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

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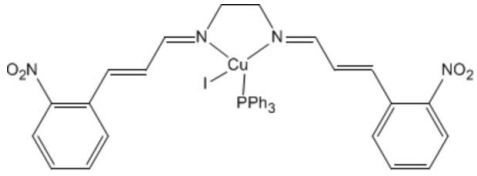
Key indicators: single-crystal X-ray study; T = 200 K; mean σ(C–C) = 0.003 Å; R factor = 0.022; wR factor = 0.051; data-to-parameter ratio = 18.8.

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

Related literature

For related literature, see: Amirnasr *et al.* (2003, 2005, 2006); Balogh-Heregovich *et al.* (1999); Barron *et al.* (1988); Kickelbick *et al.* (2002, 2003); Meghdadi *et al.* (2002).



Experimental

Crystal data

$[CuI(C_{20}H_{18}N_4O_4)(C_{18}H_{15}P)]$
M_r = 831.09
Monoclinic, $C2/c$
a = 31.64 (2) Å
b = 15.586 (10) Å
c = 17.638 (11) Å
β = 122.54 (2)°
V = 7333 (8) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.53 mm^{-1}
T = 200 (2) K
0.35 × 0.35 × 0.12 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: numerical (*ABSCOR*; Higashi, 1999)
T_{min} = 0.617, T_{max} = 0.838
31361 measured reflections
8296 independent reflections
6482 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.051
S = 0.94
8296 reflections
442 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.51 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: BT2493).

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supplementary materials

Acta Cryst. (2007). E**63**, m2472 [**doi:10.1107/S1600536807042493**]

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

M. H. Habibi, A. Lalegani, R. Mokhtari and T. Suzuki

Comment

Cinnamaldehyde and its derivatives condense with ethylenediamine to furnish a range of Schiff base compounds; a small number of such bis(cinnamaldehyde)ethylenediimine ligands have been used to furnish adducts with transition metals (Amirnasr *et al.*, 2005; Amirnasr *et al.*, 2006). 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. Among such complexes whose structures have been described are, for example, the copper(I) iodide (Kickelbick *et al.*, 2002), (triphenylphosphine)(halogen/pseudohalogeno)copper(I) (Kickelbick *et al.*, 2003), copper(I) perchlorate (Meghdadi *et al.*, 2002), and the cobalt(II) chloride, cobalt(II) bromide and nickel bromide (Amirnasr *et al.*, 2003) adducts. Here, we report the result of the reaction of Cu^I with *N*,*N*'-bis(2-nitrocinnamaldehyde)ethylenediamine and triphenylphosphane, which forms a copper Schiff base complex (Fig. 1). However, the Cu(1)—I(1) bond length of 2.6145 (12) Å is slightly longer than reported (Barron, *et al.*,1988). The Cu(1)—P(1) distance [2.2119 (13) Å] is slightly longer than in other tetrahedral copper(I) phosphine complexes (Balogh-Heregovich, *et al.*, 1999). 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 82.40 (5)°. The I(1)—Cu(1)—P(1) angle is 115.08 (4)°, being somewhat larger than the values for a tetrahedron (Table 1). The longer Cu(1)—I(1) and Cu(1)—P(1) distances and the larger deviations of angles from the ideal tetrahedral angle in this complex may be attributed to the mutual steric effects between the bulky I atom and the PPh_3 ligand. The single bond distance of C(3)—C(4), 1.448 (2) Å being slightly shorter than C(1)—C(2), 1.509 (2) Å indicates the existence of an extended electron delocalization in this complex.

Experimental

To a solution of 190 mg (1 mmol) CuI 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 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 distances in the range 0.95–0.99 Å, with $U_{iso}(H) = 1.2\ U_{eq}(C)$.

Figures

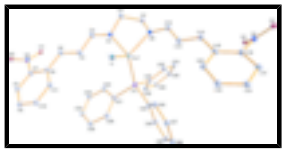


Fig. 1. The molecular structure of compound, with atom labels and 50% probability displacement ellipsoids.

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

Crystal data

$[CuI(C_{20}H_{18}N_4O_4)(C_{18}H_{15}P)]$	F_{000} = 3344
M_r = 831.09	D_x = 1.506 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71075 Å
Hall symbol: -C 2yc	Cell parameters from 25590 reflections
a = 31.64 (2) Å	θ = 3.0–27.4º
b = 15.586 (10) Å	μ = 1.53 mm^{-1}
c = 17.638 (11) Å	*T* = 200 (2) K
β = 122.54 (2)º	Plate, red
V = 7333 (8) Å^3	0.35 × 0.35 × 0.12 mm
Z = 8	

Data collection

Rigaku R-AXIS RAPID diffractometer	8296 independent reflections
Radiation source: fine-focus sealed tube	6482 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.021
Detector resolution: 10.00 pixels mm^{-1}	θ_{max} = 27.4º
T = 200(2) K	θ_{min} = 3.0º
ω scans	*h* = −39→40
Absorption correction: numerical (ABSCOR; Higashi, 1999)	*k* = −20→20
T_{min} = 0.617, T_{max} = 0.838	*l* = −22→22
31361 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
$R[F^2 > 2\sigma(F^2)]$ = 0.022	H-atom parameters constrained
$wR(F^2)$ = 0.051	$w = 1/[\sigma^2(F_o^2) + (0.028P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.94	$(\Delta/\sigma)_{max}$ = 0.003

8296 reflections	$\Delta\rho_{max}$ = 0.51 e Å^{-3}
442 parameters	$\Delta\rho_{min}$ = −0.50 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}
I1	0.741268 (5)	0.210954 (8)	0.272139 (8)	0.04254 (5)
Cu1	0.665571 (7)	0.104414 (12)	0.197272 (12)	0.02385 (5)
P1	0.602273 (16)	0.13979 (3)	0.21093 (3)	0.02384 (9)
O1	0.54983 (8)	0.29902 (10)	−0.24211 (10)	0.0804 (6)
O2	0.55500 (10)	0.42014 (12)	−0.29098 (11)	0.1098 (9)
O3	0.74378 (5)	−0.20177 (8)	0.56025 (9)	0.0411 (3)
O4	0.82068 (6)	−0.22481 (9)	0.66928 (10)	0.0545 (4)
N1	0.65513 (5)	0.07761 (8)	0.07246 (8)	0.0251 (3)
N2	0.68869 (5)	−0.02248 (8)	0.22191 (9)	0.0290 (3)
N3	0.56134 (7)	0.37400 (12)	−0.23069 (11)	0.0527 (5)
N4	0.78614 (6)	−0.17751 (10)	0.61675 (10)	0.0353 (4)
C1	0.67300 (7)	−0.00953 (11)	0.07208 (11)	0.0333 (4)
H1A	0.7087	−0.0074	0.0916	0.040*
H1B	0.6536	−0.0333	0.0104	0.040*
C2	0.66692 (7)	−0.06655 (11)	0.13471 (11)	0.0351 (4)
H2A	0.6309	−0.0784	0.1090	0.042*
H2B	0.6843	−0.1219	0.1429	0.042*
C3	0.64407 (6)	0.12722 (11)	0.00678 (10)	0.0285 (4)
H3	0.6455	0.1056	−0.0421	0.034*
C4	0.62934 (6)	0.21555 (10)	0.00470 (11)	0.0295 (4)
H4	0.6265	0.2360	0.0526	0.035*
C5	0.61952 (6)	0.26939 (11)	−0.06169 (11)	0.0299 (4)
H5	0.6202	0.2472	−0.1112	0.036*
C6	0.60769 (7)	0.36057 (11)	−0.06315 (11)	0.0328 (4)
C7	0.58224 (7)	0.41167 (11)	−0.14084 (12)	0.0389 (4)
C8	0.57386 (9)	0.49842 (13)	−0.13877 (16)	0.0573 (6)
H8	0.5567	0.5306	−0.1930	0.069*
C9	0.59048 (11)	0.53764 (14)	−0.05806 (17)	0.0706 (7)
H9	0.5841	0.5969	−0.0559	0.085*
C10	0.61655 (12)	0.49031 (14)	0.02022 (17)	0.0735 (8)
H10	0.6287	0.5176	0.0765	0.088*
C11	0.62508 (9)	0.40430 (13)	0.01776 (14)	0.0524 (6)
H11	0.6434	0.3735	0.0727	0.063*
C12	0.71458 (7)	−0.06699 (11)	0.29366 (11)	0.0327 (4)
H12	0.7203	−0.1261	0.2892	0.039*
C13	0.73532 (7)	−0.02857 (11)	0.38146 (11)	0.0333 (4)
H13	0.7314	0.0314	0.3849	0.040*
C14	0.75971 (6)	−0.07328 (11)	0.45771 (10)	0.0305 (4)
H14	0.7628	−0.1335	0.4536	0.037*
C15	0.78219 (6)	−0.03567 (11)	0.54816 (11)	0.0303 (4)

C16	0.79631 (7)	−0.08451 (11)	0.62468 (11)	0.0316 (4)
C17	0.81817 (8)	−0.04998 (13)	0.70979 (12)	0.0492 (5)
H17	0.8283	−0.0858	0.7603	0.059*
C18	0.82500 (10)	0.03758 (14)	0.71991 (13)	0.0626 (7)
H18	0.8387	0.0629	0.7775	0.075*
C19	0.81202 (9)	0.08860 (13)	0.64653 (13)	0.0533 (6)
H19	0.8168	0.1489	0.6537	0.064*
C20	0.79210 (7)	0.05210 (12)	0.56304 (12)	0.0404 (5)
H20	0.7848	0.0878	0.5138	0.049*
C21	0.56236 (6)	0.22665 (11)	0.13685 (10)	0.0278 (4)
C22	0.53365 (7)	0.21306 (12)	0.04435 (11)	0.0406 (5)
H22	0.5331	0.1577	0.0212	0.049*
C23	0.50589 (8)	0.27885 (13)	−0.01449 (12)	0.0479 (5)
H23	0.4863	0.2682	−0.0774	0.057*
C24	0.50664 (8)	0.35903 (14)	0.01767 (13)	0.0509 (6)
H24	0.4875	0.4040	−0.0228	0.061*
C25	0.53513 (9)	0.37449 (13)	0.10860 (14)	0.0548 (6)
H25	0.5360	0.4304	0.1309	0.066*
C26	0.56272 (8)	0.30846 (12)	0.16804 (12)	0.0415 (5)
H26	0.5821	0.3196	0.2309	0.050*
C27	0.55921 (6)	0.05006 (11)	0.18611 (10)	0.0276 (4)
C28	0.50778 (7)	0.05445 (13)	0.13479 (14)	0.0481 (5)
H28	0.4918	0.1077	0.1091	0.058*
C29	0.47879 (8)	−0.01857 (16)	0.11998 (15)	0.0613 (7)
H29	0.4433	−0.0146	0.0840	0.074*
C30	0.50081 (9)	−0.09547 (14)	0.15654 (14)	0.0508 (6)
H30	0.4809	−0.1450	0.1462	0.061*
C31	0.55200 (9)	−0.10058 (13)	0.20832 (16)	0.0554 (6)
H31	0.5677	−0.1539	0.2344	0.067*
C32	0.58105 (8)	−0.02865 (12)	0.22291 (14)	0.0452 (5)
H32	0.6165	−0.0333	0.2587	0.054*
C33	0.61629 (6)	0.17460 (10)	0.32143 (10)	0.0246 (3)
C34	0.57868 (7)	0.18986 (12)	0.33787 (12)	0.0366 (4)
H34	0.5448	0.1789	0.2919	0.044*
C35	0.58985 (7)	0.22083 (12)	0.42039 (12)	0.0380 (4)
H35	0.5637	0.2320	0.4303	0.046*
C36	0.63915 (7)	0.23546 (11)	0.48822 (11)	0.0332 (4)
H36	0.6469	0.2569	0.5447	0.040*
C37	0.67701 (7)	0.21905 (11)	0.47403 (11)	0.0335 (4)
H37	0.7109	0.2285	0.5210	0.040*
C38	0.66594 (6)	0.18855 (11)	0.39087 (11)	0.0287 (4)
H38	0.6923	0.1772	0.3815	0.034*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.04742 (8)	0.05158 (9)	0.03810 (7)	−0.02797 (6)	0.02926 (6)	−0.02206 (6)
Cu1	0.0270 (1)	0.0217 (1)	0.0231 (1)	−0.00045 (8)	0.01369 (8)	−0.00149 (8)

P1	0.0238 (2)	0.0245 (2)	0.02155 (19)	−0.00206 (17)	0.01104 (17)	−0.00331 (17)
O1	0.1126 (15)	0.0405 (10)	0.0416 (9)	0.0017 (9)	0.0107 (9)	−0.0032 (7)
O2	0.185 (2)	0.0629 (12)	0.0351 (9)	−0.0072 (13)	0.0281 (12)	0.0173 (9)
O3	0.0509 (9)	0.0362 (8)	0.0422 (7)	−0.0087 (6)	0.0291 (7)	−0.0072 (6)
O4	0.0648 (10)	0.0503 (9)	0.0553 (9)	0.0256 (8)	0.0369 (8)	0.0212 (7)
N1	0.0266 (7)	0.0241 (7)	0.0231 (7)	−0.0026 (6)	0.0124 (6)	−0.0016 (6)
N2	0.0380 (8)	0.0218 (7)	0.0240 (7)	0.0012 (6)	0.0146 (6)	−0.0004 (6)
N3	0.0571 (11)	0.0413 (10)	0.0346 (9)	0.0051 (9)	0.0081 (8)	0.0060 (9)
N4	0.0489 (10)	0.0345 (8)	0.0353 (8)	0.0080 (8)	0.0310 (8)	0.0060 (7)
C1	0.0441 (11)	0.0275 (9)	0.0293 (9)	0.0042 (8)	0.0204 (8)	−0.0030 (8)
C2	0.0479 (11)	0.0240 (9)	0.0281 (9)	0.0011 (8)	0.0170 (8)	−0.0027 (8)
C3	0.0313 (9)	0.0318 (9)	0.0230 (8)	−0.0037 (7)	0.0150 (7)	−0.0037 (7)
C4	0.0335 (9)	0.0302 (9)	0.0252 (8)	−0.0023 (8)	0.0161 (7)	−0.0019 (7)
C5	0.0310 (9)	0.0323 (10)	0.0264 (8)	−0.0017 (8)	0.0154 (7)	−0.0007 (8)
C6	0.0388 (10)	0.0288 (9)	0.0341 (9)	−0.0037 (8)	0.0218 (8)	0.0008 (8)
C7	0.0406 (11)	0.0304 (10)	0.0380 (10)	−0.0011 (8)	0.0160 (9)	0.0009 (9)
C8	0.0653 (15)	0.0331 (12)	0.0591 (14)	0.0033 (10)	0.0239 (12)	0.0098 (11)
C9	0.105 (2)	0.0278 (12)	0.0800 (18)	0.0040 (13)	0.0506 (17)	−0.0032 (12)
C10	0.128 (2)	0.0386 (13)	0.0591 (15)	−0.0027 (15)	0.0533 (16)	−0.0112 (12)
C11	0.0841 (17)	0.0353 (11)	0.0418 (11)	−0.0010 (11)	0.0365 (12)	0.0014 (9)
C12	0.0420 (10)	0.0241 (9)	0.0301 (9)	0.0058 (8)	0.0181 (8)	0.0013 (8)
C13	0.0414 (10)	0.0254 (9)	0.0301 (9)	0.0058 (8)	0.0171 (8)	0.0002 (8)
C14	0.0370 (10)	0.0258 (9)	0.0279 (9)	0.0044 (8)	0.0169 (8)	0.0019 (7)
C15	0.0293 (9)	0.0319 (10)	0.0271 (8)	0.0005 (7)	0.0134 (7)	0.0013 (7)
C16	0.0338 (10)	0.0314 (10)	0.0294 (9)	−0.0027 (8)	0.0170 (8)	0.0002 (8)
C17	0.0647 (14)	0.0488 (13)	0.0277 (9)	−0.0079 (11)	0.0207 (10)	0.0031 (9)
C18	0.0921 (18)	0.0526 (14)	0.0318 (11)	−0.0282 (13)	0.0260 (12)	−0.0148 (10)
C19	0.0733 (16)	0.0362 (12)	0.0413 (11)	−0.0206 (11)	0.0248 (11)	−0.0078 (10)
C20	0.0494 (12)	0.0338 (10)	0.0336 (10)	−0.0071 (9)	0.0193 (9)	0.0012 (8)
C21	0.0245 (9)	0.0306 (9)	0.0261 (8)	0.0001 (7)	0.0122 (7)	−0.0012 (7)
C22	0.0468 (12)	0.0417 (11)	0.0276 (9)	0.0086 (9)	0.0163 (8)	−0.0040 (8)
C23	0.0513 (13)	0.0538 (13)	0.0253 (9)	0.0135 (10)	0.0118 (9)	0.0040 (9)
C24	0.0585 (14)	0.0451 (13)	0.0387 (11)	0.0187 (11)	0.0193 (10)	0.0137 (10)
C25	0.0743 (16)	0.0311 (11)	0.0460 (12)	0.0093 (11)	0.0237 (12)	0.0000 (10)
C26	0.0506 (12)	0.0318 (10)	0.0297 (9)	0.0006 (9)	0.0133 (9)	−0.0026 (8)
C27	0.0304 (9)	0.0287 (9)	0.0260 (8)	−0.0065 (7)	0.0167 (7)	−0.0082 (7)
C28	0.0324 (11)	0.0413 (12)	0.0564 (13)	−0.0063 (9)	0.0146 (10)	−0.0064 (10)
C29	0.0358 (12)	0.0669 (16)	0.0631 (15)	−0.0264 (11)	0.0147 (11)	−0.0160 (13)
C30	0.0626 (15)	0.0465 (13)	0.0512 (12)	−0.0306 (11)	0.0359 (12)	−0.0217 (11)
C31	0.0691 (16)	0.0365 (12)	0.0708 (15)	−0.0124 (11)	0.0443 (13)	0.0026 (11)
C32	0.0375 (11)	0.0393 (11)	0.0579 (12)	−0.0066 (9)	0.0251 (10)	0.0061 (10)
C33	0.0295 (9)	0.0208 (8)	0.0234 (8)	−0.0032 (7)	0.0143 (7)	−0.0025 (7)
C34	0.0318 (10)	0.0437 (11)	0.0352 (9)	−0.0068 (8)	0.0185 (8)	−0.0109 (8)
C35	0.0446 (11)	0.0396 (11)	0.0409 (10)	−0.0035 (9)	0.0302 (9)	−0.0078 (9)
C36	0.0531 (12)	0.0235 (9)	0.0255 (8)	−0.0022 (8)	0.0227 (8)	−0.0013 (7)
C37	0.0372 (10)	0.0331 (10)	0.0224 (8)	−0.0042 (8)	0.0110 (7)	−0.0013 (8)
C38	0.0289 (9)	0.0300 (9)	0.0273 (8)	−0.0010 (7)	0.0151 (7)	0.0007 (7)

Geometric parameters (Å, °)

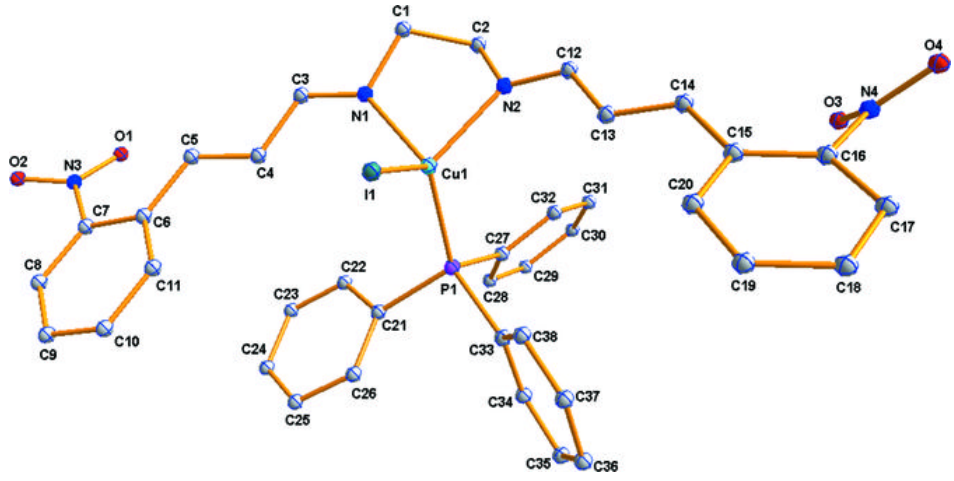
I1—Cu1	2.6145 (12)	C15—C20	1.396 (3)
Cu1—N2	2.0721 (18)	C15—C16	1.397 (2)
Cu1—N1	2.0851 (19)	C16—C17	1.380 (3)
Cu1—P1	2.2119 (13)	C17—C18	1.378 (3)
P1—C33	1.8329 (19)	C17—H17	0.9500
P1—C21	1.8329 (18)	C18—C19	1.380 (3)
P1—C27	1.8337 (19)	C18—H18	0.9500
O1—N3	1.208 (2)	C19—C20	1.375 (3)
O2—N3	1.208 (2)	C19—H19	0.9500
O3—N4	1.223 (2)	C20—H20	0.9500
O4—N4	1.228 (2)	C21—C26	1.386 (2)
N1—C3	1.275 (2)	C21—C22	1.392 (2)
N1—C1	1.472 (2)	C22—C23	1.386 (3)
N2—C12	1.280 (2)	C22—H22	0.9500
N2—C2	1.474 (2)	C23—C24	1.367 (3)
N3—C7	1.472 (3)	C23—H23	0.9500
N4—C16	1.475 (2)	C24—C25	1.374 (3)
C1—C2	1.509 (2)	C24—H24	0.9500
C1—H1A	0.9900	C25—C26	1.391 (3)
C1—H1B	0.9900	C25—H25	0.9500
C2—H2A	0.9900	C26—H26	0.9500
C2—H2B	0.9900	C27—C28	1.374 (3)
C3—C4	1.448 (2)	C27—C32	1.386 (3)
C3—H3	0.9500	C28—C29	1.395 (3)
C4—C5	1.334 (2)	C28—H28	0.9500
C4—H4	0.9500	C29—C30	1.362 (3)
C5—C6	1.466 (3)	C29—H29	0.9500
C5—H5	0.9500	C30—C31	1.368 (3)
C6—C11	1.400 (3)	C30—H30	0.9500
C6—C7	1.405 (3)	C31—C32	1.383 (3)
C7—C8	1.382 (3)	C31—H31	0.9500
C8—C9	1.368 (3)	C32—H32	0.9500
C8—H8	0.9500	C33—C34	1.389 (3)
C9—C10	1.381 (3)	C33—C38	1.395 (2)
C9—H9	0.9500	C34—C35	1.387 (3)
C10—C11	1.373 (3)	C34—H34	0.9500
C10—H10	0.9500	C35—C36	1.382 (3)
C11—H11	0.9500	C35—H35	0.9500
C12—C13	1.447 (2)	C36—C37	1.373 (3)
C12—H12	0.9500	C36—H36	0.9500
C13—C14	1.332 (2)	C37—C38	1.395 (2)
C13—H13	0.9500	C37—H37	0.9500
C14—C15	1.474 (2)	C38—H38	0.9500
C14—H14	0.9500		
N2—Cu1—N1	82.40 (5)	C20—C15—C16	115.43 (16)
N2—Cu1—P1	116.96 (4)	C20—C15—C14	121.45 (15)

N1—Cu1—P1	121.76 (5)	C16—C15—C14	123.10 (16)
N2—Cu1—I1	112.09 (6)	C17—C16—C15	123.44 (18)
N1—Cu1—I1	104.03 (4)	C17—C16—N4	116.27 (16)
P1—Cu1—I1	115.08 (4)	C15—C16—N4	120.25 (15)
C33—P1—C21	102.67 (8)	C18—C17—C16	118.62 (18)
C33—P1—C27	101.74 (7)	C18—C17—H17	120.7
C21—P1—C27	104.74 (9)	C16—C17—H17	120.7
C33—P1—Cu1	118.30 (6)	C17—C18—C19	120.15 (18)
C21—P1—Cu1	115.06 (7)	C17—C18—H18	119.9
C27—P1—Cu1	112.58 (7)	C19—C18—H18	119.9
C3—N1—C1	118.26 (14)	C20—C19—C18	120.0 (2)
C3—N1—Cu1	130.38 (12)	C20—C19—H19	120.0
C1—N1—Cu1	110.27 (10)	C18—C19—H19	120.0
C12—N2—C2	118.06 (15)	C19—C20—C15	122.27 (17)
C12—N2—Cu1	133.68 (12)	C19—C20—H20	118.9
C2—N2—Cu1	108.17 (10)	C15—C20—H20	118.9
O2—N3—O1	122.45 (19)	C26—C21—C22	117.78 (15)
O2—N3—C7	118.44 (19)	C26—C21—P1	122.75 (13)
O1—N3—C7	119.07 (17)	C22—C21—P1	119.22 (13)
O3—N4—O4	124.75 (17)	C23—C22—C21	121.09 (17)
O3—N4—C16	117.94 (15)	C23—C22—H22	119.5
O4—N4—C16	117.27 (16)	C21—C22—H22	119.5
N1—C1—C2	109.84 (14)	C24—C23—C22	120.21 (18)
N1—C1—H1A	109.7	C24—C23—H23	119.9
C2—C1—H1A	109.7	C22—C23—H23	119.9
N1—C1—H1B	109.7	C23—C24—C25	119.91 (18)
C2—C1—H1B	109.7	C23—C24—H24	120.0
H1A—C1—H1B	108.2	C25—C24—H24	120.0
N2—C2—C1	108.51 (15)	C24—C25—C26	120.12 (19)
N2—C2—H2A	110.0	C24—C25—H25	119.9
C1—C2—H2A	110.0	C26—C25—H25	119.9
N2—C2—H2B	110.0	C21—C26—C25	120.89 (17)
C1—C2—H2B	110.0	C21—C26—H26	119.6
H2A—C2—H2B	108.4	C25—C26—H26	119.6
N1—C3—C4	121.80 (15)	C28—C27—C32	117.91 (17)
N1—C3—H3	119.1	C28—C27—P1	125.74 (15)
C4—C3—H3	119.1	C32—C27—P1	116.35 (14)
C5—C4—C3	122.70 (16)	C27—C28—C29	120.6 (2)
C5—C4—H4	118.7	C27—C28—H28	119.7
C3—C4—H4	118.7	C29—C28—H28	119.7
C4—C5—C6	124.17 (16)	C30—C29—C28	120.8 (2)
C4—C5—H5	117.9	C30—C29—H29	119.6
C6—C5—H5	117.9	C28—C29—H29	119.6
C11—C6—C7	115.05 (18)	C29—C30—C31	119.20 (19)
C11—C6—C5	119.83 (16)	C29—C30—H30	120.4
C7—C6—C5	124.99 (16)	C31—C30—H30	120.4
C8—C7—C6	123.11 (18)	C30—C31—C32	120.4 (2)
C8—C7—N3	115.92 (17)	C30—C31—H31	119.8
C6—C7—N3	120.94 (17)	C32—C31—H31	119.8

C9—C8—C7	119.5 (2)	C31—C32—C27	121.1 (2)
C9—C8—H8	120.2	C31—C32—H32	119.5
C7—C8—H8	120.2	C27—C32—H32	119.5
C8—C9—C10	119.4 (2)	C34—C33—C38	118.49 (15)
C8—C9—H9	120.3	C34—C33—P1	121.89 (13)
C10—C9—H9	120.3	C38—C33—P1	119.60 (13)
C11—C10—C9	120.8 (2)	C35—C34—C33	121.02 (17)
C11—C10—H10	119.6	C35—C34—H34	119.5
C9—C10—H10	119.6	C33—C34—H34	119.5
C10—C11—C6	122.1 (2)	C36—C35—C34	119.88 (18)
C10—C11—H11	118.9	C36—C35—H35	120.1
C6—C11—H11	118.9	C34—C35—H35	120.1
N2—C12—C13	120.96 (16)	C37—C36—C35	120.04 (16)
N2—C12—H12	119.5	C37—C36—H36	120.0
C13—C12—H12	119.5	C35—C36—H36	120.0
C14—C13—C12	123.18 (17)	C36—C37—C38	120.31 (16)
C14—C13—H13	118.4	C36—C37—H37	119.8
C12—C13—H13	118.4	C38—C37—H37	119.8
C13—C14—C15	124.41 (17)	C33—C38—C37	120.23 (17)
C13—C14—H14	117.8	C33—C38—H38	119.9
C15—C14—H14	117.8	C37—C38—H38	119.9
N2—Cu1—P1—C33	89.15 (8)	C20—C15—C16—N4	177.93 (17)
N1—Cu1—P1—C33	−172.78 (7)	C14—C15—C16—N4	−3.8 (3)
I1—Cu1—P1—C33	−45.59 (6)	O3—N4—C16—C17	128.03 (19)
N2—Cu1—P1—C21	−149.07 (7)	O4—N4—C16—C17	−50.1 (2)
N1—Cu1—P1—C21	−51.00 (8)	O3—N4—C16—C15	−49.5 (2)
I1—Cu1—P1—C21	76.20 (8)	O4—N4—C16—C15	132.40 (18)
N2—Cu1—P1—C27	−29.16 (7)	C15—C16—C17—C18	2.3 (3)
N1—Cu1—P1—C27	68.91 (7)	N4—C16—C17—C18	−175.2 (2)
I1—Cu1—P1—C27	−163.90 (6)	C16—C17—C18—C19	−2.7 (4)
N2—Cu1—N1—C3	−172.34 (16)	C17—C18—C19—C20	0.2 (4)
P1—Cu1—N1—C3	70.57 (15)	C18—C19—C20—C15	2.9 (4)
I1—Cu1—N1—C3	−61.38 (15)	C16—C15—C20—C19	−3.2 (3)
N2—Cu1—N1—C1	−4.73 (11)	C14—C15—C20—C19	178.53 (19)
P1—Cu1—N1—C1	−121.81 (10)	C33—P1—C21—C26	22.44 (18)
I1—Cu1—N1—C1	106.23 (11)	C27—P1—C21—C26	128.39 (16)
N1—Cu1—N2—C12	161.61 (18)	Cu1—P1—C21—C26	−107.47 (16)
P1—Cu1—N2—C12	−76.52 (19)	C33—P1—C21—C22	−163.50 (15)
I1—Cu1—N2—C12	59.50 (18)	C27—P1—C21—C22	−57.56 (16)
N1—Cu1—N2—C2	−21.93 (11)	Cu1—P1—C21—C22	66.59 (16)
P1—Cu1—N2—C2	99.94 (12)	C26—C21—C22—C23	−0.8 (3)
I1—Cu1—N2—C2	−124.04 (11)	P1—C21—C22—C23	−175.12 (16)
C3—N1—C1—C2	−160.48 (15)	C21—C22—C23—C24	0.6 (3)
Cu1—N1—C1—C2	30.21 (17)	C22—C23—C24—C25	0.2 (4)
C12—N2—C2—C1	−138.64 (17)	C23—C24—C25—C26	−0.8 (4)
Cu1—N2—C2—C1	44.27 (17)	C22—C21—C26—C25	0.2 (3)
N1—C1—C2—N2	−49.66 (19)	P1—C21—C26—C25	174.32 (18)
C1—N1—C3—C4	−175.95 (16)	C24—C25—C26—C21	0.6 (4)
Cu1—N1—C3—C4	−9.2 (2)	C33—P1—C27—C28	96.54 (17)

N1—C3—C4—C5	177.32 (17)	C21—P1—C27—C28	−10.09 (18)
C3—C4—C5—C6	−175.87 (16)	Cu1—P1—C27—C28	−135.81 (16)
C4—C5—C6—C11	25.8 (3)	C33—P1—C27—C32	−83.40 (15)
C4—C5—C6—C7	−158.64 (19)	C21—P1—C27—C32	169.97 (14)
C11—C6—C7—C8	−1.2 (3)	Cu1—P1—C27—C32	44.25 (15)
C5—C6—C7—C8	−176.9 (2)	C32—C27—C28—C29	−0.5 (3)
C11—C6—C7—N3	−179.21 (19)	P1—C27—C28—C29	179.55 (16)
C5—C6—C7—N3	5.1 (3)	C27—C28—C29—C30	0.5 (3)
O2—N3—C7—C8	26.0 (3)	C28—C29—C30—C31	0.0 (4)
O1—N3—C7—C8	−151.9 (2)	C29—C30—C31—C32	−0.4 (3)
O2—N3—C7—C6	−155.9 (2)	C30—C31—C32—C27	0.4 (3)
O1—N3—C7—C6	26.3 (3)	C28—C27—C32—C31	0.1 (3)
C6—C7—C8—C9	−0.5 (4)	P1—C27—C32—C31	−179.95 (16)
N3—C7—C8—C9	177.6 (2)	C21—P1—C33—C34	58.50 (16)
C7—C8—C9—C10	1.7 (4)	C27—P1—C33—C34	−49.74 (16)
C8—C9—C10—C11	−1.3 (4)	Cu1—P1—C33—C34	−173.61 (12)
C9—C10—C11—C6	−0.5 (4)	C21—P1—C33—C38	−119.77 (14)
C7—C6—C11—C10	1.7 (3)	C27—P1—C33—C38	131.98 (14)
C5—C6—C11—C10	177.7 (2)	Cu1—P1—C33—C38	8.11 (15)
C2—N2—C12—C13	−177.47 (16)	C38—C33—C34—C35	2.0 (3)
Cu1—N2—C12—C13	−1.3 (3)	P1—C33—C34—C35	−176.30 (14)
N2—C12—C13—C14	175.53 (18)	C33—C34—C35—C36	−1.2 (3)
C12—C13—C14—C15	178.60 (17)	C34—C35—C36—C37	−0.2 (3)
C13—C14—C15—C20	−18.4 (3)	C35—C36—C37—C38	0.8 (3)
C13—C14—C15—C16	163.49 (19)	C34—C33—C38—C37	−1.5 (2)
C20—C15—C16—C17	0.6 (3)	P1—C33—C38—C37	176.88 (13)
C14—C15—C16—C17	178.83 (19)	C36—C37—C38—C33	0.1 (3)

Fig. 1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