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Iodidotris(triphenylphosphine)copper(I) acetonitrile solvate

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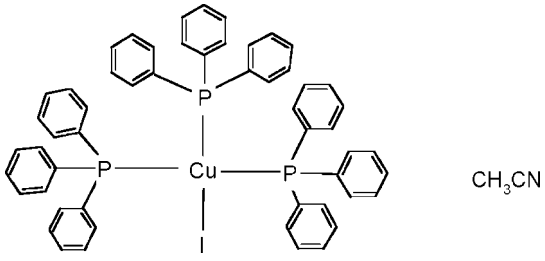
Key indicators: single-crystal X-ray study; T = 115 K; mean σ(C–C) = 0.004 Å; R factor = 0.033; wR factor = 0.068; data-to-parameter ratio = 28.5.

The title compound, $[CuI(C_{18}H_{15}P)_3]\cdot C_2H_3N$, was obtained from the reaction of triphenylphosphine and copper(I) iodide in acetonitrile. The monomeric form of the complex has slightly distorted coordination of Cu by the I atom and three P atoms. The crystal structure is stabilized by C—H$\cdots\pi$ interactions between phenyl H atoms and phenyl rings. In addition, the complex molecules exhibit C—H$\cdots$N hydrogen bonds between phenyl H atoms and acetonitrile N atoms. The crystal used was an inversion twin, with nearly equal component populations of 0.522 (8) and 0.478 (8).

Related literature

For details of the crystal structures of organophosphine-copper(I) halide derivatives, see: Caulton *et al.* (1990); Bowmaker *et al.* (2000); Eller *et al.* (1977); Hamel *et al.* (2002); Hanna *et al.* (2005); Venkatraman *et al.* (2006); Barron *et al.* (1987); Kräuter & Newmüller (1996).



Experimental

Crystal data

$[CuI(C_{18}H_{15}P)_3]\cdot C_2H_3N$
M_r = 1018.30
Orthorhombic, $Pna2_1$
a = 18.5726 (10) Å
b = 20.2631 (12) Å
c = 12.7839 (5) Å
V = 4811.2 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.23 mm^{-1}
T = 115 (2) K
0.30 × 0.25 × 0.17 mm

Data collection

Nonius KappaCCD diffractometer with an Oxford Cryosystems Cryostream cooler
Absorption correction: multi-scan (*SCALEPACK*; Otwinowski & Minor, 1997)
T_{min} = 0.709, T_{max} = 0.818
156685 measured reflections
15969 independent reflections
13488 reflections with $I > 2\sigma(I)$

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.068
S = 1.03
15969 reflections
561 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.62 e Å^{-3}
$\Delta\rho_{min}$ = −0.66 e Å^{-3}
Absolute structure: Flack (1983), 7443 Friedel pairs
Flack parameter: 0.478 (8)

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C9—H9$\cdots Cg1^{i}$	0.95	2.94	3.732	141
C40—H40$\cdots Cg2^{i}$	0.95	2.94	3.696	137
C39—H39$\cdots$N1S^{ii}	0.95	2.58	3.468 (4)	157

Symmetry codes: (i) $-x, -y+1, z-\frac{1}{2}$; (ii) $x, y, z-1$. $Cg1$ and $Cg2$ are the centroids of the C1–C6 and C7–C12 phenyl rings, respectively.

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LX2043).

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S1. Comment

Organophosphinecopper (I) halides have widely investigated system due to the formation of varying types of crystal structures (Caulton *et al.*, 1990). Eller *et al.* (1977) used the organophosphinecopper (I) systems for the direct Cu–SO_2 adduct formation. Recently Hanna *et al.* (2005) reported the structural and solid state NMR studies of the four coordinate copper (I) complexes with different cations except iodide. During our study on the interaction of heterocyclic thiosemicarbazones with copper (I) halides, we were able to isolate the title compound (1), Venkatraman *et al.*, (2006).

The structure consists of $CuI(PPh_3)_3$ unit similar to the structure described by Eller *et al.* (1977) for $CuI(PPh_2Me)_3$. The asymmetric unit of (1) contains one formula unit of the complex with no crystallographically imposed symmetry (Fig.1), and one acetonitrile solvent molecule. The Cu atom is surrounded by three phosphorus atoms and the iodide atom in a distorted tetrahedral geometry. The three independent Cu—P distances are not grossly different (2.3421 (6), 2.3463 (6), and 2.3295 (7) Å) for P1, P2, and P3, respectively, and the Cu—I distance is 2.6843 (3) Å. The Cu—P bond lengths in compound (1) are similar to values recorded for a range of other [Cu-$(PPh3)_3X$] complexes [Bowmaker *et al.*, (2000)]. The three P—Cu—I angles are 104.75 (2), 113.66 (2), and 97.69 (2)°, for P1, P2, and P3, respectively, [average 105.2°], and sums to 316.0°. The wide range of P—Cu—P/I angles indicate an irregular tetrahedral structure.

The molecular packing (Fig. 2) is stabilized by CH_2—H···π interactions between the hydrogen of phenyl group and the phenyl ring, with C9—H9···*Cg*1^{i} and C40—H40···*Cg*2^{i} separations of 2.94 Å (Fig. 2 & Table 1) (*Cg*1 and *Cg*2 are the centroids of C1—C6 and C7—C12 phenyl rings, respectively). Further stability comes from weak C—H···N1S^{ii} hydrogen bond in Fig. 2 and Table 1. A l l symmetry codes as in Table 1.

S2. Experimental

To a solution of copper (I) iodide (Aldrich; 0.190 g, 1 mmol) in acetonitrile (Aldrich; 50 ml) was added solid triphenylphosphine (Aldrich; 0.262 g, 2 mmol) in presence 0.5 ml HCl. The resulting mixture was stirred overnight. The clear solution was filtered and allowed to evaporate at room temperature in the presence of air. A colorless crystalline product suitable for X-ray diffraction was formed (yield *ca* 70%).

S3. Refinement

All H atoms were positioned geometrically and refined using a riding model, with C—H = 0.95 Å for aromatic H atoms and 0.98 Å for methyl H atoms, respectively, and with U_{iso}(H) = 1.2Ueq(C) for aromatic H atoms and U_{iso}(H) = 1.5Ueq(C) for methyl H atoms. A torsional parameter was refined for the methyl group. Refinement of the Flack (1983) parameter, using 7443 Friedel pairs indicated that the crystal used was an inversion twin with approximately equal components.

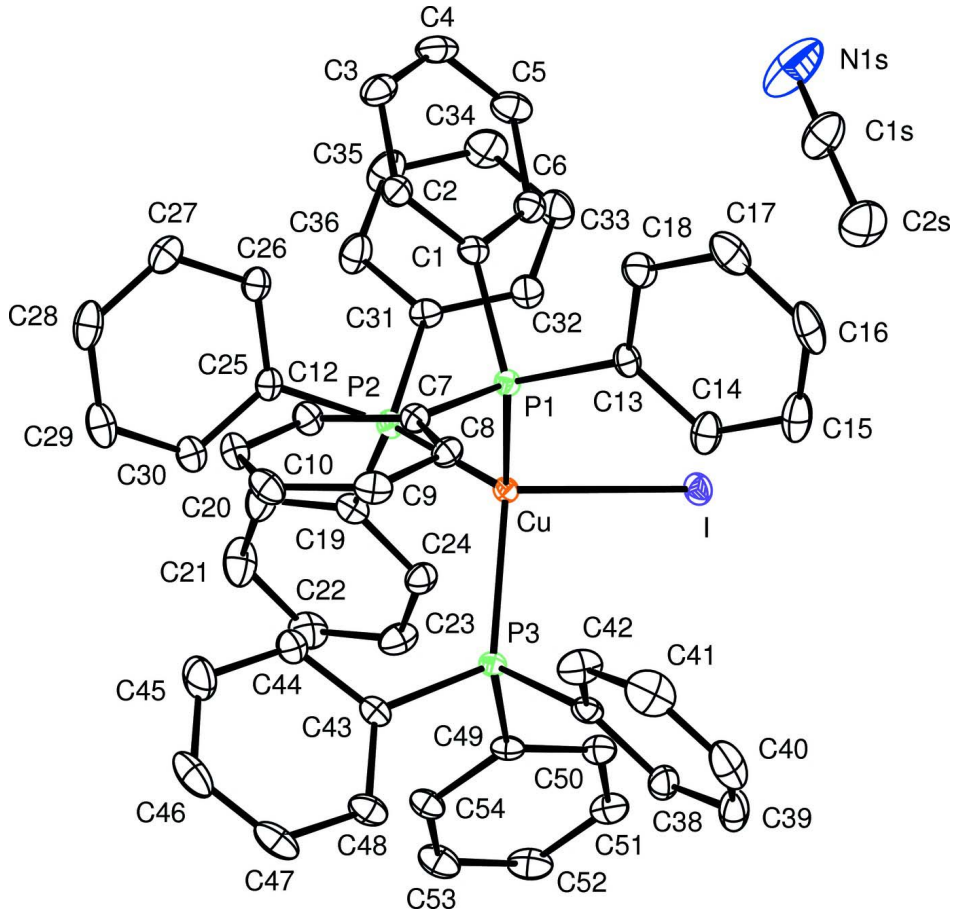

Figure 1

Numbering scheme and ellipsoids at the 50% level. H atoms are not shown.

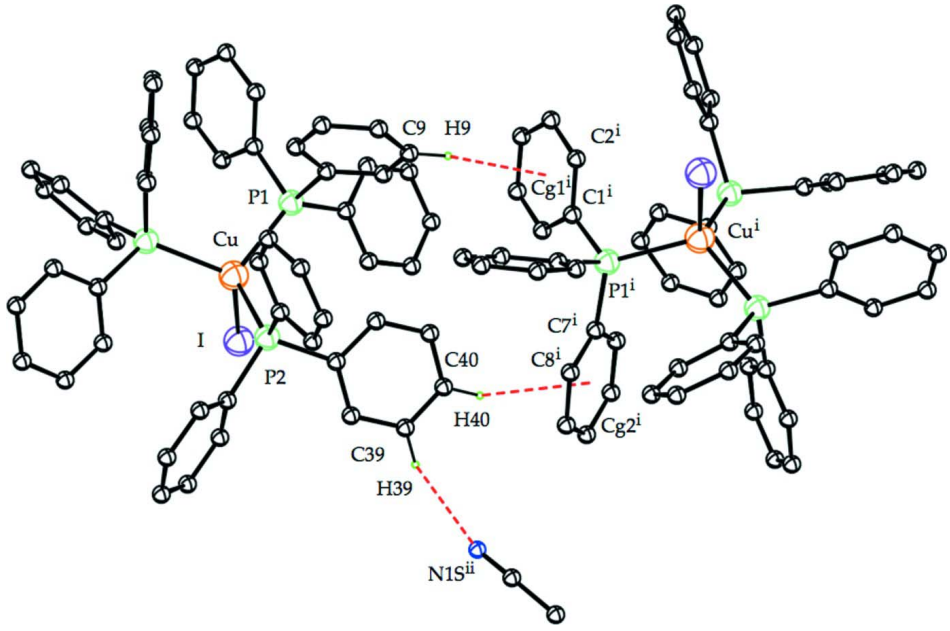

Figure 2

C—H···N and C—H···π interactions. Geometric parameters and symmetry operations are given in the Table 1.

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Crystal data

$[CuI(C_{18}H_{15}P)_3]\cdot C_2H_3N$
M_r = 1018.30
Orthorhombic, $Pna2_1$
Hall symbol: P 2c -2n
a = 18.573 (1) Å
b = 20.263 (1) Å
c = 12.7839 (5) Å
V = 4811.2 (4) Å^3
Z = 4
$F(000)$ = 2072
D_x = 1.406 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 8935 reflections
θ = 2.5–31.8°
μ = 1.23 mm^{-1}
T = 115 K
Fragment, colorless
0.30 × 0.25 × 0.17 mm

Data collection

Nonius KappaCCD diffractometer (with an Oxford Cryosystems Cryostream cooler)
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans with κ offsets
Absorption correction: multi-scan (*SCALEPACK*; Otwinowski & Minor, 1997)
T_{min} = 0.709, T_{max} = 0.818
156685 measured reflections
15969 independent reflections
13488 reflections with $I > 2\sigma(I)$
R_{int} = 0.000
θ_{max} = 31.8°, θ_{min} = 2.8°
h = −27→27
k = −29→30
l = −18→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.068
S = 1.03
15969 reflections
561 parameters
1 restraint
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

$w = 1/[\sigma^2(F_o^2) + (0.0253P)^2 + 3.4731P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.62$ e Å^{-3}
$\Delta\rho_{min} = -0.66$ e Å^{-3}
Absolute structure: Flack (1983)
Absolute structure parameter: 0.478 (8)

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
I	0.217564 (7)	0.266851 (6)	0.441186 (16)	0.02077 (3)
Cu	0.240945 (12)	0.397554 (11)	0.44517 (3)	0.01359 (5)
P1	0.13455 (3)	0.44254 (3)	0.51291 (5)	0.01432 (10)
P2	0.33677 (3)	0.42893 (3)	0.55393 (5)	0.01575 (11)
P3	0.25929 (3)	0.41255 (3)	0.26648 (4)	0.01450 (10)
C1	0.13962 (12)	0.45371 (12)	0.65502 (18)	0.0178 (4)
C2	0.12435 (12)	0.51230 (12)	0.70821 (19)	0.0207 (5)
H2	0.1108	0.5506	0.6700	0.025*
C3	0.12884 (14)	0.51494 (14)	0.8170 (2)	0.0273 (6)
H3	0.1185	0.5549	0.8527	0.033*
C4	0.14844 (14)	0.45912 (16)	0.8732 (2)	0.0301 (6)
H4	0.1513	0.4609	0.9473	0.036*
C5	0.16373 (14)	0.40114 (15)	0.8213 (2)	0.0283 (6)
H5	0.1773	0.3630	0.8598	0.034*
C6	0.15930 (14)	0.39828 (13)	0.7130 (2)	0.0217 (5)
H6	0.1698	0.3581	0.6779	0.026*
C7	0.11119 (12)	0.52434 (11)	0.46264 (16)	0.0175 (5)
C8	0.05030 (12)	0.53500 (12)	0.40169 (18)	0.0191 (4)
H8	0.0173	0.4999	0.3900	0.023*
C9	0.03727 (13)	0.59699 (13)	0.3575 (2)	0.0228 (5)
H9	−0.0040	0.6036	0.3148	0.027*
C10	0.08404 (14)	0.64869 (13)	0.3755 (2)	0.0249 (5)
H10	0.0749	0.6908	0.3455	0.030*
C11	0.14434 (11)	0.63916 (10)	0.4375 (3)	0.0234 (4)
H11	0.1760	0.6750	0.4509	0.028*
C12	0.15866 (13)	0.57737 (12)	0.48005 (19)	0.0205 (5)
H12	0.2007	0.5709	0.5211	0.025*
C13	0.04853 (12)	0.39823 (11)	0.50234 (19)	0.0186 (4)
C14	0.03752 (13)	0.35252 (12)	0.4235 (2)	0.0268 (6)

H14	0.0753	0.3423	0.3762	0.032*
C15	−0.02950 (15)	0.32139 (13)	0.4135 (2)	0.0336 (7)
H15	−0.0372	0.2908	0.3584	0.040*
C16	−0.08436 (15)	0.33469 (14)	0.4829 (3)	0.0360 (7)
H16	−0.1295	0.3130	0.4758	0.043*
C17	−0.07363 (14)	0.37963 (15)	0.5628 (2)	0.0337 (6)
H17	−0.1112	0.3885	0.6113	0.040*
C18	−0.00801 (13)	0.41170 (14)	0.5719 (2)	0.0256 (5)
H18	−0.0012	0.4432	0.6261	0.031*
C19	0.42750 (12)	0.41851 (12)	0.49989 (19)	0.0196 (5)
C20	0.48602 (14)	0.45677 (13)	0.5321 (2)	0.0300 (6)
H20	0.4792	0.4912	0.5816	0.036*
C21	0.55453 (14)	0.44453 (15)	0.4916 (3)	0.0359 (7)
H21	0.5939	0.4715	0.5121	0.043*
C22	0.56534 (14)	0.39352 (14)	0.4220 (2)	0.0314 (7)
H22	0.6121	0.3852	0.3950	0.038*
C23	0.50823 (15)	0.35457 (15)	0.3917 (2)	0.0293 (6)
H23	0.5159	0.3191	0.3445	0.035*
C24	0.43900 (12)	0.36709 (12)	0.4301 (2)	0.0230 (5)
H24	0.3998	0.3403	0.4084	0.028*
C25	0.33421 (12)	0.51645 (11)	0.59215 (19)	0.0176 (4)
C26	0.29808 (12)	0.53569 (12)	0.6835 (2)	0.0205 (5)
H26	0.2781	0.5032	0.7284	0.025*
C27	0.29136 (14)	0.60257 (14)	0.7087 (2)	0.0266 (6)
H27	0.2668	0.6153	0.7706	0.032*
C28	0.32047 (15)	0.65019 (13)	0.6435 (2)	0.0313 (6)
H28	0.3166	0.6955	0.6615	0.038*
C29	0.35523 (14)	0.63185 (13)	0.5523 (2)	0.0297 (6)
H29	0.3743	0.6647	0.5070	0.036*
C30	0.36235 (13)	0.56523 (12)	0.5268 (2)	0.0226 (5)
H30	0.3866	0.5529	0.4643	0.027*
C31	0.34799 (14)	0.38716 (13)	0.6806 (2)	0.0192 (5)
C32	0.31740 (14)	0.32518 (13)	0.6941 (2)	0.0232 (5)
H32	0.2918	0.3052	0.6381	0.028*
C33	0.32387 (16)	0.29223 (14)	0.7889 (2)	0.0319 (6)
H33	0.3025	0.2500	0.7977	0.038*
C34	0.36150 (18)	0.32092 (15)	0.8706 (2)	0.0377 (7)
H34	0.3649	0.2989	0.9361	0.045*
C35	0.39419 (18)	0.38161 (14)	0.8570 (2)	0.0372 (7)
H35	0.4210	0.4008	0.9125	0.045*
C36	0.38781 (16)	0.41478 (14)	0.7618 (2)	0.0302 (6)
H36	0.4107	0.4563	0.7524	0.036*
C37	0.18119 (13)	0.38725 (13)	0.18883 (19)	0.0193 (5)
C38	0.18054 (15)	0.33782 (12)	0.1132 (2)	0.0261 (5)
H38	0.2234	0.3143	0.0971	0.031*
C39	0.11603 (19)	0.32291 (14)	0.0607 (2)	0.0367 (7)
H39	0.1155	0.2893	0.0089	0.044*
C40	0.05379 (17)	0.35655 (16)	0.0839 (3)	0.0403 (8)

H40	0.0102	0.3453	0.0492	0.048*
C41	0.05425 (16)	0.40674 (18)	0.1574 (3)	0.0413 (8)
H41	0.0114	0.4305	0.1726	0.050*
C42	0.11817 (14)	0.42195 (16)	0.2089 (2)	0.0303 (6)
H42	0.1187	0.4567	0.2587	0.036*
C43	0.26948 (12)	0.49703 (12)	0.21873 (19)	0.0182 (4)
C44	0.28124 (15)	0.54660 (13)	0.2903 (2)	0.0262 (5)
H44	0.2849	0.5360	0.3625	0.031*
C45	0.28790 (17)	0.61243 (14)	0.2582 (3)	0.0380 (7)
H45	0.2969	0.6462	0.3081	0.046*
C46	0.28136 (16)	0.62768 (15)	0.1545 (3)	0.0367 (7)
H46	0.2858	0.6723	0.1325	0.044*
C47	0.26847 (14)	0.57923 (15)	0.0817 (2)	0.0320 (6)
H47	0.2632	0.5906	0.0100	0.038*
C48	0.26316 (14)	0.51345 (14)	0.1126 (2)	0.0253 (5)
H48	0.2553	0.4799	0.0620	0.030*
C49	0.33584 (14)	0.36919 (13)	0.20742 (19)	0.0182 (5)
C50	0.33779 (14)	0.30007 (13)	0.2073 (2)	0.0228 (5)
H50	0.2983	0.2759	0.2350	0.027*
C51	0.39711 (15)	0.26645 (13)	0.1669 (2)	0.0260 (5)
H51	0.3976	0.2196	0.1663	0.031*
C52	0.45517 (15)	0.30119 (15)	0.1277 (2)	0.0299 (6)
H52	0.4953	0.2783	0.0994	0.036*
C53	0.45462 (15)	0.36930 (15)	0.1297 (2)	0.0299 (6)
H53	0.4950	0.3932	0.1042	0.036*
C54	0.39532 (13)	0.40330 (13)	0.1690 (2)	0.0218 (5)
H54	0.3955	0.4502	0.1696	0.026*
N1S	0.0790 (2)	0.23273 (17)	0.8365 (3)	0.0715 (12)
C1S	0.05774 (19)	0.22818 (15)	0.7540 (3)	0.0409 (7)
C2S	0.0311 (2)	0.22160 (19)	0.6481 (3)	0.0474 (8)
H21S	0.0714	0.2250	0.5989	0.071*
H22S	−0.0038	0.2567	0.6338	0.071*
H23S	0.0077	0.1786	0.6400	0.071*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I	0.02420 (6)	0.01553 (5)	0.02259 (6)	−0.00050 (5)	−0.00066 (8)	0.00298 (8)
Cu	0.01321 (10)	0.01381 (10)	0.01374 (10)	0.00034 (8)	−0.00041 (14)	0.00155 (13)
P1	0.0120 (2)	0.0155 (2)	0.0155 (2)	−0.0003 (2)	−0.0003 (2)	0.0000 (2)
P2	0.0126 (2)	0.0172 (3)	0.0174 (3)	−0.0001 (2)	−0.0028 (2)	0.0018 (2)
P3	0.0143 (2)	0.0160 (2)	0.0132 (2)	0.0010 (2)	0.0002 (2)	0.0014 (2)
C1	0.0116 (10)	0.0240 (11)	0.0179 (11)	−0.0007 (8)	0.0006 (8)	−0.0002 (9)
C2	0.0157 (10)	0.0236 (12)	0.0230 (12)	−0.0015 (9)	0.0021 (9)	−0.0027 (9)
C3	0.0206 (12)	0.0366 (15)	0.0249 (13)	−0.0027 (10)	0.0038 (10)	−0.0104 (11)
C4	0.0241 (13)	0.0509 (18)	0.0154 (12)	−0.0049 (12)	0.0013 (10)	−0.0033 (11)
C5	0.0244 (13)	0.0401 (15)	0.0206 (12)	0.0013 (11)	−0.0017 (10)	0.0055 (11)
C6	0.0206 (12)	0.0228 (12)	0.0218 (12)	−0.0005 (10)	−0.0002 (10)	0.0006 (10)

C7	0.0169 (9)	0.0173 (9)	0.0185 (14)	0.0015 (7)	0.0008 (8)	0.0002 (8)
C8	0.0177 (10)	0.0211 (11)	0.0185 (10)	0.0006 (9)	−0.0022 (8)	−0.0024 (9)
C9	0.0200 (12)	0.0283 (13)	0.0203 (11)	0.0055 (9)	−0.0036 (9)	0.0039 (10)
C10	0.0249 (12)	0.0218 (12)	0.0280 (13)	0.0035 (10)	0.0030 (10)	0.0092 (10)
C11	0.0222 (9)	0.0189 (9)	0.0291 (11)	−0.0037 (7)	0.0009 (13)	0.0022 (13)
C12	0.0157 (10)	0.0226 (11)	0.0232 (11)	−0.0019 (9)	−0.0031 (8)	0.0029 (9)
C13	0.0150 (10)	0.0178 (10)	0.0230 (12)	−0.0018 (8)	−0.0027 (9)	0.0026 (9)
C14	0.0248 (11)	0.0211 (10)	0.0346 (18)	−0.0005 (9)	−0.0096 (11)	−0.0008 (10)
C15	0.0322 (14)	0.0226 (12)	0.0459 (19)	−0.0054 (10)	−0.0181 (12)	0.0014 (11)
C16	0.0229 (14)	0.0332 (14)	0.0518 (18)	−0.0130 (11)	−0.0144 (12)	0.0186 (13)
C17	0.0171 (12)	0.0432 (17)	0.0407 (16)	−0.0053 (11)	0.0000 (11)	0.0120 (13)
C18	0.0177 (11)	0.0324 (13)	0.0267 (13)	−0.0043 (10)	−0.0006 (10)	0.0006 (10)
C19	0.0142 (10)	0.0236 (11)	0.0209 (12)	0.0029 (8)	−0.0005 (8)	0.0045 (9)
C20	0.0173 (11)	0.0271 (13)	0.0456 (17)	0.0003 (10)	−0.0036 (11)	−0.0096 (12)
C21	0.0156 (11)	0.0315 (14)	0.061 (2)	−0.0016 (10)	−0.0024 (12)	−0.0061 (13)
C22	0.0188 (11)	0.0398 (14)	0.0358 (19)	0.0023 (10)	0.0044 (10)	−0.0006 (12)
C23	0.0265 (13)	0.0368 (15)	0.0247 (13)	0.0042 (11)	0.0009 (10)	−0.0074 (11)
C24	0.0200 (10)	0.0278 (11)	0.0211 (13)	−0.0018 (8)	−0.0040 (10)	−0.0030 (11)
C25	0.0142 (10)	0.0173 (10)	0.0215 (11)	−0.0003 (8)	−0.0056 (8)	0.0005 (9)
C26	0.0177 (11)	0.0200 (11)	0.0240 (12)	−0.0007 (8)	−0.0041 (9)	−0.0008 (9)
C27	0.0230 (13)	0.0271 (14)	0.0297 (14)	0.0015 (10)	−0.0045 (10)	−0.0076 (11)
C28	0.0274 (13)	0.0167 (12)	0.0500 (18)	0.0026 (10)	−0.0110 (12)	−0.0033 (11)
C29	0.0251 (13)	0.0199 (12)	0.0442 (16)	−0.0019 (10)	−0.0048 (11)	0.0080 (11)
C30	0.0181 (11)	0.0213 (11)	0.0283 (13)	−0.0004 (9)	−0.0017 (9)	0.0027 (10)
C31	0.0204 (12)	0.0199 (12)	0.0173 (11)	0.0055 (9)	−0.0024 (9)	0.0031 (9)
C32	0.0242 (13)	0.0236 (12)	0.0218 (12)	0.0003 (10)	−0.0057 (10)	0.0040 (10)
C33	0.0407 (16)	0.0260 (13)	0.0291 (14)	−0.0029 (12)	−0.0073 (12)	0.0101 (11)
C34	0.0523 (19)	0.0359 (16)	0.0248 (14)	0.0049 (14)	−0.0123 (13)	0.0097 (12)
C35	0.055 (2)	0.0293 (15)	0.0269 (14)	0.0028 (13)	−0.0216 (14)	−0.0001 (11)
C36	0.0380 (15)	0.0233 (13)	0.0292 (14)	−0.0009 (11)	−0.0147 (13)	0.0009 (11)
C37	0.0191 (12)	0.0250 (12)	0.0139 (11)	−0.0024 (9)	−0.0014 (9)	0.0040 (9)
C38	0.0346 (14)	0.0217 (12)	0.0221 (12)	−0.0049 (10)	−0.0064 (11)	0.0021 (10)
C39	0.0541 (19)	0.0272 (14)	0.0288 (15)	−0.0167 (13)	−0.0190 (13)	0.0082 (11)
C40	0.0323 (15)	0.0476 (18)	0.0408 (17)	−0.0187 (13)	−0.0207 (13)	0.0226 (15)
C41	0.0196 (13)	0.062 (2)	0.0425 (18)	0.0019 (13)	−0.0091 (12)	0.0101 (16)
C42	0.0207 (12)	0.0451 (17)	0.0250 (13)	0.0064 (12)	−0.0041 (10)	−0.0021 (12)
C43	0.0148 (10)	0.0194 (11)	0.0206 (11)	0.0020 (8)	0.0017 (8)	0.0049 (9)
C44	0.0335 (14)	0.0195 (11)	0.0257 (13)	−0.0020 (10)	0.0028 (11)	0.0022 (9)
C45	0.0489 (18)	0.0183 (12)	0.0467 (19)	−0.0020 (12)	0.0093 (15)	0.0025 (12)
C46	0.0321 (15)	0.0252 (15)	0.053 (2)	0.0040 (12)	0.0123 (14)	0.0181 (14)
C47	0.0240 (13)	0.0397 (16)	0.0324 (15)	0.0034 (11)	0.0027 (11)	0.0208 (12)
C48	0.0224 (12)	0.0327 (14)	0.0209 (12)	0.0016 (10)	−0.0015 (9)	0.0092 (10)
C49	0.0180 (11)	0.0224 (12)	0.0141 (11)	0.0052 (9)	0.0027 (9)	0.0012 (9)
C50	0.0251 (12)	0.0241 (13)	0.0193 (12)	0.0030 (10)	0.0008 (9)	0.0009 (10)
C51	0.0329 (14)	0.0241 (12)	0.0209 (12)	0.0097 (11)	0.0000 (10)	0.0006 (10)
C52	0.0266 (13)	0.0379 (15)	0.0252 (13)	0.0155 (11)	0.0063 (10)	0.0027 (11)
C53	0.0222 (12)	0.0368 (15)	0.0308 (14)	0.0056 (11)	0.0082 (10)	0.0077 (12)
C54	0.0184 (11)	0.0246 (12)	0.0224 (12)	0.0034 (9)	0.0043 (10)	0.0053 (10)

N1S	0.106 (3)	0.055 (2)	0.053 (2)	0.026 (2)	−0.039 (2)	−0.0197 (17)
C1S	0.0500 (19)	0.0309 (15)	0.0418 (18)	0.0090 (13)	−0.0135 (15)	−0.0073 (13)
C2S	0.054 (2)	0.052 (2)	0.0363 (18)	−0.0011 (16)	−0.0160 (15)	0.0016 (15)

Geometric parameters (Å, º)

Cu—I	2.6843 (3)	C26—C27	1.398 (4)
Cu—P1	2.3421 (6)	C26—H26	0.9500
Cu—P2	2.3463 (6)	C27—C28	1.385 (4)
Cu—P3	2.3295 (7)	C27—H27	0.9500
P1—C7	1.830 (2)	C28—C29	1.384 (4)
P1—C1	1.833 (2)	C28—H28	0.9500
P1—C13	1.838 (2)	C29—C30	1.395 (4)
P2—C19	1.833 (2)	C29—H29	0.9500
P2—C31	1.839 (3)	C30—H30	0.9500
P2—C25	1.840 (2)	C31—C32	1.389 (4)
P3—C43	1.827 (2)	C31—C36	1.392 (4)
P3—C37	1.831 (3)	C32—C33	1.389 (4)
P3—C49	1.834 (3)	C32—H32	0.9500
C1—C6	1.394 (3)	C33—C34	1.385 (4)
C1—C2	1.397 (3)	C33—H33	0.9500
C2—C3	1.395 (4)	C34—C35	1.383 (4)
C2—H2	0.9500	C34—H34	0.9500
C3—C4	1.388 (4)	C35—C36	1.395 (4)
C3—H3	0.9500	C35—H35	0.9500
C4—C5	1.378 (4)	C36—H36	0.9500
C4—H4	0.9500	C37—C42	1.389 (4)
C5—C6	1.389 (4)	C37—C38	1.392 (4)
C5—H5	0.9500	C38—C39	1.406 (4)
C6—H6	0.9500	C38—H38	0.9500
C7—C8	1.390 (3)	C39—C40	1.374 (5)
C7—C12	1.408 (3)	C39—H39	0.9500
C8—C9	1.399 (3)	C40—C41	1.385 (5)
C8—H8	0.9500	C40—H40	0.9500
C9—C10	1.380 (4)	C41—C42	1.392 (4)
C9—H9	0.9500	C41—H41	0.9500
C10—C11	1.385 (4)	C42—H42	0.9500
C10—H10	0.9500	C43—C44	1.376 (4)
C11—C12	1.391 (3)	C43—C48	1.402 (3)
C11—H11	0.9500	C44—C45	1.401 (4)
C12—H12	0.9500	C44—H44	0.9500
C13—C14	1.384 (3)	C45—C46	1.367 (5)
C13—C18	1.403 (4)	C45—H45	0.9500
C14—C15	1.401 (3)	C46—C47	1.374 (5)
C14—H14	0.9500	C46—H46	0.9500
C15—C16	1.377 (4)	C47—C48	1.394 (4)
C15—H15	0.9500	C47—H47	0.9500
C16—C17	1.383 (5)	C48—H48	0.9500

C16—H16	0.9500	C49—C54	1.393 (4)
C17—C18	1.386 (4)	C49—C50	1.401 (4)
C17—H17	0.9500	C50—C51	1.395 (4)
C18—H18	0.9500	C50—H50	0.9500
C19—C24	1.388 (4)	C51—C52	1.382 (4)
C19—C20	1.397 (3)	C51—H51	0.9500
C20—C21	1.396 (4)	C52—C53	1.380 (4)
C20—H20	0.9500	C52—H52	0.9500
C21—C22	1.378 (4)	C53—C54	1.393 (4)
C21—H21	0.9500	C53—H53	0.9500
C22—C23	1.378 (4)	C54—H54	0.9500
C22—H22	0.9500	N1S—C1S	1.130 (5)
C23—C24	1.400 (3)	C1S—C2S	1.447 (5)
C23—H23	0.9500	C2S—H21S	0.9800
C24—H24	0.9500	C2S—H22S	0.9800
C25—C30	1.396 (3)	C2S—H23S	0.9800
C25—C26	1.402 (3)		

P1—Cu—P2	108.39 (2)	C30—C25—P2	120.9 (2)
P3—Cu—P1	115.80 (2)	C26—C25—P2	120.1 (2)
P3—Cu—P2	115.77 (2)	C27—C26—C25	120.3 (2)
P1—Cu—I	104.75 (2)	C27—C26—H26	119.9
P2—Cu—I	113.66 (2)	C25—C26—H26	119.9
P3—Cu—I	97.69 (2)	C28—C27—C26	120.1 (3)
C7—P1—C1	104.4 (1)	C28—C27—H27	119.9
C7—P1—C13	102.2 (1)	C26—C27—H27	119.9
C1—P1—C13	100.2 (1)	C29—C28—C27	120.1 (3)
C7—P1—Cu	115.01 (7)	C29—C28—H28	119.9
C1—P1—Cu	111.79 (8)	C27—C28—H28	119.9
C13—P1—Cu	121.07 (8)	C28—C29—C30	120.1 (3)
C19—P2—C31	100.1 (1)	C28—C29—H29	120.0
C19—P2—C25	103.6 (1)	C30—C29—H29	120.0
C31—P2—C25	102.3 (1)	C29—C30—C25	120.7 (2)
C19—P2—Cu	116.27 (8)	C29—C30—H30	119.7
C31—P2—Cu	118.89 (9)	C25—C30—H30	119.7
C25—P2—Cu	113.51 (7)	C32—C31—C36	119.2 (2)
C43—P3—C37	99.4 (1)	C32—C31—P2	118.7 (2)
C43—P3—C49	103.4 (1)	C36—C31—P2	122.1 (2)
C37—P3—C49	104.9 (1)	C33—C32—C31	120.5 (3)
C43—P3—Cu	117.71 (8)	C33—C32—H32	119.7
C37—P3—Cu	112.29 (8)	C31—C32—H32	119.7
C49—P3—Cu	117.04 (8)	C34—C33—C32	120.0 (3)
C6—C1—C2	118.6 (2)	C34—C33—H33	120.0
C6—C1—P1	116.1 (2)	C32—C33—H33	120.0
C2—C1—P1	125.2 (2)	C35—C34—C33	120.0 (3)
C3—C2—C1	120.4 (2)	C35—C34—H34	120.0
C3—C2—H2	119.8	C33—C34—H34	120.0
C1—C2—H2	119.8	C34—C35—C36	120.1 (3)

C4—C3—C2	120.0 (2)	C34—C35—H35	120.0
C4—C3—H3	120.0	C36—C35—H35	120.0
C2—C3—H3	120.0	C31—C36—C35	120.1 (3)
C5—C4—C3	120.0 (2)	C31—C36—H36	119.9
C5—C4—H4	120.0	C35—C36—H36	119.9
C3—C4—H4	120.0	C42—C37—C38	119.0 (2)
C4—C5—C6	120.2 (3)	C42—C37—P3	115.2 (2)
C4—C5—H5	119.9	C38—C37—P3	125.8 (2)
C6—C5—H5	119.9	C37—C38—C39	119.5 (3)
C5—C6—C1	120.8 (2)	C37—C38—H38	120.2
C5—C6—H6	119.6	C39—C38—H38	120.2
C1—C6—H6	119.6	C40—C39—C38	120.5 (3)
C8—C7—C12	118.7 (2)	C40—C39—H39	119.7
C8—C7—P1	122.0 (2)	C38—C39—H39	119.7
C12—C7—P1	119.2 (2)	C39—C40—C41	120.3 (3)
C7—C8—C9	120.4 (2)	C39—C40—H40	119.8
C7—C8—H8	119.8	C41—C40—H40	119.8
C9—C8—H8	119.8	C40—C41—C42	119.3 (3)
C10—C9—C8	120.3 (2)	C40—C41—H41	120.4
C10—C9—H9	119.8	C42—C41—H41	120.4
C8—C9—H9	119.8	C37—C42—C41	121.3 (3)
C9—C10—C11	119.9 (2)	C37—C42—H42	119.4
C9—C10—H10	120.0	C41—C42—H42	119.4
C11—C10—H10	120.0	C44—C43—C48	118.9 (2)
C10—C11—C12	120.3 (2)	C44—C43—P3	118.6 (2)
C10—C11—H11	119.9	C48—C43—P3	122.5 (2)
C12—C11—H11	119.9	C43—C44—C45	121.0 (3)
C11—C12—C7	120.4 (2)	C43—C44—H44	119.5
C11—C12—H12	119.8	C45—C44—H44	119.5
C7—C12—H12	119.8	C46—C45—C44	119.4 (3)
C14—C13—C18	118.8 (2)	C46—C45—H45	120.3
C14—C13—P1	120.6 (2)	C44—C45—H45	120.3
C18—C13—P1	120.6 (2)	C45—C46—C47	120.7 (3)
C13—C14—C15	119.9 (3)	C45—C46—H46	119.6
C13—C14—H14	120.1	C47—C46—H46	119.6
C15—C14—H14	120.1	C46—C47—C48	120.2 (3)
C16—C15—C14	120.7 (3)	C46—C47—H47	119.9
C16—C15—H15	119.6	C48—C47—H47	119.9
C14—C15—H15	119.6	C47—C48—C43	119.7 (3)
C15—C16—C17	119.8 (2)	C47—C48—H48	120.1
C15—C16—H16	120.1	C43—C48—H48	120.1
C17—C16—H16	120.1	C54—C49—C50	118.4 (2)
C16—C17—C18	119.9 (3)	C54—C49—P3	121.5 (2)
C16—C17—H17	120.1	C50—C49—P3	120.0 (2)
C18—C17—H17	120.1	C51—C50—C49	120.6 (2)
C17—C18—C13	120.9 (3)	C51—C50—H50	119.7
C17—C18—H18	119.6	C49—C50—H50	119.7
C13—C18—H18	119.6	C52—C51—C50	120.1 (2)

C24—C19—C20	119.1 (2)	C52—C51—H51	119.9
C24—C19—P2	118.0 (2)	C50—C51—H51	119.9
C20—C19—P2	122.7 (2)	C53—C52—C51	119.8 (2)
C21—C20—C19	120.1 (3)	C53—C52—H52	120.1
C21—C20—H20	120.0	C51—C52—H52	120.1
C19—C20—H20	120.0	C52—C53—C54	120.5 (2)
C22—C21—C20	120.4 (3)	C52—C53—H53	119.8
C22—C21—H21	119.8	C54—C53—H53	119.8
C20—C21—H21	119.8	C49—C54—C53	120.6 (2)
C23—C22—C21	119.9 (2)	C49—C54—H54	119.7
C23—C22—H22	120.0	C53—C54—H54	119.7
C21—C22—H22	120.0	N1S—C1S—C2S	179.3 (4)
C22—C23—C24	120.3 (2)	C1S—C2S—H21S	109.5
C22—C23—H23	119.8	C1S—C2S—H22S	109.5
C24—C23—H23	119.8	H21S—C2S—H22S	109.5
C19—C24—C23	120.2 (2)	C1S—C2S—H23S	109.5
C19—C24—H24	119.9	H21S—C2S—H23S	109.5
C23—C24—H24	119.9	H22S—C2S—H23S	109.5
C30—C25—C26	118.7 (2)		

P3—Cu—P1—C7	−41.42 (8)	C19—C20—C21—C22	−1.9 (5)
P2—Cu—P1—C7	90.62 (8)	C20—C21—C22—C23	0.4 (5)
I—Cu—P1—C7	−147.73 (8)	C21—C22—C23—C24	0.9 (4)
P3—Cu—P1—C1	−160.21 (9)	C20—C19—C24—C23	−0.9 (4)
P2—Cu—P1—C1	−28.18 (9)	P2—C19—C24—C23	−176.1 (2)
I—Cu—P1—C1	93.47 (9)	C22—C23—C24—C19	−0.6 (4)
P3—Cu—P1—C13	82.11 (9)	C19—P2—C25—C30	43.1 (2)
P2—Cu—P1—C13	−145.85 (9)	C31—P2—C25—C30	146.78 (19)
I—Cu—P1—C13	−24.20 (9)	Cu—P2—C25—C30	−83.89 (19)
P3—Cu—P2—C19	−32.45 (9)	C19—P2—C25—C26	−142.59 (19)
P1—Cu—P2—C19	−164.50 (9)	C31—P2—C25—C26	−38.9 (2)
I—Cu—P2—C19	79.49 (9)	Cu—P2—C25—C26	90.42 (19)
P3—Cu—P2—C31	−152.11 (10)	C30—C25—C26—C27	−0.8 (3)
P1—Cu—P2—C31	75.84 (10)	P2—C25—C26—C27	−175.18 (18)
I—Cu—P2—C31	−40.17 (10)	C25—C26—C27—C28	−0.1 (4)
P3—Cu—P2—C25	87.57 (9)	C26—C27—C28—C29	1.1 (4)
P1—Cu—P2—C25	−44.48 (9)	C27—C28—C29—C30	−1.3 (4)
I—Cu—P2—C25	−160.49 (8)	C28—C29—C30—C25	0.5 (4)
P1—Cu—P3—C43	63.46 (9)	C26—C25—C30—C29	0.6 (3)
P2—Cu—P3—C43	−65.03 (9)	P2—C25—C30—C29	174.95 (19)
I—Cu—P3—C43	173.98 (8)	C19—P2—C31—C32	−105.8 (2)
P1—Cu—P3—C37	−51.02 (10)	C25—P2—C31—C32	147.8 (2)
P2—Cu—P3—C37	−179.52 (9)	Cu—P2—C31—C32	21.9 (2)
I—Cu—P3—C37	59.50 (9)	C19—P2—C31—C36	72.3 (3)
P1—Cu—P3—C49	−172.41 (10)	C25—P2—C31—C36	−34.1 (3)
P2—Cu—P3—C49	59.10 (10)	Cu—P2—C31—C36	−160.0 (2)
I—Cu—P3—C49	−61.89 (10)	C36—C31—C32—C33	2.6 (4)
C7—P1—C1—C6	−177.91 (18)	P2—C31—C32—C33	−179.3 (2)

C13—P1—C1—C6	76.6 (2)	C31—C32—C33—C34	−0.5 (5)
Cu—P1—C1—C6	−53.0 (2)	C32—C33—C34—C35	−1.6 (5)
C7—P1—C1—C2	3.1 (2)	C33—C34—C35—C36	1.6 (5)
C13—P1—C1—C2	−102.4 (2)	C32—C31—C36—C35	−2.7 (4)
Cu—P1—C1—C2	128.07 (19)	P2—C31—C36—C35	179.3 (2)
C6—C1—C2—C3	0.0 (3)	C34—C35—C36—C31	0.6 (5)
P1—C1—C2—C3	178.94 (19)	C43—P3—C37—C42	−63.8 (2)
C1—C2—C3—C4	−0.1 (4)	C49—P3—C37—C42	−170.4 (2)
C2—C3—C4—C5	0.3 (4)	Cu—P3—C37—C42	61.5 (2)
C3—C4—C5—C6	−0.3 (4)	C43—P3—C37—C38	115.7 (2)
C4—C5—C6—C1	0.2 (4)	C49—P3—C37—C38	9.1 (3)
C2—C1—C6—C5	0.0 (4)	Cu—P3—C37—C38	−119.0 (2)
P1—C1—C6—C5	−179.1 (2)	C42—C37—C38—C39	−1.6 (4)
C1—P1—C7—C8	−122.92 (19)	P3—C37—C38—C39	178.9 (2)
C13—P1—C7—C8	−18.9 (2)	C37—C38—C39—C40	−0.2 (4)
Cu—P1—C7—C8	114.23 (18)	C38—C39—C40—C41	1.6 (4)
C1—P1—C7—C12	61.5 (2)	C39—C40—C41—C42	−1.1 (5)
C13—P1—C7—C12	165.52 (19)	C38—C37—C42—C41	2.2 (4)
Cu—P1—C7—C12	−61.40 (19)	P3—C37—C42—C41	−178.3 (2)
C12—C7—C8—C9	0.9 (3)	C40—C41—C42—C37	−0.8 (5)
P1—C7—C8—C9	−174.72 (18)	C37—P3—C43—C44	135.0 (2)
C7—C8—C9—C10	−1.3 (4)	C49—P3—C43—C44	−117.1 (2)
C8—C9—C10—C11	0.2 (4)	Cu—P3—C43—C44	13.6 (2)
C9—C10—C11—C12	1.2 (4)	C37—P3—C43—C48	−42.6 (2)
C10—C11—C12—C7	−1.5 (4)	C49—P3—C43—C48	65.2 (2)
C8—C7—C12—C11	0.4 (4)	Cu—P3—C43—C48	−164.05 (17)
P1—C7—C12—C11	176.2 (2)	C48—C43—C44—C45	−0.9 (4)
C7—P1—C13—C14	104.3 (2)	P3—C43—C44—C45	−178.6 (2)
C1—P1—C13—C14	−148.4 (2)	C43—C44—C45—C46	1.1 (4)
Cu—P1—C13—C14	−25.1 (2)	C44—C45—C46—C47	−0.1 (5)
C7—P1—C13—C18	−73.6 (2)	C45—C46—C47—C48	−1.2 (4)
C1—P1—C13—C18	33.7 (2)	C46—C47—C48—C43	1.4 (4)
Cu—P1—C13—C18	157.04 (17)	C44—C43—C48—C47	−0.3 (4)
C18—C13—C14—C15	0.9 (4)	P3—C43—C48—C47	177.28 (19)
P1—C13—C14—C15	−177.04 (19)	C43—P3—C49—C54	18.8 (2)
C13—C14—C15—C16	−1.4 (4)	C37—P3—C49—C54	122.4 (2)
C14—C15—C16—C17	0.5 (4)	Cu—P3—C49—C54	−112.4 (2)
C15—C16—C17—C18	0.8 (4)	C43—P3—C49—C50	−166.1 (2)
C16—C17—C18—C13	−1.3 (4)	C37—P3—C49—C50	−62.4 (2)
C14—C13—C18—C17	0.5 (4)	Cu—P3—C49—C50	62.8 (2)
P1—C13—C18—C17	178.4 (2)	C54—C49—C50—C51	−1.8 (4)
C31—P2—C19—C24	98.0 (2)	P3—C49—C50—C51	−177.1 (2)
C25—P2—C19—C24	−156.6 (2)	C49—C50—C51—C52	0.9 (4)
Cu—P2—C19—C24	−31.4 (2)	C50—C51—C52—C53	0.7 (4)
C31—P2—C19—C20	−77.0 (2)	C51—C52—C53—C54	−1.4 (4)
C25—P2—C19—C20	28.4 (2)	C50—C49—C54—C53	1.2 (4)
Cu—P2—C19—C20	153.61 (19)	P3—C49—C54—C53	176.4 (2)
C24—C19—C20—C21	2.1 (4)	C52—C53—C54—C49	0.4 (4)

P2—C19—C20—C21	177.1 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9···*Cg*1^{i}	0.95	2.94	3.732	141
C40—H40···*Cg*2^{i}	0.95	2.94	3.696	137
C39—H39···N1*S*^{ii}	0.95	2.58	3.468 (4)	157

Symmetry codes: (i) −*x*, −*y*+1, *z*−1/2; (ii) *x*, *y*, *z*−1.