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Tris[diphenyl(4-tolyl)phosphane]-1κ^2P,2κP-μ-di-iodido-1:2κ^4I-dicopper(I)

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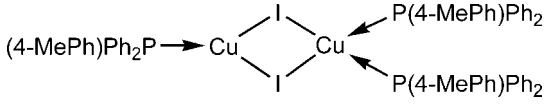
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.007 Å; disorder in main residue; R factor = 0.034; wR factor = 0.076; data-to-parameter ratio = 18.9.

The title complex, $[Cu_2I_2(C_{19}H_{17}P)_3]$, was obtained by refluxing two equivalents of P(4-TolPh$_2$) (4-Tol is 4-tolyl) with one equivalent of CuI in acetonitrile. Two distinct copper(I) centres are bridged by two iodide atoms with a Cu···Cu separation of 2.7807 (9) Å, one with a trigonal coordination geometry and one Cu—P bond of 2.2209 (11) Å, and the second with a distorted tetrahedral coordination geometry and two Cu—P bonds of 2.2562 (12) and 2.2601 (11) Å. No hydrogen bonding, intercalation or stacking interactions were found in the crystal structure. One I atom is disordered over two positions, with occupancies of *ca* 0.79 and 0.21, and the H atoms of the methyl groups are each disordered equally over two positions.

Related literature

Structurally related μ-iodido copper(I) complexes have been reported for PPh_3 (Eller *et al.*, 1977; Liang *et al.*, 1999) and P(4-Tol)$_3$ (Meijboom, 2006).



Experimental

Crystal data

$[Cu_2I_2(C_{19}H_{17}P)_3]$
M_r = 1209.77
Triclinic, $P\overline{1}$
a = 13.984 (2) Å
b = 14.092 (5) Å
c = 16.084 (3) Å
α = 103.948 (2)°
β = 101.743 (3)°
γ = 117.769 (4)°
V = 2531.1 (11) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.19 mm^{-1}
T = 100 (2) K
0.16 × 0.15 × 0.07 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.721, T_{max} = 0.862
44264 measured reflections
11001 independent reflections
8657 reflections with $I > 2\sigma(I)$
R_{int} = 0.047

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.077
S = 1.03
11001 reflections
581 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.89 e Å^{-3}
$\Delta\rho_{min}$ = −0.98 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

I1—Cu2	2.561 (4)	Cu2—P3	2.2209 (11)
I1—Cu1	2.747 (4)	Cu2—Cu1	2.7807 (9)
I2—Cu2	2.5421 (10)	Cu1—P2	2.2562 (12)
I2—Cu1	2.7033 (8)	Cu1—P1	2.2601 (12)
Cu2—I1—Cu1	63.07 (9)	Cu2—I2—Cu1	63.941 (18)

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT-Plus* (Bruker, 2004); data reduction: *SAINT-Plus* and *XPREP* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2006); 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: CV2286).

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supplementary materials

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Tris[diphenyl(4-tolyl)phosphane]-1κ^2P,2κP-μ-di-iodido-1:2κ^4I-dicopper(I)

G. Steyl

Comment

The title complex, (I), is an extension of the previously investigated PPh_3 (Eller *et al.*, 1977; Liang *et al.*, 1999) and P(4-Tol)$_3$ (Meijboom, 2006) derivatives. The complex forms part of a range of copper(I) complexes with an iodido molecule coordinated to the metal centre. The range of coordination modes in which the iodido moiety can coordinate to the metal range from single to three centered interactions (*i.e.* cubane structures).

The title complex presents the most commonly observed coordination pattern for iodido copper(I) complexes, with two distinct copper(I) centres linked *via* an iodido bridge, see Fig. 1. Compared to previously published structures of the PPh_3 (Eller *et al.*, 1977; Liang *et al.*, 1999) and P(4-Tol)$_3$ (Meijboom, 2006) complexes no significant structural effect could be observed when one of the aryl substituents is functionalized. There are no significant intercalation or stacking interactions in the title compound.

Experimental

The title compound was obtained by refluxing two equivalents of P(4-TolPh_2) with one equivalent of CuI in acetonitrile for six hours. On cooling crystals suitable for X-ray crystallography were obtained. (Yield: 50%)

Refinement

H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93–0.96 Å and with U_{iso}(H) = 1.2 times U_{eq}(C aromatic) and U_{iso}(H) = 1.5 times U_{eq}(C methyl).

Atom I1 has been treated as disordered between two positions with the refined occupancies of 0.79 (4) and 0.21 (4), respectively.

Figures

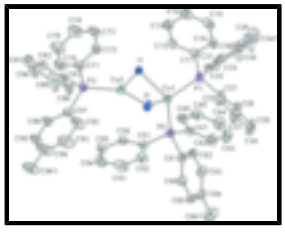


Fig. 1. The molecular structure of (I), with atom labels and 50% probability displacement ellipsoids for non-H atoms. Only the major component of the disordered atom I1 is shown. Hydrogen atoms are omitted for clarity.

Tris[diphenyl(4-tolyl)phosphane]-1κ^2*P*,2κ*P*-μ-di-iodido-1:2κ^4*I*-dicopper(I)

Crystal data

$[Cu_2I_2(C_{19}H_{17}P)_3]$	$Z = 2$
$M_r = 1209.77$	$F_{000} = 1204$
Triclinic, $P\overline{1}$	$D_x = 1.587$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 13.984$ (2) Å	Cell parameters from 9818 reflections
$b = 14.092$ (5) Å	$\theta = 2.6$–27.6º
$c = 16.084$ (3) Å	$\mu = 2.19$ mm^{-1}
$\alpha = 103.948$ (2)º	$T = 100$ (2) K
$\beta = 101.743$ (3)º	Block, colourless
$\gamma = 117.769$ (4)º	0.16 × 0.15 × 0.07 mm
$V = 2531.1$ (11) Å^3	

Data collection

Bruker SMART 1K CCD area-detector diffractometer	11001 independent reflections
Radiation source: fine-focus sealed tube	8657 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.047$
Detector resolution: 512 pixels mm^{-1}	$\theta_{max} = 27.0$º
$T = 100(2)$ K	$\theta_{min} = 2.2$º
φ and ω scans	$h = -17\rightarrow17$
Absorption correction: multi-scan (SADABS; Bruker, 1998)	$k = -18\rightarrow18$
$T_{min} = 0.721$, $T_{max} = 0.862$	$l = -20\rightarrow20$
44264 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.034$	H-atom parameters constrained
$wR(F^2) = 0.077$	$w = 1/[\sigma^2(F_o^2) + (0.0282P)^2 + 2.0291P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} = 0.010$
11001 reflections	$\Delta\rho_{max} = 0.89$ e Å^{-3}
581 parameters	$\Delta\rho_{min} = -0.97$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Experimental. A disorder is observed on the methyl moieties of the tolyl group as well as one of the iodido groups.

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}	Occ. (<1)
I1	0.7341 (3)	0.5527 (3)	0.3950 (3)	0.0229 (3)	0.79 (4)
I2	0.71959 (2)	0.307168 (19)	0.154947 (17)	0.03187 (7)	
Cu2	0.79801 (3)	0.51480 (3)	0.25878 (3)	0.02518 (10)	
Cu1	0.59671 (3)	0.33342 (3)	0.25824 (3)	0.02458 (10)	
P2	0.43984 (7)	0.31991 (8)	0.16951 (6)	0.0260 (2)	
P1	0.57986 (8)	0.20772 (8)	0.32759 (7)	0.0274 (2)	
P3	0.94695 (7)	0.65489 (8)	0.24280 (6)	0.0264 (2)	
C11	0.7117 (3)	0.2117 (3)	0.3774 (2)	0.0267 (7)	
C41	0.3348 (3)	0.3020 (3)	0.2255 (2)	0.0289 (8)	
C31	0.5205 (3)	0.2125 (3)	0.4187 (3)	0.0326 (8)	
C72	1.0760 (3)	0.5883 (3)	0.3379 (3)	0.0343 (9)	
H72	1.0138	0.5555	0.3569	0.041*	
C21	0.4767 (3)	0.0587 (3)	0.2438 (3)	0.0332 (8)	
C46	0.3639 (3)	0.3952 (3)	0.3024 (2)	0.0337 (8)	
H46	0.4328	0.4666	0.3209	0.040*	
C51	0.4678 (3)	0.4474 (3)	0.1426 (2)	0.0287 (8)	
C34	0.4276 (3)	0.2242 (3)	0.5571 (3)	0.0391 (9)	
C15	0.8127 (4)	0.1300 (4)	0.4397 (3)	0.0391 (9)	
H15	0.8105	0.0689	0.4537	0.047*	
C56	0.5720 (3)	0.5111 (3)	0.1320 (2)	0.0310 (8)	
H56	0.6243	0.4877	0.1380	0.037*	
C61	0.3544 (3)	0.1981 (3)	0.0583 (2)	0.0287 (8)	
C26	0.3589 (3)	0.0108 (3)	0.2253 (3)	0.0416 (10)	
H26	0.3344	0.0501	0.2614	0.050*	
C91	0.9365 (3)	0.6554 (3)	0.1282 (2)	0.0313 (8)	
C43	0.1619 (4)	0.1836 (4)	0.2508 (3)	0.0500 (11)	
H43	0.0940	0.1118	0.2336	0.060*	
C16	0.7105 (3)	0.1195 (3)	0.3960 (3)	0.0336 (8)	
H16	0.6399	0.0501	0.3787	0.040*	
C81	0.9948 (3)	0.8033 (3)	0.3089 (2)	0.0334 (8)	
C32	0.4914 (3)	0.2935 (3)	0.4438 (2)	0.0266 (7)	

H32	0.5032	0.3451	0.4144	0.032*	
C22	0.5116 (3)	−0.0002 (3)	0.1875 (3)	0.0421 (10)	
H22	0.5902	0.0323	0.1979	0.051*	
C12	0.8182 (3)	0.3118 (3)	0.4001 (2)	0.0320 (8)	
H12	0.8212	0.3738	0.3874	0.038*	
C64	0.2260 (3)	0.0081 (3)	−0.1122 (3)	0.0381 (9)	
C94	0.9349 (4)	0.6509 (6)	−0.0475 (3)	0.0674 (11)	
C84	1.0531 (7)	1.0281 (4)	0.3995 (4)	0.085 (2)	
H84	1.0729	1.1031	0.4314	0.102*	
C14	0.9178 (4)	0.2301 (4)	0.4626 (3)	0.0394 (9)	
H14	0.9867	0.2371	0.4919	0.047*	
C45	0.2910 (3)	0.3828 (4)	0.3517 (3)	0.0411 (10)	
H45	0.3103	0.4462	0.4020	0.049*	
C44	0.1903 (4)	0.2768 (4)	0.3260 (3)	0.0509 (11)	
H44	0.1417	0.2681	0.3593	0.061*	
C62	0.3765 (3)	0.1103 (3)	0.0388 (2)	0.0320 (8)	
H62	0.4350	0.1148	0.0826	0.038*	
C33	0.4449 (3)	0.2995 (3)	0.5119 (2)	0.0303 (8)	
H33	0.4253	0.3543	0.5273	0.036*	
C54	0.5225 (4)	0.6445 (4)	0.1023 (3)	0.0469 (11)	
H54	0.5408	0.7104	0.0892	0.056*	
C13	0.9202 (3)	0.3201 (3)	0.4416 (3)	0.0370 (9)	
H13	0.9912	0.3873	0.4556	0.044*	
C66	0.2666 (3)	0.1889 (3)	−0.0092 (3)	0.0339 (8)	
H66	0.2502	0.2465	0.0023	0.041*	
C96	0.9597 (3)	0.7513 (4)	0.1066 (3)	0.0400 (9)	
H96	0.9762	0.8186	0.1511	0.048*	
C63	0.3125 (3)	0.0162 (3)	−0.0451 (3)	0.0366 (9)	
H63	0.3277	−0.0423	−0.0565	0.044*	
C341	0.3806 (4)	0.2300 (4)	0.6334 (3)	0.0543 (12)	
H34A	0.3660	0.2912	0.6432	0.081*	0.50
H34B	0.4364	0.2453	0.6890	0.081*	0.50
H34C	0.3094	0.1572	0.6166	0.081*	0.50
H34D	0.3752	0.1713	0.6560	0.081*	0.50
H34E	0.3049	0.2172	0.6101	0.081*	0.50
H34F	0.4318	0.3053	0.6826	0.081*	0.50
C36	0.4995 (5)	0.1357 (4)	0.4628 (4)	0.0637 (15)	
H36	0.5164	0.0789	0.4464	0.076*	
C52	0.3906 (3)	0.4840 (4)	0.1322 (3)	0.0393 (9)	
H52	0.3200	0.4428	0.1391	0.047*	
C71	1.0733 (3)	0.6445 (3)	0.2791 (3)	0.0338 (8)	
C65	0.2040 (3)	0.0956 (3)	−0.0927 (3)	0.0373 (9)	
H65	0.1458	0.0912	−0.1367	0.045*	
C83	1.1370 (5)	1.0091 (4)	0.3875 (3)	0.0772 (18)	
H83	1.2136	1.0716	0.4093	0.093*	
C76	1.1659 (3)	0.6917 (4)	0.2500 (3)	0.0545 (13)	
H76	1.1643	0.7290	0.2097	0.065*	
C73	1.1714 (4)	0.5807 (4)	0.3689 (3)	0.0485 (11)	
H73	1.1739	0.5440	0.4095	0.058*	

C23	0.4298 (4)	−0.1069 (3)	0.1161 (3)	0.0500 (11)	
H23	0.4539	−0.1470	0.0803	0.060*	
C24	0.3130 (4)	−0.1541 (4)	0.0979 (3)	0.0545 (12)	
H24	0.2583	−0.2247	0.0488	0.065*	
C42	0.2340 (3)	0.1957 (4)	0.2002 (3)	0.0399 (9)	
H42	0.2141	0.1322	0.1495	0.048*	
C93	0.9070 (5)	0.5532 (5)	−0.0271 (3)	0.0646 (14)	
H93	0.8876	0.4852	−0.0725	0.077*	
C92	0.9076 (4)	0.5550 (4)	0.0590 (3)	0.0538 (12)	
H92	0.8885	0.4884	0.0709	0.065*	
C74	1.2623 (4)	0.6276 (5)	0.3394 (4)	0.0650 (15)	
H74	1.3256	0.6214	0.3594	0.078*	
C95	0.9587 (4)	0.7487 (4)	0.0200 (3)	0.0503 (11)	
H95	0.9744	0.8142	0.0071	0.060*	
C25	0.2777 (3)	−0.0957 (4)	0.1531 (3)	0.0505 (11)	
H25	0.1989	−0.1280	0.1417	0.061*	
C53	0.4185 (4)	0.5809 (4)	0.1118 (3)	0.0495 (11)	
H53	0.3658	0.6038	0.1044	0.059*	
C82	1.1094 (4)	0.8966 (4)	0.3427 (3)	0.0513 (12)	
H82	1.1674	0.8841	0.3356	0.062*	
C75	1.2603 (4)	0.6834 (5)	0.2808 (4)	0.0665 (15)	
H75	1.3225	0.7157	0.2618	0.080*	
C55	0.5994 (4)	0.6088 (3)	0.1126 (3)	0.0399 (9)	
H55	0.6703	0.6510	0.1065	0.048*	
C35	0.4539 (5)	0.1422 (4)	0.5305 (4)	0.0652 (15)	
H35	0.4406	0.0895	0.5590	0.078*	
C85	0.9388 (6)	0.9366 (4)	0.3647 (4)	0.0785 (18)	
H85	0.8813	0.9504	0.3712	0.094*	
C941	0.9443 (4)	0.6557 (5)	−0.1376 (3)	0.0674 (11)	
H94A	0.9252	0.5815	−0.1774	0.101*	0.50
H94B	1.0222	0.7144	−0.1274	0.101*	0.50
H94C	0.8913	0.6741	−0.1659	0.101*	0.50
H94D	0.9673	0.7318	−0.1364	0.101*	0.50
H94E	0.8703	0.5989	−0.1864	0.101*	0.50
H94F	1.0012	0.6392	−0.1479	0.101*	0.50
C86	0.9093 (4)	0.8241 (4)	0.3200 (3)	0.0518 (12)	
H86	0.8322	0.7624	0.2973	0.062*	
C641	0.1583 (4)	−0.0910 (4)	−0.2036 (3)	0.0666 (14)	
H64A	0.1027	−0.0816	−0.2405	0.100*	0.50
H64B	0.1185	−0.1626	−0.1951	0.100*	0.50
H64C	0.2102	−0.0926	−0.2340	0.100*	0.50
H64D	0.1849	−0.1429	−0.2059	0.100*	0.50
H64E	0.1691	−0.0619	−0.2513	0.100*	0.50
H64F	0.0774	−0.1320	−0.2124	0.100*	0.50
I3	0.722 (2)	0.5469 (15)	0.381 (2)	0.032 (2)	0.21 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.0197 (5)	0.0244 (4)	0.0226 (8)	0.0103 (4)	0.0102 (5)	0.0076 (5)
I2	0.02803 (13)	0.02857 (12)	0.03736 (15)	0.01492 (10)	0.01749 (11)	0.00656 (10)
Cu2	0.0211 (2)	0.0268 (2)	0.0296 (2)	0.01260 (18)	0.01282 (18)	0.01188 (18)
Cu1	0.0204 (2)	0.0253 (2)	0.0295 (2)	0.01191 (18)	0.01177 (18)	0.01153 (17)
P2	0.0199 (4)	0.0307 (5)	0.0274 (5)	0.0134 (4)	0.0108 (4)	0.0103 (4)
P1	0.0255 (5)	0.0243 (4)	0.0364 (5)	0.0127 (4)	0.0175 (4)	0.0142 (4)
P3	0.0201 (4)	0.0342 (5)	0.0292 (5)	0.0140 (4)	0.0132 (4)	0.0167 (4)
C11	0.0314 (19)	0.0310 (18)	0.0241 (18)	0.0186 (16)	0.0150 (15)	0.0128 (15)
C41	0.0267 (18)	0.039 (2)	0.0270 (19)	0.0203 (17)	0.0122 (15)	0.0156 (16)
C31	0.031 (2)	0.0285 (19)	0.045 (2)	0.0149 (17)	0.0230 (18)	0.0194 (17)
C72	0.0271 (19)	0.048 (2)	0.036 (2)	0.0200 (18)	0.0178 (17)	0.0240 (18)
C21	0.030 (2)	0.0240 (18)	0.042 (2)	0.0104 (16)	0.0158 (17)	0.0147 (16)
C46	0.032 (2)	0.045 (2)	0.030 (2)	0.0241 (18)	0.0125 (16)	0.0164 (17)
C51	0.0289 (19)	0.0340 (19)	0.0253 (19)	0.0191 (17)	0.0092 (15)	0.0109 (15)
C34	0.035 (2)	0.042 (2)	0.045 (2)	0.0176 (19)	0.0267 (19)	0.0211 (19)
C15	0.056 (3)	0.048 (2)	0.037 (2)	0.039 (2)	0.023 (2)	0.0245 (19)
C56	0.030 (2)	0.036 (2)	0.0268 (19)	0.0179 (17)	0.0081 (16)	0.0133 (16)
C61	0.0206 (17)	0.0327 (19)	0.031 (2)	0.0111 (15)	0.0133 (15)	0.0127 (15)
C26	0.033 (2)	0.035 (2)	0.060 (3)	0.0150 (18)	0.024 (2)	0.025 (2)
C91	0.0231 (18)	0.052 (2)	0.031 (2)	0.0232 (18)	0.0162 (16)	0.0229 (18)
C43	0.033 (2)	0.049 (3)	0.063 (3)	0.015 (2)	0.029 (2)	0.022 (2)
C16	0.040 (2)	0.0307 (19)	0.037 (2)	0.0187 (18)	0.0224 (18)	0.0175 (16)
C81	0.037 (2)	0.032 (2)	0.028 (2)	0.0117 (17)	0.0124 (17)	0.0189 (16)
C32	0.0214 (17)	0.0294 (18)	0.0263 (19)	0.0112 (15)	0.0092 (14)	0.0122 (15)
C22	0.034 (2)	0.034 (2)	0.046 (3)	0.0110 (18)	0.0178 (19)	0.0087 (18)
C12	0.034 (2)	0.0312 (19)	0.037 (2)	0.0185 (17)	0.0172 (17)	0.0169 (16)
C64	0.026 (2)	0.040 (2)	0.029 (2)	0.0082 (17)	0.0095 (16)	0.0056 (17)
C94	0.069 (2)	0.130 (3)	0.050 (2)	0.073 (3)	0.0374 (19)	0.054 (2)
C84	0.146 (6)	0.032 (3)	0.055 (3)	0.024 (4)	0.058 (4)	0.018 (2)
C14	0.041 (2)	0.052 (3)	0.039 (2)	0.033 (2)	0.0169 (19)	0.0219 (19)
C45	0.042 (2)	0.061 (3)	0.036 (2)	0.035 (2)	0.0214 (19)	0.021 (2)
C44	0.042 (3)	0.067 (3)	0.059 (3)	0.032 (2)	0.036 (2)	0.030 (2)
C62	0.0234 (18)	0.040 (2)	0.030 (2)	0.0169 (17)	0.0099 (16)	0.0108 (16)
C33	0.0219 (18)	0.035 (2)	0.030 (2)	0.0142 (16)	0.0089 (15)	0.0089 (16)
C54	0.061 (3)	0.042 (2)	0.049 (3)	0.033 (2)	0.021 (2)	0.024 (2)
C13	0.032 (2)	0.040 (2)	0.041 (2)	0.0200 (18)	0.0159 (18)	0.0168 (18)
C66	0.0263 (19)	0.035 (2)	0.037 (2)	0.0137 (17)	0.0114 (17)	0.0148 (17)
C96	0.031 (2)	0.059 (3)	0.044 (2)	0.026 (2)	0.0173 (18)	0.033 (2)
C63	0.029 (2)	0.037 (2)	0.036 (2)	0.0175 (18)	0.0109 (17)	0.0058 (17)
C341	0.063 (3)	0.052 (3)	0.069 (3)	0.036 (2)	0.045 (3)	0.031 (2)
C36	0.101 (4)	0.063 (3)	0.104 (4)	0.064 (3)	0.086 (4)	0.067 (3)
C52	0.040 (2)	0.058 (3)	0.041 (2)	0.035 (2)	0.0236 (19)	0.025 (2)
C71	0.0265 (19)	0.051 (2)	0.033 (2)	0.0224 (18)	0.0168 (16)	0.0226 (18)
C65	0.0251 (19)	0.041 (2)	0.033 (2)	0.0138 (18)	0.0045 (16)	0.0105 (17)

C83	0.084 (4)	0.043 (3)	0.040 (3)	−0.005 (3)	0.002 (3)	0.017 (2)
C76	0.034 (2)	0.098 (4)	0.059 (3)	0.038 (3)	0.028 (2)	0.058 (3)
C73	0.043 (2)	0.080 (3)	0.050 (3)	0.042 (2)	0.022 (2)	0.043 (2)
C23	0.046 (3)	0.036 (2)	0.044 (3)	0.010 (2)	0.018 (2)	0.0043 (19)
C24	0.046 (3)	0.034 (2)	0.048 (3)	0.002 (2)	0.009 (2)	0.009 (2)
C42	0.032 (2)	0.047 (2)	0.047 (2)	0.0217 (19)	0.0223 (19)	0.0200 (19)
C93	0.094 (4)	0.099 (4)	0.042 (3)	0.076 (4)	0.037 (3)	0.031 (3)
C92	0.072 (3)	0.076 (3)	0.045 (3)	0.052 (3)	0.033 (2)	0.036 (2)
C74	0.039 (3)	0.117 (4)	0.077 (4)	0.054 (3)	0.030 (3)	0.062 (3)
C95	0.040 (2)	0.086 (3)	0.051 (3)	0.039 (2)	0.027 (2)	0.048 (3)
C25	0.024 (2)	0.039 (2)	0.066 (3)	0.0012 (18)	0.014 (2)	0.023 (2)
C53	0.067 (3)	0.063 (3)	0.048 (3)	0.054 (3)	0.026 (2)	0.025 (2)
C82	0.043 (3)	0.044 (3)	0.041 (3)	0.008 (2)	0.001 (2)	0.023 (2)
C75	0.041 (3)	0.123 (5)	0.078 (4)	0.053 (3)	0.039 (3)	0.069 (3)
C55	0.044 (2)	0.040 (2)	0.036 (2)	0.021 (2)	0.0130 (19)	0.0207 (18)
C35	0.104 (4)	0.064 (3)	0.102 (4)	0.064 (3)	0.085 (4)	0.067 (3)
C85	0.126 (5)	0.048 (3)	0.100 (4)	0.050 (3)	0.088 (4)	0.043 (3)
C941	0.069 (2)	0.130 (3)	0.050 (2)	0.073 (3)	0.0374 (19)	0.054 (2)
C86	0.068 (3)	0.038 (2)	0.069 (3)	0.030 (2)	0.050 (3)	0.029 (2)
C641	0.046 (3)	0.069 (3)	0.064 (3)	0.027 (3)	0.013 (2)	0.008 (3)
I3	0.034 (4)	0.0266 (16)	0.030 (5)	0.012 (2)	0.015 (4)	0.008 (2)

Geometric parameters (Å, °)

I1—Cu2	2.561 (4)	C84—H84	0.9300
I1—Cu1	2.747 (4)	C14—C13	1.376 (5)
I2—Cu2	2.5421 (10)	C14—H14	0.9300
I2—Cu1	2.7033 (8)	C45—C44	1.375 (6)
Cu2—P3	2.2209 (11)	C45—H45	0.9300
Cu2—I3	2.469 (17)	C44—H44	0.9300
Cu2—Cu1	2.7807 (9)	C62—C63	1.385 (5)
Cu1—P2	2.2562 (12)	C62—H62	0.9300
Cu1—P1	2.2601 (12)	C33—H33	0.9300
Cu1—I3	2.62 (2)	C54—C53	1.373 (6)
P2—C61	1.820 (4)	C54—C55	1.382 (5)
P2—C41	1.826 (3)	C54—H54	0.9300
P2—C51	1.832 (4)	C13—H13	0.9300
P1—C11	1.824 (4)	C66—C65	1.377 (5)
P1—C21	1.825 (4)	C66—H66	0.9300
P1—C31	1.828 (4)	C96—C95	1.382 (5)
P3—C81	1.813 (4)	C96—H96	0.9300
P3—C91	1.822 (4)	C63—H63	0.9300
P3—C71	1.829 (4)	C341—H34A	0.9600
C11—C12	1.383 (5)	C341—H34B	0.9600
C11—C16	1.395 (5)	C341—H34C	0.9600
C41—C42	1.379 (5)	C341—H34D	0.9600
C41—C46	1.391 (5)	C341—H34E	0.9600
C31—C32	1.382 (5)	C341—H34F	0.9600
C31—C36	1.386 (5)	C36—C35	1.373 (6)

C72—C71	1.378 (5)	C36—H36	0.9300
C72—C73	1.389 (5)	C52—C53	1.377 (6)
C72—H72	0.9300	C52—H52	0.9300
C21—C26	1.388 (5)	C71—C76	1.390 (5)
C21—C22	1.394 (5)	C65—H65	0.9300
C46—C45	1.388 (5)	C83—C82	1.395 (7)
C46—H46	0.9300	C83—H83	0.9300
C51—C56	1.384 (5)	C76—C75	1.381 (6)
C51—C52	1.396 (5)	C76—H76	0.9300
C34—C35	1.371 (5)	C73—C74	1.376 (6)
C34—C33	1.384 (5)	C73—H73	0.9300
C34—C341	1.508 (5)	C23—C24	1.377 (6)
C15—C14	1.372 (5)	C23—H23	0.9300
C15—C16	1.380 (5)	C24—C25	1.384 (6)
C15—H15	0.9300	C24—H24	0.9300
C56—C55	1.379 (5)	C42—H42	0.9300
C56—H56	0.9300	C93—C92	1.377 (6)
C61—C62	1.390 (5)	C93—H93	0.9300
C61—C66	1.395 (5)	C92—H92	0.9300
C26—C25	1.387 (6)	C74—C75	1.369 (6)
C26—H26	0.9300	C74—H74	0.9300
C91—C96	1.384 (5)	C95—H95	0.9300
C91—C92	1.389 (6)	C25—H25	0.9300
C43—C44	1.378 (6)	C53—H53	0.9300
C43—C42	1.397 (5)	C82—H82	0.9300
C43—H43	0.9300	C75—H75	0.9300
C16—H16	0.9300	C55—H55	0.9300
C81—C82	1.389 (5)	C35—H35	0.9300
C81—C86	1.392 (5)	C85—C86	1.386 (6)
C32—C33	1.389 (5)	C85—H85	0.9300
C32—H32	0.9300	C941—H94A	0.9600
C22—C23	1.385 (5)	C941—H94B	0.9600
C22—H22	0.9300	C941—H94C	0.9600
C12—C13	1.383 (5)	C941—H94D	0.9600
C12—H12	0.9300	C941—H94E	0.9600
C64—C65	1.385 (5)	C941—H94F	0.9600
C64—C63	1.387 (5)	C86—H86	0.9300
C64—C641	1.490 (6)	C641—H64A	0.9600
C94—C95	1.376 (7)	C641—H64B	0.9600
C94—C93	1.387 (7)	C641—H64C	0.9600
C94—C941	1.496 (6)	C641—H64D	0.9600
C84—C83	1.359 (8)	C641—H64E	0.9600
C84—C85	1.378 (8)	C641—H64F	0.9600
Cu2—I1—Cu1	63.07 (9)	C95—C96—H96	119.5
Cu2—I2—Cu1	63.941 (18)	C91—C96—H96	119.5
P3—Cu2—I3	124.3 (4)	C62—C63—C64	120.8 (4)
P3—Cu2—I2	116.50 (3)	C62—C63—H63	119.6
I3—Cu2—I2	118.7 (4)	C64—C63—H63	119.6
P3—Cu2—I1	122.44 (9)	C34—C341—H34A	109.5

I3—Cu2—I1	4.6 (7)	C34—C341—H34B	109.5
I2—Cu2—I1	119.85 (9)	H34A—C341—H34B	109.5
P3—Cu2—Cu1	173.43 (3)	C34—C341—H34C	109.5
I3—Cu2—Cu1	59.4 (5)	H34A—C341—H34C	109.5
I2—Cu2—Cu1	60.85 (2)	H34B—C341—H34C	109.5
I1—Cu2—Cu1	61.74 (9)	C34—C341—H34D	109.5
P2—Cu1—P1	121.94 (4)	H34A—C341—H34D	141.1
P2—Cu1—I3	104.5 (6)	H34B—C341—H34D	56.3
P1—Cu1—I3	110.1 (6)	H34C—C341—H34D	56.3
P2—Cu1—I2	109.14 (4)	C34—C341—H34E	109.5
P1—Cu1—I2	102.33 (3)	H34A—C341—H34E	56.3
I3—Cu1—I2	108.3 (3)	H34B—C341—H34E	141.1
P2—Cu1—I1	107.95 (9)	H34C—C341—H34E	56.3
P1—Cu1—I1	106.56 (11)	H34D—C341—H34E	109.5
I3—Cu1—I1	3.8 (7)	C34—C341—H34F	109.5
I2—Cu1—I1	108.23 (7)	H34A—C341—H34F	56.3
P2—Cu1—Cu2	109.66 (4)	H34B—C341—H34F	56.3
P1—Cu1—Cu2	128.35 (3)	H34C—C341—H34F	141.1
I3—Cu1—Cu2	54.4 (3)	H34D—C341—H34F	109.5
I2—Cu1—Cu2	55.21 (2)	H34E—C341—H34F	109.5
I1—Cu1—Cu2	55.19 (8)	C35—C36—C31	120.9 (4)
C61—P2—C41	103.73 (16)	C35—C36—H36	119.6
C61—P2—C51	104.49 (16)	C31—C36—H36	119.6
C41—P2—C51	103.13 (16)	C53—C52—C51	120.3 (4)
C61—P2—Cu1	116.33 (12)	C53—C52—H52	119.9
C41—P2—Cu1	111.73 (12)	C51—C52—H52	119.9
C51—P2—Cu1	115.91 (11)	C72—C71—C76	119.4 (3)
C11—P1—C21	104.78 (16)	C72—C71—P3	118.2 (3)
C11—P1—C31	104.50 (17)	C76—C71—P3	122.4 (3)
C21—P1—C31	102.44 (17)	C66—C65—C64	121.2 (4)
C11—P1—Cu1	116.45 (12)	C66—C65—H65	119.4
C21—P1—Cu1	109.69 (13)	C64—C65—H65	119.4
C31—P1—Cu1	117.40 (12)	C84—C83—C82	120.6 (5)
C81—P3—C91	102.06 (17)	C84—C83—H83	119.7
C81—P3—C71	105.71 (18)	C82—C83—H83	119.7
C91—P3—C71	102.79 (16)	C75—C76—C71	120.1 (4)
C81—P3—Cu2	116.76 (12)	C75—C76—H76	119.9
C91—P3—Cu2	119.02 (12)	C71—C76—H76	119.9
C71—P3—Cu2	108.92 (13)	C74—C73—C72	119.7 (4)
C12—C11—C16	118.2 (3)	C74—C73—H73	120.1
C12—C11—P1	118.7 (3)	C72—C73—H73	120.1
C16—C11—P1	123.1 (3)	C24—C23—C22	120.5 (4)
C42—C41—C46	119.2 (3)	C24—C23—H23	119.8
C42—C41—P2	121.8 (3)	C22—C23—H23	119.8
C46—C41—P2	118.6 (3)	C23—C24—C25	119.5 (4)
C32—C31—C36	117.5 (3)	C23—C24—H24	120.2
C32—C31—P1	119.4 (3)	C25—C24—H24	120.2
C36—C31—P1	123.0 (3)	C41—C42—C43	119.8 (4)
C71—C72—C73	120.1 (3)	C41—C42—H42	120.1

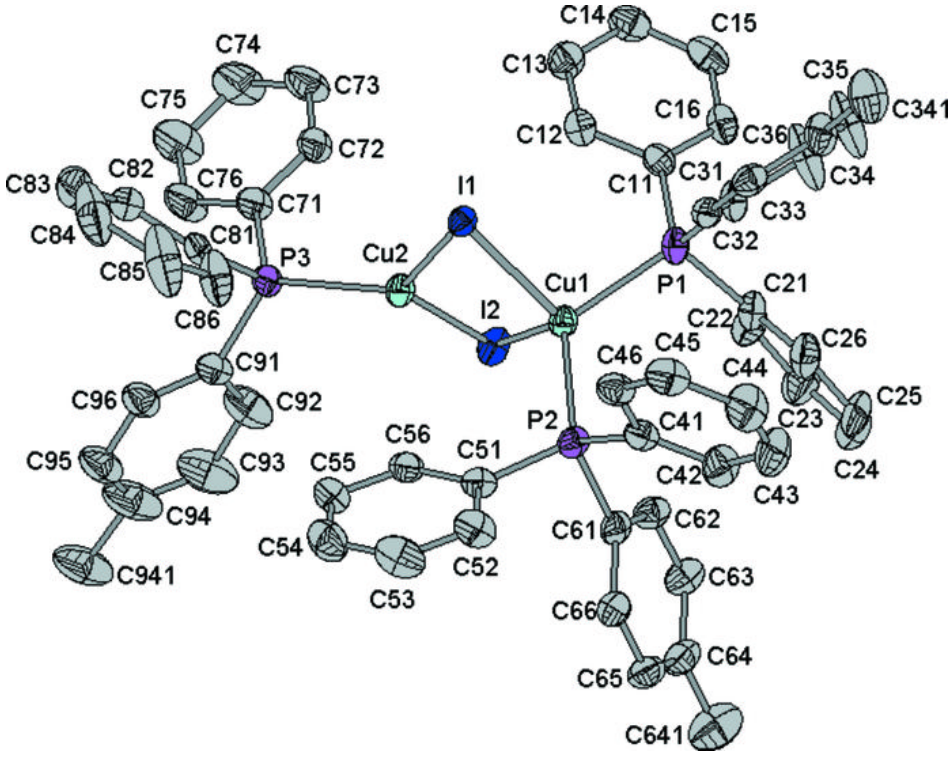
C71—C72—H72	119.9	C43—C42—H42	120.1
C73—C72—H72	119.9	C92—C93—C94	121.3 (5)
C26—C21—C22	119.1 (3)	C92—C93—H93	119.4
C26—C21—P1	118.8 (3)	C94—C93—H93	119.4
C22—C21—P1	121.3 (3)	C93—C92—C91	120.7 (4)
C45—C46—C41	120.7 (4)	C93—C92—H92	119.7
C45—C46—H46	119.7	C91—C92—H92	119.7
C41—C46—H46	119.7	C75—C74—C73	120.5 (4)
C56—C51—C52	118.1 (3)	C75—C74—H74	119.7
C56—C51—P2	117.9 (3)	C73—C74—H74	119.7
C52—C51—P2	124.0 (3)	C94—C95—C96	121.2 (5)
C35—C34—C33	118.1 (4)	C94—C95—H95	119.4
C35—C34—C341	119.9 (4)	C96—C95—H95	119.4
C33—C34—C341	122.0 (4)	C24—C25—C26	120.5 (4)
C14—C15—C16	120.4 (4)	C24—C25—H25	119.8
C14—C15—H15	119.8	C26—C25—H25	119.8
C16—C15—H15	119.8	C54—C53—C52	121.4 (4)
C55—C56—C51	121.0 (3)	C54—C53—H53	119.3
C55—C56—H56	119.5	C52—C53—H53	119.3
C51—C56—H56	119.5	C81—C82—C83	119.8 (5)
C62—C61—C66	118.0 (3)	C81—C82—H82	120.1
C62—C61—P2	119.5 (3)	C83—C82—H82	120.1
C66—C61—P2	122.4 (3)	C74—C75—C76	120.0 (4)
C25—C26—C21	120.1 (4)	C74—C75—H75	120.0
C25—C26—H26	119.9	C76—C75—H75	120.0
C21—C26—H26	119.9	C56—C55—C54	120.6 (4)
C96—C91—C92	117.9 (4)	C56—C55—H55	119.7
C96—C91—P3	123.9 (3)	C54—C55—H55	119.7
C92—C91—P3	118.1 (3)	C34—C35—C36	121.7 (4)
C44—C43—C42	120.8 (4)	C34—C35—H35	119.1
C44—C43—H43	119.6	C36—C35—H35	119.1
C42—C43—H43	119.6	C84—C85—C86	120.1 (5)
C15—C16—C11	120.8 (4)	C84—C85—H85	119.9
C15—C16—H16	119.6	C86—C85—H85	119.9
C11—C16—H16	119.6	C94—C941—H94A	109.5
C82—C81—C86	119.1 (4)	C94—C941—H94B	109.5
C82—C81—P3	123.7 (3)	H94A—C941—H94B	109.5
C86—C81—P3	117.0 (3)	C94—C941—H94C	109.5
C31—C32—C33	121.4 (3)	H94A—C941—H94C	109.5
C31—C32—H32	119.3	H94B—C941—H94C	109.5
C33—C32—H32	119.3	C94—C941—H94D	109.5
C23—C22—C21	120.3 (4)	H94A—C941—H94D	141.1
C23—C22—H22	119.9	H94B—C941—H94D	56.3
C21—C22—H22	119.9	H94C—C941—H94D	56.3
C13—C12—C11	120.5 (3)	C94—C941—H94E	109.5
C13—C12—H12	119.8	H94A—C941—H94E	56.3
C11—C12—H12	119.8	H94B—C941—H94E	141.1
C65—C64—C63	118.3 (3)	H94C—C941—H94E	56.3
C65—C64—C641	120.2 (4)	H94D—C941—H94E	109.5

C63—C64—C641	121.5 (4)	C94—C941—H94F	109.5
C95—C94—C93	117.9 (4)	H94A—C941—H94F	56.3
C95—C94—C941	119.1 (5)	H94B—C941—H94F	56.3
C93—C94—C941	123.0 (5)	H94C—C941—H94F	141.1
C83—C84—C85	120.3 (5)	H94D—C941—H94F	109.5
C83—C84—H84	119.9	H94E—C941—H94F	109.5
C85—C84—H84	119.9	C85—C86—C81	120.1 (5)
C15—C14—C13	119.3 (4)	C85—C86—H86	119.9
C15—C14—H14	120.3	C81—C86—H86	119.9
C13—C14—H14	120.3	C64—C641—H64A	109.5
C44—C45—C46	120.0 (4)	C64—C641—H64B	109.5
C44—C45—H45	120.0	H64A—C641—H64B	109.5
C46—C45—H45	120.0	C64—C641—H64C	109.5
C45—C44—C43	119.6 (4)	H64A—C641—H64C	109.5
C45—C44—H44	120.2	H64B—C641—H64C	109.5
C43—C44—H44	120.2	C64—C641—H64D	109.5
C63—C62—C61	120.8 (3)	H64A—C641—H64D	141.1
C63—C62—H62	119.6	H64B—C641—H64D	56.3
C61—C62—H62	119.6	H64C—C641—H64D	56.3
C34—C33—C32	120.3 (3)	C64—C641—H64E	109.5
C34—C33—H33	119.9	H64A—C641—H64E	56.3
C32—C33—H33	119.9	H64B—C641—H64E	141.1
C53—C54—C55	118.7 (4)	H64C—C641—H64E	56.3
C53—C54—H54	120.7	H64D—C641—H64E	109.5
C55—C54—H54	120.7	C64—C641—H64F	109.5
C14—C13—C12	120.8 (4)	H64A—C641—H64F	56.3
C14—C13—H13	119.6	H64B—C641—H64F	56.3
C12—C13—H13	119.6	H64C—C641—H64F	141.1
C65—C66—C61	120.8 (3)	H64D—C641—H64F	109.5
C65—C66—H66	119.6	H64E—C641—H64F	109.5
C61—C66—H66	119.6	Cu2—I3—Cu1	66.2 (5)
C95—C96—C91	121.0 (4)		
Cu1—I2—Cu2—P3	−173.20 (4)	C41—P2—C61—C66	67.2 (3)
Cu1—I2—Cu2—I3	14.0 (8)	C51—P2—C61—C66	−40.5 (3)
Cu1—I2—Cu2—I1	19.07 (12)	Cu1—P2—C61—C66	−169.7 (3)
Cu1—I1—Cu2—P3	174.12 (4)	C22—C21—C26—C25	1.6 (6)
Cu1—I1—Cu2—I3	58 (6)	P1—C21—C26—C25	170.9 (3)
Cu1—I1—Cu2—I2	−18.90 (11)	C81—P3—C91—C96	−1.2 (3)
Cu2—I2—Cu1—P2	101.10 (4)	C71—P3—C91—C96	−110.6 (3)
Cu2—I2—Cu1—P1	−128.43 (4)	Cu2—P3—C91—C96	129.0 (3)
Cu2—I2—Cu1—I3	−12.1 (7)	C81—P3—C91—C92	176.4 (3)
Cu2—I2—Cu1—I1	−16.15 (11)	C71—P3—C91—C92	67.0 (3)
Cu2—I1—Cu1—P2	−101.86 (7)	Cu2—P3—C91—C92	−53.4 (3)
Cu2—I1—Cu1—P1	125.57 (7)	C14—C15—C16—C11	−2.5 (6)
Cu2—I1—Cu1—I3	−76 (5)	C12—C11—C16—C15	3.0 (5)
Cu2—I1—Cu1—I2	16.15 (10)	P1—C11—C16—C15	−175.4 (3)
I3—Cu2—Cu1—P2	94.1 (8)	C91—P3—C81—C82	−80.2 (3)
I2—Cu2—Cu1—P2	−100.12 (4)	C71—P3—C81—C82	26.9 (4)
I1—Cu2—Cu1—P2	98.64 (12)	Cu2—P3—C81—C82	148.2 (3)

I3—Cu2—Cu1—P1	−88.4 (8)	C91—P3—C81—C86	95.2 (3)
I2—Cu2—Cu1—P1	77.40 (4)	C71—P3—C81—C86	−157.6 (3)
I1—Cu2—Cu1—P1	−83.83 (12)	Cu2—P3—C81—C86	−36.4 (4)
I2—Cu2—Cu1—I3	165.8 (8)	C36—C31—C32—C33	1.2 (6)
I1—Cu2—Cu1—I3	4.5 (8)	P1—C31—C32—C33	179.3 (3)
I3—Cu2—Cu1—I2	−165.8 (8)	C26—C21—C22—C23	−2.2 (6)
I1—Cu2—Cu1—I2	−161.24 (12)	P1—C21—C22—C23	−171.2 (3)
I3—Cu2—Cu1—I1	−4.5 (8)	C16—C11—C12—C13	−1.2 (5)
I2—Cu2—Cu1—I1	161.24 (12)	P1—C11—C12—C13	177.2 (3)
P1—Cu1—P2—C61	−71.29 (14)	C16—C15—C14—C13	0.1 (6)
I3—Cu1—P2—C61	163.3 (4)	C41—C46—C45—C44	1.6 (6)
I2—Cu1—P2—C61	47.57 (13)	C46—C45—C44—C43	−0.6 (7)
I1—Cu1—P2—C61	164.99 (15)	C42—C43—C44—C45	−0.2 (7)
Cu2—Cu1—P2—C61	106.42 (13)	C66—C61—C62—C63	−0.5 (5)
P1—Cu1—P2—C41	47.54 (13)	P2—C61—C62—C63	179.7 (3)
I3—Cu1—P2—C41	−77.9 (4)	C35—C34—C33—C32	−2.1 (6)
I2—Cu1—P2—C41	166.41 (13)	C341—C34—C33—C32	178.2 (4)
I1—Cu1—P2—C41	−76.17 (16)	C31—C32—C33—C34	0.6 (5)
Cu2—Cu1—P2—C41	−134.74 (13)	C15—C14—C13—C12	1.6 (6)
P1—Cu1—P2—C51	165.29 (12)	C11—C12—C13—C14	−1.1 (6)
I3—Cu1—P2—C51	39.9 (4)	C62—C61—C66—C65	0.0 (5)
I2—Cu1—P2—C51	−75.85 (12)	P2—C61—C66—C65	179.8 (3)
I1—Cu1—P2—C51	41.57 (15)	C92—C91—C96—C95	−2.5 (5)
Cu2—Cu1—P2—C51	−17.00 (13)	P3—C91—C96—C95	175.0 (3)
P2—Cu1—P1—C11	168.14 (12)	C61—C62—C63—C64	1.1 (6)
I3—Cu1—P1—C11	−69.0 (4)	C65—C64—C63—C62	−1.0 (6)
I2—Cu1—P1—C11	46.01 (12)	C641—C64—C63—C62	178.5 (4)
I1—Cu1—P1—C11	−67.51 (14)	C32—C31—C36—C35	−1.5 (7)
Cu2—Cu1—P1—C11	−9.12 (13)	P1—C31—C36—C35	−179.5 (4)
P2—Cu1—P1—C21	49.40 (13)	C56—C51—C52—C53	0.0 (6)
I3—Cu1—P1—C21	172.3 (4)	P2—C51—C52—C53	−179.9 (3)
I2—Cu1—P1—C21	−72.73 (13)	C73—C72—C71—C76	1.0 (6)
I1—Cu1—P1—C21	173.76 (14)	C73—C72—C71—P3	−178.5 (3)
Cu2—Cu1—P1—C21	−127.85 (12)	C81—P3—C71—C72	103.8 (3)
P2—Cu1—P1—C31	−66.91 (15)	C91—P3—C71—C72	−149.5 (3)
I3—Cu1—P1—C31	56.0 (4)	Cu2—P3—C71—C72	−22.4 (3)
I2—Cu1—P1—C31	170.96 (14)	C81—P3—C71—C76	−75.7 (4)
I1—Cu1—P1—C31	57.44 (16)	C91—P3—C71—C76	31.0 (4)
Cu2—Cu1—P1—C31	115.84 (14)	Cu2—P3—C71—C76	158.1 (3)
I3—Cu2—P3—C81	−13.1 (8)	C61—C66—C65—C64	0.0 (6)
I2—Cu2—P3—C81	174.51 (13)	C63—C64—C65—C66	0.5 (6)
I1—Cu2—P3—C81	−18.10 (19)	C641—C64—C65—C66	−179.0 (4)
I3—Cu2—P3—C91	−136.3 (8)	C85—C84—C83—C82	−2.3 (8)
I2—Cu2—P3—C91	51.32 (14)	C72—C71—C76—C75	−0.7 (7)
I1—Cu2—P3—C91	−141.29 (18)	P3—C71—C76—C75	178.8 (4)
I3—Cu2—P3—C71	106.5 (8)	C71—C72—C73—C74	−1.1 (7)
I2—Cu2—P3—C71	−65.93 (13)	C21—C22—C23—C24	2.3 (7)
I1—Cu2—P3—C71	101.46 (18)	C22—C23—C24—C25	−1.8 (7)
C21—P1—C11—C12	143.9 (3)	C46—C41—C42—C43	1.0 (6)

C31—P1—C11—C12	−108.8 (3)	P2—C41—C42—C43	173.7 (3)
Cu1—P1—C11—C12	22.5 (3)	C44—C43—C42—C41	0.0 (7)
C21—P1—C11—C16	−37.8 (3)	C95—C94—C93—C92	−2.6 (7)
C31—P1—C11—C16	69.6 (3)	C941—C94—C93—C92	175.2 (5)
Cu1—P1—C11—C16	−159.2 (2)	C94—C93—C92—C91	−0.1 (7)
C61—P2—C41—C42	22.6 (4)	C96—C91—C92—C93	2.6 (6)
C51—P2—C41—C42	131.4 (3)	P3—C91—C92—C93	−175.0 (4)
Cu1—P2—C41—C42	−103.4 (3)	C72—C73—C74—C75	1.0 (8)
C61—P2—C41—C46	−164.6 (3)	C93—C94—C95—C96	2.7 (7)
C51—P2—C41—C46	−55.9 (3)	C941—C94—C95—C96	−175.2 (4)
Cu1—P2—C41—C46	69.3 (3)	C91—C96—C95—C94	−0.1 (6)
C11—P1—C31—C32	128.9 (3)	C23—C24—C25—C26	1.2 (7)
C21—P1—C31—C32	−122.0 (3)	C21—C26—C25—C24	−1.1 (7)
Cu1—P1—C31—C32	−1.8 (3)	C55—C54—C53—C52	0.7 (7)
C11—P1—C31—C36	−53.1 (4)	C51—C52—C53—C54	−0.8 (6)
C21—P1—C31—C36	55.9 (4)	C86—C81—C82—C83	0.3 (6)
Cu1—P1—C31—C36	176.1 (4)	P3—C81—C82—C83	175.6 (3)
C11—P1—C21—C26	150.4 (3)	C84—C83—C82—C81	1.0 (7)
C31—P1—C21—C26	41.6 (4)	C73—C74—C75—C76	−0.8 (9)
Cu1—P1—C21—C26	−83.9 (3)	C71—C76—C75—C74	0.6 (8)
C11—P1—C21—C22	−40.5 (4)	C51—C56—C55—C54	−0.8 (6)
C31—P1—C21—C22	−149.4 (3)	C53—C54—C55—C56	0.1 (6)
Cu1—P1—C21—C22	85.2 (3)	C33—C34—C35—C36	1.8 (8)
C42—C41—C46—C45	−1.8 (6)	C341—C34—C35—C36	−178.4 (5)
P2—C41—C46—C45	−174.7 (3)	C31—C36—C35—C34	0.0 (9)
C61—P2—C51—C56	−95.7 (3)	C83—C84—C85—C86	2.3 (9)
C41—P2—C51—C56	156.2 (3)	C84—C85—C86—C81	−1.0 (8)
Cu1—P2—C51—C56	33.8 (3)	C82—C81—C86—C85	−0.3 (7)
C61—P2—C51—C52	84.3 (3)	P3—C81—C86—C85	−176.0 (4)
C41—P2—C51—C52	−23.9 (4)	P3—Cu2—I3—Cu1	173.59 (9)
Cu1—P2—C51—C52	−146.3 (3)	I2—Cu2—I3—Cu1	−14.2 (8)
C52—C51—C56—C55	0.7 (5)	I1—Cu2—I3—Cu1	−119 (6)
P2—C51—C56—C55	−179.3 (3)	P2—Cu1—I3—Cu2	−104.0 (4)
C41—P2—C61—C62	−113.0 (3)	P1—Cu1—I3—Cu2	123.4 (4)
C51—P2—C61—C62	139.2 (3)	I2—Cu1—I3—Cu2	12.3 (7)
Cu1—P2—C61—C62	10.1 (3)	I1—Cu1—I3—Cu2	101 (5)

Fig. 1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