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{*N*′-[1-(2-Pyridyl)ethylidene-κ*N*]benzohydrazidato-κ^2*N*′,*O*}{*N*′-[1-(2-pyridyl)ethylidene-κ*N*]benzohydrazide-κ^2*N*′,*O*}copper(II) trichloroacetate

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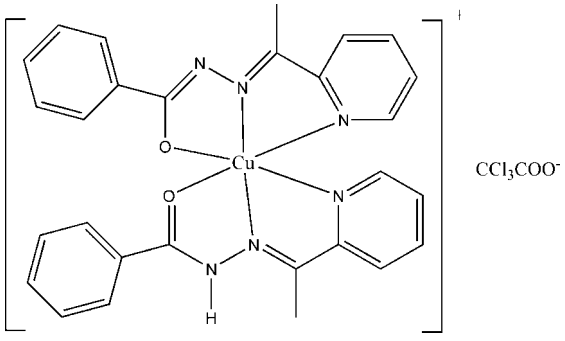
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.006 Å; R factor = 0.059; wR factor = 0.189; data-to-parameter ratio = 15.5.

In the title complex, [Cu(C$_{14}$H$_{13}$N$_3$O)(C$_{14}$H$_{12}$N$_3$O)](CCl$_3$COO), the central Cu(II) ion exhibits a distorted octahedral geometry with the two ligands coordinating in an meridional format. The N$_4$O$_2$ ligand environment is defined by two benzoyl O atoms, two pyridyl N atoms and imino N atoms. As evidenced by the bond lengths, the two benzohydrazone ligands exist in distinctively different forms, one of them as a regular neutral ligand and the other as an anionic enolate arising from deprotonation. The much longer Cu—O bond and longer Cu—N bond lengths in the neutral benzohydrazone ligand imply weak ligation in comparison with the anionic enolate form. The acute angles of the five-membered rings cause a significant deviation from a regular octahedral geometry.

Related literature

For related complexes of the same precursor ligand, see: Patole *et al.* (2003); Sen *et al.* (2005, 2007*a*,*b*); Ray *et al.* (2008); Datta *et al.* (2010).



Experimental

Crystal data

[Cu(C$_{14}$H$_{13}$N$_3$O)(C$_{14}$H$_{12}$N$_3$O)](C$_2$Cl$_3$O$_2$)
M_r = 703.45
Triclinic, $P\overline{1}$
a = 8.3341 (6) Å
b = 13.0470 (9) Å
c = 16.0729 (12) Å
α = 107.737 (1)°
β = 102.541 (1)°
γ = 95.259 (1)°
V = 1601.3 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.98 mm^{-1}
T = 295 K
0.30 × 0.27 × 0.25 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.799, T_{max} = 0.875
9034 measured reflections
6180 independent reflections
4962 reflections with $I > 2\sigma(I)$
R_{int} = 0.016

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.189
S = 1.03
6180 reflections
399 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.52 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu—N1	2.046 (3)	Cu—N5	2.088 (3)
Cu—N2	1.938 (3)	Cu—O1	1.996 (3)
Cu—N4	2.196 (3)	Cu—O2	2.420 (2)

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZK2027).

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supporting information

Acta Cryst. (2011). E**67**, m1388 [https://doi.org/10.1107/S1600536811036592]

{*N*′-[1-(2-Pyridyl)ethylidene-κN]benzohydrazidato-$\kappa^2 N',O$}{*N*′-[1-(2-pyridyl)-ethylidene-κN]benzohydrazide-$\kappa^2 N',O$}copper(II) trichloroacetate

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S1. Comment

The title complex is consisted of two tridentate benzohydrazone ligands oriented in a meridional fashion. One ligand coordinates in the deprotonated enolate form and acts as a monoanion. The other ligand coordinates in the regular neutral form. The nonequivalent coordination of these two ligands is proved by the bond distances surrounding the cuprous ion. The Cu—O distance for neutral ligand (2.420 (2) Å) is much longer than that of deprotonated ligand, 1.996 (3) Å. Contrarily, the C—O bond distance of the neutral ligand (1.228 (4) Å) is shorter than that of the deprotonated enolate form (1.280 (4) Å). The Cu—N bond distances of the enolate ligand (2.046 (3) and 1.938 (3) Å) are also shorter than those of the neutral ligand (2.196 (3) and 2.088 (3) Å). Nevertheless, the Cu—O and Cu—N bond distances (Table 1) are comparable with the literature reported complexes under the same ligand mode(Patole *et al.*, 2003, Sen *et al.*, 2005, 2007*a*,b, Ray *et al.*, 2008. Datta *et al.*, 2010). The distortion from regular octahedral symmetry is relatively large considering that the bond angles surrounding cuprous ion lie between 71.3 (1) and 163.0 (1)°. The equatorial plane can be defined by O1, N1, N2 and N5 atoms and, accordingly, the axial sites are occupied by O2 and N4 atoms. The Cu(II) ion deviates from the equatorial plane towards the axial N4 atom by 0.1421 (4) Å. The dihedral angles between two pyridine rings and two benzene rings are 86.1 (2)° and 81.7 (2)°, respectively.

S2. Experimental

The ligand precursor, $[C_6H_5C(O)NHN{=}C(CH_3)C_5H_4N]$ was prepared according to a literature procedure (Sen *et al.*, 2005). To the ligand (2 mmol), methanolic solution (20 ml) of anhydrous copper trichloroacetate (0.388 g, 1 mmol) was added with constant stirring and was kept at room temperature yielding light green square-shaped crystals suitable for X-ray diffraction after few days. Crystals were filtered and were air-dried.

S3. Refinement

All the H atoms were positioned geometrically and refined as riding atoms, with C_{aryl}—H = 0.93, C_{methyl}—H = 0.96 Å, while *Uiso*(H) = 1.5 *Ueq*(C) for the methyl H atoms and 1.2 *Ueq* (C) for all the other H atoms are used in the final refinement. A disagreeable reflection with delta(F2)/ e.s.d. >10 was omitted.

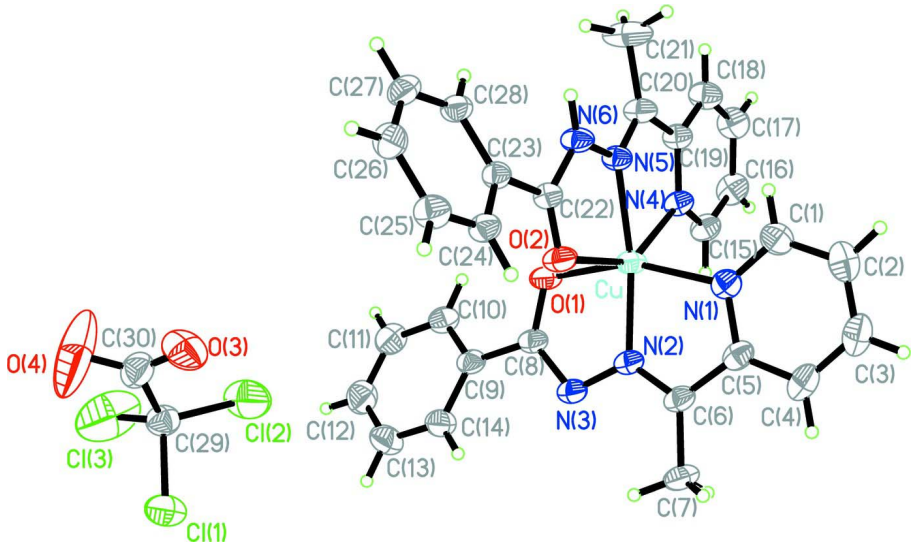

Figure 1

The molecular structure of the title complex, showing 30% displacement ellipsoids.

{*N*′-[1-(2-Pyridyl)ethylidene-κN]benzohydrazidato-$\kappa^2 N'$,*O*}{*N*′-[1-(2-pyridyl)ethylidene-κN]benzohydrazide-$\kappa^2 N'$,*O*}copper(II) trichloroacetate

Crystal data

$[Cu(C_{14}H_{13}N_3O)(C_{14}H_{12}N_3O)](C_2Cl_3O_2)$
$M_r = 703.45$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.3341$ (6) Å
$b = 13.0470$ (9) Å
$c = 16.0729$ (12) Å
$\alpha = 107.737$ (1)°
$\beta = 102.541$ (1)°
$\gamma = 95.259$ (1)°
$V = 1601.3$ (2) Å^3
$Z = 2$
$F(000) = 718$
$D_x = 1.459$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$\mu = 0.98$ mm^{-1}
$T = 295$ K
Square, green
0.30 × 0.27 × 0.25 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.799$, $T_{max} = 0.875$
9034 measured reflections
6180 independent reflections
4962 reflections with $I > 2\sigma(I)$
$R_{int} = 0.016$
$\theta_{max} = 26.0°$, $\theta_{min} = 2.5°$
$h = -10 \rightarrow 10$
$k = -15 \rightarrow 16$
$l = -17 \rightarrow 19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.059$
$wR(F^2) = 0.189$
$S = 1.03$
6180 reflections
399 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1266P)^2 + 0.7166P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.16$ e Å^{-3}
$\Delta\rho_{min} = -0.52$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.8662 (5)	0.7231 (4)	0.8172 (3)	0.0642 (10)
H1	0.9207	0.7952	0.8428	0.077*
C2	0.8171 (6)	0.6703 (5)	0.8729 (3)	0.0779 (12)
H2	0.8365	0.7069	0.9346	0.094*
C3	0.7401 (6)	0.5639 (5)	0.8359 (4)	0.0810 (14)
H3	0.7067	0.5271	0.8722	0.097*
C4	0.7121 (5)	0.5114 (4)	0.7440 (3)	0.0707 (12)
H4	0.6604	0.4387	0.7180	0.085*
C5	0.7614 (4)	0.5676 (3)	0.6908 (3)	0.0524 (8)
C6	0.7387 (4)	0.5210 (3)	0.5918 (3)	0.0521 (8)
C7	0.6495 (6)	0.4074 (3)	0.5377 (3)	0.0740 (12)
H7A	0.6098	0.4019	0.4755	0.111*
H7B	0.5568	0.3907	0.5606	0.111*
H7C	0.7247	0.3567	0.5422	0.111*
C8	0.8707 (4)	0.6479 (3)	0.4554 (2)	0.0478 (7)
C9	0.8752 (4)	0.6359 (3)	0.3610 (2)	0.0501 (8)
C10	1.0003 (5)	0.7006 (3)	0.3449 (3)	0.0596 (9)
H10	1.0787	0.7523	0.3933	0.072*
C11	1.0075 (6)	0.6879 (4)	0.2581 (3)	0.0723 (11)
H11	1.0934	0.7292	0.2479	0.087*
C12	0.8891 (7)	0.6145 (4)	0.1860 (3)	0.0810 (13)
H12	0.8925	0.6080	0.1272	0.097*
C13	0.7658 (7)	0.5509 (4)	0.2012 (3)	0.0834 (14)
H13	0.6871	0.5002	0.1524	0.100*
C14	0.7575 (5)	0.5614 (3)	0.2868 (3)	0.0642 (10)
H14	0.6723	0.5183	0.2960	0.077*
C15	1.2778 (5)	0.7146 (3)	0.7063 (3)	0.0568 (9)
H15	1.2450	0.6421	0.6691	0.068*
C16	1.4413 (5)	0.7497 (4)	0.7564 (3)	0.0677 (11)
H16	1.5173	0.7016	0.7527	0.081*
C17	1.4910 (5)	0.8573 (4)	0.8123 (3)	0.0693 (11)
H17	1.6000	0.8826	0.8478	0.083*

C18	1.3744 (5)	0.9265 (3)	0.8142 (3)	0.0622 (10)
H18	1.4044	0.9996	0.8505	0.075*
C19	1.2123 (4)	0.8857 (3)	0.7613 (2)	0.0490 (8)
C20	1.0801 (4)	0.9549 (3)	0.7556 (3)	0.0533 (8)
C21	1.1254 (6)	1.0762 (3)	0.8015 (4)	0.0950 (19)
H21A	1.2375	1.1002	0.8011	0.142*
H21B	1.1173	1.0944	0.8628	0.142*
H21C	1.0503	1.1118	0.7700	0.142*
C22	0.6592 (4)	0.9005 (3)	0.6336 (2)	0.0445 (7)
C23	0.5230 (4)	0.9641 (3)	0.6162 (2)	0.0428 (7)
C24	0.3589 (4)	0.9092 (3)	0.5859 (2)	0.0496 (8)
H24	0.3367	0.8353	0.5785	0.060*
C25	0.2288 (5)	0.9639 (3)	0.5669 (3)	0.0595 (9)
H25	0.1193	0.9275	0.5484	0.071*
C26	0.2622 (5)	1.0744 (3)	0.5757 (3)	0.0634 (10)
H26	0.1751	1.1113	0.5622	0.076*
C27	0.4247 (5)	1.1279 (3)	0.6045 (3)	0.0624 (10)
H27	0.4472	1.2013	0.6105	0.075*
C28	0.5548 (5)	1.0737 (3)	0.6245 (3)	0.0520 (8)
H28	0.6641	1.1107	0.6437	0.062*
C29	0.3176 (6)	0.7394 (4)	0.0606 (3)	0.0661 (10)
C30	0.2374 (6)	0.8395 (4)	0.1034 (4)	0.0753 (12)
N1	0.8380 (4)	0.6743 (3)	0.7289 (2)	0.0526 (7)
N2	0.8012 (3)	0.5880 (2)	0.5580 (2)	0.0468 (6)
N3	0.7924 (4)	0.5618 (2)	0.4679 (2)	0.0521 (7)
N4	1.1651 (3)	0.7807 (2)	0.7093 (2)	0.0478 (6)
N5	0.9358 (3)	0.9034 (2)	0.70525 (19)	0.0456 (6)
N6	0.8058 (3)	0.9593 (2)	0.6930 (2)	0.0500 (7)
H6	0.8162	1.0281	0.7214	0.060*
O1	0.9407 (3)	0.73837 (19)	0.51784 (18)	0.0564 (6)
O2	0.6418 (3)	0.80149 (19)	0.59581 (19)	0.0558 (6)
O3	0.2322 (5)	0.8536 (3)	0.1794 (3)	0.1018 (12)
O4	0.1930 (14)	0.8931 (8)	0.0589 (6)	0.261 (5)
Cu	0.90049 (5)	0.73603 (3)	0.63528 (3)	0.05047 (18)
Cl1	0.16329 (19)	0.61979 (11)	0.01824 (10)	0.0956 (4)
Cl2	0.4774 (2)	0.71845 (14)	0.14101 (15)	0.1265 (7)
Cl3	0.3983 (5)	0.7551 (2)	−0.02666 (19)	0.1990 (15)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.057 (2)	0.068 (2)	0.061 (2)	0.0066 (18)	0.0097 (18)	0.017 (2)
C2	0.078 (3)	0.097 (4)	0.063 (3)	0.021 (3)	0.013 (2)	0.034 (3)
C3	0.081 (3)	0.096 (4)	0.087 (3)	0.021 (3)	0.023 (3)	0.059 (3)
C4	0.071 (3)	0.067 (3)	0.091 (3)	0.017 (2)	0.024 (2)	0.047 (2)
C5	0.0419 (17)	0.0469 (18)	0.074 (2)	0.0123 (14)	0.0144 (16)	0.0269 (17)
C6	0.0478 (18)	0.0364 (17)	0.070 (2)	0.0089 (14)	0.0104 (16)	0.0179 (16)
C7	0.085 (3)	0.0380 (19)	0.088 (3)	−0.0057 (19)	0.010 (2)	0.018 (2)

C8	0.0435 (17)	0.0360 (16)	0.059 (2)	0.0079 (13)	0.0117 (15)	0.0091 (14)
C9	0.0549 (19)	0.0355 (16)	0.057 (2)	0.0135 (14)	0.0140 (16)	0.0098 (14)
C10	0.064 (2)	0.0476 (19)	0.066 (2)	0.0114 (17)	0.0211 (19)	0.0144 (17)
C11	0.087 (3)	0.065 (3)	0.074 (3)	0.018 (2)	0.036 (2)	0.024 (2)
C12	0.110 (4)	0.077 (3)	0.064 (3)	0.024 (3)	0.034 (3)	0.025 (2)
C13	0.103 (4)	0.069 (3)	0.057 (3)	0.011 (3)	0.005 (2)	0.003 (2)
C14	0.066 (2)	0.052 (2)	0.064 (2)	0.0067 (18)	0.0079 (19)	0.0127 (18)
C15	0.056 (2)	0.0482 (19)	0.071 (2)	0.0183 (16)	0.0217 (18)	0.0201 (18)
C16	0.054 (2)	0.068 (3)	0.088 (3)	0.0254 (19)	0.021 (2)	0.031 (2)
C17	0.044 (2)	0.077 (3)	0.082 (3)	0.0107 (19)	0.0065 (19)	0.026 (2)
C18	0.0436 (19)	0.060 (2)	0.072 (2)	0.0040 (16)	0.0085 (17)	0.0109 (19)
C19	0.0405 (17)	0.0453 (18)	0.058 (2)	0.0058 (13)	0.0128 (14)	0.0125 (15)
C20	0.0430 (18)	0.0400 (17)	0.065 (2)	0.0068 (14)	0.0089 (16)	0.0049 (16)
C21	0.056 (2)	0.045 (2)	0.143 (5)	0.0061 (18)	0.001 (3)	−0.008 (3)
C22	0.0430 (16)	0.0393 (16)	0.0497 (18)	0.0053 (13)	0.0122 (14)	0.0132 (14)
C23	0.0410 (16)	0.0403 (16)	0.0454 (17)	0.0072 (12)	0.0109 (13)	0.0121 (13)
C24	0.0452 (17)	0.0432 (17)	0.058 (2)	0.0037 (14)	0.0114 (15)	0.0161 (15)
C25	0.0426 (18)	0.060 (2)	0.072 (2)	0.0059 (16)	0.0120 (17)	0.0183 (19)
C26	0.058 (2)	0.062 (2)	0.069 (2)	0.0254 (18)	0.0090 (19)	0.020 (2)
C27	0.069 (2)	0.0408 (18)	0.074 (3)	0.0121 (17)	0.008 (2)	0.0217 (18)
C28	0.0500 (19)	0.0409 (17)	0.058 (2)	0.0009 (14)	0.0075 (15)	0.0135 (15)
C29	0.077 (3)	0.059 (2)	0.062 (2)	0.008 (2)	0.025 (2)	0.0147 (19)
C30	0.086 (3)	0.066 (3)	0.082 (3)	0.024 (2)	0.022 (3)	0.030 (2)
N1	0.0419 (15)	0.0540 (17)	0.0612 (18)	0.0060 (12)	0.0107 (13)	0.0206 (14)
N2	0.0452 (15)	0.0338 (13)	0.0583 (17)	0.0058 (11)	0.0126 (12)	0.0118 (12)
N3	0.0571 (17)	0.0368 (14)	0.0568 (17)	0.0048 (12)	0.0127 (14)	0.0099 (12)
N4	0.0423 (14)	0.0393 (14)	0.0611 (17)	0.0074 (11)	0.0156 (13)	0.0143 (13)
N5	0.0413 (14)	0.0385 (14)	0.0512 (15)	0.0087 (11)	0.0106 (12)	0.0073 (12)
N6	0.0418 (14)	0.0362 (14)	0.0612 (17)	0.0111 (11)	0.0069 (12)	0.0043 (12)
O1	0.0632 (15)	0.0387 (12)	0.0574 (15)	−0.0042 (11)	0.0175 (12)	0.0046 (11)
O2	0.0510 (13)	0.0346 (12)	0.0705 (16)	0.0058 (10)	0.0059 (12)	0.0087 (11)
O3	0.109 (3)	0.096 (3)	0.079 (2)	0.042 (2)	0.023 (2)	−0.008 (2)
O4	0.395 (13)	0.307 (10)	0.265 (9)	0.269 (10)	0.187 (9)	0.224 (9)
Cu	0.0526 (3)	0.0376 (3)	0.0532 (3)	−0.00343 (18)	0.0129 (2)	0.00748 (19)
Cl1	0.0939 (9)	0.0706 (8)	0.0948 (9)	−0.0064 (6)	0.0015 (7)	0.0103 (7)
Cl2	0.0788 (9)	0.0975 (11)	0.1661 (17)	0.0305 (8)	−0.0130 (10)	0.0181 (11)
Cl3	0.336 (4)	0.1402 (18)	0.171 (2)	0.017 (2)	0.189 (3)	0.0433 (16)

Geometric parameters (Å, º)

Cu—N1	2.046 (3)	C14—H14	0.9300
N2—N3	1.367 (4)	C15—N4	1.330 (4)
Cu—N2	1.938 (3)	C15—C16	1.378 (6)
Cu—N4	2.196 (3)	C15—H15	0.9300
N5—N6	1.373 (4)	C16—C17	1.383 (6)
Cu—N5	2.088 (3)	C16—H16	0.9300
N6—H6	0.8600	C17—C18	1.385 (6)
Cu—O1	1.996 (3)	C17—H17	0.9300

Cu—O2	2.420 (2)	C18—C19	1.388 (5)
C1—N1	1.324 (5)	C18—H18	0.9300
C1—C2	1.389 (6)	C19—N4	1.338 (4)
C1—H1	0.9300	C19—C20	1.493 (5)
C2—C3	1.364 (7)	C20—N5	1.285 (4)
C2—H2	0.9300	C20—C21	1.500 (5)
C3—C4	1.383 (7)	C21—H21A	0.9600
C3—H3	0.9300	C21—H21B	0.9600
C4—C5	1.385 (6)	C21—H21C	0.9600
C4—H4	0.9300	C22—O2	1.228 (4)
C5—N1	1.367 (5)	C22—N6	1.367 (4)
C5—C6	1.481 (6)	C22—C23	1.494 (4)
C6—N2	1.289 (5)	C23—C28	1.390 (5)
C6—C7	1.496 (5)	C23—C24	1.393 (5)
C7—H7A	0.9600	C24—C25	1.382 (5)
C7—H7B	0.9600	C24—H24	0.9300
C7—H7C	0.9600	C25—C26	1.400 (6)
O1—C8	1.280 (4)	C25—H25	0.9300
C8—N3	1.338 (4)	C26—C27	1.376 (6)
C8—C9	1.485 (5)	C26—H26	0.9300
C9—C14	1.393 (5)	C27—C28	1.381 (5)
C9—C10	1.398 (5)	C27—H27	0.9300
C10—C11	1.370 (6)	C28—H28	0.9300
C10—H10	0.9300	C29—C30	1.561 (6)
C11—C12	1.374 (7)	C29—Cl3	1.738 (4)
C11—H11	0.9300	C29—Cl2	1.747 (5)
C12—C13	1.370 (7)	C29—Cl1	1.777 (5)
C12—H12	0.9300	C30—O4	1.173 (7)
C13—C14	1.360 (7)	C30—O3	1.189 (6)
C13—H13	0.9300		

N1—C1—C2	122.2 (4)	C20—C21—H21C	109.5
N1—C1—H1	118.9	H21A—C21—H21C	109.5
C2—C1—H1	118.9	H21B—C21—H21C	109.5
C3—C2—C1	119.1 (5)	O2—C22—N6	121.8 (3)
C3—C2—H2	120.5	O2—C22—C23	122.1 (3)
C1—C2—H2	120.5	N6—C22—C23	116.1 (3)
C2—C3—C4	119.4 (4)	C28—C23—C24	119.3 (3)
C2—C3—H3	120.3	C28—C23—C22	122.4 (3)
C4—C3—H3	120.3	C24—C23—C22	118.2 (3)
C3—C4—C5	119.6 (4)	C25—C24—C23	120.3 (3)
C3—C4—H4	120.2	C25—C24—H24	119.9
C5—C4—H4	120.2	C23—C24—H24	119.9
N1—C5—C4	120.3 (4)	C24—C25—C26	120.0 (3)
N1—C5—C6	114.8 (3)	C24—C25—H25	120.0
C4—C5—C6	125.0 (4)	C26—C25—H25	120.0
N2—C6—C5	113.4 (3)	C27—C26—C25	119.5 (3)
N2—C6—C7	124.2 (4)	C27—C26—H26	120.3

C5—C6—C7	122.4 (3)	C25—C26—H26	120.3
C6—C7—H7A	109.5	C26—C27—C28	120.7 (3)
C6—C7—H7B	109.5	C26—C27—H27	119.7
H7A—C7—H7B	109.5	C28—C27—H27	119.7
C6—C7—H7C	109.5	C27—C28—C23	120.3 (3)
H7A—C7—H7C	109.5	C27—C28—H28	119.9
H7B—C7—H7C	109.5	C23—C28—H28	119.9
O1—C8—N3	125.2 (3)	C30—C29—Cl3	111.7 (3)
O1—C8—C9	118.4 (3)	C30—C29—Cl2	111.6 (3)
N3—C8—C9	116.4 (3)	Cl3—C29—Cl2	108.5 (3)
C14—C9—C10	118.2 (4)	C30—C29—Cl1	108.9 (3)
C14—C9—C8	121.9 (3)	Cl3—C29—Cl1	109.4 (3)
C10—C9—C8	119.9 (3)	Cl2—C29—Cl1	106.7 (2)
C11—C10—C9	120.1 (4)	O4—C30—O3	127.5 (6)
C11—C10—H10	119.9	O4—C30—C29	117.5 (6)
C9—C10—H10	119.9	O3—C30—C29	115.0 (4)
C10—C11—C12	120.6 (4)	C1—N1—C5	119.5 (3)
C10—C11—H11	119.7	C1—N1—Cu	128.5 (3)
C12—C11—H11	119.7	C5—N1—Cu	112.0 (2)
C13—C12—C11	119.7 (5)	C6—N2—N3	122.9 (3)
C13—C12—H12	120.2	C6—N2—Cu	119.6 (3)
C11—C12—H12	120.2	N3—N2—Cu	117.4 (2)
C14—C13—C12	120.7 (5)	C8—N3—N2	107.9 (3)
C14—C13—H13	119.7	C15—N4—C19	119.1 (3)
C12—C13—H13	119.7	C15—N4—Cu	126.5 (2)
C13—C14—C9	120.7 (4)	C19—N4—Cu	114.4 (2)
C13—C14—H14	119.6	C20—N5—N6	120.0 (3)
C9—C14—H14	119.6	C20—N5—Cu	120.5 (2)
N4—C15—C16	122.4 (4)	N6—N5—Cu	119.4 (2)
N4—C15—H15	118.8	C22—N6—N5	116.8 (3)
C16—C15—H15	118.8	C22—N6—H6	121.6
C15—C16—C17	119.2 (4)	N5—N6—H6	121.6
C15—C16—H16	120.4	C8—O1—Cu	109.8 (2)
C17—C16—H16	120.4	C22—O2—Cu	110.6 (2)
C16—C17—C18	118.4 (4)	N2—Cu—O1	79.25 (11)
C16—C17—H17	120.8	N2—Cu—N1	80.17 (12)
C18—C17—H17	120.8	O1—Cu—N1	159.01 (12)
C17—C18—C19	119.2 (4)	N2—Cu—N5	162.98 (12)
C17—C18—H18	120.4	O1—Cu—N5	100.25 (11)
C19—C18—H18	120.4	N1—Cu—N5	100.64 (12)
N4—C19—C18	121.7 (3)	N2—Cu—N4	122.15 (11)
N4—C19—C20	115.2 (3)	O1—Cu—N4	94.88 (11)
C18—C19—C20	123.1 (3)	N1—Cu—N4	92.52 (11)
N5—C20—C19	115.0 (3)	N5—Cu—N4	74.87 (10)
N5—C20—C21	125.4 (3)	N2—Cu—O2	91.71 (10)
C19—C20—C21	119.4 (3)	O1—Cu—O2	88.33 (11)
C20—C21—H21A	109.5	N1—Cu—O2	96.41 (11)
C20—C21—H21B	109.5	N5—Cu—O2	71.28 (9)

H21A—C21—H21B	109.5	N4—Cu—O2	146.02 (9)