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Di-μ-iodo-1κI:2κI-tris(tri-*m*-tolylphosphine)-1$\kappa^2 P,P'$:2$\kappa P''$-dicopper(I): a new polymorph

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Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.004 Å
R factor = 0.031
wR factor = 0.075
Data-to-parameter ratio = 20.3

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

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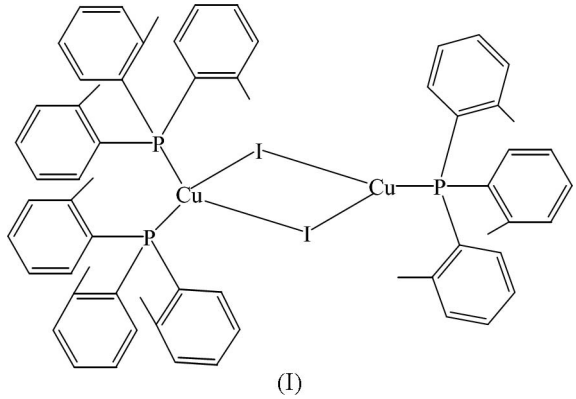
The structure of the title compound, $[Cu_2I_2(C_{21}H_{21}P)_3]$, was redetermined at low temperature (150 K) and shown to be a new triclinic polymorph.

Comment

The title compound, (I), is a binuclear copper(I) complex, in which the Cu atoms are bridged by two I atoms. A total of three molecules of tri-*m*-tolylphosphine are coordinated to the two copper centres. The structure of the same compound was reported by Akrivos *et al.* (1993) and shown also to be triclinic, space group $P\overline{1}$. This polymorph, (II), has a significantly longer *c* axis [24.635 Å compared to 19.0630 (3) Å for the present structure, (I)] and slightly smaller cell angles, considering the reduced cells of both polymorphs.



(I)

The molecular structure of (I) is illustrated in Fig. 1 and selected bond distances and angles are given in Table 1. In (I), atom Cu1 is coordinated by one P atom (P1), and atom Cu2 is coordinated by two P atoms (P2 and P3). The copper centres are bridged by two I atoms. The intramolecular Cu···Cu distance of 2.9551 (4) Å is decreased by *ca* 0.05 Å compared with that in (II). An interesting difference between the two polymorphs is that the Cu—I distances are inverted. That is, in (I), the Cu1—I distances average 2.5544 (1) Å and the Cu2—I distances average 2.750 (1) Å. This is exactly the opposite situation in polymorph (II) where the corresponding average distances are 2.767 and 2.549 Å, respectively. The Cu—I—Cu angles are very similar. The dihedral angle between the Cu1/I1/I2 and Cu2/I1/I2 planes of 3.75 (12)° is smaller than the value of 8.56° in polymorph (II).

Experimental

A suspension of tri-*m*-tolylphosphine (0.310 g, 1 mmol) and copper(I) iodide (0.382 g, 2 mmol) in 2-propanol (50 ml) was refluxed

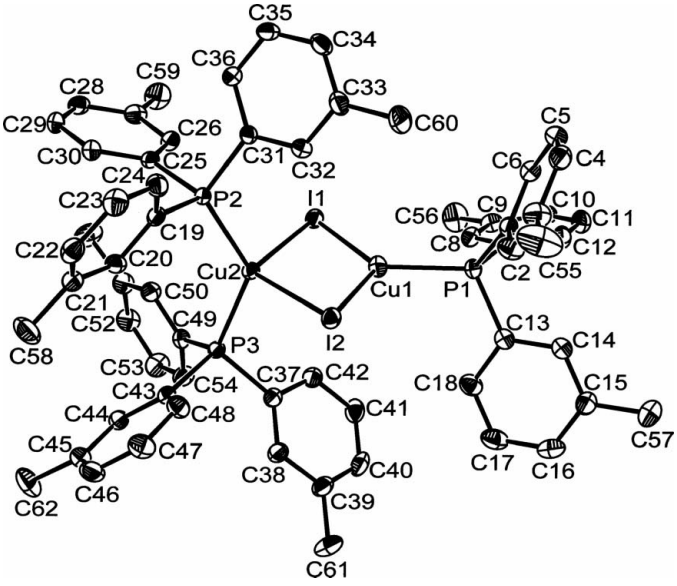


Figure 1
View of the molecular structure of compound (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity.

for 16 h. The resulting solution was filtered while hot. Slow evaporation of the solvent at room temperature gave colourless crystals of (I).

Crystal data

$[Cu_2I_2(C_{21}H_{21}P)_3]$
M_r = 1293.92
Triclinic, $P\overline{1}$
a = 11.6770 (1) Å
b = 13.5461 (1) Å
c = 19.0630 (3) Å
α = 86.0220 (5)°
β = 86.1216 (5)°
γ = 72.6081 (5)°
V = 2867.07 (6) Å^3
Z = 2
D_x = 1.499 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 12975 reflections
θ = 2.9–27.5°
μ = 1.94 mm^{-1}
T = 150 (2) K
Prism, colourless
0.20 × 0.15 × 0.15 mm

Data collection

Nonius KappaCCD diffractometer
ω scans
Absorption correction: multi-scan (Blessing, 1995)
T_{min} = 0.690, T_{max} = 0.749
40258 measured reflections
12975 independent reflections
11475 reflections with $I > 2\sigma(I)$
R_{int} = 0.045
θ_{max} = 27.6°
$h = -15 \rightarrow 15$
$k = -17 \rightarrow 17$
$l = -24 \rightarrow 24$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.075
S = 1.03
12975 reflections
640 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0251P)^2 + 3.1211P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.70 e Å^{-3}
$\Delta\rho_{min}$ = −1.18 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1···Cu2	2.9551 (4)	Cu1—I2	2.5481 (4)
Cu1—P1	2.2298 (7)	Cu2—P3	2.2737 (7)
Cu2—P2	2.2687 (7)	Cu2—I2	2.7454 (3)
Cu1—I1	2.5403 (3)	Cu2—I1	2.7548 (3)
P1—Cu1—I1	126.33 (2)	P2—Cu2—I1	102.441 (19)
P1—Cu1—I2	114.78 (2)	P3—Cu2—I1	106.48 (2)
I1—Cu1—I2	118.859 (12)	I2—Cu2—I1	105.603 (10)
P2—Cu2—P3	130.66 (2)	Cu1—I1—Cu2	67.706 (10)
P2—Cu2—I2	109.470 (19)	Cu1—I2—Cu2	67.750 (10)
P3—Cu2—I2	100.138 (19)		

The H atoms were placed in calculated positions (aromatic C—H = 0.95 Å and methyl C—H = 0.98 Å), and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(aromatic C) and 1.5U_{eq}(methyl C). The deepest electron-density hole lies 0.86 Å from atom I2.

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, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP3* for Windows (Farrugia, 1997); software used to prepare material for publication: *WinGX* publication routines (Farrugia, 1999).

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$h = -15 \rightarrow 15$
$k = -17 \rightarrow 17$
$l = -24 \rightarrow 24$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.075$
$S = 1.04$
12975 reflections
640 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
$w = 1/[\sigma^2(F_o^2) + (0.0251P)^2 + 3.1211P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.70$ e Å^{-3}
$\Delta\rho_{min} = -1.18$ 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}
Cu1	0.02400 (3)	0.68868 (2)	0.222661 (17)	0.02206 (7)
Cu2	0.18389 (3)	0.47977 (2)	0.259583 (15)	0.01785 (7)
I1	0.227543 (14)	0.621073 (12)	0.158303 (8)	0.02103 (5)
I2	−0.043049 (14)	0.570632 (12)	0.315865 (8)	0.02136 (5)
P1	−0.11002 (6)	0.84307 (5)	0.20347 (3)	0.01869 (13)
P2	0.18148 (5)	0.34616 (4)	0.19479 (3)	0.01582 (12)
P3	0.29469 (5)	0.48396 (5)	0.35232 (3)	0.01645 (12)
C1	−0.2436 (2)	0.83248 (18)	0.16363 (13)	0.0198 (5)
C2	−0.3266 (2)	0.7964 (2)	0.20524 (15)	0.0283 (6)
H2	−0.3144	0.7807	0.2540	0.034*
C3	−0.4274 (3)	0.7826 (2)	0.17687 (16)	0.0320 (6)
C4	−0.4430 (2)	0.8056 (2)	0.10510 (16)	0.0298 (6)
H4	−0.5118	0.7977	0.0850	0.036*
C5	−0.3608 (2)	0.8396 (2)	0.06292 (15)	0.0277 (6)
H5	−0.3725	0.8538	0.0140	0.033*
C6	−0.2601 (2)	0.8534 (2)	0.09170 (14)	0.0239 (5)
H6	−0.2032	0.8768	0.0625	0.029*
C7	−0.0631 (2)	0.94051 (19)	0.14778 (13)	0.0212 (5)
C8	0.0591 (2)	0.9217 (2)	0.13164 (14)	0.0231 (5)
H8	0.1136	0.8579	0.1473	0.028*
C9	0.1032 (2)	0.9950 (2)	0.09279 (14)	0.0260 (5)
C10	0.0222 (3)	1.0862 (2)	0.06877 (14)	0.0271 (6)
H10	0.0507	1.1358	0.0410	0.033*
C11	−0.1000 (3)	1.1064 (2)	0.08466 (15)	0.0301 (6)
H11	−0.1545	1.1696	0.0681	0.036*
C12	−0.1426 (2)	1.0346 (2)	0.12452 (15)	0.0264 (6)
H12	−0.2262	1.0493	0.1362	0.032*
C13	−0.1705 (2)	0.91254 (19)	0.28297 (13)	0.0209 (5)
C14	−0.2815 (3)	0.9893 (2)	0.28606 (14)	0.0281 (6)
H14	−0.3308	1.0025	0.2468	0.034*
C15	−0.3212 (3)	1.0467 (2)	0.34530 (15)	0.0300 (6)
C16	−0.2471 (3)	1.0253 (2)	0.40261 (15)	0.0329 (6)
H16	−0.2724	1.0637	0.4436	0.039*
C17	−0.1380 (3)	0.9494 (2)	0.40034 (15)	0.0341 (7)
H17	−0.0889	0.9361	0.4397	0.041*

C18	−0.0991 (2)	0.8920 (2)	0.34097 (14)	0.0269 (6)
H18	−0.0242	0.8391	0.3400	0.032*
C19	0.1394 (2)	0.24248 (18)	0.24624 (13)	0.0180 (5)
C20	0.2018 (2)	0.20238 (19)	0.30726 (13)	0.0213 (5)
H20	0.2592	0.2329	0.3218	0.026*
C21	0.1811 (2)	0.11864 (19)	0.34683 (14)	0.0243 (5)
C22	0.0925 (3)	0.0782 (2)	0.32641 (15)	0.0269 (6)
H22	0.0764	0.0217	0.3533	0.032*
C23	0.0276 (3)	0.1189 (2)	0.26755 (16)	0.0287 (6)
H23	−0.0332	0.0911	0.2548	0.034*
C24	0.0515 (2)	0.20046 (19)	0.22717 (14)	0.0243 (5)
H24	0.0077	0.2277	0.1864	0.029*
C25	0.3255 (2)	0.27565 (18)	0.15097 (13)	0.0185 (5)
C26	0.3856 (2)	0.33232 (19)	0.10718 (13)	0.0226 (5)
H26	0.3516	0.4053	0.1016	0.027*
C27	0.4941 (2)	0.2855 (2)	0.07115 (14)	0.0250 (5)
C28	0.5417 (2)	0.1781 (2)	0.08010 (14)	0.0268 (6)
H28	0.6153	0.1441	0.0558	0.032*
C29	0.4840 (2)	0.1204 (2)	0.12348 (14)	0.0265 (6)
H29	0.5185	0.0475	0.1292	0.032*
C30	0.3752 (2)	0.16838 (19)	0.15912 (14)	0.0234 (5)
H30	0.3352	0.1283	0.1887	0.028*
C31	0.0775 (2)	0.37619 (17)	0.12307 (13)	0.0182 (5)
C32	−0.0362 (2)	0.44460 (19)	0.13600 (13)	0.0222 (5)
H32	−0.0546	0.4772	0.1796	0.027*
C33	−0.1240 (2)	0.4663 (2)	0.08607 (14)	0.0255 (6)
C34	−0.0950 (3)	0.4191 (2)	0.02232 (15)	0.0277 (6)
H34	−0.1538	0.4327	−0.0121	0.033*
C35	0.0187 (3)	0.3524 (2)	0.00824 (14)	0.0275 (6)
H35	0.0375	0.3214	−0.0359	0.033*
C36	0.1053 (2)	0.33065 (19)	0.05824 (13)	0.0229 (5)
H36	0.1831	0.2849	0.0483	0.027*
C37	0.2461 (2)	0.60925 (19)	0.39297 (13)	0.0197 (5)
C38	0.2003 (2)	0.6222 (2)	0.46267 (14)	0.0253 (5)
H38	0.1951	0.5635	0.4916	0.030*
C39	0.1622 (2)	0.7206 (2)	0.49025 (15)	0.0294 (6)
C40	0.1715 (2)	0.8049 (2)	0.44737 (16)	0.0305 (6)
H40	0.1461	0.8719	0.4656	0.037*
C41	0.2171 (2)	0.7934 (2)	0.37836 (16)	0.0288 (6)
H41	0.2236	0.8521	0.3499	0.035*
C42	0.2533 (2)	0.69572 (19)	0.35087 (14)	0.0236 (5)
H42	0.2830	0.6880	0.3033	0.028*
C43	0.2905 (2)	0.39208 (18)	0.42685 (13)	0.0194 (5)
C44	0.3925 (2)	0.33842 (19)	0.46361 (13)	0.0222 (5)
H44	0.4681	0.3478	0.4490	0.027*
C45	0.3844 (3)	0.2713 (2)	0.52159 (14)	0.0269 (6)
C46	0.2734 (3)	0.2609 (2)	0.54365 (14)	0.0297 (6)
H46	0.2666	0.2173	0.5840	0.036*

C47	0.1710 (3)	0.3134 (2)	0.50753 (15)	0.0315 (6)
H47	0.0952	0.3054	0.5232	0.038*
C48	0.1800 (2)	0.3773 (2)	0.44865 (14)	0.0254 (5)
H48	0.1108	0.4111	0.4231	0.031*
C49	0.4546 (2)	0.46600 (18)	0.33277 (13)	0.0197 (5)
C50	0.5121 (2)	0.4002 (2)	0.27961 (14)	0.0225 (5)
H50	0.4666	0.3686	0.2540	0.027*
C51	0.6352 (2)	0.3798 (2)	0.26323 (15)	0.0271 (6)
C52	0.6989 (2)	0.4300 (2)	0.29944 (16)	0.0312 (6)
H52	0.7821	0.4187	0.2880	0.037*
C53	0.6430 (2)	0.4965 (2)	0.35200 (17)	0.0323 (6)
H53	0.6880	0.5303	0.3761	0.039*
C54	0.5215 (2)	0.5139 (2)	0.36954 (15)	0.0271 (6)
H54	0.4839	0.5580	0.4063	0.033*
C55	−0.5157 (3)	0.7432 (4)	0.2231 (2)	0.0585 (11)
H55A	−0.4722	0.6821	0.2516	0.088*
H55B	−0.5708	0.7244	0.1937	0.088*
H55C	−0.5616	0.7974	0.2542	0.088*
C56	0.2361 (3)	0.9739 (3)	0.07822 (19)	0.0426 (8)
H56A	0.2563	1.0393	0.0759	0.064*
H56B	0.2596	0.9407	0.0332	0.064*
H56C	0.2792	0.9279	0.1160	0.064*
C57	−0.4407 (3)	1.1296 (3)	0.34772 (19)	0.0551 (10)
H57A	−0.4822	1.1301	0.3046	0.083*
H57B	−0.4278	1.1972	0.3514	0.083*
H57C	−0.4899	1.1153	0.3887	0.083*
C58	0.2519 (3)	0.0731 (2)	0.41054 (17)	0.0416 (8)
H58A	0.3213	0.0152	0.3969	0.062*
H58B	0.2007	0.0481	0.4459	0.062*
H58C	0.2796	0.1263	0.4303	0.062*
C59	0.5570 (3)	0.3484 (3)	0.02395 (18)	0.0385 (7)
H59A	0.5100	0.3758	−0.0175	0.058*
H59B	0.6368	0.3044	0.0090	0.058*
H59C	0.5654	0.4059	0.0496	0.058*
C60	−0.2461 (3)	0.5430 (2)	0.10116 (18)	0.0379 (7)
H60A	−0.2386	0.5924	0.1344	0.057*
H60B	−0.3016	0.5058	0.1216	0.057*
H60C	−0.2770	0.5803	0.0572	0.057*
C61	0.1116 (3)	0.7333 (3)	0.56531 (17)	0.0474 (9)
H61A	0.1730	0.7411	0.5953	0.071*
H61B	0.0874	0.6721	0.5821	0.071*
H61C	0.0415	0.7950	0.5673	0.071*
C62	0.4954 (3)	0.2123 (3)	0.55996 (18)	0.0446 (8)
H62A	0.4802	0.2219	0.6106	0.067*
H62B	0.5626	0.2384	0.5429	0.067*
H62C	0.5155	0.1385	0.5513	0.067*
C63	0.6979 (3)	0.3029 (3)	0.20892 (18)	0.0413 (8)
H63A	0.7559	0.3297	0.1801	0.062*

H63B	0.6384	0.2923	0.1787	0.062*
H63C	0.7402	0.2369	0.2327	0.062*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.01968 (15)	0.01962 (15)	0.02568 (17)	−0.00387 (12)	−0.00322 (12)	0.00026 (12)
Cu2	0.01795 (14)	0.01681 (14)	0.01847 (15)	−0.00368 (11)	−0.00283 (11)	−0.00348 (11)
I1	0.02303 (9)	0.01757 (8)	0.02112 (8)	−0.00433 (6)	0.00092 (6)	−0.00102 (6)
I2	0.01693 (8)	0.02201 (8)	0.02323 (9)	−0.00336 (6)	0.00141 (6)	−0.00133 (6)
P1	0.0156 (3)	0.0181 (3)	0.0212 (3)	−0.0033 (2)	−0.0020 (2)	0.0004 (2)
P2	0.0165 (3)	0.0140 (3)	0.0158 (3)	−0.0024 (2)	−0.0021 (2)	−0.0013 (2)
P3	0.0150 (3)	0.0169 (3)	0.0170 (3)	−0.0035 (2)	−0.0018 (2)	−0.0030 (2)
C1	0.0179 (11)	0.0183 (11)	0.0217 (12)	−0.0026 (9)	−0.0019 (9)	−0.0031 (9)
C2	0.0273 (14)	0.0367 (15)	0.0240 (14)	−0.0139 (12)	−0.0036 (11)	0.0000 (11)
C3	0.0280 (14)	0.0401 (16)	0.0310 (15)	−0.0146 (13)	−0.0012 (12)	−0.0036 (12)
C4	0.0227 (13)	0.0302 (14)	0.0357 (16)	−0.0038 (11)	−0.0075 (11)	−0.0092 (12)
C5	0.0280 (14)	0.0292 (14)	0.0245 (13)	−0.0046 (11)	−0.0069 (11)	−0.0040 (11)
C6	0.0236 (13)	0.0235 (12)	0.0229 (13)	−0.0042 (10)	−0.0002 (10)	−0.0033 (10)
C7	0.0247 (12)	0.0196 (11)	0.0186 (12)	−0.0053 (10)	−0.0012 (10)	−0.0016 (9)
C8	0.0221 (12)	0.0207 (12)	0.0261 (13)	−0.0051 (10)	−0.0005 (10)	−0.0035 (10)
C9	0.0287 (14)	0.0273 (13)	0.0234 (13)	−0.0101 (11)	0.0011 (11)	−0.0046 (10)
C10	0.0400 (16)	0.0219 (12)	0.0215 (13)	−0.0133 (12)	0.0008 (11)	0.0012 (10)
C11	0.0353 (15)	0.0201 (12)	0.0323 (15)	−0.0036 (11)	−0.0056 (12)	0.0007 (11)
C12	0.0242 (13)	0.0219 (12)	0.0297 (14)	−0.0017 (11)	−0.0033 (11)	0.0011 (10)
C13	0.0203 (12)	0.0206 (12)	0.0229 (13)	−0.0078 (10)	−0.0025 (10)	0.0009 (10)
C14	0.0285 (14)	0.0285 (14)	0.0231 (13)	−0.0015 (11)	−0.0049 (11)	−0.0006 (11)
C15	0.0320 (15)	0.0255 (13)	0.0272 (14)	−0.0010 (12)	0.0017 (11)	−0.0018 (11)
C16	0.0426 (17)	0.0374 (15)	0.0214 (14)	−0.0157 (14)	0.0031 (12)	−0.0080 (11)
C17	0.0341 (15)	0.0475 (17)	0.0236 (14)	−0.0151 (14)	−0.0070 (12)	−0.0036 (12)
C18	0.0221 (13)	0.0346 (14)	0.0247 (13)	−0.0093 (11)	−0.0032 (10)	0.0007 (11)
C19	0.0188 (11)	0.0151 (11)	0.0189 (12)	−0.0030 (9)	0.0008 (9)	−0.0028 (9)
C20	0.0250 (12)	0.0214 (12)	0.0182 (12)	−0.0075 (10)	−0.0030 (10)	−0.0016 (9)
C21	0.0296 (14)	0.0202 (12)	0.0203 (12)	−0.0034 (11)	0.0010 (10)	−0.0011 (10)
C22	0.0324 (14)	0.0193 (12)	0.0283 (14)	−0.0085 (11)	0.0068 (11)	−0.0008 (10)
C23	0.0274 (14)	0.0253 (13)	0.0368 (16)	−0.0121 (11)	−0.0038 (11)	−0.0030 (11)
C24	0.0259 (13)	0.0212 (12)	0.0266 (13)	−0.0071 (11)	−0.0068 (10)	−0.0004 (10)
C25	0.0180 (11)	0.0191 (11)	0.0171 (11)	−0.0024 (9)	−0.0034 (9)	−0.0041 (9)
C26	0.0215 (12)	0.0204 (12)	0.0236 (13)	−0.0025 (10)	−0.0004 (10)	−0.0039 (10)
C27	0.0192 (12)	0.0332 (14)	0.0230 (13)	−0.0075 (11)	−0.0010 (10)	−0.0048 (11)
C28	0.0172 (12)	0.0347 (14)	0.0219 (13)	0.0039 (11)	−0.0012 (10)	−0.0087 (11)
C29	0.0257 (13)	0.0213 (12)	0.0253 (13)	0.0051 (11)	−0.0039 (11)	−0.0032 (10)
C30	0.0245 (13)	0.0198 (12)	0.0228 (13)	−0.0013 (10)	−0.0031 (10)	−0.0013 (10)
C31	0.0233 (12)	0.0133 (10)	0.0178 (11)	−0.0048 (9)	−0.0040 (9)	0.0005 (9)
C32	0.0244 (13)	0.0221 (12)	0.0193 (12)	−0.0043 (10)	−0.0052 (10)	−0.0022 (9)
C33	0.0237 (13)	0.0220 (12)	0.0297 (14)	−0.0044 (11)	−0.0087 (11)	0.0022 (10)
C34	0.0335 (15)	0.0241 (13)	0.0260 (14)	−0.0074 (11)	−0.0144 (11)	0.0028 (10)
C35	0.0401 (16)	0.0248 (13)	0.0173 (12)	−0.0078 (12)	−0.0059 (11)	−0.0035 (10)

C36	0.0283 (13)	0.0181 (11)	0.0203 (12)	−0.0030 (10)	−0.0037 (10)	−0.0028 (9)
C37	0.0138 (11)	0.0225 (12)	0.0229 (12)	−0.0035 (9)	−0.0049 (9)	−0.0052 (10)
C38	0.0227 (13)	0.0267 (13)	0.0241 (13)	−0.0021 (11)	−0.0025 (10)	−0.0067 (10)
C39	0.0234 (13)	0.0326 (14)	0.0288 (14)	0.0006 (11)	−0.0058 (11)	−0.0136 (11)
C40	0.0223 (13)	0.0234 (13)	0.0435 (17)	0.0013 (11)	−0.0092 (12)	−0.0155 (12)
C41	0.0287 (14)	0.0204 (12)	0.0376 (16)	−0.0058 (11)	−0.0095 (12)	−0.0035 (11)
C42	0.0221 (12)	0.0231 (12)	0.0264 (13)	−0.0063 (10)	−0.0050 (10)	−0.0041 (10)
C43	0.0211 (12)	0.0173 (11)	0.0184 (12)	−0.0025 (10)	−0.0026 (9)	−0.0040 (9)
C44	0.0214 (12)	0.0225 (12)	0.0217 (12)	−0.0037 (10)	−0.0029 (10)	−0.0032 (10)
C45	0.0314 (14)	0.0244 (13)	0.0221 (13)	−0.0026 (11)	−0.0063 (11)	−0.0015 (10)
C46	0.0398 (16)	0.0301 (14)	0.0198 (13)	−0.0118 (12)	−0.0029 (11)	0.0026 (11)
C47	0.0294 (14)	0.0389 (16)	0.0279 (15)	−0.0134 (13)	−0.0007 (11)	0.0005 (12)
C48	0.0225 (12)	0.0295 (13)	0.0242 (13)	−0.0076 (11)	−0.0035 (10)	0.0018 (10)
C49	0.0175 (11)	0.0187 (11)	0.0220 (12)	−0.0040 (9)	−0.0018 (9)	0.0003 (9)
C50	0.0180 (12)	0.0247 (12)	0.0246 (13)	−0.0057 (10)	−0.0019 (10)	−0.0026 (10)
C51	0.0170 (12)	0.0336 (14)	0.0286 (14)	−0.0046 (11)	0.0002 (10)	−0.0023 (11)
C52	0.0167 (12)	0.0423 (16)	0.0342 (16)	−0.0080 (12)	−0.0018 (11)	−0.0026 (12)
C53	0.0216 (13)	0.0373 (15)	0.0413 (17)	−0.0115 (12)	−0.0054 (12)	−0.0081 (13)
C54	0.0214 (13)	0.0298 (14)	0.0298 (14)	−0.0054 (11)	−0.0015 (11)	−0.0088 (11)
C55	0.046 (2)	0.104 (3)	0.044 (2)	−0.051 (2)	−0.0043 (16)	0.003 (2)
C56	0.0286 (15)	0.0477 (19)	0.052 (2)	−0.0152 (14)	0.0056 (14)	0.0049 (15)
C57	0.054 (2)	0.050 (2)	0.0401 (19)	0.0180 (18)	0.0011 (16)	−0.0104 (16)
C58	0.060 (2)	0.0352 (16)	0.0309 (16)	−0.0160 (16)	−0.0163 (15)	0.0131 (13)
C59	0.0325 (16)	0.0418 (17)	0.0397 (18)	−0.0117 (14)	0.0107 (13)	−0.0016 (14)
C60	0.0269 (15)	0.0383 (16)	0.0429 (18)	0.0019 (13)	−0.0136 (13)	−0.0050 (14)
C61	0.055 (2)	0.0480 (19)	0.0313 (17)	−0.0004 (17)	0.0033 (15)	−0.0199 (15)
C62	0.0409 (18)	0.0473 (19)	0.0396 (18)	−0.0045 (15)	−0.0161 (15)	0.0151 (15)
C63	0.0239 (14)	0.053 (2)	0.0442 (19)	−0.0048 (14)	0.0050 (13)	−0.0191 (15)

Geometric parameters (Å, º)

Cu1—Cu2	2.9551 (4)	C30—H30	0.9500
Cu1—P1	2.2298 (7)	C31—C32	1.391 (3)
Cu2—P2	2.2687 (7)	C31—C36	1.395 (3)
Cu1—I1	2.5403 (3)	C32—C33	1.399 (3)
Cu1—I2	2.5481 (4)	C32—H32	0.9500
Cu1—Cu2	2.9551 (4)	C33—C34	1.387 (4)
Cu2—P3	2.2737 (7)	C33—C60	1.514 (4)
Cu2—I2	2.7454 (3)	C34—C35	1.385 (4)
Cu2—I1	2.7548 (3)	C34—H34	0.9500
P1—C7	1.824 (3)	C35—C36	1.390 (4)
P1—C13	1.827 (3)	C35—H35	0.9500
P1—C1	1.827 (3)	C36—H36	0.9500
P2—C19	1.825 (3)	C37—C42	1.394 (4)
P2—C31	1.833 (2)	C37—C38	1.401 (4)
P2—C25	1.844 (2)	C38—C39	1.401 (4)
P3—C49	1.826 (3)	C38—H38	0.9500
P3—C37	1.830 (2)	C39—C40	1.384 (4)

P3—C43	1.831 (3)	C39—C61	1.512 (4)
C1—C2	1.391 (4)	C40—C41	1.387 (4)
C1—C6	1.395 (4)	C40—H40	0.9500
C2—C3	1.394 (4)	C41—C42	1.391 (4)
C2—H2	0.9500	C41—H41	0.9500
C3—C4	1.394 (4)	C42—H42	0.9500
C3—C55	1.505 (5)	C43—C48	1.396 (4)
C4—C5	1.375 (4)	C43—C44	1.401 (3)
C4—H4	0.9500	C44—C45	1.399 (4)
C5—C6	1.397 (4)	C44—H44	0.9500
C5—H5	0.9500	C45—C46	1.380 (4)
C6—H6	0.9500	C45—C62	1.511 (4)
C7—C8	1.389 (4)	C46—C47	1.394 (4)
C7—C12	1.398 (3)	C46—H46	0.9500
C8—C9	1.396 (4)	C47—C48	1.387 (4)
C8—H8	0.9500	C47—H47	0.9500
C9—C10	1.383 (4)	C48—H48	0.9500
C9—C56	1.502 (4)	C49—C50	1.395 (3)
C10—C11	1.387 (4)	C49—C54	1.401 (4)
C10—H10	0.9500	C50—C51	1.399 (4)
C11—C12	1.380 (4)	C50—H50	0.9500
C11—H11	0.9500	C51—C52	1.388 (4)
C12—H12	0.9500	C51—C63	1.511 (4)
C13—C18	1.393 (4)	C52—C53	1.388 (4)
C13—C14	1.399 (4)	C52—H52	0.9500
C14—C15	1.389 (4)	C53—C54	1.388 (4)
C14—H14	0.9500	C53—H53	0.9500
C15—C16	1.400 (4)	C54—H54	0.9500
C15—C57	1.507 (4)	C55—H55A	0.9800
C16—C17	1.378 (4)	C55—H55B	0.9800
C16—H16	0.9500	C55—H55C	0.9800
C17—C18	1.390 (4)	C56—H56A	0.9800
C17—H17	0.9500	C56—H56B	0.9800
C18—H18	0.9500	C56—H56C	0.9800
C19—C24	1.392 (4)	C57—H57A	0.9800
C19—C20	1.404 (3)	C57—H57B	0.9800
C20—C21	1.391 (4)	C57—H57C	0.9800
C20—H20	0.9500	C58—H58A	0.9800
C21—C22	1.394 (4)	C58—H58B	0.9800
C21—C58	1.505 (4)	C58—H58C	0.9800
C22—C23	1.385 (4)	C59—H59A	0.9800
C22—H22	0.9500	C59—H59B	0.9800
C23—C24	1.388 (4)	C59—H59C	0.9800
C23—H23	0.9500	C60—H60A	0.9800
C24—H24	0.9500	C60—H60B	0.9800
C25—C26	1.390 (4)	C60—H60C	0.9800
C25—C30	1.396 (3)	C61—H61A	0.9800
C26—C27	1.394 (4)	C61—H61B	0.9800

C26—H26	0.9500	C61—H61C	0.9800
C27—C28	1.396 (4)	C62—H62A	0.9800
C27—C59	1.501 (4)	C62—H62B	0.9800
C28—C29	1.378 (4)	C62—H62C	0.9800
C28—H28	0.9500	C63—H63A	0.9800
C29—C30	1.397 (4)	C63—H63B	0.9800
C29—H29	0.9500	C63—H63C	0.9800

P1—Cu1—I1	126.33 (2)	C32—C31—C36	119.2 (2)
P1—Cu1—I2	114.78 (2)	C32—C31—P2	117.46 (18)
I1—Cu1—I2	118.859 (12)	C36—C31—P2	123.32 (19)
P1—Cu1—Cu2	174.07 (2)	C31—C32—C33	121.3 (2)
I1—Cu1—Cu2	59.603 (9)	C31—C32—H32	119.3
I2—Cu1—Cu2	59.302 (9)	C33—C32—H32	119.3
P2—Cu2—P3	130.66 (2)	C34—C33—C32	118.5 (2)
P2—Cu2—I2	109.470 (19)	C34—C33—C60	121.4 (2)
P3—Cu2—I2	100.138 (19)	C32—C33—C60	120.0 (2)
P2—Cu2—I1	102.441 (19)	C35—C34—C33	120.7 (2)
P3—Cu2—I1	106.48 (2)	C35—C34—H34	119.6
I2—Cu2—I1	105.603 (10)	C33—C34—H34	119.6
P2—Cu2—Cu1	118.613 (19)	C34—C35—C36	120.5 (2)
P3—Cu2—Cu1	110.716 (19)	C34—C35—H35	119.8
I2—Cu2—Cu1	52.948 (9)	C36—C35—H35	119.8
I1—Cu2—Cu1	52.691 (9)	C35—C36—C31	119.8 (2)
Cu1—I1—Cu2	67.706 (10)	C35—C36—H36	120.1
Cu1—I2—Cu2	67.750 (10)	C31—C36—H36	120.1
C7—P1—C13	102.16 (11)	C42—C37—C38	119.3 (2)
C7—P1—C1	104.81 (12)	C42—C37—P3	117.19 (19)
C13—P1—C1	103.52 (11)	C38—C37—P3	123.5 (2)
C7—P1—Cu1	118.29 (8)	C37—C38—C39	120.8 (3)
C13—P1—Cu1	114.52 (8)	C37—C38—H38	119.6
C1—P1—Cu1	111.95 (8)	C39—C38—H38	119.6
C19—P2—C31	102.78 (11)	C40—C39—C38	118.7 (3)
C19—P2—C25	102.26 (11)	C40—C39—C61	121.3 (3)
C31—P2—C25	102.94 (11)	C38—C39—C61	120.1 (3)
C19—P2—Cu2	113.61 (8)	C39—C40—C41	121.3 (2)
C31—P2—Cu2	116.89 (8)	C39—C40—H40	119.3
C25—P2—Cu2	116.38 (8)	C41—C40—H40	119.3
C49—P3—C37	102.41 (11)	C40—C41—C42	119.8 (3)
C49—P3—C43	104.20 (11)	C40—C41—H41	120.1
C37—P3—C43	103.00 (11)	C42—C41—H41	120.1
C49—P3—Cu2	116.33 (8)	C41—C42—C37	120.1 (3)
C37—P3—Cu2	112.46 (8)	C41—C42—H42	119.9
C43—P3—Cu2	116.65 (8)	C37—C42—H42	119.9
C2—C1—C6	119.4 (2)	C48—C43—C44	119.0 (2)
C2—C1—P1	119.05 (19)	C48—C43—P3	118.13 (18)
C6—C1—P1	121.4 (2)	C44—C43—P3	122.8 (2)
C1—C2—C3	121.4 (3)	C45—C44—C43	120.9 (3)

C1—C2—H2	119.3	C45—C44—H44	119.6
C3—C2—H2	119.3	C43—C44—H44	119.6
C2—C3—C4	118.2 (3)	C46—C45—C44	119.0 (2)
C2—C3—C55	120.3 (3)	C46—C45—C62	120.7 (3)
C4—C3—C55	121.5 (3)	C44—C45—C62	120.4 (3)
C5—C4—C3	121.2 (3)	C45—C46—C47	120.9 (3)
C5—C4—H4	119.4	C45—C46—H46	119.5
C3—C4—H4	119.4	C47—C46—H46	119.5
C4—C5—C6	120.3 (3)	C48—C47—C46	119.9 (3)
C4—C5—H5	119.9	C48—C47—H47	120.0
C6—C5—H5	119.9	C46—C47—H47	120.0
C1—C6—C5	119.5 (3)	C47—C48—C43	120.2 (2)
C1—C6—H6	120.2	C47—C48—H48	119.9
C5—C6—H6	120.2	C43—C48—H48	119.9
C8—C7—C12	119.0 (2)	C50—C49—C54	119.2 (2)
C8—C7—P1	117.51 (19)	C50—C49—P3	117.99 (19)
C12—C7—P1	123.4 (2)	C54—C49—P3	122.79 (19)
C7—C8—C9	121.2 (2)	C49—C50—C51	121.3 (2)
C7—C8—H8	119.4	C49—C50—H50	119.3
C9—C8—H8	119.4	C51—C50—H50	119.3
C10—C9—C8	118.6 (3)	C52—C51—C50	118.3 (3)
C10—C9—C56	121.5 (3)	C52—C51—C63	120.9 (2)
C8—C9—C56	119.9 (3)	C50—C51—C63	120.8 (3)
C9—C10—C11	121.0 (3)	C53—C52—C51	121.1 (3)
C9—C10—H10	119.5	C53—C52—H52	119.4
C11—C10—H10	119.5	C51—C52—H52	119.4
C12—C11—C10	120.1 (2)	C54—C53—C52	120.3 (3)
C12—C11—H11	120.0	C54—C53—H53	119.8
C10—C11—H11	120.0	C52—C53—H53	119.8
C11—C12—C7	120.2 (3)	C53—C54—C49	119.7 (3)
C11—C12—H12	119.9	C53—C54—H54	120.1
C7—C12—H12	119.9	C49—C54—H54	120.1
C18—C13—C14	119.3 (2)	C3—C55—H55A	109.5
C18—C13—P1	117.98 (19)	C3—C55—H55B	109.5
C14—C13—P1	122.60 (19)	H55A—C55—H55B	109.5
C15—C14—C13	121.5 (2)	C3—C55—H55C	109.5
C15—C14—H14	119.3	H55A—C55—H55C	109.5
C13—C14—H14	119.3	H55B—C55—H55C	109.5
C14—C15—C16	118.1 (3)	C9—C56—H56A	109.5
C14—C15—C57	120.9 (3)	C9—C56—H56B	109.5
C16—C15—C57	121.0 (3)	H56A—C56—H56B	109.5
C17—C16—C15	120.9 (3)	C9—C56—H56C	109.5
C17—C16—H16	119.5	H56A—C56—H56C	109.5
C15—C16—H16	119.5	H56B—C56—H56C	109.5
C16—C17—C18	120.6 (3)	C15—C57—H57A	109.5
C16—C17—H17	119.7	C15—C57—H57B	109.5
C18—C17—H17	119.7	H57A—C57—H57B	109.5
C17—C18—C13	119.6 (3)	C15—C57—H57C	109.5

C17—C18—H18	120.2	H57A—C57—H57C	109.5
C13—C18—H18	120.2	H57B—C57—H57C	109.5
C24—C19—C20	119.1 (2)	C21—C58—H58A	109.5
C24—C19—P2	123.49 (19)	C21—C58—H58B	109.5
C20—C19—P2	117.40 (19)	H58A—C58—H58B	109.5
C21—C20—C19	121.1 (2)	C21—C58—H58C	109.5
C21—C20—H20	119.5	H58A—C58—H58C	109.5
C19—C20—H20	119.5	H58B—C58—H58C	109.5
C20—C21—C22	118.5 (2)	C27—C59—H59A	109.5
C20—C21—C58	120.9 (3)	C27—C59—H59B	109.5
C22—C21—C58	120.7 (3)	H59A—C59—H59B	109.5
C23—C22—C21	121.1 (2)	C27—C59—H59C	109.5
C23—C22—H22	119.4	H59A—C59—H59C	109.5
C21—C22—H22	119.4	H59B—C59—H59C	109.5
C22—C23—C24	120.0 (3)	C33—C60—H60A	109.5
C22—C23—H23	120.0	C33—C60—H60B	109.5
C24—C23—H23	120.0	H60A—C60—H60B	109.5
C23—C24—C19	120.2 (2)	C33—C60—H60C	109.5
C23—C24—H24	119.9	H60A—C60—H60C	109.5
C19—C24—H24	119.9	H60B—C60—H60C	109.5
C26—C25—C30	119.1 (2)	C39—C61—H61A	109.5
C26—C25—P2	118.06 (18)	C39—C61—H61B	109.5
C30—C25—P2	122.8 (2)	H61A—C61—H61B	109.5
C25—C26—C27	122.1 (2)	C39—C61—H61C	109.5
C25—C26—H26	119.0	H61A—C61—H61C	109.5
C27—C26—H26	119.0	H61B—C61—H61C	109.5
C26—C27—C28	117.7 (3)	C45—C62—H62A	109.5
C26—C27—C59	121.1 (3)	C45—C62—H62B	109.5
C28—C27—C59	121.2 (2)	H62A—C62—H62B	109.5
C29—C28—C27	121.2 (2)	C45—C62—H62C	109.5
C29—C28—H28	119.4	H62A—C62—H62C	109.5
C27—C28—H28	119.4	H62B—C62—H62C	109.5
C28—C29—C30	120.5 (2)	C51—C63—H63A	109.5
C28—C29—H29	119.8	C51—C63—H63B	109.5
C30—C29—H29	119.8	H63A—C63—H63B	109.5
C25—C30—C29	119.5 (3)	C51—C63—H63C	109.5
C25—C30—H30	120.3	H63A—C63—H63C	109.5
C29—C30—H30	120.3	H63B—C63—H63C	109.5