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Tetra-μ_3-iodo-tetrakis[(cyclohexyldiphenylphosphine-κP)copper(I)]

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Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.011 Å
R factor = 0.061
wR factor = 0.125
Data-to-parameter ratio = 24.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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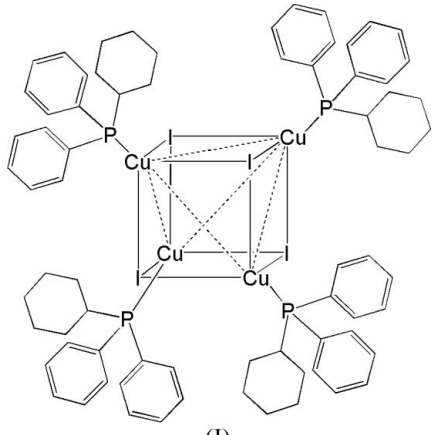
The molecule of the title compound, $[Cu_4I_4(C_{18}H_{21}P)_4]$, which lies on a crystallographic twofold rotation axis, displays a cubane-like Cu_4I_4 core.

Comment

Phosphine complexes of copper(I) halides $[(CuXL_n)_m]$ (X = halogen and L = phosphine), which display a wide range of coordination geometries, are useful as catalysts, as precursors to organocopper reagents (Taylor, 1994) and as starting materials for the preparation of heterometallic complexes (Albano *et al.*, 1995; Kudinov *et al.*, 1993). It was proposed that the title complex, (I), has an irregular cubane structure (Churchill & Kalra, 1974*a*,*b*,*c*; Churchill & Rotella, 1977), which is confirmed in the present study. The tetranuclear molecule lies on a crystallographic twofold rotation axis (Fig. 1).



(I)

The Cu_4I_4 core is a slightly irregular cubane with alternating copper(I) and iodide ions. The Cu atom exists in a tetrahedral environment, being linked to three I atoms and to the P atom of the cyclohexyldiphenylphosphine ligand.

The copper–iodine bond lengths show a significant range of values. The average of the bond lengths is in good agreement with the values of 2.6837 (13) and 2.6767 (15) Å in the Cu_4I_4 cores of other regular cubane-like adducts (Churchill & Kalra, 1974*a*,*b*,*c*; Churchill & Rotella, 1977). The six copper–copper contact distances are similar to reported values. The iodine–iodine contacts are also comparable to reported values, as are the copper–phosphorus bond distances.

There are van der Waals repulsive forces that may be responsible for the distortion of the six faces of the cubane core; the distortion manifests itself in the small Cu—I—Cu angles and in the non-planarity of the four-membered rings defining the faces of the cube.

Experimental

Cyclohexyldiphenylphosphine (0.235 g, 1 mmol) and copper(I) iodide (0.135 g, 2 mmol) were dissolved in 30 ml of acetone. After refluxing the mixture for one day, the hot solution was filtered. Cuboidal crystals were obtained upon recrystallization from the same solvent.

Crystal data

$[Cu_4I_4(C_{18}H_{21}P)_4]$
M_r = 1835.03
Monoclinic, $C2/c$
a = 22.7712 (3) Å
b = 15.6704 (3) Å
c = 21.9311 (5) Å
β = 116.054 (1)°
V = 7030.5 (2) Å^3
Z = 4
D_x = 1.734 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 3.08 mm^{-1}
T = 150 (2) K
Cuboid, colorless
0.26 × 0.22 × 0.20 mm

Data collection

Nonius KappaCCD diffractometer
ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.501, T_{max} = 0.578
(expected range = 0.469–0.540)
63740 measured reflections
8032 independent reflections
6289 reflections with $I > 2\sigma(I)$
R_{int} = 0.127
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.125
S = 1.21
8032 reflections
331 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + 97.862P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.00 e Å^{-3}
$\Delta\rho_{min}$ = −0.92 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

I1—Cu1	2.6976 (11)	I2—Cu2^{i}	2.7667 (11)
I1—Cu1^{i}	2.6849 (10)	Cu1—Cu2	2.8631 (13)
I1—Cu2	2.6645 (10)	Cu1—Cu2^{i}	3.0292 (13)
I2—Cu2	2.6543 (11)	Cu2—Cu2^{i}	3.0570 (18)
I2—Cu1	2.7077 (10)		
Cu1^{i}—I1—Cu1	70.07 (4)	I2—Cu2—I1	115.10 (4)
Cu2—I1—Cu1^{i}	68.98 (3)	I2—Cu2—I2^{i}	104.49 (3)
Cu2—I1—Cu1	64.54 (3)	I1—Cu2—I2^{i}	106.78 (4)
Cu2—I2—Cu1	64.54 (3)	I2—Cu2—Cu1	58.64 (3)
Cu2—I2—Cu2^{i}	68.62 (3)	I1—Cu2—Cu1	58.29 (3)
Cu1—I2—Cu2^{i}	67.18 (3)	I2^{i}—Cu2—Cu1	107.27 (4)
I1^{i}—Cu1—I1	103.98 (3)	I2—Cu2—Cu1^{i}	105.64 (4)
I1^{i}—Cu1—I2	107.90 (3)	I1—Cu2—Cu1^{i}	55.83 (3)
I1—Cu1—I2	112.27 (4)	I2^{i}—Cu2—Cu1^{i}	55.48 (3)
I1^{i}—Cu1—Cu2	107.34 (4)	Cu1—Cu2—Cu1^{i}	63.18 (4)
I1—Cu1—Cu2	57.17 (3)	I2—Cu2—Cu2^{i}	57.43 (3)
I2—Cu1—Cu2	56.83 (3)	I1—Cu2—Cu2^{i}	102.56 (2)
I1^{i}—Cu1—Cu2^{i}	55.19 (3)	I2^{i}—Cu2—Cu2^{i}	53.95 (3)
I1—Cu1—Cu2^{i}	102.49 (4)	Cu1—Cu2—Cu2^{i}	61.45 (3)
I2—Cu1—Cu2^{i}	57.34 (3)	Cu1^{i}—Cu2—Cu2^{i}	56.12 (3)
Cu2—Cu1—Cu2^{i}	62.43 (4)		

Symmetry code: (i) $-x+1, y, -z+\frac{3}{2}$.

The data did not diffract well and the mosaicity was high so the R_{int} value was high. H atoms were placed in calculated positions (C—H = **0.95–1.00** Å) and included as riding atoms, with U_{iso}(H) values of $1.2U_{eq}$ of the attached C atoms. The final difference Fourier map had a large peak/hole 1.00 Å from atom C14..

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

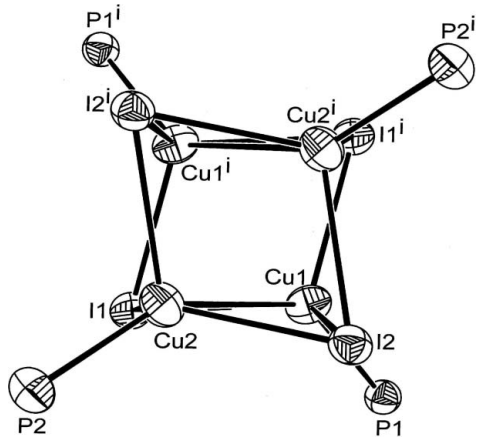


Figure 1
The central coren of (I), showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level. The symmetry code is given in Table 1.

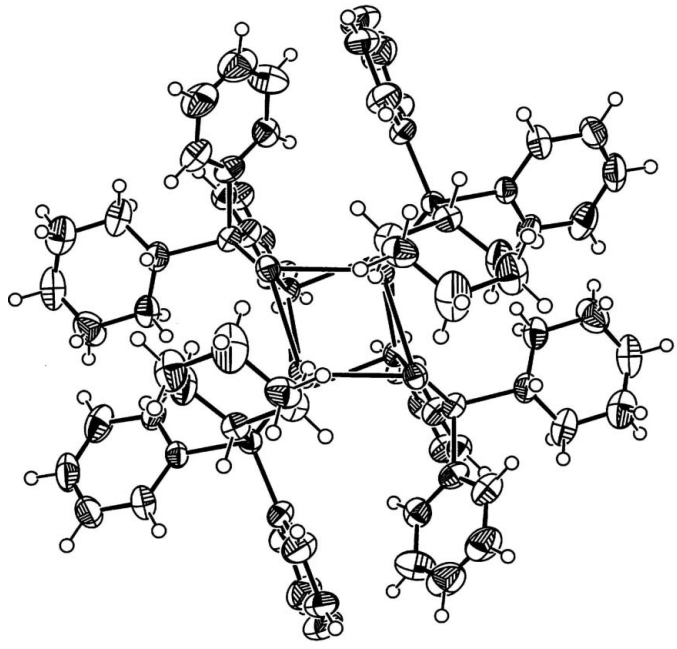


Figure 2
The molecular structure of complex (I). Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented by circles of arbitrary size.

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References

Albano, V. G., Busetto, L., Sabatino, M. C., Schmitz, P. & Zanotti, V. (1995). *J. Chem. Soc. Dalton Trans.* pp. 287–2093.
Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.
Churchill, M. R. & Kalra, K. L. (1974*a*). *Inorg. Chem.* **13**, 1065–1071.
Churchill, M. R. & Kalra, K. L. (1974*b*). *Inorg. Chem.* **13**, 1427–1434.

Churchill, M. R. & Kalra, K. L. (1974*c*). *Inorg. Chem.* **13**, 1899–1904.
Churchill, M. R. & Rotella, F. J. (1977). *Inorg. Chem.* **16**, 3267–3273.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Kudinov, A., Muratov, D., Rybinskaya, M. & Turpeinen, U. (1993). *Mendeleev Commun.* **2**, 39–40.
Nonius (2000). *COLLECT*. Nonius BV, Delft, The Netherlands.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Taylor, R. J. K. (1994). *Organocopper Reagents. A Practical Approach*. Oxford University Press.

supporting information

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Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 22.7712$ (3) Å
$b = 15.6704$ (3) Å
$c = 21.9311$ (5) Å
$\beta = 116.054$ (1)°
$V = 7030.5$ (2) Å^3
$Z = 4$
$F(000) = 3616$
$D_x = 1.734$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 8077 reflections
$\theta = 2.9$–$27.5°$
$\mu = 3.08$ mm^{-1}
$T = 150$ K
Cuboid, colorless
0.26 × 0.22 × 0.20 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan
$T_{min} = 0.501$, $T_{max} = 0.578$
63740 measured reflections
8032 independent reflections
6289 reflections with $I > 2\sigma(I)$
$R_{int} = 0.127$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.0°$
$h = -29 \rightarrow 29$
$k = -20 \rightarrow 19$
$l = -28 \rightarrow 28$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.061$
$wR(F^2) = 0.125$
$S = 1.21$
8032 reflections
331 parameters
24 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
$w = 1/[\sigma^2(F_o^2) + 97.862P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.01$ e Å^{-3}
$\Delta\rho_{min} = -0.92$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
I1	0.50557 (2)	0.49256 (3)	0.65599 (2)	0.03452 (13)
I2	0.39523 (2)	0.69922 (3)	0.70308 (2)	0.03321 (12)
Cu1	0.42457 (5)	0.53083 (6)	0.71218 (5)	0.0394 (2)
Cu2	0.49587 (5)	0.65787 (6)	0.67853 (5)	0.0381 (2)
P1	0.33129 (9)	0.45435 (12)	0.66404 (9)	0.0316 (4)
P2	0.51053 (10)	0.72918 (12)	0.59690 (10)	0.0360 (4)
C1	0.2712 (2)	0.4907 (3)	0.58054 (19)	0.0334 (16)
C2	0.2911 (2)	0.5474 (3)	0.5445 (2)	0.046 (2)
H2	0.3349	0.5672	0.5636	0.055*
C3	0.2467 (3)	0.5752 (3)	0.4806 (2)	0.064 (3)
H3	0.2603	0.6140	0.4560	0.076*
C4	0.1825 (3)	0.5463 (4)	0.4526 (2)	0.064 (3)
H4	0.1522	0.5653	0.4089	0.076*
C5	0.1626 (2)	0.4896 (4)	0.4886 (3)	0.056 (2)
H5	0.1187	0.4698	0.4695	0.068*
C6	0.2069 (2)	0.4618 (3)	0.5526 (2)	0.050 (2)
H6	0.1934	0.4230	0.5772	0.060*
C7	0.2815 (3)	0.4538 (3)	0.7114 (3)	0.0413 (18)
C8	0.2564 (3)	0.5324 (3)	0.7178 (3)	0.053 (2)
H8	0.2666	0.5822	0.6997	0.063*
C9	0.2163 (3)	0.5379 (4)	0.7505 (3)	0.071 (3)
H9	0.1991	0.5916	0.7549	0.085*
C10	0.2013 (3)	0.4650 (5)	0.7769 (3)	0.078 (3)
H10	0.1740	0.4688	0.7993	0.094*
C11	0.2265 (3)	0.3864 (4)	0.7706 (3)	0.061 (3)
H11	0.2162	0.3365	0.7886	0.073*
C12	0.2665 (3)	0.3808 (3)	0.7378 (3)	0.059 (2)
H12	0.2837	0.3271	0.7335	0.071*
C13	0.3412 (3)	0.3405 (4)	0.6489 (3)	0.0362 (16)
H13	0.3001	0.3109	0.6426	0.043*
C14	0.3493 (5)	0.3264 (4)	0.5848 (3)	0.056 (2)
H14A	0.3879	0.3585	0.5878	0.067*
H14B	0.3103	0.3487	0.5455	0.067*
C15	0.3578 (5)	0.2322 (5)	0.5734 (3)	0.063 (3)
H15A	0.3662	0.2259	0.5330	0.075*
H15B	0.3170	0.2012	0.5645	0.075*
C16	0.4143 (5)	0.1931 (6)	0.6349 (4)	0.077 (3)
H16A	0.4171	0.1313	0.6272	0.093*
H16B	0.4559	0.2200	0.6412	0.093*
C17	0.4044 (4)	0.2062 (4)	0.6986 (3)	0.051 (2)

H17A	0.3648	0.1748	0.6939	0.061*
H17B	0.4423	0.1826	0.7383	0.061*
C18	0.3967 (4)	0.3002 (4)	0.7104 (3)	0.0455 (19)
H18A	0.4381	0.3304	0.7200	0.055*
H18B	0.3879	0.3065	0.7505	0.055*
C19	0.5802 (2)	0.6838 (3)	0.5874 (3)	0.045 (2)
C20	0.5708 (3)	0.6110 (3)	0.5480 (3)	0.055 (2)
H20	0.5281	0.5886	0.5230	0.066*
C21	0.6240 (4)	0.5710 (3)	0.5451 (3)	0.070 (3)
H21	0.6176	0.5212	0.5181	0.084*
C22	0.6866 (3)	0.6037 (4)	0.5816 (4)	0.081 (4)
H22	0.7229	0.5764	0.5797	0.097*
C23	0.6959 (2)	0.6765 (4)	0.6210 (3)	0.072 (3)
H23	0.7387	0.6989	0.6460	0.086*
C24	0.6427 (3)	0.7166 (3)	0.6239 (3)	0.048 (2)
H24	0.6491	0.7663	0.6509	0.057*
C25	0.5256 (3)	0.8451 (2)	0.6111 (3)	0.047 (2)
C26	0.5547 (3)	0.8937 (3)	0.5788 (3)	0.0433 (19)
H26	0.5708	0.8668	0.5504	0.052*
C27	0.5602 (3)	0.9816 (3)	0.5881 (3)	0.054 (2)
H27	0.5801	1.0147	0.5661	0.065*
C28	0.5366 (3)	1.0209 (2)	0.6297 (3)	0.048 (2)
H28	0.5404	1.0810	0.6361	0.057*
C29	0.5075 (3)	0.9724 (3)	0.6620 (3)	0.052 (2)
H29	0.4913	0.9993	0.6904	0.062*
C30	0.5019 (3)	0.8845 (3)	0.6526 (3)	0.0422 (19)
H30	0.4820	0.8513	0.6747	0.051*
C31	0.4444 (3)	0.7277 (6)	0.5117 (3)	0.051 (2)
H31	0.4358	0.6652	0.5034	0.062*
C32	0.4591 (4)	0.7531 (6)	0.4546 (3)	0.060 (3)
H32A	0.4936	0.7148	0.4543	0.072*
H32B	0.4770	0.8117	0.4631	0.072*
C33	0.4022 (4)	0.7507 (6)	0.3855 (3)	0.068 (3)
H33A	0.4137	0.7838	0.3539	0.081*
H33B	0.3949	0.6909	0.3695	0.081*
C34	0.3397 (4)	0.7850 (6)	0.3821 (4)	0.074 (3)
H34A	0.3035	0.7676	0.3384	0.088*
H34B	0.3418	0.8481	0.3826	0.088*
C35	0.3240 (3)	0.7565 (7)	0.4384 (4)	0.075 (3)
H35A	0.2887	0.7930	0.4387	0.090*
H35C	0.3072	0.6973	0.4291	0.090*
C36	0.3807 (3)	0.7593 (6)	0.5073 (3)	0.052 (2)
H36C	0.3867	0.8191	0.5236	0.062*
H36A	0.3696	0.7250	0.5387	0.062*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.0349 (3)	0.0310 (2)	0.0335 (2)	−0.0004 (2)	0.0113 (2)	−0.00226 (19)
I2	0.0356 (3)	0.0336 (2)	0.0289 (2)	0.0052 (2)	0.01262 (19)	0.00124 (19)
Cu1	0.0346 (5)	0.0368 (5)	0.0397 (5)	−0.0026 (4)	0.0099 (4)	−0.0012 (4)
Cu2	0.0452 (6)	0.0348 (5)	0.0365 (5)	−0.0001 (4)	0.0199 (4)	0.0016 (4)
P1	0.0307 (10)	0.0329 (9)	0.0297 (9)	0.0001 (8)	0.0118 (8)	−0.0014 (8)
P2	0.0447 (12)	0.0320 (10)	0.0338 (10)	−0.0043 (9)	0.0196 (9)	−0.0018 (8)
C1	0.033 (4)	0.035 (4)	0.028 (3)	0.002 (3)	0.010 (3)	−0.002 (3)
C2	0.051 (5)	0.054 (5)	0.030 (4)	0.000 (4)	0.016 (4)	0.004 (4)
C3	0.087 (8)	0.063 (6)	0.039 (5)	0.011 (6)	0.026 (5)	0.015 (4)
C4	0.065 (7)	0.076 (7)	0.032 (4)	0.027 (5)	0.004 (4)	−0.005 (4)
C5	0.038 (5)	0.071 (6)	0.049 (5)	0.003 (5)	0.009 (4)	−0.014 (5)
C6	0.047 (5)	0.056 (5)	0.034 (4)	−0.001 (4)	0.006 (4)	−0.001 (4)
C7	0.043 (5)	0.052 (5)	0.034 (4)	−0.003 (4)	0.021 (4)	−0.004 (4)
C8	0.063 (6)	0.054 (5)	0.050 (5)	0.003 (5)	0.033 (5)	−0.004 (4)
C9	0.082 (8)	0.078 (7)	0.066 (7)	0.010 (6)	0.044 (6)	−0.003 (6)
C10	0.071 (8)	0.109 (9)	0.080 (8)	0.009 (7)	0.055 (7)	0.000 (7)
C11	0.045 (5)	0.089 (7)	0.057 (6)	0.006 (5)	0.030 (5)	0.014 (5)
C12	0.066 (7)	0.064 (6)	0.059 (6)	0.005 (5)	0.038 (5)	0.005 (5)
C13	0.040 (4)	0.031 (4)	0.038 (4)	−0.002 (3)	0.018 (3)	−0.001 (3)
C14	0.069 (6)	0.052 (5)	0.036 (4)	0.009 (5)	0.013 (4)	−0.006 (4)
C15	0.076 (7)	0.048 (5)	0.051 (5)	0.011 (5)	0.016 (5)	−0.018 (4)
C16	0.094 (8)	0.058 (6)	0.062 (6)	0.032 (6)	0.017 (6)	−0.004 (5)
C17	0.043 (5)	0.045 (5)	0.063 (6)	0.015 (4)	0.022 (4)	0.015 (4)
C18	0.051 (5)	0.038 (4)	0.046 (5)	−0.001 (4)	0.021 (4)	0.001 (4)
C19	0.061 (6)	0.035 (4)	0.051 (5)	−0.002 (4)	0.036 (4)	−0.002 (4)
C20	0.078 (7)	0.049 (5)	0.051 (5)	−0.002 (5)	0.039 (5)	−0.005 (4)
C21	0.091 (9)	0.058 (6)	0.072 (7)	0.021 (6)	0.046 (7)	−0.005 (5)
C22	0.098 (10)	0.083 (8)	0.080 (8)	0.039 (7)	0.056 (8)	0.019 (7)
C23	0.060 (7)	0.060 (6)	0.103 (9)	0.001 (5)	0.041 (6)	0.004 (6)
C24	0.053 (5)	0.041 (4)	0.045 (5)	0.006 (4)	0.019 (4)	0.009 (4)
C25	0.062 (6)	0.036 (4)	0.048 (5)	−0.006 (4)	0.030 (4)	−0.003 (4)
C26	0.050 (5)	0.039 (4)	0.044 (5)	−0.008 (4)	0.023 (4)	−0.006 (4)
C27	0.075 (7)	0.038 (4)	0.060 (5)	−0.002 (4)	0.040 (5)	0.008 (4)
C28	0.048 (5)	0.034 (4)	0.056 (5)	−0.012 (4)	0.017 (4)	−0.007 (4)
C29	0.074 (6)	0.035 (4)	0.060 (5)	0.006 (4)	0.042 (5)	−0.002 (4)
C30	0.059 (5)	0.035 (4)	0.045 (5)	−0.006 (4)	0.034 (4)	0.000 (3)
C31	0.053 (5)	0.064 (6)	0.033 (4)	−0.013 (5)	0.016 (4)	0.001 (4)
C32	0.088 (8)	0.049 (5)	0.039 (5)	−0.001 (5)	0.024 (5)	−0.001 (4)
C33	0.089 (8)	0.055 (6)	0.054 (6)	−0.020 (6)	0.027 (6)	0.004 (5)
C34	0.100 (9)	0.050 (6)	0.042 (5)	−0.003 (6)	0.005 (5)	−0.004 (4)
C35	0.057 (6)	0.084 (8)	0.067 (7)	0.003 (6)	0.010 (5)	0.024 (6)
C36	0.059 (6)	0.047 (5)	0.042 (5)	−0.008 (4)	0.015 (4)	−0.007 (4)

Geometric parameters (Å, º)

I1—Cu1	2.6976 (11)	C15—H15A	0.9900
I1—Cu1^{i}	2.6849 (10)	C15—H15B	0.9900
I1—Cu2	2.6645 (10)	C16—C17	1.523 (8)
I2—Cu2	2.6543 (11)	C16—H16A	0.9900
I2—Cu1	2.7077 (10)	C16—H16B	0.9900
I2—Cu2^{i}	2.7667 (11)	C17—C18	1.519 (7)
Cu1—P1	2.257 (2)	C17—H17A	0.9900
Cu1—I1^{i}	2.6849 (10)	C17—H17B	0.9900
Cu1—Cu2	2.8631 (13)	C18—H18A	0.9900
Cu1—Cu2^{i}	3.0292 (13)	C18—H18B	0.9900
Cu2—P2	2.256 (2)	C19—C20	1.3900
Cu2—I2^{i}	2.7667 (11)	C19—C24	1.3900
Cu2—Cu1^{i}	3.0292 (13)	C20—C21	1.3900
Cu2—Cu2^{i}	3.0570 (18)	C20—H20	0.9500
P1—C1	1.830 (4)	C21—C22	1.3900
P1—C7	1.844 (4)	C21—H21	0.9500
P1—C13	1.846 (6)	C22—C23	1.3900
P2—C31	1.814 (7)	C22—H22	0.9500
P2—C19	1.831 (5)	C23—C24	1.3900
P2—C25	1.849 (4)	C23—H23	0.9500
C1—C2	1.3900	C24—H24	0.9500
C1—C6	1.3900	C25—C26	1.3900
C2—C3	1.3900	C25—C30	1.3900
C2—H2	0.9500	C26—C27	1.3900
C3—C4	1.3900	C26—H26	0.9500
C3—H3	0.9500	C27—C28	1.3900
C4—C5	1.3900	C27—H27	0.9500
C4—H4	0.9500	C28—C29	1.3900
C5—C6	1.3900	C28—H28	0.9500
C5—H5	0.9500	C29—C30	1.3900
C6—H6	0.9500	C29—H29	0.9500
C7—C8	1.3900	C30—H30	0.9500
C7—C12	1.3900	C31—C32	1.485 (7)
C8—C9	1.3900	C31—C36	1.494 (7)
C8—H8	0.9500	C31—H31	1.0000
C9—C10	1.3900	C32—C33	1.500 (7)
C9—H9	0.9500	C32—H32A	0.9900
C10—C11	1.3900	C32—H32B	0.9900
C10—H10	0.9500	C33—C34	1.491 (8)
C11—C12	1.3900	C33—H33A	0.9900
C11—H11	0.9500	C33—H33B	0.9900
C12—H12	0.9500	C34—C35	1.496 (8)
C13—C14	1.511 (7)	C34—H34A	0.9900
C13—C18	1.523 (7)	C34—H34B	0.9900
C13—H13	1.0000	C35—C36	1.496 (7)
C14—C15	1.523 (7)	C35—H35A	0.9900

C14—H14A	0.9900	C35—H35C	0.9900
C14—H14B	0.9900	C36—H36C	0.9900
C15—C16	1.526 (8)	C36—H36A	0.9900
Cu1^{i}—I1—Cu1	70.07 (4)	C13—C14—H14B	109.3
Cu2—I1—Cu1^{i}	68.98 (3)	C15—C14—H14B	109.3
Cu2—I1—Cu1	64.54 (3)	H14A—C14—H14B	107.9
Cu2—I2—Cu1	64.54 (3)	C14—C15—C16	111.3 (6)
Cu2—I2—Cu2^{i}	68.62 (3)	C14—C15—H15A	109.4
Cu1—I2—Cu2^{i}	67.18 (3)	C16—C15—H15A	109.4
P1—Cu1—I1^{i}	112.08 (6)	C14—C15—H15B	109.4
P1—Cu1—I1	111.11 (6)	C16—C15—H15B	109.4
I1^{i}—Cu1—I1	103.98 (3)	H15A—C15—H15B	108.0
P1—Cu1—I2	109.39 (6)	C17—C16—C15	110.4 (6)
I1^{i}—Cu1—I2	107.90 (3)	C17—C16—H16A	109.6
I1—Cu1—I2	112.27 (4)	C15—C16—H16A	109.6
P1—Cu1—Cu2	140.58 (6)	C17—C16—H16B	109.6
I1^{i}—Cu1—Cu2	107.34 (4)	C15—C16—H16B	109.6
I1—Cu1—Cu2	57.17 (3)	H16A—C16—H16B	108.1
I2—Cu1—Cu2	56.83 (3)	C18—C17—C16	111.1 (5)
P1—Cu1—Cu2^{i}	146.32 (7)	C18—C17—H17A	109.4
I1^{i}—Cu1—Cu2^{i}	55.19 (3)	C16—C17—H17A	109.4
I1—Cu1—Cu2^{i}	102.49 (4)	C18—C17—H17B	109.4
I2—Cu1—Cu2^{i}	57.34 (3)	C16—C17—H17B	109.4
Cu2—Cu1—Cu2^{i}	62.43 (4)	H17A—C17—H17B	108.0
P2—Cu2—I2	118.81 (7)	C17—C18—C13	111.4 (5)
P2—Cu2—I1	106.33 (6)	C17—C18—H18A	109.4
I2—Cu2—I1	115.10 (4)	C13—C18—H18A	109.4
P2—Cu2—I2^{i}	104.17 (6)	C17—C18—H18B	109.4
I2—Cu2—I2^{i}	104.49 (3)	C13—C18—H18B	109.4
I1—Cu2—I2^{i}	106.78 (4)	H18A—C18—H18B	108.0
P2—Cu2—Cu1	147.91 (7)	C20—C19—C24	120.0
I2—Cu2—Cu1	58.64 (3)	C20—C19—P2	119.1 (3)
I1—Cu2—Cu1	58.29 (3)	C24—C19—P2	120.7 (3)
I2^{i}—Cu2—Cu1	107.27 (4)	C19—C20—C21	120.0
P2—Cu2—Cu1^{i}	135.06 (7)	C19—C20—H20	120.0
I2—Cu2—Cu1^{i}	105.64 (4)	C21—C20—H20	120.0
I1—Cu2—Cu1^{i}	55.83 (3)	C20—C21—C22	120.0
I2^{i}—Cu2—Cu1^{i}	55.48 (3)	C20—C21—H21	120.0
Cu1—Cu2—Cu1^{i}	63.18 (4)	C22—C21—H21	120.0
P2—Cu2—Cu2^{i}	148.19 (6)	C23—C22—C21	120.0
I2—Cu2—Cu2^{i}	57.43 (3)	C23—C22—H22	120.0
I1—Cu2—Cu2^{i}	102.56 (2)	C21—C22—H22	120.0
I2^{i}—Cu2—Cu2^{i}	53.95 (3)	C22—C23—C24	120.0
Cu1—Cu2—Cu2^{i}	61.45 (3)	C22—C23—H23	120.0
Cu1^{i}—Cu2—Cu2^{i}	56.12 (3)	C24—C23—H23	120.0
C1—P1—C7	101.0 (3)	C23—C24—C19	120.0
C1—P1—C13	102.6 (3)	C23—C24—H24	120.0

C7—P1—C13	104.6 (3)	C19—C24—H24	120.0
C1—P1—Cu1	116.07 (18)	C26—C25—C30	120.0
C7—P1—Cu1	115.1 (2)	C26—C25—P2	123.1 (3)
C13—P1—Cu1	115.6 (2)	C30—C25—P2	116.7 (3)
C31—P2—C19	104.2 (3)	C27—C26—C25	120.0
C31—P2—C25	101.2 (4)	C27—C26—H26	120.0
C19—P2—C25	107.2 (3)	C25—C26—H26	120.0
C31—P2—Cu2	117.8 (3)	C28—C27—C26	120.0
C19—P2—Cu2	109.6 (2)	C28—C27—H27	120.0
C25—P2—Cu2	115.74 (18)	C26—C27—H27	120.0
C2—C1—C6	120.0	C27—C28—C29	120.0
C2—C1—P1	118.7 (3)	C27—C28—H28	120.0
C6—C1—P1	121.3 (3)	C29—C28—H28	120.0
C3—C2—C1	120.0	C30—C29—C28	120.0
C3—C2—H2	120.0	C30—C29—H29	120.0
C1—C2—H2	120.0	C28—C29—H29	120.0
C4—C3—C2	120.0	C29—C30—C25	120.0
C4—C3—H3	120.0	C29—C30—H30	120.0
C2—C3—H3	120.0	C25—C30—H30	120.0
C5—C4—C3	120.0	C32—C31—C36	115.4 (5)
C5—C4—H4	120.0	C32—C31—P2	118.2 (5)
C3—C4—H4	120.0	C36—C31—P2	113.9 (5)
C4—C5—C6	120.0	C32—C31—H31	101.9
C4—C5—H5	120.0	C36—C31—H31	101.9
C6—C5—H5	120.0	P2—C31—H31	101.9
C5—C6—C1	120.0	C31—C32—C33	115.5 (6)
C5—C6—H6	120.0	C31—C32—H32A	108.4
C1—C6—H6	120.0	C33—C32—H32A	108.4
C8—C7—C12	120.0	C31—C32—H32B	108.4
C8—C7—P1	115.7 (3)	C33—C32—H32B	108.4
C12—C7—P1	124.2 (3)	H32A—C32—H32B	107.5
C9—C8—C7	120.0	C34—C33—C32	115.1 (6)
C9—C8—H8	120.0	C34—C33—H33A	108.5
C7—C8—H8	120.0	C32—C33—H33A	108.5
C10—C9—C8	120.0	C34—C33—H33B	108.5
C10—C9—H9	120.0	C32—C33—H33B	108.5
C8—C9—H9	120.0	H33A—C33—H33B	107.5
C9—C10—C11	120.0	C33—C34—C35	114.8 (6)
C9—C10—H10	120.0	C33—C34—H34A	108.6
C11—C10—H10	120.0	C35—C34—H34A	108.6
C10—C11—C12	120.0	C33—C34—H34B	108.6
C10—C11—H11	120.0	C35—C34—H34B	108.6
C12—C11—H11	120.0	H34A—C34—H34B	107.6
C11—C12—C7	120.0	C36—C35—C34	114.3 (6)
C11—C12—H12	120.0	C36—C35—H35A	108.7
C7—C12—H12	120.0	C34—C35—H35A	108.7
C14—C13—C18	111.7 (5)	C36—C35—H35C	108.7
C14—C13—P1	112.6 (4)	C34—C35—H35C	108.7

C18—C13—P1	111.2 (4)	H35A—C35—H35C	107.6
C14—C13—H13	107.0	C31—C36—C35	115.9 (5)
C18—C13—H13	107.0	C31—C36—H36C	108.3
P1—C13—H13	107.0	C35—C36—H36C	108.3
C13—C14—C15	111.8 (6)	C31—C36—H36A	108.3
C13—C14—H14A	109.3	C35—C36—H36A	108.3
C15—C14—H14A	109.3	H36C—C36—H36A	107.4

Cu2—I1—Cu1—P1	137.42 (7)	I2—Cu2—P2—C25	62.0 (2)
Cu1^{i}—I1—Cu1—P1	−147.05 (6)	I1—Cu2—P2—C25	−166.3 (2)
Cu2—I1—Cu1—I1^{i}	−101.82 (4)	I2^{i}—Cu2—P2—C25	−53.7 (2)
Cu1^{i}—I1—Cu1—I1^{i}	−26.29 (4)	Cu1—Cu2—P2—C25	138.1 (2)
Cu2—I1—Cu1—I2	14.56 (3)	Cu1^{i}—Cu2—P2—C25	−108.6 (2)
Cu1^{i}—I1—Cu1—I2	90.08 (3)	Cu2^{i}—Cu2—P2—C25	−11.8 (3)
Cu1^{i}—I1—Cu1—Cu2	75.53 (3)	C7—P1—C1—C2	140.6 (3)
Cu2—I1—Cu1—Cu2^{i}	−45.01 (4)	C13—P1—C1—C2	−111.6 (4)
Cu1^{i}—I1—Cu1—Cu2^{i}	30.52 (4)	Cu1—P1—C1—C2	15.5 (4)
Cu2—I2—Cu1—P1	−138.44 (7)	C7—P1—C1—C6	−40.3 (4)
Cu2^{i}—I2—Cu1—P1	145.31 (7)	C13—P1—C1—C6	67.5 (4)
Cu2—I2—Cu1—I1^{i}	99.38 (4)	Cu1—P1—C1—C6	−165.4 (2)
Cu2^{i}—I2—Cu1—I1^{i}	23.13 (3)	C6—C1—C2—C3	0.0
Cu2—I2—Cu1—I1	−14.61 (3)	P1—C1—C2—C3	179.1 (4)
Cu2^{i}—I2—Cu1—I1	−90.86 (4)	C1—C2—C3—C4	0.0
Cu2^{i}—I2—Cu1—Cu2	−76.25 (4)	C2—C3—C4—C5	0.0
Cu2—I2—Cu1—Cu2^{i}	76.25 (4)	C3—C4—C5—C6	0.0
Cu1—I2—Cu2—P2	142.86 (8)	C4—C5—C6—C1	0.0
Cu2^{i}—I2—Cu2—P2	−143.09 (7)	C2—C1—C6—C5	0.0
Cu1—I2—Cu2—I1	15.13 (3)	P1—C1—C6—C5	−179.1 (4)
Cu2^{i}—I2—Cu2—I1	89.18 (3)	C1—P1—C7—C8	−61.8 (4)
Cu1—I2—Cu2—I2^{i}	−101.63 (4)	C13—P1—C7—C8	−168.0 (3)
Cu2^{i}—I2—Cu2—I2^{i}	−27.58 (4)	Cu1—P1—C7—C8	64.0 (3)
Cu2^{i}—I2—Cu2—Cu1	74.05 (3)	C1—P1—C7—C12	115.8 (4)
Cu1—I2—Cu2—Cu1^{i}	−44.01 (4)	C13—P1—C7—C12	9.6 (4)
Cu2^{i}—I2—Cu2—Cu1^{i}	30.04 (4)	Cu1—P1—C7—C12	−118.4 (3)
Cu1—I2—Cu2—Cu2^{i}	−74.05 (3)	C12—C7—C8—C9	0.0
Cu1^{i}—I1—Cu2—P2	133.84 (7)	P1—C7—C8—C9	177.7 (4)
Cu1—I1—Cu2—P2	−148.96 (7)	C7—C8—C9—C10	0.0
Cu1^{i}—I1—Cu2—I2	−92.39 (4)	C8—C9—C10—C11	0.0
Cu1—I1—Cu2—I2	−15.19 (3)	C9—C10—C11—C12	0.0
Cu1^{i}—I1—Cu2—I2^{i}	23.07 (3)	C10—C11—C12—C7	0.0
Cu1—I1—Cu2—I2^{i}	100.27 (4)	C8—C7—C12—C11	0.0
Cu1^{i}—I1—Cu2—Cu1	−77.20 (4)	P1—C7—C12—C11	−177.5 (5)
Cu1—I1—Cu2—Cu1^{i}	77.20 (4)	C1—P1—C13—C14	46.0 (6)
Cu1^{i}—I1—Cu2—Cu2^{i}	−32.70 (4)	C7—P1—C13—C14	151.1 (5)
Cu1—I1—Cu2—Cu2^{i}	44.50 (4)	Cu1—P1—C13—C14	−81.3 (6)
P1—Cu1—Cu2—P2	−14.99 (18)	C1—P1—C13—C18	172.3 (5)
I1^{i}—Cu1—Cu2—P2	164.42 (12)	C7—P1—C13—C18	−82.7 (5)
I1—Cu1—Cu2—P2	68.70 (13)	Cu1—P1—C13—C18	45.0 (5)

I2—Cu1—Cu2—P2	−95.17 (13)	C18—C13—C14—C15	53.7 (9)
Cu2^{i}—Cu1—Cu2—P2	−162.46 (14)	P1—C13—C14—C15	179.7 (6)
P1—Cu1—Cu2—I2	80.18 (10)	C13—C14—C15—C16	−54.8 (11)
I1^{i}—Cu1—Cu2—I2	−100.41 (4)	C14—C15—C16—C17	56.0 (11)
I1—Cu1—Cu2—I2	163.87 (4)	C15—C16—C17—C18	−56.7 (10)
Cu2^{i}—Cu1—Cu2—I2	−67.29 (3)	C16—C17—C18—C13	55.9 (9)
P1—Cu1—Cu2—I1	−83.69 (10)	C14—C13—C18—C17	−54.3 (8)
I1^{i}—Cu1—Cu2—I1	95.73 (4)	P1—C13—C18—C17	179.0 (5)
I2—Cu1—Cu2—I1	−163.87 (4)	C31—P2—C19—C20	−44.7 (4)
Cu2^{i}—Cu1—Cu2—I1	128.84 (4)	C25—P2—C19—C20	−151.5 (3)
P1—Cu1—Cu2—I2^{i}	176.92 (9)	Cu2—P2—C19—C20	82.2 (3)
I1^{i}—Cu1—Cu2—I2^{i}	−3.67 (5)	C31—P2—C19—C24	141.2 (4)
I1—Cu1—Cu2—I2^{i}	−99.39 (4)	C25—P2—C19—C24	34.5 (4)
I2—Cu1—Cu2—I2^{i}	96.74 (4)	Cu2—P2—C19—C24	−91.8 (3)
Cu2^{i}—Cu1—Cu2—I2^{i}	29.45 (3)	C24—C19—C20—C21	0.0
P1—Cu1—Cu2—Cu1^{i}	−148.38 (11)	P2—C19—C20—C21	−174.1 (4)
I1^{i}—Cu1—Cu2—Cu1^{i}	31.03 (4)	C19—C20—C21—C22	0.0
I1—Cu1—Cu2—Cu1^{i}	−64.69 (3)	C20—C21—C22—C23	0.0
I2—Cu1—Cu2—Cu1^{i}	131.44 (4)	C21—C22—C23—C24	0.0
Cu2^{i}—Cu1—Cu2—Cu1^{i}	64.15 (4)	C22—C23—C24—C19	0.0
P1—Cu1—Cu2—Cu2^{i}	147.47 (11)	C20—C19—C24—C23	0.0
I1^{i}—Cu1—Cu2—Cu2^{i}	−33.12 (4)	P2—C19—C24—C23	174.0 (4)
I1—Cu1—Cu2—Cu2^{i}	−128.84 (4)	C31—P2—C25—C26	−71.7 (4)
I2—Cu1—Cu2—Cu2^{i}	67.29 (3)	C19—P2—C25—C26	37.2 (4)
I1^{i}—Cu1—P1—C1	166.9 (2)	Cu2—P2—C25—C26	159.8 (3)
I1—Cu1—P1—C1	−77.2 (2)	C31—P2—C25—C30	103.8 (4)
I2—Cu1—P1—C1	47.3 (2)	C19—P2—C25—C30	−147.3 (3)
Cu2—Cu1—P1—C1	−13.7 (2)	Cu2—P2—C25—C30	−24.7 (4)
Cu2^{i}—Cu1—P1—C1	107.0 (2)	C30—C25—C26—C27	0.0
I1^{i}—Cu1—P1—C7	49.3 (2)	P2—C25—C26—C27	175.4 (5)
I1—Cu1—P1—C7	165.2 (2)	C25—C26—C27—C28	0.0
I2—Cu1—P1—C7	−70.3 (2)	C26—C27—C28—C29	0.0
Cu2—Cu1—P1—C7	−131.3 (2)	C27—C28—C29—C30	0.0
Cu2^{i}—Cu1—P1—C7	−10.6 (3)	C28—C29—C30—C25	0.0
I1^{i}—Cu1—P1—C13	−72.9 (2)	C26—C25—C30—C29	0.0
I1—Cu1—P1—C13	43.0 (2)	P2—C25—C30—C29	−175.6 (4)
I2—Cu1—P1—C13	167.5 (2)	C19—P2—C31—C32	−41.9 (8)
Cu2—Cu1—P1—C13	106.5 (2)	C25—P2—C31—C32	69.2 (7)
Cu2^{i}—Cu1—P1—C13	−132.7 (2)	Cu2—P2—C31—C32	−163.6 (6)
I2—Cu2—P2—C31	−57.8 (3)	C19—P2—C31—C36	177.8 (6)
I1—Cu2—P2—C31	73.9 (3)	C25—P2—C31—C36	−71.1 (6)
I2^{i}—Cu2—P2—C31	−173.5 (3)	Cu2—P2—C31—C36	56.1 (7)
Cu1—Cu2—P2—C31	18.2 (4)	C36—C31—C32—C33	−40.0 (11)
Cu1^{i}—Cu2—P2—C31	131.5 (3)	P2—C31—C32—C33	−179.8 (7)
Cu2^{i}—Cu2—P2—C31	−131.6 (3)	C31—C32—C33—C34	42.1 (11)
I2—Cu2—P2—C19	−176.71 (19)	C32—C33—C34—C35	−44.2 (12)
I1—Cu2—P2—C19	−45.0 (2)	C33—C34—C35—C36	44.2 (12)
I2^{i}—Cu2—P2—C19	67.6 (2)	C32—C31—C36—C35	40.6 (11)

Cu1—Cu2—P2—C19	−100.7 (2)	P2—C31—C36—C35	−177.9 (7)
Cu1^{i}—Cu2—P2—C19	12.7 (2)	C34—C35—C36—C31	−42.5 (12)
Cu2^{i}—Cu2—P2—C19	109.5 (2)		

Symmetry code: (i) −*x*+1, *y*, −*z*+3/2.