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{*N*,*N*′-Bis[3-(2-nitrophenyl)prop-2-enylidene]ethylenediamine-κ^2N,N'}chlorido(triphenylphosphine-κP)copper(I)

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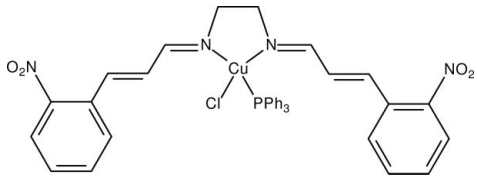
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.007 Å; R factor = 0.051; wR factor = 0.132; data-to-parameter ratio = 38.2.

The title complex, $[CuCl(C_{20}H_{18}N_4O_4)(C_{18}H_{15}P)]$, has two molecules in the asymmetric unit. The Cu atom is four-coordinate in a distorted tetrahedral geometry, bonded to two imine N atoms of the Schiff base, Cl and PPh_3; the main distortion is the small bite angle of the chelating Schiff base ligand. One triphenylphospine ligand adopts an approximate propeller conformation, with dihedral angles of 69.36 (14), 77.02 (12) and 82.44 (15)° for pairs of benzene rings, the normals of which make angles of 37.8, 65.4 and 72.6° with the P—Cu bond; the arrangement in the other triphenylphosphine ligand is rather less symmetrical, with dihedral angles of 63.41 (15), 70.67 (12) and 78.11 (12)° and angles of 20.3, 78.6 and 83.2° between the ring plane normals and the P—Cu bond. There are intermolecular C—H···Cl and C—H···O interactions. The crystal was a non-merohedral twin, with approximately equal contributions of the two domains.

Related literature

For related literature, see: Yamada (1999); Goswami & Eichhorn (1999); Rybak-Akimova *et al.* (1998); Amirnasr *et al.* (2005, 2006); Liu *et al.* (2005); Khalaji *et al.* (2007); Barron *et al.* (1988).



Experimental

Crystal data

$[CuCl(C_{20}H_{18}N_4O_4)(C_{18}H_{15}P)]$
M_r = 739.64
Triclinic, $P\overline{1}$
a = 8.4684 (10) Å
b = 16.5749 (19) Å
c = 26.321 (3) Å
α = 100.338 (3)°
β = 90.767 (3)°
γ = 103.499 (3)°
V = 3528.2 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.79 mm^{-1}
T = 150 (2) K
0.34 × 0.10 × 0.10 mm

Data collection

Bruker SMART 1K CCD diffractometer
Absorption correction: multi-scan (*TWINABS*; Bruker, 2005)
T_{min} = 0.753, T_{max} = 0.901
56982 measured reflections
33770 independent reflections
21591 reflections with $I > 2\sigma(I)$
R_{int} = 0.047

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.132
S = 1.10
33770 reflections
884 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.59 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—Cl1	2.3332 (11)	Cu2—Cl2	2.3253 (11)
Cu1—P1	2.1762 (11)	Cu2—P2	2.1730 (11)
Cu1—N2	2.121 (3)	Cu2—N6	2.127 (3)
Cu1—N3	2.077 (3)	Cu2—N7	2.080 (3)
Cl1—Cu1—P1	115.98 (5)	Cl2—Cu2—P2	117.85 (4)
Cl1—Cu1—N2	101.81 (9)	Cl2—Cu2—N6	96.77 (9)
Cl1—Cu1—N3	98.19 (9)	Cl2—Cu2—N7	104.00 (9)
P1—Cu1—N2	121.16 (9)	P2—Cu2—N6	121.11 (9)
P1—Cu1—N3	129.82 (9)	P2—Cu2—N7	126.11 (9)
N2—Cu1—N3	82.70 (12)	N6—Cu2—N7	82.97 (12)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7···Cl2^{i}	0.95	2.82	3.683 (4)	151
C9—H9···Cl2^{i}	0.95	2.69	3.585 (4)	158
C12—H12···O8^{ii}	0.95	2.53	3.263 (5)	134
C24—H24···O2^{iii}	0.95	2.56	3.377 (5)	145
C30—H30···O3^{iii}	0.95	2.52	3.245 (6)	133
C37—H37···O5^{iv}	0.95	2.52	3.114 (6)	121
C50—H50···Cl1	0.95	2.73	3.595 (4)	153
C67—H67···O4^{v}	0.95	2.59	3.372 (6)	140
C72—H72···Cl2	0.95	2.80	3.716 (4)	163
C74—H74···O6^{iii}	0.95	2.46	3.237 (6)	139

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

Data collection: *GEMINI* and *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2005); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and local programs.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2559).

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supplementary materials

Acta Cryst. (2007). E**63**, m2933-m2934 [**doi:10.1107/S1600536807056267**]

{*N*,*N*'-Bis[3-(2-nitrophenyl)prop-2-enylidene]ethylenediamine-$\kappa^2 N,N'$}chlorido(triphenylphosphine-κP)copper(I)

M. H. Habibi, M. Montazerozohori, A. Lalegani, R. Mokhtari, R. W. Harrington and W. Clegg

Comment

Transition metal complexes containing Schiff base ligands have been of great interest for many years (Yamada, 1999). These complexes play an important role in coordination chemistry related to catalysis and enzymatic reactions, magnetism and molecular architectures (Goswami & Eichhorn, 1999; Rybak-Akimova *et al.*, 1998). The study of the variety of products in self-assembly processes between labile metal ions and flexible multidentate ligands is an interesting topic in supramolecular chemistry. The balance between the formation of different structures is often subtle. Factors that affect the coordination topology include not only the highly influential factors of metal and ligand coordination preferences, but also solvent-based influences, which have been extensively studied for silver(I) complexes (Amirnasr *et al.*, 2006; Liu *et al.*, 2005; Amirnasr *et al.*, 2005; Khalaji *et al.*, 2007). Here we report the results of the reaction of CuCl with *N*,*N*′-bis(2-nitrocinnamaldehyde)ethylenediamine and triphenylphosphine, which forms a copper(I) Schiff base complex, the crystal structure of which we have determined. The title complex is stable in dichloromethane for at least 24 h, but is decomposed in methanol much faster. A methanol solution exposed to the air slowly turns violet and finally green within 2 h. The complex is stable in air in the solid state for 2–3 weeks.

The asymmetric unit (Fig. 1) contains two complex molecules with essentially identical geometry. The bond lengths and angles around the Cu atoms are in good agreement with those found in similar copper(I) complexes (Barron *et al.*, 1988). While a tetrahedral geometry is common for a four-coordinate copper(I) centre, the coordination in this complex is distorted by the restricted bite angle of the chelating ligand. The bond lengths in the chains of the ligand are consistent with extended electron delocalization.

The four nitro groups in the two independent molecules are twisted somewhat out of the planes of the benzene rings, with absolute O—N—C—C torsion angles in the range 17.2 (6)–33.6 (6)°. Dihedral angles between pairs of phenyl groups in the triphenylphosphine ligand are 82.44 (15), 77.02 (12) and 69.36 (14)° in one molecule, and 63.41 (15), 78.11 (12) and 70.67 (12)° in the other. Inspection shows that these rings form approximately a propeller arrangement in one molecule (angles between their normals and the P—Cu bond are 37.8, 65.4 and 72.6°), but a much less symmetrical arrangement in the other (corresponding angles are 20.3, 78.6 and 83.2°).

Molecules are linked *via* C—H···Cl and C—H···O interactions.

Experimental

To a solution of 99 mg (1 mmol) CuCl in 5 ml acetonitrile a solution of 261 mg (1 mmol) of PPh_3 in 5 ml acetonitrile was added. The mixture was stirred for 5 min and then 378 mg (1 mmol) of *N*,*N*'-bis(2-nitrocinnamaldehyde)ethylenediamine in 5 ml acetonitrile was added and the solution stirred for an additional 60 min. The volume of the solvent was reduced under vacuum to about 5 ml. The diffusion of diethyl ether vapour into the concentrated solution gave needle-like red crystals suitable for X-ray studies. The crystals were collected and dried *in vacuo*.

Refinement

All H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H = 0.95–0.99 Å, and with U_{iso}(H) = 1.2U_{eq}(C).

The crystal was found to be a non-merohedral twin, with symmetry-inequivalent reflections overlapping in the diffraction pattern, making it impossible to merge all equivalent reflections before the refinement. The deposited structure factors are in the format generated by the undocumented LIST 7 instruction of *SHELXTL*, in which the contributions of the twin components are identified following refinement of the twin fraction; this was 0.5095:0.4905 (6). The twin law (obtained as part of the cell and orientation matrix refinement and given to 3 decimal places) is: 1.009 0.019 0.013 / −0.059 0.999 0.030 / −0.140 − 0.098 0.986.

Figures

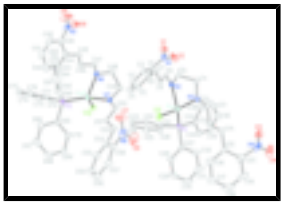


Fig. 1. The asymmetric unit, with atom labels and 40% probability displacement ellipsoids. H atoms have been omitted for clarity.

{*N*,*N*'-Bis[3-(2-nitrophenyl)prop-2-enylidene]ethylenediamine- κ^2*N*,*N*'}chlorido(triphenylphosphine-κ*P*)copper(I)

Crystal data

[CuCl($C_{20}H_{18}N_4O_4$)($C_{18}H_{15}P$)]	Z = 4
M_r = 739.64	F_{000} = 1528
Triclinic, $P\overline{1}$	D_x = 1.392 Mg m^{-3}
a = 8.4684 (10) Å	Mo $K\alpha$ radiation λ = 0.71073 Å
b = 16.5749 (19) Å	Cell parameters from 6328 reflections
c = 26.321 (3) Å	θ = 2.5–26.5º
α = 100.338 (3)º	μ = 0.79 mm^{-1}
β = 90.767 (3)º	T = 150 (2) K
γ = 103.499 (3)º	Rod, red
V = 3528.2 (7) Å^3	0.34 × 0.10 × 0.10 mm

Data collection

Bruker SMART 1K CCD diffractometer	33770 independent reflections
Radiation source: sealed tube	21591 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.047
T = 150(2) K	θ_{max} = 28.4º

thin–slice ω scans	θ_{min} = 1.4º
Absorption correction: multi-scan (TWINABS; Bruker, 2005)	h = −11→11
T_{min} = 0.753, T_{max} = 0.901	k = −22→21
56982 measured reflections	l = −34→35

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.051	H-atom parameters constrained
$wR(F^2)$ = 0.132	$w = 1/[\sigma^2(F_o^2) + (0.0326P)^2 + 12.0057P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.10	$(\Delta/\sigma)_{max}$ = 0.001
33770 reflections	$\Delta\rho_{max}$ = 0.59 e Å^{-3}
884 parameters	$\Delta\rho_{min}$ = −0.53 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Cu1	0.83930 (6)	0.34287 (3)	0.286307 (18)	0.02188 (11)
Cl1	0.75924 (14)	0.43883 (7)	0.35090 (4)	0.0358 (3)
P1	0.64450 (12)	0.24294 (6)	0.24358 (4)	0.0224 (2)
O1	1.0781 (5)	0.3844 (3)	−0.03731 (13)	0.0585 (10)
O2	1.1042 (4)	0.3616 (3)	0.03932 (13)	0.0568 (10)
O3	1.1143 (5)	0.1011 (2)	0.45215 (13)	0.0517 (9)
O4	1.0924 (5)	0.0893 (3)	0.53202 (13)	0.0673 (12)
N1	1.0290 (4)	0.3818 (2)	0.00601 (13)	0.0339 (8)
N2	1.0061 (4)	0.42440 (19)	0.24764 (11)	0.0191 (6)
N3	1.0506 (4)	0.3350 (2)	0.32407 (12)	0.0235 (7)
N4	1.0422 (6)	0.1050 (2)	0.49193 (15)	0.0448 (10)
C1	0.8713 (5)	0.4016 (2)	0.01746 (15)	0.0256 (9)
C2	0.7680 (6)	0.3977 (3)	−0.02449 (16)	0.0336 (10)
H2	0.8032	0.3880	−0.0587	0.040*
C3	0.6144 (6)	0.4082 (3)	−0.01604 (18)	0.0409 (12)
H3	0.5425	0.4063	−0.0445	0.049*
C4	0.5639 (5)	0.4213 (3)	0.03352 (18)	0.0411 (12)
H4	0.4553	0.4256	0.0391	0.049*
C5	0.6702 (5)	0.4284 (3)	0.07542 (17)	0.0346 (10)
H5	0.6345	0.4396	0.1095	0.042*
C6	0.8286 (5)	0.4194 (3)	0.06863 (15)	0.0266 (9)
C7	0.9412 (5)	0.4376 (2)	0.11454 (14)	0.0229 (8)
H7	1.0504	0.4668	0.1113	0.028*
C8	0.9034 (5)	0.4169 (2)	0.16037 (14)	0.0226 (8)
H8	0.7985	0.3837	0.1648	0.027*

C9	1.0244 (4)	0.4455 (2)	0.20336 (14)	0.0203 (8)
H9	1.1243	0.4826	0.1982	0.024*
C10	1.1457 (5)	0.4580 (2)	0.28535 (14)	0.0226 (8)
H10A	1.1164	0.4960	0.3153	0.027*
H10B	1.2383	0.4907	0.2693	0.027*
C11	1.1923 (5)	0.3841 (2)	0.30284 (16)	0.0254 (9)
H11A	1.2282	0.3482	0.2732	0.030*
H11B	1.2832	0.4049	0.3296	0.030*
C12	1.0730 (5)	0.3071 (2)	0.36506 (15)	0.0240 (8)
H12	1.1806	0.3186	0.3799	0.029*
C13	0.9426 (5)	0.2589 (2)	0.38981 (15)	0.0253 (9)
H13	0.8338	0.2496	0.3765	0.030*
C14	0.9718 (5)	0.2269 (2)	0.43105 (15)	0.0280 (9)
H14	1.0824	0.2355	0.4425	0.034*
C15	0.8494 (5)	0.1802 (3)	0.46016 (15)	0.0307 (10)
C16	0.6903 (6)	0.1909 (3)	0.46014 (18)	0.0402 (11)
H16	0.6606	0.2265	0.4390	0.048*
C17	0.5754 (7)	0.1512 (3)	0.4900 (2)	0.0514 (14)
H17	0.4680	0.1593	0.4889	0.062*
C18	0.6156 (8)	0.0994 (3)	0.5217 (2)	0.0566 (16)
H18	0.5370	0.0735	0.5429	0.068*
C19	0.7692 (7)	0.0860 (3)	0.52203 (19)	0.0513 (14)
H19	0.7975	0.0500	0.5431	0.062*
C20	0.8817 (6)	0.1251 (3)	0.49173 (16)	0.0364 (11)
C21	0.5196 (4)	0.2838 (2)	0.20235 (16)	0.0251 (9)
C22	0.5105 (4)	0.3673 (2)	0.21791 (15)	0.0229 (8)
H22	0.5700	0.4004	0.2484	0.028*
C23	0.4149 (4)	0.4027 (2)	0.18919 (15)	0.0249 (8)
H23	0.4096	0.4597	0.2001	0.030*
C24	0.3283 (5)	0.3553 (3)	0.14503 (17)	0.0372 (11)
H24	0.2624	0.3794	0.1256	0.045*
C25	0.3372 (6)	0.2727 (3)	0.1291 (2)	0.0568 (16)
H25	0.2769	0.2399	0.0986	0.068*
C26	0.4333 (6)	0.2373 (3)	0.1570 (2)	0.0500 (14)
H26	0.4405	0.1807	0.1452	0.060*
C27	0.4928 (5)	0.1833 (2)	0.28019 (17)	0.0306 (10)
C28	0.3288 (6)	0.1827 (3)	0.2772 (2)	0.0466 (13)
H28	0.2898	0.2127	0.2542	0.056*
C29	0.2206 (7)	0.1381 (3)	0.3078 (3)	0.068 (2)
H29	0.1086	0.1383	0.3056	0.082*
C30	0.2747 (8)	0.0944 (3)	0.3407 (2)	0.0664 (19)
H30	0.2003	0.0641	0.3613	0.080*
C31	0.4375 (8)	0.0938 (3)	0.3442 (2)	0.0561 (16)
H31	0.4752	0.0632	0.3671	0.067*
C32	0.5456 (6)	0.1383 (3)	0.31390 (17)	0.0394 (11)
H32	0.6575	0.1379	0.3163	0.047*
C33	0.7079 (5)	0.1586 (2)	0.20031 (15)	0.0250 (9)
C34	0.6046 (6)	0.0798 (3)	0.18249 (18)	0.0379 (11)
H34	0.4959	0.0686	0.1930	0.045*

C35	0.6569 (7)	0.0172 (3)	0.14974 (17)	0.0438 (12)
H35	0.5847	−0.0365	0.1380	0.053*
C36	0.8133 (7)	0.0332 (3)	0.13436 (18)	0.0480 (14)
H36	0.8496	−0.0092	0.1116	0.058*
C37	0.9172 (6)	0.1104 (4)	0.1519 (2)	0.0571 (16)
H37	1.0258	0.1210	0.1414	0.068*
C38	0.8655 (5)	0.1734 (3)	0.18492 (17)	0.0373 (11)
H38	0.9388	0.2267	0.1969	0.045*
Cu2	0.48633 (6)	0.68749 (3)	0.219149 (18)	0.02083 (11)
Cl2	0.33758 (12)	0.58831 (6)	0.15118 (4)	0.0274 (2)
P2	0.38212 (12)	0.79103 (6)	0.25379 (4)	0.0202 (2)
O5	0.9162 (6)	0.9170 (3)	−0.04751 (15)	0.0868 (16)
O6	0.9493 (5)	0.8923 (2)	0.02872 (15)	0.0607 (10)
O7	0.7323 (4)	0.6617 (3)	0.47157 (14)	0.0558 (10)
O8	0.6781 (5)	0.5964 (2)	0.53537 (13)	0.0609 (11)
N5	0.8623 (6)	0.8960 (3)	−0.00768 (16)	0.0504 (12)
N6	0.7106 (4)	0.7103 (2)	0.18252 (12)	0.0226 (7)
N7	0.6010 (4)	0.61720 (19)	0.25880 (11)	0.0192 (6)
N8	0.6364 (5)	0.6220 (3)	0.49759 (14)	0.0396 (9)
C39	0.6849 (6)	0.8767 (3)	−0.00442 (16)	0.0394 (11)
C40	0.5976 (9)	0.9098 (3)	−0.0364 (2)	0.0591 (16)
H40	0.6521	0.9428	−0.0599	0.071*
C41	0.4332 (9)	0.8953 (4)	−0.0344 (2)	0.0669 (19)
H41	0.3727	0.9179	−0.0565	0.080*
C42	0.3541 (7)	0.8476 (4)	−0.0002 (2)	0.0568 (15)
H42	0.2394	0.8381	0.0016	0.068*
C43	0.4423 (6)	0.8134 (3)	0.03156 (18)	0.0402 (11)
H43	0.3865	0.7799	0.0545	0.048*
C44	0.6106 (6)	0.8273 (3)	0.03047 (15)	0.0309 (10)
C45	0.6958 (5)	0.7858 (3)	0.06340 (16)	0.0295 (9)
H45	0.7908	0.7699	0.0507	0.035*
C46	0.6514 (5)	0.7686 (2)	0.10935 (15)	0.0258 (9)
H46	0.5569	0.7834	0.1233	0.031*
C47	0.7452 (5)	0.7276 (2)	0.13830 (15)	0.0251 (9)
H47	0.8383	0.7128	0.1233	0.030*
C48	0.8224 (5)	0.6720 (3)	0.20750 (16)	0.0270 (9)
H48A	0.8813	0.7124	0.2379	0.032*
H48B	0.9033	0.6570	0.1830	0.032*
C49	0.7239 (4)	0.5931 (2)	0.22429 (14)	0.0226 (8)
H49A	0.6702	0.5513	0.1937	0.027*
H49B	0.7962	0.5672	0.2426	0.027*
C50	0.6007 (4)	0.5961 (2)	0.30332 (14)	0.0204 (8)
H50	0.6753	0.5640	0.3101	0.024*
C51	0.4960 (4)	0.6171 (2)	0.34397 (14)	0.0210 (8)
H51	0.4176	0.6479	0.3387	0.025*
C52	0.5109 (5)	0.5926 (2)	0.38895 (14)	0.0231 (8)
H52	0.5981	0.5667	0.3929	0.028*
C53	0.4080 (5)	0.6011 (2)	0.43307 (15)	0.0251 (9)
C54	0.2416 (5)	0.5938 (3)	0.42456 (17)	0.0339 (10)

H54	0.1993	0.5913	0.3906	0.041*
C55	0.1368 (6)	0.5901 (3)	0.4644 (2)	0.0442 (12)
H55	0.0248	0.5870	0.4577	0.053*
C56	0.1947 (7)	0.5908 (3)	0.51386 (18)	0.0448 (13)
H56	0.1216	0.5852	0.5408	0.054*
C57	0.3585 (6)	0.5997 (3)	0.52404 (17)	0.0396 (11)
H57	0.3997	0.6013	0.5581	0.047*
C58	0.4614 (5)	0.6063 (3)	0.48434 (15)	0.0300 (9)
C59	0.5387 (5)	0.8755 (2)	0.29209 (16)	0.0260 (9)
C60	0.5591 (5)	0.8865 (3)	0.34516 (17)	0.0399 (11)
H60	0.4832	0.8530	0.3638	0.048*
C61	0.6920 (6)	0.9472 (4)	0.3714 (2)	0.0571 (16)
H61	0.7036	0.9559	0.4081	0.068*
C62	0.8057 (6)	0.9941 (4)	0.3450 (2)	0.0579 (16)
H62	0.8959	1.0349	0.3632	0.069*
C63	0.7883 (6)	0.9819 (3)	0.2919 (2)	0.0516 (14)
H63	0.8668	1.0141	0.2733	0.062*
C64	0.6567 (5)	0.9226 (3)	0.26561 (19)	0.0374 (11)
H64	0.6465	0.9139	0.2289	0.045*
C65	0.2164 (5)	0.7695 (2)	0.29703 (15)	0.0237 (8)
C66	0.1528 (5)	0.8326 (3)	0.32549 (18)	0.0387 (11)
H66	0.1985	0.8901	0.3237	0.046*
C67	0.0240 (6)	0.8127 (3)	0.35622 (19)	0.0474 (13)
H67	−0.0199	0.8561	0.3750	0.057*
C68	−0.0414 (5)	0.7288 (3)	0.35961 (18)	0.0414 (12)
H68	−0.1272	0.7150	0.3818	0.050*
C69	0.0179 (5)	0.6664 (3)	0.33113 (18)	0.0345 (10)
H69	−0.0289	0.6091	0.3329	0.041*
C70	0.1455 (5)	0.6858 (3)	0.29972 (16)	0.0273 (9)
H70	0.1851	0.6416	0.2799	0.033*
C71	0.2946 (4)	0.8436 (2)	0.20901 (15)	0.0229 (8)
C72	0.2333 (5)	0.7960 (3)	0.16073 (15)	0.0264 (9)
H72	0.2440	0.7395	0.1514	0.032*
C73	0.1567 (5)	0.8307 (3)	0.12622 (17)	0.0355 (10)
H73	0.1157	0.7979	0.0933	0.043*
C74	0.1396 (5)	0.9125 (3)	0.1395 (2)	0.0428 (12)
H74	0.0875	0.9362	0.1157	0.051*
C75	0.1982 (6)	0.9595 (3)	0.1873 (2)	0.0437 (12)
H75	0.1853	1.0156	0.1965	0.052*
C76	0.2759 (5)	0.9262 (3)	0.22211 (18)	0.0335 (10)
H76	0.3165	0.9595	0.2550	0.040*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0202 (2)	0.0233 (2)	0.0237 (2)	0.00567 (19)	0.00173 (19)	0.0080 (2)
Cl1	0.0520 (7)	0.0422 (6)	0.0244 (5)	0.0289 (5)	0.0130 (5)	0.0118 (5)
P1	0.0201 (5)	0.0194 (5)	0.0292 (5)	0.0062 (4)	0.0052 (4)	0.0065 (4)

O1	0.071 (3)	0.086 (3)	0.0298 (19)	0.039 (2)	0.0203 (18)	0.0127 (19)
O2	0.047 (2)	0.105 (3)	0.0319 (19)	0.044 (2)	0.0029 (16)	0.015 (2)
O3	0.074 (3)	0.064 (2)	0.0325 (19)	0.032 (2)	0.0181 (18)	0.0263 (17)
O4	0.114 (4)	0.079 (3)	0.0304 (19)	0.054 (3)	0.006 (2)	0.0242 (19)
N1	0.038 (2)	0.040 (2)	0.0225 (19)	0.0122 (17)	0.0043 (16)	0.0006 (16)
N2	0.0204 (16)	0.0194 (16)	0.0179 (16)	0.0042 (13)	0.0009 (13)	0.0051 (13)
N3	0.0242 (17)	0.0225 (17)	0.0256 (17)	0.0077 (14)	0.0021 (14)	0.0062 (14)
N4	0.075 (3)	0.037 (2)	0.030 (2)	0.021 (2)	0.005 (2)	0.0156 (18)
C1	0.029 (2)	0.028 (2)	0.0202 (19)	0.0060 (17)	−0.0012 (17)	0.0063 (17)
C2	0.049 (3)	0.032 (2)	0.019 (2)	0.008 (2)	−0.0046 (19)	0.0050 (18)
C3	0.042 (3)	0.048 (3)	0.032 (3)	0.008 (2)	−0.018 (2)	0.009 (2)
C4	0.027 (2)	0.055 (3)	0.043 (3)	0.009 (2)	−0.007 (2)	0.015 (2)
C5	0.026 (2)	0.051 (3)	0.029 (2)	0.010 (2)	0.0010 (18)	0.011 (2)
C6	0.025 (2)	0.032 (2)	0.024 (2)	0.0051 (17)	0.0009 (17)	0.0097 (17)
C7	0.0190 (19)	0.030 (2)	0.0208 (19)	0.0049 (16)	0.0016 (16)	0.0073 (16)
C8	0.0194 (19)	0.029 (2)	0.0203 (19)	0.0056 (16)	0.0045 (16)	0.0085 (16)
C9	0.0202 (19)	0.0208 (19)	0.0207 (19)	0.0047 (15)	0.0036 (15)	0.0061 (15)
C10	0.023 (2)	0.023 (2)	0.0200 (19)	0.0009 (16)	−0.0012 (16)	0.0051 (16)
C11	0.020 (2)	0.032 (2)	0.027 (2)	0.0070 (17)	0.0005 (16)	0.0129 (18)
C12	0.028 (2)	0.023 (2)	0.022 (2)	0.0068 (16)	−0.0039 (16)	0.0066 (16)
C13	0.028 (2)	0.026 (2)	0.023 (2)	0.0060 (17)	0.0007 (17)	0.0066 (17)
C14	0.034 (2)	0.024 (2)	0.025 (2)	0.0043 (18)	−0.0008 (18)	0.0061 (17)
C15	0.042 (3)	0.025 (2)	0.021 (2)	0.0008 (19)	0.0024 (19)	0.0033 (17)
C16	0.044 (3)	0.035 (3)	0.037 (3)	0.001 (2)	0.005 (2)	0.005 (2)
C17	0.045 (3)	0.053 (3)	0.045 (3)	−0.005 (3)	0.012 (2)	−0.001 (3)
C18	0.073 (4)	0.047 (3)	0.036 (3)	−0.012 (3)	0.025 (3)	0.004 (2)
C19	0.081 (4)	0.039 (3)	0.031 (3)	0.004 (3)	0.020 (3)	0.014 (2)
C20	0.059 (3)	0.028 (2)	0.020 (2)	0.006 (2)	0.005 (2)	0.0061 (18)
C21	0.0173 (19)	0.025 (2)	0.033 (2)	0.0060 (16)	0.0014 (17)	0.0047 (17)
C22	0.0156 (18)	0.025 (2)	0.027 (2)	0.0010 (15)	0.0039 (16)	0.0069 (17)
C23	0.020 (2)	0.025 (2)	0.032 (2)	0.0073 (16)	0.0054 (17)	0.0097 (17)
C24	0.029 (2)	0.051 (3)	0.035 (2)	0.021 (2)	−0.003 (2)	0.004 (2)
C25	0.057 (3)	0.058 (3)	0.051 (3)	0.029 (3)	−0.031 (3)	−0.020 (3)
C26	0.053 (3)	0.037 (3)	0.056 (3)	0.022 (2)	−0.024 (3)	−0.014 (2)
C27	0.033 (2)	0.0165 (19)	0.039 (2)	0.0021 (17)	0.015 (2)	0.0012 (18)
C28	0.034 (3)	0.025 (2)	0.082 (4)	0.007 (2)	0.026 (3)	0.010 (2)
C29	0.047 (3)	0.032 (3)	0.123 (6)	0.008 (2)	0.054 (4)	0.005 (3)
C30	0.080 (5)	0.033 (3)	0.072 (4)	−0.006 (3)	0.057 (4)	−0.003 (3)
C31	0.083 (4)	0.036 (3)	0.036 (3)	−0.012 (3)	0.013 (3)	0.004 (2)
C32	0.049 (3)	0.032 (2)	0.029 (2)	−0.006 (2)	0.008 (2)	0.0038 (19)
C33	0.029 (2)	0.026 (2)	0.026 (2)	0.0138 (17)	0.0073 (17)	0.0112 (17)
C34	0.049 (3)	0.024 (2)	0.042 (3)	0.009 (2)	0.020 (2)	0.008 (2)
C35	0.078 (4)	0.030 (2)	0.031 (2)	0.024 (3)	0.012 (2)	0.009 (2)
C36	0.070 (4)	0.058 (3)	0.028 (2)	0.047 (3)	0.000 (2)	−0.003 (2)
C37	0.036 (3)	0.092 (5)	0.046 (3)	0.035 (3)	0.008 (2)	−0.006 (3)
C38	0.029 (2)	0.050 (3)	0.033 (2)	0.014 (2)	0.005 (2)	0.003 (2)
Cu2	0.0235 (2)	0.0225 (2)	0.0186 (2)	0.00857 (19)	0.00131 (19)	0.00512 (19)
Cl2	0.0316 (5)	0.0251 (5)	0.0226 (5)	−0.0003 (4)	−0.0066 (4)	0.0066 (4)
P2	0.0199 (5)	0.0207 (5)	0.0203 (5)	0.0054 (4)	−0.0003 (4)	0.0041 (4)

O5	0.111 (4)	0.091 (3)	0.037 (2)	−0.025 (3)	0.031 (2)	0.019 (2)
O6	0.058 (2)	0.069 (3)	0.051 (2)	−0.001 (2)	0.018 (2)	0.022 (2)
O7	0.038 (2)	0.084 (3)	0.039 (2)	−0.0008 (19)	−0.0085 (16)	0.019 (2)
O8	0.084 (3)	0.063 (2)	0.039 (2)	0.024 (2)	−0.026 (2)	0.0117 (18)
N5	0.076 (3)	0.034 (2)	0.032 (2)	−0.008 (2)	0.023 (2)	0.0073 (19)
N6	0.0194 (16)	0.0241 (17)	0.0228 (17)	0.0009 (13)	0.0000 (13)	0.0061 (14)
N7	0.0200 (16)	0.0194 (16)	0.0183 (16)	0.0040 (13)	0.0025 (13)	0.0047 (13)
N8	0.050 (3)	0.045 (2)	0.0229 (19)	0.014 (2)	−0.0131 (18)	0.0021 (17)
C39	0.069 (3)	0.028 (2)	0.020 (2)	0.009 (2)	0.008 (2)	0.0053 (18)
C40	0.115 (6)	0.038 (3)	0.030 (3)	0.027 (3)	0.005 (3)	0.013 (2)
C41	0.115 (6)	0.064 (4)	0.037 (3)	0.051 (4)	−0.012 (3)	0.012 (3)
C42	0.069 (4)	0.065 (4)	0.047 (3)	0.039 (3)	−0.008 (3)	0.008 (3)
C43	0.048 (3)	0.043 (3)	0.035 (3)	0.018 (2)	0.001 (2)	0.012 (2)
C44	0.049 (3)	0.027 (2)	0.018 (2)	0.011 (2)	0.0038 (19)	0.0059 (17)
C45	0.029 (2)	0.029 (2)	0.029 (2)	0.0047 (18)	0.0056 (18)	0.0071 (18)
C46	0.026 (2)	0.028 (2)	0.023 (2)	0.0042 (17)	0.0033 (17)	0.0074 (17)
C47	0.021 (2)	0.029 (2)	0.026 (2)	0.0025 (16)	0.0068 (17)	0.0103 (17)
C48	0.018 (2)	0.036 (2)	0.029 (2)	0.0054 (17)	0.0016 (17)	0.0140 (19)
C49	0.022 (2)	0.028 (2)	0.0200 (19)	0.0099 (16)	0.0035 (16)	0.0064 (16)
C50	0.0179 (19)	0.0212 (19)	0.0218 (19)	0.0024 (15)	−0.0027 (15)	0.0068 (15)
C51	0.0203 (19)	0.026 (2)	0.0167 (18)	0.0048 (16)	−0.0005 (15)	0.0061 (15)
C52	0.0197 (19)	0.028 (2)	0.0204 (19)	0.0027 (16)	−0.0016 (15)	0.0047 (16)
C53	0.031 (2)	0.026 (2)	0.0178 (19)	0.0068 (17)	0.0010 (17)	0.0039 (16)
C54	0.033 (2)	0.040 (3)	0.028 (2)	0.008 (2)	0.0029 (19)	0.0035 (19)
C55	0.034 (3)	0.047 (3)	0.050 (3)	0.007 (2)	0.015 (2)	0.006 (2)
C56	0.063 (4)	0.037 (3)	0.033 (3)	0.009 (2)	0.028 (2)	0.006 (2)
C57	0.062 (3)	0.035 (3)	0.021 (2)	0.011 (2)	0.010 (2)	0.0061 (19)
C58	0.041 (3)	0.028 (2)	0.021 (2)	0.0070 (19)	0.0013 (18)	0.0058 (17)
C59	0.020 (2)	0.024 (2)	0.033 (2)	0.0088 (16)	−0.0026 (17)	0.0009 (17)
C60	0.027 (2)	0.058 (3)	0.031 (2)	0.009 (2)	−0.0029 (19)	−0.002 (2)
C61	0.033 (3)	0.083 (4)	0.042 (3)	0.013 (3)	−0.012 (2)	−0.021 (3)
C62	0.021 (2)	0.066 (4)	0.067 (4)	0.002 (2)	−0.006 (3)	−0.027 (3)
C63	0.030 (3)	0.048 (3)	0.063 (4)	−0.005 (2)	0.002 (2)	−0.007 (3)
C64	0.030 (2)	0.034 (2)	0.043 (3)	−0.0004 (19)	0.002 (2)	0.003 (2)
C65	0.021 (2)	0.028 (2)	0.023 (2)	0.0056 (16)	−0.0009 (16)	0.0049 (16)
C66	0.034 (3)	0.034 (3)	0.041 (3)	0.003 (2)	0.010 (2)	−0.003 (2)
C67	0.040 (3)	0.059 (3)	0.037 (3)	0.011 (2)	0.012 (2)	−0.006 (2)
C68	0.023 (2)	0.066 (3)	0.033 (3)	0.003 (2)	0.0040 (19)	0.012 (2)
C69	0.021 (2)	0.042 (3)	0.044 (3)	0.0036 (19)	−0.0019 (19)	0.025 (2)
C70	0.020 (2)	0.031 (2)	0.033 (2)	0.0052 (17)	−0.0043 (17)	0.0125 (18)
C71	0.0150 (18)	0.024 (2)	0.032 (2)	0.0053 (15)	0.0015 (16)	0.0096 (17)
C72	0.025 (2)	0.029 (2)	0.028 (2)	0.0074 (17)	0.0019 (17)	0.0107 (18)
C73	0.026 (2)	0.051 (3)	0.033 (2)	0.010 (2)	−0.0045 (19)	0.013 (2)
C74	0.030 (2)	0.055 (3)	0.056 (3)	0.019 (2)	0.002 (2)	0.031 (3)
C75	0.041 (3)	0.036 (3)	0.064 (3)	0.019 (2)	0.002 (3)	0.022 (2)
C76	0.029 (2)	0.028 (2)	0.045 (3)	0.0078 (18)	−0.003 (2)	0.008 (2)

Geometric parameters (Å, °)

Cu1—Cl1	2.3332 (11)	Cu2—Cl2	2.3253 (11)
Cu1—P1	2.1762 (11)	Cu2—P2	2.1730 (11)
Cu1—N2	2.121 (3)	Cu2—N6	2.127 (3)
Cu1—N3	2.077 (3)	Cu2—N7	2.080 (3)
P1—C21	1.823 (4)	P2—C59	1.823 (4)
P1—C27	1.827 (4)	P2—C65	1.829 (4)
P1—C33	1.826 (4)	P2—C71	1.829 (4)
O1—N1	1.223 (4)	O5—N5	1.224 (5)
O2—N1	1.216 (4)	O6—N5	1.220 (5)
O3—N4	1.218 (5)	O7—N8	1.220 (5)
O4—N4	1.224 (5)	O8—N8	1.227 (5)
N1—C1	1.470 (5)	N5—C39	1.468 (7)
N2—C9	1.277 (5)	N6—C47	1.270 (5)
N2—C10	1.468 (5)	N6—C48	1.465 (5)
N3—C11	1.462 (5)	N7—C49	1.469 (5)
N3—C12	1.277 (5)	N7—C50	1.282 (4)
N4—C20	1.473 (6)	N8—C58	1.470 (6)
C1—C2	1.382 (5)	C39—C40	1.377 (7)
C1—C6	1.397 (5)	C39—C44	1.398 (6)
C2—H2	0.950	C40—H40	0.950
C2—C3	1.368 (6)	C40—C41	1.360 (9)
C3—H3	0.950	C41—H41	0.950
C3—C4	1.374 (7)	C41—C42	1.381 (8)
C4—H4	0.950	C42—H42	0.950
C4—C5	1.385 (6)	C42—C43	1.388 (6)
C5—H5	0.950	C43—H43	0.950
C5—C6	1.394 (6)	C43—C44	1.391 (6)
C6—C7	1.471 (5)	C44—C45	1.475 (6)
C7—H7	0.950	C45—H45	0.950
C7—C8	1.336 (5)	C45—C46	1.331 (5)
C8—H8	0.950	C46—H46	0.950
C8—C9	1.451 (5)	C46—C47	1.447 (5)
C9—H9	0.950	C47—H47	0.950
C10—H10A	0.990	C48—H48A	0.990
C10—H10B	0.990	C48—H48B	0.990
C10—C11	1.514 (5)	C48—C49	1.520 (5)
C11—H11A	0.990	C49—H49A	0.990
C11—H11B	0.990	C49—H49B	0.990
C12—H12	0.950	C50—H50	0.950
C12—C13	1.440 (5)	C50—C51	1.445 (5)
C13—H13	0.950	C51—H51	0.950
C13—C14	1.334 (5)	C51—C52	1.332 (5)
C14—H14	0.950	C52—H52	0.950
C14—C15	1.456 (6)	C52—C53	1.467 (5)
C15—C16	1.400 (6)	C53—C54	1.398 (6)
C15—C20	1.407 (6)	C53—C58	1.399 (5)

C16—H16	0.950	C54—H54	0.950
C16—C17	1.381 (7)	C54—C55	1.383 (6)
C17—H17	0.950	C55—H55	0.950
C17—C18	1.390 (8)	C55—C56	1.382 (7)
C18—H18	0.950	C56—H56	0.950
C18—C19	1.370 (8)	C56—C57	1.378 (7)
C19—H19	0.950	C57—H57	0.950
C19—C20	1.371 (6)	C57—C58	1.373 (6)
C21—C22	1.391 (5)	C59—C60	1.379 (6)
C21—C26	1.390 (6)	C59—C64	1.395 (6)
C22—H22	0.950	C60—H60	0.950
C22—C23	1.390 (5)	C60—C61	1.398 (6)
C23—H23	0.950	C61—H61	0.950
C23—C24	1.373 (6)	C61—C62	1.371 (8)
C24—H24	0.950	C62—H62	0.950
C24—C25	1.377 (7)	C62—C63	1.376 (8)
C25—H25	0.950	C63—H63	0.950
C25—C26	1.383 (6)	C63—C64	1.382 (6)
C26—H26	0.950	C64—H64	0.950
C27—C28	1.388 (6)	C65—C66	1.392 (6)
C27—C32	1.388 (6)	C65—C70	1.393 (5)
C28—H28	0.950	C66—H66	0.950
C28—C29	1.396 (7)	C66—C67	1.380 (6)
C29—H29	0.950	C67—H67	0.950
C29—C30	1.362 (9)	C67—C68	1.391 (7)
C30—H30	0.950	C68—H68	0.950
C30—C31	1.383 (8)	C68—C69	1.363 (6)
C31—H31	0.950	C69—H69	0.950
C31—C32	1.391 (6)	C69—C70	1.382 (6)
C32—H32	0.950	C70—H70	0.950
C33—C34	1.388 (6)	C71—C72	1.392 (5)
C33—C38	1.379 (6)	C71—C76	1.397 (5)
C34—H34	0.950	C72—H72	0.950
C34—C35	1.385 (6)	C72—C73	1.386 (5)
C35—H35	0.950	C73—H73	0.950
C35—C36	1.370 (7)	C73—C74	1.381 (6)
C36—H36	0.950	C74—H74	0.950
C36—C37	1.369 (8)	C74—C75	1.373 (7)
C37—H37	0.950	C75—H75	0.950
C37—C38	1.391 (7)	C75—C76	1.383 (6)
C38—H38	0.950	C76—H76	0.950
Cl1—Cu1—P1	115.98 (5)	Cl2—Cu2—P2	117.85 (4)
Cl1—Cu1—N2	101.81 (9)	Cl2—Cu2—N6	96.77 (9)
Cl1—Cu1—N3	98.19 (9)	Cl2—Cu2—N7	104.00 (9)
P1—Cu1—N2	121.16 (9)	P2—Cu2—N6	121.11 (9)
P1—Cu1—N3	129.82 (9)	P2—Cu2—N7	126.11 (9)
N2—Cu1—N3	82.70 (12)	N6—Cu2—N7	82.97 (12)
Cu1—P1—C21	111.74 (13)	Cu2—P2—C59	110.15 (13)
Cu1—P1—C27	118.29 (15)	Cu2—P2—C65	118.41 (13)

Cu1—P1—C33	115.99 (14)	Cu2—P2—C71	116.39 (13)
C21—P1—C27	102.3 (2)	C59—P2—C65	105.04 (18)
C21—P1—C33	104.83 (18)	C59—P2—C71	104.04 (18)
C27—P1—C33	101.88 (18)	C65—P2—C71	101.26 (17)
O1—N1—O2	122.2 (4)	O5—N5—O6	122.8 (5)
O1—N1—C1	118.6 (4)	O5—N5—C39	117.1 (5)
O2—N1—C1	119.2 (3)	O6—N5—C39	120.1 (4)
Cu1—N2—C9	140.3 (3)	Cu2—N6—C47	131.6 (3)
Cu1—N2—C10	103.3 (2)	Cu2—N6—C48	108.0 (2)
C9—N2—C10	116.1 (3)	C47—N6—C48	117.0 (3)
Cu1—N3—C11	109.7 (2)	Cu2—N7—C49	104.9 (2)
Cu1—N3—C12	131.3 (3)	Cu2—N7—C50	138.7 (3)
C11—N3—C12	118.1 (3)	C49—N7—C50	116.2 (3)
O3—N4—O4	123.6 (4)	O7—N8—O8	123.4 (4)
O3—N4—C20	119.0 (4)	O7—N8—C58	118.6 (4)
O4—N4—C20	117.4 (4)	O8—N8—C58	117.9 (4)
N1—C1—C2	116.7 (4)	N5—C39—C40	117.3 (5)
N1—C1—C6	120.2 (3)	N5—C39—C44	120.3 (4)
C2—C1—C6	123.0 (4)	C40—C39—C44	122.4 (5)
C1—C2—H2	120.5	C39—C40—H40	120.1
C1—C2—C3	119.0 (4)	C39—C40—C41	119.8 (5)
H2—C2—C3	120.5	H40—C40—C41	120.1
C2—C3—H3	120.0	C40—C41—H41	120.0
C2—C3—C4	120.1 (4)	C40—C41—C42	120.1 (5)
H3—C3—C4	120.0	H41—C41—C42	120.0
C3—C4—H4	119.8	C41—C42—H42	120.0
C3—C4—C5	120.5 (4)	C41—C42—C43	119.9 (6)
H4—C4—C5	119.8	H42—C42—C43	120.0
C4—C5—H5	119.4	C42—C43—H43	119.3
C4—C5—C6	121.3 (4)	C42—C43—C44	121.4 (5)
H5—C5—C6	119.4	H43—C43—C44	119.3
C1—C6—C5	116.0 (4)	C39—C44—C43	116.4 (4)
C1—C6—C7	125.2 (4)	C39—C44—C45	124.9 (4)
C5—C6—C7	118.5 (4)	C43—C44—C45	118.6 (4)
C6—C7—H7	117.2	C44—C45—H45	117.1
C6—C7—C8	125.7 (4)	C44—C45—C46	125.7 (4)
H7—C7—C8	117.2	H45—C45—C46	117.1
C7—C8—H8	120.4	C45—C46—H46	119.6
C7—C8—C9	119.2 (4)	C45—C46—C47	120.8 (4)
H8—C8—C9	120.4	H46—C46—C47	119.6
N2—C9—C8	124.6 (4)	N6—C47—C46	124.0 (4)
N2—C9—H9	117.7	N6—C47—H47	118.0
C8—C9—H9	117.7	C46—C47—H47	118.0
N2—C10—H10A	110.1	N6—C48—H48A	110.0
N2—C10—H10B	110.1	N6—C48—H48B	110.0
N2—C10—C11	108.0 (3)	N6—C48—C49	108.4 (3)
H10A—C10—H10B	108.4	H48A—C48—H48B	108.4
H10A—C10—C11	110.1	H48A—C48—C49	110.0
H10B—C10—C11	110.1	H48B—C48—C49	110.0

N3—C11—C10	108.6 (3)	N7—C49—C48	108.4 (3)
N3—C11—H11A	110.0	N7—C49—H49A	110.0
N3—C11—H11B	110.0	N7—C49—H49B	110.0
C10—C11—H11A	110.0	C48—C49—H49A	110.0
C10—C11—H11B	110.0	C48—C49—H49B	110.0
H11A—C11—H11B	108.4	H49A—C49—H49B	108.4
N3—C12—H12	118.5	N7—C50—H50	117.3
N3—C12—C13	123.1 (4)	N7—C50—C51	125.3 (3)
H12—C12—C13	118.5	H50—C50—C51	117.3
C12—C13—H13	119.3	C50—C51—H51	120.4
C12—C13—C14	121.3 (4)	C50—C51—C52	119.1 (4)
H13—C13—C14	119.3	H51—C51—C52	120.4
C13—C14—H14	117.0	C51—C52—H52	116.3
C13—C14—C15	125.9 (4)	C51—C52—C53	127.4 (4)
H14—C14—C15	117.0	H52—C52—C53	116.3
C14—C15—C16	120.9 (4)	C52—C53—C54	119.9 (4)
C14—C15—C20	123.8 (4)	C52—C53—C58	123.9 (4)
C16—C15—C20	115.3 (4)	C54—C53—C58	115.7 (4)
C15—C16—H16	119.2	C53—C54—H54	119.2
C15—C16—C17	121.7 (5)	C53—C54—C55	121.7 (4)
H16—C16—C17	119.2	H54—C54—C55	119.2
C16—C17—H17	119.7	C54—C55—H55	119.9
C16—C17—C18	120.5 (5)	C54—C55—C56	120.2 (5)
H17—C17—C18	119.7	H55—C55—C56	119.9
C17—C18—H18	120.2	C55—C56—H56	120.1
C17—C18—C19	119.5 (5)	C55—C56—C57	119.9 (4)
H18—C18—C19	120.2	H56—C56—C57	120.1
C18—C19—H19	120.3	C56—C57—H57	120.5
C18—C19—C20	119.4 (5)	C56—C57—C58	119.0 (4)
H19—C19—C20	120.3	H57—C57—C58	120.5
N4—C20—C15	119.6 (4)	N8—C58—C53	119.4 (4)
N4—C20—C19	116.8 (4)	N8—C58—C57	117.2 (4)
C15—C20—C19	123.6 (5)	C53—C58—C57	123.4 (4)
P1—C21—C22	117.0 (3)	P2—C59—C60	123.0 (3)
P1—C21—C26	124.5 (3)	P2—C59—C64	117.7 (3)
C22—C21—C26	118.4 (4)	C60—C59—C64	118.6 (4)
C21—C22—H22	119.7	C59—C60—H60	120.1
C21—C22—C23	120.6 (4)	C59—C60—C61	119.8 (5)
H22—C22—C23	119.7	H60—C60—C61	120.1
C22—C23—H23	119.9	C60—C61—H61	119.5
C22—C23—C24	120.2 (4)	C60—C61—C62	120.9 (5)
H23—C23—C24	119.9	H61—C61—C62	119.5
C23—C24—H24	120.1	C61—C62—H62	120.2
C23—C24—C25	119.7 (4)	C61—C62—C63	119.6 (5)
H24—C24—C25	120.1	H62—C62—C63	120.2
C24—C25—H25	119.8	C62—C63—H63	120.0
C24—C25—C26	120.5 (4)	C62—C63—C64	120.0 (5)
H25—C25—C26	119.8	H63—C63—C64	120.0
C21—C26—C25	120.5 (4)	C59—C64—C63	121.0 (5)

C21—C26—H26	119.7	C59—C64—H64	119.5
C25—C26—H26	119.7	C63—C64—H64	119.5
P1—C27—C28	123.5 (4)	P2—C65—C66	123.1 (3)
P1—C27—C32	118.1 (3)	P2—C65—C70	118.4 (3)
C28—C27—C32	118.4 (4)	C66—C65—C70	118.4 (4)
C27—C28—H28	119.8	C65—C66—H66	119.6
C27—C28—C29	120.4 (5)	C65—C66—C67	120.7 (4)
H28—C28—C29	119.8	H66—C66—C67	119.6
C28—C29—H29	119.8	C66—C67—H67	120.1
C28—C29—C30	120.4 (5)	C66—C67—C68	119.8 (5)
H29—C29—C30	119.8	H67—C67—C68	120.1
C29—C30—H30	119.8	C67—C68—H68	120.0
C29—C30—C31	120.3 (5)	C67—C68—C69	119.9 (4)
H30—C30—C31	119.8	H68—C68—C69	120.0
C30—C31—H31	120.3	C68—C69—H69	119.7
C30—C31—C32	119.4 (6)	C68—C69—C70	120.7 (4)
H31—C31—C32	120.3	H69—C69—C70	119.7
C27—C32—C31	121.1 (5)	C65—C70—C69	120.4 (4)
C27—C32—H32	119.5	C65—C70—H70	119.8
C31—C32—H32	119.5	C69—C70—H70	119.8
P1—C33—C34	122.8 (3)	P2—C71—C72	117.5 (3)
P1—C33—C38	118.7 (3)	P2—C71—C76	123.5 (3)
C34—C33—C38	118.5 (4)	C72—C71—C76	118.8 (4)
C33—C34—H34	119.4	C71—C72—H72	119.8
C33—C34—C35	121.3 (5)	C71—C72—C73	120.3 (4)
H34—C34—C35	119.4	H72—C72—C73	119.8
C34—C35—H35	120.2	C72—C73—H73	119.8
C34—C35—C36	119.6 (5)	C72—C73—C74	120.3 (4)
H35—C35—C36	120.2	H73—C73—C74	119.8
C35—C36—H36	120.1	C73—C74—H74	120.2
C35—C36—C37	119.9 (4)	C73—C74—C75	119.7 (4)
H36—C36—C37	120.1	H74—C74—C75	120.2
C36—C37—H37	119.6	C74—C75—H75	119.6
C36—C37—C38	120.8 (5)	C74—C75—C76	120.8 (4)
H37—C37—C38	119.6	H75—C75—C76	119.6
C33—C38—C37	120.0 (5)	C71—C76—C75	120.0 (4)
C33—C38—H38	120.0	C71—C76—H76	120.0
C37—C38—H38	120.0	C75—C76—H76	120.0
Cl1—Cu1—P1—C21	69.27 (15)	Cl2—Cu2—P2—C59	−163.61 (15)
Cl1—Cu1—P1—C27	−49.16 (16)	Cl2—Cu2—P2—C65	75.53 (15)
Cl1—Cu1—P1—C33	−170.66 (14)	Cl2—Cu2—P2—C71	−45.55 (15)
N2—Cu1—P1—C21	−54.84 (17)	N6—Cu2—P2—C59	−45.27 (18)
N2—Cu1—P1—C27	−173.26 (18)	N6—Cu2—P2—C65	−166.13 (17)
N2—Cu1—P1—C33	65.24 (17)	N6—Cu2—P2—C71	72.80 (17)
N3—Cu1—P1—C21	−162.95 (18)	N7—Cu2—P2—C59	59.99 (18)
N3—Cu1—P1—C27	78.6 (2)	N7—Cu2—P2—C65	−60.86 (18)
N3—Cu1—P1—C33	−42.88 (19)	N7—Cu2—P2—C71	178.06 (17)
Cl1—Cu1—N2—C9	−117.2 (4)	Cl2—Cu2—N6—C47	50.1 (4)
Cl1—Cu1—N2—C10	70.1 (2)	Cl2—Cu2—N6—C48	−108.1 (2)

P1—Cu1—N2—C9	13.3 (4)	P2—Cu2—N6—C47	−78.3 (4)
P1—Cu1—N2—C10	−159.42 (19)	P2—Cu2—N6—C48	123.5 (2)
N3—Cu1—N2—C9	145.9 (4)	N7—Cu2—N6—C47	153.4 (4)
N3—Cu1—N2—C10	−26.8 (2)	N7—Cu2—N6—C48	−4.8 (2)
Cl1—Cu1—N3—C11	−103.5 (2)	Cl2—Cu2—N7—C49	70.3 (2)
Cl1—Cu1—N3—C12	64.8 (4)	Cl2—Cu2—N7—C50	−115.7 (4)
P1—Cu1—N3—C11	122.3 (2)	P2—Cu2—N7—C49	−148.61 (19)
P1—Cu1—N3—C12	−69.4 (4)	P2—Cu2—N7—C50	25.4 (4)
N2—Cu1—N3—C11	−2.6 (2)	N6—Cu2—N7—C49	−24.9 (2)
N2—Cu1—N3—C12	165.7 (4)	N6—Cu2—N7—C50	149.1 (4)
O1—N1—C1—C2	18.3 (6)	O5—N5—C39—C40	−21.5 (6)
O1—N1—C1—C6	−164.6 (4)	O5—N5—C39—C44	159.1 (4)
O2—N1—C1—C2	−159.9 (4)	O6—N5—C39—C40	157.2 (5)
O2—N1—C1—C6	17.2 (6)	O6—N5—C39—C44	−22.1 (6)
N1—C1—C2—C3	174.2 (4)	N5—C39—C40—C41	−178.8 (5)
C6—C1—C2—C3	−2.8 (7)	C44—C39—C40—C41	0.5 (8)
C1—C2—C3—C4	−0.7 (7)	C39—C40—C41—C42	0.1 (8)
C2—C3—C4—C5	3.3 (7)	C40—C41—C42—C43	−0.9 (9)
C3—C4—C5—C6	−2.4 (7)	C41—C42—C43—C44	1.0 (8)
C4—C5—C6—C1	−1.0 (6)	C42—C43—C44—C39	−0.4 (7)
C4—C5—C6—C7	172.8 (4)	C42—C43—C44—C45	−177.1 (4)
N1—C1—C6—C5	−173.3 (4)	N5—C39—C44—C43	178.9 (4)
N1—C1—C6—C7	13.4 (6)	N5—C39—C44—C45	−4.6 (6)
C2—C1—C6—C5	3.6 (6)	C40—C39—C44—C43	−0.4 (7)
C2—C1—C6—C7	−169.7 (4)	C40—C39—C44—C45	176.1 (4)
C1—C6—C7—C8	−146.7 (4)	C39—C44—C45—C46	151.1 (4)
C5—C6—C7—C8	40.1 (6)	C43—C44—C45—C46	−32.5 (6)
C6—C7—C8—C9	−174.8 (4)	C44—C45—C46—C47	−179.9 (4)
Cu1—N2—C9—C8	5.8 (6)	Cu2—N6—C47—C46	25.9 (6)
C10—N2—C9—C8	177.9 (3)	C48—N6—C47—C46	−177.5 (4)
C7—C8—C9—N2	−174.6 (4)	C45—C46—C47—N6	179.2 (4)
Cu1—N2—C10—C11	51.4 (3)	Cu2—N6—C48—C49	33.0 (4)
C9—N2—C10—C11	−123.4 (3)	C47—N6—C48—C49	−128.8 (4)
Cu1—N3—C11—C10	31.3 (4)	Cu2—N7—C49—C48	50.5 (3)
C12—N3—C11—C10	−138.7 (3)	C50—N7—C49—C48	−125.1 (3)
N2—C10—C11—N3	−57.1 (4)	N6—C48—C49—N7	−57.3 (4)
Cu1—N3—C12—C13	11.8 (6)	Cu2—N7—C50—C51	3.2 (6)
C11—N3—C12—C13	179.3 (3)	C49—N7—C50—C51	176.8 (3)
N3—C12—C13—C14	176.4 (4)	N7—C50—C51—C52	−178.5 (4)
C12—C13—C14—C15	177.6 (4)	C50—C51—C52—C53	−174.3 (4)
C13—C14—C15—C16	−24.5 (6)	C51—C52—C53—C54	34.6 (6)
C13—C14—C15—C20	158.6 (4)	C51—C52—C53—C58	−153.5 (4)
C14—C15—C16—C17	−175.9 (4)	C52—C53—C54—C55	171.2 (4)
C20—C15—C16—C17	1.2 (6)	C58—C53—C54—C55	−1.4 (6)
C15—C16—C17—C18	0.7 (7)	C53—C54—C55—C56	−2.1 (7)
C16—C17—C18—C19	−1.9 (8)	C54—C55—C56—C57	3.4 (7)
C17—C18—C19—C20	1.1 (8)	C55—C56—C57—C58	−1.1 (7)
C18—C19—C20—N4	−177.2 (4)	C56—C57—C58—N8	175.7 (4)
C18—C19—C20—C15	0.9 (7)	C56—C57—C58—C53	−2.7 (7)

C14—C15—C20—N4	−6.9 (6)	C52—C53—C58—N8	13.3 (6)
C14—C15—C20—C19	175.0 (4)	C52—C53—C58—C57	−168.4 (4)
C16—C15—C20—N4	176.0 (4)	C54—C53—C58—N8	−174.5 (4)
C16—C15—C20—C19	−2.1 (6)	C54—C53—C58—C57	3.8 (6)
O3—N4—C20—C15	−33.6 (6)	O7—N8—C58—C53	28.6 (6)
O3—N4—C20—C19	144.6 (5)	O7—N8—C58—C57	−149.8 (4)
O4—N4—C20—C15	149.7 (4)	O8—N8—C58—C53	−153.6 (4)
O4—N4—C20—C19	−32.1 (6)	O8—N8—C58—C57	28.0 (6)
Cu1—P1—C21—C22	−27.4 (3)	Cu2—P2—C59—C60	−99.6 (4)
Cu1—P1—C21—C26	152.9 (4)	Cu2—P2—C59—C64	70.7 (3)
C27—P1—C21—C22	100.1 (3)	C65—P2—C59—C60	28.9 (4)
C27—P1—C21—C26	−79.6 (4)	C65—P2—C59—C64	−160.8 (3)
C33—P1—C21—C22	−153.9 (3)	C71—P2—C59—C60	134.9 (4)
C33—P1—C21—C26	26.5 (5)	C71—P2—C59—C64	−54.8 (4)
P1—C21—C22—C23	−178.6 (3)	P2—C59—C60—C61	173.4 (4)
C26—C21—C22—C23	1.1 (6)	C64—C59—C60—C61	3.2 (7)
C21—C22—C23—C24	0.0 (6)	C59—C60—C61—C62	−2.2 (8)
C22—C23—C24—C25	−0.5 (7)	C60—C61—C62—C63	0.4 (8)
C23—C24—C25—C26	−0.3 (8)	C61—C62—C63—C64	0.1 (8)
C24—C25—C26—C21	1.5 (9)	C62—C63—C64—C59	1.0 (8)
P1—C21—C26—C25	177.8 (4)	P2—C59—C64—C63	−173.4 (4)
C22—C21—C26—C25	−1.8 (8)	C60—C59—C64—C63	−2.7 (7)
Cu1—P1—C27—C28	117.3 (4)	Cu2—P2—C65—C66	173.0 (3)
Cu1—P1—C27—C32	−60.7 (4)	Cu2—P2—C65—C70	−10.2 (3)
C21—P1—C27—C28	−5.9 (4)	C59—P2—C65—C66	49.5 (4)
C21—P1—C27—C32	176.0 (3)	C59—P2—C65—C70	−133.6 (3)
C33—P1—C27—C28	−114.2 (4)	C71—P2—C65—C66	−58.5 (4)
C33—P1—C27—C32	67.8 (4)	C71—P2—C65—C70	118.3 (3)
P1—C27—C28—C29	−177.6 (4)	P2—C65—C66—C67	177.8 (4)
C32—C27—C28—C29	0.4 (7)	C70—C65—C66—C67	0.9 (7)
C27—C28—C29—C30	−0.4 (8)	C65—C66—C67—C68	1.2 (7)
C28—C29—C30—C31	0.1 (9)	C66—C67—C68—C69	−2.5 (7)
C29—C30—C31—C32	0.1 (8)	C67—C68—C69—C70	1.6 (7)
P1—C27—C32—C31	177.9 (4)	C68—C69—C70—C65	0.5 (6)
C28—C27—C32—C31	−0.3 (7)	P2—C65—C70—C69	−178.8 (3)
C30—C31—C32—C27	0.0 (7)	C66—C65—C70—C69	−1.8 (6)
Cu1—P1—C33—C34	160.3 (3)	Cu2—P2—C71—C72	28.3 (3)
Cu1—P1—C33—C38	−19.2 (4)	Cu2—P2—C71—C76	−156.5 (3)
C21—P1—C33—C34	−75.9 (4)	C59—P2—C71—C72	149.6 (3)
C21—P1—C33—C38	104.5 (3)	C59—P2—C71—C76	−35.2 (4)
C27—P1—C33—C34	30.4 (4)	C65—P2—C71—C72	−101.6 (3)
C27—P1—C33—C38	−149.1 (3)	C65—P2—C71—C76	73.6 (4)
P1—C33—C34—C35	−179.9 (3)	P2—C71—C72—C73	176.1 (3)
C38—C33—C34—C35	−0.4 (7)	C76—C71—C72—C73	0.7 (6)
C33—C34—C35—C36	−0.3 (7)	C71—C72—C73—C74	−0.4 (6)
C34—C35—C36—C37	0.7 (7)	C72—C73—C74—C75	−0.3 (7)
C35—C36—C37—C38	−0.5 (8)	C73—C74—C75—C76	0.7 (7)
P1—C33—C38—C37	−179.9 (4)	C74—C75—C76—C71	−0.4 (7)
C34—C33—C38—C37	0.6 (7)	P2—C71—C76—C75	−175.5 (3)

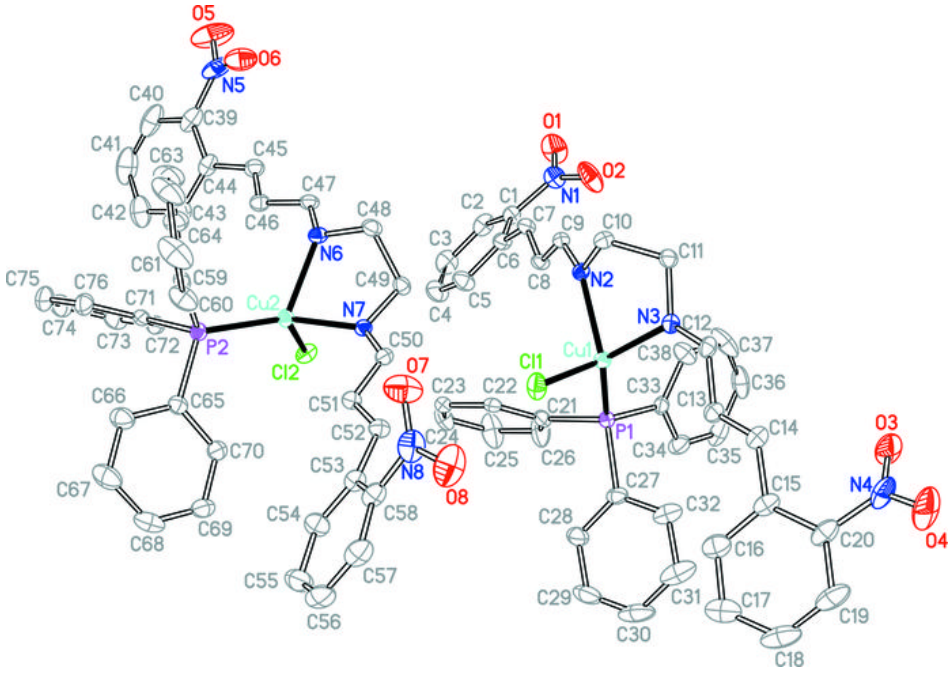
C36—C37—C38—C33	−0.1 (8)	C72—C71—C76—C75	−0.3 (6)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···Cl2^{i}	0.95	2.82	3.683 (4)	151
C9—H9···Cl2^{i}	0.95	2.69	3.585 (4)	158
C12—H12···O8^{ii}	0.95	2.53	3.263 (5)	134
C24—H24···O2^{iii}	0.95	2.56	3.377 (5)	145
C30—H30···O3^{iii}	0.95	2.52	3.245 (6)	133
C37—H37···O5^{iv}	0.95	2.52	3.114 (6)	121
C50—H50···Cl1	0.95	2.73	3.595 (4)	153
C67—H67···O4^{v}	0.95	2.59	3.372 (6)	140
C72—H72···Cl2	0.95	2.80	3.716 (4)	163
C74—H74···O6^{iii}	0.95	2.46	3.237 (6)	139

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

Fig. 1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O6
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C40
C39
C41
C63
C45
C44
C47
C42
C43
C46
C48
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C61
C59
C49
C75
C76
C71
C60
Cu2
N7
C74
C73
C72
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Cl2
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O7
C66
C65
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C23
C22
C52
C24
C70
C53
N8
O8
C67
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C58
C69
C68
C55
C57
C56
O1
O2
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C54
C58
C16
C20
O4
C67
C69
C68
C29
C31
C17
C19
C55
C57
C30
C56
C18