Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

[*N*′-(4-Methoxy-2-oxidobenzylidene)-4-nitrobenzohydrazidato-κ^3O,N,O']-(pyridine-κN)copper(II)

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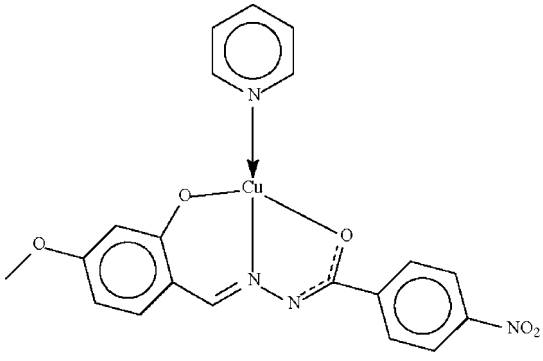
Received 15 December 2008; accepted 16 December 2008

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.028; wR factor = 0.087; data-to-parameter ratio = 14.5.

The pyridine-coordinated Cu^{II} atom in the title Schiff base complex, $[Cu(C_{15}H_{11}N_3O_5)(C_5H_5N)]$, is O,N,O'-chelated by the doubly deprotonated Schiff base ligand. The metal centre is in a square-planar coordination geometry.

Related literature

For the pyridine adducts of copper derivatives of similar ligands, see: Ali *et al.* (2004); Chen & Liu (2004); Das & Pal (2005); Fariati *et al.* (2002); Lu & Liu (2005); Lu *et al.* (2003).



Experimental

Crystal data

$[Cu(C_{15}H_{11}N_3O_5)(C_5H_5N)]$
M_r = 455.91
Triclinic, $P\overline{1}$
a = 6.3529 (1) Å
b = 9.8409 (2) Å
c = 15.1303 (3) Å
α = 98.063 (1)°
β = 92.011 (1)°
γ = 107.088 (1)°
V = 892.31 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.27 mm^{-1}
T = 100 (2) K
0.40 × 0.10 × 0.05 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.807, T_{max} = 1.000
(expected range = 0.757–0.939)
6268 measured reflections
3942 independent reflections
3605 reflections with $I > 2\sigma(I)$
R_{int} = 0.013

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.087
S = 1.09
3942 reflections
272 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

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: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

We thank the University of Malaya for funding this study (Science Fund grants 12–02-03–2031, 12–02-03–2051).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2838).

References

Ali, H., Khamis, N. A., Basirun, W. J. & Yamin, B. M. (2004). *Acta Cryst.* E**60**, m982–m983.
Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Bruker (2007). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Chen, W.-H. & Liu, S.-X. (2004). *Chin. J. Inorg. Chem.* **20**, 668–670.
Das, S. & Pal, S. (2005). *J. Mol. Struct.* **753**, 68–79.
Fariati, F., Caruso, U., Centore, R., Marcolli, W., De Maria, A., Panunzi, B., Roviello, A. & Tuzi, A. (2002). *Inorg. Chem.* **41**, 6597–6603.
Lu, W.-G., Feng, X.-L., Liu, H.-W. & Wang, S.-L. (2003). *Chin. J. Inorg. Chem.* **19**, 206–210.
Lu, W.-G. & Liu, H.-W. (2005). *Chin. J. Struct. Chem.* **24**, 1078–1082.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2009). *publCIF*. In preparation.

supporting information

Acta Cryst. (2009). E**65**, m121 [doi:10.1107/S1600536808042803]

[*N*′-(4-Methoxy-2-oxidobenzylidene)4-nitrobenzohydrazidato-κ^3O,N,O'](pyridine-κN)copper(II)

Nooraziah Mohd Lair, Hapipah Mohd Ali and Seik Weng Ng

S1. Experimental

N′-2-Hydroxy-3-methoxybenzylidene)-nitrobenzohydrazide (0.30 g, 1 mmol) and copper acetate (0.20 g, 1 mmol) were heated in a ethanol (50 ml) for 2 hours. The solvent was removed and the resulting compound recrystallized from pyridine.

S2. Refinement

Hydrogen atoms were placed at calculated positions ($C_{aromatic}$–H 0.95 Å, C_{methyl}–H 0.98 Å) and were treated as riding on their parent carbon atoms, with U(H) set to 1.2Ueq($C_{aromatic}$) or 1.5Ueq(C_{methyl}).

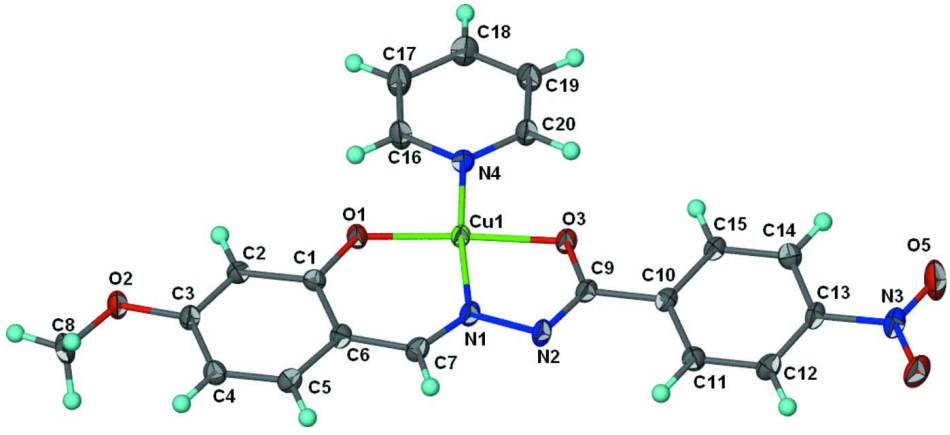


Figure 1

Displacement ellipsoid plot (Barbour, 2001) of Cu(C_5H_5N)($C_{15}H_{11}N_3O_5$) at the 70% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius.

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Crystal data

[Cu($C_{15}H_{11}N_3O_5$)(C_5H_5N)]
M_r = 455.91
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 6.3529 (1) Å
b = 9.8409 (2) Å
c = 15.1303 (3) Å
α = 98.063 (1)°
β = 92.011 (1)°
γ = 107.088 (1)°
V = 892.31 (3) Å^3
Z = 2
F(000) = 466
D_x = 1.697 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3716 reflections
θ = 2.4–29.2°
μ = 1.27 mm^{-1}

T = 100 K
Block, brown

0.40 × 0.10 × 0.05 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.807, T_{max} = 1.000

6268 measured reflections
3942 independent reflections
3605 reflections with $I > 2\sigma(I)$
R_{int} = 0.013
θ_{max} = 27.5°, θ_{min} = 1.4°
h = −6→8
k = −12→12
l = −19→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.087
S = 1.09
3942 reflections
272 parameters
0 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0494P)^2 + 0.535P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	1.14506 (4)	0.70062 (2)	0.728016 (14)	0.01312 (9)
N1	0.9381 (3)	0.64556 (17)	0.62386 (11)	0.0150 (3)
N2	1.0273 (3)	0.68298 (18)	0.54424 (10)	0.0159 (3)
N3	1.7555 (3)	0.93172 (18)	0.27544 (11)	0.0189 (4)
N4	1.3792 (3)	0.78081 (17)	0.82931 (11)	0.0145 (3)
O1	0.9305 (2)	0.61658 (15)	0.80405 (9)	0.0163 (3)
O2	0.2533 (2)	0.39329 (16)	0.90700 (9)	0.0199 (3)
O3	1.3444 (2)	0.77637 (15)	0.64095 (9)	0.0159 (3)
O4	1.6632 (3)	0.91481 (17)	0.20033 (9)	0.0247 (3)
O5	1.9560 (3)	0.9856 (2)	0.29243 (11)	0.0311 (4)
C1	0.7183 (3)	0.5521 (2)	0.78294 (13)	0.0139 (4)
C2	0.5869 (3)	0.5009 (2)	0.85092 (13)	0.0152 (4)
H2	0.6540	0.5120	0.9097	0.018*
C3	0.3615 (3)	0.4346 (2)	0.83442 (13)	0.0149 (4)
C4	0.2562 (3)	0.4147 (2)	0.74829 (13)	0.0151 (4)
H4	0.1016	0.3693	0.7371	0.018*
C5	0.3837 (3)	0.4630 (2)	0.68048 (13)	0.0146 (4)
H5	0.3142	0.4495	0.6219	0.018*
C6	0.6124 (3)	0.5313 (2)	0.69468 (12)	0.0140 (4)
C7	0.7290 (3)	0.5785 (2)	0.61964 (12)	0.0149 (4)
H7	0.6471	0.5592	0.5631	0.018*
C8	0.0219 (3)	0.3204 (3)	0.89270 (15)	0.0247 (5)
H8A	−0.0352	0.2939	0.9492	0.037*

H8B	−0.0038	0.2333	0.8484	0.037*
H8C	−0.0540	0.3840	0.8707	0.037*
C9	1.2393 (3)	0.7493 (2)	0.56222 (12)	0.0140 (4)
C10	1.3714 (3)	0.79538 (19)	0.48671 (12)	0.0142 (4)
C11	1.2684 (3)	0.7902 (2)	0.40223 (13)	0.0162 (4)
H11	1.1119	0.7555	0.3927	0.019*
C12	1.3932 (3)	0.8352 (2)	0.33284 (13)	0.0174 (4)
H12	1.3242	0.8321	0.2755	0.021*
C13	1.6204 (3)	0.8849 (2)	0.34864 (12)	0.0149 (4)
C14	1.7277 (3)	0.8905 (2)	0.43096 (13)	0.0162 (4)
H14	1.8844	0.9243	0.4396	0.019*
C15	1.6016 (3)	0.8457 (2)	0.50049 (12)	0.0146 (4)
H15	1.6720	0.8492	0.5576	0.017*
C16	1.3332 (3)	0.7615 (2)	0.91374 (13)	0.0189 (4)
H16	1.1851	0.7146	0.9246	0.023*
C17	1.4910 (3)	0.8068 (2)	0.98487 (13)	0.0219 (4)
H17	1.4524	0.7913	1.0435	0.026*
C18	1.7074 (3)	0.8753 (2)	0.96950 (14)	0.0210 (4)
H18	1.8197	0.9079	1.0175	0.025*
C19	1.7569 (3)	0.8955 (2)	0.88305 (13)	0.0189 (4)
H19	1.9041	0.9416	0.8707	0.023*
C20	1.5893 (3)	0.8476 (2)	0.81504 (13)	0.0161 (4)
H20	1.6239	0.8625	0.7559	0.019*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.01168 (13)	0.01707 (13)	0.00996 (13)	0.00263 (9)	0.00095 (8)	0.00366 (8)
N1	0.0165 (8)	0.0172 (8)	0.0117 (7)	0.0044 (6)	0.0032 (6)	0.0046 (6)
N2	0.0166 (8)	0.0193 (8)	0.0109 (7)	0.0027 (7)	0.0034 (6)	0.0048 (6)
N3	0.0245 (9)	0.0184 (8)	0.0147 (8)	0.0060 (7)	0.0075 (7)	0.0047 (6)
N4	0.0133 (8)	0.0162 (8)	0.0137 (8)	0.0039 (6)	0.0007 (6)	0.0032 (6)
O1	0.0109 (6)	0.0234 (7)	0.0136 (6)	0.0025 (5)	0.0012 (5)	0.0057 (5)
O2	0.0136 (7)	0.0297 (8)	0.0154 (7)	0.0027 (6)	0.0032 (5)	0.0082 (6)
O3	0.0139 (7)	0.0218 (7)	0.0110 (6)	0.0028 (5)	0.0006 (5)	0.0046 (5)
O4	0.0325 (9)	0.0307 (8)	0.0127 (7)	0.0103 (7)	0.0053 (6)	0.0074 (6)
O5	0.0224 (8)	0.0431 (10)	0.0229 (8)	−0.0003 (7)	0.0092 (7)	0.0092 (7)
C1	0.0131 (9)	0.0140 (8)	0.0154 (9)	0.0050 (7)	0.0014 (7)	0.0030 (7)
C2	0.0143 (9)	0.0192 (9)	0.0130 (9)	0.0056 (8)	0.0009 (7)	0.0041 (7)
C3	0.0156 (9)	0.0160 (9)	0.0141 (9)	0.0048 (7)	0.0042 (7)	0.0046 (7)
C4	0.0125 (9)	0.0156 (9)	0.0157 (9)	0.0025 (7)	0.0007 (7)	0.0018 (7)
C5	0.0167 (9)	0.0141 (8)	0.0124 (8)	0.0041 (7)	−0.0001 (7)	0.0011 (7)
C6	0.0156 (9)	0.0133 (8)	0.0127 (8)	0.0040 (7)	0.0021 (7)	0.0021 (7)
C7	0.0164 (9)	0.0153 (9)	0.0115 (8)	0.0027 (7)	−0.0009 (7)	0.0024 (7)
C8	0.0126 (10)	0.0395 (13)	0.0216 (10)	0.0032 (9)	0.0058 (8)	0.0122 (9)
C9	0.0169 (9)	0.0146 (9)	0.0116 (8)	0.0055 (7)	0.0025 (7)	0.0038 (7)
C10	0.0171 (9)	0.0129 (8)	0.0130 (9)	0.0046 (7)	0.0022 (7)	0.0034 (7)
C11	0.0146 (9)	0.0202 (9)	0.0135 (9)	0.0045 (7)	0.0005 (7)	0.0033 (7)

C12	0.0211 (10)	0.0199 (9)	0.0111 (9)	0.0057 (8)	0.0007 (7)	0.0033 (7)
C13	0.0197 (10)	0.0138 (9)	0.0116 (8)	0.0048 (7)	0.0055 (7)	0.0035 (7)
C14	0.0154 (9)	0.0159 (9)	0.0166 (9)	0.0035 (7)	0.0019 (7)	0.0021 (7)
C15	0.0168 (9)	0.0163 (9)	0.0111 (8)	0.0050 (7)	0.0014 (7)	0.0037 (7)
C16	0.0148 (10)	0.0249 (10)	0.0147 (9)	0.0021 (8)	0.0019 (7)	0.0031 (8)
C17	0.0193 (10)	0.0293 (11)	0.0125 (9)	0.0008 (9)	0.0010 (8)	0.0029 (8)
C18	0.0186 (10)	0.0248 (10)	0.0149 (9)	0.0007 (8)	−0.0034 (8)	0.0013 (8)
C19	0.0143 (9)	0.0197 (10)	0.0199 (10)	0.0008 (8)	0.0009 (8)	0.0033 (8)
C20	0.0156 (9)	0.0176 (9)	0.0143 (9)	0.0033 (7)	0.0026 (7)	0.0036 (7)

Geometric parameters (Å, º)

Cu1—O1	1.8922 (14)	C6—C7	1.435 (3)
Cu1—N1	1.9239 (16)	C7—H7	0.9500
Cu1—O3	1.9320 (14)	C8—H8A	0.9800
Cu1—N4	1.9989 (16)	C8—H8B	0.9800
N1—C7	1.293 (3)	C8—H8C	0.9800
N1—N2	1.399 (2)	C9—C10	1.485 (3)
N2—C9	1.312 (3)	C10—C15	1.397 (3)
N3—O5	1.229 (2)	C10—C11	1.403 (3)
N3—O4	1.227 (2)	C11—C12	1.382 (3)
N3—C13	1.467 (2)	C11—H11	0.9500
N4—C20	1.343 (3)	C12—C13	1.381 (3)
N4—C16	1.347 (2)	C12—H12	0.9500
O1—C1	1.316 (2)	C13—C14	1.385 (3)
O2—C3	1.363 (2)	C14—C15	1.387 (3)
O2—C8	1.427 (2)	C14—H14	0.9500
O3—C9	1.299 (2)	C15—H15	0.9500
C1—C2	1.403 (3)	C16—C17	1.375 (3)
C1—C6	1.434 (3)	C16—H16	0.9500
C2—C3	1.385 (3)	C17—C18	1.386 (3)
C2—H2	0.9500	C17—H17	0.9500
C3—C4	1.405 (3)	C18—C19	1.384 (3)
C4—C5	1.380 (3)	C18—H18	0.9500
C4—H4	0.9500	C19—C20	1.381 (3)
C5—C6	1.404 (3)	C19—H19	0.9500
C5—H5	0.9500	C20—H20	0.9500
O1—Cu1—N1	93.57 (6)	O2—C8—H8B	109.5
O1—Cu1—O3	174.58 (6)	H8A—C8—H8B	109.5
N1—Cu1—O3	81.17 (6)	O2—C8—H8C	109.5
O1—Cu1—N4	92.67 (6)	H8A—C8—H8C	109.5
N1—Cu1—N4	172.51 (7)	H8B—C8—H8C	109.5
O3—Cu1—N4	92.68 (6)	O3—C9—N2	125.19 (17)
C7—N1—N2	117.25 (16)	O3—C9—C10	117.01 (17)
C7—N1—Cu1	127.41 (13)	N2—C9—C10	117.79 (16)
N2—N1—Cu1	115.34 (12)	C15—C10—C11	119.71 (17)
C9—N2—N1	108.05 (15)	C15—C10—C9	119.31 (16)

O5—N3—O4	123.25 (17)	C11—C10—C9	120.98 (18)
O5—N3—C13	118.27 (16)	C12—C11—C10	120.41 (18)
O4—N3—C13	118.47 (17)	C12—C11—H11	119.8
C20—N4—C16	117.86 (17)	C10—C11—H11	119.8
C20—N4—Cu1	121.38 (13)	C11—C12—C13	118.53 (17)
C16—N4—Cu1	120.64 (14)	C11—C12—H12	120.7
C1—O1—Cu1	127.54 (12)	C13—C12—H12	120.7
C3—O2—C8	117.33 (15)	C12—C13—C14	122.62 (18)
C9—O3—Cu1	110.23 (12)	C12—C13—N3	119.26 (17)
O1—C1—C2	118.11 (17)	C14—C13—N3	118.12 (18)
O1—C1—C6	124.11 (17)	C15—C14—C13	118.62 (18)
C2—C1—C6	117.78 (17)	C15—C14—H14	120.7
C3—C2—C1	121.55 (17)	C13—C14—H14	120.7
C3—C2—H2	119.2	C14—C15—C10	120.11 (17)
C1—C2—H2	119.2	C14—C15—H15	119.9
O2—C3—C2	115.33 (17)	C10—C15—H15	119.9
O2—C3—C4	123.65 (18)	N4—C16—C17	122.91 (19)
C2—C3—C4	121.01 (18)	N4—C16—H16	118.5
C5—C4—C3	118.12 (18)	C17—C16—H16	118.5
C5—C4—H4	120.9	C16—C17—C18	118.84 (19)
C3—C4—H4	120.9	C16—C17—H17	120.6
C4—C5—C6	122.53 (17)	C18—C17—H17	120.6
C4—C5—H5	118.7	C19—C18—C17	118.81 (19)
C6—C5—H5	118.7	C19—C18—H18	120.6
C5—C6—C1	119.00 (17)	C17—C18—H18	120.6
C5—C6—C7	117.98 (17)	C20—C19—C18	119.05 (19)
C1—C6—C7	123.02 (17)	C20—C19—H19	120.5
N1—C7—C6	124.30 (17)	C18—C19—H19	120.5
N1—C7—H7	117.9	N4—C20—C19	122.52 (18)
C6—C7—H7	117.9	N4—C20—H20	118.7
O2—C8—H8A	109.5	C19—C20—H20	118.7

O1—Cu1—N1—C7	1.77 (18)	C5—C6—C7—N1	178.35 (18)
O3—Cu1—N1—C7	−179.56 (18)	C1—C6—C7—N1	−1.0 (3)
O1—Cu1—N1—N2	−178.07 (13)	Cu1—O3—C9—N2	1.5 (2)
O3—Cu1—N1—N2	0.60 (12)	Cu1—O3—C9—C10	−177.59 (12)
C7—N1—N2—C9	−179.91 (17)	N1—N2—C9—O3	−1.0 (3)
Cu1—N1—N2—C9	−0.05 (19)	N1—N2—C9—C10	178.08 (15)
O1—Cu1—N4—C20	174.53 (15)	O3—C9—C10—C15	9.0 (3)
O3—Cu1—N4—C20	−4.54 (15)	N2—C9—C10—C15	−170.09 (17)
O1—Cu1—N4—C16	−1.39 (16)	O3—C9—C10—C11	−170.48 (17)
O3—Cu1—N4—C16	179.54 (15)	N2—C9—C10—C11	10.4 (3)
N1—Cu1—O1—C1	−2.34 (16)	C15—C10—C11—C12	−0.4 (3)
N4—Cu1—O1—C1	173.51 (16)	C9—C10—C11—C12	179.15 (17)
N1—Cu1—O3—C9	−1.01 (12)	C10—C11—C12—C13	0.1 (3)
N4—Cu1—O3—C9	−176.72 (13)	C11—C12—C13—C14	0.4 (3)
Cu1—O1—C1—C2	−178.09 (13)	C11—C12—C13—N3	179.37 (17)
Cu1—O1—C1—C6	1.7 (3)	O5—N3—C13—C12	174.64 (18)

O1—C1—C2—C3	178.63 (17)	O4—N3—C13—C12	−5.6 (3)
C6—C1—C2—C3	−1.1 (3)	O5—N3—C13—C14	−6.3 (3)
C8—O2—C3—C2	−178.07 (18)	O4—N3—C13—C14	173.44 (18)
C8—O2—C3—C4	2.8 (3)	C12—C13—C14—C15	−0.6 (3)
C1—C2—C3—O2	−178.47 (17)	N3—C13—C14—C15	−179.62 (16)
C1—C2—C3—C4	0.7 (3)	C13—C14—C15—C10	0.4 (3)
O2—C3—C4—C5	179.17 (17)	C11—C10—C15—C14	0.1 (3)
C2—C3—C4—C5	0.0 (3)	C9—C10—C15—C14	−179.40 (17)
C3—C4—C5—C6	−0.4 (3)	C20—N4—C16—C17	−0.1 (3)
C4—C5—C6—C1	−0.1 (3)	Cu1—N4—C16—C17	175.93 (16)
C4—C5—C6—C7	−179.44 (17)	N4—C16—C17—C18	0.0 (3)
O1—C1—C6—C5	−178.95 (17)	C16—C17—C18—C19	−0.1 (3)
C2—C1—C6—C5	0.8 (3)	C17—C18—C19—C20	0.4 (3)
O1—C1—C6—C7	0.4 (3)	C16—N4—C20—C19	0.4 (3)
C2—C1—C6—C7	−179.86 (17)	Cu1—N4—C20—C19	−175.60 (15)
N2—N1—C7—C6	179.34 (16)	C18—C19—C20—N4	−0.6 (3)
Cu1—N1—C7—C6	−0.5 (3)		