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{Bis[2-(diphenylphosphanyl)phenyl] ether-κ^2P,P'}(1,1′-dibenzyl-1*H*,1′*H*-4,4′-bi-1,2,3-triazole-$\kappa^2N^3,N^{3'}$)copper(I) hexafluoridophosphate dichloromethane hemisolvate

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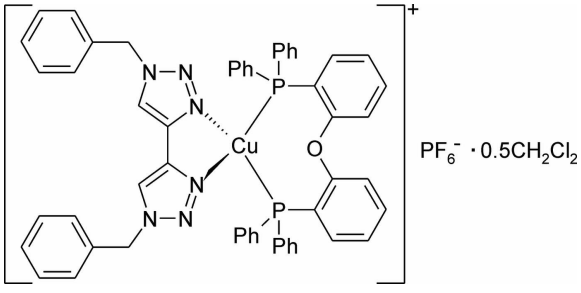
Key indicators: single-crystal X-ray study; T = 123 K; mean σ(C–C) = 0.005 Å; some non-H atoms missing; disorder in solvent or counterion; R factor = 0.045; wR factor = 0.109; data-to-parameter ratio = 16.3.

In the crystal structure of the title compound, $[Cu(C_{18}H_{16}N_6)(C_{36}H_{28}OP_2)]PF_6{\cdot}0.5CH_2Cl_2$ or [Cu(DPEPhos)(Bn-bta)]$PF_6{\cdot}0.5CH_2Cl_2$ {DPEPhos = bis[(diphenylphosphanyl)phenyl] ether and Bn-bta = 1,1′-dibenzyl-1*H*,1′*H*-4,4′-bi-1,2,3triazole}, the Cu atom is coordinated by two N and two P atoms of the ligands in a strongly distorted tetrahedral environment. There are two crystallographically independent complex cations present, which differ significantly in their geometrical parameters. The solvent molecule is disordered but satisfactory atomic positions could not be determined.

Related literature

For related literature, see: Monkowius *et al.* (2007) and references therein; Cosier & Glazer (1986). For the treatment of disordered solvent, see: Spek (2003).



Experimental

Crystal data

$[Cu(C_{18}H_{16}N_6)(C_{36}H_{28}OP_2)]PF_6{\cdot}0.5CH_2Cl_2$
M_r = 1105.88
Triclinic, $P\overline{1}$
a = 13.566 (1) Å
b = 14.371 (1) Å
c = 29.021 (3) Å
α = 83.30 (1)°
β = 87.33 (1)°
γ = 71.99 (1)°
V = 5343.3 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.61 mm^{-1}
T = 123 K
0.39 × 0.22 × 0.14 mm

Data collection

Stoe IPDS diffractometer
Absorption correction: analytical (*X-SHAPE* and *X-RED* in *IPDS Software*; Stoe & Cie, 1998)
T_{min} = 0.846, T_{max} = 0.942
49713 measured reflections
21326 independent reflections
12619 reflections with $I > 2\sigma(I)$
R_{int} = 0.050

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.109
S = 0.83
21326 reflections
1306 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.65 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu1—P1	2.2573 (9)	Cu2—P4	2.3070 (10)
Cu1—P2	2.2922 (11)	Cu2—N7	2.194 (3)
Cu1—N1	2.169 (3)	Cu2—N10	2.063 (3)
Cu1—N4	2.103 (2)	Cu2—P3	2.2252 (8)

Data collection: *IPDS Software* (Stoe & Cie, 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*.

Parts of this work were supported by the Bundesministerium für Bildung und Forschung (BMBF). We also acknowledge financial support from the DFG (SPP 1118). SR thanks the Elitenetzwerk Bayern for a graduate fellowship.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IM2049).

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supplementary materials

Acta Cryst. (2008). E**64**, m195 [**doi:10.1107/S1600536807066342**]

{Bis[2-(diphenylphosphanyl)phenyl] ether-κ^2P,P'}(1,1'-dibenzyl-1*H*,1'*H*-4,4'bi-1,2,3-triazole-$\kappa^2N^3,N^{3'}$)copper(I) hexafluoridophosphate dichloromethane hemisolvate

U. Monkowius, S. Ritter, B. König, H. Yersin and M. Zabel

Comment

The title compound crystallizes in two forms from dichloromethane/diethyl ether: one form contains solvent molecules, the other not. The latter structure was recently published (Monkowius *et al.*, 2007), the former is now reported in this paper. The asymmetric unit of the title compound consists of two complex cations $[(DPEPhos)(Bn\text{-}bta)Cu]^+$, two anions $[PF_6]^-$, and one molecule CH_2Cl_2 (Fig. 1). Additional partially occupied and/or disordered solvent molecules were also found, but satisfactory atomic positions could not be determined. These disordered solvent molecules were treated as a diffuse contribution using the SQUEEZE routine in *PLATON* software package (Spek, 2003). SQUEEZE calculated 310.0 $Å^3$ void space per unit cell and 19.8 electrons. Both cations significantly differ in their geometrical parameters: The Cu—P bond lengths are 2.2579 (9)/2.2923 (11) Å for Cu1—P1/Cu1—P2 and 2.2253 (9)/2.3072 (10) Å for Cu2—P3/Cu2—P4; the Cu—N bond lengths are 2.171 (3)/2.102 (3) Å (Cu1—N1/Cu1—N4) and 2.195 (3)/2.063 (3) Å (Cu2—N7/Cu2—N10). Furthermore, the bis-triazolyl moiety deviates considerably from planarity in the case of the cation containing Cu1 [Cu1: ⟨ (N1—C38—C39—N4) = -15.7 (5)°; Cu2: ⟨ (N7—C92—C93—N10) = -3.9 (5)°]. The bite angles of the Bn-bta ligands are 79.68 (10) and 78.95 (10) (N1—Cu1—N4 and N7—Cu2—N10, respectively). There are no close contacts between the oxygen atoms of the phosphine ligands and the copper atoms. The complex cations in the crystal structure of the crystal containing *no* solvent molecules display comparable sturctural characteristics (Monkowius *et al.*, 2007).

Experimental

The preparation of the title compound was published recently (Monkowius *et al.*, 2007).

Refinement

The data were collected at 123 K using an Oxford Cryosystems Cooler (Cosier & Glazer, 1986). The structure was solved by direct methods (*SIR97*) and refined by full-matrix anisotropic least squares (*SHELXL97*). The H-atoms were calculated geometrically and a riding model with $U_{iso}(H) = 1.2\ U_{eq}(C)$ the was used during refinement process.

Figures

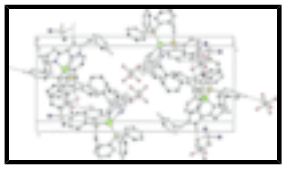


Fig. 1. : Excerpt from a cell plott depicting the hydrogen-bond pattern in crystals of the title compound. Hydrogen bonds are indicated by dashed lines. Only the participating H atoms are shown for clarity.

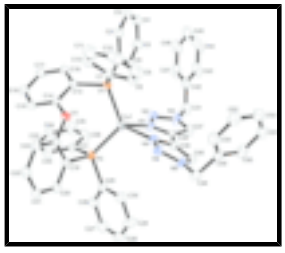


Fig. 2. : *ORTEP* drawing of the structure of the cation containing Cu1 in crystals of the title compound (H atoms have been omitted for clarity). Displacement ellipsoids for non-H atoms are drawn at the 50% probability level.

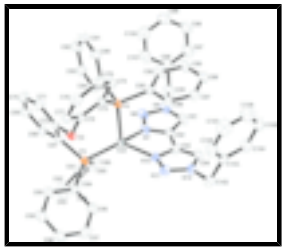


Fig. 3. : *ORTEP* drawing of the structure of the cation containing Cu2. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level.

{Bis[2-(diphenylphosphanyl)phenyl] ether-κ^2*P,P'*}(1,1'-dibenzyl-1*H*,1'*H*-4,4'-bi- 1,2,3-triazole-κ^2*N,N'*)copper(I) hexafluoridophosphate dichloromethane hemisolvate

Crystal data

$[Cu(C_{18}H_{16}N_6)(C_{36}H_{28}OP_2)]PF_6 \cdot 0.5CH_2Cl_2$	$Z = 4$
$M_r = 1105.88$	$F_{000} = 2268$
Triclinic, $P\bar{1}$	Cell parameters were determined by indexing 8000 reflections with I/sigma limit 6.0.
Hall symbol: -P 1	$D_x = 1.375$ Mg m^{-3}
$a = 13.566$ (1) Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$b = 14.371$ (1) Å	Cell parameters from 8000 reflections
$c = 29.021$ (3) Å	$\theta = 2.0$–26.9º
$\alpha = 83.30$ (1)º	$\mu = 0.61$ mm^{-1}
$\beta = 87.33$ (1)º	$T = 123$ K
$\gamma = 71.99$ (1)º	Prism, colourless
$V = 5343.3$ (9) Å^3	0.39 × 0.22 × 0.14 mm

Data collection

Stoe IPDS diffractometer	21326 independent reflections
Radiation source: fine-focus sealed tube	12619 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.050$
$T = 123$(1) K	$\theta_{max} = 26.9$º
rotation scans	$\theta_{min} = 2.0$º
Absorption correction: analytical (X-SHAPE and X-RED; Stoe, 1998)	$h = -16 \rightarrow 16$
$T_{min} = 0.846$, $T_{max} = 0.942$	$k = -18 \rightarrow 18$
49713 measured reflections	$l = -36 \rightarrow 36$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.045$	H-atom parameters constrained
$wR(F^2) = 0.109$	$w = 1/[\sigma^2(F_o^2) + (0.0577P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.83$	$(\Delta/\sigma)_{max} = 0.007$
21326 reflections	$\Delta\rho_{max} = 1.65$ e Å^{-3}
1306 parameters	$\Delta\rho_{min} = -0.32$ 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] 65 Phi movement mode Oscillation Phi incr. [degrees] 0.8 Number of exposures 267 Irradiation / exposure [min] 3.00

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 $F^2 > \sigma(F^2)$ 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)
Cu1	0.08178 (3)	0.83015 (3)	0.62926 (1)	0.0234 (1)	
P1	0.06724 (6)	0.90146 (5)	0.69560 (3)	0.0218 (3)	
P2	−0.07224 (7)	0.85071 (5)	0.59389 (3)	0.0222 (3)	
O1	−0.12401 (17)	0.85545 (14)	0.69674 (7)	0.0233 (7)	
N1	0.1978 (2)	0.86079 (17)	0.58112 (8)	0.0241 (8)	
N2	0.2278 (2)	0.93689 (18)	0.56365 (9)	0.0292 (9)	
N3	0.3227 (2)	0.90056 (19)	0.54609 (9)	0.0309 (9)	
N4	0.1838 (2)	0.68704 (17)	0.62619 (8)	0.0235 (8)	
N5	0.1833 (2)	0.59678 (17)	0.64103 (9)	0.0253 (8)	
N6	0.2585 (2)	0.53654 (17)	0.61677 (8)	0.0251 (8)	
C1	0.1501 (3)	0.9759 (2)	0.70609 (10)	0.0242 (10)	
C2	0.1715 (3)	0.9926 (2)	0.75051 (11)	0.0291 (10)	
C3	0.2320 (3)	1.0536 (2)	0.75602 (12)	0.0334 (11)	

C4	0.2701 (3)	1.0978 (2)	0.71769 (13)	0.0362 (11)
C5	0.2483 (3)	1.0828 (2)	0.67349 (12)	0.0333 (11)
C6	0.1885 (3)	1.0219 (2)	0.66762 (11)	0.0289 (10)
C7	0.0814 (3)	0.8151 (2)	0.74817 (10)	0.0253 (10)
C8	0.1611 (3)	0.7264 (2)	0.74880 (11)	0.0308 (10)
C9	0.1757 (3)	0.6576 (3)	0.78806 (13)	0.0423 (13)
C10	0.1115 (3)	0.6758 (3)	0.82587 (13)	0.0457 (14)
C11	0.0315 (3)	0.7626 (3)	0.82560 (13)	0.0483 (15)
C12	0.0166 (3)	0.8332 (3)	0.78661 (11)	0.0365 (11)
C13	−0.0616 (3)	0.9903 (2)	0.69879 (10)	0.0235 (9)
C14	−0.1471 (3)	0.9575 (2)	0.69471 (10)	0.0226 (9)
C15	−0.2468 (3)	1.0205 (2)	0.68926 (11)	0.0287 (10)
C16	−0.2617 (3)	1.1208 (2)	0.68710 (12)	0.0357 (11)
C17	−0.1791 (3)	1.1567 (2)	0.69129 (12)	0.0335 (10)
C18	−0.0798 (3)	1.0921 (2)	0.69751 (11)	0.0285 (10)
C19	−0.1749 (2)	0.8102 (2)	0.62608 (10)	0.0208 (9)
C20	−0.2389 (3)	0.7669 (2)	0.60517 (11)	0.0266 (10)
C21	−0.3138 (3)	0.7345 (2)	0.63056 (11)	0.0273 (10)
C22	−0.3267 (3)	0.7451 (2)	0.67766 (11)	0.0262 (10)
C23	−0.2646 (3)	0.7873 (2)	0.69950 (10)	0.0243 (10)
C24	−0.1901 (2)	0.81893 (19)	0.67367 (10)	0.0211 (9)
C25	−0.0621 (3)	0.7876 (2)	0.54184 (10)	0.0271 (10)
C26	−0.1143 (3)	0.8307 (3)	0.50116 (11)	0.0353 (11)
C27	−0.1095 (3)	0.7747 (3)	0.46449 (12)	0.0441 (15)
C28	−0.0523 (4)	0.6758 (3)	0.46820 (13)	0.0465 (15)
C29	0.0027 (3)	0.6331 (3)	0.50845 (13)	0.0443 (13)
C30	−0.0022 (3)	0.6882 (2)	0.54508 (12)	0.0352 (11)
C31	−0.1371 (3)	0.9810 (2)	0.57467 (10)	0.0252 (10)
C32	−0.2444 (3)	1.0235 (2)	0.57567 (11)	0.0323 (10)
C33	−0.2885 (3)	1.1239 (2)	0.56287 (12)	0.0390 (11)
C34	−0.2262 (3)	1.1825 (2)	0.54878 (11)	0.0359 (13)
C35	−0.1207 (3)	1.1411 (2)	0.54718 (13)	0.0400 (13)
C36	−0.0756 (3)	1.0409 (2)	0.56031 (12)	0.0354 (11)
C37	0.3557 (3)	0.8006 (2)	0.55155 (11)	0.0312 (10)
C38	0.2745 (3)	0.7762 (2)	0.57419 (10)	0.0235 (9)
C39	0.2597 (3)	0.6839 (2)	0.59330 (10)	0.0228 (9)
C40	0.3078 (3)	0.5871 (2)	0.58689 (10)	0.0254 (10)
C41	0.3822 (3)	0.9668 (3)	0.52656 (13)	0.0409 (13)
C42	0.4164 (3)	1.0154 (2)	0.56338 (13)	0.0369 (11)
C43	0.4702 (3)	0.9603 (3)	0.60265 (16)	0.0460 (13)
C44	0.5030 (3)	1.0048 (3)	0.63588 (18)	0.0562 (16)
C45	0.4845 (3)	1.1064 (3)	0.63014 (18)	0.0547 (16)
C46	0.4326 (3)	1.1615 (3)	0.59124 (16)	0.0493 (15)
C47	0.3986 (3)	1.1170 (2)	0.55825 (14)	0.0420 (11)
C48	0.2881 (3)	0.4291 (2)	0.62911 (11)	0.0309 (10)
C49	0.3839 (3)	0.3955 (2)	0.65930 (11)	0.0284 (10)
C50	0.4805 (3)	0.3919 (2)	0.64060 (12)	0.0345 (10)
C51	0.5676 (3)	0.3680 (2)	0.66892 (14)	0.0397 (11)
C52	0.5574 (3)	0.3449 (2)	0.71581 (13)	0.0391 (13)

C53	0.4614 (3)	0.3464 (2)	0.73532 (13)	0.0384 (13)
C54	0.3741 (3)	0.3725 (2)	0.70684 (12)	0.0345 (10)
Cu2	0.68648 (3)	0.66119 (2)	0.85537 (1)	0.0238 (1)
P3	0.60262 (7)	0.80514 (5)	0.88099 (3)	0.0214 (2)
P4	0.58030 (7)	0.58939 (5)	0.82256 (2)	0.0210 (2)
O2	0.47952 (17)	0.80736 (14)	0.80196 (7)	0.0223 (7)
N7	0.7667 (2)	0.53225 (18)	0.90283 (9)	0.0267 (8)
N8	0.7430 (2)	0.47872 (18)	0.93939 (9)	0.0303 (9)
N9	0.8175 (2)	0.39114 (18)	0.94200 (9)	0.0309 (9)
N10	0.8277 (2)	0.61348 (17)	0.82183 (9)	0.0249 (8)
N11	0.8674 (2)	0.63858 (18)	0.78170 (9)	0.0286 (9)
N12	0.9532 (2)	0.56495 (19)	0.77455 (9)	0.0296 (9)
C55	0.6148 (3)	0.9171 (2)	0.84762 (10)	0.0234 (9)
C56	0.7129 (3)	0.9196 (2)	0.83269 (11)	0.0319 (10)
C57	0.7260 (3)	1.0051 (3)	0.80918 (13)	0.0398 (12)
C58	0.6421 (3)	1.0874 (2)	0.79934 (12)	0.0386 (13)
C59	0.5439 (3)	1.0847 (2)	0.81310 (13)	0.0408 (13)
C60	0.5299 (3)	1.0007 (2)	0.83731 (11)	0.0311 (10)
C61	0.6284 (3)	0.8201 (2)	0.94064 (10)	0.0234 (10)
C62	0.6104 (3)	0.9117 (2)	0.95593 (11)	0.0341 (12)
C63	0.6315 (3)	0.9207 (2)	1.00104 (12)	0.0426 (13)
C64	0.6701 (3)	0.8374 (3)	1.03208 (11)	0.0382 (13)
C65	0.6876 (3)	0.7454 (3)	1.01748 (12)	0.0385 (13)
C66	0.6684 (3)	0.7363 (2)	0.97189 (11)	0.0313 (10)
C67	0.4633 (3)	0.8221 (2)	0.88250 (10)	0.0230 (9)
C68	0.4016 (3)	0.8335 (2)	0.92249 (10)	0.0269 (10)
C69	0.3000 (3)	0.8331 (2)	0.92225 (11)	0.0313 (10)
C70	0.2571 (3)	0.8187 (2)	0.88182 (11)	0.0329 (11)
C71	0.3166 (3)	0.8085 (2)	0.84090 (10)	0.0274 (10)
C72	0.4169 (3)	0.81180 (19)	0.84159 (10)	0.0212 (9)
C73	0.5048 (2)	0.6523 (2)	0.77096 (10)	0.0219 (9)
C74	0.4900 (3)	0.6036 (2)	0.73396 (10)	0.0260 (10)
C75	0.4367 (3)	0.6565 (2)	0.69435 (10)	0.0274 (10)
C76	0.3968 (3)	0.7580 (2)	0.69095 (10)	0.0278 (10)
C77	0.4099 (3)	0.8081 (2)	0.72751 (10)	0.0244 (10)
C78	0.4623 (2)	0.7555 (2)	0.76678 (10)	0.0217 (9)
C79	0.4860 (3)	0.5575 (2)	0.86309 (10)	0.0235 (9)
C80	0.4121 (3)	0.5156 (2)	0.84982 (11)	0.0288 (10)
C81	0.3425 (3)	0.4922 (2)	0.88201 (12)	0.0353 (11)
C82	0.3453 (3)	0.5102 (2)	0.92784 (12)	0.0366 (11)
C83	0.4175 (3)	0.5511 (2)	0.94151 (11)	0.0342 (10)
C84	0.4875 (3)	0.5752 (2)	0.90953 (10)	0.0274 (10)
C85	0.6603 (3)	0.4718 (2)	0.80445 (10)	0.0228 (9)
C86	0.7293 (3)	0.4708 (2)	0.76711 (11)	0.0270 (10)
C87	0.8036 (3)	0.3847 (2)	0.75765 (11)	0.0313 (10)
C88	0.8111 (3)	0.2974 (2)	0.78581 (12)	0.0338 (10)
C89	0.7432 (3)	0.2969 (2)	0.82270 (12)	0.0364 (13)
C90	0.6676 (3)	0.3836 (2)	0.83178 (10)	0.0287 (10)
C91	0.8881 (3)	0.3871 (2)	0.90763 (11)	0.0313 (10)

C92	0.8553 (3)	0.4788 (2)	0.88251 (10)	0.0257 (10)	
C93	0.8901 (3)	0.5229 (2)	0.84000 (11)	0.0256 (10)	
C94	0.9703 (3)	0.4918 (2)	0.80964 (11)	0.0301 (10)	
C95	0.8054 (3)	0.3102 (2)	0.97643 (12)	0.0413 (13)	
C96	0.7343 (3)	0.2593 (2)	0.95748 (11)	0.0368 (13)	
C97	0.7739 (4)	0.1628 (3)	0.94661 (13)	0.0433 (13)	
C98	0.7094 (4)	0.1176 (3)	0.92957 (14)	0.0470 (13)	
C99	0.6050 (4)	0.1677 (3)	0.92261 (14)	0.0506 (14)	
C100	0.5648 (4)	0.2627 (3)	0.93351 (13)	0.0459 (14)	
C101	0.6279 (3)	0.3083 (2)	0.95093 (12)	0.0429 (13)	
C102	1.0130 (3)	0.5656 (3)	0.73054 (12)	0.0360 (11)	
C103	0.9964 (3)	0.4935 (2)	0.70019 (11)	0.0285 (10)	
C104	1.0547 (3)	0.3949 (2)	0.70620 (12)	0.0338 (11)	
C105	1.0361 (3)	0.3285 (3)	0.67962 (13)	0.0387 (13)	
C106	0.9596 (4)	0.3594 (3)	0.64657 (12)	0.0453 (14)	
C107	0.9012 (3)	0.4578 (3)	0.63981 (12)	0.0456 (13)	
C108	0.9191 (3)	0.5246 (2)	0.66651 (12)	0.0369 (11)	
P5	0.63201 (9)	0.59126 (9)	0.52066 (4)	0.0483 (4)	
F1	0.7155 (3)	0.5663 (2)	0.55921 (11)	0.0879 (11)	
F2	0.6077 (2)	0.70671 (18)	0.52607 (8)	0.0619 (10)	
F3	0.5437 (3)	0.5895 (2)	0.55735 (11)	0.0797 (11)	
F4	0.5515 (3)	0.6202 (3)	0.47934 (11)	0.1106 (16)	
F5	0.6534 (3)	0.4778 (2)	0.51565 (11)	0.0946 (14)	
F6	0.7181 (3)	0.5989 (4)	0.48236 (12)	0.126 (2)	
P6	0.75858 (8)	0.72327 (6)	0.16583 (3)	0.0336 (3)	
F7	0.8165 (2)	0.68433 (16)	0.11945 (7)	0.0575 (9)	
F8	0.78290 (17)	0.61105 (13)	0.18930 (7)	0.0420 (7)	
F9	0.86676 (17)	0.72705 (14)	0.18517 (8)	0.0451 (8)	
F10	0.73427 (18)	0.83487 (14)	0.14342 (7)	0.0435 (7)	
F11	0.70162 (19)	0.76077 (15)	0.21269 (7)	0.0462 (8)	
F12	0.65161 (19)	0.71926 (15)	0.14669 (8)	0.0544 (8)	
Cl1	1.0766 (2)	0.10331 (18)	0.92882 (9)	0.0663 (9)	0.500
Cl2	0.9733 (2)	0.0499 (2)	0.85498 (10)	0.0752 (10)	0.500
C109	1.0701 (8)	0.0833 (6)	0.8737 (3)	0.055 (3)	0.500
H2	0.14490	0.96240	0.77700	0.0350*	
H3	0.24690	1.06440	0.78630	0.0400*	
H4	0.31150	1.13880	0.72150	0.0430*	
H5	0.27420	1.11410	0.64710	0.0400*	
H6	0.17380	1.01170	0.63730	0.0350*	
H8	0.20570	0.71270	0.72250	0.0370*	
H9	0.23080	0.59760	0.78850	0.0510*	
H10	0.12210	0.62850	0.85240	0.0550*	
H11	−0.01360	0.77470	0.85170	0.0580*	
H12	−0.03800	0.89340	0.78660	0.0440*	
H15	−0.30360	0.99590	0.68700	0.0340*	
H16	−0.32950	1.16560	0.68270	0.0430*	
H17	−0.19060	1.22560	0.68990	0.0400*	
H18	−0.02360	1.11690	0.70090	0.0340*	
H20	−0.23080	0.75960	0.57300	0.0320*	

H21	−0.35590	0.70510	0.61580	0.0330*
H22	−0.37820	0.72340	0.69500	0.0310*
H23	−0.27310	0.79430	0.73170	0.0290*
H26	−0.15340	0.89850	0.49820	0.0420*
H27	−0.14580	0.80460	0.43670	0.0530*
H28	−0.05080	0.63760	0.44340	0.0560*
H29	0.04370	0.56590	0.51090	0.0530*
H30	0.03520	0.65850	0.57260	0.0420*
H32	−0.28770	0.98380	0.58510	0.0390*
H33	−0.36170	1.15230	0.56380	0.0470*
H34	−0.25640	1.25100	0.54030	0.0430*
H35	−0.07800	1.18110	0.53700	0.0480*
H36	−0.00230	1.01330	0.55950	0.0420*
H37	0.41990	0.75770	0.54200	0.0370*
H40	0.36320	0.56140	0.56610	0.0300*
H41A	0.33870	1.01820	0.50390	0.0490*
H41B	0.44400	0.92850	0.50980	0.0490*
H43	0.48420	0.89090	0.60640	0.0550*
H44	0.53810	0.96650	0.66260	0.0670*
H45	0.50740	1.13770	0.65280	0.0660*
H46	0.42030	1.23070	0.58720	0.0590*
H47	0.36280	1.15590	0.53180	0.0500*
H48A	0.30260	0.39540	0.60050	0.0370*
H48B	0.23030	0.41150	0.64610	0.0370*
H50	0.48790	0.40580	0.60800	0.0410*
H51	0.63320	0.36790	0.65580	0.0480*
H52	0.61650	0.32760	0.73510	0.0470*
H53	0.45490	0.32980	0.76770	0.0460*
H54	0.30820	0.37460	0.72010	0.0410*
H10D	1.08770	0.54820	0.73750	0.0430*
H10E	0.99120	0.63260	0.71370	0.0430*
H56	0.77110	0.86280	0.83860	0.0380*
H57	0.79360	1.00670	0.79980	0.0480*
H58	0.65150	1.14550	0.78320	0.0470*
H59	0.48570	1.14090	0.80590	0.0490*
H60	0.46220	0.99990	0.84690	0.0370*
H62	0.58300	0.96920	0.93510	0.0410*
H63	0.61960	0.98410	1.01080	0.0510*
H64	0.68440	0.84350	1.06310	0.0460*
H65	0.71280	0.68810	1.03870	0.0460*
H66	0.68240	0.67280	0.96190	0.0380*
H68	0.43010	0.84180	0.95050	0.0320*
H69	0.25900	0.84270	0.94970	0.0380*
H70	0.18800	0.81590	0.88210	0.0390*
H71	0.28810	0.79940	0.81310	0.0330*
H74	0.51640	0.53390	0.73580	0.0310*
H75	0.42780	0.62230	0.66950	0.0330*
H76	0.36080	0.79350	0.66390	0.0330*
H77	0.38300	0.87780	0.72550	0.0290*

H80	0.40990	0.50330	0.81850	0.0350*	
H81	0.29290	0.46390	0.87270	0.0420*	
H82	0.29740	0.49440	0.94990	0.0440*	
H83	0.41930	0.56280	0.97300	0.0410*	
H84	0.53660	0.60380	0.91910	0.0330*	
H86	0.72510	0.53030	0.74800	0.0320*	
H87	0.84960	0.38490	0.73190	0.0370*	
H88	0.86290	0.23820	0.77960	0.0400*	
H89	0.74810	0.23740	0.84190	0.0440*	
H90	0.62040	0.38260	0.85690	0.0350*	
H91	0.94720	0.33330	0.90190	0.0370*	
H94	1.02580	0.43190	0.81260	0.0360*	
H95A	0.77560	0.33720	1.00560	0.0500*	
H95B	0.87420	0.26170	0.98340	0.0500*	
H97	0.84540	0.12810	0.95090	0.0520*	
H98	0.73660	0.05140	0.92250	0.0560*	
H99	0.56140	0.13630	0.91030	0.0610*	
H100	0.49330	0.29690	0.92900	0.0550*	
H101	0.59940	0.37370	0.95870	0.0510*	
H104	1.10780	0.37290	0.72880	0.0400*	
H105	1.07630	0.26110	0.68410	0.0470*	
H106	0.94700	0.31330	0.62850	0.0540*	
H107	0.84900	0.47940	0.61690	0.0550*	
H108	0.87870	0.59190	0.66200	0.0440*	
H10A	1.07090	0.14450	0.85430	0.0650*	0.500
H10B	1.13520	0.03200	0.86670	0.0650*	0.500

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0207 (2)	0.0232 (2)	0.0257 (2)	−0.0052 (2)	0.0000 (2)	−0.0044 (1)
P1	0.0183 (5)	0.0214 (4)	0.0252 (4)	−0.0046 (3)	−0.0033 (3)	−0.0039 (3)
P2	0.0219 (5)	0.0241 (4)	0.0209 (4)	−0.0080 (3)	−0.0011 (3)	−0.0010 (3)
O1	0.0208 (13)	0.0217 (10)	0.0267 (11)	−0.0051 (9)	−0.0056 (9)	−0.0019 (8)
N1	0.0257 (17)	0.0223 (12)	0.0235 (13)	−0.0075 (11)	0.0013 (11)	0.0009 (10)
N2	0.0290 (19)	0.0251 (13)	0.0313 (14)	−0.0075 (12)	0.0069 (12)	0.0005 (11)
N3	0.0294 (19)	0.0275 (13)	0.0339 (15)	−0.0090 (12)	0.0089 (12)	0.0016 (11)
N4	0.0251 (17)	0.0194 (11)	0.0250 (13)	−0.0057 (11)	−0.0004 (11)	−0.0019 (9)
N5	0.0260 (17)	0.0237 (12)	0.0262 (13)	−0.0072 (11)	−0.0006 (11)	−0.0036 (10)
N6	0.0273 (17)	0.0213 (12)	0.0258 (13)	−0.0054 (11)	−0.0023 (11)	−0.0035 (10)
C1	0.0182 (19)	0.0226 (14)	0.0306 (16)	−0.0030 (12)	−0.0030 (13)	−0.0055 (12)
C2	0.025 (2)	0.0279 (15)	0.0333 (17)	−0.0054 (14)	−0.0029 (14)	−0.0058 (13)
C3	0.031 (2)	0.0357 (17)	0.0366 (18)	−0.0109 (15)	−0.0064 (15)	−0.0118 (14)
C4	0.029 (2)	0.0323 (17)	0.051 (2)	−0.0114 (15)	−0.0030 (16)	−0.0132 (15)
C5	0.031 (2)	0.0334 (17)	0.0392 (19)	−0.0151 (15)	0.0024 (15)	−0.0049 (14)
C6	0.026 (2)	0.0296 (16)	0.0322 (17)	−0.0085 (14)	−0.0039 (14)	−0.0064 (13)
C7	0.024 (2)	0.0276 (15)	0.0259 (15)	−0.0093 (13)	−0.0072 (13)	−0.0024 (12)
C8	0.029 (2)	0.0315 (16)	0.0331 (17)	−0.0103 (14)	−0.0056 (14)	−0.0029 (13)

C9	0.047 (3)	0.0312 (18)	0.047 (2)	−0.0099 (17)	−0.0224 (19)	0.0057 (15)
C10	0.054 (3)	0.046 (2)	0.039 (2)	−0.022 (2)	−0.022 (2)	0.0145 (17)
C11	0.045 (3)	0.067 (3)	0.0333 (19)	−0.021 (2)	−0.0055 (18)	0.0051 (18)
C12	0.030 (2)	0.0434 (19)	0.0304 (18)	−0.0045 (16)	−0.0039 (15)	0.0016 (14)
C13	0.024 (2)	0.0246 (14)	0.0202 (14)	−0.0041 (13)	−0.0033 (12)	−0.0042 (11)
C14	0.023 (2)	0.0229 (14)	0.0218 (14)	−0.0051 (13)	−0.0012 (12)	−0.0071 (11)
C15	0.023 (2)	0.0325 (16)	0.0329 (17)	−0.0089 (14)	−0.0051 (14)	−0.0103 (13)
C16	0.025 (2)	0.0292 (16)	0.047 (2)	0.0058 (14)	−0.0096 (16)	−0.0157 (14)
C17	0.034 (2)	0.0226 (15)	0.0421 (19)	−0.0024 (14)	−0.0094 (16)	−0.0099 (13)
C18	0.029 (2)	0.0256 (15)	0.0329 (17)	−0.0088 (14)	−0.0038 (14)	−0.0090 (12)
C19	0.0195 (19)	0.0197 (13)	0.0215 (14)	−0.0051 (12)	0.0004 (12)	0.0014 (11)
C20	0.028 (2)	0.0261 (15)	0.0249 (15)	−0.0075 (13)	−0.0048 (13)	0.0003 (12)
C21	0.023 (2)	0.0236 (14)	0.0360 (17)	−0.0080 (13)	−0.0038 (14)	−0.0023 (12)
C22	0.021 (2)	0.0240 (14)	0.0327 (17)	−0.0079 (13)	0.0020 (13)	0.0021 (12)
C23	0.022 (2)	0.0242 (14)	0.0247 (15)	−0.0053 (13)	0.0006 (13)	−0.0001 (11)
C24	0.0189 (19)	0.0182 (13)	0.0244 (15)	−0.0034 (12)	−0.0050 (12)	0.0001 (11)
C25	0.028 (2)	0.0324 (16)	0.0233 (15)	−0.0130 (14)	0.0011 (13)	−0.0029 (12)
C26	0.035 (2)	0.0459 (19)	0.0239 (16)	−0.0114 (16)	0.0020 (14)	−0.0025 (14)
C27	0.045 (3)	0.071 (3)	0.0214 (17)	−0.025 (2)	0.0014 (16)	−0.0063 (16)
C28	0.057 (3)	0.063 (3)	0.0328 (19)	−0.034 (2)	0.0092 (18)	−0.0199 (17)
C29	0.060 (3)	0.0355 (18)	0.043 (2)	−0.0193 (18)	0.0033 (19)	−0.0156 (16)
C30	0.040 (2)	0.0338 (17)	0.0340 (18)	−0.0137 (16)	−0.0027 (16)	−0.0047 (14)
C31	0.028 (2)	0.0272 (15)	0.0215 (15)	−0.0110 (14)	−0.0001 (13)	−0.0007 (12)
C32	0.032 (2)	0.0310 (16)	0.0309 (17)	−0.0085 (15)	0.0046 (14)	0.0041 (13)
C33	0.032 (2)	0.0365 (18)	0.0373 (19)	0.0020 (16)	0.0062 (16)	0.0035 (15)
C34	0.049 (3)	0.0251 (16)	0.0280 (17)	−0.0055 (16)	0.0045 (15)	0.0020 (13)
C35	0.045 (3)	0.0329 (18)	0.044 (2)	−0.0188 (18)	−0.0040 (18)	0.0083 (15)
C36	0.029 (2)	0.0348 (18)	0.0416 (19)	−0.0118 (15)	0.0007 (16)	0.0039 (15)
C37	0.028 (2)	0.0305 (16)	0.0323 (17)	−0.0060 (14)	0.0058 (14)	−0.0024 (13)
C38	0.025 (2)	0.0238 (14)	0.0207 (14)	−0.0062 (13)	−0.0019 (12)	−0.0012 (11)
C39	0.022 (2)	0.0233 (14)	0.0207 (14)	−0.0040 (12)	−0.0017 (12)	−0.0005 (11)
C40	0.027 (2)	0.0257 (15)	0.0215 (15)	−0.0050 (13)	0.0024 (13)	−0.0045 (12)
C41	0.036 (3)	0.0326 (18)	0.052 (2)	−0.0131 (16)	0.0185 (17)	0.0039 (15)
C42	0.023 (2)	0.0291 (17)	0.057 (2)	−0.0089 (15)	0.0105 (16)	0.0004 (15)
C43	0.023 (2)	0.0289 (17)	0.083 (3)	−0.0082 (15)	−0.005 (2)	0.0089 (18)
C44	0.030 (3)	0.048 (2)	0.091 (3)	−0.0153 (19)	−0.019 (2)	0.007 (2)
C45	0.029 (3)	0.053 (2)	0.089 (3)	−0.021 (2)	−0.005 (2)	−0.010 (2)
C46	0.033 (3)	0.0292 (18)	0.088 (3)	−0.0145 (17)	0.007 (2)	−0.0049 (19)
C47	0.027 (2)	0.0308 (17)	0.062 (2)	−0.0059 (16)	0.0139 (18)	0.0055 (16)
C48	0.038 (2)	0.0206 (14)	0.0348 (17)	−0.0091 (14)	−0.0027 (15)	−0.0051 (12)
C49	0.031 (2)	0.0175 (14)	0.0345 (17)	−0.0040 (13)	−0.0026 (14)	−0.0030 (12)
C50	0.036 (2)	0.0256 (16)	0.0369 (18)	−0.0036 (15)	0.0033 (16)	−0.0011 (13)
C51	0.029 (2)	0.0265 (16)	0.059 (2)	−0.0028 (15)	−0.0003 (18)	−0.0022 (15)
C52	0.038 (3)	0.0200 (15)	0.056 (2)	−0.0019 (14)	−0.0156 (19)	−0.0040 (14)
C53	0.051 (3)	0.0229 (15)	0.0387 (19)	−0.0073 (16)	−0.0091 (18)	−0.0001 (13)
C54	0.038 (2)	0.0241 (15)	0.0401 (19)	−0.0090 (15)	−0.0020 (16)	0.0010 (13)
Cu2	0.0236 (2)	0.0197 (2)	0.0271 (2)	−0.0033 (2)	−0.0046 (2)	−0.0055 (1)
P3	0.0233 (5)	0.0188 (3)	0.0216 (4)	−0.0045 (3)	−0.0036 (3)	−0.0041 (3)
P4	0.0237 (5)	0.0187 (3)	0.0200 (4)	−0.0051 (3)	−0.0041 (3)	−0.0026 (3)

O2	0.0235 (14)	0.0226 (10)	0.0205 (10)	−0.0054 (9)	−0.0018 (9)	−0.0056 (8)
N7	0.0298 (18)	0.0245 (12)	0.0238 (13)	−0.0046 (11)	−0.0059 (11)	−0.0024 (10)
N8	0.0374 (19)	0.0236 (13)	0.0277 (14)	−0.0058 (12)	−0.0058 (12)	−0.0017 (10)
N9	0.039 (2)	0.0206 (12)	0.0302 (14)	−0.0047 (12)	−0.0092 (13)	0.0006 (10)
N10	0.0260 (17)	0.0224 (12)	0.0271 (13)	−0.0074 (11)	−0.0053 (11)	−0.0034 (10)
N11	0.0274 (18)	0.0280 (13)	0.0311 (14)	−0.0090 (12)	−0.0012 (12)	−0.0045 (11)
N12	0.0250 (18)	0.0284 (13)	0.0360 (15)	−0.0075 (12)	0.0009 (12)	−0.0087 (11)
C55	0.024 (2)	0.0238 (14)	0.0217 (14)	−0.0045 (13)	−0.0010 (12)	−0.0070 (11)
C56	0.027 (2)	0.0293 (16)	0.0359 (18)	−0.0043 (14)	−0.0003 (15)	−0.0015 (13)
C57	0.031 (2)	0.042 (2)	0.046 (2)	−0.0149 (17)	0.0095 (16)	0.0032 (16)
C58	0.045 (3)	0.0266 (16)	0.042 (2)	−0.0122 (16)	0.0070 (17)	0.0051 (14)
C59	0.043 (3)	0.0235 (16)	0.048 (2)	−0.0022 (15)	0.0010 (18)	0.0054 (14)
C60	0.028 (2)	0.0255 (15)	0.0366 (18)	−0.0047 (14)	0.0022 (14)	−0.0017 (13)
C61	0.023 (2)	0.0253 (14)	0.0227 (15)	−0.0076 (13)	−0.0036 (12)	−0.0034 (11)
C62	0.050 (3)	0.0230 (15)	0.0272 (16)	−0.0073 (15)	−0.0072 (15)	−0.0024 (12)
C63	0.068 (3)	0.0308 (17)	0.0305 (18)	−0.0147 (18)	−0.0042 (18)	−0.0094 (14)
C64	0.052 (3)	0.0438 (19)	0.0226 (16)	−0.0182 (18)	−0.0054 (16)	−0.0071 (14)
C65	0.051 (3)	0.0351 (18)	0.0297 (17)	−0.0151 (17)	−0.0103 (16)	0.0043 (14)
C66	0.042 (2)	0.0251 (15)	0.0277 (16)	−0.0112 (15)	−0.0081 (15)	−0.0005 (12)
C67	0.027 (2)	0.0180 (13)	0.0233 (15)	−0.0058 (12)	−0.0034 (13)	−0.0007 (11)
C68	0.030 (2)	0.0252 (15)	0.0252 (15)	−0.0075 (13)	−0.0032 (13)	−0.0035 (12)
C69	0.033 (2)	0.0352 (17)	0.0252 (16)	−0.0100 (15)	0.0056 (14)	−0.0053 (13)
C70	0.026 (2)	0.0358 (17)	0.0360 (18)	−0.0091 (15)	0.0000 (15)	−0.0020 (14)
C71	0.026 (2)	0.0312 (16)	0.0247 (15)	−0.0074 (14)	−0.0048 (13)	−0.0035 (12)
C72	0.026 (2)	0.0157 (13)	0.0203 (14)	−0.0042 (12)	−0.0017 (12)	−0.0012 (10)
C73	0.0207 (19)	0.0225 (14)	0.0225 (14)	−0.0065 (12)	−0.0020 (12)	−0.0018 (11)
C74	0.029 (2)	0.0227 (14)	0.0280 (16)	−0.0094 (13)	−0.0043 (13)	−0.0043 (12)
C75	0.027 (2)	0.0364 (17)	0.0225 (15)	−0.0126 (14)	−0.0051 (13)	−0.0080 (13)
C76	0.027 (2)	0.0328 (16)	0.0224 (15)	−0.0082 (14)	−0.0048 (13)	0.0005 (12)
C77	0.0193 (19)	0.0253 (14)	0.0274 (16)	−0.0054 (13)	−0.0020 (13)	−0.0009 (12)
C78	0.0218 (19)	0.0227 (14)	0.0216 (14)	−0.0072 (12)	−0.0011 (12)	−0.0046 (11)
C79	0.025 (2)	0.0187 (13)	0.0241 (15)	−0.0027 (12)	−0.0033 (13)	−0.0016 (11)
C80	0.032 (2)	0.0273 (15)	0.0271 (16)	−0.0077 (14)	−0.0035 (14)	−0.0061 (12)
C81	0.036 (2)	0.0293 (16)	0.044 (2)	−0.0152 (16)	0.0006 (16)	−0.0035 (14)
C82	0.035 (2)	0.0326 (17)	0.0392 (19)	−0.0087 (16)	0.0105 (16)	−0.0004 (14)
C83	0.038 (2)	0.0346 (17)	0.0265 (16)	−0.0060 (16)	0.0023 (15)	−0.0049 (13)
C84	0.029 (2)	0.0266 (15)	0.0256 (16)	−0.0063 (14)	−0.0014 (13)	−0.0051 (12)
C85	0.024 (2)	0.0230 (14)	0.0215 (14)	−0.0058 (12)	−0.0049 (12)	−0.0044 (11)
C86	0.030 (2)	0.0241 (15)	0.0295 (16)	−0.0116 (14)	0.0007 (14)	−0.0041 (12)
C87	0.027 (2)	0.0372 (17)	0.0329 (17)	−0.0114 (15)	0.0042 (14)	−0.0138 (14)
C88	0.035 (2)	0.0258 (15)	0.0373 (18)	−0.0016 (14)	−0.0056 (15)	−0.0096 (13)
C89	0.048 (3)	0.0231 (15)	0.0327 (18)	−0.0036 (15)	−0.0032 (16)	0.0002 (13)
C90	0.035 (2)	0.0269 (15)	0.0222 (15)	−0.0070 (14)	0.0013 (13)	−0.0025 (12)
C91	0.031 (2)	0.0248 (15)	0.0330 (18)	0.0004 (14)	−0.0072 (15)	−0.0048 (13)
C92	0.025 (2)	0.0219 (14)	0.0289 (16)	−0.0030 (13)	−0.0096 (13)	−0.0058 (12)
C93	0.023 (2)	0.0251 (15)	0.0292 (16)	−0.0057 (13)	−0.0072 (13)	−0.0066 (12)
C94	0.025 (2)	0.0284 (16)	0.0360 (18)	−0.0056 (14)	−0.0047 (14)	−0.0053 (13)
C95	0.056 (3)	0.0283 (17)	0.0327 (18)	−0.0055 (17)	−0.0075 (17)	0.0064 (14)
C96	0.052 (3)	0.0293 (16)	0.0244 (16)	−0.0084 (16)	0.0005 (16)	0.0042 (13)

C97	0.052 (3)	0.0320 (18)	0.041 (2)	−0.0084 (17)	0.0067 (18)	0.0000 (15)
C98	0.060 (3)	0.0288 (17)	0.053 (2)	−0.0154 (19)	0.012 (2)	−0.0080 (16)
C99	0.061 (3)	0.040 (2)	0.055 (2)	−0.024 (2)	0.000 (2)	0.0007 (17)
C100	0.045 (3)	0.049 (2)	0.041 (2)	−0.0159 (19)	0.0025 (18)	0.0089 (17)
C101	0.065 (3)	0.0280 (17)	0.0289 (18)	−0.0056 (18)	0.0027 (17)	−0.0013 (14)
C102	0.031 (2)	0.0388 (18)	0.0406 (19)	−0.0144 (16)	0.0096 (16)	−0.0078 (15)
C103	0.024 (2)	0.0312 (16)	0.0293 (16)	−0.0091 (14)	0.0071 (14)	−0.0006 (13)
C104	0.028 (2)	0.0350 (17)	0.0347 (18)	−0.0058 (15)	0.0048 (15)	−0.0019 (14)
C105	0.038 (3)	0.0310 (17)	0.045 (2)	−0.0080 (16)	0.0146 (17)	−0.0082 (15)
C106	0.058 (3)	0.052 (2)	0.0327 (19)	−0.025 (2)	0.0117 (18)	−0.0148 (16)
C107	0.045 (3)	0.063 (2)	0.0286 (18)	−0.018 (2)	−0.0049 (17)	0.0012 (17)
C108	0.038 (2)	0.0316 (17)	0.0346 (18)	−0.0039 (15)	−0.0007 (16)	0.0040 (14)
P5	0.0426 (7)	0.0663 (7)	0.0377 (5)	−0.0153 (5)	−0.0039 (5)	−0.0153 (5)
F1	0.082 (2)	0.0759 (18)	0.089 (2)	0.0149 (15)	−0.0483 (18)	−0.0312 (15)
F2	0.069 (2)	0.0614 (15)	0.0564 (15)	−0.0254 (13)	−0.0063 (13)	0.0066 (12)
F3	0.078 (2)	0.0642 (16)	0.090 (2)	−0.0206 (15)	0.0336 (17)	0.0029 (14)
F4	0.130 (3)	0.147 (3)	0.077 (2)	−0.078 (3)	−0.058 (2)	0.020 (2)
F5	0.111 (3)	0.080 (2)	0.097 (2)	−0.0184 (18)	−0.010 (2)	−0.0524 (18)
F6	0.115 (4)	0.209 (4)	0.083 (2)	−0.081 (3)	0.050 (2)	−0.072 (3)
P6	0.0363 (6)	0.0299 (4)	0.0314 (4)	−0.0031 (4)	−0.0105 (4)	−0.0059 (3)
F7	0.073 (2)	0.0477 (12)	0.0398 (12)	0.0020 (12)	0.0014 (11)	−0.0134 (10)
F8	0.0439 (15)	0.0325 (10)	0.0479 (12)	−0.0087 (9)	−0.0114 (10)	−0.0020 (9)
F9	0.0395 (15)	0.0371 (11)	0.0573 (13)	−0.0106 (9)	−0.0181 (11)	0.0044 (9)
F10	0.0555 (16)	0.0330 (10)	0.0344 (11)	−0.0018 (10)	−0.0125 (10)	−0.0005 (8)
F11	0.0559 (17)	0.0439 (11)	0.0396 (11)	−0.0137 (11)	0.0017 (10)	−0.0133 (9)
F12	0.0451 (16)	0.0426 (12)	0.0727 (15)	−0.0012 (10)	−0.0276 (12)	−0.0182 (11)
Cl1	0.0591 (18)	0.0735 (14)	0.0746 (15)	−0.0256 (12)	0.0009 (12)	−0.0276 (12)
Cl2	0.0491 (17)	0.1032 (19)	0.0864 (18)	−0.0296 (14)	0.0163 (13)	−0.0522 (15)
C109	0.084 (7)	0.040 (4)	0.057 (5)	−0.043 (5)	−0.004 (5)	−0.004 (4)

Geometric parameters (Å, °)

Cu1—P1	2.2573 (9)	C22—H22	0.9500
Cu1—P2	2.2922 (11)	C23—H23	0.9500
Cu1—N1	2.169 (3)	C26—H26	0.9500
Cu1—N4	2.103 (2)	C27—H27	0.9500
Cu2—P4	2.3070 (10)	C28—H28	0.9500
Cu2—N7	2.194 (3)	C29—H29	0.9500
Cu2—N10	2.063 (3)	C30—H30	0.9500
Cu2—P3	2.2252 (8)	C32—H32	0.9500
Cl1—C109	1.669 (9)	C33—H33	0.9500
Cl2—C109	1.664 (11)	C34—H34	0.9500
P1—C7	1.828 (3)	C35—H35	0.9500
P1—C1	1.831 (4)	C36—H36	0.9500
P1—C13	1.824 (4)	C37—H37	0.9500
P2—C31	1.837 (3)	C40—H40	0.9500
P2—C19	1.845 (3)	C41—H41A	0.9900
P2—C25	1.829 (3)	C41—H41B	0.9900
P3—C67	1.829 (4)	C43—H43	0.9500

P3—C61	1.832 (3)	C44—H44	0.9500
P3—C55	1.828 (3)	C45—H45	0.9500
P4—C85	1.825 (3)	C46—H46	0.9500
P4—C73	1.834 (3)	C47—H47	0.9500
P4—C79	1.824 (4)	C48—H48A	0.9900
P5—F5	1.588 (3)	C48—H48B	0.9900
P5—F4	1.590 (4)	C50—H50	0.9500
P5—F3	1.569 (4)	C51—H51	0.9500
P5—F6	1.594 (4)	C52—H52	0.9500
P5—F1	1.561 (4)	C53—H53	0.9500
P5—F2	1.614 (3)	C54—H54	0.9500
P6—F7	1.596 (2)	C55—C60	1.397 (5)
P6—F10	1.598 (2)	C55—C56	1.390 (6)
P6—F8	1.615 (2)	C56—C57	1.391 (5)
P6—F9	1.614 (3)	C57—C58	1.377 (5)
P6—F11	1.598 (2)	C58—C59	1.384 (6)
P6—F12	1.598 (3)	C59—C60	1.385 (5)
O1—C14	1.396 (3)	C61—C66	1.398 (4)
O1—C24	1.399 (4)	C61—C62	1.385 (4)
O2—C72	1.393 (4)	C62—C63	1.382 (5)
O2—C78	1.400 (3)	C63—C64	1.387 (5)
N1—N2	1.321 (4)	C64—C65	1.382 (6)
N1—C38	1.362 (4)	C65—C66	1.389 (5)
N2—N3	1.332 (4)	C67—C68	1.394 (5)
N3—C41	1.478 (5)	C67—C72	1.413 (5)
N3—C37	1.358 (4)	C68—C69	1.380 (6)
N4—C39	1.365 (4)	C69—C70	1.398 (5)
N4—N5	1.320 (3)	C70—C71	1.400 (5)
N5—N6	1.347 (4)	C71—C72	1.377 (6)
N6—C40	1.352 (4)	C73—C74	1.402 (4)
N6—C48	1.475 (4)	C73—C78	1.408 (4)
N7—C92	1.361 (4)	C74—C75	1.399 (4)
N7—N8	1.323 (4)	C75—C76	1.383 (4)
N8—N9	1.345 (4)	C76—C77	1.397 (4)
N9—C91	1.344 (5)	C77—C78	1.385 (4)
N9—C95	1.487 (4)	C79—C84	1.403 (4)
N10—N11	1.319 (4)	C79—C80	1.407 (5)
N10—C93	1.375 (4)	C80—C81	1.385 (5)
N11—N12	1.336 (4)	C81—C82	1.389 (5)
N12—C102	1.481 (5)	C82—C83	1.382 (5)
N12—C94	1.348 (4)	C83—C84	1.389 (5)
C1—C2	1.398 (4)	C85—C90	1.393 (4)
C1—C6	1.393 (5)	C85—C86	1.397 (5)
C2—C3	1.399 (5)	C86—C87	1.380 (4)
C3—C4	1.376 (5)	C87—C88	1.393 (4)
C4—C5	1.385 (5)	C88—C89	1.380 (5)
C5—C6	1.393 (5)	C89—C90	1.391 (4)
C7—C12	1.386 (5)	C91—C92	1.382 (4)
C7—C8	1.392 (4)	C92—C93	1.447 (5)

C8—C9	1.397 (5)	C93—C94	1.364 (5)
C9—C10	1.367 (6)	C95—C96	1.532 (5)
C10—C11	1.377 (6)	C96—C97	1.392 (5)
C11—C12	1.406 (5)	C96—C101	1.408 (6)
C13—C18	1.403 (4)	C97—C98	1.378 (7)
C13—C14	1.395 (6)	C98—C99	1.388 (7)
C14—C15	1.380 (5)	C99—C100	1.373 (6)
C15—C16	1.387 (4)	C100—C101	1.372 (6)
C16—C17	1.386 (6)	C102—C103	1.509 (5)
C17—C18	1.385 (5)	C103—C108	1.400 (5)
C19—C24	1.401 (4)	C103—C104	1.388 (4)
C19—C20	1.407 (5)	C104—C105	1.381 (5)
C20—C21	1.391 (5)	C105—C106	1.379 (6)
C21—C22	1.390 (4)	C106—C107	1.387 (6)
C22—C23	1.391 (5)	C107—C108	1.384 (5)
C23—C24	1.387 (5)	C56—H56	0.9500
C25—C30	1.403 (4)	C57—H57	0.9500
C25—C26	1.384 (5)	C58—H58	0.9500
C26—C27	1.395 (5)	C59—H59	0.9500
C27—C28	1.387 (6)	C60—H60	0.9500
C28—C29	1.389 (6)	C62—H62	0.9500
C29—C30	1.385 (5)	C63—H63	0.9500
C31—C32	1.394 (6)	C64—H64	0.9500
C31—C36	1.392 (5)	C65—H65	0.9500
C32—C33	1.393 (4)	C66—H66	0.9500
C33—C34	1.385 (5)	C68—H68	0.9500
C34—C35	1.370 (6)	C69—H69	0.9500
C35—C36	1.394 (4)	C70—H70	0.9500
C37—C38	1.373 (6)	C71—H71	0.9500
C38—C39	1.446 (4)	C74—H74	0.9500
C39—C40	1.372 (4)	C75—H75	0.9500
C41—C42	1.505 (5)	C76—H76	0.9500
C42—C43	1.403 (6)	C77—H77	0.9500
C42—C47	1.395 (4)	C80—H80	0.9500
C43—C44	1.377 (6)	C81—H81	0.9500
C44—C45	1.394 (6)	C82—H82	0.9500
C45—C46	1.385 (7)	C83—H83	0.9500
C46—C47	1.380 (6)	C84—H84	0.9500
C48—C49	1.520 (5)	C86—H86	0.9500
C49—C54	1.391 (5)	C87—H87	0.9500
C49—C50	1.383 (6)	C88—H88	0.9500
C50—C51	1.401 (6)	C89—H89	0.9500
C51—C52	1.374 (5)	C90—H90	0.9500
C52—C53	1.391 (6)	C91—H91	0.9500
C53—C54	1.404 (6)	C94—H94	0.9500
C2—H2	0.9500	C95—H95B	0.9900
C3—H3	0.9500	C95—H95A	0.9900
C4—H4	0.9500	C97—H97	0.9500
C5—H5	0.9500	C98—H98	0.9500

C6—H6	0.9500	C99—H99	0.9500
C8—H8	0.9500	C100—H100	0.9500
C9—H9	0.9500	C101—H101	0.9500
C10—H10	0.9500	C102—H10E	0.9900
C11—H11	0.9500	C102—H10D	0.9900
C12—H12	0.9500	C104—H104	0.9500
C15—H15	0.9500	C105—H105	0.9500
C16—H16	0.9500	C106—H106	0.9500
C17—H17	0.9500	C107—H107	0.9500
C18—H18	0.9500	C108—H108	0.9500
C20—H20	0.9500	C109—H10A	0.9900
C21—H21	0.9500	C109—H10B	0.9900
Cu1···O1	3.285 (2)	C46···H33^{ii}	2.8300
Cu2···O2	3.271 (2)	C46···H5	2.8300
Cu1···H6	3.2600	C47···H5	3.0200
Cu1···H30	3.3500	C47···H41B^{iii}	2.8200
Cu1···H36	3.0700	C51···H16^{ix}	2.8000
Cu1···H8	3.2600	C52···H74	2.7300
Cu2···H84	2.9300	C52···H16^{ix}	2.8100
Cu2···H66	3.1100	C53···H74	3.0100
Cu2···H56	3.4100	C55···H62	2.7100
Cl1···H97	3.0900	C59···H99^{xi}	3.0400
P2···C14	3.429 (3)	C60···H62	2.9100
P3···P4	3.7994 (11)	C61···H68	2.6200
P4···N7	3.364 (3)	C62···H98^{xi}	3.0700
P4···N10	3.478 (3)	C62···H68	2.9300
P4···C72	3.369 (3)	C65···H100^{xii}	3.0200
P4···P3	3.7994 (11)	C67···H84	3.0600
P6···H94^{i}	3.1200	C67···H60	2.6400
F1···C21^{ii}	3.284 (4)	C70···H10B^{viii}	2.9900
F2···C21^{ii}	3.367 (4)	C72···H60	2.9700
F2···C37	3.346 (5)	C73···H22^{ii}	2.9300
F2···C47^{iii}	3.294 (4)	C73···H86	3.0500
F3···C40	3.284 (6)	C73···H80	3.0000
F3···C37	3.297 (4)	C74···H22^{ii}	2.9500
F5···C40^{iv}	3.194 (4)	C74···H80	3.0300
F6···C48^{iv}	3.314 (5)	C74···H86	3.0600
F8···C94^{i}	3.215 (5)	C75···H22^{ii}	2.9500
F9···C94^{i}	3.228 (4)	C75···H8	3.0800
F11···C53^{iv}	3.285 (5)	C76···H22^{ii}	2.9400
F11···C54^{iv}	3.182 (4)	C76···H8	2.9400
F11···C4^{iii}	3.142 (4)	C77···H71	2.9300
F11···C3^{iii}	3.298 (4)	C77···H22^{ii}	2.9100
F12···C81^{iv}	3.220 (4)	C78···H71	2.6000

F1···H107	2.4600	C78···H22^{ii}	2.9000
F1···H21^{ii}	2.6500	C79···H90	2.6300
F2···H37	2.4600	C80···H90	2.8800
F2···H21^{ii}	2.6700	C80···H9	2.9500
F2···H47^{iii}	2.5600	C82···H100	3.1000
F3···H37	2.4800	C83···H95A^{xii}	3.0700
F3···H40	2.6000	C83···H101	2.9600
F4···H50^{iv}	2.7100	C84···H101	3.0400
F4···H46^{iii}	2.8200	C85···H74	2.7300
F5···H40^{iv}	2.5400	C86···H74	2.9000
F6···H48A^{iv}	2.4200	C87···H52	3.0200
F7···H65^{v}	2.7800	C88···H17^{ix}	3.0800
F7···H64^{v}	2.8300	C88···H52	2.9700
F8···H94^{i}	2.4700	C89···H52	3.0500
F8···H54^{iv}	2.8500	C96···H69^{xii}	2.9000
F8···H81^{iv}	2.6000	C97···H69^{xii}	3.0200
F9···H94^{i}	2.2900	C98···H89	3.0200
F9···H104^{i}	2.7100	C99···H62^{xiii}	2.9400
F10···H64^{v}	2.4400	C100···H90	2.8700
F10···H3^{iii}	2.7000	C101···H83^{xii}	2.9700
F11···H3^{iii}	2.8100	C101···H90	2.8100
F11···H53^{iv}	2.8200	C103···H87	2.9400
F11···H54^{iv}	2.6200	C104···H87	2.8900
F11···H4^{iii}	2.4900	C104···H48B^{ii}	2.9400
F12···H81^{iv}	2.6300	C105···H87	2.8300
O1···Cu1	3.285 (2)	C106···H28^{iv}	2.8400
O1···C7	3.085 (5)	C106···H87	2.8300
O1···C12	3.230 (4)	C107···H87	2.8900
O2···Cu2	3.271 (2)	C108···H87	2.9400
O2···C55	3.180 (4)	H2···C7	2.7400
O2···C60	3.338 (4)	H2···C12	2.9000
N1···C39	2.406 (4)	H3···F10^{iii}	2.7000
N1···N4	2.737 (3)	H3···F11^{iii}	2.8100
N2···C6	3.345 (4)	H4···F11^{iii}	2.4900
N3···C33^{vi}	3.292 (4)	H5···C47	3.0200
N4···N1	2.737 (3)	H5···C46	2.8300
N4···C38	2.405 (4)	H5···C44	3.0400
N7···N10	2.711 (4)	H5···C45	2.8400
N7···C93	2.404 (5)	H6···Cu1	3.2600
N7···P4	3.364 (3)	H6···N1	2.7900
N8···C101	3.267 (4)	H6···N2	2.4800
N8···C84	3.423 (5)	H8···Cu1	3.2600
N10···C86	3.340 (4)	H8···C76	2.9400

N10···N7	2.711 (4)	H8···N4	2.9000
N10···P4	3.478 (3)	H8···C75	3.0800
N10···C92	2.409 (4)	H9···C80	2.9500
N11···C23^{ii}	3.211 (4)	H9···H80	2.5300
N1···H6	2.7900	H10A···F9^{i}	2.4100
N2···H26^{vi}	2.7500	H10A···F10^{i}	2.7500
N2···H6	2.4800	H10D···C9^{ii}	2.8100
N3···H43	2.8300	H10D···C8^{ii}	3.0800
N4···H30	2.7600	H10D···H104	2.4900
N4···H8	2.9000	H10E···H108	2.4300
N5···H30	2.7600	H12···C13	2.7400
N7···H66	2.7400	H12···C14	3.0200
N8···H66	2.8000	H12···H57^{vii}	2.4000
N8···H101	2.8100	H15···C23	2.8600
N8···H84	2.8700	H15···H44^{vii}	2.4600
N11···H23^{ii}	2.7600	H15···C44^{vii}	3.0400
C2···C77	3.584 (5)	H15···C24	2.6000
C3···F11^{iii}	3.298 (4)	H16···C51^{viii}	2.8000
C4···F11^{iii}	3.142 (4)	H16···C52^{viii}	2.8100
C5···C44	3.453 (6)	H16···H45^{vii}	2.5700
C5···C45	3.487 (6)	H17···C88^{viii}	3.0800
C6···C18	3.558 (6)	H18···C6	2.9500
C6···N2	3.345 (4)	H18···C2	3.0200
C7···O1	3.085 (5)	H18···C1	2.5900
C8···C102^{vii}	3.594 (6)	H20···C25	2.5500
C9···C102^{vii}	3.474 (6)	H20···C26	2.8400
C12···C14	3.496 (5)	H20···C30	3.0500
C12···O1	3.230 (4)	H21···F1^{vii}	2.6500
C14···P2	3.429 (3)	H21···F2^{vii}	2.6700
C14···C12	3.496 (5)	H22···C78^{vii}	2.9000
C14···C31	3.461 (4)	H22···C75^{vii}	2.9500
C15···C57^{vii}	3.471 (5)	H22···C76^{vii}	2.9400
C15···C32	3.291 (4)	H22···C77^{vii}	2.9100
C15···C19	3.571 (4)	H22···C74^{vii}	2.9500
C15···C58^{vii}	3.574 (5)	H22···C73^{vii}	2.9300
C15···C23	3.412 (4)	H23···N11^{vii}	2.7600
C16···C58^{vii}	3.488 (5)	H26···H41A^{vi}	2.4300
C16···C51^{viii}	3.585 (4)	H26···C32	3.0200
C16···C52^{viii}	3.555 (4)	H26···N2^{vi}	2.7500
C17···C88^{viii}	3.567 (5)	H26···C31	2.6800
C18···C6	3.558 (6)	H28···C106^{iv}	2.8400
C19···C15	3.571 (4)	H30···N4	2.7600
C20···C26	3.556 (5)	H30···Cu1	3.3500

C20···C30	3.510 (5)	H30···N5	2.7600
C21···F2^{vii}	3.367 (4)	H32···C44^{vii}	3.0800
C21···F1^{vii}	3.284 (4)	H32···C20	2.9700
C23···C15	3.412 (4)	H32···C19	2.6600
C23···N11^{vii}	3.211 (4)	H33···C46^{vii}	2.8300
C26···C20	3.556 (5)	H33···C45^{vii}	2.9500
C26···C35^{vi}	3.542 (6)	H35···C26^{vi}	2.7500
C28···C106^{iv}	3.541 (5)	H35···C25^{vi}	2.9900
C30···C20	3.510 (5)	H35···C28^{vi}	3.0900
C31···C14	3.461 (4)	H35···C27^{vi}	2.8000
C32···C41^{vi}	3.546 (5)	H36···Cu1	3.0700
C32···C15	3.291 (4)	H37···F3	2.4800
C33···C37^{vi}	3.445 (5)	H37···F2	2.4600
C33···N3^{vi}	3.292 (4)	H40···H50	2.5600
C33···C41^{vi}	3.489 (5)	H40···F3	2.6000
C34···C37^{vi}	3.416 (5)	H40···F5^{iv}	2.5400
C35···C26^{vi}	3.542 (6)	H41A···H47	2.3400
C37···C34^{vi}	3.416 (5)	H41A···H26^{vi}	2.4300
C37···C33^{vi}	3.445 (5)	H41A···C32^{vi}	2.9000
C37···F2	3.346 (5)	H41B···C47^{iii}	2.8200
C37···F3	3.297 (4)	H41B···C42^{iii}	2.9900
C40···F3	3.284 (6)	H43···C21^{ii}	3.0100
C40···F5^{iv}	3.194 (4)	H43···N3	2.8300
C40···C50	3.323 (5)	H43···C37	3.0700
C41···C32^{vi}	3.546 (5)	H44···H15^{ii}	2.4600
C41···C33^{vi}	3.489 (5)	H45···H16^{ii}	2.5700
C44···C5	3.453 (6)	H46···F4^{iii}	2.8200
C45···C5	3.487 (6)	H46···H48A^{xi}	2.4700
C47···F2^{iii}	3.294 (4)	H47···F2^{iii}	2.5600
C48···F6^{iv}	3.314 (5)	H47···H41A	2.3400
C50···C40	3.323 (5)	H48A···H50	2.5800
C51···C16^{ix}	3.585 (4)	H48A···F6^{iv}	2.4200
C52···C16^{ix}	3.555 (4)	H48A···H46^{xiii}	2.4700
C53···F11^{iv}	3.285 (5)	H48B···C104^{vii}	2.9400
C54···F11^{iv}	3.182 (4)	H48B···H54	2.3700
C55···O2	3.180 (4)	H50···H48A	2.5800
C57···C15^{ii}	3.471 (5)	H50···F4^{iv}	2.7100
C58···C15^{ii}	3.574 (5)	H50···H40	2.5600
C58···C16^{ii}	3.488 (5)	H50···C40	2.9900
C60···C72	3.495 (5)	H52···C89	3.0500
C60···O2	3.338 (4)	H52···C87	3.0200
C62···C68	3.565 (6)	H52···C88	2.9700

C63···C63^{x}	3.590 (5)	H53···F11^{iv}	2.8200
C67···C84	3.459 (4)	H54···H48B	2.3700
C68···C62	3.565 (6)	H54···F11^{iv}	2.6200
C68···C84	3.590 (4)	H54···F8^{iv}	2.8500
C71···C77	3.470 (4)	H56···Cu2	3.4100
C71···C73	3.566 (4)	H57···H12^{ii}	2.4000
C72···C79	3.468 (4)	H58···C16^{ii}	2.9900
C72···C60	3.495 (5)	H59···F12^{iii}	2.7400
C72···P4	3.369 (3)	H59···F11^{iii}	2.5400
C73···C71	3.566 (4)	H60···C67	2.6400
C74···C86	3.337 (5)	H60···C72	2.9700
C77···C2	3.584 (5)	H62···C55	2.7100
C77···C71	3.470 (4)	H62···C60	2.9100
C79···C72	3.468 (4)	H62···C99^{xi}	2.9400
C80···C90	3.447 (5)	H62···H99^{xi}	2.3600
C81···F12^{iv}	3.220 (4)	H64···F7^{xiv}	2.8300
C84···C67	3.459 (4)	H64···F10^{xiv}	2.4400
C84···C68	3.590 (4)	H65···F7^{xiv}	2.7800
C84···N8	3.423 (5)	H66···Cu2	3.1100
C85···C92	3.594 (5)	H66···N7	2.7400
C86···C93	3.407 (5)	H66···N8	2.8000
C86···N10	3.340 (4)	H68···C61	2.6200
C86···C74	3.337 (5)	H68···C62	2.9300
C87···C94	3.574 (5)	H69···C96^{xii}	2.9000
C88···C17^{ix}	3.567 (5)	H69···C97^{xii}	3.0200
C90···C80	3.447 (5)	H70···C11	3.0700
C90···C101	3.568 (5)	H71···C8	3.0700
C92···C85	3.594 (5)	H71···C77	2.9300
C93···C86	3.407 (5)	H71···C78	2.6000
C94···F8^{i}	3.215 (5)	H71···C9	3.0600
C94···F9^{i}	3.228 (4)	H74···C85	2.7300
C94···C104	3.454 (5)	H74···C86	2.9000
C94···C87	3.574 (5)	H74···C52	2.7300
C1···H77	3.0800	H74···C53	3.0100
C1···H18	2.5900	H76···C38	2.9700
C101···C90	3.568 (5)	H77···C1	3.0800
C101···N8	3.267 (4)	H77···C2	2.9400
C102···C8^{ii}	3.594 (6)	H77···C4	3.0400
C2···H18	3.0200	H77···C3	2.9200
C2···H77	2.9400	H80···C74	3.0300
C102···C9^{ii}	3.474 (6)	H80···H9	2.5300
C3···H77	2.9200	H80···C73	3.0000
C4···H77	3.0400	H81···F8^{iv}	2.6000
C104···C94	3.454 (5)	H81···F12^{iv}	2.6300
C4···H105^{viii}	3.0400	H83···H101^{xii}	2.2500

C5···H105^{viii}	2.9200	H83···C101^{xii}	2.9700
C6···H18	2.9500	H84···C67	3.0600
C106···C28^{iv}	3.541 (5)	H84···Cu2	2.9300
C7···H2	2.7400	H84···N8	2.8700
C8···H10D^{vii}	3.0800	H86···C73	3.0500
C8···H71	3.0700	H86···C74	3.0600
C9···H71	3.0600	H87···C108	2.9400
C109···F10^{i}	3.216 (11)	H87···C103	2.9400
C9···H10D^{vii}	2.8100	H87···C104	2.8900
C109···F9^{i}	3.362 (9)	H87···C105	2.8300
C11···H70	3.0700	H87···C106	2.8300
C12···H2	2.9000	H87···C107	2.8900
C13···H12	2.7400	H88···C17^{ix}	3.0800
C14···H12	3.0200	H89···C98	3.0200
C16···H58^{vii}	2.9900	H90···C79	2.6300
C17···H88^{viii}	3.0800	H90···C80	2.8800
C19···H32	2.6600	H90···C101	2.8100
C19···H108^{vii}	3.0600	H90···C100	2.8700
C20···H108^{vii}	2.9000	H94···F8^{i}	2.4700
C20···H32	2.9700	H94···P6^{i}	3.1200
C21···H43^{vii}	3.0100	H94···F9^{i}	2.2900
C21···H108^{vii}	2.8900	H95A···C83^{xii}	3.0700
C22···H108^{vii}	3.0200	H95B···H97	2.3800
C23···H15	2.8600	H97···H95B	2.3800
C24···H15	2.6000	H97···Cl1	3.0900
C25···H20	2.5500	H98···C62^{xiii}	3.0700
C25···H35^{vi}	2.9900	H99···C59^{xiii}	3.0400
C26···H20	2.8400	H99···H62^{xiii}	2.3600
C26···H35^{vi}	2.7500	H100···C65^{xii}	3.0200
C27···H35^{vi}	2.8000	H100···C82	3.1000
C28···H106^{iv}	3.1000	H101···N8	2.8100
C28···H35^{vi}	3.0900	H101···C83	2.9600
C30···H20	3.0500	H101···C84	3.0400
C31···H26	2.6800	H101···H83^{xii}	2.2500
C32···H41A^{vi}	2.9000	H104···H10D	2.4900
C32···H26	3.0200	H104···F9^{i}	2.7100
C37···H43	3.0700	H105···C4^{ix}	3.0400
C38···H76	2.9700	H105···C5^{ix}	2.9200
C40···H50	2.9900	H106···C28^{iv}	3.1000
C42···H41B^{iii}	2.9900	H107···F1	2.4600
C44···H5	3.0400	H108···C19^{ii}	3.0600
C44···H32^{ii}	3.0800	H108···C20^{ii}	2.9000

C44···H15^{ii}	3.0400	H108···C21^{ii}	2.8900
C45···H5	2.8400	H108···C22^{ii}	3.0200
C45···H33^{ii}	2.9500	H108···H10E	2.4300
P1—Cu1—P2	114.87 (4)	C25—C30—H30	120.00
P1—Cu1—N1	114.00 (7)	C33—C32—H32	120.00
P1—Cu1—N4	119.47 (7)	C31—C32—H32	120.00
P2—Cu1—N1	112.53 (7)	C32—C33—H33	120.00
P2—Cu1—N4	111.50 (8)	C34—C33—H33	120.00
N1—Cu1—N4	79.66 (10)	C33—C34—H34	120.00
P3—Cu2—N10	131.32 (7)	C35—C34—H34	120.00
P4—Cu2—N7	96.69 (7)	C36—C35—H35	120.00
P4—Cu2—N10	105.32 (8)	C34—C35—H35	120.00
N7—Cu2—N10	79.04 (10)	C31—C36—H36	120.00
P3—Cu2—P4	113.92 (4)	C35—C36—H36	120.00
P3—Cu2—N7	121.67 (7)	C38—C37—H37	128.00
C1—P1—C13	101.54 (15)	N3—C37—H37	128.00
Cu1—P1—C1	120.97 (11)	N6—C40—H40	128.00
Cu1—P1—C7	113.88 (10)	C39—C40—H40	128.00
Cu1—P1—C13	108.99 (11)	C42—C41—H41B	109.00
C1—P1—C7	103.58 (15)	C42—C41—H41A	109.00
C7—P1—C13	106.41 (16)	H41A—C41—H41B	108.00
C25—P2—C31	104.88 (14)	N3—C41—H41B	109.00
Cu1—P2—C19	119.85 (10)	N3—C41—H41A	109.00
Cu1—P2—C25	115.28 (13)	C44—C43—H43	119.00
C19—P2—C31	103.54 (16)	C42—C43—H43	119.00
C19—P2—C25	100.26 (16)	C43—C44—H44	120.00
Cu1—P2—C31	111.27 (13)	C45—C44—H44	120.00
C55—P3—C61	103.64 (14)	C46—C45—H45	120.00
Cu2—P3—C67	109.47 (10)	C44—C45—H45	120.00
Cu2—P3—C61	116.82 (10)	C45—C46—H46	120.00
Cu2—P3—C55	118.22 (11)	C47—C46—H46	120.00
C55—P3—C67	104.27 (16)	C42—C47—H47	120.00
C61—P3—C67	102.65 (16)	C46—C47—H47	120.00
Cu2—P4—C73	120.05 (10)	N6—C48—H48A	110.00
Cu2—P4—C79	113.76 (11)	N6—C48—H48B	110.00
Cu2—P4—C85	108.35 (13)	C49—C48—H48B	110.00
C73—P4—C79	104.56 (15)	H48A—C48—H48B	108.00
C73—P4—C85	104.27 (13)	C49—C48—H48A	110.00
C79—P4—C85	104.45 (15)	C49—C50—H50	119.00
F2—P5—F3	87.99 (15)	C51—C50—H50	120.00
F1—P5—F2	89.42 (15)	C52—C51—H51	120.00
F1—P5—F3	92.0 (2)	C50—C51—H51	120.00
F1—P5—F4	176.3 (2)	C53—C52—H52	120.00
F1—P5—F5	91.19 (18)	C51—C52—H52	120.00
F1—P5—F6	89.7 (2)	C52—C53—H53	120.00
F5—P5—F6	91.6 (2)	C54—C53—H53	120.00
F3—P5—F6	176.9 (2)	C49—C54—H54	120.00
F3—P5—F4	91.3 (2)	C53—C54—H54	120.00

F3—P5—F5	90.90 (18)	P3—C55—C60	122.7 (3)
F2—P5—F5	178.8 (2)	C56—C55—C60	118.8 (3)
F4—P5—F5	90.5 (2)	P3—C55—C56	118.5 (2)
F4—P5—F6	86.9 (2)	C55—C56—C57	120.2 (3)
F2—P5—F6	89.5 (2)	C56—C57—C58	120.7 (4)
F2—P5—F4	88.99 (18)	C57—C58—C59	119.4 (3)
F7—P6—F9	89.78 (14)	C58—C59—C60	120.5 (3)
F7—P6—F8	89.80 (11)	C55—C60—C59	120.3 (4)
F11—P6—F12	90.21 (14)	P3—C61—C66	119.1 (2)
F7—P6—F12	90.16 (14)	P3—C61—C62	122.3 (2)
F8—P6—F9	89.85 (12)	C62—C61—C66	118.6 (3)
F8—P6—F10	179.08 (12)	C61—C62—C63	121.1 (3)
F8—P6—F11	89.43 (11)	C62—C63—C64	120.2 (3)
F9—P6—F11	89.85 (13)	C63—C64—C65	119.5 (3)
F7—P6—F10	91.06 (12)	C64—C65—C66	120.3 (3)
F7—P6—F11	179.14 (13)	C61—C66—C65	120.4 (3)
F10—P6—F12	90.30 (13)	P3—C67—C68	124.5 (3)
F9—P6—F12	179.87 (12)	P3—C67—C72	117.9 (3)
F10—P6—F11	89.71 (11)	C68—C67—C72	117.2 (4)
F8—P6—F12	90.03 (12)	C67—C68—C69	121.3 (3)
F9—P6—F10	89.82 (12)	C68—C69—C70	120.4 (3)
C14—O1—C24	117.6 (2)	C69—C70—C71	119.6 (4)
C72—O2—C78	117.9 (2)	C70—C71—C72	119.0 (3)
Cu1—N1—N2	138.63 (19)	O2—C72—C71	122.7 (3)
Cu1—N1—C38	110.6 (2)	O2—C72—C67	114.9 (3)
N2—N1—C38	109.1 (3)	C67—C72—C71	122.4 (3)
N1—N2—N3	106.7 (2)	P4—C73—C78	119.1 (2)
N2—N3—C37	111.9 (3)	P4—C73—C74	123.5 (2)
C37—N3—C41	127.3 (3)	C74—C73—C78	117.3 (3)
N2—N3—C41	120.7 (3)	C73—C74—C75	120.8 (3)
N5—N4—C39	109.8 (2)	C74—C75—C76	120.7 (3)
Cu1—N4—C39	112.37 (18)	C75—C76—C77	119.6 (3)
Cu1—N4—N5	136.3 (2)	C76—C77—C78	119.6 (3)
N4—N5—N6	106.0 (2)	O2—C78—C77	118.7 (2)
N5—N6—C40	111.9 (2)	O2—C78—C73	119.1 (2)
C40—N6—C48	127.4 (3)	C73—C78—C77	122.1 (3)
N5—N6—C48	120.0 (2)	C80—C79—C84	118.6 (3)
Cu2—N7—C92	110.05 (19)	P4—C79—C80	122.8 (2)
N8—N7—C92	109.6 (2)	P4—C79—C84	118.6 (3)
Cu2—N7—N8	137.6 (2)	C79—C80—C81	120.6 (3)
N7—N8—N9	106.1 (2)	C80—C81—C82	119.9 (4)
C91—N9—C95	128.6 (3)	C81—C82—C83	120.3 (3)
N8—N9—C91	112.0 (2)	C82—C83—C84	120.4 (3)
N8—N9—C95	118.8 (3)	C79—C84—C83	120.2 (3)
Cu2—N10—N11	135.5 (2)	P4—C85—C90	121.1 (2)
N11—N10—C93	108.8 (3)	C86—C85—C90	118.5 (3)
Cu2—N10—C93	114.3 (2)	P4—C85—C86	119.4 (2)
N10—N11—N12	106.7 (2)	C85—C86—C87	120.9 (3)
C94—N12—C102	127.0 (3)	C86—C87—C88	120.0 (3)

N11—N12—C102	120.9 (3)	C87—C88—C89	119.9 (3)
N11—N12—C94	111.8 (3)	C88—C89—C90	119.9 (3)
P1—C1—C2	123.1 (3)	C85—C90—C89	120.8 (3)
C2—C1—C6	119.1 (3)	N9—C91—C92	104.4 (3)
P1—C1—C6	117.8 (2)	N7—C92—C93	117.7 (3)
C1—C2—C3	120.2 (3)	C91—C92—C93	134.3 (3)
C2—C3—C4	120.1 (3)	N7—C92—C91	107.8 (3)
C3—C4—C5	120.3 (3)	N10—C93—C92	117.3 (3)
C4—C5—C6	120.1 (3)	N10—C93—C94	108.1 (3)
C1—C6—C5	120.3 (3)	C92—C93—C94	134.4 (3)
P1—C7—C8	117.5 (2)	N12—C94—C93	104.6 (3)
P1—C7—C12	123.4 (3)	N9—C95—C96	110.4 (3)
C8—C7—C12	119.1 (3)	C95—C96—C97	120.4 (4)
C7—C8—C9	120.0 (3)	C95—C96—C101	121.1 (3)
C8—C9—C10	120.7 (4)	C97—C96—C101	118.5 (4)
C9—C10—C11	120.1 (4)	C96—C97—C98	120.0 (5)
C10—C11—C12	120.0 (4)	C97—C98—C99	120.7 (4)
C7—C12—C11	120.2 (4)	C98—C99—C100	119.9 (5)
P1—C13—C14	118.0 (2)	C99—C100—C101	120.0 (5)
P1—C13—C18	123.7 (3)	C96—C101—C100	120.9 (3)
C14—C13—C18	117.5 (3)	N12—C102—C103	111.1 (3)
O1—C14—C15	122.4 (3)	C102—C103—C104	120.8 (3)
O1—C14—C13	114.7 (3)	C104—C103—C108	118.9 (3)
C13—C14—C15	122.9 (3)	C102—C103—C108	120.3 (3)
C14—C15—C16	118.1 (4)	C103—C104—C105	120.5 (4)
C15—C16—C17	121.0 (3)	C104—C105—C106	120.4 (4)
C16—C17—C18	120.0 (3)	C105—C106—C107	119.9 (4)
C13—C18—C17	120.5 (4)	C106—C107—C108	120.0 (4)
C20—C19—C24	116.8 (3)	C103—C108—C107	120.3 (3)
P2—C19—C20	122.7 (2)	C57—C56—H56	120.00
P2—C19—C24	120.4 (2)	C55—C56—H56	120.00
C19—C20—C21	121.5 (3)	C56—C57—H57	120.00
C20—C21—C22	119.8 (3)	C58—C57—H57	120.00
C21—C22—C23	120.3 (3)	C59—C58—H58	120.00
C22—C23—C24	119.2 (3)	C57—C58—H58	120.00
C19—C24—C23	122.4 (3)	C58—C59—H59	120.00
O1—C24—C23	118.4 (3)	C60—C59—H59	120.00
O1—C24—C19	119.1 (2)	C59—C60—H60	120.00
P2—C25—C30	116.9 (2)	C55—C60—H60	120.00
C26—C25—C30	119.2 (3)	C61—C62—H62	119.00
P2—C25—C26	123.8 (3)	C63—C62—H62	120.00
C25—C26—C27	120.0 (4)	C64—C63—H63	120.00
C26—C27—C28	120.7 (4)	C62—C63—H63	120.00
C27—C28—C29	119.4 (4)	C63—C64—H64	120.00
C28—C29—C30	120.2 (4)	C65—C64—H64	120.00
C25—C30—C29	120.5 (3)	C66—C65—H65	120.00
C32—C31—C36	118.6 (3)	C64—C65—H65	120.00
P2—C31—C36	118.2 (3)	C61—C66—H66	120.00
P2—C31—C32	123.2 (3)	C65—C66—H66	120.00

C31—C32—C33	120.4 (3)	C67—C68—H68	119.00
C32—C33—C34	120.3 (4)	C69—C68—H68	119.00
C33—C34—C35	119.7 (3)	C70—C69—H69	120.00
C34—C35—C36	120.5 (3)	C68—C69—H69	120.00
C31—C36—C35	120.5 (4)	C71—C70—H70	120.00
N3—C37—C38	103.8 (3)	C69—C70—H70	120.00
N1—C38—C39	117.9 (3)	C70—C71—H71	120.00
C37—C38—C39	133.5 (3)	C72—C71—H71	121.00
N1—C38—C37	108.5 (3)	C73—C74—H74	120.00
N4—C39—C40	108.0 (3)	C75—C74—H74	120.00
C38—C39—C40	134.4 (3)	C76—C75—H75	120.00
N4—C39—C38	117.6 (3)	C74—C75—H75	120.00
N6—C40—C39	104.4 (3)	C77—C76—H76	120.00
N3—C41—C42	112.3 (3)	C75—C76—H76	120.00
C41—C42—C47	120.3 (3)	C78—C77—H77	120.00
C43—C42—C47	118.2 (4)	C76—C77—H77	120.00
C41—C42—C43	121.5 (3)	C79—C80—H80	120.00
C42—C43—C44	121.4 (4)	C81—C80—H80	120.00
C43—C44—C45	119.7 (4)	C82—C81—H81	120.00
C44—C45—C46	119.6 (4)	C80—C81—H81	120.00
C45—C46—C47	120.7 (4)	C83—C82—H82	120.00
C42—C47—C46	120.5 (4)	C81—C82—H82	120.00
N6—C48—C49	109.9 (3)	C84—C83—H83	120.00
C48—C49—C50	121.0 (3)	C82—C83—H83	120.00
C50—C49—C54	119.2 (4)	C79—C84—H84	120.00
C48—C49—C54	119.8 (3)	C83—C84—H84	120.00
C49—C50—C51	121.0 (3)	C87—C86—H86	120.00
C50—C51—C52	119.4 (4)	C85—C86—H86	120.00
C51—C52—C53	120.6 (4)	C86—C87—H87	120.00
C52—C53—C54	119.6 (3)	C88—C87—H87	120.00
C49—C54—C53	120.1 (4)	C87—C88—H88	120.00
C1—C2—H2	120.00	C89—C88—H88	120.00
C3—C2—H2	120.00	C90—C89—H89	120.00
C4—C3—H3	120.00	C88—C89—H89	120.00
C2—C3—H3	120.00	C85—C90—H90	120.00
C5—C4—H4	120.00	C89—C90—H90	120.00
C3—C4—H4	120.00	N9—C91—H91	128.00
C4—C5—H5	120.00	C92—C91—H91	128.00
C6—C5—H5	120.00	N12—C94—H94	128.00
C5—C6—H6	120.00	C93—C94—H94	128.00
C1—C6—H6	120.00	N9—C95—H95B	110.00
C9—C8—H8	120.00	N9—C95—H95A	110.00
C7—C8—H8	120.00	H95A—C95—H95B	108.00
C10—C9—H9	120.00	C96—C95—H95A	110.00
C8—C9—H9	120.00	C96—C95—H95B	110.00
C11—C10—H10	120.00	C96—C97—H97	120.00
C9—C10—H10	120.00	C98—C97—H97	120.00
C12—C11—H11	120.00	C99—C98—H98	120.00
C10—C11—H11	120.00	C97—C98—H98	120.00

C7—C12—H12	120.00	C98—C99—H99	120.00
C11—C12—H12	120.00	C100—C99—H99	120.00
C14—C15—H15	121.00	C101—C100—H100	120.00
C16—C15—H15	121.00	C99—C100—H100	120.00
C17—C16—H16	119.00	C96—C101—H101	120.00
C15—C16—H16	120.00	C100—C101—H101	120.00
C16—C17—H17	120.00	N12—C102—H10E	109.00
C18—C17—H17	120.00	N12—C102—H10D	109.00
C17—C18—H18	120.00	H10D—C102—H10E	108.00
C13—C18—H18	120.00	C103—C102—H10D	109.00
C19—C20—H20	119.00	C103—C102—H10E	109.00
C21—C20—H20	119.00	C103—C104—H104	120.00
C22—C21—H21	120.00	C105—C104—H104	120.00
C20—C21—H21	120.00	C106—C105—H105	120.00
C21—C22—H22	120.00	C104—C105—H105	120.00
C23—C22—H22	120.00	C105—C106—H106	120.00
C24—C23—H23	120.00	C107—C106—H106	120.00
C22—C23—H23	120.00	C108—C107—H107	120.00
C27—C26—H26	120.00	C106—C107—H107	120.00
C25—C26—H26	120.00	C107—C108—H108	120.00
C28—C27—H27	120.00	C103—C108—H108	120.00
C26—C27—H27	120.00	Cl1—C109—Cl2	121.8 (6)
C29—C28—H28	120.00	Cl1—C109—H10A	107.00
C27—C28—H28	120.00	Cl1—C109—H10B	107.00
C28—C29—H29	120.00	Cl2—C109—H10A	107.00
C30—C29—H29	120.00	Cl2—C109—H10B	107.00
C29—C30—H30	120.00	H10A—C109—H10B	107.00
P2—Cu1—P1—C1	−133.00 (12)	N11—N10—C93—C92	−175.4 (3)
P2—Cu1—P1—C7	102.59 (15)	Cu2—N10—C93—C94	168.1 (2)
P2—Cu1—P1—C13	−16.04 (12)	Cu2—N10—N11—N12	−164.6 (2)
N1—Cu1—P1—C1	−1.03 (14)	C93—N10—N11—N12	0.2 (3)
N1—Cu1—P1—C7	−125.44 (16)	Cu2—N10—C93—C92	−7.0 (4)
N1—Cu1—P1—C13	115.93 (14)	N11—N10—C93—C94	−0.3 (4)
N4—Cu1—P1—C1	90.46 (15)	N10—N11—N12—C94	−0.1 (4)
N4—Cu1—P1—C7	−33.95 (17)	N10—N11—N12—C102	175.2 (3)
N4—Cu1—P1—C13	−152.59 (14)	C94—N12—C102—C103	68.9 (5)
P1—Cu1—P2—C19	−56.89 (11)	N11—N12—C102—C103	−105.6 (4)
P1—Cu1—P2—C25	−176.78 (11)	N11—N12—C94—C93	−0.1 (4)
P1—Cu1—P2—C31	63.98 (12)	C102—N12—C94—C93	−175.0 (3)
N1—Cu1—P2—C19	170.44 (12)	C6—C1—C2—C3	−0.9 (5)
N1—Cu1—P2—C25	50.56 (13)	P1—C1—C2—C3	−177.3 (3)
N1—Cu1—P2—C31	−68.68 (13)	P1—C1—C6—C5	177.3 (3)
N4—Cu1—P2—C19	83.05 (13)	C2—C1—C6—C5	0.7 (5)
N4—Cu1—P2—C25	−36.83 (13)	C1—C2—C3—C4	0.4 (5)
N4—Cu1—P2—C31	−156.08 (13)	C2—C3—C4—C5	0.4 (5)
P1—Cu1—N1—N2	−45.5 (3)	C3—C4—C5—C6	−0.7 (5)
P1—Cu1—N1—C38	117.1 (2)	C4—C5—C6—C1	0.1 (5)
P2—Cu1—N1—N2	87.6 (3)	P1—C7—C8—C9	179.9 (3)
P2—Cu1—N1—C38	−109.9 (2)	C8—C7—C12—C11	−0.1 (6)

N4—Cu1—N1—N2	−163.2 (3)	C12—C7—C8—C9	−0.8 (6)
N4—Cu1—N1—C38	−0.7 (2)	P1—C7—C12—C11	179.2 (3)
P1—Cu1—N4—N5	77.3 (3)	C7—C8—C9—C10	0.9 (6)
P1—Cu1—N4—C39	−119.0 (2)	C8—C9—C10—C11	−0.1 (6)
P2—Cu1—N4—N5	−60.6 (3)	C9—C10—C11—C12	−0.8 (6)
P2—Cu1—N4—C39	103.1 (2)	C10—C11—C12—C7	0.9 (6)
N1—Cu1—N4—N5	−170.9 (3)	P1—C13—C14—C15	−169.5 (2)
N1—Cu1—N4—C39	−7.2 (2)	P1—C13—C14—O1	10.8 (3)
N7—Cu2—P4—C73	−169.37 (13)	C18—C13—C14—C15	0.4 (4)
N7—Cu2—P4—C79	65.76 (13)	P1—C13—C18—C17	167.8 (3)
N7—Cu2—P4—C85	−49.91 (12)	C18—C13—C14—O1	−179.3 (3)
N10—Cu2—P4—C73	−88.94 (13)	C14—C13—C18—C17	−1.5 (5)
N10—Cu2—P4—C79	146.19 (13)	C13—C14—C15—C16	1.0 (5)
N10—Cu2—P4—C85	30.52 (13)	O1—C14—C15—C16	−179.3 (3)
P3—Cu2—N7—N8	58.2 (3)	C14—C15—C16—C17	−1.4 (5)
P3—Cu2—N7—C92	−143.6 (2)	C15—C16—C17—C18	0.3 (5)
P4—Cu2—N7—N8	−65.3 (3)	C16—C17—C18—C13	1.2 (5)
P4—Cu2—N7—C92	93.0 (2)	C20—C19—C24—C23	−0.3 (4)
N10—Cu2—N7—N8	−169.7 (3)	C20—C19—C24—O1	175.8 (2)
N10—Cu2—N7—C92	−11.4 (2)	P2—C19—C20—C21	178.2 (2)
P3—Cu2—N10—N11	−63.2 (3)	C24—C19—C20—C21	0.1 (4)
P3—Cu2—N10—C93	132.7 (2)	P2—C19—C24—O1	−2.3 (4)
P4—Cu2—N10—N11	80.0 (3)	P2—C19—C24—C23	−178.4 (2)
P4—Cu2—N10—C93	−84.2 (2)	C19—C20—C21—C22	0.3 (5)
N7—Cu2—N10—N11	174.0 (3)	C20—C21—C22—C23	−0.4 (5)
N7—Cu2—N10—C93	9.9 (2)	C21—C22—C23—C24	0.3 (5)
N10—Cu2—P3—C55	34.68 (18)	C22—C23—C24—C19	0.1 (4)
P4—Cu2—P3—C55	−106.10 (15)	C22—C23—C24—O1	−176.0 (3)
P4—Cu2—P3—C61	129.06 (14)	C30—C25—C26—C27	1.9 (6)
P4—Cu2—P3—C67	13.02 (11)	P2—C25—C26—C27	−174.3 (3)
N7—Cu2—P3—C55	138.86 (17)	C26—C25—C30—C29	−1.6 (6)
N7—Cu2—P3—C61	14.01 (17)	P2—C25—C30—C29	174.9 (3)
N7—Cu2—P3—C67	−102.03 (14)	C25—C26—C27—C28	−0.3 (6)
P3—Cu2—P4—C73	61.56 (12)	C26—C27—C28—C29	−1.6 (7)
N10—Cu2—P3—C61	−90.16 (18)	C27—C28—C29—C30	2.0 (7)
N10—Cu2—P3—C67	153.79 (14)	C28—C29—C30—C25	−0.4 (7)
P3—Cu2—P4—C79	−63.31 (11)	P2—C31—C36—C35	−177.4 (3)
P3—Cu2—P4—C85	−178.99 (10)	C32—C31—C36—C35	−0.1 (5)
C7—P1—C1—C2	−27.7 (3)	P2—C31—C32—C33	176.7 (2)
Cu1—P1—C1—C2	−156.8 (2)	C36—C31—C32—C33	−0.5 (5)
Cu1—P1—C1—C6	26.7 (3)	C31—C32—C33—C34	0.3 (5)
C7—P1—C13—C18	122.1 (3)	C32—C33—C34—C35	0.4 (5)
C7—P1—C1—C6	155.8 (3)	C33—C34—C35—C36	−1.0 (5)
C13—P1—C1—C2	82.5 (3)	C34—C35—C36—C31	0.9 (5)
C13—P1—C1—C6	−93.9 (3)	N3—C37—C38—N1	0.1 (4)
Cu1—P1—C7—C8	43.9 (3)	N3—C37—C38—C39	−175.3 (3)
Cu1—P1—C7—C12	−135.4 (3)	N1—C38—C39—N4	−15.8 (5)
C1—P1—C7—C8	−89.4 (3)	N1—C38—C39—C40	166.1 (4)
C1—P1—C7—C12	91.3 (4)	C37—C38—C39—N4	159.3 (4)

C13—P1—C7—C8	164.0 (3)	C37—C38—C39—C40	−18.8 (7)
C13—P1—C7—C12	−15.3 (4)	N4—C39—C40—N6	−0.5 (4)
Cu1—P1—C13—C14	54.6 (2)	C38—C39—C40—N6	177.8 (4)
Cu1—P1—C13—C18	−114.7 (3)	N3—C41—C42—C43	52.2 (5)
C1—P1—C13—C14	−176.7 (2)	N3—C41—C42—C47	−130.3 (4)
C1—P1—C13—C18	14.1 (3)	C41—C42—C43—C44	178.8 (4)
C7—P1—C13—C14	−68.7 (3)	C47—C42—C43—C44	1.3 (6)
Cu1—P2—C19—C20	−142.3 (2)	C41—C42—C47—C46	−178.0 (4)
Cu1—P2—C31—C36	32.8 (3)	C43—C42—C47—C46	−0.5 (6)
C19—P2—C31—C32	−14.3 (3)	C42—C43—C44—C45	−1.3 (7)
C19—P2—C31—C36	162.8 (2)	C43—C44—C45—C46	0.5 (7)
Cu1—P2—C19—C24	35.7 (3)	C44—C45—C46—C47	0.3 (7)
C25—P2—C19—C20	−15.1 (3)	C45—C46—C47—C42	−0.3 (7)
C25—P2—C19—C24	162.9 (2)	N6—C48—C49—C50	−73.4 (3)
C31—P2—C19—C20	93.1 (3)	N6—C48—C49—C54	103.4 (3)
C31—P2—C19—C24	−88.9 (2)	C48—C49—C50—C51	175.2 (3)
Cu1—P2—C25—C26	−135.2 (3)	C54—C49—C50—C51	−1.7 (4)
Cu1—P2—C25—C30	48.6 (3)	C48—C49—C54—C53	−176.7 (3)
C19—P2—C25—C26	94.7 (4)	C50—C49—C54—C53	0.3 (4)
C19—P2—C25—C30	−81.6 (3)	C49—C50—C51—C52	2.0 (4)
C31—P2—C25—C26	−12.4 (4)	C50—C51—C52—C53	−0.9 (4)
C31—P2—C25—C30	171.3 (3)	C51—C52—C53—C54	−0.5 (4)
Cu1—P2—C31—C32	−144.4 (2)	C52—C53—C54—C49	0.8 (4)
C25—P2—C31—C32	90.4 (3)	P3—C55—C56—C57	−176.8 (3)
C25—P2—C31—C36	−92.5 (3)	C60—C55—C56—C57	2.0 (5)
C61—P3—C55—C56	84.8 (3)	P3—C55—C60—C59	178.0 (3)
Cu2—P3—C55—C56	−46.3 (3)	C56—C55—C60—C59	−0.7 (5)
Cu2—P3—C55—C60	134.9 (2)	C55—C56—C57—C58	−1.7 (5)
C67—P3—C55—C56	−168.1 (2)	C56—C57—C58—C59	0.1 (5)
C67—P3—C55—C60	13.1 (3)	C57—C58—C59—C60	1.2 (5)
Cu2—P3—C61—C62	158.3 (3)	C58—C59—C60—C55	−0.8 (5)
Cu2—P3—C61—C66	−21.3 (4)	P3—C61—C62—C63	−179.4 (3)
C55—P3—C61—C62	26.3 (4)	C66—C61—C62—C63	0.1 (6)
C55—P3—C61—C66	−153.2 (3)	P3—C61—C66—C65	−179.3 (3)
C67—P3—C61—C62	−82.0 (4)	C62—C61—C66—C65	1.2 (6)
C67—P3—C61—C66	98.5 (3)	C61—C62—C63—C64	−0.8 (6)
Cu2—P3—C67—C68	119.3 (2)	C62—C63—C64—C65	0.2 (6)
Cu2—P3—C67—C72	−53.1 (2)	C63—C64—C65—C66	1.1 (6)
C55—P3—C67—C68	−113.3 (3)	C64—C65—C66—C61	−1.8 (6)
C55—P3—C67—C72	74.3 (2)	P3—C67—C68—C69	−171.4 (2)
C61—P3—C67—C68	−5.5 (3)	C72—C67—C68—C69	1.0 (4)
C61—P3—C67—C72	−177.8 (2)	P3—C67—C72—O2	−11.2 (3)
C61—P3—C55—C60	−94.0 (3)	P3—C67—C72—C71	170.1 (2)
C79—P4—C73—C74	−90.3 (3)	C68—C67—C72—O2	175.8 (2)
C79—P4—C73—C78	92.4 (2)	C68—C67—C72—C71	−2.9 (4)
C85—P4—C73—C74	19.1 (3)	C67—C68—C69—C70	1.6 (4)
C85—P4—C73—C78	−158.2 (2)	C68—C69—C70—C71	−2.5 (4)
Cu2—P4—C79—C80	178.2 (2)	C69—C70—C71—C72	0.7 (4)
Cu2—P4—C79—C84	−2.1 (3)	C70—C71—C72—O2	−176.6 (2)

C73—P4—C79—C80	45.4 (3)	C70—C71—C72—C67	2.0 (4)
C73—P4—C79—C84	−134.9 (2)	P4—C73—C74—C75	−176.2 (3)
C85—P4—C79—C80	−63.9 (3)	C78—C73—C74—C75	1.2 (5)
C85—P4—C79—C84	115.9 (3)	P4—C73—C78—O2	0.5 (4)
Cu2—P4—C85—C86	−69.6 (3)	P4—C73—C78—C77	176.0 (3)
Cu2—P4—C85—C90	99.0 (3)	C74—C73—C78—O2	−177.0 (3)
C73—P4—C85—C86	59.4 (3)	C74—C73—C78—C77	−1.5 (5)
C73—P4—C85—C90	−132.1 (3)	C73—C74—C75—C76	−0.4 (6)
Cu2—P4—C73—C74	140.6 (3)	C74—C75—C76—C77	0.0 (6)
Cu2—P4—C73—C78	−36.7 (3)	C75—C76—C77—C78	−0.3 (6)
C79—P4—C85—C86	168.8 (3)	C76—C77—C78—O2	176.6 (3)
C79—P4—C85—C90	−22.6 (4)	C76—C77—C78—C73	1.1 (5)
C14—O1—C24—C19	83.8 (3)	P4—C79—C80—C81	179.6 (2)
C14—O1—C24—C23	−99.9 (3)	C84—C79—C80—C81	−0.1 (4)
C24—O1—C14—C13	−152.5 (3)	P4—C79—C84—C83	−179.4 (2)
C24—O1—C14—C15	27.7 (4)	C80—C79—C84—C83	0.3 (4)
C72—O2—C78—C73	−81.3 (3)	C79—C80—C81—C82	0.1 (5)
C78—O2—C72—C67	152.0 (2)	C80—C81—C82—C83	−0.2 (5)
C72—O2—C78—C77	103.1 (3)	C81—C82—C83—C84	0.4 (5)
C78—O2—C72—C71	−29.4 (4)	C82—C83—C84—C79	−0.5 (5)
Cu1—N1—C38—C37	−167.8 (2)	P4—C85—C86—C87	168.4 (3)
Cu1—N1—C38—C39	8.5 (4)	C90—C85—C86—C87	−0.5 (6)
Cu1—N1—N2—N3	162.4 (2)	P4—C85—C90—C89	−167.4 (3)
C38—N1—N2—N3	−0.3 (3)	C86—C85—C90—C89	1.3 (6)
N2—N1—C38—C37	0.1 (4)	C85—C86—C87—C88	−0.6 (6)
N2—N1—C38—C39	176.4 (3)	C86—C87—C88—C89	1.0 (6)
N1—N2—N3—C37	0.4 (3)	C87—C88—C89—C90	−0.2 (6)
N1—N2—N3—C41	−175.7 (3)	C88—C89—C90—C85	−1.0 (6)
N2—N3—C41—C42	69.8 (4)	N9—C91—C92—N7	−0.6 (4)
N2—N3—C37—C38	−0.3 (4)	N9—C91—C92—C93	−175.3 (4)
C41—N3—C37—C38	175.5 (3)	N7—C92—C93—N10	−3.7 (5)
C37—N3—C41—C42	−105.7 (4)	N7—C92—C93—C94	−177.1 (4)
N5—N4—C39—C38	−177.7 (3)	C91—C92—C93—N10	170.7 (4)
C39—N4—N5—N6	−0.9 (3)	C91—C92—C93—C94	−2.7 (8)
N5—N4—C39—C40	0.9 (4)	N10—C93—C94—N12	0.2 (4)
Cu1—N4—N5—N6	163.0 (2)	C92—C93—C94—N12	174.1 (4)
Cu1—N4—C39—C38	14.2 (4)	N9—C95—C96—C97	112.2 (3)
Cu1—N4—C39—C40	−167.2 (2)	N9—C95—C96—C101	−68.2 (4)
N4—N5—N6—C48	172.0 (3)	C95—C96—C97—C98	−180.0 (3)
N4—N5—N6—C40	0.6 (3)	C101—C96—C97—C98	0.4 (5)
N5—N6—C48—C49	−97.9 (3)	C95—C96—C101—C100	179.3 (3)
N5—N6—C40—C39	−0.1 (4)	C97—C96—C101—C100	−1.1 (5)
C48—N6—C40—C39	−170.7 (3)	C96—C97—C98—C99	0.7 (6)
C40—N6—C48—C49	72.1 (4)	C97—C98—C99—C100	−1.1 (6)
Cu2—N7—N8—N9	158.4 (2)	C98—C99—C100—C101	0.5 (6)
N8—N7—C92—C93	176.1 (3)	C99—C100—C101—C96	0.6 (6)
Cu2—N7—C92—C91	−164.3 (2)	N12—C102—C103—C104	−84.6 (4)
Cu2—N7—C92—C93	11.5 (4)	N12—C102—C103—C108	93.2 (4)
C92—N7—N8—N9	0.1 (3)	C102—C103—C104—C105	177.2 (4)

N8—N7—C92—C91	0.3 (4)	C108—C103—C104—C105	−0.5 (6)
N7—N8—N9—C91	−0.5 (4)	C102—C103—C108—C107	−177.6 (4)
N7—N8—N9—C95	−172.6 (3)	C104—C103—C108—C107	0.2 (6)
C95—N9—C91—C92	171.8 (3)	C103—C104—C105—C106	0.3 (6)
N8—N9—C91—C92	0.7 (4)	C104—C105—C106—C107	0.3 (7)
C91—N9—C95—C96	−89.1 (4)	C105—C106—C107—C108	−0.6 (6)
N8—N9—C95—C96	81.5 (3)	C106—C107—C108—C103	0.4 (6)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···F11^{iii}	0.95	2.49	3.142 (4)	126
C6—H6···N2	0.95	2.48	3.345 (4)	151
C109—H10A···F9^{i}	0.9900	2.4100	3.362 (9)	161.00
C37—H37···F2	0.95	2.46	3.346 (5)	155
C37—H37···F3	0.95	2.48	3.297 (4)	144
C40—H40···F5^{iv}	0.95	2.54	3.194 (4)	126
C48—H48A···F6^{iv}	0.99	2.42	3.314 (5)	149
C59—H59···F11^{iii}	0.95	2.54	3.443 (4)	158
C64—H64···F10^{xiv}	0.95	2.44	3.379 (4)	172
C94—H94···F8^{i}	0.95	2.47	3.215 (5)	135
C94—H94···F9^{i}	0.95	2.29	3.228 (4)	167
C107—H107···F1	0.95	2.46	3.394 (5)	169

Symmetry codes: (iii) −*x*+1, −*y*+2, −*z*+1; (i) −*x*+2, −*y*+1, −*z*+1; (iv) −*x*+1, −*y*+1, −*z*+1; (xiv) *x*, *y*, *z*+1.

Fig. 1

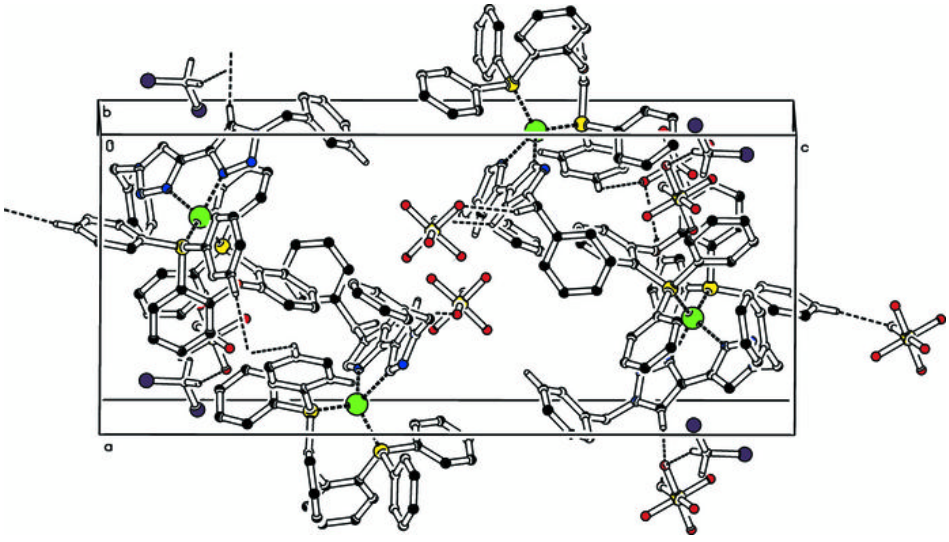
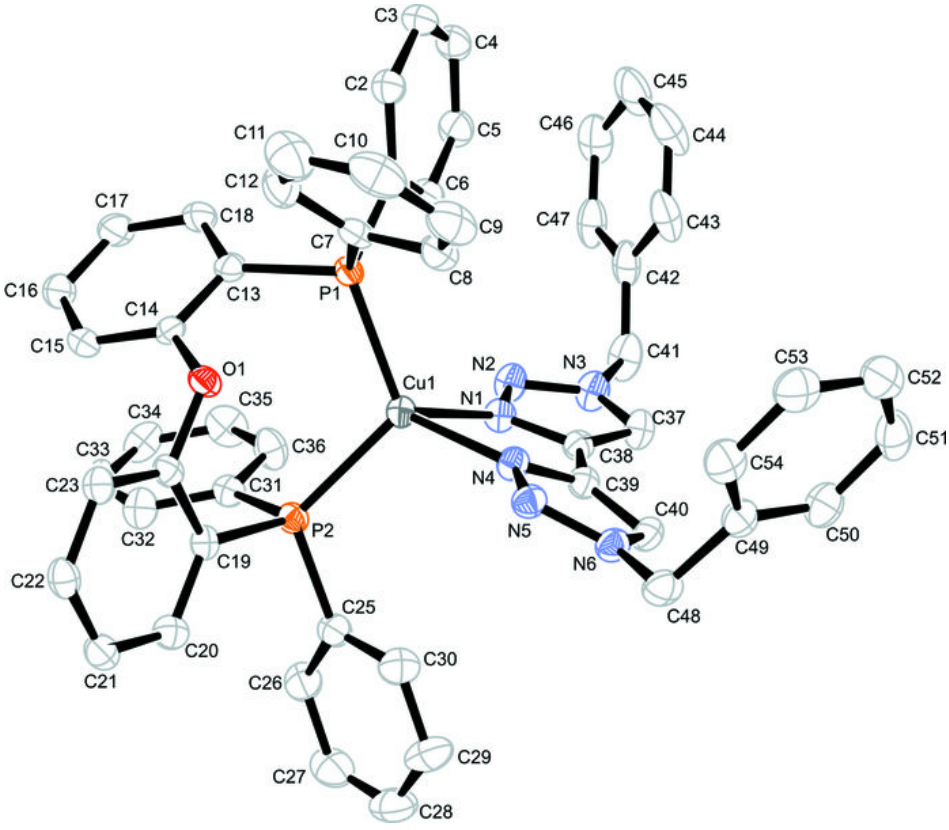


Fig. 2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C14
C15
O1
Cu1
N2
N3
C41
C45
C46
C44
C47
C43
C42
C53
C52
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C51
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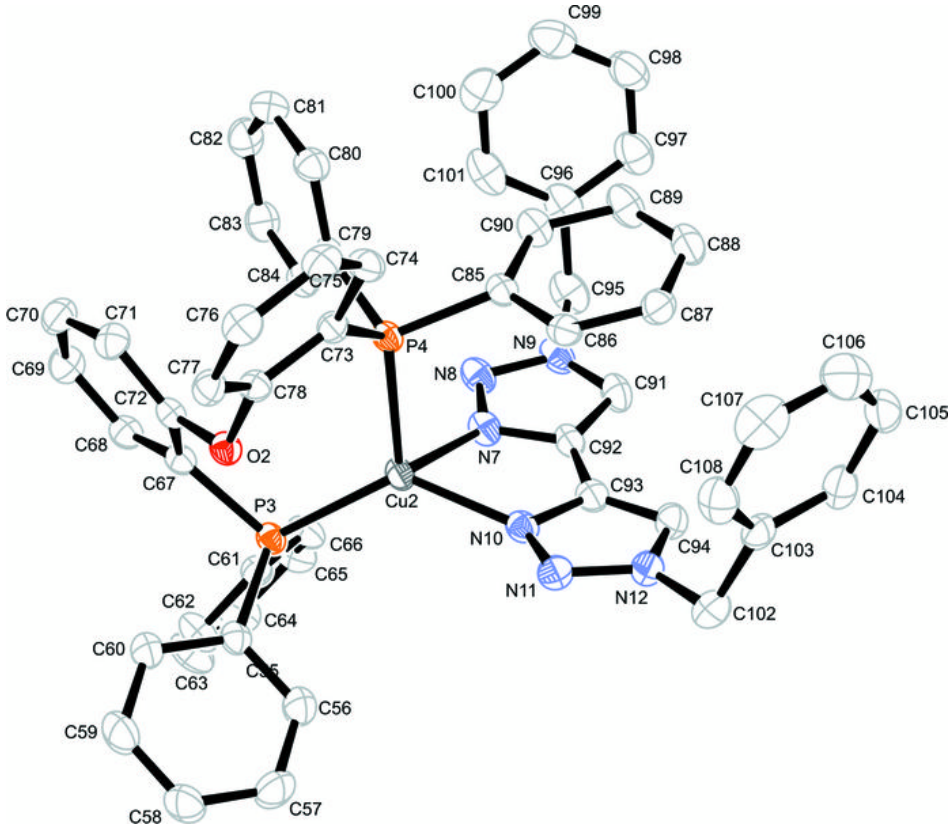
C28

Fig. 3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C65
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C57