For coordination compounds of 3*d* metals with sulfonylamidophosphate ligands, see: Moroz *et al.* (2009); Trush *et al.* (2011). For the coordination mode of structural analogs of $\beta$-diketones, see: Gawryszewska *et al.* (2011); Yizhak *et al.* (2013); Kariaka *et al.* (2013); Amirkhanov *et al.* (2014).




## Experimental

### Crystal data

$[Cu(C_8H_{11}NO_5PS)(C_{18}H_{15}P)_2]$
$M_r$ = 852.29
Monoclinic, $P2_1/c$
$a$ = 12.8657 (12) Å
$b$ = 26.281 (3) Å
$c$ = 13.971 (3) Å
$\beta$ = 121.875 (10)°
$V$ = 4011.6 (11) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.76 mm$^{-1}$
$T$ = 100 K
0.40 × 0.30 × 0.10 mm

### Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
$T_{min}$ = 0.74, $T_{max}$ = 0.90
27134 measured reflections
9293 independent reflections
4739 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.137

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.086
$wR(F^2)$ = 0.120
$S$ = 1.04
9293 reflections
438 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.48 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.56 e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Cu1—O3 | 2.065 (3) | Cu1—P2 | 2.2345 (15) |
| Cu1—O1 | 2.263 (3) | Cu1—P3 | 2.2381 (14) |

Data collection: *COLLECT* (Nonius, 1999); cell refinement: *DENZO/SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO/SCALEPACK*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

The authors are grateful to Dr Y. S. Moroz for kind assistance in solving and refining the structure.

Supporting information for this paper is available from the IUCr electronic archives (Reference: HB7222).

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# supplementary materials

*Acta Cryst.* (2014). E**70**, m209–m210 [doi:10.1107/S1600536814010095]

# {Dimethyl [(phenylsulfonyl)amido]phosphato-$\kappa^2O,O'$}bis(triphenylphosphane-$\kappa P$)copper(I)

**Olesia V. Moroz, Viktor A. Trush, Tatiana Yu. Sliva, Kateryna O. Znovjyak and Vladimir M. Amirkhanov**

## 1. Introduction

Coordination chemistry of structural analogs of *β*-diketones has been widely studied during last 30 years. Among them, sulfonyl phosphoramides (SAPh) bearing a $S(O)_2NHP(O)$ structural fragment and different substituents at sulfur and phosphorus atoms were first synthesized by Kirsanov (Kirsanov, 1965). These compounds are extensively used in medicine as bactericidal agents (Xu & Angell, 2000) and in agriculture as pesticides (Kishino & Saito, 1979). Recently, coordination compounds of lanthanides and 3*d* metals with SAPhs behaving as bidentate O,O-donor chelating ligands have been reported (Moroz, *et al.*, 2009; Moroz, *et al.*, 2012; Trush, *et al.*, 2011). As our contribution to the study of coordination compounds of 3*d* metals based on SAPh, we synthesized and structurally characterized a copper(I)-containing complex $[Cu(\boldsymbol{L})(PPh_3)_2]$ (**I**) {where, H***L*** is dimethyl(phenylsulfonyl)amidophosphate ($C_6H_5S(O)_2NHP(O)(OCH_3)_2$) and $PPh_3$ is triphenylphosphane}. Complexes of $Cu^I$ have useful luminescent properties, they can be used in microelectronics and as catalysts of homolytic C–Hal (Hal = Cl, Br) bond cleavage in polyhaloalkanes (Nagashima, *et al.*, 1993; Nondek, *et al.*, 1987; Tarkhanova, *et al.*, 2001; Zazybin, *et al.*, 2006). Triphenylphosphane molecule was used to prevent cluster formation during complexation reaction.

The molecular structure of **I** is shown in Figure1. Van der Waals contacts exist between molecules of **I** in the crystal structure. The coordination environment of the Cu ion is a distorted tetrahedron (2+2). The values for the bond angles around the central atom are in the range from 88.9 (1)° to 129.94 (6)°. The coordination polyhedron consists of two phosphorus atoms from $PPh_3$ molecules and two oxygen atoms from the phosphoryl and the sulfonyl groups of $\boldsymbol{L}^-$, which is coordinated in bidentate chelate mode forming with central ion a six-membered chelate ring. The later coordination mode is typical for the deprotonated structural analogs of *β*-diketones, SAPh and CAPh (carbacylamidophosphates) (Gawryszewska, *et al.*, 2011; Yizhak, *et al.*, 2013; Kariaka, *et al.*, 2013; Amirkhanov, *et al.*, 2014). It has already been observed for $[Cu(PPh_3)_nL_1]$ based on N-acylamidophosphinate ligands (Verat, *et al.*, 2006) and for $(PPh_3)_3CuI$ (Barron, *et al.*, 1987) that the number of the coordinated $PPh_3$ molecules to the central ion has the main influence on the Cu–P bond lengths. As in the present compound the $Cu^I$ atom coordinates two $PPh_3$, the Cu–P distances of 2.234 (1), 2.238 (1)Å are in good agreement with the values observed for the complexes containing two $PPh_3$ ligands (Yang, *et al.*, 2001; Zabirov, *et al.*, 2003; Verat, *et al.*, 2006).

The Cu–O(S) and Cu–O(P) bond lengths (2.263 (3) and 2.066 (3)Å, respectively) (Table1) are similar to the reported values for the complexes of 3*d*-metals with H***L*** (Moroz, *et al.*, 2009; Trush, *et al.*, 2011). The amide nitrogen atom of the ligand is deprotonated that leads to decreasing the S–N, N–P and increasing the P–O, S–O bond length values (Table1) compared with those for H***L*** (Moroz, *et al.*, 2009). Such changes may be related to the occurrence of the *π*-coupling in O—S—N—P—O fragment and are usual for SAPh ligands (Moroz, *et al.*, 2009; Trush, *et al.*, 2011). The value of the O(1)

—Cu(1)—O(3) angle of 88.9 (1)° is typical for the coordination compounds with O- donor SAPh and CAPh ligands. The phosphorus and sulfur atoms of **I** have distorted tetrahedral configurations (Table1). Oxygen atoms of the phosphoryl O(3) and the sulfonyl O(2) groups of the O—S—N—P—O structural fragment adopt an anticlinal conformation (the dihedral angle between O(2)—S(1)—P(1) and O(3)—P(1)—S(1) planes is 106.3°). The six-membered Cu—O—P—N—S—O metallocycle has a distorted boat conformation with the deviations of N(1) and Cu(1) from the mean plane of 0.40Å and 0.26Å, respectively.

## 2. Experimental

The synthesis of H***L*** was carried out according to previously published procedure (Moroz, *et al.*, 2009).

Compound **I** was prepared according to the following scheme:

$4H\boldsymbol{L} + 4Cu + 8PPh_3 + O_2 \rightarrow 4[Cu(\boldsymbol{L})(PPh_3)_2] + 2H_2O$

Briefly, a heterogeneous mixture of copper powder (0.065g, 1mmol), triphenylphosphane (0.524g, 2mmol) and H***L*** (0.287g, 1mmol) in 40mL of acetone was stirred for 4 days upon heating with a reflux condenser. Decreasing of the powder was observed simultaneously with gradual appearance of white precipitate. The later was filtered off, washed thoroughly with chilled isopropanol, dried and dissolved in minimal amount of DMF to remove the residual copper powder. The resulting solution was left at ambient temperature for crystallization in air. The colorless crystals were collected by filtration after 2 days, washed with chilled isopropanol and dried on filter. Yield: 0.64g (75%). The compound is soluble in methanol, acetonitrile, chloroform, DMSO and DMF. Anal. calc. for $C_{44}H_{41}NO_5P_3SCu$: C61.81, H4.71, N1.61, S3.54%; found: C62.00, H4.85, N1.64, S3.76%; IR (KBr, $cm^{-1}$): 1225, 1250 (s, $SO_2$) and 1180 (s, PO); $^1$H NMR (400 MHz, $CDCl_3$): 3.28 (d, 6H, $CH_3$, $^3J_{P–H}$ = 12Hz), 7.09 (m, $H_\beta$, 2H, $C_6H_5(\boldsymbol{L}^-)$), 7.27 (m, $H_\beta$, 12H, $C_6H_5(PPh_3)$), 7.33 (s, $H_\gamma$, 1H, $C_6H_5(\boldsymbol{L}^-)$), 7.39 (m, $H_{\alpha+\gamma}$, 18H, $C_6H_5(PPh_3)$) 7.62 (m, $H_\alpha$, 2H, $C_6H_5(\boldsymbol{L}^-)$) ppm. $^{31}$P NMR (162.1 MHz, $CDCl_3$): 0.8 (g, $^3J_{P–H}$ = 12Hz, $\boldsymbol{L}^-$), -4.3 (s, $PPh_3$) ppm.

## 3. Refinement

The H atoms were attached to carbon atoms geometrically. The H atoms were refined with riding constraints (C—H in the range 0.93–0.98Å, and $U_{iso}$(H) lie in the range 1.2-1.5 times $U_{eq}$ of the parent atom). Crystal data, data collection and structure refinement details are summarized in Table 1.

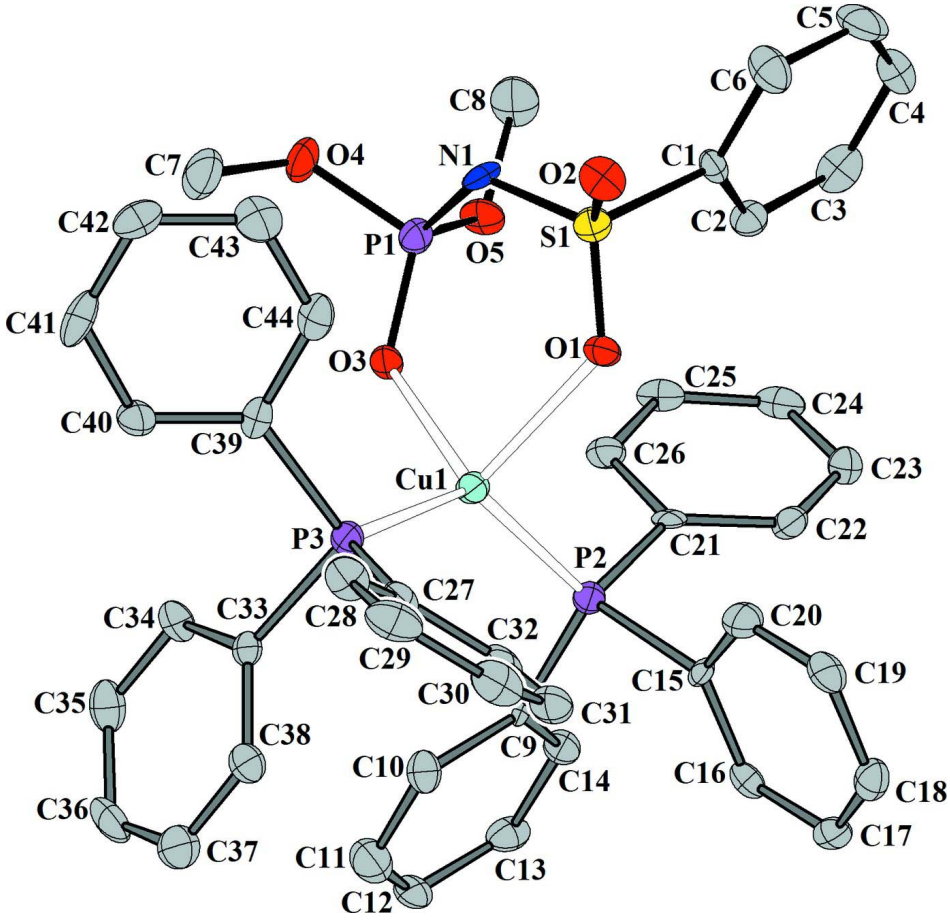


**Figure 1**

Structural representation of **I** with atom numbering scheme and 50% probability thermal ellipsoid. The H atoms are omitted for clarity.

**{Dimethyl [(phenylsulfonyl)amido]phosphato-$\kappa^2O,O'$}bis(triphenylphosphane-$\kappa P$)copper(I)**

*Crystal data*

$[Cu(C_8H_{11}NO_5PS)(C_{18}H_{15}P)_2]$
$M_r$ = 852.29
Monoclinic, $P2_1/c$
$a$ = 12.8657 (12) Å
$b$ = 26.281 (3) Å
$c$ = 13.971 (3) Å
$\beta$ = 121.875 (10)°
$V$ = 4011.6 (11) Å$^3$
$Z$ = 4
$F(000)$ = 1768
$D_x$ = 1.411 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 27134 reflections
$\theta$ = 2.9–28.5°
$\mu$ = 0.76 mm$^{-1}$
$T$ = 100 K
Needle, colourless
0.40 × 0.30 × 0.10 mm

*Data collection*

Nonius KappaCCD diffractometer
Radiation source: sealed X-ray tube
Detector resolution: 9 pixels mm$^{-1}$
$\varphi$ scans and $\omega$ scans with $\kappa$ offset
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
$T_{min}$ = 0.74, $T_{max}$ = 0.90
27134 measured reflections
9293 independent reflections
4739 reflections with $I > 2\sigma(I)$

$R_{int}$ = 0.137
$\theta_{max}$ = 28.5°, $\theta_{min}$ = 2.9°
$h$ = −16→16
$k$ = −33→34
$l$ = −18→18

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.086
$wR(F^2)$ = 0.120
$S$ = 1.04
9293 reflections
438 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0188P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.48 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.56 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 $F^2 > 2\sigma(F^2)$ 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 (Å²)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.7620 (4) | 0.16461 (19) | 1.0173 (4) | 0.0134 (12) |
| C2 | 0.7765 (5) | 0.15558 (19) | 0.9275 (4) | 0.0195 (13) |
| H68 | 0.7094 | 0.1479 | 0.8566 | 0.023* |
| C3 | 0.8930 (5) | 0.1582 (2) | 0.9452 (5) | 0.0257 (14) |
| H102 | 0.9034 | 0.1531 | 0.8848 | 0.031* |
| C4 | 0.9933 (5) | 0.1682 (2) | 1.0499 (5) | 0.0260 (14) |
| H106 | 1.0707 | 0.1698 | 1.0602 | 0.031* |
| C5 | 0.9789 (5) | 0.1758 (2) | 1.1401 (5) | 0.0323 (16) |
| H19 | 1.0468 | 0.1822 | 1.2115 | 0.039* |
| C6 | 0.8614 (5) | 0.1740 (2) | 1.1237 (5) | 0.0277 (15) |
| H57 | 0.8509 | 0.1790 | 1.1840 | 0.033* |
| C7 | 0.3285 (5) | 0.2987 (2) | 0.8180 (5) | 0.0375 (17) |
| H74A | 0.2652 | 0.2749 | 0.7708 | 0.056* |
| H74B | 0.3002 | 0.3327 | 0.7928 | 0.056* |
| H74C | 0.3493 | 0.2948 | 0.8945 | 0.056* |
| C8 | 0.6702 (5) | 0.2749 (2) | 0.8269 (5) | 0.0303 (15) |
| H7A | 0.6423 | 0.3079 | 0.8330 | 0.045* |
| H7B | 0.7084 | 0.2774 | 0.7838 | 0.045* |
| H7C | 0.7283 | 0.2622 | 0.9008 | 0.045* |
| C9 | 0.2961 (5) | 0.06859 (19) | 0.5000 (4) | 0.0203 (5) |
| C10 | 0.1706 (5) | 0.06746 (19) | 0.4622 (4) | 0.0203 (5) |
| H25 | 0.1469 | 0.0701 | 0.5144 | 0.024* |
| C11 | 0.0819 (5) | 0.06245 (18) | 0.3490 (4) | 0.0203 (5) |
| H21 | −0.0003 | 0.0612 | 0.3260 | 0.024* |

| | | | | |
|---|---|---|---|---|
| C12 | 0.1160 (5) | 0.05931 (19) | 0.2692 (4) | 0.0203 (5) |
| H16 | 0.0567 | 0.0560 | 0.1930 | 0.024* |
| C13 | 0.2384 (5) | 0.06113 (19) | 0.3045 (4) | 0.0203 (5) |
| H15 | 0.2613 | 0.0599 | 0.2515 | 0.024* |
| C14 | 0.3274 (5) | 0.06484 (19) | 0.4179 (4) | 0.0203 (5) |
| H35 | 0.4095 | 0.0648 | 0.4403 | 0.024* |
| C15 | 0.4477 (4) | 0.00831 (18) | 0.6988 (4) | 0.0132 (12) |
| C16 | 0.4271 (4) | −0.03269 (19) | 0.6270 (4) | 0.0147 (12) |
| H20 | 0.3927 | −0.0268 | 0.5504 | 0.018* |
| C17 | 0.4570 (5) | −0.0819 (2) | 0.6678 (5) | 0.0189 (13) |
| H6 | 0.4437 | −0.1088 | 0.6192 | 0.023* |
| C18 | 0.5070 (5) | −0.0910 (2) | 0.7817 (5) | 0.0215 (14) |
| H56 | 0.5264 | −0.1241 | 0.8093 | 0.026* |
| C19 | 0.5283 (5) | −0.0510 (2) | 0.8547 (5) | 0.0242 (14) |
| H8 | 0.5628 | −0.0573 | 0.9311 | 0.029* |
| C20 | 0.4987 (5) | −0.0024 (2) | 0.8145 (5) | 0.0236 (14) |
| H31 | 0.5123 | 0.0241 | 0.8640 | 0.028* |
| C21 | 0.5434 (5) | 0.09651 (19) | 0.6489 (4) | 0.0141 (12) |
| C22 | 0.6453 (5) | 0.0664 (2) | 0.6779 (4) | 0.0184 (13) |
| H60 | 0.6493 | 0.0333 | 0.7032 | 0.022* |
| C23 | 0.7411 (5) | 0.0854 (2) | 0.6694 (4) | 0.0229 (14) |
| H29 | 0.8085 | 0.0650 | 0.6888 | 0.027* |
| C24 | 0.7358 (5) | 0.1347 (2) | 0.6320 (4) | 0.0243 (14) |
| H54 | 0.7988 | 0.1472 | 0.6245 | 0.029* |
| C25 | 0.6370 (5) | 0.1655 (2) | 0.6057 (4) | 0.0191 (13) |
| H70 | 0.6346 | 0.1988 | 0.5822 | 0.023* |
| C26 | 0.5425 (5) | 0.14690 (19) | 0.6142 (4) | 0.0191 (13) |
| H67 | 0.4767 | 0.1680 | 0.5966 | 0.023* |
| C27 | 0.1898 (4) | 0.0599 (2) | 0.8496 (4) | 0.0177 (13) |
| C28 | 0.1400 (5) | 0.0630 (2) | 0.9169 (4) | 0.0232 (14) |
| H105 | 0.1078 | 0.0938 | 0.9224 | 0.028* |
| C29 | 0.1375 (5) | 0.0207 (2) | 0.9761 (5) | 0.0324 (16) |
| H1 | 0.1021 | 0.0229 | 1.0193 | 0.039* |
| C30 | 0.1891 (5) | −0.0249 (2) | 0.9696 (5) | 0.0332 (16) |
| H45 | 0.1901 | −0.0531 | 1.0104 | 0.040* |
| C31 | 0.2386 (5) | −0.0284 (2) | 0.9029 (5) | 0.0285 (15) |
| H72 | 0.2710 | −0.0591 | 0.8975 | 0.034* |
| C32 | 0.2400 (5) | 0.01393 (19) | 0.8440 (4) | 0.0209 (14) |
| H38 | 0.2748 | 0.0115 | 0.8003 | 0.025* |
| C33 | 0.0584 (4) | 0.11361 (19) | 0.6394 (4) | 0.0143 (12) |
| C34 | 0.0297 (5) | 0.1559 (2) | 0.5668 (4) | 0.0191 (13) |
| H61 | 0.0792 | 0.1847 | 0.5923 | 0.023* |
| C35 | −0.0716 (5) | 0.1547 (2) | 0.4583 (5) | 0.0251 (15) |
| H107 | −0.0912 | 0.1832 | 0.4124 | 0.030* |
| C36 | −0.1443 (5) | 0.1115 (2) | 0.4168 (5) | 0.0275 (15) |
| H47 | −0.2106 | 0.1104 | 0.3429 | 0.033* |
| C37 | −0.1168 (5) | 0.0703 (2) | 0.4865 (5) | 0.0275 (15) |
| H66 | −0.1659 | 0.0415 | 0.4594 | 0.033* |
| C38 | −0.0173 (5) | 0.0709 (2) | 0.5966 (4) | 0.0194 (13) |

| | | | | |
|---|---|---|---|---|
| H62 | −0.0008 | 0.0425 | 0.6423 | 0.023* |
| C39 | 0.1906 (5) | 0.1685 (2) | 0.8525 (5) | 0.0235 (6) |
| C40 | 0.0861 (5) | 0.19774 (19) | 0.8175 (5) | 0.0235 (6) |
| H13 | 0.0132 | 0.1899 | 0.7510 | 0.028* |
| C41 | 0.0923 (5) | 0.2386 (2) | 0.8830 (4) | 0.0235 (6) |
| H28 | 0.0230 | 0.2585 | 0.8589 | 0.028* |
| C42 | 0.1968 (5) | 0.2504 (2) | 0.9812 (5) | 0.0235 (6) |
| H65 | 0.1984 | 0.2777 | 1.0242 | 0.028* |
| C43 | 0.3019 (5) | 0.2214 (2) | 1.0173 (5) | 0.0235 (6) |
| H14 | 0.3742 | 0.2291 | 1.0845 | 0.028* |
| C44 | 0.2972 (5) | 0.1810 (2) | 0.9521 (4) | 0.0235 (6) |
| H75 | 0.3673 | 0.1617 | 0.9757 | 0.028* |
| Cu1 | 0.36062 (6) | 0.12135 (2) | 0.75302 (5) | 0.01638 (18) |
| N1 | 0.5554 (4) | 0.21783 (15) | 0.9479 (3) | 0.0169 (10) |
| O1 | 0.5448 (3) | 0.12269 (13) | 0.9166 (3) | 0.0198 (9) |
| O2 | 0.6296 (3) | 0.15752 (13) | 1.1063 (3) | 0.0246 (9) |
| O3 | 0.3780 (3) | 0.19846 (12) | 0.7364 (3) | 0.0173 (9) |
| O4 | 0.4335 (3) | 0.28906 (12) | 0.8119 (3) | 0.0268 (10) |
| O5 | 0.5671 (3) | 0.24042 (13) | 0.7711 (3) | 0.0227 (9) |
| P1 | 0.48025 (13) | 0.23250 (5) | 0.81736 (13) | 0.0190 (4) |
| P2 | 0.41040 (12) | 0.07398 (5) | 0.65026 (12) | 0.0153 (3) |
| P3 | 0.20168 (12) | 0.11467 (5) | 0.77600 (12) | 0.0162 (3) |
| S1 | 0.61185 (12) | 0.16414 (5) | 0.99649 (12) | 0.0183 (3) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.008 (3) | 0.014 (3) | 0.015 (3) | 0.000 (2) | 0.004 (3) | 0.003 (2) |
| C2 | 0.022 (4) | 0.019 (3) | 0.018 (3) | −0.001 (3) | 0.011 (3) | −0.001 (3) |
| C3 | 0.034 (4) | 0.026 (3) | 0.026 (4) | 0.003 (3) | 0.022 (3) | 0.001 (3) |
| C4 | 0.015 (3) | 0.032 (4) | 0.027 (4) | 0.002 (3) | 0.008 (3) | 0.001 (3) |
| C5 | 0.021 (4) | 0.045 (4) | 0.023 (4) | −0.007 (3) | 0.006 (3) | −0.013 (3) |
| C6 | 0.022 (4) | 0.042 (4) | 0.021 (4) | 0.000 (3) | 0.013 (3) | −0.002 (3) |
| C7 | 0.029 (4) | 0.025 (4) | 0.067 (5) | 0.002 (3) | 0.031 (4) | −0.005 (3) |
| C8 | 0.025 (4) | 0.027 (4) | 0.041 (4) | −0.007 (3) | 0.020 (3) | 0.008 (3) |
| C9 | 0.0184 (14) | 0.0199 (12) | 0.0188 (14) | 0.0008 (11) | 0.0072 (12) | −0.0007 (11) |
| C10 | 0.0184 (14) | 0.0199 (12) | 0.0188 (14) | 0.0008 (11) | 0.0072 (12) | −0.0007 (11) |
| C11 | 0.0184 (14) | 0.0199 (12) | 0.0188 (14) | 0.0008 (11) | 0.0072 (12) | −0.0007 (11) |
| C12 | 0.0184 (14) | 0.0199 (12) | 0.0188 (14) | 0.0008 (11) | 0.0072 (12) | −0.0007 (11) |
| C13 | 0.0184 (14) | 0.0199 (12) | 0.0188 (14) | 0.0008 (11) | 0.0072 (12) | −0.0007 (11) |
| C14 | 0.0184 (14) | 0.0199 (12) | 0.0188 (14) | 0.0008 (11) | 0.0072 (12) | −0.0007 (11) |
| C15 | 0.011 (3) | 0.010 (3) | 0.022 (3) | 0.000 (2) | 0.011 (3) | −0.004 (2) |
| C16 | 0.012 (3) | 0.020 (3) | 0.014 (3) | −0.002 (2) | 0.008 (3) | 0.002 (3) |
| C17 | 0.018 (3) | 0.018 (3) | 0.027 (4) | −0.005 (3) | 0.016 (3) | −0.006 (3) |
| C18 | 0.020 (3) | 0.019 (3) | 0.028 (4) | 0.004 (3) | 0.015 (3) | 0.002 (3) |
| C19 | 0.019 (3) | 0.029 (4) | 0.013 (3) | 0.002 (3) | 0.000 (3) | 0.002 (3) |
| C20 | 0.025 (4) | 0.021 (3) | 0.017 (3) | 0.002 (3) | 0.005 (3) | −0.003 (3) |
| C21 | 0.012 (3) | 0.018 (3) | 0.010 (3) | −0.004 (2) | 0.005 (3) | −0.008 (2) |
| C22 | 0.019 (3) | 0.015 (3) | 0.026 (4) | −0.001 (3) | 0.016 (3) | −0.003 (3) |
| C23 | 0.016 (3) | 0.024 (3) | 0.028 (4) | 0.001 (3) | 0.011 (3) | −0.006 (3) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C24 | 0.027 (4) | 0.030 (4) | 0.022 (3) | −0.013 (3) | 0.017 (3) | −0.007 (3) |
| C25 | 0.023 (4) | 0.021 (3) | 0.018 (3) | −0.010 (3) | 0.015 (3) | −0.005 (3) |
| C26 | 0.020 (3) | 0.015 (3) | 0.021 (3) | −0.004 (3) | 0.010 (3) | −0.003 (3) |
| C27 | 0.011 (3) | 0.021 (3) | 0.017 (3) | −0.004 (3) | 0.005 (3) | 0.000 (3) |
| C28 | 0.020 (3) | 0.024 (3) | 0.025 (4) | −0.002 (3) | 0.011 (3) | 0.006 (3) |
| C29 | 0.028 (4) | 0.037 (4) | 0.031 (4) | −0.014 (3) | 0.014 (3) | −0.001 (3) |
| C30 | 0.033 (4) | 0.024 (4) | 0.025 (4) | −0.007 (3) | 0.004 (3) | 0.015 (3) |
| C31 | 0.023 (4) | 0.021 (4) | 0.033 (4) | −0.003 (3) | 0.009 (3) | 0.000 (3) |
| C32 | 0.013 (3) | 0.017 (3) | 0.017 (3) | −0.001 (3) | −0.002 (3) | 0.004 (3) |
| C33 | 0.013 (3) | 0.015 (3) | 0.018 (3) | 0.000 (2) | 0.011 (3) | −0.002 (3) |
| C34 | 0.010 (3) | 0.027 (3) | 0.025 (4) | −0.003 (3) | 0.012 (3) | 0.002 (3) |
| C35 | 0.019 (4) | 0.032 (4) | 0.029 (4) | 0.006 (3) | 0.015 (3) | 0.007 (3) |
| C36 | 0.011 (3) | 0.045 (4) | 0.023 (4) | −0.002 (3) | 0.007 (3) | −0.003 (3) |
| C37 | 0.023 (4) | 0.026 (4) | 0.035 (4) | −0.002 (3) | 0.016 (3) | −0.006 (3) |
| C38 | 0.013 (3) | 0.024 (3) | 0.019 (3) | 0.000 (3) | 0.008 (3) | 0.000 (3) |
| C39 | 0.0276 (15) | 0.0243 (14) | 0.0243 (15) | 0.0026 (12) | 0.0176 (13) | −0.0019 (11) |
| C40 | 0.0276 (15) | 0.0243 (14) | 0.0243 (15) | 0.0026 (12) | 0.0176 (13) | −0.0019 (11) |
| C41 | 0.0276 (15) | 0.0243 (14) | 0.0243 (15) | 0.0026 (12) | 0.0176 (13) | −0.0019 (11) |
| C42 | 0.0276 (15) | 0.0243 (14) | 0.0243 (15) | 0.0026 (12) | 0.0176 (13) | −0.0019 (11) |
| C43 | 0.0276 (15) | 0.0243 (14) | 0.0243 (15) | 0.0026 (12) | 0.0176 (13) | −0.0019 (11) |
| C44 | 0.0276 (15) | 0.0243 (14) | 0.0243 (15) | 0.0026 (12) | 0.0176 (13) | −0.0019 (11) |
| Cu1 | 0.0157 (4) | 0.0148 (4) | 0.0206 (4) | −0.0015 (3) | 0.0109 (3) | −0.0025 (3) |
| N1 | 0.025 (3) | 0.009 (2) | 0.017 (3) | −0.002 (2) | 0.012 (2) | −0.004 (2) |
| O1 | 0.016 (2) | 0.016 (2) | 0.021 (2) | −0.0027 (18) | 0.0045 (18) | −0.0015 (18) |
| O2 | 0.027 (2) | 0.030 (2) | 0.019 (2) | −0.0022 (19) | 0.014 (2) | 0.0023 (19) |
| O3 | 0.014 (2) | 0.012 (2) | 0.024 (2) | −0.0024 (17) | 0.0090 (19) | 0.0023 (17) |
| O4 | 0.024 (2) | 0.012 (2) | 0.041 (3) | 0.0049 (18) | 0.016 (2) | 0.0027 (19) |
| O5 | 0.021 (2) | 0.022 (2) | 0.028 (2) | −0.0081 (18) | 0.015 (2) | −0.0018 (19) |
| P1 | 0.0175 (9) | 0.0135 (8) | 0.0252 (9) | −0.0002 (7) | 0.0108 (8) | 0.0006 (7) |
| P2 | 0.0143 (8) | 0.0137 (8) | 0.0186 (9) | −0.0004 (6) | 0.0093 (7) | −0.0005 (7) |
| P3 | 0.0144 (8) | 0.0150 (8) | 0.0211 (8) | −0.0007 (7) | 0.0106 (7) | −0.0002 (7) |
| S1 | 0.0198 (9) | 0.0175 (8) | 0.0189 (8) | −0.0015 (7) | 0.0110 (7) | 0.0002 (7) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C6 | 1.378 (7) | C24—H54 | 0.9300 |
| C1—C2 | 1.384 (6) | C25—C26 | 1.373 (6) |
| C1—S1 | 1.795 (5) | C25—H70 | 0.9300 |
| C2—C3 | 1.386 (7) | C26—H67 | 0.9300 |
| C2—H68 | 0.9300 | C27—C28 | 1.392 (6) |
| C3—C4 | 1.371 (7) | C27—C32 | 1.392 (7) |
| C3—H102 | 0.9300 | C27—P3 | 1.821 (5) |
| C4—C5 | 1.381 (7) | C28—C29 | 1.396 (7) |
| C4—H106 | 0.9300 | C28—H105 | 0.9300 |
| C5—C6 | 1.405 (7) | C29—C30 | 1.396 (7) |
| C5—H19 | 0.9300 | C29—H1 | 0.9300 |
| C6—H57 | 0.9300 | C30—C31 | 1.382 (7) |
| C7—O4 | 1.419 (5) | C30—H45 | 0.9300 |
| C7—H74A | 0.9600 | C31—C32 | 1.390 (7) |
| C7—H74B | 0.9600 | C31—H72 | 0.9300 |

| | | | |
|---|---|---|---|
| C7—H74C | 0.9600 | C32—H38 | 0.9300 |
| C8—O5 | 1.448 (5) | C33—C38 | 1.397 (6) |
| C8—H7A | 0.9600 | C33—C34 | 1.416 (6) |
| C8—H7B | 0.9600 | C33—P3 | 1.824 (5) |
| C8—H7C | 0.9600 | C34—C35 | 1.382 (7) |
| C9—C14 | 1.406 (6) | C34—H61 | 0.9300 |
| C9—C10 | 1.409 (6) | C35—C36 | 1.390 (7) |
| C9—P2 | 1.824 (5) | C35—H107 | 0.9300 |
| C10—C11 | 1.383 (6) | C36—C37 | 1.370 (7) |
| C10—H25 | 0.9300 | C36—H47 | 0.9300 |
| C11—C12 | 1.400 (6) | C37—C38 | 1.387 (7) |
| C11—H21 | 0.9300 | C37—H66 | 0.9300 |
| C12—C13 | 1.380 (6) | C38—H62 | 0.9300 |
| C12—H16 | 0.9300 | C39—C44 | 1.382 (7) |
| C13—C14 | 1.384 (6) | C39—C40 | 1.394 (7) |
| C13—H15 | 0.9300 | C39—P3 | 1.823 (5) |
| C14—H35 | 0.9300 | C40—C41 | 1.386 (7) |
| C15—C16 | 1.399 (6) | C40—H13 | 0.9300 |
| C15—C20 | 1.415 (7) | C41—C42 | 1.355 (7) |
| C15—P2 | 1.824 (5) | C41—H28 | 0.9300 |
| C16—C17 | 1.385 (6) | C42—C43 | 1.394 (6) |
| C16—H20 | 0.9300 | C42—H65 | 0.9300 |
| C17—C18 | 1.386 (7) | C43—C44 | 1.380 (7) |
| C17—H6 | 0.9300 | C43—H14 | 0.9300 |
| C18—C19 | 1.388 (7) | C44—H75 | 0.9300 |
| C18—H56 | 0.9300 | Cu1—O3 | 2.065 (3) |
| C19—C20 | 1.366 (7) | Cu1—O1 | 2.263 (3) |
| C19—H8 | 0.9300 | Cu1—P2 | 2.2345 (15) |
| C20—H31 | 0.9300 | Cu1—P3 | 2.2381 (14) |
| C21—C22 | 1.395 (6) | N1—S1 | 1.568 (4) |
| C21—C26 | 1.409 (6) | N1—P1 | 1.596 (4) |
| C21—P2 | 1.820 (5) | O1—S1 | 1.470 (3) |
| C22—C23 | 1.391 (6) | O2—S1 | 1.438 (3) |
| C22—H60 | 0.9300 | O3—P1 | 1.496 (3) |
| C23—C24 | 1.386 (7) | O4—P1 | 1.590 (3) |
| C23—H29 | 0.9300 | O5—P1 | 1.572 (3) |
| C24—C25 | 1.382 (7) | | |

| | | | |
|---|---|---|---|
| C6—C1—C2 | 121.0 (5) | C27—C28—C29 | 121.1 (5) |
| C6—C1—S1 | 118.9 (4) | C27—C28—H105 | 119.5 |
| C2—C1—S1 | 120.1 (4) | C29—C28—H105 | 119.5 |
| C1—C2—C3 | 118.8 (5) | C28—C29—C30 | 119.0 (5) |
| C1—C2—H68 | 120.6 | C28—C29—H1 | 120.5 |
| C3—C2—H68 | 120.6 | C30—C29—H1 | 120.5 |
| C4—C3—C2 | 121.2 (5) | C31—C30—C29 | 120.3 (5) |
| C4—C3—H102 | 119.4 | C31—C30—H45 | 119.8 |
| C2—C3—H102 | 119.4 | C29—C30—H45 | 119.8 |
| C3—C4—C5 | 119.9 (5) | C30—C31—C32 | 120.1 (5) |
| C3—C4—H106 | 120.1 | C30—C31—H72 | 120.0 |

| | | | |
|---|---|---|---|
| C5—C4—H106 | 120.1 | C32—C31—H72 | 120.0 |
| C4—C5—C6 | 119.8 (6) | C31—C32—C27 | 120.7 (5) |
| C4—C5—H19 | 120.1 | C31—C32—H38 | 119.7 |
| C6—C5—H19 | 120.1 | C27—C32—H38 | 119.7 |
| C1—C6—C5 | 119.2 (5) | C38—C33—C34 | 117.7 (5) |
| C1—C6—H57 | 120.4 | C38—C33—P3 | 123.5 (4) |
| C5—C6—H57 | 120.4 | C34—C33—P3 | 118.3 (4) |
| O4—C7—H74A | 109.5 | C35—C34—C33 | 120.4 (5) |
| O4—C7—H74B | 109.5 | C35—C34—H61 | 119.8 |
| H74A—C7—H74B | 109.5 | C33—C34—H61 | 119.8 |
| O4—C7—H74C | 109.5 | C34—C35—C36 | 120.8 (5) |
| H74A—C7—H74C | 109.5 | C34—C35—H107 | 119.6 |
| H74B—C7—H74C | 109.5 | C36—C35—H107 | 119.6 |
| O5—C8—H7A | 109.5 | C37—C36—C35 | 119.0 (5) |
| O5—C8—H7B | 109.5 | C37—C36—H47 | 120.5 |
| H7A—C8—H7B | 109.5 | C35—C36—H47 | 120.5 |
| O5—C8—H7C | 109.5 | C36—C37—C38 | 121.3 (5) |
| H7A—C8—H7C | 109.5 | C36—C37—H66 | 119.3 |
| H7B—C8—H7C | 109.5 | C38—C37—H66 | 119.3 |
| C14—C9—C10 | 117.3 (5) | C37—C38—C33 | 120.6 (5) |
| C14—C9—P2 | 122.7 (4) | C37—C38—H62 | 119.7 |
| C10—C9—P2 | 120.1 (4) | C33—C38—H62 | 119.7 |
| C11—C10—C9 | 121.3 (5) | C44—C39—C40 | 118.9 (5) |
| C11—C10—H25 | 119.3 | C44—C39—P3 | 115.5 (4) |
| C9—C10—H25 | 119.3 | C40—C39—P3 | 125.6 (4) |
| C10—C11—C12 | 120.0 (5) | C41—C40—C39 | 119.2 (5) |
| C10—C11—H21 | 120.0 | C41—C40—H13 | 120.4 |
| C12—C11—H21 | 120.0 | C39—C40—H13 | 120.4 |
| C13—C12—C11 | 119.5 (5) | C42—C41—C40 | 121.7 (5) |
| C13—C12—H16 | 120.3 | C42—C41—H28 | 119.1 |
| C11—C12—H16 | 120.3 | C40—C41—H28 | 119.1 |
| C12—C13—C14 | 120.6 (5) | C41—C42—C43 | 119.7 (5) |
| C12—C13—H15 | 119.7 | C41—C42—H65 | 120.1 |
| C14—C13—H15 | 119.7 | C43—C42—H65 | 120.1 |
| C13—C14—C9 | 121.3 (5) | C44—C43—C42 | 119.0 (5) |
| C13—C14—H35 | 119.4 | C44—C43—H14 | 120.5 |
| C9—C14—H35 | 119.4 | C42—C43—H14 | 120.5 |
| C16—C15—C20 | 117.6 (5) | C43—C44—C39 | 121.5 (5) |
| C16—C15—P2 | 123.3 (4) | C43—C44—H75 | 119.3 |
| C20—C15—P2 | 119.0 (4) | C39—C44—H75 | 119.3 |
| C17—C16—C15 | 121.2 (5) | O3—Cu1—P2 | 112.93 (9) |
| C17—C16—H20 | 119.4 | O3—Cu1—P3 | 104.75 (9) |
| C15—C16—H20 | 119.4 | P2—Cu1—P3 | 129.95 (6) |
| C16—C17—C18 | 119.6 (5) | O3—Cu1—O1 | 88.88 (13) |
| C16—C17—H6 | 120.2 | P2—Cu1—O1 | 98.93 (9) |
| C18—C17—H6 | 120.2 | P3—Cu1—O1 | 113.89 (9) |
| C17—C18—C19 | 120.3 (5) | S1—N1—P1 | 125.1 (3) |
| C17—C18—H56 | 119.9 | S1—O1—Cu1 | 131.3 (2) |
| C19—C18—H56 | 119.9 | P1—O3—Cu1 | 127.3 (2) |

| | | | |
|---|---|---|---|
| C20—C19—C18 | 120.2 (5) | C7—O4—P1 | 120.7 (3) |
| C20—C19—H8 | 119.9 | C8—O5—P1 | 120.7 (3) |
| C18—C19—H8 | 119.9 | O3—P1—O5 | 107.5 (2) |
| C19—C20—C15 | 121.1 (5) | O3—P1—O4 | 111.3 (2) |
| C19—C20—H31 | 119.5 | O5—P1—O4 | 100.9 (2) |
| C15—C20—H31 | 119.5 | O3—P1—N1 | 118.7 (2) |
| C22—C21—C26 | 117.9 (5) | O5—P1—N1 | 111.6 (2) |
| C22—C21—P2 | 123.9 (4) | O4—P1—N1 | 105.4 (2) |
| C26—C21—P2 | 118.2 (4) | C21—P2—C15 | 104.3 (2) |
| C23—C22—C21 | 120.7 (5) | C21—P2—C9 | 101.8 (2) |
| C23—C22—H60 | 119.6 | C15—P2—C9 | 104.4 (2) |
| C21—C22—H60 | 119.6 | C21—P2—Cu1 | 114.54 (16) |
| C24—C23—C22 | 119.9 (5) | C15—P2—Cu1 | 113.38 (17) |
| C24—C23—H29 | 120.1 | C9—P2—Cu1 | 116.87 (17) |
| C22—C23—H29 | 120.1 | C27—P3—C39 | 103.1 (2) |
| C25—C24—C23 | 120.2 (5) | C27—P3—C33 | 103.8 (2) |
| C25—C24—H54 | 119.9 | C39—P3—C33 | 106.1 (2) |
| C23—C24—H54 | 119.9 | C27—P3—Cu1 | 119.89 (17) |
| C26—C25—C24 | 120.1 (5) | C39—P3—Cu1 | 112.55 (18) |
| C26—C25—H70 | 120.0 | C33—P3—Cu1 | 110.26 (16) |
| C24—C25—H70 | 120.0 | O2—S1—O1 | 114.8 (2) |
| C25—C26—C21 | 121.2 (5) | O2—S1—N1 | 110.3 (2) |
| C25—C26—H67 | 119.4 | O1—S1—N1 | 112.7 (2) |
| C21—C26—H67 | 119.4 | O2—S1—C1 | 106.1 (2) |
| C28—C27—C32 | 118.8 (5) | O1—S1—C1 | 106.2 (2) |
| C28—C27—P3 | 122.7 (4) | N1—S1—C1 | 106.1 (2) |
| C32—C27—P3 | 118.3 (4) | | |

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| C6—C1—C2—C3 | −2.7 (8) | Cu1—O3—P1—N1 | −27.4 (3) |
| S1—C1—C2—C3 | 177.4 (4) | C8—O5—P1—O3 | 175.3 (3) |
| C1—C2—C3—C4 | 1.8 (8) | C8—O5—P1—O4 | 58.6 (4) |
| C2—C3—C4—C5 | 0.0 (8) | C8—O5—P1—N1 | −53.0 (4) |
| C3—C4—C5—C6 | −0.8 (9) | C7—O4—P1—O3 | 49.6 (4) |
| C2—C1—C6—C5 | 1.9 (8) | C7—O4—P1—O5 | 163.5 (4) |
| S1—C1—C6—C5 | −178.2 (4) | C7—O4—P1—N1 | −80.3 (4) |
| C4—C5—C6—C1 | −0.1 (8) | S1—N1—P1—O3 | 49.7 (4) |
| C14—C9—C10—C11 | 0.5 (7) | S1—N1—P1—O5 | −76.2 (3) |
| P2—C9—C10—C11 | −178.8 (4) | S1—N1—P1—O4 | 175.1 (3) |
| C9—C10—C11—C12 | −1.2 (8) | C22—C21—P2—C15 | 1.3 (5) |
| C10—C11—C12—C13 | 0.1 (8) | C26—C21—P2—C15 | 179.7 (4) |
| C11—C12—C13—C14 | 1.5 (8) | C22—C21—P2—C9 | −107.1 (4) |
| C12—C13—C14—C9 | −2.2 (8) | C26—C21—P2—C9 | 71.4 (4) |
| C10—C9—C14—C13 | 1.2 (8) | C22—C21—P2—Cu1 | 125.8 (4) |
| P2—C9—C14—C13 | −179.6 (4) | C26—C21—P2—Cu1 | −55.7 (4) |
| C20—C15—C16—C17 | −0.8 (7) | C16—C15—P2—C21 | −85.1 (4) |
| P2—C15—C16—C17 | 180.0 (4) | C20—C15—P2—C21 | 95.7 (4) |
| C15—C16—C17—C18 | 0.7 (7) | C16—C15—P2—C9 | 21.4 (5) |
| C16—C17—C18—C19 | −0.7 (7) | C20—C15—P2—C9 | −157.8 (4) |
| C17—C18—C19—C20 | 0.8 (8) | C16—C15—P2—Cu1 | 149.7 (4) |

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| C18—C19—C20—C15 | −0.9 (8) | C20—C15—P2—Cu1 | −29.5 (4) |
| C16—C15—C20—C19 | 0.9 (8) | C14—C9—P2—C21 | 20.4 (5) |
| P2—C15—C20—C19 | −179.9 (4) | C10—C9—P2—C21 | −160.3 (4) |
| C26—C21—C22—C23 | −1.8 (7) | C14—C9—P2—C15 | −87.9 (5) |
| P2—C21—C22—C23 | 176.6 (4) | C10—C9—P2—C15 | 91.3 (4) |
| C21—C22—C23—C24 | 0.1 (8) | C14—C9—P2—Cu1 | 146.0 (4) |
| C22—C23—C24—C25 | 1.5 (8) | C10—C9—P2—Cu1 | −34.8 (5) |
| C23—C24—C25—C26 | −1.4 (8) | C28—C27—P3—C39 | 20.0 (5) |
| C24—C25—C26—C21 | −0.3 (8) | C32—C27—P3—C39 | −155.7 (4) |
| C22—C21—C26—C25 | 1.9 (7) | C28—C27—P3—C33 | −90.5 (5) |
| P2—C21—C26—C25 | −176.6 (4) | C32—C27—P3—C33 | 93.8 (4) |
| C32—C27—C28—C29 | −1.4 (8) | C28—C27—P3—Cu1 | 146.0 (4) |
| P3—C27—C28—C29 | −177.0 (4) | C32—C27—P3—Cu1 | −29.7 (5) |
| C27—C28—C29—C30 | 1.7 (8) | C44—C39—P3—C27 | 80.6 (4) |
| C28—C29—C30—C31 | −1.8 (8) | C40—C39—P3—C27 | −100.9 (5) |
| C29—C30—C31—C32 | 1.6 (8) | C44—C39—P3—C33 | −170.6 (4) |
| C30—C31—C32—C27 | −1.2 (8) | C40—C39—P3—C33 | 7.9 (5) |
| C28—C27—C32—C31 | 1.1 (8) | C44—C39—P3—Cu1 | −50.0 (4) |
| P3—C27—C32—C31 | 176.9 (4) | C40—C39—P3—Cu1 | 128.5 (4) |
| C38—C33—C34—C35 | 1.3 (7) | C38—C33—P3—C27 | −17.6 (5) |
| P3—C33—C34—C35 | 173.5 (4) | C34—C33—P3—C27 | 170.6 (4) |
| C33—C34—C35—C36 | −2.5 (7) | C38—C33—P3—C39 | −125.8 (4) |
| C34—C35—C36—C37 | 2.2 (8) | C34—C33—P3—C39 | 62.4 (4) |
| C35—C36—C37—C38 | −0.8 (8) | C38—C33—P3—Cu1 | 112.0 (4) |
| C36—C37—C38—C33 | −0.3 (8) | C34—C33—P3—Cu1 | −59.7 (4) |
| C34—C33—C38—C37 | 0.1 (7) | Cu1—O1—S1—O2 | 115.2 (3) |
| P3—C33—C38—C37 | −171.7 (4) | Cu1—O1—S1—N1 | −12.2 (3) |
| C44—C39—C40—C41 | 0.4 (7) | Cu1—O1—S1—C1 | −127.9 (3) |
| P3—C39—C40—C41 | −178.1 (4) | P1—N1—S1—O2 | −157.4 (3) |
| C39—C40—C41—C42 | −1.1 (8) | P1—N1—S1—O1 | −27.6 (4) |
| C40—C41—C42—C43 | 1.0 (8) | P1—N1—S1—C1 | 88.2 (3) |
| C41—C42—C43—C44 | −0.2 (8) | C6—C1—S1—O2 | −18.7 (5) |
| C42—C43—C44—C39 | −0.5 (8) | C2—C1—S1—O2 | 161.2 (4) |
| C40—C39—C44—C43 | 0.4 (8) | C6—C1—S1—O1 | −141.2 (4) |
| P3—C39—C44—C43 | 179.0 (4) | C2—C1—S1—O1 | 38.7 (5) |
| Cu1—O3—P1—O5 | 100.4 (2) | C6—C1—S1—N1 | 98.7 (4) |
| Cu1—O3—P1—O4 | −150.0 (2) | C2—C1—S1—N1 | −81.5 (5) |