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Tetrakis(triphenylarsine)copper(I) hexafluoridophosphate

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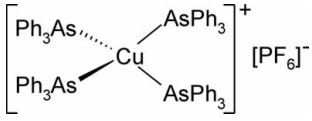
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.007 Å; R factor = 0.037; wR factor = 0.097; data-to-parameter ratio = 15.9.

In the crystal structure of the title compound, $[Cu(C_{18}H_{15}As)_4]PF_6$, the Cu atom is coordinated by four As atoms of triphenylarsine ligands in a tetrahedral geometry. The complex cation is located on a crystallographic threefold axis. Both PF_6^- anions are located on special positions of site symmetry $\overline{3}$. The Cu—As bond of the independent arsine ligand is shorter than the Cu—As bonds of the three symmetry-related arsine ligands.

Related literature

For related literature, see: Bowmaker *et al.* (1990); Engelhardt *et al.* (1985).



Experimental

Crystal data

$[Cu(C_{18}H_{15}As)_4]PF_6$
M_r = 1433.40
Trigonal, $R\overline{3}$
a = 14.4025 (10) Å
c = 52.015 (4) Å
V = 9344.1 (12) Å^3
Z = 6
Mo $K\alpha$ radiation
μ = 2.55 mm^{-1}
T = 296 K
0.14 × 0.12 × 0.10 mm

Data collection

Stoe IPDS diffractometer
Absorption correction: refined from ΔF (Walker & Stuart, 1983)
T_{min} = 0.349, T_{max} = 0.769
23664 measured reflections
4049 independent reflections
3118 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.097
S = 1.04
4049 reflections
254 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.77 e Å^{-3}
$\Delta\rho_{min}$ = −0.62 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

As1—Cu1	2.5472 (5)	As1—C13	1.958 (5)
As1—C1	1.959 (4)	As2—Cu1	2.5044 (9)
As1—C7	1.956 (3)	As2—C19	1.950 (4)
Cu1—As1—C1	112.61 (13)	C7—As1—C13	99.85 (17)
Cu1—As1—C7	117.80 (13)	Cu1—As2—C19	117.96 (10)
Cu1—As1—C13	122.35 (11)	C19—As2—C19^{i}	99.81 (18)
C1—As1—C7	101.64 (15)	As1—Cu1—As2	109.30 (2)
C1—As1—C13	99.19 (17)	As1—Cu1—As1^{i}	109.65 (2)

Symmetry codes: (i) $-y+1, x-y, z$; (ii) $-y, x-y, z$; (iii) $-x, -y, -z$; (iv) $-x+y+2, -x+2, z$; (v) $x-y+\frac{2}{3}, x-\frac{2}{3}, -z+\frac{1}{3}$.

Data collection: *IPDS Software* (Stoe, 1998); cell refinement: *IPDS Software*; data reduction: *IPDS Software*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2651).

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supplementary materials

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Tetrakis(triphenylarsine)copper(I) hexafluoridophosphate

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Comment

Crystals of the title compound were obtained as a side-product in the preparation of [(Ph-BIAN)Cu(I)(Ph_3As)$_2$][PF_6] (Ph-BIAN = Bis(phenyl-imino)acenaphthene) in methylene chloride solution. To identify this compound a single-crystal structure analysis was performed.

The title compound contains $[(Ph_3As)_4Cu]^+$ ions which are disposed about crystallographic threefold axes, the metal atom lying on a special position of symmetry *3* is coordinated by two independent ligands. One of it is totally independent, whereas the other three are symmetry-related completing the nearly regular tetrahedral environment of the copper atom. The bond angles are 109.30 (2) and 109.65 (2) ° for As1—Cu1—As2 and As1—Cu1—As1', respectively. Two independent phosphorus and fluorine atoms are found. The Cu—As2 bond of the independent (axial) arsine ligand is significantly shorter than the value for the off-axis Cu—As1 bonds (2.5044 (9) *versus* 2.5472 (5) Å). A similar distortion was previously found for the analogous salts $[(Ph_3P)_4Cu]^+$ (with ClO_4^- or PF_6^- as anions), which also crystallize in the same space group (Bowmaker *et al.*, 1990, Engelhardt *et al.*, 1985).

Experimental

The title compound was isolated as a side-product in the preparation of [(Ph-BIAN)Cu(I)(Ph_3As)$_2$][PF_6] (Ph-BIAN = Bis(phenyl-imino)acenaphthene). [Cu(NCMe)$_4$]PF_6 (50 mg, 0.13 mmol) and Ph_3As (93 mg, 0.30 mmol) was stirred in methylene chloride (10 ml) for 2 h. Ph-BIAN (51 mg, 0.15 mmol) was added and stirring was continued for another 2 h. The product was precipitated with pentane. Slow diffusion of diethyl ether into a methylene chloride solution of the product mixture yielded a dark powder and the title compound as colourless crystals. To identify the colourless crystals a single-crystal analysis was performed.

Refinement

The H-atoms were calculated geometrically and refined using a riding model with C—H = 0.93Å and U(H) = 1.2U_{eq}(C).

Figures

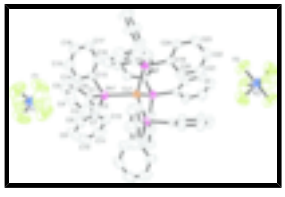


Fig. 1. : View of the title compound with the atom numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level.

Tetrakis(triphenylarsine)copper(I) hexafluoridophosphate

Crystal data

$[Cu(C_{18}H_{15}As)_4]PF_6$	$Z = 6$
$M_r = 1433.40$	$F_{000} = 4332$
Trigonal, $R\overline{3}$	Cell parameters were determined by indexing 8000 reflections with I/sigma limit 6.0.
Hall symbol: -R 3	$D_x = 1.528$ Mg m^{-3}
$a = 14.4025$ (10) Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$b = 14.4025$ (10) Å	Cell parameters from 8000 reflections
$c = 52.015$ (4) Å	$\theta = 2.4$–25.9º
$\alpha = 90$º	$\mu = 2.55$ mm^{-1}
$\beta = 90$º	$T = 296$ K
$\gamma = 120$º	Prism, light yellow, translucent
$V = 9344.1$ (12) Å^3	0.14 × 0.12 × 0.10 mm

Data collection

Stoe IPDS diffractometer	4049 independent reflections
Radiation source: fine-focus sealed tube	3118 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.032$
$T = 296(1)$ K	$\theta_{max} = 25.9$º
rotation scans	$\theta_{min} = 2.4$º
Absorption correction: part of the refinement model (ΔF) refined from delta-F (Walker & Stuart, 1983)	$h = -17 \rightarrow 17$
$T_{min} = 0.349$, $T_{max} = 0.769$	$k = -17 \rightarrow 17$
23664 measured reflections	$l = -63 \rightarrow 61$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.037$	H-atom parameters constrained
$wR(F^2) = 0.097$	$w = 1/[\sigma^2(F_o^2) + (0.P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} = 0.001$
4049 reflections	$\Delta\rho_{max} = 1.77$ e Å^{-3}
254 parameters	$\Delta\rho_{min} = -0.62$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Experimental. Data were collected applying an imaging plate system (Stoe) with the following measurement parameters:

Detector distance [mm] 70 Phi movement mode Oscillation Phi incr. [degrees] 1.0 Number of exposures 192 Irradiation / exposure [min] 2.50

For a detailed description of the method see: Sheldrick, G·*M*., Paulus, E. Vertesy, *L*. & Hahn, F. (1995) Acta Cryst. B51, 89–98.

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

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 $F^2 > 2\text{sigma}(F^2)$ 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}
As1	0.47917 (3)	0.20088 (3)	0.06525 (1)	0.0440 (1)
As2	0.66667	0.33333	0.12958 (1)	0.0398 (1)
Cu1	0.66667	0.33333	0.08144 (1)	0.0466 (2)
C1	0.4361 (3)	0.0520 (3)	0.07350 (6)	0.0448 (10)
C2	0.5099 (3)	0.0188 (3)	0.06918 (8)	0.0610 (14)
C3	0.4877 (4)	−0.0818 (4)	0.07706 (10)	0.0771 (19)
C4	0.3929 (4)	−0.1499 (3)	0.08911 (9)	0.0730 (16)
C5	0.3189 (4)	−0.1186 (3)	0.09291 (9)	0.0699 (16)
C6	0.3402 (3)	−0.0175 (3)	0.08519 (7)	0.0564 (12)
C7	0.4540 (3)	0.1926 (3)	0.02816 (6)	0.0491 (11)
C8	0.3857 (4)	0.0974 (4)	0.01602 (8)	0.0779 (18)
C9	0.3650 (6)	0.0970 (5)	−0.00996 (10)	0.106 (3)
C10	0.4128 (6)	0.1912 (5)	−0.02384 (9)	0.096 (2)
C11	0.4819 (5)	0.2846 (5)	−0.01205 (9)	0.082 (2)
C12	0.5020 (3)	0.2858 (3)	0.01399 (7)	0.0604 (12)
C13	0.3514 (3)	0.2028 (3)	0.07735 (6)	0.0457 (10)
C14	0.2602 (3)	0.1674 (4)	0.06245 (8)	0.0648 (14)
C15	0.1694 (4)	0.1644 (4)	0.07263 (9)	0.0786 (19)
C16	0.1697 (4)	0.1970 (4)	0.09752 (9)	0.0730 (17)
C17	0.2590 (4)	0.2334 (4)	0.11206 (8)	0.0699 (16)
C18	0.3503 (3)	0.2367 (3)	0.10222 (7)	0.0584 (12)
C19	0.7988 (3)	0.4342 (3)	0.14716 (6)	0.0420 (10)
C20	0.8947 (3)	0.4451 (3)	0.13850 (7)	0.0541 (11)
C21	0.9898 (3)	0.5153 (3)	0.15034 (9)	0.0653 (16)
C22	0.9904 (4)	0.5749 (4)	0.17108 (9)	0.0732 (17)
C23	0.8955 (4)	0.5649 (4)	0.17971 (9)	0.0786 (17)
C24	0.7999 (3)	0.4955 (3)	0.16784 (7)	0.0620 (14)
P1	0.00000	0.00000	0.00000	0.0713 (7)

F1	0.0013 (5)	0.0885 (4)	0.01719 (9)	0.185 (3)
P2	1.33333	0.66667	0.16667	0.0504 (6)
F2	1.2304 (2)	0.6030 (3)	0.18418 (6)	0.0990 (11)
H2	0.57430	0.06430	0.06100	0.0730*
H3	0.53770	−0.10360	0.07420	0.0930*
H4	0.37920	−0.21700	0.09470	0.0880*
H5	0.25380	−0.16520	0.10070	0.0830*
H6	0.28950	0.00340	0.08790	0.0680*
H8	0.35360	0.03350	0.02530	0.0940*
H9	0.31860	0.03270	−0.01810	0.1270*
H10	0.39760	0.19070	−0.04120	0.1160*
H11	0.51590	0.34790	−0.02150	0.0990*
H12	0.54850	0.35030	0.02200	0.0730*
H14	0.25960	0.14560	0.04560	0.0780*
H15	0.10820	0.14010	0.06260	0.0940*
H16	0.10850	0.19410	0.10430	0.0870*
H17	0.25940	0.25630	0.12880	0.0840*
H18	0.41120	0.26190	0.11240	0.0700*
H20	0.89480	0.40460	0.12460	0.0650*
H21	1.05390	0.52250	0.14430	0.0780*
H22	1.05460	0.62170	0.17920	0.0880*
H23	0.89590	0.60540	0.19370	0.0950*
H24	0.73620	0.48980	0.17370	0.0740*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
As1	0.0427 (2)	0.0399 (2)	0.0462 (2)	0.0183 (2)	−0.0025 (1)	−0.0001 (1)
As2	0.0426 (2)	0.0426 (2)	0.0341 (3)	0.0213 (1)	0.0000	0.0000
Cu1	0.0483 (3)	0.0483 (3)	0.0431 (4)	0.0241 (1)	0.0000	0.0000
C1	0.0454 (19)	0.0368 (17)	0.0476 (17)	0.0171 (15)	−0.0056 (14)	−0.0021 (13)
C2	0.051 (2)	0.050 (2)	0.081 (3)	0.0245 (19)	0.0029 (19)	0.0043 (19)
C3	0.079 (3)	0.063 (3)	0.106 (4)	0.048 (3)	0.000 (3)	0.002 (2)
C4	0.087 (3)	0.043 (2)	0.087 (3)	0.031 (2)	−0.010 (2)	0.003 (2)
C5	0.064 (3)	0.047 (2)	0.083 (3)	0.016 (2)	0.012 (2)	0.012 (2)
C6	0.050 (2)	0.045 (2)	0.070 (2)	0.0205 (18)	0.0069 (17)	0.0076 (17)
C7	0.049 (2)	0.053 (2)	0.0471 (17)	0.0269 (17)	−0.0011 (14)	−0.0021 (15)
C8	0.102 (4)	0.061 (3)	0.055 (2)	0.029 (3)	−0.014 (2)	−0.0080 (19)
C9	0.148 (6)	0.099 (4)	0.065 (3)	0.058 (4)	−0.034 (3)	−0.032 (3)
C10	0.145 (5)	0.129 (5)	0.047 (2)	0.093 (5)	−0.008 (3)	−0.002 (3)
C11	0.110 (4)	0.099 (4)	0.061 (3)	0.070 (4)	0.017 (3)	0.024 (3)
C12	0.061 (2)	0.060 (2)	0.060 (2)	0.030 (2)	0.0038 (18)	0.0097 (18)
C13	0.0430 (18)	0.0395 (18)	0.0536 (18)	0.0199 (15)	−0.0032 (14)	0.0017 (14)
C14	0.059 (2)	0.080 (3)	0.061 (2)	0.039 (2)	−0.0094 (19)	−0.009 (2)
C15	0.056 (3)	0.105 (4)	0.085 (3)	0.048 (3)	−0.013 (2)	−0.004 (3)
C16	0.067 (3)	0.076 (3)	0.087 (3)	0.044 (3)	0.015 (2)	0.010 (2)
C17	0.079 (3)	0.071 (3)	0.063 (2)	0.040 (3)	0.011 (2)	−0.002 (2)
C18	0.055 (2)	0.058 (2)	0.058 (2)	0.025 (2)	−0.0021 (17)	−0.0078 (17)

C19	0.0421 (18)	0.0405 (17)	0.0400 (15)	0.0181 (15)	0.0002 (13)	0.0029 (13)
C20	0.054 (2)	0.058 (2)	0.0539 (19)	0.0306 (19)	−0.0005 (16)	−0.0032 (16)
C21	0.041 (2)	0.067 (3)	0.088 (3)	0.027 (2)	0.0015 (19)	0.005 (2)
C22	0.054 (3)	0.065 (3)	0.093 (3)	0.024 (2)	−0.020 (2)	−0.014 (2)
C23	0.067 (3)	0.080 (3)	0.081 (3)	0.031 (3)	−0.020 (2)	−0.039 (2)
C24	0.051 (2)	0.069 (3)	0.062 (2)	0.027 (2)	−0.0027 (17)	−0.0179 (19)
P1	0.0817 (12)	0.0817 (12)	0.0507 (13)	0.0409 (6)	0.0000	0.0000
F1	0.229 (6)	0.182 (5)	0.173 (4)	0.124 (5)	−0.008 (4)	−0.076 (4)
P2	0.0409 (7)	0.0409 (7)	0.0694 (14)	0.0205 (4)	0.0000	0.0000
F2	0.0655 (17)	0.101 (2)	0.117 (2)	0.0315 (17)	0.0315 (16)	0.0196 (18)

Geometric parameters (Å, °)

As1—Cu1	2.5472 (5)	C13—C14	1.384 (6)
As1—C1	1.959 (4)	C13—C18	1.386 (5)
As1—C7	1.956 (3)	C14—C15	1.391 (8)
As1—C13	1.958 (5)	C15—C16	1.376 (7)
As2—Cu1	2.5044 (9)	C16—C17	1.352 (8)
As2—C19	1.950 (4)	C17—C18	1.390 (8)
As2—C19^{i}	1.950 (5)	C19—C20	1.385 (7)
As2—C19^{ii}	1.950 (4)	C19—C24	1.387 (5)
P1—F1^{iii}	1.549 (8)	C20—C21	1.376 (6)
P1—F1^{iv}	1.549 (5)	C21—C22	1.376 (7)
P1—F1^{v}	1.549 (7)	C22—C23	1.376 (9)
P1—F1^{vi}	1.549 (8)	C23—C24	1.378 (7)
P1—F1^{vii}	1.549 (7)	C2—H2	0.9300
P1—F1	1.549 (5)	C3—H3	0.9300
P2—F2^{viii}	1.584 (5)	C4—H4	0.9300
P2—F2	1.584 (3)	C5—H5	0.9300
P2—F2^{ix}	1.583 (5)	C6—H6	0.9300
P2—F2^{x}	1.585 (3)	C8—H8	0.9300
P2—F2^{xi}	1.584 (3)	C9—H9	0.9300
P2—F2^{xii}	1.584 (3)	C10—H10	0.9300
C1—C2	1.385 (7)	C11—H11	0.9300
C1—C6	1.377 (6)	C12—H12	0.9300
C2—C3	1.381 (6)	C14—H14	0.9300
C3—C4	1.371 (8)	C15—H15	0.9300
C4—C5	1.363 (8)	C16—H16	0.9300
C5—C6	1.389 (6)	C17—H17	0.9300
C7—C8	1.378 (6)	C18—H18	0.9300
C7—C12	1.377 (5)	C20—H20	0.9300
C8—C9	1.383 (7)	C21—H21	0.9300
C9—C10	1.379 (8)	C22—H22	0.9300
C10—C11	1.356 (9)	C23—H23	0.9300
C11—C12	1.383 (6)	C24—H24	0.9300
As1···H2^{ii}	3.1700	C14···H9^{vi}	3.0700

Cu1···H2	3.5700	C19···H24^{ii}	2.6000
Cu1···H12	3.6000	C19···H18^{ii}	2.6700
Cu1···H18	3.6600	C20···H24^{ii}	3.0000
Cu1···H20	3.6800	C20···H18^{ii}	2.8000
Cu1···H2^{i}	3.5700	C21···H22^{x}	2.9700
Cu1···H12^{i}	3.6000	C24···H24^{ii}	3.0700
Cu1···H18^{i}	3.6600	H2···Cu1	3.5700
Cu1···H20^{i}	3.6800	H2···C13^{i}	2.9300
Cu1···H2^{ii}	3.5700	H2···As1^{i}	3.1700
Cu1···H12^{ii}	3.6000	H3···H10^{xiii}	2.5600
Cu1···H18^{ii}	3.6600	H4···H4^{xiv}	2.5300
Cu1···H20^{ii}	3.6800	H4···H4^{xv}	2.5300
F2···C22	3.343 (7)	H6···C14	2.9200
F1···H14^{vii}	2.7500	H6···C13	2.6000
F1···H15	2.7100	H8···C1	2.7300
F2···H22	2.6900	H8···C11^{v}	3.0300
C6···C14	3.590 (7)	H9···C14^{v}	3.0700
C8···C14	3.455 (7)	H10···H3^{xiii}	2.5600
C14···C8	3.455 (7)	H12···Cu1	3.6000
C14···C6	3.590 (7)	H12···C12^{ii}	3.0000
C18···C19^{i}	3.574 (6)	H12···C7^{ii}	2.8000
C18···C20^{i}	3.551 (6)	H14···C7	2.6900
C19···C18^{ii}	3.574 (5)	H14···C8	2.7200
C20···C24^{ii}	3.590 (6)	H14···F1^{iii}	2.7500
C20···C18^{ii}	3.551 (6)	H15···F1	2.7100
C22···F2	3.343 (7)	H18···C20^{i}	2.8000
C24···C20^{i}	3.590 (7)	H18···Cu1	3.6600
C1···H8	2.7300	H18···C19^{i}	2.6700
C1···H20^{ii}	2.8200	H20···C1^{i}	2.8200
C6···H20^{ii}	3.0000	H20···C6^{i}	3.0000
C7···H12^{i}	2.8000	H20···Cu1	3.6800
C7···H14	2.6900	H21···H22^{x}	2.3900
C8···H14	2.7200	H22···F2	2.6900
C11···H8^{vi}	3.0300	H22···C21^{ix}	2.9700
C12···H12^{i}	3.0000	H22···H21^{ix}	2.3900
C13···H6	2.6000	H24···C20^{i}	3.0000
C13···H2^{ii}	2.9300	H24···C24^{i}	3.0700
C14···H6	2.9200	H24···C19^{i}	2.6000
Cu1—As1—C1	112.61 (13)	C8—C9—C10	120.5 (5)
Cu1—As1—C7	117.80 (13)	C9—C10—C11	119.8 (5)
Cu1—As1—C13	122.35 (11)	C10—C11—C12	120.0 (5)
C1—As1—C7	101.64 (15)	C7—C12—C11	120.8 (4)

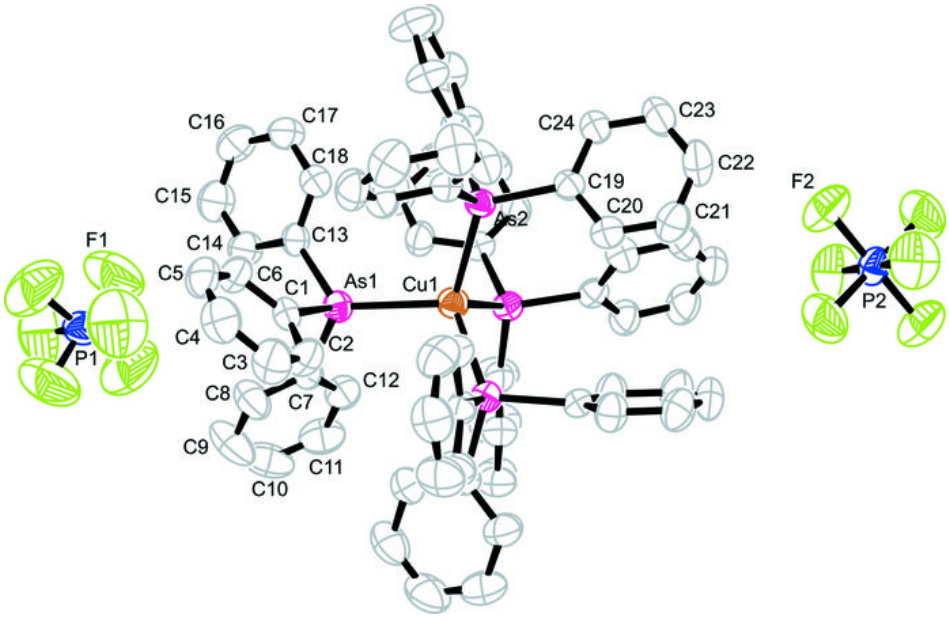
C1—As1—C13	99.19 (17)	As1—C13—C18	118.8 (3)
C7—As1—C13	99.85 (17)	C14—C13—C18	118.5 (4)
Cu1—As2—C19	117.96 (10)	As1—C13—C14	122.7 (3)
Cu1—As2—C19^{i}	117.96 (11)	C13—C14—C15	120.2 (4)
Cu1—As2—C19^{ii}	117.96 (10)	C14—C15—C16	120.3 (5)
C19—As2—C19^{i}	99.81 (18)	C15—C16—C17	119.9 (6)
C19—As2—C19^{ii}	99.81 (18)	C16—C17—C18	120.5 (4)
C19^{i}—As2—C19^{ii}	99.8 (2)	C13—C18—C17	120.6 (4)
As1—Cu1—As2	109.30 (2)	As2—C19—C24	122.3 (4)
As1—Cu1—As1^{i}	109.65 (2)	C20—C19—C24	119.1 (4)
As1—Cu1—As1^{ii}	109.65 (2)	As2—C19—C20	118.6 (3)
As1^{i}—Cu1—As2	109.30 (2)	C19—C20—C21	120.5 (4)
As1^{ii}—Cu1—As2	109.30 (2)	C20—C21—C22	120.2 (5)
As1^{i}—Cu1—As1^{ii}	109.65 (2)	C21—C22—C23	119.6 (5)
F1^{vii}—P1—F1^{iv}	90.0 (3)	C22—C23—C24	120.6 (4)
F1^{vii}—P1—F1^{v}	180.00	C19—C24—C23	119.9 (5)
F1^{vii}—P1—F1^{vi}	90.0 (3)	C1—C2—H2	120.00
F1^{iii}—P1—F1^{iv}	90.0 (3)	C3—C2—H2	120.00
F1^{iii}—P1—F1^{v}	90.0 (3)	C4—C3—H3	120.00
F1^{iii}—P1—F1^{vi}	180.00	C2—C3—H3	120.00
F1^{iv}—P1—F1^{v}	90.0 (3)	C3—C4—H4	120.00
F1^{iv}—P1—F1^{vi}	90.0 (3)	C5—C4—H4	120.00
F1^{v}—P1—F1^{vi}	90.0 (3)	C4—C5—H5	120.00
F1—P1—F1^{vii}	90.0 (3)	C6—C5—H5	120.00
F1—P1—F1^{iii}	90.0 (3)	C1—C6—H6	120.00
F1—P1—F1^{iv}	180.00	C5—C6—H6	120.00
F1—P1—F1^{v}	90.0 (3)	C9—C8—H8	120.00
F1—P1—F1^{vi}	90.0 (3)	C7—C8—H8	120.00
F1^{vii}—P1—F1^{iii}	90.0 (3)	C8—C9—H9	120.00
F2^{viii}—P2—F2^{ix}	180.00	C10—C9—H9	120.00
F2^{viii}—P2—F2^{x}	89.8 (2)	C11—C10—H10	120.00
F2^{xi}—P2—F2^{xii}	89.8 (2)	C9—C10—H10	120.00
F2^{xi}—P2—F2^{ix}	89.8 (2)	C10—C11—H11	120.00
F2^{xi}—P2—F2^{x}	180.00	C12—C11—H11	120.00
F2^{xii}—P2—F2^{ix}	90.2 (2)	C7—C12—H12	120.00
F2^{xii}—P2—F2^{x}	90.2 (2)	C11—C12—H12	120.00
F2^{ix}—P2—F2^{x}	90.2 (2)	C15—C14—H14	120.00
F2^{viii}—P2—F2^{xii}	89.8 (2)	C13—C14—H14	120.00
F2—P2—F2^{viii}	90.2 (2)	C16—C15—H15	120.00
F2—P2—F2^{xi}	90.2 (2)	C14—C15—H15	120.00
F2—P2—F2^{xii}	180.00	C15—C16—H16	120.00

F2—P2—F2^{ix}	89.8 (2)	C17—C16—H16	120.00
F2—P2—F2^{x}	89.8 (2)	C16—C17—H17	120.00
F2^{viii}—P2—F2^{xi}	90.2 (2)	C18—C17—H17	120.00
C2—C1—C6	119.0 (4)	C17—C18—H18	120.00
As1—C1—C2	117.7 (3)	C13—C18—H18	120.00
As1—C1—C6	123.1 (3)	C19—C20—H20	120.00
C1—C2—C3	120.0 (4)	C21—C20—H20	120.00
C2—C3—C4	120.8 (5)	C22—C21—H21	120.00
C3—C4—C5	119.6 (4)	C20—C21—H21	120.00
C4—C5—C6	120.4 (4)	C21—C22—H22	120.00
C1—C6—C5	120.3 (5)	C23—C22—H22	120.00
As1—C7—C8	122.1 (3)	C24—C23—H23	120.00
C8—C7—C12	119.1 (3)	C22—C23—H23	120.00
As1—C7—C12	118.8 (3)	C23—C24—H24	120.00
C7—C8—C9	119.8 (5)	C19—C24—H24	120.00
C1—As1—Cu1—As2	−66.60 (12)	Cu1—As2—C19—C24	134.7 (3)
C7—As1—Cu1—As2	175.59 (14)	C19^{i}—As2—C19—C24	5.6 (3)
C13—As1—Cu1—As2	51.33 (12)	C19^{ii}—As2—C19—C24	−96.2 (3)
C1—As1—Cu1—As1^{i}	53.18 (12)	As1—C1—C2—C3	173.5 (3)
C7—As1—Cu1—As1^{i}	−64.63 (15)	As1—C1—C6—C5	−173.4 (3)
C13—As1—Cu1—As1^{i}	171.12 (12)	C2—C1—C6—C5	1.1 (6)
C1—As1—Cu1—As1^{ii}	173.61 (12)	C6—C1—C2—C3	−1.4 (6)
C7—As1—Cu1—As1^{ii}	55.80 (15)	C1—C2—C3—C4	0.2 (7)
C13—As1—Cu1—As1^{ii}	−68.45 (13)	C2—C3—C4—C5	1.3 (7)
C13—As1—C1—C2	−176.1 (3)	C3—C4—C5—C6	−1.5 (7)
Cu1—As1—C1—C6	129.4 (3)	C4—C5—C6—C1	0.3 (6)
Cu1—As1—C13—C14	151.9 (3)	C12—C7—C8—C9	−1.1 (9)
C1—As1—C13—C14	−83.8 (4)	As1—C7—C8—C9	175.6 (6)
C7—As1—C13—C14	19.8 (4)	C8—C7—C12—C11	0.3 (8)
Cu1—As1—C1—C2	−45.2 (3)	As1—C7—C12—C11	−176.5 (5)
C7—As1—C1—C2	81.8 (3)	C7—C8—C9—C10	0.4 (12)
C13—As1—C7—C8	−80.5 (5)	C8—C9—C10—C11	1.1 (13)
Cu1—As1—C7—C12	−38.7 (4)	C9—C10—C11—C12	−1.8 (13)
C7—As1—C1—C6	−103.6 (3)	C10—C11—C12—C7	1.2 (10)
C13—As1—C1—C6	−1.5 (3)	As1—C13—C14—C15	176.0 (4)
C13—As1—C7—C12	96.2 (4)	C14—C13—C18—C17	1.1 (6)
Cu1—As1—C7—C8	144.6 (4)	C18—C13—C14—C15	−1.2 (7)
C1—As1—C7—C8	21.1 (5)	As1—C13—C18—C17	−176.2 (3)
C1—As1—C13—C18	93.4 (3)	C13—C14—C15—C16	0.3 (7)
Cu1—As1—C13—C18	−30.9 (3)	C14—C15—C16—C17	0.8 (8)
C1—As1—C7—C12	−162.2 (4)	C15—C16—C17—C18	−1.0 (7)
C7—As1—C13—C18	−163.0 (3)	C16—C17—C18—C13	0.0 (7)
C19^{ii}—As2—C19—C20	84.2 (3)	As2—C19—C20—C21	−180.0 (3)
C19^{ii}—As2—Cu1—As1	63.5 (2)	C24—C19—C20—C21	0.4 (6)
C19—As2—Cu1—As1	−176.49 (15)	As2—C19—C24—C23	179.4 (3)
C19—As2—Cu1—As1^{ii}	−56.49 (15)	C20—C19—C24—C23	−1.0 (6)

C19^{i}—As2—Cu1—As1	−56.49 (17)	C19—C20—C21—C22	0.5 (6)
C19—As2—Cu1—As1^{i}	63.51 (15)	C20—C21—C22—C23	−0.8 (7)
Cu1—As2—C19—C20	−44.9 (3)	C21—C22—C23—C24	0.2 (7)
C19^{i}—As2—C19—C20	−174.0 (3)	C22—C23—C24—C19	0.7 (7)

Symmetry codes: (i) −*y*+1, *x*−*y*, *z*; (ii) −*x*+*y*+1, −*x*+1, *z*; (iii) −*x*+*y*, −*x*, *z*; (iv) −*x*, −*y*, −*z*; (v) *y*, −*x*+*y*, −*z*; (vi) *x*−*y*, *x*, −*z*; (vii) −*y*, *x*−*y*, *z*; (viii) −*y*+2, *x*−*y*, *z*; (ix) *y*+2/3, −*x*+*y*+4/3, −*z*+1/3; (x) *x*−*y*+2/3, *x*−2/3, −*z*+1/3; (xi) −*x*+*y*+2, −*x*+2, *z*; (xii) −*x*+8/3, −*y*+4/3, −*z*+1/3; (xiii) −*x*+1, −*y*, −*z*; (xiv) −*y*, *x*−*y*−1, *z*; (xv) −*x*+*y*+1, −*x*, *z*.

Fig. 1


C16
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P2