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(Bromido)[*N*,*N*′-bis(2-nitrocinnamaldehyde)ethylenediamine](triphenylphosphine)copper(I)

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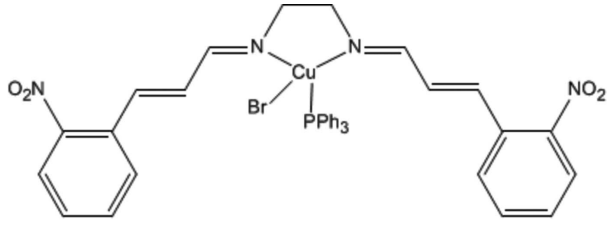
Key indicators: single-crystal X-ray study; T = 200 K; mean σ(C–C) = 0.004 Å; R factor = 0.027; wR factor = 0.059; data-to-parameter ratio = 18.3.

In the title mononuclear Cu^{I} complex, $C_{38}H_{33}CuBrN_4O_4P$ or $[CuBr(C_{18}H_{15}P)(C_9H_7NO_2)_2(C_2H_4N_2)]$, the Cu^{I} ion is coordinated by two imine N atoms of a Schiff base ligand, a Br$^-$ anion and a PPh_3 ligand in a distorted tetrahedral geometry. The N—Cu—N angle is only 82.15 (7)°, but the Br—Cu—P angle is 114.54 (4)°.

Related literature

For general background, see: Bren *et al.* (1991); Horvath (1994); Striejewske (1998). For related structures, see: Barron *et al.* (1988).



Experimental

Crystal data

$[CuBr(C_{18}H_{15}P)(C_9H_7NO_2)_2(C_2H_4N_2)]$
M_r = 784.10
Monoclinic, $C2/c$
a = 31.288 (19) Å
b = 15.486 (9) Å
c = 17.381 (10) Å
β = 122.34 (2)°
V = 7116 (7) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.83 mm^{-1}
T = 200 (2) K
0.26 × 0.20 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.635, T_{max} = 0.720
24792 measured reflections
8101 independent reflections
5147 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.059
S = 1.02
8101 reflections
443 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—Br1	2.4411 (11)	N2—C2	1.473 (3)
Cu1—N1	2.086 (2)	N3—C7	1.470 (3)
Cu1—N2	2.078 (2)	N4—C16	1.482 (3)
Cu1—P1	2.2069 (13)	C1—C2	1.490 (3)
P1—C33	1.831 (2)	C3—C4	1.446 (3)
P1—C27	1.832 (2)	C4—C5	1.333 (3)
P1—C21	1.833 (2)	C5—C6	1.464 (3)
N1—C3	1.275 (2)	C12—C13	1.439 (3)
N1—C1	1.473 (3)	C13—C14	1.335 (3)
N2—C12	1.277 (3)	C14—C15	1.459 (3)
N2—Cu1—N1	82.15 (7)	N2—Cu1—Br1	113.00 (7)
N2—Cu1—P1	117.29 (5)	N1—Cu1—Br1	106.03 (5)
N1—Cu1—P1	119.52 (6)	P1—Cu1—Br1	114.54 (4)

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: XU2320).

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supplementary materials

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(Bromido)[*N*,*N*'-bis(2-nitrocinnamaldehyde)ethylenediamine](triphenylphosphine)copper(I)

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Comment

The coordination chemistry of copper(I) complexes has received increased attention over the last decades. This is mainly due to the potential application of these complexes in catalytic processes (Striejewske, 1998) photosensitization reactions (Bren *et al.*, 1991) and light harvesting studies (Horvath, 1994). 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. Here, we reported the results of the reaction of Cu(I) with *N*,*N*'-bis(2-nitrocinnamaldehyde)ethylenediamine and triphenylphosphine, which forms a copper Schiff base complex (Fig. 1).

The bond lengths and angles (Table 1) around the Cu in (I) are good agreement with the found in similar copper complexes. The Cu(1)—Br(1) bond lengths of 2.4411 (11) Å agree well with the same distance in other tetrahedral copper(I) complexes. The Cu(1)—P(1) distances are 2.2069 (13) Å which agree well with the same distances in other tetrahedral copper(I) phosphine complexes (Barron *et al.*, 1988). While a tetrahedral geometry might be expected for a four coordinated copper(I) center the coordination sphere around copper(I) in this complex is distorted by the restricting bite angle of the chelating ligand. The N(1)—Cu(1)—N(2) angle is only 82.15 (7)°. The Br(1)—Cu(1)—P(1)angle is 114.54 (4)°, being somewhat larger than the values for a tetrahedron (Table 1). The single bond distance of C(3)—C(4), 1.446 (3) Å being slightly shorter than C(1)—C(2), 1.490 (3) Å indicates the existence of an extended electron delocalization in this complex.

Experimental

To a solution of 143 mg (1 mmol) CuBr in 5 ml acetonitril a solution of 261 mg (1 mmol) of PPh_3 in 5 ml aetonitril 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 acetonitril were added and stirred for an additional 60 min. The volume of the solvent was reduced under vacuum to about 5 ml. The diffusion of diethyl ether vapor into the concentrated solution gave needle like red crystals suitable for X-ray studies. The crystals were collectedand 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 (aromatic) or 0.99 Å (methylene), U_{iso}(H) = 1.2 U_{eq}(C).

Figures

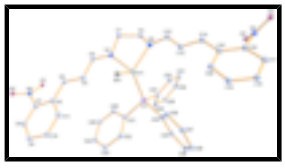


Fig. 1. The molecular structure of compound, with atom labels and 50% probability displacement ellipsoids.

(Bromido)[*N*,*N*'-bis(2-nitrocinnamaldehyde)ethylenediamine] (triphenylphosphine)copper(I)

Crystal data

$[CuBr(C_{18}H_{15}P)(C_9H_7NO_2)_2(C_2H_4N_2)]$	F_{000} = 3200
M_r = 784.10	D_x = 1.464 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71075 Å
Hall symbol: -C 2yc	Cell parameters from 17438 reflections
a = 31.288 (19) Å	θ = 3.0–27.4º
b = 15.486 (9) Å	μ = 1.83 mm^{-1}
c = 17.381 (10) Å	*T* = 200 (2) K
β = 122.34 (2)º	Block, red
V = 7116 (7) Å^3	0.26 × 0.20 × 0.18 mm
Z = 8	

Data collection

Rigaku R-AXIS RAPID IP diffractometer	8101 independent reflections
Radiation source: fine-focus sealed tube	5147 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.027
Detector resolution: 10.00 pixels mm^{-1}	θ_{max} = 27.4º
T = 200(2) K	θ_{min} = 3.0º
ω scans	*h* = −40→40
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	*k* = −20→19
T_{min} = 0.635, T_{max} = 0.720	*l* = −22→18
24792 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
$R[F^2 > 2\sigma(F^2)]$ = 0.027	H-atom parameters constrained
$wR(F^2)$ = 0.059	$w = 1/[\sigma^2(F_o^2) + (0.022P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.03	$(\Delta/\sigma)_{max}$ = 0.003

8101 reflections	$\Delta\rho_{max} = 0.45$ e Å^{-3}
443 parameters	$\Delta\rho_{min} = -0.36$ 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}
Br1	0.73895 (1)	0.21194 (2)	0.27023 (2)	0.04174 (8)
Cu1	0.66984 (1)	0.10741 (2)	0.20239 (2)	0.02458 (7)
P1	0.60586 (2)	0.14022 (3)	0.21692 (4)	0.02312 (13)
O1	0.54777 (9)	0.29990 (12)	−0.25066 (12)	0.0780 (7)
O2	0.56141 (11)	0.41867 (13)	−0.29544 (14)	0.1012 (9)
O3	0.74427 (7)	−0.20459 (10)	0.56309 (12)	0.0417 (4)
O4	0.82159 (7)	−0.22703 (11)	0.67454 (12)	0.0562 (5)
N1	0.65620 (6)	0.07940 (10)	0.07370 (11)	0.0241 (4)
N2	0.69483 (7)	−0.01979 (11)	0.22714 (12)	0.0292 (4)
N3	0.56248 (9)	0.37427 (14)	−0.23709 (14)	0.0498 (6)
N4	0.78663 (9)	−0.18000 (12)	0.62149 (14)	0.0357 (5)
C1	0.67318 (10)	−0.00878 (13)	0.07142 (15)	0.0370 (6)
H1A	0.7082	−0.0068	0.0849	0.044*
H1B	0.6511	−0.0334	0.0097	0.044*
C2	0.67151 (10)	−0.06515 (14)	0.13921 (15)	0.0428 (6)
H2A	0.6360	−0.0798	0.1174	0.051*
H2B	0.6900	−0.1196	0.1468	0.051*
C3	0.64364 (8)	0.12863 (13)	0.00597 (14)	0.0276 (5)
H3	0.6436	0.1062	−0.0449	0.033*
C4	0.62938 (8)	0.21775 (13)	0.00451 (14)	0.0276 (5)
H4	0.6291	0.2396	0.0553	0.033*
C5	0.61667 (8)	0.27048 (13)	−0.06515 (14)	0.0283 (5)
H5	0.6157	0.2468	−0.1165	0.034*
C6	0.60404 (8)	0.36203 (14)	−0.06876 (15)	0.0296 (5)
C7	0.58057 (9)	0.41257 (13)	−0.14738 (15)	0.0317 (5)
C8	0.57179 (10)	0.49984 (15)	−0.14772 (18)	0.0477 (7)
H8	0.5563	0.5317	−0.2029	0.057*
C9	0.58561 (11)	0.53990 (16)	−0.0676 (2)	0.0589 (8)
H9	0.5794	0.5999	−0.0668	0.071*
C10	0.60830 (13)	0.49345 (17)	0.0113 (2)	0.0689 (9)
H10	0.6176	0.5212	0.0669	0.083*
C11	0.61791 (11)	0.40660 (15)	0.01102 (17)	0.0487 (7)
H11	0.6345	0.3761	0.0671	0.058*
C12	0.72131 (9)	−0.06427 (14)	0.29956 (15)	0.0314 (5)
H12	0.7277	−0.1234	0.2948	0.038*
C13	0.74164 (8)	−0.02660 (14)	0.38822 (15)	0.0302 (5)
H13	0.7385	0.0340	0.3920	0.036*
C14	0.76468 (8)	−0.07209 (14)	0.46547 (14)	0.0294 (5)
H14	0.7683	−0.1325	0.4611	0.035*
C15	0.78476 (8)	−0.03598 (14)	0.55608 (15)	0.0288 (5)

C16	0.79624 (8)	−0.08569 (13)	0.63139 (15)	0.0290 (5)
C17	0.81345 (10)	−0.05208 (16)	0.71668 (16)	0.0470 (7)
H17	0.8209	−0.0888	0.7661	0.056*
C18	0.81954 (11)	0.03615 (17)	0.72838 (17)	0.0588 (8)
H18	0.8301	0.0611	0.7858	0.071*
C19	0.81029 (10)	0.08818 (16)	0.65625 (17)	0.0476 (7)
H19	0.8152	0.1488	0.6647	0.057*
C20	0.79407 (9)	0.05265 (15)	0.57269 (16)	0.0371 (6)
H20	0.7890	0.0893	0.5246	0.044*
C21	0.56473 (8)	0.22662 (13)	0.14153 (14)	0.0259 (5)
C22	0.56463 (9)	0.30877 (14)	0.17307 (16)	0.0374 (6)
H22	0.5843	0.3204	0.2366	0.045*
C23	0.53600 (10)	0.37431 (15)	0.11253 (17)	0.0527 (8)
H23	0.5367	0.4306	0.1348	0.063*
C24	0.50679 (10)	0.35815 (16)	0.02082 (17)	0.0441 (7)
H24	0.4869	0.4030	−0.0203	0.053*
C25	0.50631 (9)	0.27697 (15)	−0.01143 (16)	0.0419 (6)
H25	0.4862	0.2656	−0.0749	0.050*
C26	0.53508 (9)	0.21187 (15)	0.04829 (15)	0.0347 (6)
H26	0.5346	0.1560	0.0253	0.042*
C27	0.56290 (8)	0.04926 (13)	0.19192 (14)	0.0243 (5)
C28	0.51085 (9)	0.05384 (16)	0.14222 (16)	0.0401 (6)
H28	0.4947	0.1079	0.1187	0.048*
C29	0.48189 (10)	−0.01954 (17)	0.12612 (18)	0.0493 (7)
H29	0.4460	−0.0154	0.0914	0.059*
C30	0.50445 (10)	−0.09786 (16)	0.15978 (17)	0.0436 (7)
H30	0.4844	−0.1480	0.1484	0.052*
C31	0.55592 (11)	−0.10335 (16)	0.20979 (18)	0.0493 (7)
H31	0.5718	−0.1575	0.2336	0.059*
C32	0.58499 (9)	−0.03061 (14)	0.22597 (16)	0.0385 (6)
H32	0.6208	−0.0353	0.2611	0.046*
C33	0.62006 (8)	0.17584 (12)	0.32871 (13)	0.0232 (5)
C34	0.58210 (8)	0.18790 (14)	0.34743 (15)	0.0322 (5)
H34	0.5480	0.1745	0.3022	0.039*
C35	0.59388 (9)	0.21907 (14)	0.43110 (15)	0.0337 (6)
H35	0.5678	0.2280	0.4428	0.040*
C36	0.64343 (9)	0.23719 (13)	0.49750 (15)	0.0318 (6)
H36	0.6514	0.2592	0.5547	0.038*
C37	0.68139 (9)	0.22356 (13)	0.48133 (14)	0.0303 (5)
H37	0.7155	0.2351	0.5277	0.036*
C38	0.66975 (8)	0.19283 (13)	0.39707 (14)	0.0264 (5)
H38	0.6961	0.1834	0.3862	0.032*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0467 (2)	0.0473 (2)	0.0391 (1)	−0.0234 (1)	0.0282 (1)	−0.0204 (1)
Cu1	0.0291 (2)	0.0222 (1)	0.0232 (1)	0.0003 (1)	0.0145 (1)	−0.0010 (1)

P1	0.0246 (3)	0.0226 (3)	0.0205 (3)	−0.0019 (2)	0.0110 (3)	−0.0027 (2)
O1	0.1120 (19)	0.0389 (12)	0.0386 (12)	0.0062 (12)	0.0105 (13)	−0.0057 (9)
O2	0.185 (3)	0.0627 (15)	0.0401 (14)	0.0130 (16)	0.0493 (16)	0.0177 (11)
O3	0.0517 (12)	0.0331 (10)	0.0443 (11)	−0.0100 (9)	0.0284 (10)	−0.0077 (8)
O4	0.0698 (14)	0.0464 (11)	0.0583 (13)	0.0251 (10)	0.0382 (12)	0.0217 (10)
N1	0.0282 (11)	0.0232 (9)	0.0216 (10)	−0.0019 (8)	0.0138 (9)	−0.0008 (8)
N2	0.0399 (12)	0.0248 (10)	0.0227 (11)	0.0037 (9)	0.0167 (10)	−0.0008 (8)
N3	0.0670 (17)	0.0371 (13)	0.0280 (13)	0.0115 (12)	0.0139 (12)	0.0051 (11)
N4	0.0510 (15)	0.0319 (11)	0.0374 (13)	0.0073 (11)	0.0324 (13)	0.0071 (10)
C1	0.0563 (18)	0.0240 (12)	0.0286 (14)	0.0024 (12)	0.0212 (14)	−0.0029 (10)
C2	0.0640 (19)	0.0249 (13)	0.0306 (14)	0.0034 (13)	0.0193 (14)	−0.0036 (11)
C3	0.0304 (14)	0.0277 (13)	0.0220 (12)	−0.0025 (10)	0.0122 (11)	−0.0032 (10)
C4	0.0298 (13)	0.0295 (12)	0.0240 (12)	−0.0022 (10)	0.0147 (11)	−0.0022 (10)
C5	0.0329 (14)	0.0301 (13)	0.0233 (12)	−0.0002 (10)	0.0159 (12)	−0.0008 (10)
C6	0.0323 (14)	0.0255 (12)	0.0290 (13)	−0.0023 (10)	0.0150 (12)	−0.0014 (10)
C7	0.0327 (14)	0.0278 (13)	0.0298 (14)	0.0004 (11)	0.0135 (12)	−0.0013 (10)
C8	0.0587 (19)	0.0295 (14)	0.0453 (17)	0.0062 (13)	0.0214 (16)	0.0077 (12)
C9	0.078 (2)	0.0256 (14)	0.065 (2)	0.0047 (15)	0.0322 (19)	−0.0057 (14)
C10	0.113 (3)	0.0371 (17)	0.0447 (19)	0.0046 (17)	0.034 (2)	−0.0119 (14)
C11	0.077 (2)	0.0341 (15)	0.0359 (16)	0.0030 (14)	0.0309 (16)	−0.0019 (12)
C12	0.0428 (15)	0.0213 (12)	0.0295 (14)	0.0063 (11)	0.0190 (13)	0.0019 (10)
C13	0.0361 (15)	0.0245 (12)	0.0310 (14)	0.0040 (11)	0.0186 (13)	0.0008 (10)
C14	0.0345 (14)	0.0243 (12)	0.0290 (13)	0.0017 (10)	0.0166 (12)	0.0018 (10)
C15	0.0238 (13)	0.0300 (13)	0.0269 (13)	0.0004 (10)	0.0099 (12)	0.0017 (10)
C16	0.0323 (14)	0.0296 (13)	0.0281 (13)	−0.0008 (10)	0.0181 (12)	0.0010 (10)
C17	0.0655 (19)	0.0460 (16)	0.0254 (14)	−0.0055 (14)	0.0215 (15)	0.0030 (12)
C18	0.088 (2)	0.0463 (17)	0.0291 (16)	−0.0205 (16)	0.0231 (17)	−0.0127 (13)
C19	0.0615 (19)	0.0357 (15)	0.0388 (16)	−0.0153 (13)	0.0224 (15)	−0.0070 (12)
C20	0.0401 (16)	0.0324 (14)	0.0310 (14)	−0.0070 (12)	0.0139 (13)	0.0017 (11)
C21	0.0239 (13)	0.0281 (12)	0.0233 (12)	0.0004 (10)	0.0110 (11)	0.0012 (10)
C22	0.0506 (17)	0.0265 (13)	0.0244 (13)	0.0009 (12)	0.0129 (13)	−0.0024 (11)
C23	0.079 (2)	0.0283 (15)	0.0369 (17)	0.0120 (14)	0.0212 (16)	0.0005 (12)
C24	0.0541 (18)	0.0396 (15)	0.0339 (16)	0.0157 (13)	0.0204 (15)	0.0114 (12)
C25	0.0453 (16)	0.0479 (16)	0.0220 (13)	0.0089 (13)	0.0110 (13)	0.0013 (12)
C26	0.0417 (15)	0.0331 (13)	0.0259 (13)	0.0055 (12)	0.0159 (12)	−0.0039 (11)
C27	0.0282 (13)	0.0251 (12)	0.0251 (13)	−0.0057 (10)	0.0180 (12)	−0.0079 (10)
C28	0.0323 (16)	0.0351 (14)	0.0455 (16)	−0.0053 (12)	0.0159 (14)	−0.0054 (12)
C29	0.0287 (16)	0.0554 (18)	0.0514 (18)	−0.0173 (14)	0.0131 (14)	−0.0148 (15)
C30	0.0582 (19)	0.0388 (16)	0.0444 (16)	−0.0257 (14)	0.0346 (16)	−0.0168 (13)
C31	0.060 (2)	0.0283 (14)	0.0591 (19)	−0.0071 (14)	0.0311 (17)	0.0033 (13)
C32	0.0345 (15)	0.0352 (14)	0.0471 (16)	−0.0045 (12)	0.0226 (14)	0.0050 (12)
C33	0.0276 (13)	0.0177 (11)	0.0198 (12)	−0.0008 (9)	0.0098 (11)	0.0004 (9)
C34	0.0270 (14)	0.0361 (13)	0.0320 (14)	−0.0058 (11)	0.0147 (12)	−0.0063 (11)
C35	0.0426 (16)	0.0303 (13)	0.0345 (14)	−0.0008 (12)	0.0248 (13)	−0.0035 (11)
C36	0.0526 (17)	0.0210 (12)	0.0229 (13)	−0.0025 (11)	0.0210 (13)	−0.0015 (10)
C37	0.0320 (14)	0.0316 (13)	0.0231 (12)	−0.0043 (11)	0.0120 (12)	−0.0017 (10)
C38	0.0311 (14)	0.0250 (12)	0.0269 (13)	−0.0010 (10)	0.0181 (12)	0.0013 (10)

Geometric parameters (Å, °)

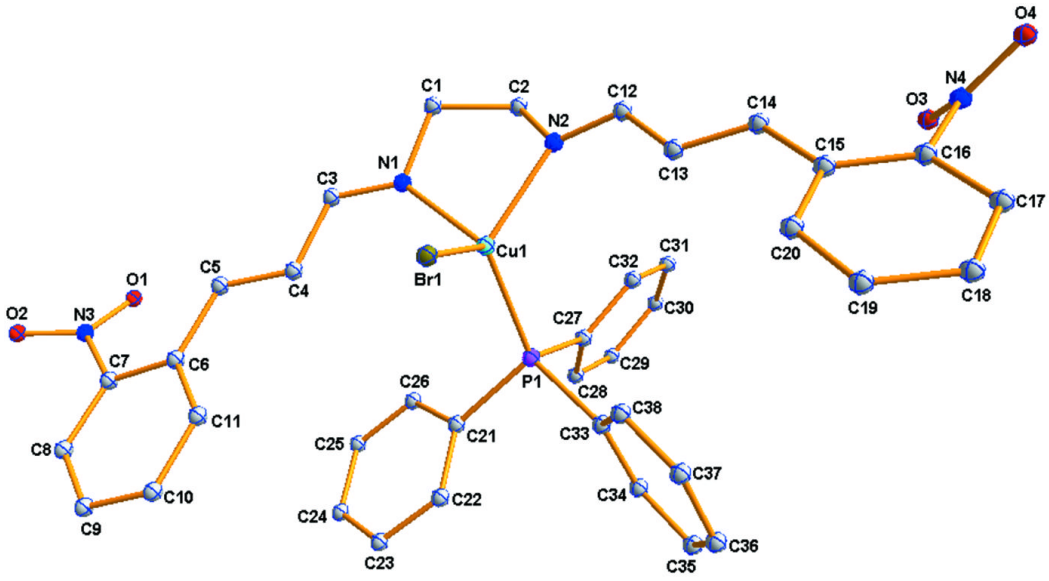
Cu1—Br1	2.4411 (11)	C15—C16	1.390 (3)
Cu1—N1	2.086 (2)	C15—C20	1.401 (3)
Cu1—N2	2.078 (2)	C16—C17	1.380 (3)
Cu1—P1	2.2069 (13)	C17—C18	1.380 (3)
P1—C33	1.831 (2)	C17—H17	0.9500
P1—C27	1.832 (2)	C18—C19	1.384 (3)
P1—C21	1.833 (2)	C18—H18	0.9500
O1—N3	1.216 (3)	C19—C20	1.371 (3)
O2—N3	1.211 (3)	C19—H19	0.9500
O3—N4	1.222 (2)	C20—H20	0.9500
O4—N4	1.224 (2)	C21—C22	1.386 (3)
N1—C3	1.275 (2)	C21—C26	1.390 (3)
N1—C1	1.473 (3)	C22—C23	1.390 (3)
N2—C12	1.277 (3)	C22—H22	0.9500
N2—C2	1.473 (3)	C23—C24	1.371 (3)
N3—C7	1.470 (3)	C23—H23	0.9500
N4—C16	1.482 (3)	C24—C25	1.373 (3)
C1—C2	1.490 (3)	C24—H24	0.9500
C1—H1A	0.9900	C25—C26	1.380 (3)
C1—H1B	0.9900	C25—H25	0.9500
C2—H2A	0.9900	C26—H26	0.9500
C2—H2B	0.9900	C27—C28	1.378 (3)
C3—C4	1.446 (3)	C27—C32	1.386 (3)
C3—H3	0.9500	C28—C29	1.385 (3)
C4—C5	1.333 (3)	C28—H28	0.9500
C4—H4	0.9500	C29—C30	1.367 (3)
C5—C6	1.464 (3)	C29—H29	0.9500
C5—H5	0.9500	C30—C31	1.363 (4)
C6—C11	1.394 (3)	C30—H30	0.9500
C6—C7	1.395 (3)	C31—C32	1.379 (3)
C7—C8	1.379 (3)	C31—H31	0.9500
C8—C9	1.367 (3)	C32—H32	0.9500
C8—H8	0.9500	C33—C38	1.386 (3)
C9—C10	1.363 (4)	C33—C34	1.402 (3)
C9—H9	0.9500	C34—C35	1.382 (3)
C10—C11	1.379 (3)	C34—H34	0.9500
C10—H10	0.9500	C35—C36	1.378 (3)
C11—H11	0.9500	C35—H35	0.9500
C12—C13	1.439 (3)	C36—C37	1.375 (3)
C12—H12	0.9500	C36—H36	0.9500
C13—C14	1.335 (3)	C37—C38	1.390 (3)
C13—H13	0.9500	C37—H37	0.9500
C14—C15	1.459 (3)	C38—H38	0.9500
C14—H14	0.9500		
N2—Cu1—N1	82.15 (7)	C16—C15—C20	115.3 (2)
N2—Cu1—P1	117.29 (5)	C16—C15—C14	123.3 (2)

N1—Cu1—P1	119.52 (6)	C20—C15—C14	121.33 (19)
N2—Cu1—Br1	113.00 (7)	C17—C16—C15	124.0 (2)
N1—Cu1—Br1	106.03 (5)	C17—C16—N4	115.76 (19)
P1—Cu1—Br1	114.54 (4)	C15—C16—N4	120.14 (19)
C33—P1—C27	102.37 (9)	C18—C17—C16	118.4 (2)
C33—P1—C21	102.58 (10)	C18—C17—H17	120.8
C27—P1—C21	104.26 (11)	C16—C17—H17	120.8
C33—P1—Cu1	118.08 (8)	C17—C18—C19	119.8 (2)
C27—P1—Cu1	113.04 (7)	C17—C18—H18	120.1
C21—P1—Cu1	114.78 (7)	C19—C18—H18	120.1
C3—N1—C1	117.83 (17)	C20—C19—C18	120.3 (2)
C3—N1—Cu1	130.59 (15)	C20—C19—H19	119.8
C1—N1—Cu1	110.58 (12)	C18—C19—H19	119.8
C12—N2—C2	117.77 (18)	C19—C20—C15	122.0 (2)
C12—N2—Cu1	133.60 (15)	C19—C20—H20	119.0
C2—N2—Cu1	108.34 (13)	C15—C20—H20	119.0
O2—N3—O1	122.5 (2)	C22—C21—C26	118.1 (2)
O2—N3—C7	118.8 (2)	C22—C21—P1	122.45 (17)
O1—N3—C7	118.6 (2)	C26—C21—P1	119.29 (17)
O3—N4—O4	125.1 (2)	C21—C22—C23	120.5 (2)
O3—N4—C16	117.8 (2)	C21—C22—H22	119.7
O4—N4—C16	117.0 (2)	C23—C22—H22	119.7
N1—C1—C2	110.86 (17)	C24—C23—C22	120.4 (2)
N1—C1—H1A	109.5	C24—C23—H23	119.8
C2—C1—H1A	109.5	C22—C23—H23	119.8
N1—C1—H1B	109.5	C23—C24—C25	119.8 (2)
C2—C1—H1B	109.5	C23—C24—H24	120.1
H1A—C1—H1B	108.1	C25—C24—H24	120.1
N2—C2—C1	109.49 (19)	C24—C25—C26	120.1 (2)
N2—C2—H2A	109.8	C24—C25—H25	120.0
C1—C2—H2A	109.8	C26—C25—H25	120.0
N2—C2—H2B	109.8	C25—C26—C21	121.1 (2)
C1—C2—H2B	109.8	C25—C26—H26	119.4
H2A—C2—H2B	108.2	C21—C26—H26	119.4
N1—C3—C4	121.76 (19)	C28—C27—C32	117.8 (2)
N1—C3—H3	119.1	C28—C27—P1	125.49 (18)
C4—C3—H3	119.1	C32—C27—P1	116.74 (17)
C5—C4—C3	122.67 (19)	C27—C28—C29	120.7 (2)
C5—C4—H4	118.7	C27—C28—H28	119.6
C3—C4—H4	118.7	C29—C28—H28	119.6
C4—C5—C6	125.1 (2)	C30—C29—C28	120.6 (2)
C4—C5—H5	117.5	C30—C29—H29	119.7
C6—C5—H5	117.5	C28—C29—H29	119.7
C11—C6—C7	114.7 (2)	C31—C30—C29	119.4 (2)
C11—C6—C5	120.2 (2)	C31—C30—H30	120.3
C7—C6—C5	125.0 (2)	C29—C30—H30	120.3
C8—C7—C6	123.6 (2)	C30—C31—C32	120.3 (2)
C8—C7—N3	115.4 (2)	C30—C31—H31	119.9
C6—C7—N3	121.02 (19)	C32—C31—H31	119.9

C9—C8—C7	119.1 (2)	C31—C32—C27	121.2 (2)
C9—C8—H8	120.4	C31—C32—H32	119.4
C7—C8—H8	120.4	C27—C32—H32	119.4
C10—C9—C8	119.7 (2)	C38—C33—C34	118.48 (19)
C10—C9—H9	120.1	C38—C33—P1	119.40 (15)
C8—C9—H9	120.1	C34—C33—P1	122.11 (17)
C9—C10—C11	120.6 (3)	C35—C34—C33	120.6 (2)
C9—C10—H10	119.7	C35—C34—H34	119.7
C11—C10—H10	119.7	C33—C34—H34	119.7
C10—C11—C6	122.2 (2)	C36—C35—C34	120.0 (2)
C10—C11—H11	118.9	C36—C35—H35	120.0
C6—C11—H11	118.9	C34—C35—H35	120.0
N2—C12—C13	121.3 (2)	C37—C36—C35	120.3 (2)
N2—C12—H12	119.4	C37—C36—H36	119.8
C13—C12—H12	119.4	C35—C36—H36	119.8
C14—C13—C12	123.7 (2)	C36—C37—C38	120.0 (2)
C14—C13—H13	118.2	C36—C37—H37	120.0
C12—C13—H13	118.2	C38—C37—H37	120.0
C13—C14—C15	124.9 (2)	C33—C38—C37	120.62 (19)
C13—C14—H14	117.5	C33—C38—H38	119.7
C15—C14—H14	117.5	C37—C38—H38	119.7
N2—Cu1—P1—C33	89.94 (10)	C20—C15—C16—N4	178.3 (2)
N1—Cu1—P1—C33	−173.43 (9)	C14—C15—C16—N4	−2.1 (3)
Br1—Cu1—P1—C33	−46.02 (8)	O3—N4—C16—C17	123.0 (2)
N2—Cu1—P1—C27	−29.44 (10)	O4—N4—C16—C17	−55.0 (3)
N1—Cu1—P1—C27	67.19 (9)	O3—N4—C16—C15	−52.8 (3)
Br1—Cu1—P1—C27	−165.40 (7)	O4—N4—C16—C15	129.3 (2)
N2—Cu1—P1—C21	−148.85 (9)	C15—C16—C17—C18	0.2 (4)
N1—Cu1—P1—C21	−52.22 (10)	N4—C16—C17—C18	−175.3 (2)
Br1—Cu1—P1—C21	75.19 (9)	C16—C17—C18—C19	−2.5 (4)
N2—Cu1—N1—C3	−170.9 (2)	C17—C18—C19—C20	1.4 (4)
P1—Cu1—N1—C3	72.10 (19)	C18—C19—C20—C15	2.0 (4)
Br1—Cu1—N1—C3	−59.15 (19)	C16—C15—C20—C19	−4.0 (3)
N2—Cu1—N1—C1	−2.85 (14)	C14—C15—C20—C19	176.3 (2)
P1—Cu1—N1—C1	−119.84 (14)	C33—P1—C21—C22	22.2 (2)
Br1—Cu1—N1—C1	108.90 (14)	C27—P1—C21—C22	128.66 (18)
N1—Cu1—N2—C12	164.7 (2)	Cu1—P1—C21—C22	−107.14 (18)
P1—Cu1—N2—C12	−76.1 (2)	C33—P1—C21—C26	−162.58 (17)
Br1—Cu1—N2—C12	60.5 (2)	C27—P1—C21—C26	−56.14 (19)
N1—Cu1—N2—C2	−21.89 (14)	Cu1—P1—C21—C26	68.06 (19)
P1—Cu1—N2—C2	97.35 (14)	C26—C21—C22—C23	−0.7 (3)
Br1—Cu1—N2—C2	−126.03 (13)	P1—C21—C22—C23	174.56 (19)
C3—N1—C1—C2	−163.0 (2)	C21—C22—C23—C24	1.1 (4)
Cu1—N1—C1—C2	27.2 (2)	C22—C23—C24—C25	−0.8 (4)
C12—N2—C2—C1	−142.5 (2)	C23—C24—C25—C26	0.1 (4)
Cu1—N2—C2—C1	42.9 (2)	C24—C25—C26—C21	0.3 (4)
N1—C1—C2—N2	−46.8 (3)	C22—C21—C26—C25	0.0 (3)
C1—N1—C3—C4	−176.3 (2)	P1—C21—C26—C25	−175.39 (18)
Cu1—N1—C3—C4	−8.9 (3)	C33—P1—C27—C28	94.3 (2)

N1—C3—C4—C5	179.2 (2)	C21—P1—C27—C28	−12.3 (2)
C3—C4—C5—C6	−177.2 (2)	Cu1—P1—C27—C28	−137.58 (18)
C4—C5—C6—C11	18.0 (3)	C33—P1—C27—C32	−85.85 (17)
C4—C5—C6—C7	−165.5 (2)	C21—P1—C27—C32	167.55 (16)
C11—C6—C7—C8	0.5 (4)	Cu1—P1—C27—C32	42.24 (18)
C5—C6—C7—C8	−176.1 (2)	C32—C27—C28—C29	−0.9 (3)
C11—C6—C7—N3	−178.3 (2)	P1—C27—C28—C29	178.95 (17)
C5—C6—C7—N3	5.1 (3)	C27—C28—C29—C30	0.4 (4)
O2—N3—C7—C8	30.4 (4)	C28—C29—C30—C31	0.2 (4)
O1—N3—C7—C8	−147.5 (3)	C29—C30—C31—C32	−0.3 (4)
O2—N3—C7—C6	−150.7 (3)	C30—C31—C32—C27	−0.2 (4)
O1—N3—C7—C6	31.4 (3)	C28—C27—C32—C31	0.8 (3)
C6—C7—C8—C9	−1.4 (4)	P1—C27—C32—C31	−179.06 (18)
N3—C7—C8—C9	177.4 (2)	C27—P1—C33—C38	133.75 (17)
C7—C8—C9—C10	0.8 (4)	C21—P1—C33—C38	−118.36 (17)
C8—C9—C10—C11	0.7 (5)	Cu1—P1—C33—C38	8.93 (19)
C9—C10—C11—C6	−1.6 (5)	C27—P1—C33—C34	−47.24 (19)
C7—C6—C11—C10	1.0 (4)	C21—P1—C33—C34	60.65 (19)
C5—C6—C11—C10	177.8 (3)	Cu1—P1—C33—C34	−172.06 (14)
C2—N2—C12—C13	−174.4 (2)	C38—C33—C34—C35	2.4 (3)
Cu1—N2—C12—C13	−1.4 (3)	P1—C33—C34—C35	−176.67 (16)
N2—C12—C13—C14	172.3 (2)	C33—C34—C35—C36	−1.1 (3)
C12—C13—C14—C15	−178.7 (2)	C34—C35—C36—C37	−0.7 (3)
C13—C14—C15—C16	162.4 (2)	C35—C36—C37—C38	1.2 (3)
C13—C14—C15—C20	−18.0 (3)	C34—C33—C38—C37	−1.9 (3)
C20—C15—C16—C17	2.9 (3)	P1—C33—C38—C37	177.19 (15)
C14—C15—C16—C17	−177.5 (2)	C36—C37—C38—C33	0.1 (3)

Fig. 1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