Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# *catena*-Poly[[(isoquinoline-$\kappa N$)(triphenylphospane-$\kappa P$)copper(I)]-$\mu$-thiocyanato-$\kappa^2 N$:$S$]

**Jian-Bao Li,[a] Li-Li Zhou,[b] Man-Hua Wu,[a] Qiong-Hua Jin[a]* and Cun-Lin Zhang[c]**

[a]Department of Chemistry, Capital Normal University, Beijing 100048, People's Republic of China, [b]Research Center for Import-Export Chemicals Safety of the General Administration of Quality Supervision, Inspection and Quarantine of the People's Republic of China (AQSIQ), Beijing 100123, People's Republic of China, and [c]Key Laboratory of Terahertz Optoelectronics of the Ministry of Education, Department of Physics, Capital Normal University, Beijing 100048, People's Republic of China
Correspondence e-mail: jinqh204@163.com

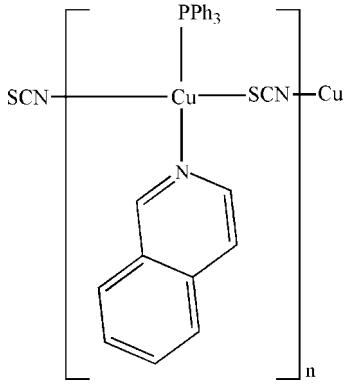
Received 24 January 2012; accepted 4 February 2012

Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.007 Å; $R$ factor = 0.041; $wR$ factor = 0.108; data-to-parameter ratio = 14.5.

In the title coordination compound, $[Cu(NCS)(C_9H_7N)(C_{18}H_{15}P)]_n$, the $Cu^I$ atom is tetrahedrally coordinated by one N atom from an isoquinoline ligand, one P atom from a triphenylphospane ligand, and one N and one S atom from two thiocyanate anions. The thiocyanide anions bridge the $Cu^I$ atoms into a chain along [100]. $\pi$–$\pi$ interactions between the pyridine and benzene rings of the isoquinoline ligands connect the chains [centroid-to-centroid distance = 3.722 (3) Å].

## Related literature

For background to the applications of copper(I) complexes, see: Dai *et al.* (2010); Jin *et al.* (2010); Lu *et al.* (1997); Song *et al.* (2010). For related structures, see: Jin *et al.* (1999); Li, Wu *et al.* (2011); Li, Xiao *et al.* (2011).




## Experimental

### Crystal data

$[Cu(NCS)(C_9H_7N)(C_{18}H_{15}P)]$
$M_r$ = 513.05
Monoclinic, $P2_1/c$
$a$ = 12.9573 (13) Å
$b$ = 10.5506 (11) Å
$c$ = 18.9241 (18) Å
$\beta$ = 108.961 (1)°
$V$ = 2446.7 (4) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 1.06 mm$^{-1}$
$T$ = 298 K
0.32 × 0.21 × 0.19 mm

### Data collection

Bruker SMART 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min}$ = 0.727, $T_{max}$ = 0.824
12067 measured reflections
4313 independent reflections
2656 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.042

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.108
$S$ = 1.05
4313 reflections
298 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.41 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.25 e Å$^{-3}$

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

| | | | |
|---|---|---|---|
| Cu1—N1 | 2.087 (3) | Cu1—P1 | 2.2282 (11) |
| Cu1—N2$^{i}$ | 1.991 (4) | Cu1—S1 | 2.3781 (12) |

Symmetry code: (i) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT-Plus* (Bruker, 2007); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

This work was supported by the National Natural Science Foundation of China (grant No. 21171119), the CAIQ Basic Research Program (No. 2010JK022), the National Keystone Basic Research Program (973 Program) under grant Nos. 2007CB310408 and 2006CB302901, and the Funding Project for Academic Human Resources Development in Institutions of Higher Learning under the Jurisdiction of Beijing Municipality. It was also supported by the State Key Laboratory of Functional Materials for Informatics, Shanghai Institute of Microsystem and Information Technology, Chinese Academy of Sciences.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2511).

## References

Brandenburg, K. (1999). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Bruker (2001). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2007). *SMART* and *SAINT-Plus*. Bruker AXS Inc., Madison, Wisconsin, USA.
Dai, Y.-C., Jin, Q.-H., Cui, L.-N., Xu, L.-J. & Zhang, C.-L. (2010). *Acta Cryst.* E**66**, m1124–m1125.
Jin, Q.-H., Hu, K.-Y., Song, L.-L., Wang, R., Zhang, C.-L., Zuo, X. & Lu, X.-M. (2010). *Polyhedron*, **29**, 441–445.

Jin, Q.-H., Wang, Y.-X. & Xin, X.-L. (1999). *Acta Cryst.* C**55**, 341–343.
Li, J.-B., Wu, M.-H., Wen, J., Jiang, Y.-H., Jin, Q.-H. & Gong, H.-L. (2011). *Z. Kristallogr. New Cryst. Struct.* **226**, 109–111.
Li, J.-B., Xiao, Y.-L., Wu, M.-H., Jiang, Y.-H., Jin, Q.-H. & Zhang, C.-L. (2011). *Z. Kristallogr. New Cryst. Struct.* **226**, 97–98.
Lu, J., Crisci, G., Niu, T. Y. & Jacobson, A. J. (1997). *Inorg. Chem.* **36**, 5140–5141.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Song, L.-L., Cui, L.-N., Jin, Q.-H. & Zhang, C.-L. (2010). *Acta Cryst.* E**66**, m1237–m1238.

# supplementary materials

*Acta Cryst.* (2012). E**68**, m283–m284 [doi:10.1107/S1600536812004837]

## *catena*-Poly[[(isoquinoline-$\kappa N$)(triphenylphospane-$\kappa P$)copper(I)]-$\mu$-thiocyanato-$\kappa^2 N$:$S$]

**Jian-Bao Li, Li-Li Zhou, Man-Hua Wu, Qiong-Hua Jin and Cun-Lin Zhang**

### Comment

Many research efforts have been devoted to copper(I) complexes due to their interesting coordination chemistry and potential applications in photography, electrochemical processes, antimicrobial and antitumor activities (Dai *et al.*, 2010; Jin *et al.*, 2010; Lu *et al.*, 1997; Song *et al.*, 2010). Recently, we obtained some copper(I) complexes containing phosphine and isoquinoline (iq) ligands and coordinated anions (Li, Wu *et al.*, 2011; Li, Xiao *et al.*, 2011). Continuing these efforts, we report here the title compound, (I).

The compound was synthesized by the reaction of copper(I) salt with triphenylphospane ($PPh_3$) and iq in a mixed solution of dichloromethane and methanol. The molar ratio of Cu(I):$PPh_3$ (1:1) and the excess of iq are very important for the generation of this compound. The excess of iq facilitates its coordination to Cu(I) atom because the coordination ability of iq is weaker than that of $PPh_3$ and $SCN^-$ anion.

The $Cu^I$ atom is bonded to one N atom from an iq ligand, one P atom from a $PPh_3$ ligand, one S and one N atom from two $SCN^-$ anions (Fig. 1). The $SCN^-$ anion behaves as a bridging ligand. The structure of the title compound is similar to that of $[CuBr(PPh_3)_2(iq)]$ (II) (Li, Wu *et al.*, 2011), $[CuCl(PPh_3)(iq)]_2$, (III) (Li, Xiao *et al.*, 2011), and $[CuI(PPh_3)(quinoline)]_2$ (IV) (Jin *et al.*, 1999). The bond length Cu1—P1 [2.2282 (11) Å] (Table 1) is shorter than the corresponding distances in (II) [2.2789 (14) Å] and (IV) [2.2466 (11) Å]. The Cu1—N1 bond length [2.087 (3) Å] is also shorter than the corresponding values in (II) [2.097 (3) Å] and (IV) [2.135 (4) Å]. The Cu1—P1 [2.1945 (8) Å] and Cu1—N1 [2.066 (2) Å] in (III) are shorter than the corresponding values in (I), (II) and (IV). The bond angle N1—Cu1—P1 [110.38 (9)°] in (I) is smaller than those in (III) [120.23 (7)°] and (IV) [117.20 (8)°] but larger than that in (II) [101.51 (12)°], while the bond angle P1—Cu1—S1 [113.85 (4)°] is smaller than those in (II) [115.88 (4)°], (III) [116.34 (3)°] and (IV) [114.70 (3)°]. The thiocyanide anions bridge the $Cu^I$ atoms into a chain along [100] (Fig. 2). $\pi$–$\pi$ interactions between the pyridine and benzene rings of the iq ligands connect the chains [centroid–centroid distance = 3.722 (3) Å].

### Experimental

The title complex was prepared by adding $PPh_3$ (0.3 mmol, 0.079 g) into a mixture of $CH_2Cl_2$ (5 ml) and MeOH (5 ml) containing CuSCN (0.3 mmol, 0.036 g) and excess iq. The stirring continued for 3 h. After slow evaporation of the filtrate at ambient temperature for several days, yellow strip-shaped crystals were obtained. Crystals suitable for single-crystal X-ray diffraction were selected directly from the sample as prepared.

### Refinement

H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 Å and with $U_{iso}(H) = 1.2U_{eq}(C)$.

### Computing details

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT-Plus* (Bruker, 2007); data reduction: *SAINT-Plus* (Bruker, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

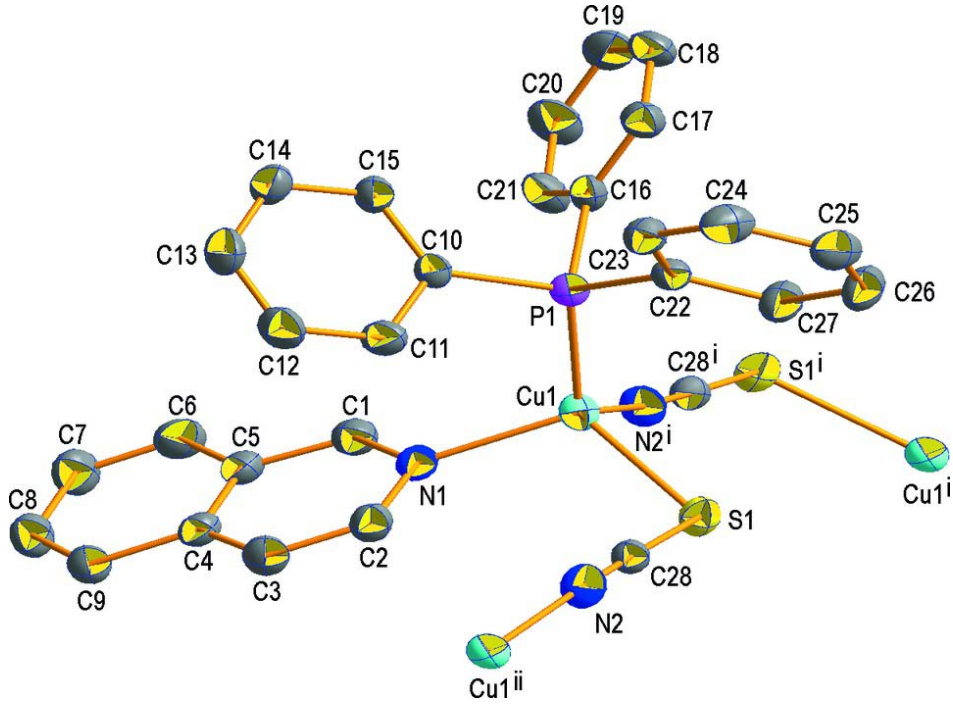



**Figure 1**

The asymmetric unit of the title complex. Displacement ellipsoids are shown at the 30% probability level. H atoms are omitted for clarity. [Symmetry codes: (i) 1 - *x*, -1/2 + *y*, 1/2 - *z*; (ii) 1 - *x*, 1/2 + *y*, 1/2 - *z*.]

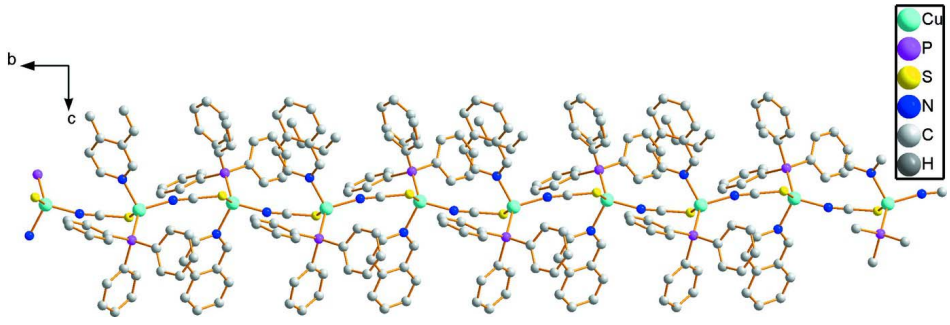



**Figure 2**

A view of the chain structure in the title compound.

**_catena_-Poly[[(isoquinoline-$\kappa N$)(triphenylphospane- $\kappa P$)copper(I)]-$\mu$-thiocyanato-$\kappa^2 N$:$S$]**

*Crystal data*

$[Cu(NCS)(C_9H_7N)(C_{18}H_{15}P)]$
$M_r$ = 513.05
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a$ = 12.9573 (13) Å
$b$ = 10.5506 (11) Å

$c$ = 18.9241 (18) Å
$\beta$ = 108.961 (1)°
$V$ = 2446.7 (4) Å$^3$
$Z$ = 4
$F$(000) = 1056
$D_x$ = 1.393 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å

Cell parameters from 2854 reflections
$\theta$ = 2.6–22.5°
$\mu$ = 1.06 mm$^{-1}$
$T$ = 298 K
Prism, yellow
0.32 × 0.21 × 0.19 mm

*Data collection*

Bruker SMART 1000 CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min}$ = 0.727, $T_{max}$ = 0.824

12067 measured reflections
4313 independent reflections
2656 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.042
$\theta_{max}$ = 25.0°, $\theta_{min}$ = 2.6°
$h$ = −15→15
$k$ = −12→12
$l$ = −22→18

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.108
$S$ = 1.05
4313 reflections
298 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0387P)^2 + 1.2684P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.41 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.25 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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cu1 | 0.60682 (4) | 0.39666 (4) | 0.25965 (3) | 0.04929 (17) |
| P1 | 0.75772 (8) | 0.43807 (9) | 0.35473 (6) | 0.0449 (3) |
| S1 | 0.44293 (9) | 0.45262 (10) | 0.28281 (7) | 0.0572 (3) |
| N1 | 0.6132 (3) | 0.4852 (3) | 0.16249 (18) | 0.0523 (9) |
| N2 | 0.4224 (3) | 0.7158 (3) | 0.2701 (2) | 0.0638 (10) |
| C1 | 0.6628 (3) | 0.4305 (4) | 0.1208 (2) | 0.0575 (11) |
| H1 | 0.6942 | 0.3515 | 0.1357 | 0.069* |
| C2 | 0.5675 (3) | 0.6006 (4) | 0.1397 (2) | 0.0581 (11) |
| H2 | 0.5312 | 0.6408 | 0.1685 | 0.070* |
| C3 | 0.5719 (4) | 0.6601 (4) | 0.0774 (3) | 0.0629 (12) |

| | | | | |
|---|---|---|---|---|
| H3 | 0.5406 | 0.7398 | 0.0650 | 0.076* |
| C4 | 0.6232 (3) | 0.6021 (4) | 0.0322 (2) | 0.0499 (10) |
| C5 | 0.6721 (3) | 0.4842 (4) | 0.0535 (2) | 0.0486 (10) |
| C6 | 0.7248 (4) | 0.4218 (5) | 0.0107 (3) | 0.0700 (13) |
| H6 | 0.7581 | 0.3440 | 0.0262 | 0.084* |
| C7 | 0.7275 (4) | 0.4745 (5) | −0.0540 (3) | 0.0770 (14) |
| H7 | 0.7627 | 0.4329 | −0.0830 | 0.092* |
| C8 | 0.6774 (4) | 0.5913 (5) | −0.0770 (3) | 0.0744 (14) |
| H8 | 0.6794 | 0.6257 | −0.1218 | 0.089* |
| C9 | 0.6265 (4) | 0.6557 (5) | −0.0369 (3) | 0.0653 (12) |
| H9 | 0.5939 | 0.7335 | −0.0535 | 0.078* |
| C10 | 0.8397 (3) | 0.5678 (3) | 0.3374 (2) | 0.0437 (9) |
| C11 | 0.7862 (3) | 0.6785 (4) | 0.3058 (2) | 0.0566 (11) |
| H11 | 0.7108 | 0.6840 | 0.2942 | 0.068* |
| C12 | 0.8432 (4) | 0.7799 (4) | 0.2916 (3) | 0.0689 (13) |
| H12 | 0.8066 | 0.8541 | 0.2716 | 0.083* |
| C13 | 0.9535 (4) | 0.7718 (4) | 0.3067 (3) | 0.0694 (13) |
| H13 | 0.9915 | 0.8398 | 0.2959 | 0.083* |
| C14 | 1.0081 (4) | 0.6638 (4) | 0.3376 (2) | 0.0641 (12) |
| H14 | 1.0833 | 0.6588 | 0.3486 | 0.077* |
| C15 | 0.9514 (3) | 0.5630 (4) | 0.3524 (2) | 0.0546 (11) |
| H15 | 0.9891 | 0.4897 | 0.3731 | 0.065* |
| C16 | 0.8556 (3) | 0.3077 (3) | 0.3805 (2) | 0.0475 (10) |
| C17 | 0.9200 (3) | 0.2820 (4) | 0.4534 (2) | 0.0564 (11) |
| H17 | 0.9139 | 0.3318 | 0.4924 | 0.068* |
| C18 | 0.9935 (4) | 0.1819 (4) | 0.4680 (3) | 0.0672 (13) |
| H18 | 1.0364 | 0.1647 | 0.5170 | 0.081* |
| C19 | 1.0033 (4) | 0.1087 (4) | 0.4113 (3) | 0.0755 (15) |
| H19 | 1.0534 | 0.0425 | 0.4216 | 0.091* |
| C20 | 0.9398 (4) | 0.1320 (4) | 0.3393 (3) | 0.0807 (15) |
| H20 | 0.9462 | 0.0814 | 0.3007 | 0.097* |
| C21 | 0.8663 (4) | 0.2305 (4) | 0.3241 (3) | 0.0645 (12) |
| H21 | 0.8230 | 0.2456 | 0.2750 | 0.077* |
| C22 | 0.7412 (3) | 0.4807 (4) | 0.4436 (2) | 0.0457 (10) |
| C23 | 0.8026 (3) | 0.5724 (4) | 0.4911 (2) | 0.0563 (11) |
| H23 | 0.8544 | 0.6179 | 0.4772 | 0.068* |
| C24 | 0.7881 (4) | 0.5973 (4) | 0.5587 (2) | 0.0674 (13) |
| H24 | 0.8301 | 0.6592 | 0.5900 | 0.081* |
| C25 | 0.7125 (4) | 0.5319 (5) | 0.5801 (3) | 0.0747 (14) |
| H25 | 0.7030 | 0.5491 | 0.6258 | 0.090* |
| C26 | 0.6510 (4) | 0.4414 (5) | 0.5342 (3) | 0.0824 (15) |
| H26 | 0.6001 | 0.3957 | 0.5489 | 0.099* |
| C27 | 0.6640 (4) | 0.4169 (4) | 0.4657 (3) | 0.0682 (13) |
| H27 | 0.6200 | 0.3565 | 0.4342 | 0.082* |
| C28 | 0.4320 (3) | 0.6079 (4) | 0.2756 (2) | 0.0466 (10) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cu1 | 0.0578 (3) | 0.0447 (3) | 0.0480 (3) | −0.0041 (2) | 0.0207 (2) | −0.0004 (2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| P1 | 0.0494 (6) | 0.0434 (6) | 0.0444 (6) | −0.0001 (5) | 0.0187 (5) | 0.0021 (5) |
| S1 | 0.0612 (7) | 0.0445 (6) | 0.0755 (8) | 0.0004 (5) | 0.0353 (6) | 0.0060 (5) |
| N1 | 0.051 (2) | 0.061 (2) | 0.048 (2) | −0.0058 (17) | 0.0210 (18) | −0.0031 (17) |
| N2 | 0.076 (3) | 0.050 (2) | 0.073 (3) | −0.0087 (19) | 0.035 (2) | −0.0070 (19) |
| C1 | 0.057 (3) | 0.058 (3) | 0.057 (3) | −0.003 (2) | 0.019 (2) | −0.002 (2) |
| C2 | 0.061 (3) | 0.060 (3) | 0.062 (3) | 0.003 (2) | 0.033 (2) | 0.002 (2) |
| C3 | 0.071 (3) | 0.055 (3) | 0.072 (3) | 0.007 (2) | 0.035 (3) | 0.006 (2) |
| C4 | 0.042 (2) | 0.057 (3) | 0.050 (3) | −0.008 (2) | 0.016 (2) | −0.007 (2) |
| C5 | 0.043 (2) | 0.054 (3) | 0.051 (3) | −0.0049 (19) | 0.018 (2) | −0.007 (2) |
| C6 | 0.069 (3) | 0.077 (3) | 0.070 (3) | 0.009 (2) | 0.031 (3) | −0.004 (3) |
| C7 | 0.089 (4) | 0.094 (4) | 0.058 (3) | −0.005 (3) | 0.037 (3) | −0.004 (3) |
| C8 | 0.081 (3) | 0.101 (4) | 0.047 (3) | −0.014 (3) | 0.027 (3) | 0.003 (3) |
| C9 | 0.066 (3) | 0.075 (3) | 0.056 (3) | −0.009 (2) | 0.021 (3) | 0.009 (2) |
| C10 | 0.053 (2) | 0.043 (2) | 0.038 (2) | −0.0006 (18) | 0.020 (2) | −0.0005 (17) |
| C11 | 0.054 (3) | 0.053 (3) | 0.061 (3) | 0.000 (2) | 0.016 (2) | 0.003 (2) |
| C12 | 0.084 (4) | 0.047 (3) | 0.081 (4) | 0.006 (2) | 0.034 (3) | 0.014 (2) |
| C13 | 0.087 (4) | 0.053 (3) | 0.080 (4) | −0.014 (3) | 0.043 (3) | 0.005 (2) |
| C14 | 0.061 (3) | 0.066 (3) | 0.075 (3) | −0.007 (2) | 0.035 (3) | 0.005 (3) |
| C15 | 0.059 (3) | 0.053 (3) | 0.060 (3) | 0.004 (2) | 0.031 (2) | 0.010 (2) |
| C16 | 0.056 (3) | 0.041 (2) | 0.050 (3) | −0.0028 (19) | 0.024 (2) | 0.0048 (19) |
| C17 | 0.061 (3) | 0.051 (3) | 0.057 (3) | −0.003 (2) | 0.019 (2) | 0.005 (2) |
| C18 | 0.066 (3) | 0.058 (3) | 0.072 (3) | 0.004 (2) | 0.013 (3) | 0.023 (3) |
| C19 | 0.076 (3) | 0.053 (3) | 0.105 (5) | 0.019 (2) | 0.039 (3) | 0.023 (3) |
| C20 | 0.108 (4) | 0.063 (3) | 0.082 (4) | 0.027 (3) | 0.046 (3) | 0.013 (3) |
| C21 | 0.089 (3) | 0.055 (3) | 0.055 (3) | 0.017 (2) | 0.030 (3) | 0.012 (2) |
| C22 | 0.046 (2) | 0.050 (2) | 0.043 (2) | 0.0034 (19) | 0.017 (2) | 0.0042 (19) |
| C23 | 0.058 (3) | 0.061 (3) | 0.055 (3) | −0.001 (2) | 0.025 (2) | −0.002 (2) |
| C24 | 0.068 (3) | 0.081 (3) | 0.054 (3) | 0.006 (3) | 0.021 (3) | −0.014 (2) |
| C25 | 0.069 (3) | 0.111 (4) | 0.054 (3) | 0.016 (3) | 0.033 (3) | 0.000 (3) |
| C26 | 0.070 (3) | 0.127 (5) | 0.062 (3) | −0.021 (3) | 0.037 (3) | 0.002 (3) |
| C27 | 0.064 (3) | 0.091 (4) | 0.054 (3) | −0.020 (3) | 0.025 (2) | −0.005 (2) |
| C28 | 0.049 (2) | 0.052 (3) | 0.042 (2) | −0.002 (2) | 0.0204 (19) | 0.002 (2) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cu1—N1 | 2.087 (3) | C11—H11 | 0.9300 |
| Cu1—N2$^{i}$ | 1.991 (4) | C12—C13 | 1.366 (6) |
| Cu1—P1 | 2.2282 (11) | C12—H12 | 0.9300 |
| Cu1—S1 | 2.3781 (12) | C13—C14 | 1.369 (6) |
| P1—C22 | 1.820 (4) | C13—H13 | 0.9300 |
| P1—C16 | 1.826 (4) | C14—C15 | 1.372 (5) |
| P1—C10 | 1.826 (4) | C14—H14 | 0.9300 |
| S1—C28 | 1.647 (4) | C15—H15 | 0.9300 |
| N1—C1 | 1.303 (5) | C16—C21 | 1.385 (5) |
| N1—C2 | 1.362 (5) | C16—C17 | 1.387 (5) |
| N2—C28 | 1.146 (4) | C17—C18 | 1.389 (6) |
| C1—C5 | 1.435 (6) | C17—H17 | 0.9300 |
| C1—H1 | 0.9300 | C18—C19 | 1.361 (6) |
| C2—C3 | 1.352 (6) | C18—H18 | 0.9300 |
| C2—H2 | 0.9300 | C19—C20 | 1.366 (6) |

| | | | |
|---|---|---|---|
| C3—C4 | 1.385 (5) | C19—H19 | 0.9300 |
| C3—H3 | 0.9300 | C20—C21 | 1.376 (6) |
| C4—C5 | 1.395 (5) | C20—H20 | 0.9300 |
| C4—C9 | 1.438 (6) | C21—H21 | 0.9300 |
| C5—C6 | 1.384 (6) | C22—C27 | 1.378 (5) |
| C6—C7 | 1.355 (6) | C22—C23 | 1.383 (5) |
| C6—H6 | 0.9300 | C23—C24 | 1.378 (6) |
| C7—C8 | 1.394 (6) | C23—H23 | 0.9300 |
| C7—H7 | 0.9300 | C24—C25 | 1.361 (6) |
| C8—C9 | 1.340 (6) | C24—H24 | 0.9300 |
| C8—H8 | 0.9300 | C25—C26 | 1.361 (6) |
| C9—H9 | 0.9300 | C25—H25 | 0.9300 |
| C10—C15 | 1.382 (5) | C26—C27 | 1.385 (6) |
| C10—C11 | 1.390 (5) | C26—H26 | 0.9300 |
| C11—C12 | 1.376 (6) | C27—H27 | 0.9300 |

| | | | |
|---|---|---|---|
| $N2^{i}$—Cu1—N1 | 103.75 (14) | C13—C12—C11 | 120.2 (4) |
| $N2^{i}$—Cu1—P1 | 116.93 (11) | C13—C12—H12 | 119.9 |
| N1—Cu1—P1 | 110.38 (9) | C11—C12—H12 | 119.9 |
| $N2^{i}$—Cu1—S1 | 101.00 (11) | C12—C13—C14 | 120.1 (4) |
| N1—Cu1—S1 | 110.14 (10) | C12—C13—H13 | 120.0 |
| P1—Cu1—S1 | 113.85 (4) | C14—C13—H13 | 120.0 |
| C22—P1—C16 | 102.65 (18) | C13—C14—C15 | 119.8 (4) |
| C22—P1—C10 | 103.35 (17) | C13—C14—H14 | 120.1 |
| C16—P1—C10 | 102.60 (17) | C15—C14—H14 | 120.1 |
| C22—P1—Cu1 | 117.32 (13) | C14—C15—C10 | 121.6 (4) |
| C16—P1—Cu1 | 114.77 (13) | C14—C15—H15 | 119.2 |
| C10—P1—Cu1 | 114.27 (13) | C10—C15—H15 | 119.2 |
| C28—S1—Cu1 | 106.87 (14) | C21—C16—C17 | 118.2 (4) |
| C1—N1—C2 | 116.9 (4) | C21—C16—P1 | 118.2 (3) |
| C1—N1—Cu1 | 120.3 (3) | C17—C16—P1 | 123.7 (3) |
| C2—N1—Cu1 | 122.8 (3) | C16—C17—C18 | 120.0 (4) |
| N1—C1—C5 | 124.3 (4) | C16—C17—H17 | 120.0 |
| N1—C1—H1 | 117.8 | C18—C17—H17 | 120.0 |
| C5—C1—H1 | 117.8 | C19—C18—C17 | 120.5 (4) |
| C3—C2—N1 | 123.6 (4) | C19—C18—H18 | 119.7 |
| C3—C2—H2 | 118.2 | C17—C18—H18 | 119.7 |
| N1—C2—H2 | 118.2 | C18—C19—C20 | 120.3 (4) |
| C2—C3—C4 | 119.9 (4) | C18—C19—H19 | 119.8 |
| C2—C3—H3 | 120.0 | C20—C19—H19 | 119.8 |
| C4—C3—H3 | 120.0 | C19—C20—C21 | 119.7 (5) |
| C3—C4—C5 | 118.6 (4) | C19—C20—H20 | 120.1 |
| C3—C4—C9 | 123.4 (4) | C21—C20—H20 | 120.1 |
| C5—C4—C9 | 117.9 (4) | C20—C21—C16 | 121.3 (4) |
| C6—C5—C4 | 121.3 (4) | C20—C21—H21 | 119.3 |
| C6—C5—C1 | 122.2 (4) | C16—C21—H21 | 119.3 |
| C4—C5—C1 | 116.5 (4) | C27—C22—C23 | 117.8 (4) |
| C7—C6—C5 | 119.7 (5) | C27—C22—P1 | 118.3 (3) |
| C7—C6—H6 | 120.1 | C23—C22—P1 | 123.9 (3) |

| | | | |
|---|---|---|---|
| C5—C6—H6 | 120.1 | C24—C23—C22 | 120.9 (4) |
| C6—C7—C8 | 119.9 (5) | C24—C23—H23 | 119.6 |
| C6—C7—H7 | 120.1 | C22—C23—H23 | 119.6 |
| C8—C7—H7 | 120.1 | C25—C24—C23 | 120.5 (5) |
| C9—C8—C7 | 122.4 (5) | C25—C24—H24 | 119.8 |
| C9—C8—H8 | 118.8 | C23—C24—H24 | 119.8 |
| C7—C8—H8 | 118.8 | C26—C25—C24 | 119.7 (5) |
| C8—C9—C4 | 118.7 (4) | C26—C25—H25 | 120.2 |
| C8—C9—H9 | 120.6 | C24—C25—H25 | 120.2 |
| C4—C9—H9 | 120.6 | C25—C26—C27 | 120.3 (5) |
| C15—C10—C11 | 117.5 (4) | C25—C26—H26 | 119.9 |
| C15—C10—P1 | 124.6 (3) | C27—C26—H26 | 119.9 |
| C11—C10—P1 | 117.9 (3) | C22—C27—C26 | 120.9 (4) |
| C12—C11—C10 | 120.8 (4) | C22—C27—H27 | 119.6 |
| C12—C11—H11 | 119.6 | C26—C27—H27 | 119.6 |
| C10—C11—H11 | 119.6 | N2—C28—S1 | 178.8 (4) |

| | | | |
|---|---|---|---|
| N2$^{i}$—Cu1—P1—C22 | −106.25 (18) | Cu1—P1—C10—C15 | −132.9 (3) |
| N1—Cu1—P1—C22 | 135.50 (18) | C22—P1—C10—C11 | −82.6 (3) |
| S1—Cu1—P1—C22 | 11.04 (15) | C16—P1—C10—C11 | 170.9 (3) |
| N2$^{i}$—Cu1—P1—C16 | 14.40 (19) | Cu1—P1—C10—C11 | 46.0 (3) |
| N1—Cu1—P1—C16 | −103.84 (18) | C15—C10—C11—C12 | −1.2 (6) |
| S1—Cu1—P1—C16 | 131.69 (14) | P1—C10—C11—C12 | 179.8 (3) |
| N2$^{i}$—Cu1—P1—C10 | 132.54 (18) | C10—C11—C12—C13 | 1.7 (7) |
| N1—Cu1—P1—C10 | 14.30 (17) | C11—C12—C13—C14 | −1.5 (7) |
| S1—Cu1—P1—C10 | −110.16 (14) | C12—C13—C14—C15 | 1.0 (7) |
| N2$^{i}$—Cu1—S1—C28 | −158.11 (19) | C13—C14—C15—C10 | −0.6 (7) |
| N1—Cu1—S1—C28 | −48.89 (18) | C11—C10—C15—C14 | 0.7 (6) |
| P1—Cu1—S1—C28 | 75.70 (15) | P1—C10—C15—C14 | 179.6 (3) |
| N2$^{i}$—Cu1—N1—C1 | −41.4 (3) | C22—P1—C16—C21 | 163.7 (3) |
| P1—Cu1—N1—C1 | 84.6 (3) | C10—P1—C16—C21 | −89.3 (3) |
| S1—Cu1—N1—C1 | −148.8 (3) | Cu1—P1—C16—C21 | 35.3 (4) |
| N2$^{i}$—Cu1—N1—C2 | 138.9 (3) | C22—P1—C16—C17 | −16.5 (4) |
| P1—Cu1—N1—C2 | −95.0 (3) | C10—P1—C16—C17 | 90.5 (4) |
| S1—Cu1—N1—C2 | 31.5 (3) | Cu1—P1—C16—C17 | −145.0 (3) |
| C2—N1—C1—C5 | 0.2 (6) | C21—C16—C17—C18 | 0.7 (6) |
| Cu1—N1—C1—C5 | −179.5 (3) | P1—C16—C17—C18 | −179.1 (3) |
| C1—N1—C2—C3 | −0.5 (6) | C16—C17—C18—C19 | 0.2 (6) |
| Cu1—N1—C2—C3 | 179.1 (3) | C17—C18—C19—C20 | −0.8 (7) |
| N1—C2—C3—C4 | 1.4 (7) | C18—C19—C20—C21 | 0.5 (8) |
| C2—C3—C4—C5 | −1.9 (6) | C19—C20—C21—C16 | 0.4 (7) |
| C2—C3—C4—C9 | 176.6 (4) | C17—C16—C21—C20 | −0.9 (6) |
| C3—C4—C5—C6 | −179.9 (4) | P1—C16—C21—C20 | 178.8 (4) |
| C9—C4—C5—C6 | 1.6 (6) | C16—P1—C22—C27 | −87.1 (3) |
| C3—C4—C5—C1 | 1.5 (5) | C10—P1—C22—C27 | 166.4 (3) |
| C9—C4—C5—C1 | −177.0 (3) | Cu1—P1—C22—C27 | 39.7 (4) |
| N1—C1—C5—C6 | −179.3 (4) | C16—P1—C22—C23 | 92.0 (3) |
| N1—C1—C5—C4 | −0.7 (6) | C10—P1—C22—C23 | −14.5 (4) |
| C4—C5—C6—C7 | −1.2 (7) | Cu1—P1—C22—C23 | −141.2 (3) |

| | | | |
|---|---|---|---|
| C1—C5—C6—C7 | 177.4 (4) | C27—C22—C23—C24 | 1.1 (6) |
| C5—C6—C7—C8 | 0.0 (7) | P1—C22—C23—C24 | −178.0 (3) |
| C6—C7—C8—C9 | 0.6 (8) | C22—C23—C24—C25 | −0.1 (7) |
| C7—C8—C9—C4 | −0.2 (7) | C23—C24—C25—C26 | 0.0 (7) |
| C3—C4—C9—C8 | −179.4 (4) | C24—C25—C26—C27 | −0.9 (8) |
| C5—C4—C9—C8 | −1.0 (6) | C23—C22—C27—C26 | −2.0 (6) |
| C22—P1—C10—C15 | 98.4 (4) | P1—C22—C27—C26 | 177.2 (4) |
| C16—P1—C10—C15 | −8.1 (4) | C25—C26—C27—C22 | 1.9 (8) |

Symmetry code: (i) $-x+1, y-1/2, -z+1/2$.