

Bis(*N,N*-dimethylformamide- κ O)-bis(2,4,6-trinitrophenolato- κ^2 O¹,O²)-copper(II)

Bai-Yu Li, Jun-Feng Tong, Wen-Kui Dong,* Jian Yao and Jian-Chao Wu

School of Chemical and Biological Engineering, Lanzhou Jiaotong University, Lanzhou 730070, People's Republic of China

Correspondence e-mail: dongwk@mail.lzjtu.cn

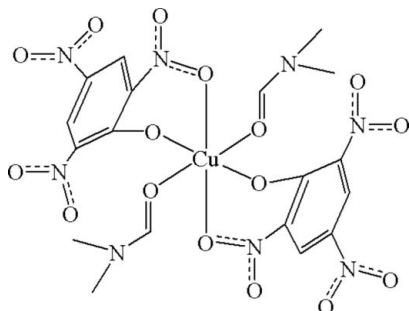
Received 13 November 2008; accepted 26 November 2008

Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.030; wR factor = 0.078; data-to-parameter ratio = 11.0.

The molecule of the title complex, $[\text{Cu}(\text{C}_6\text{H}_2\text{N}_3\text{O}_7)_2(\text{C}_3\text{H}_7\text{NO})_2]$, is disposed about a crystallographic centre of symmetry. The Cu^{II} cation is six-coordinated by two phenolate O atoms and two *ortho*-nitro O atoms of two picrate units and by two carbonyl O atoms from two coordinated dimethylformamide molecules, forming a distorted octahedral geometry.

Related literature

For background to 2,4,6-trinitrophenoxides, see: Arnaud-Neu *et al.* (2005); Dong *et al.* (1998, 2007*a,b*); Harrowfield *et al.* (1995, 1998); Liu *et al.* (2008); Marchand *et al.* (2003); Muthamizhchelvan *et al.* (2005); Song *et al.* (2007); Talanova *et al.* (1999); Venkatasubramanian *et al.* (1985); Wang *et al.* (2003).



Experimental

Crystal data

$[\text{Cu}(\text{C}_6\text{H}_2\text{N}_3\text{O}_7)_2(\text{C}_3\text{H}_7\text{NO})_2]$	$b = 8.3361$ (11) Å
$M_r = 665.94$	$c = 9.8429$ (14) Å
Triclinic, $P\bar{1}$	$\alpha = 73.945$ (1)°
$a = 8.0620$ (10) Å	$\beta = 88.796$ (2)°

$\gamma = 87.968$ (2)°
 $V = 635.25$ (15) Å³
 $Z = 1$
 Mo $K\alpha$ radiation

$\mu = 0.96$ mm⁻¹
 $T = 298$ (2) K
 $0.45 \times 0.42 \times 0.30$ mm

Data collection

Siemens SMART 1000 CCD diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\text{min}} = 0.673$, $T_{\text{max}} = 0.762$

3320 measured reflections
 2198 independent reflections
 1973 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.019$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.030$
 $wR(F^2) = 0.078$
 $S = 1.08$
 2198 reflections

199 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.22$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.36$ e Å⁻³

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); 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.

This work was supported by the Foundation of the Education Department of Gansu Province (No. 0604-01) and the 'Qing Lan' Talent Engineering Funds of Lanzhou Jiaotong University (No. QL-05-19 A), which are gratefully acknowledged.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2446).

References

- Arnaud-Neu, F., Harrowfield, J. M., Michel, S., Skelton, B. W. & White, A. H. (2005). *Supramol. Chem.* **17**, 609–615.
- Dong, W. K., Feng, J. H., Wang, L., Xu, L., Zhao, L., Yang, X. Q. & Yu, T. Z. (2007*a*). *Transition Met. Chem.* **32**, 1101–1105.
- Dong, W. K., Song, X. Q., Sun, Y. X. & Wu, H. L. (2007*b*). *Chin. J. Inorg. Chem.* **23**, 1809–1811.
- Dong, W., Yang, R. & Yu, K. (1998). *Acta Cryst.* **C54**, 1416–1418.
- Harrowfield, J. M., Sharma, R. P., Skelton, B. W. & White, A. H. (1998). *Aust. J. Chem.* **51**, 735–746.
- Harrowfield, J. M., Skelton, B. W. & White, A. H. (1995). *Aust. J. Chem.* **48**, 1311–1331.
- Liu, Z. Q., Li, Y. T., Wu, Z. Y. & Song, Y. L. (2008). *Inorg. Chim. Acta*, **361**, 226–232.
- Marchand, A. P., Hazlewood, A., Huang, Z., Vadlakonda, S. K., Rocha, J. D. R., Power, T. D., Majerski, K. M., Klalic, L., Kragol, G. & Bryan, J. C. (2003). *Struct. Chem.* **14**, 279–288.
- Muthamizhchelvan, C., Saminathan, K., Fraanje, J., Peschar, R. & Sivakumar, K. (2005). *Acta Cryst.* **E61**, o1153–o1155.
- Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Siemens (1996). SMART and SAINT. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
- Song, X. Q., Dou, W., Liu, W. S. & Ma, J. X. (2007). *Inorg. Chem. Commun.* **10**, 419–422.
- Talanova, G. G., Elkirim, N. S. A., Talanov, V. S., Hanes, R. E. Jr, Hwang, H.-S., Bartsch, R. A. & Rogers, R. D. (1999). *J. Am. Chem. Soc.* **121**, 11281–11290.
- Venkatasubramanian, K., Joshi, K., Poonia, N. S., Montfort, W. R., Ernst, S. R. & Hackert, M. L. (1985). *J. Incl. Phenom. Macro.* **3**, 453–459.
- Wang, Y. W., Liu, W. S., Tang, N., Tan, M. Y. & Yu, K. B. (2003). *J. Mol. Struct.* **660**, 41–47.

supporting information

Acta Cryst. (2009). E65, m1 [doi:10.1107/S1600536808039846]

Bis(*N,N*-dimethylformamide- κ O)bis(2,4,6-trinitrophenolato- κ^2 O¹,O²)copper(II)

Bai-Yu Li, Jun-Feng Tong, Wen-Kui Dong, Jian Yao and Jian-Chao Wu

S1. Comment

2,4,6-Trinitrophenoxides, 'picrates', play an important role in the modern coordination chemistry (Dong *et al.*, 1998; Dong *et al.*, 2007a). Picrate anion with extraordinary varieties in the binding of complexes, has great potential in building coordination networks (Liu *et al.*, 2008). They can act as the bridging mono- (Arnaud-Neu *et al.*, 2005; Wang *et al.*, 2003), di- (Marchand *et al.*, 2003; Song *et al.*, 2007), tri- (Harrowfield *et al.*, 1995; Dong *et al.*, 1998; Dong *et al.*, 2007a), tetra- (Venkatasubramanian *et al.*, 1985) or penta- (Dong *et al.*, 2007b; Harrowfield *et al.*, 1998) dentate ligands *via* the phenolic oxygen, *ortho*-nitro oxygen and *para*-nitro oxygen atoms to build coordination networks as well as interlink the one-dimensional or two-dimensional molecules into frameworks *via* the hydrogen bonds (Muthamizchelvan *et al.*, 2005) or π - π stacking interactions (Talanova *et al.*, 1999). Here, in continuation of our previous studies on synthesis and structural characterization of transition metal complexes with salen-type bisoxime chelating ligands, a single-crystal of unexpected complex, bis(*N,N*-dimethylformamide- κ O)bis(2,4,6-trinitrophenolato- κ^2 O,^{*O'*})copper(II), was obtained and structurally characterized by X-ray crystallography.

The crystal structure of the title complex consists of discrete C₁₈H₁₈CuN₈O₁₆ molecules (Fig. 1), in which all bond lengths are in normal ranges. The two benzene rings in each molecule of the title complex are parallel and the distance between them is 2.115 (2)Å. The central Cu^{II} atom is located on a crystallographic inversion center. The carbonyl oxygens O8, O8^{*i*} and the phenoxy oxygens O1, O1^{*i*}(symmetry code (*i*) -x=1, -y+1, -z+1) coordinate to the copper atom to form a distorted square planar structure with Cu1-O2 and Cu1-O8 bond lengths of 1.9226 (15) and 1.9401 (15)Å respectively. The two *ortho*-nitro oxygen atoms (O2 and O2^{*i*}) occupy axial positions with Cu1-O2 = 2.659 (2)Å to give a distorted octahedral coordination geometry around the copper atom.

S2. Experimental

Copper(II) picrate tetrahydrate and 5,5'-dihydroxy-2,2'-[1,1'-(propane-1,3-diylldioxydinitrilo)diethylidene]diphenol were synthesized by an analogous method (Dong *et al.*, 2007a). A ethyl acetate-*N,N*-dimethylformamide mixed solution (2 ml) of 5,5'-dihydroxy-2,2'-[1,1'-(propane-1,3-diylldioxydinitrilo)diethylidene]diphenol (4.1 mg, 0.01 mmol) was added dropwise to a acetone solution (2 ml) of copper(II) picrate tetrahydrate (6.1 mg, 0.01 mmol) at room temperature. The brilliant yellow solution obtained was placed in n-hexane sphere and allowed to stand at room temperature for about several weeks. Along with diffusion of n-hexane into the mixed solution of the complex, Green block-like single crystals of bis(*N,N*-dimethylformamide- κ O)bis(2,4,6-trinitrophenolato- κ^2 O,^{*O'*})copper(II) complex suitable for X-ray crystallographic analysis were obtained. Anal. Calc. for C₁₈H₁₈CuN₈O₁₆: C, 34.51; H, 3.48; N, 16.10; Cu, 9.13%. Found: C, 34.73; H, 3.51; N, 16.17; Cu, 9.01%.

S3. Refinement

Non-H atoms were refined anisotropically. H atoms were treated as riding atoms with distances C—H = 0.96 (CH₃), 0.97 (CH₂), 0.93 Å (CH), $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$ and $1.5 U_{\text{eq}}(\text{C})$.

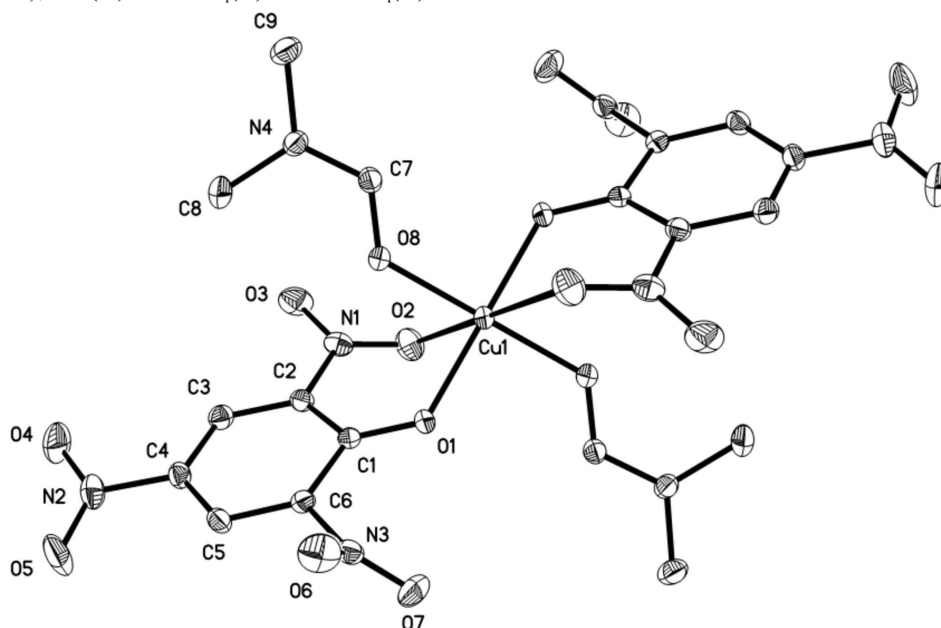


Figure 1

The molecule structure of the title complex with atom numbering scheme [Symmetry codes: $-x + 1, -y + 1, -z + 1$]. Displacement ellipsoids for non-hydrogen atoms are drawn at the 30% probability level.

Bis(*N,N*-dimethylformamide- κ O)bis(2,4,6-trinitrophenolato- κ^2 O¹,O²)copper(II)

Crystal data

[Cu(C₆H₂N₃O₇)₂(C₃H₇NO)₂]

$M_r = 665.94$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 8.062$ (1) Å

$b = 8.3361$ (11) Å

$c = 9.8429$ (14) Å

$\alpha = 73.945$ (1)°

$\beta = 88.796$ (2)°

$\gamma = 87.968$ (2)°

$V = 635.25$ (15) Å³

$Z = 1$

$F(000) = 339$

$D_x = 1.741$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 2174 reflections

$\theta = 2.5$ – 27.5 °

$\mu = 0.96$ mm⁻¹

$T = 298$ K

Block-like, green

$0.45 \times 0.42 \times 0.30$ mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Sheldrick, 1996)

$T_{\text{min}} = 0.673$, $T_{\text{max}} = 0.762$

3320 measured reflections

2198 independent reflections

1973 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.020$

$\theta_{\text{max}} = 25.0$ °, $\theta_{\text{min}} = 2.2$ °

$h = -9 \rightarrow 9$

$k = -9 \rightarrow 6$

$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.030$
 $wR(F^2) = 0.078$
 $S = 1.08$
 2198 reflections
 199 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
 $w = 1/[\sigma^2(F_o^2) + (0.036P)^2 + 0.273P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.22 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.36 \text{ e } \text{\AA}^{-3}$
 Extinction correction: *SHELXL97* (Sheldrick,
 2008), $F_c^* = kF_c[1 + 0.001xF_c^2\lambda^3/\sin(2\theta)]^{-1/4}$
 Extinction coefficient: 0.141 (6)

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	0.5000	0.5000	0.5000	0.02554 (17)
N1	0.5597 (3)	0.5206 (2)	0.1667 (2)	0.0339 (5)
N2	0.8515 (3)	1.0013 (3)	-0.1186 (2)	0.0407 (5)
N3	0.5610 (3)	1.0497 (2)	0.3079 (2)	0.0341 (5)
N4	0.9697 (2)	0.3374 (2)	0.4240 (2)	0.0289 (4)
O1	0.4863 (2)	0.71913 (19)	0.36927 (16)	0.0332 (4)
O2	0.4407 (2)	0.4683 (2)	0.2441 (2)	0.0497 (5)
O3	0.6381 (3)	0.4363 (2)	0.1017 (2)	0.0496 (5)
O4	0.9214 (3)	0.9088 (3)	-0.1814 (2)	0.0587 (6)
O5	0.8672 (3)	1.1525 (3)	-0.1527 (2)	0.0639 (6)
O6	0.6713 (3)	1.1133 (3)	0.3553 (2)	0.0552 (5)
O7	0.4137 (3)	1.0653 (2)	0.3315 (2)	0.0556 (5)
O8	0.72371 (18)	0.47226 (19)	0.43167 (16)	0.0306 (4)
C1	0.5606 (3)	0.7778 (3)	0.2512 (2)	0.0255 (5)
C2	0.6088 (3)	0.6916 (3)	0.1486 (2)	0.0265 (5)
C3	0.7030 (3)	0.7633 (3)	0.0293 (2)	0.0301 (5)
H3	0.7350	0.7018	-0.0331	0.036*
C4	0.7490 (3)	0.9268 (3)	0.0041 (2)	0.0298 (5)
C5	0.7014 (3)	1.0223 (3)	0.0951 (2)	0.0287 (5)
H5	0.7312	1.1331	0.0767	0.034*
C6	0.6098 (3)	0.9480 (3)	0.2118 (2)	0.0259 (5)
C7	0.8263 (3)	0.3548 (3)	0.4840 (2)	0.0278 (5)
H7	0.7989	0.2774	0.5687	0.033*

C8	1.0134 (3)	0.4484 (4)	0.2868 (3)	0.0434 (6)
H8A	0.9757	0.4034	0.2134	0.065*
H8B	1.1317	0.4587	0.2795	0.065*
H8C	0.9615	0.5564	0.2768	0.065*
C9	1.0878 (3)	0.2028 (3)	0.4895 (3)	0.0402 (6)
H9A	1.0476	0.1441	0.5817	0.060*
H9B	1.1933	0.2489	0.4979	0.060*
H9C	1.1001	0.1270	0.4320	0.060*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0244 (2)	0.0238 (2)	0.0255 (2)	-0.00033 (15)	0.00563 (15)	-0.00252 (15)
N1	0.0396 (12)	0.0273 (11)	0.0347 (11)	-0.0003 (9)	-0.0077 (9)	-0.0081 (9)
N2	0.0390 (12)	0.0539 (15)	0.0278 (11)	-0.0100 (11)	0.0067 (9)	-0.0084 (10)
N3	0.0480 (13)	0.0224 (10)	0.0299 (10)	0.0035 (9)	0.0070 (9)	-0.0051 (8)
N4	0.0255 (10)	0.0290 (10)	0.0325 (10)	0.0012 (8)	0.0019 (8)	-0.0097 (8)
O1	0.0358 (9)	0.0260 (8)	0.0316 (9)	0.0026 (7)	0.0142 (7)	0.0011 (7)
O2	0.0463 (11)	0.0393 (10)	0.0610 (12)	-0.0169 (9)	0.0065 (9)	-0.0085 (9)
O3	0.0708 (14)	0.0310 (10)	0.0510 (12)	0.0033 (9)	-0.0010 (10)	-0.0187 (9)
O4	0.0601 (13)	0.0758 (15)	0.0440 (12)	-0.0094 (11)	0.0237 (10)	-0.0236 (11)
O5	0.0878 (17)	0.0495 (13)	0.0479 (12)	-0.0253 (12)	0.0274 (11)	-0.0019 (10)
O6	0.0705 (14)	0.0512 (12)	0.0538 (12)	-0.0025 (11)	-0.0067 (10)	-0.0306 (10)
O7	0.0498 (13)	0.0475 (12)	0.0714 (14)	0.0092 (9)	0.0224 (10)	-0.0225 (10)
O8	0.0249 (8)	0.0303 (9)	0.0318 (9)	0.0019 (7)	0.0065 (6)	-0.0015 (7)
C1	0.0218 (11)	0.0253 (11)	0.0256 (11)	0.0035 (9)	-0.0002 (9)	-0.0013 (9)
C2	0.0273 (12)	0.0235 (11)	0.0274 (11)	0.0003 (9)	-0.0013 (9)	-0.0047 (9)
C3	0.0316 (12)	0.0328 (13)	0.0262 (12)	0.0031 (10)	0.0000 (9)	-0.0088 (9)
C4	0.0286 (12)	0.0348 (13)	0.0226 (11)	-0.0015 (10)	0.0024 (9)	-0.0026 (9)
C5	0.0300 (12)	0.0239 (11)	0.0292 (12)	-0.0041 (9)	0.0008 (9)	-0.0020 (9)
C6	0.0268 (11)	0.0247 (11)	0.0259 (11)	0.0031 (9)	0.0010 (9)	-0.0069 (9)
C7	0.0284 (12)	0.0273 (12)	0.0267 (11)	-0.0027 (9)	0.0025 (9)	-0.0060 (9)
C8	0.0360 (14)	0.0516 (16)	0.0381 (14)	-0.0010 (12)	0.0132 (11)	-0.0059 (12)
C9	0.0323 (13)	0.0369 (14)	0.0517 (16)	0.0065 (11)	-0.0001 (11)	-0.0135 (12)

Geometric parameters (Å, °)

Cu1—O1 ⁱ	1.9226 (15)	O1—C1	1.275 (3)
Cu1—O1	1.9226 (15)	O8—C7	1.261 (3)
Cu1—O8	1.9401 (15)	C1—C6	1.431 (3)
Cu1—O8 ⁱ	1.9401 (15)	C1—C2	1.432 (3)
Cu1—O2	2.659 (2)	C2—C3	1.385 (3)
N1—O3	1.226 (3)	C3—C4	1.379 (3)
N1—O2	1.228 (3)	C3—H3	0.9300
N1—C2	1.455 (3)	C4—C5	1.393 (3)
N2—O5	1.222 (3)	C5—C6	1.361 (3)
N2—O4	1.230 (3)	C5—H5	0.9300
N2—C4	1.452 (3)	C7—H7	0.9300

N3—O6	1.215 (3)	C8—H8A	0.9600
N3—O7	1.215 (3)	C8—H8B	0.9600
N3—C6	1.474 (3)	C8—H8C	0.9600
N4—C7	1.310 (3)	C9—H9A	0.9600
N4—C8	1.455 (3)	C9—H9B	0.9600
N4—C9	1.459 (3)	C9—H9C	0.9600
O1 ⁱ —Cu1—O1	180.0	C3—C2—N1	116.6 (2)
O1 ⁱ —Cu1—O8	90.87 (6)	C1—C2—N1	120.38 (19)
O1—Cu1—O8	89.13 (6)	C4—C3—C2	119.3 (2)
O1 ⁱ —Cu1—O8 ⁱ	89.13 (6)	C4—C3—H3	120.4
O1—Cu1—O8 ⁱ	90.87 (6)	C2—C3—H3	120.4
O8—Cu1—O8 ⁱ	180.000 (1)	C3—C4—C5	121.5 (2)
O1 ⁱ —Cu1—O2	108.49 (7)	C3—C4—N2	119.6 (2)
O1—Cu1—O2	71.51 (7)	C5—C4—N2	118.9 (2)
O8—Cu1—O2	78.81 (6)	C6—C5—C4	117.8 (2)
O8 ⁱ —Cu1—O2	101.19 (6)	C6—C5—H5	121.1
O3—N1—O2	123.1 (2)	C4—C5—H5	121.1
O3—N1—C2	118.1 (2)	C5—C6—C1	125.5 (2)
O2—N1—C2	118.8 (2)	C5—C6—N3	117.3 (2)
O5—N2—O4	123.1 (2)	C1—C6—N3	117.15 (18)
O5—N2—C4	118.4 (2)	O8—C7—N4	122.7 (2)
O4—N2—C4	118.5 (2)	O8—C7—H7	118.7
O6—N3—O7	125.3 (2)	N4—C7—H7	118.7
O6—N3—C6	117.4 (2)	N4—C8—H8A	109.5
O7—N3—C6	117.3 (2)	N4—C8—H8B	109.5
C7—N4—C8	120.7 (2)	H8A—C8—H8B	109.5
C7—N4—C9	121.3 (2)	N4—C8—H8C	109.5
C8—N4—C9	117.95 (19)	H8A—C8—H8C	109.5
C1—O1—Cu1	130.29 (14)	H8B—C8—H8C	109.5
N1—O2—Cu1	108.53 (14)	N4—C9—H9A	109.5
C7—O8—Cu1	126.60 (14)	N4—C9—H9B	109.5
O1—C1—C6	119.4 (2)	H9A—C9—H9B	109.5
O1—C1—C2	127.7 (2)	N4—C9—H9C	109.5
C6—C1—C2	112.79 (19)	H9A—C9—H9C	109.5
C3—C2—C1	123.0 (2)	H9B—C9—H9C	109.5
O8—Cu1—O1—C1	27.0 (2)	N1—C2—C3—C4	178.0 (2)
O8 ⁱ —Cu1—O1—C1	-153.0 (2)	C2—C3—C4—C5	-0.7 (3)
O2—Cu1—O1—C1	-51.52 (19)	C2—C3—C4—N2	178.4 (2)
O3—N1—O2—Cu1	123.9 (2)	O5—N2—C4—C3	167.6 (2)
C2—N1—O2—Cu1	-57.3 (2)	O4—N2—C4—C3	-14.0 (3)
O1 ⁱ —Cu1—O2—N1	-115.98 (15)	O5—N2—C4—C5	-13.3 (3)
O1—Cu1—O2—N1	64.02 (15)	O4—N2—C4—C5	165.1 (2)
O8—Cu1—O2—N1	-28.83 (15)	C3—C4—C5—C6	1.1 (3)
O8 ⁱ —Cu1—O2—N1	151.17 (15)	N2—C4—C5—C6	-177.9 (2)
O1 ⁱ —Cu1—O8—C7	-8.81 (18)	C4—C5—C6—C1	1.4 (3)
O1—Cu1—O8—C7	171.19 (18)	C4—C5—C6—N3	179.6 (2)

O2—Cu1—O8—C7	-117.49 (19)	O1—C1—C6—C5	174.3 (2)
Cu1—O1—C1—C6	-144.15 (17)	C2—C1—C6—C5	-3.9 (3)
Cu1—O1—C1—C2	33.8 (3)	O1—C1—C6—N3	-3.9 (3)
O1—C1—C2—C3	-173.8 (2)	C2—C1—C6—N3	177.93 (19)
C6—C1—C2—C3	4.3 (3)	O6—N3—C6—C5	-56.1 (3)
O1—C1—C2—N1	5.9 (3)	O7—N3—C6—C5	122.8 (2)
C6—C1—C2—N1	-176.03 (19)	O6—N3—C6—C1	122.2 (2)
O3—N1—C2—C3	19.5 (3)	O7—N3—C6—C1	-58.9 (3)
O2—N1—C2—C3	-159.3 (2)	Cu1—O8—C7—N4	173.74 (16)
O3—N1—C2—C1	-160.2 (2)	C8—N4—C7—O8	-4.3 (3)
O2—N1—C2—C1	21.0 (3)	C9—N4—C7—O8	178.2 (2)
C1—C2—C3—C4	-2.2 (3)		

Symmetry code: (i) $-x+1, -y+1, -z+1$.