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Azido{*N*,*N*′-bis[3-(2-nitrophenyl)prop-2-enylidene]ethylenediamine}(triphenylphosphine)copper(I) chloroform solvate

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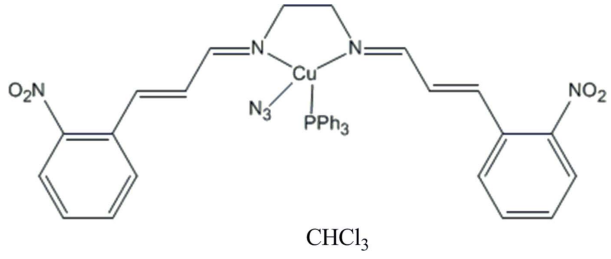
Key indicators: single-crystal X-ray study; T = 200 K; mean σ(C–C) = 0.003 Å; R factor = 0.030; wR factor = 0.092; data-to-parameter ratio = 16.5.

The title compound, $[Cu(N_3)(C_{20}H_{18}N_4O_4)(C_{18}H_{15}P)]\cdot CHCl_3$, is mononuclear copper(I) complex. The Cu^I centre is four-coordinated in a distorted tetrahedral environment by two imine N atoms of the Schiff base, an N_3 ligand and a PPh_3 residue.

Related literature

For related literature, see: Amirnasr *et al.* (2002, 2006); Barron *et al.* (1998); Clarke *et al.* (2003); Dori & Ziolo (1973); Gorji *et al.* (2001); Gustafsson *et al.* (2005); Khalaji *et al.* (2006); Kung *et al.* (1997); Li *et al.* (2003); Suzuki (2005).



$CHCl_3$

Experimental

Crystal data

$[Cu(N_3)(C_{20}H_{18}N_4O_4)(C_{18}H_{15}P)]\cdot CHCl_3$
M_r = 865.59
Triclinic, $P\overline{1}$
a = 9.102 (6) Å
b = 14.328 (9) Å
c = 16.410 (7) Å
α = 109.51 (2)°
β = 103.29 (3)°
γ = 90.45 (3)°
V = 1954.9 (19) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.86 mm^{-1}
T = 200 (2) K
0.22 × 0.18 × 0.15 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.834, T_{max} = 0.882
15528 measured reflections
8200 independent reflections
6283 reflections with $I > 2\sigma(I)$
R_{int} = 0.016

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.092
S = 1.00
8200 reflections
497 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.64 e Å^{-3}
$\Delta\rho_{min}$ = −0.50 e Å^{-3}

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2007); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2498).

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supplementary materials

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Azido{*N*,*N*'-bis[3-(2-nitrophenyl)prop-2-enylidene]ethylenediamine}(triphenylphosphine)copper(I) chloroform solvate

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Comment

The number of ligands bound to the copper(I) ion is greatly influenced by both the chemical nature and the geometry of the ligand (Amirnasr *et al.*, 2006; Li *et al.*, 2003; Clarke *et al.*, 2003; Khalaji *et al.*, 2006) and the type of solvent (Gustafsson *et al.*, 2005). The steric, electronic, and conformational effects imparted by the coordinated ligands play an important role in modifying the properties of the prepared metal complex. A thorough understanding of these effects will serve as the basis for a rational design of complexes with specific and predictable properties. Here we report the synthesis and characterization of a new complex, (I), as well as molecular structure from single-crystal X-ray analysis. The bond lengths and angles around the Cu(I) in (I) are in good agreement with the values found in similar copper complexes (Amirnasr *et al.*, 2002). Selected geometric parameters are show in Table 1. The pseudohalides, N_3, is know to coordinate to metals in both terminal and bridging modes (Suzuki, 2005). However it act as terminal ligand and the structure of this complex consist of discrete molecules of this complex consist of discrete molecules of four-coordinated, containing the bidentate Schiff base, PPh_3 and N_3 ligand. The geometry around Cu(I) is distorted from tetrahedral to psedotetrahedral (Fig. 1). The N(1)—Cu(1)—N(2) angle is 81.39 (7)° and N(5)—Cu(1)—P(1) angle is 115.39 (6)° in complex being somewhat larger than the values for a tetrahedron (Table 1). The average Cu—N(Schiff base) distances of 2.0913 Å is similar to those in the pseudo-tetrahedral (diimine) copper(I) complexes (Barron *et al.*, 1998). The copper azido, Cu—N(5), bond lengths of 2.031 (2) Å is slightly longer than those reported for other tetrahedral copper(I) complexes containing azido ligand (Kung *et al.*, 1997). The Cu(1)—N(5)—N(6) bond angle is 128.68 (15)°. For terminal azido complexes this angle varies between 117° and 132° which is within the expected range for the sp^2 nitrogen (Dori & Ziolo, 1973; Gorji *et al.* 2001). The single bond distance of C(3)—C(4), 1.442 (3) Å being slightly shorter than C(1)—C(2), 1.520 (5) Å indicates the existence of an extended electron delocalization in this complex.

Experimental

To a solution of 105 mg (1 mmol) CuN_3 in 5 ml toluenea solution of 261 mg (1 mmol) of PPh_3 in 5 ml toluene 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 toluene were added and reflux for 60 min. Red crystals suitable for X-ray analysis were obtained by the diffusion of diethyl ether vapor into a concentrated solution of $C_{38}H_{33}CuN_7O_4P$ in chloroform. The resulting crystals of the title compound were collected and dried under vacuum.

Refinement

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

Figures

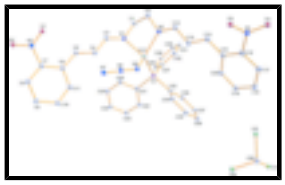

Fig. 1. The molecular structure of compound, with atom labels and 50% probability displacement ellipsoids.

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Crystal data

$[Cu(N_3)(C_{20}H_{18}N_4O_4)(C_{18}H_{15}P)]\cdot CHCl_3$	$Z = 2$
$M_r = 865.59$	$F_{000} = 888$
Triclinic, $P\overline{1}$	$D_x = 1.471$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71075$ Å
$a = 9.102$ (6) Å	Cell parameters from 11830 reflections
$b = 14.328$ (9) Å	$\theta = 3.0$–27.4°
$c = 16.410$ (7) Å	$\mu = 0.86$ mm^{-1}
$\alpha = 109.51$ (2)°	$T = 200$ (2) K
$\beta = 103.29$ (3)°	Block, red
$\gamma = 90.45$ (3)°	0.22 × 0.18 × 0.15 mm
$V = 1954.9$ (19) Å^3	

Data collection

Rigaku R-AXIS RAPID diffractometer	8200 independent reflections
Radiation source: fine-focus sealed tube	6283 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.016$
Detector resolution: 10.00 pixels mm^{-1}	$\theta_{max} = 27.4^\circ$
$T = 200(2)$ K	$\theta_{min} = 3.0^\circ$
ω scans	$h = -11\rightarrow11$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$k = -18\rightarrow18$
$T_{min} = 0.834$, $T_{max} = 0.882$	$l = -18\rightarrow20$
15528 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.030$	H-atom parameters constrained
$wR(F^2) = 0.092$	$w = 1/[\sigma^2(F_o^2) + (0.0578P)^2]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} = 0.001$
8200 reflections	$\Delta\rho_{max} = 0.64$ e Å^{-3}
497 parameters	$\Delta\rho_{min} = -0.49$ 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	0.11196 (3)	0.176702 (17)	0.178776 (13)	0.02108 (7)
Cl1	0.51266 (7)	−0.10182 (5)	0.11080 (4)	0.04100 (14)
Cl2	0.63207 (10)	−0.01236 (7)	0.30103 (5)	0.0730 (2)
Cl3	0.36468 (9)	−0.15220 (6)	0.23049 (5)	0.0630 (2)
P1	0.11027 (5)	0.28753 (4)	0.30973 (3)	0.01926 (11)
O4	−0.0400 (2)	−0.38709 (12)	0.25223 (11)	0.0491 (4)
O3	0.0440 (2)	−0.31450 (12)	0.17320 (10)	0.0428 (4)
O1	0.30874 (18)	0.27941 (12)	−0.18253 (9)	0.0370 (4)
O2	0.4708 (2)	0.37033 (14)	−0.20621 (10)	0.0493 (5)
N1	0.01363 (18)	0.21652 (12)	0.06768 (10)	0.0224 (3)
N2	−0.06478 (17)	0.06375 (12)	0.11801 (9)	0.0206 (3)
N5	0.31277 (19)	0.11851 (13)	0.16964 (11)	0.0276 (4)
N6	0.3936 (2)	0.12754 (14)	0.12657 (12)	0.0339 (4)
N7	0.4774 (3)	0.13683 (19)	0.08465 (16)	0.0579 (6)
N4	0.0176 (2)	−0.31477 (14)	0.24334 (12)	0.0335 (4)
N3	0.4224 (2)	0.33698 (13)	−0.15698 (11)	0.0293 (4)
C1	−0.1481 (2)	0.18368 (15)	0.04484 (13)	0.0261 (4)
H1A	−0.1990	0.1905	−0.0128	0.031*
H1B	−0.1959	0.2254	0.0913	0.031*
C2	−0.1655 (2)	0.07557 (15)	0.03818 (12)	0.0245 (4)
H2A	−0.2721	0.0561	0.0344	0.029*
H2B	−0.1383	0.0322	−0.0163	0.029*
C3	0.0638 (2)	0.25774 (14)	0.01996 (12)	0.0239 (4)
H3	−0.0058	0.2688	−0.0281	0.029*
C4	0.2226 (2)	0.28784 (15)	0.03691 (12)	0.0252 (4)
H4	0.2916	0.2755	0.0844	0.030*
C5	0.2773 (2)	0.33235 (15)	−0.01126 (12)	0.0245 (4)
H5	0.2075	0.3460	−0.0577	0.029*
C6	0.4394 (2)	0.36133 (14)	0.00352 (12)	0.0245 (4)
C7	0.5095 (2)	0.36755 (14)	−0.06247 (12)	0.0259 (4)
C8	0.6607 (3)	0.39891 (16)	−0.04500 (14)	0.0325 (5)
H8	0.7031	0.4016	−0.0920	0.039*
C9	0.7499 (3)	0.42631 (17)	0.04082 (15)	0.0367 (5)
H9	0.8541	0.4485	0.0536	0.044*
C10	0.6857 (3)	0.42112 (17)	0.10854 (14)	0.0356 (5)
H10	0.7462	0.4397	0.1680	0.043*
C11	0.5355 (3)	0.38933 (16)	0.08983 (14)	0.0312 (5)
H11	0.4945	0.3861	0.1372	0.037*

C12	−0.0919 (2)	−0.01417 (15)	0.13532 (12)	0.0239 (4)
H12	−0.1736	−0.0614	0.0966	0.029*
C13	−0.0012 (2)	−0.03264 (15)	0.21264 (13)	0.0257 (4)
H13	0.0815	0.0141	0.2507	0.031*
C14	−0.0301 (2)	−0.11327 (15)	0.23206 (13)	0.0266 (4)
H14	−0.1053	−0.1631	0.1898	0.032*
C15	0.0466 (2)	−0.12993 (16)	0.31449 (13)	0.0275 (4)
C16	0.0632 (2)	−0.22393 (16)	0.32232 (13)	0.0277 (4)
C17	0.1260 (3)	−0.23790 (18)	0.40255 (14)	0.0352 (5)
H17	0.1324	−0.3030	0.4052	0.042*
C18	0.1786 (3)	−0.1560 (2)	0.47803 (15)	0.0425 (6)
H18	0.2230	−0.1643	0.5332	0.051*
C19	0.1670 (3)	−0.0618 (2)	0.47363 (15)	0.0452 (6)
H19	0.2051	−0.0053	0.5257	0.054*
C20	0.0998 (3)	−0.04925 (17)	0.39331 (14)	0.0367 (5)
H20	0.0897	0.0162	0.3920	0.044*
C21	0.2127 (2)	0.40704 (14)	0.33211 (12)	0.0213 (4)
C22	0.2903 (2)	0.47090 (16)	0.41650 (13)	0.0303 (5)
H22	0.2885	0.4545	0.4678	0.036*
C23	0.3699 (3)	0.55806 (17)	0.42563 (15)	0.0376 (5)
H23	0.4220	0.6013	0.4834	0.045*
C24	0.3746 (3)	0.58271 (17)	0.35230 (15)	0.0371 (5)
H24	0.4315	0.6418	0.3590	0.044*
C25	0.2960 (3)	0.52100 (17)	0.26878 (15)	0.0381 (5)
H25	0.2974	0.5383	0.2179	0.046*
C26	0.2155 (2)	0.43458 (16)	0.25869 (13)	0.0301 (5)
H26	0.1610	0.3931	0.2008	0.036*
C27	−0.0781 (2)	0.32069 (15)	0.32397 (11)	0.0232 (4)
C28	−0.1203 (2)	0.41723 (17)	0.34369 (13)	0.0319 (5)
H28	−0.0468	0.4709	0.3564	0.038*
C29	−0.2696 (3)	0.4356 (2)	0.34482 (15)	0.0420 (6)
H29	−0.2979	0.5017	0.3578	0.050*
C30	−0.3766 (3)	0.3585 (2)	0.32731 (15)	0.0452 (6)
H30	−0.4786	0.3714	0.3278	0.054*
C31	−0.3354 (3)	0.2624 (2)	0.30894 (15)	0.0445 (6)
H31	−0.4088	0.2093	0.2978	0.053*
C32	−0.1874 (2)	0.24358 (18)	0.30673 (14)	0.0347 (5)
H32	−0.1600	0.1773	0.2933	0.042*
C33	0.1972 (2)	0.25336 (15)	0.40682 (12)	0.0244 (4)
C34	0.3130 (2)	0.19163 (16)	0.39942 (14)	0.0322 (5)
H34	0.3422	0.1674	0.3446	0.039*
C35	0.3877 (3)	0.16445 (18)	0.47098 (15)	0.0417 (6)
H35	0.4675	0.1223	0.4651	0.050*
C36	0.3450 (3)	0.19911 (19)	0.55075 (15)	0.0441 (6)
H36	0.3950	0.1803	0.5996	0.053*
C37	0.2305 (3)	0.2606 (2)	0.55940 (15)	0.0436 (6)
H37	0.2028	0.2849	0.6147	0.052*
C38	0.1543 (3)	0.28788 (18)	0.48801 (14)	0.0362 (5)
H38	0.0739	0.3295	0.4942	0.043*

C57	0.4654 (3)	−0.05803 (18)	0.21369 (15)	0.0403 (6)
H57	0.3999	−0.0022	0.2142	0.048*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0216 (1)	0.0208 (1)	0.0203 (1)	−0.00021 (9)	0.00547 (9)	0.00619 (9)
Cl1	0.0364 (3)	0.0472 (4)	0.0398 (3)	0.0053 (3)	0.0089 (2)	0.0158 (2)
Cl2	0.0757 (6)	0.0776 (6)	0.0433 (4)	−0.0086 (4)	−0.0105 (3)	0.0093 (3)
Cl3	0.0566 (5)	0.0691 (5)	0.0831 (5)	0.0109 (4)	0.0394 (4)	0.0370 (4)
P1	0.0179 (2)	0.0202 (3)	0.0197 (2)	−0.00029 (19)	0.00561 (17)	0.00637 (18)
O4	0.0557 (12)	0.0298 (9)	0.0604 (11)	−0.0070 (8)	0.0032 (8)	0.0214 (8)
O3	0.0532 (11)	0.0401 (10)	0.0342 (9)	0.0074 (8)	0.0082 (7)	0.0132 (7)
O1	0.0337 (9)	0.0427 (10)	0.0337 (8)	−0.0100 (7)	0.0073 (6)	0.0132 (7)
O2	0.0593 (12)	0.0574 (12)	0.0382 (9)	−0.0163 (9)	0.0182 (8)	0.0220 (8)
N1	0.0231 (9)	0.0209 (8)	0.0253 (8)	0.0007 (7)	0.0065 (6)	0.0101 (6)
N2	0.0193 (8)	0.0210 (8)	0.0211 (8)	0.0016 (6)	0.0053 (6)	0.0068 (6)
N5	0.0235 (9)	0.0318 (10)	0.0290 (9)	0.0112 (7)	0.0085 (7)	0.0109 (7)
N6	0.0324 (11)	0.0304 (10)	0.0374 (10)	0.0096 (8)	0.0078 (8)	0.0101 (8)
N7	0.0575 (16)	0.0663 (17)	0.0754 (16)	0.0239 (13)	0.0459 (13)	0.0370 (13)
N4	0.0325 (11)	0.0287 (10)	0.0387 (11)	0.0035 (8)	0.0016 (8)	0.0159 (8)
N3	0.0348 (11)	0.0293 (10)	0.0287 (9)	0.0007 (8)	0.0125 (7)	0.0131 (7)
C1	0.0210 (10)	0.0295 (11)	0.0298 (10)	0.0021 (8)	0.0038 (8)	0.0146 (8)
C2	0.0206 (10)	0.0278 (11)	0.0233 (10)	−0.0023 (8)	0.0012 (7)	0.0094 (8)
C3	0.0285 (11)	0.0243 (11)	0.0205 (10)	0.0035 (8)	0.0062 (7)	0.0095 (7)
C4	0.0273 (11)	0.0251 (11)	0.0257 (10)	0.0025 (8)	0.0075 (8)	0.0112 (8)
C5	0.0273 (11)	0.0244 (10)	0.0225 (10)	0.0012 (8)	0.0076 (7)	0.0079 (7)
C6	0.0284 (11)	0.0188 (10)	0.0284 (10)	0.0012 (8)	0.0092 (8)	0.0094 (7)
C7	0.0303 (12)	0.0187 (10)	0.0296 (11)	−0.0002 (8)	0.0087 (8)	0.0088 (8)
C8	0.0322 (12)	0.0280 (12)	0.0418 (12)	0.0006 (9)	0.0144 (9)	0.0144 (9)
C9	0.0255 (12)	0.0307 (12)	0.0533 (14)	−0.0017 (9)	0.0071 (10)	0.0154 (10)
C10	0.0341 (13)	0.0320 (12)	0.0359 (12)	0.0014 (10)	−0.0002 (9)	0.0112 (9)
C11	0.0334 (12)	0.0283 (12)	0.0322 (11)	0.0009 (9)	0.0077 (9)	0.0113 (8)
C12	0.0193 (10)	0.0231 (10)	0.0287 (10)	−0.0020 (8)	0.0065 (7)	0.0077 (8)
C13	0.0225 (10)	0.0240 (10)	0.0309 (10)	−0.0031 (8)	0.0044 (8)	0.0112 (8)
C14	0.0239 (11)	0.0252 (11)	0.0301 (11)	−0.0014 (8)	0.0050 (8)	0.0097 (8)
C15	0.0245 (11)	0.0292 (11)	0.0326 (11)	−0.0017 (9)	0.0084 (8)	0.0146 (8)
C16	0.0232 (11)	0.0303 (11)	0.0325 (11)	−0.0008 (9)	0.0068 (8)	0.0148 (8)
C17	0.0318 (12)	0.0408 (14)	0.0406 (13)	0.0044 (10)	0.0085 (9)	0.0241 (10)
C18	0.0401 (14)	0.0571 (17)	0.0326 (13)	−0.0006 (12)	0.0022 (10)	0.0228 (11)
C19	0.0522 (16)	0.0448 (15)	0.0329 (13)	−0.0071 (12)	0.0017 (10)	0.0119 (10)
C20	0.0441 (14)	0.0322 (13)	0.0342 (12)	−0.0029 (10)	0.0087 (9)	0.0127 (9)
C21	0.0175 (10)	0.0213 (10)	0.0261 (10)	0.0016 (8)	0.0081 (7)	0.0077 (7)
C22	0.0302 (12)	0.0295 (12)	0.0275 (11)	−0.0018 (9)	0.0030 (8)	0.0079 (8)
C23	0.0345 (13)	0.0274 (12)	0.0396 (12)	−0.0056 (10)	−0.0005 (9)	0.0035 (9)
C24	0.0306 (13)	0.0254 (12)	0.0555 (14)	−0.0046 (10)	0.0132 (10)	0.0130 (10)
C25	0.0463 (15)	0.0324 (13)	0.0428 (13)	−0.0029 (11)	0.0201 (10)	0.0164 (10)
C26	0.0327 (12)	0.0290 (12)	0.0285 (11)	−0.0032 (9)	0.0103 (8)	0.0081 (8)

C27	0.0199 (10)	0.0311 (11)	0.0183 (10)	0.0017 (8)	0.0056 (7)	0.0076 (7)
C28	0.0272 (12)	0.0343 (12)	0.0344 (11)	0.0047 (9)	0.0106 (8)	0.0101 (9)
C29	0.0341 (14)	0.0491 (16)	0.0441 (13)	0.0175 (12)	0.0162 (10)	0.0132 (11)
C30	0.0216 (12)	0.074 (2)	0.0395 (13)	0.0119 (12)	0.0123 (9)	0.0149 (12)
C31	0.0263 (13)	0.0563 (17)	0.0441 (13)	−0.0096 (11)	0.0118 (10)	0.0070 (11)
C32	0.0257 (12)	0.0361 (13)	0.0384 (12)	−0.0021 (10)	0.0126 (9)	0.0050 (9)
C33	0.0232 (10)	0.0252 (11)	0.0241 (10)	−0.0057 (8)	0.0045 (7)	0.0087 (8)
C34	0.0287 (12)	0.0325 (12)	0.0333 (11)	0.0007 (9)	0.0039 (8)	0.0112 (9)
C35	0.0336 (14)	0.0413 (14)	0.0482 (14)	0.0019 (11)	−0.0046 (10)	0.0226 (11)
C36	0.0407 (15)	0.0504 (16)	0.0404 (14)	−0.0157 (12)	−0.0115 (10)	0.0295 (11)
C37	0.0435 (15)	0.0634 (17)	0.0267 (12)	−0.0138 (13)	0.0042 (9)	0.0227 (11)
C38	0.0310 (13)	0.0479 (15)	0.0320 (12)	0.0005 (10)	0.0111 (9)	0.0146 (10)
C57	0.0438 (15)	0.0403 (14)	0.0398 (13)	0.0134 (11)	0.0107 (10)	0.0172 (10)

Geometric parameters (Å, °)

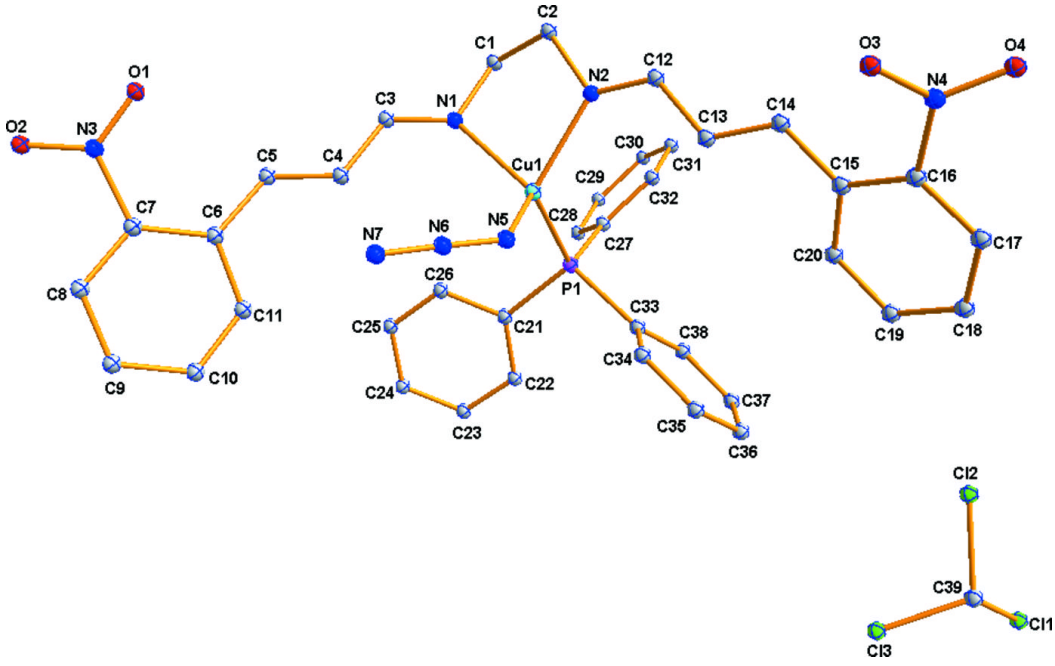
Cu1—N5	2.031 (2)	C14—C15	1.469 (3)
Cu1—N2	2.0844 (19)	C14—H14	0.9500
Cu1—N1	2.0982 (17)	C15—C20	1.396 (3)
Cu1—P1	2.2082 (11)	C15—C16	1.401 (3)
Cl1—C57	1.749 (2)	C16—C17	1.390 (3)
Cl2—C57	1.772 (3)	C17—C18	1.374 (3)
Cl3—C57	1.756 (3)	C17—H17	0.9500
P1—C21	1.826 (2)	C18—C19	1.378 (4)
P1—C27	1.828 (2)	C18—H18	0.9500
P1—C33	1.831 (2)	C19—C20	1.391 (3)
O4—N4	1.224 (2)	C19—H19	0.9500
O3—N4	1.230 (2)	C20—H20	0.9500
O1—N3	1.218 (2)	C21—C26	1.393 (3)
O2—N3	1.222 (2)	C21—C22	1.395 (3)
N1—C3	1.280 (2)	C22—C23	1.385 (3)
N1—C1	1.465 (3)	C22—H22	0.9500
N2—C12	1.276 (2)	C23—C24	1.372 (3)
N2—C2	1.478 (2)	C23—H23	0.9500
N5—N6	1.165 (2)	C24—C25	1.379 (3)
N6—N7	1.172 (3)	C24—H24	0.9500
N4—C16	1.471 (3)	C25—C26	1.375 (3)
N3—C7	1.483 (3)	C25—H25	0.9500
C1—C2	1.520 (3)	C26—H26	0.9500
C1—H1A	0.9900	C27—C28	1.390 (3)
C1—H1B	0.9900	C27—C32	1.391 (3)
C2—H2A	0.9900	C28—C29	1.389 (3)
C2—H2B	0.9900	C28—H28	0.9500
C3—C4	1.442 (3)	C29—C30	1.376 (4)
C3—H3	0.9500	C29—H29	0.9500
C4—C5	1.339 (3)	C30—C31	1.383 (4)
C4—H4	0.9500	C30—H30	0.9500
C5—C6	1.471 (3)	C31—C32	1.382 (3)
C5—H5	0.9500	C31—H31	0.9500

C6—C7	1.403 (3)	C32—H32	0.9500
C6—C11	1.406 (3)	C33—C34	1.383 (3)
C7—C8	1.378 (3)	C33—C38	1.405 (3)
C8—C9	1.377 (3)	C34—C35	1.391 (3)
C8—H8	0.9500	C34—H34	0.9500
C9—C10	1.391 (3)	C35—C36	1.383 (4)
C9—H9	0.9500	C35—H35	0.9500
C10—C11	1.369 (3)	C36—C37	1.372 (4)
C10—H10	0.9500	C36—H36	0.9500
C11—H11	0.9500	C37—C38	1.393 (3)
C12—C13	1.452 (3)	C37—H37	0.9500
C12—H12	0.9500	C38—H38	0.9500
C13—C14	1.336 (3)	C57—H57	1.0000
C13—H13	0.9500		
N5—Cu1—N2	109.65 (8)	C16—C15—C14	124.28 (19)
N5—Cu1—N1	111.99 (7)	C17—C16—C15	123.3 (2)
N2—Cu1—N1	81.39 (7)	C17—C16—N4	116.00 (19)
N5—Cu1—P1	115.39 (6)	C15—C16—N4	120.67 (17)
N2—Cu1—P1	118.36 (5)	C18—C17—C16	118.9 (2)
N1—Cu1—P1	115.48 (6)	C18—C17—H17	120.5
C21—P1—C27	103.45 (10)	C16—C17—H17	120.5
C21—P1—C33	103.54 (9)	C17—C18—C19	120.0 (2)
C27—P1—C33	104.79 (9)	C17—C18—H18	120.0
C21—P1—Cu1	113.38 (7)	C19—C18—H18	120.0
C27—P1—Cu1	114.71 (7)	C18—C19—C20	120.2 (2)
C33—P1—Cu1	115.58 (8)	C18—C19—H19	119.9
C3—N1—C1	119.46 (15)	C20—C19—H19	119.9
C3—N1—Cu1	134.93 (14)	C19—C20—C15	122.0 (2)
C1—N1—Cu1	105.59 (11)	C19—C20—H20	119.0
C12—N2—C2	117.20 (16)	C15—C20—H20	119.0
C12—N2—Cu1	130.68 (13)	C26—C21—C22	118.20 (18)
C2—N2—Cu1	111.94 (12)	C26—C21—P1	116.90 (14)
N6—N5—Cu1	128.68 (15)	C22—C21—P1	124.88 (14)
N5—N6—N7	178.7 (2)	C23—C22—C21	120.18 (19)
O4—N4—O3	123.98 (19)	C23—C22—H22	119.9
O4—N4—C16	117.87 (18)	C21—C22—H22	119.9
O3—N4—C16	118.11 (18)	C24—C23—C22	120.8 (2)
O1—N3—O2	122.97 (17)	C24—C23—H23	119.6
O1—N3—C7	119.48 (15)	C22—C23—H23	119.6
O2—N3—C7	117.55 (17)	C23—C24—C25	119.5 (2)
N1—C1—C2	108.93 (16)	C23—C24—H24	120.3
N1—C1—H1A	109.9	C25—C24—H24	120.3
C2—C1—H1A	109.9	C26—C25—C24	120.41 (19)
N1—C1—H1B	109.9	C26—C25—H25	119.8
C2—C1—H1B	109.9	C24—C25—H25	119.8
H1A—C1—H1B	108.3	C25—C26—C21	120.91 (19)
N2—C2—C1	108.89 (15)	C25—C26—H26	119.5
N2—C2—H2A	109.9	C21—C26—H26	119.5
C1—C2—H2A	109.9	C28—C27—C32	118.8 (2)

N2—C2—H2B	109.9	C28—C27—P1	123.47 (16)
C1—C2—H2B	109.9	C32—C27—P1	117.56 (16)
H2A—C2—H2B	108.3	C29—C28—C27	120.3 (2)
N1—C3—C4	121.97 (17)	C29—C28—H28	119.9
N1—C3—H3	119.0	C27—C28—H28	119.9
C4—C3—H3	119.0	C30—C29—C28	120.3 (2)
C5—C4—C3	123.01 (17)	C30—C29—H29	119.9
C5—C4—H4	118.5	C28—C29—H29	119.9
C3—C4—H4	118.5	C29—C30—C31	119.9 (2)
C4—C5—C6	123.83 (18)	C29—C30—H30	120.0
C4—C5—H5	118.1	C31—C30—H30	120.0
C6—C5—H5	118.1	C32—C31—C30	120.0 (2)
C7—C6—C11	114.83 (19)	C32—C31—H31	120.0
C7—C6—C5	125.10 (17)	C30—C31—H31	120.0
C11—C6—C5	120.02 (17)	C31—C32—C27	120.7 (2)
C8—C7—C6	123.20 (18)	C31—C32—H32	119.6
C8—C7—N3	116.32 (17)	C27—C32—H32	119.6
C6—C7—N3	120.46 (18)	C34—C33—C38	118.88 (18)
C9—C8—C7	119.78 (19)	C34—C33—P1	117.52 (15)
C9—C8—H8	120.1	C38—C33—P1	123.59 (17)
C7—C8—H8	120.1	C33—C34—C35	121.0 (2)
C8—C9—C10	119.2 (2)	C33—C34—H34	119.5
C8—C9—H9	120.4	C35—C34—H34	119.5
C10—C9—H9	120.4	C36—C35—C34	119.6 (2)
C11—C10—C9	120.22 (19)	C36—C35—H35	120.2
C11—C10—H10	119.9	C34—C35—H35	120.2
C9—C10—H10	119.9	C37—C36—C35	120.14 (19)
C10—C11—C6	122.80 (19)	C37—C36—H36	119.9
C10—C11—H11	118.6	C35—C36—H36	119.9
C6—C11—H11	118.6	C36—C37—C38	120.7 (2)
N2—C12—C13	121.77 (18)	C36—C37—H37	119.6
N2—C12—H12	119.1	C38—C37—H37	119.6
C13—C12—H12	119.1	C37—C38—C33	119.6 (2)
C14—C13—C12	122.19 (19)	C37—C38—H38	120.2
C14—C13—H13	118.9	C33—C38—H38	120.2
C12—C13—H13	118.9	Cl1—C57—Cl3	110.98 (14)
C13—C14—C15	124.30 (19)	Cl1—C57—Cl2	109.92 (14)
C13—C14—H14	117.8	Cl3—C57—Cl2	110.04 (13)
C15—C14—H14	117.8	Cl1—C57—H57	108.6
C20—C15—C16	115.48 (18)	Cl3—C57—H57	108.6
C20—C15—C14	120.10 (19)	Cl2—C57—H57	108.6
N5—Cu1—P1—C21	72.99 (10)	C20—C15—C16—C17	0.9 (3)
N2—Cu1—P1—C21	−154.22 (8)	C14—C15—C16—C17	−174.9 (2)
N1—Cu1—P1—C21	−60.28 (9)	C20—C15—C16—N4	−177.37 (19)
N5—Cu1—P1—C27	−168.46 (8)	C14—C15—C16—N4	6.8 (3)
N2—Cu1—P1—C27	−35.67 (9)	O4—N4—C16—C17	38.5 (3)
N1—Cu1—P1—C27	58.27 (9)	O3—N4—C16—C17	−139.2 (2)
N5—Cu1—P1—C33	−46.33 (9)	O4—N4—C16—C15	−143.1 (2)
N2—Cu1—P1—C33	86.46 (9)	O3—N4—C16—C15	39.2 (3)

N1—Cu1—P1—C33	−179.60 (8)	C15—C16—C17—C18	−1.8 (3)
N5—Cu1—N1—C3	−40.5 (2)	N4—C16—C17—C18	176.5 (2)
N2—Cu1—N1—C3	−148.3 (2)	C16—C17—C18—C19	0.8 (4)
P1—Cu1—N1—C3	94.30 (19)	C17—C18—C19—C20	1.1 (4)
N5—Cu1—N1—C1	137.74 (13)	C18—C19—C20—C15	−2.1 (4)
N2—Cu1—N1—C1	29.94 (12)	C16—C15—C20—C19	1.1 (3)
P1—Cu1—N1—C1	−87.45 (13)	C14—C15—C20—C19	177.1 (2)
N5—Cu1—N2—C12	60.37 (19)	C27—P1—C21—C26	−94.68 (17)
N1—Cu1—N2—C12	170.74 (18)	C33—P1—C21—C26	156.19 (16)
P1—Cu1—N2—C12	−74.88 (19)	Cu1—P1—C21—C26	30.18 (18)
N5—Cu1—N2—C2	−114.55 (13)	C27—P1—C21—C22	86.81 (19)
N1—Cu1—N2—C2	−4.18 (12)	C33—P1—C21—C22	−22.3 (2)
P1—Cu1—N2—C2	110.20 (12)	Cu1—P1—C21—C22	−148.32 (16)
N2—Cu1—N5—N6	109.6 (2)	C26—C21—C22—C23	−1.3 (3)
N1—Cu1—N5—N6	21.2 (2)	P1—C21—C22—C23	177.21 (17)
P1—Cu1—N5—N6	−113.69 (19)	C21—C22—C23—C24	−0.4 (4)
Cu1—N5—N6—N7	138 (10)	C22—C23—C24—C25	1.5 (4)
C3—N1—C1—C2	127.91 (18)	C23—C24—C25—C26	−1.1 (4)
Cu1—N1—C1—C2	−50.67 (16)	C24—C25—C26—C21	−0.6 (4)
C12—N2—C2—C1	162.44 (17)	C22—C21—C26—C25	1.8 (3)
Cu1—N2—C2—C1	−21.90 (18)	P1—C21—C26—C25	−176.84 (18)
N1—C1—C2—N2	48.7 (2)	C21—P1—C27—C28	2.31 (17)
C1—N1—C3—C4	−177.38 (18)	C33—P1—C27—C28	110.50 (16)
Cu1—N1—C3—C4	0.7 (3)	Cu1—P1—C27—C28	−121.68 (15)
N1—C3—C4—C5	−179.00 (19)	C21—P1—C27—C32	176.81 (14)
C3—C4—C5—C6	−178.40 (19)	C33—P1—C27—C32	−75.01 (16)
C4—C5—C6—C7	151.3 (2)	Cu1—P1—C27—C32	52.81 (16)
C4—C5—C6—C11	−31.3 (3)	C32—C27—C28—C29	−0.9 (3)
C11—C6—C7—C8	−0.2 (3)	P1—C27—C28—C29	173.57 (15)
C5—C6—C7—C8	177.3 (2)	C27—C28—C29—C30	0.6 (3)
C11—C6—C7—N3	177.93 (18)	C28—C29—C30—C31	0.3 (3)
C5—C6—C7—N3	−4.5 (3)	C29—C30—C31—C32	−1.1 (3)
O1—N3—C7—C8	155.6 (2)	C30—C31—C32—C27	0.8 (3)
O2—N3—C7—C8	−23.3 (3)	C28—C27—C32—C31	0.1 (3)
O1—N3—C7—C6	−22.7 (3)	P1—C27—C32—C31	−174.63 (16)
O2—N3—C7—C6	158.4 (2)	C21—P1—C33—C34	−95.15 (17)
C6—C7—C8—C9	−0.2 (3)	C27—P1—C33—C34	156.73 (16)
N3—C7—C8—C9	−178.49 (19)	Cu1—P1—C33—C34	29.44 (18)
C7—C8—C9—C10	0.4 (3)	C21—P1—C33—C38	83.61 (19)
C8—C9—C10—C11	−0.1 (3)	C27—P1—C33—C38	−24.5 (2)
C9—C10—C11—C6	−0.4 (4)	Cu1—P1—C33—C38	−151.80 (16)
C7—C6—C11—C10	0.6 (3)	C38—C33—C34—C35	−0.6 (3)
C5—C6—C11—C10	−177.1 (2)	P1—C33—C34—C35	178.23 (17)
C2—N2—C12—C13	−179.26 (17)	C33—C34—C35—C36	0.4 (3)
Cu1—N2—C12—C13	6.0 (3)	C34—C35—C36—C37	−0.5 (4)
N2—C12—C13—C14	179.0 (2)	C35—C36—C37—C38	0.9 (4)
C12—C13—C14—C15	−172.71 (19)	C36—C37—C38—C33	−1.2 (3)
C13—C14—C15—C20	30.1 (3)	C34—C33—C38—C37	1.0 (3)
C13—C14—C15—C16	−154.3 (2)	P1—C33—C38—C37	−177.78 (17)

Fig. 1


C2
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