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Bis(3-acetyl-6-methyl-2-oxo-2*H*-pyran-4-olato)bis(dimethylformamide)copper(II)

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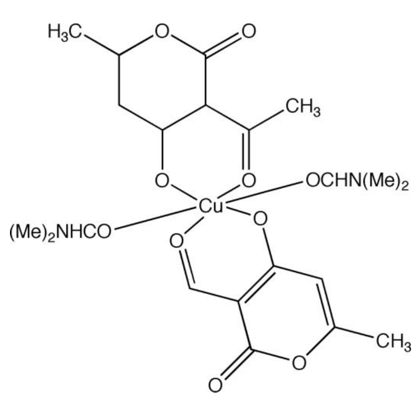
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.002 Å; R factor = 0.037; wR factor = 0.103; data-to-parameter ratio = 21.9.

The title compound, $[Cu(C_8H_7O_4)_2(C_3H_7NO)_2]$, is a mononuclear copper(II) complex where the Cu^{II} atom, lying on an inversion center, is coordinated in elongated octahedral fashion by six O atoms, four from two 3-acetyl-6-methyl-2-oxo-2*H*-pyran-4-olate ligands in equatorial positions and the remaining two from dimethylformamide molecules in axial positions.

Related literature

For related literature, see: Arndt *et al.* (1936); Casabó *et al.* (1987); Djedouani *et al.* (2006); Gelasco *et al.* (1997); Zucolotto Chalaça *et al.* (2002).



Experimental

Crystal data

$[Cu(C_8H_7O_4)_2(C_3H_7NO)_2]$	γ = 78.852 (2)°
M_r = 544.01	V = 601.93 (3) Å^3
Triclinic, $P\overline{1}$	Z = 1
a = 7.6894 (2) Å	Mo $K\alpha$ radiation
b = 8.5406 (2) Å	μ = 0.97 mm^{-1}
c = 9.3858 (3) Å	T = 173 (2) K
α = 84.870 (1)°	0.10 × 0.10 × 0.10 mm
β = 86.964 (1)°	

Data collection

Nonius KappaCCD diffractometer	3518 independent reflections
Absorption correction: none	3021 reflections with $I > 2\sigma(I)$
8024 measured reflections	R_{int} = 0.050

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037	161 parameters
$wR(F^2)$ = 0.103	H-atom parameters constrained
S = 1.05	$\Delta\rho_{max}$ = 0.36 e Å^{-3}
3518 reflections	$\Delta\rho_{min}$ = −0.55 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.9181 (11)	Cu1—O5	2.4462 (16)
Cu1—O4	1.9366 (12)		
O1—Cu1—O4	90.29 (5)	O4—Cu1—O5	87.33 (5)
O1—Cu1—O5	87.44 (6)		

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO* (Nonius, 1998); data reduction: *DENZO*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ATOMS* (Dowty, 1995); software used to prepare material for publication: *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG2087).

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supplementary materials

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Bis(3-acetyl-6-methyl-2-oxo-2*H*-pyran-4-olato)bis(dimethylformamide)copper(II)

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Comment

Dehydroacetic acid DHA, [3-acetyl-6-methyl-2*H*-pyran-2,4(3*H*)-dione], (Arndt *et al.*, 1936) is an industrial product used as a fungicide, bactericide and also as an important intermediate in organic synthesis. However, little is known on its metal complexes; those with Cu and Zn have been reported to be, respectively, a fungicide and a heat stabilizer for vinyl chloride resins. There are some other reports in the patent literature and also the stability constantes of some complexes have been measured. (Casabó *et al.*, 1987). The Cu complex has been already described in this latter report, but the characterization of the compound was based only on thermal and elemental analysis, and on IR and NMR spectroscopy.

As an extension of our work (Djedouani *et al.*, 2006), we present here the synthesis and crystal structure determination of $[Cu(DHA)_2(DMF)_2]$ (I), which molecular structure is illustrated in Fig. 1.

The Cu^{II} center, lying on an inversion center, is coordinated to six oxygen atoms forming an elongated octahedra. The equatorial plane is defined by two DHA ligands, each chelating the metal through two oxygen atoms, O2 and O3, while the two dimethylformamide molecules fill the two axial sites *via* their oxygen atom (O1), in a similar fashion to that observed in other DHA complexes (Zucolotto *et al.*, 2002) but with a larger distortion due to the Jahn-Teller effect. This can be envisaged when comparing with the Co isostructural isolog $Co(DHA)_2(DMF)_2$ (A. Gelasco, *et al.*, 1997; Casabó *et al.*, 1987): the Cu—$O_{(DMF)}$ bond length in (I), (2.446 (16) Å) is significantly longer than the corresponding Co—$O_{(DMF)}$ distance, 2.168 (2) Å, while the equatorial bonds are slightly shorter. The coordination distances in (I) are in good agreement with those found in $Cu(DHA)_2(DMSO)_2$ (DMSO: dimethylsulfoxyde, Djedouani *et al.*, 2006).

The structure of (I) is different from the $Mn(DHA)_2(H_2O)_2$ one, in which one water molecule is at the axial position and the other at the equatorial position.

The dimethylformamide molecules are involved in intermolecular hydrogen bonding *via* weak C—H···O interactions. (Figure 2),

Experimental

To a solution of copper acetate monohydrate is added, with stirring a solution of dehydroacetic acid in absolute ethanol with a 1:2 stoichiometric ratio. Complex (I) precipitated after one hour. The precipitate was filtered and recrystallized by slow evaporation in a dimethylsulfoxide solution.

Refinement

H atoms were idealized (C—H range: 0.95–0.98 Å) and refined isotropically.

Figures

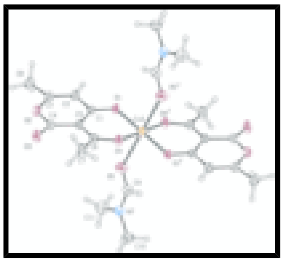

Fig. 1. *ORTEP* view of a selected part of the crystal structure of compound 2. The ellipsoids enclose 30% of the electronic density. Symmetry operators for generating equivalent positions: (*i*) −*x*,-*y*,-*z*.

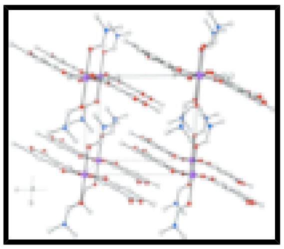

Fig. 2. View of the crystal structure of $Cu(DHA)_2(DMF)_2$ (I) in the (b,c) plane. The hydrogen atoms have been omitted for clarity.

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Crystal data

$[Cu(C_8H_7O_4)_2(C_3H_7NO)_2]$	$Z = 1$
$M_r = 544.01$	$F_{000} = 283.00$
Triclinic, $P\overline{1}$	$D_x = 1.501$ Mg m^{-3}
Hall symbol: -P 1	Mo *K*α radiation λ = 0.71069 Å
a = 7.6894 (2) Å	Cell parameters from 4486 reflections
b = 8.5406 (2) Å	θ = 1.0–30.0º
c = 9.3858 (3) Å	μ = 0.97 mm^{-1}
α = 84.8700 (10)º	*T* = 173 (2) K
β = 86.9640 (10)º	Prism, blue
γ = 78.852 (2)º	0.10 × 0.10 × 0.10 mm
V = 601.93 (3) Å^3	

Data collection

Nonius KappaCCD diffractometer	3021 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.050$
Monochromator: graphite	$\theta_{max} = 30.1$º
T = 173(2) K	$\theta_{min} = 2.2$º
π [CHECK] scans	$h = -10 \rightarrow 10$
Absorption correction: none	$k = -12 \rightarrow 11$
8024 measured reflections	$l = -13 \rightarrow 13$
3518 independent reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.037$	$w = 1/[\sigma^2(F_o^2) + (0.0542P)^2 + 0.0974P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.103$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.05$	$\Delta\rho_{max} = 0.36$ e Å^{-3}
3518 reflections	$\Delta\rho_{min} = -0.55$ e Å^{-3}
161 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.221 (11)
Secondary atom site location: difference Fourier map	

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 $F^2 > 2\text{sigma}(F^2)$ 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}
Cu1	0.0000	0.0000	0.0000	0.03279 (12)
O1	−0.09598 (15)	−0.06122 (16)	0.18483 (12)	0.0368 (3)
O2	0.15683 (17)	−0.26020 (18)	0.54467 (13)	0.0438 (3)
O3	0.41095 (18)	−0.1951 (2)	0.47529 (15)	0.0534 (4)
O4	0.21496 (15)	0.02621 (16)	0.08599 (13)	0.0375 (3)
O5	0.1369 (2)	−0.28176 (19)	−0.01498 (18)	0.0560 (4)
N1	0.3220 (2)	−0.47067 (19)	−0.13276 (18)	0.0420 (3)
C1	−0.0075 (2)	−0.1174 (2)	0.29462 (16)	0.0304 (3)
C2	−0.1011 (2)	−0.1903 (2)	0.41121 (18)	0.0379 (4)
H2	−0.2243	−0.1887	0.4047	0.045*
C3	−0.0181 (2)	−0.2601 (2)	0.52813 (18)	0.0381 (4)
C4	0.2594 (2)	−0.1858 (2)	0.44211 (18)	0.0367 (4)
C5	0.1755 (2)	−0.1125 (2)	0.31181 (16)	0.0298 (3)
C6	0.2740 (2)	−0.0303 (2)	0.20597 (17)	0.0318 (3)
C7	0.4565 (2)	−0.0019 (3)	0.2306 (2)	0.0502 (5)
H7A	0.4933	0.0685	0.1513	0.075*

H7B	0.5402	−0.1044	0.2362	0.075*
H7C	0.4551	0.0485	0.3205	0.075*
C8	−0.0964 (3)	−0.3446 (3)	0.6534 (2)	0.0540 (5)
H8A	−0.0298	−0.4546	0.6676	0.081*
H8B	−0.2205	−0.3466	0.6361	0.081*
H8C	−0.0903	−0.2885	0.7391	0.081*
C9	0.2491 (2)	−0.3213 (2)	−0.1090 (2)	0.0417 (4)
H9	0.2869	−0.2382	−0.1697	0.050*
C10	0.4528 (3)	−0.5079 (3)	−0.2474 (3)	0.0623 (6)
H10A	0.4087	−0.5726	−0.3135	0.093*
H10B	0.5635	−0.5680	−0.2074	0.093*
H10C	0.4747	−0.4083	−0.2992	0.093*
C11	0.2675 (4)	−0.6042 (3)	−0.0473 (3)	0.0635 (6)
H11A	0.3720	−0.6746	−0.0060	0.095*
H11B	0.2091	−0.6645	−0.1080	0.095*
H11C	0.1847	−0.5638	0.0299	0.095*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.02832 (16)	0.0447 (2)	0.02637 (16)	−0.01107 (11)	−0.00577 (10)	0.00369 (11)
O1	0.0273 (5)	0.0532 (8)	0.0289 (5)	−0.0080 (5)	−0.0048 (4)	0.0048 (5)
O2	0.0425 (7)	0.0554 (8)	0.0313 (6)	−0.0085 (6)	−0.0059 (5)	0.0095 (5)
O3	0.0409 (7)	0.0749 (11)	0.0439 (7)	−0.0139 (7)	−0.0169 (6)	0.0137 (7)
O4	0.0335 (6)	0.0486 (7)	0.0324 (6)	−0.0156 (5)	−0.0079 (4)	0.0073 (5)
O5	0.0567 (9)	0.0460 (8)	0.0641 (10)	−0.0085 (7)	0.0111 (7)	−0.0096 (7)
N1	0.0425 (8)	0.0368 (8)	0.0455 (8)	−0.0090 (6)	0.0026 (6)	0.0027 (6)
C1	0.0298 (7)	0.0340 (8)	0.0272 (7)	−0.0052 (6)	−0.0016 (5)	−0.0038 (6)
C2	0.0331 (8)	0.0478 (10)	0.0323 (8)	−0.0088 (7)	−0.0002 (6)	0.0004 (7)
C3	0.0397 (9)	0.0424 (10)	0.0310 (8)	−0.0072 (7)	0.0017 (6)	−0.0003 (7)
C4	0.0363 (8)	0.0410 (9)	0.0313 (8)	−0.0043 (7)	−0.0066 (6)	0.0017 (7)
C5	0.0300 (7)	0.0327 (8)	0.0268 (7)	−0.0053 (6)	−0.0055 (5)	−0.0012 (6)
C6	0.0295 (7)	0.0344 (8)	0.0323 (7)	−0.0071 (6)	−0.0066 (6)	−0.0020 (6)
C7	0.0373 (9)	0.0687 (14)	0.0480 (11)	−0.0236 (9)	−0.0146 (8)	0.0141 (9)
C8	0.0571 (12)	0.0634 (14)	0.0396 (10)	−0.0150 (10)	0.0045 (9)	0.0101 (9)
C9	0.0386 (9)	0.0372 (9)	0.0508 (10)	−0.0123 (7)	−0.0046 (8)	0.0008 (8)
C10	0.0601 (14)	0.0568 (14)	0.0621 (14)	0.0010 (10)	0.0158 (11)	0.0008 (11)
C11	0.0718 (15)	0.0436 (12)	0.0736 (16)	−0.0164 (10)	0.0133 (12)	0.0061 (11)

Geometric parameters (Å, °)

Cu1—O1	1.9181 (11)	C3—C8	1.486 (3)
Cu1—O4	1.9366 (12)	C4—C5	1.447 (2)
Cu1—O5	2.4462 (16)	C5—C6	1.433 (2)
Cu1—O1^{i}	1.9181 (11)	C6—C7	1.503 (2)
Cu1—O4^{i}	1.9366 (12)	C2—H2	0.9499
Cu1—O5^{i}	2.4462 (16)	C7—H7A	0.9793
O1—C1	1.2707 (19)	C7—H7B	0.9802

O2—C3	1.362 (2)	C7—H7C	0.9796
O2—C4	1.399 (2)	C8—H8A	0.9805
O3—C4	1.208 (2)	C8—H8B	0.9800
O4—C6	1.257 (2)	C8—H8C	0.9800
O5—C9	1.224 (2)	C9—H9	0.9501
N1—C9	1.324 (2)	C10—H10A	0.9804
N1—C10	1.447 (3)	C10—H10B	0.9795
N1—C11	1.451 (3)	C10—H10C	0.9804
C1—C2	1.439 (2)	C11—H11A	0.9808
C1—C5	1.434 (2)	C11—H11B	0.9800
C2—C3	1.333 (2)	C11—H11C	0.9800
Cu1···H11B^{ii}	3.5934	C11···O4^{xi}	3.380 (3)
Cu1···H11B^{iii}	3.5934	C4···H7C	2.8540
O1···O4	2.7325 (17)	C4···H7B	2.9629
O1···O5	3.040 (2)	C6···H8C^{ix}	2.8916
O1···C6	2.926 (2)	C8···H11C^{xii}	3.0797
O1···C7^{iv}	3.390 (2)	C9···H8C^{x}	2.9937
O1···C9^{i}	3.279 (2)	H2···O3^{iv}	2.8573
O1···O4^{i}	2.7189 (17)	H2···H7B^{iv}	2.4278
O1···O5^{i}	3.175 (2)	H2···H8B	2.4503
O2···C10^{v}	3.367 (3)	H7A···H11A^{ii}	2.5766
O2···C9^{v}	3.338 (2)	H7A···H9^{xiii}	2.4515
O3···C7	2.753 (3)	H7B···O1^{vii}	2.9016
O4···O1^{i}	2.7189 (17)	H7B···O3	2.5247
O4···O1	2.7325 (17)	H7B···C4	2.9629
O4···O5^{i}	3.190 (2)	H7B···H2^{vii}	2.4278
O4···O5	3.049 (2)	H7C···O3	2.4969
O4···C1	2.880 (2)	H7C···C4	2.8540
O4···C11^{ii}	3.380 (3)	H7C···O3^{viii}	2.7275
O5···O4^{i}	3.190 (2)	H8B···H2	2.4503
O5···C1	3.381 (2)	H8B···H10C^{xiv}	2.5316
O5···O4	3.049 (2)	H8C···C9^{v}	2.9937
O5···O1	3.040 (2)	H8C···O4^{ix}	2.8797
O5···O1^{i}	3.175 (2)	H8C···C6^{ix}	2.8916
O1···H11B^{iii}	2.8143	H8C···H11C^{xii}	2.5529
O1···H9^{i}	2.6870	H9···H10C	2.2342
O1···H7B^{iv}	2.9016	H9···O1^{i}	2.6870
O3···H10A^{vi}	2.7234	H9···H7A^{xiii}	2.4515
O3···H7B	2.5247	H10A···H11B	2.5639
O3···H2^{vii}	2.8573	H10A···O3^{vi}	2.7234
O3···H7C^{viii}	2.7275	H10B···H11A	2.5468
O3···H10C^{v}	2.6667	H10C···O3^{x}	2.6667
O3···H7C	2.4969	H10C···H8B^{xv}	2.5316

O4···H8C^{ix}	2.8797	H10C···H9	2.2342
O5···H11C	2.3680	H11A···H7A^{xi}	2.5766
C2···C4^{ix}	3.577 (2)	H11A···H10B	2.5468
C4···C2^{ix}	3.577 (2)	H11B···Cu1^{xi}	3.5934
C6···C8^{ix}	3.568 (3)	H11B···H10A	2.5639
C7···O3	2.753 (3)	H11B···Cu1^{iii}	3.5934
C7···O1^{vii}	3.390 (2)	H11B···O1^{iii}	2.8143
C8···C6^{ix}	3.568 (3)	H11C···O5	2.3680
C9···O2^{x}	3.338 (2)	H11C···C8^{xii}	3.0797
C10···O2^{x}	3.367 (3)	H11C···H8C^{xii}	2.5529
O1—Cu1—O4	90.29 (5)	C4—C5—C6	119.53 (14)
O1—Cu1—O5	87.44 (6)	O4—C6—C5	123.26 (14)
O1—Cu1—O1^{i}	180.00	O4—C6—C7	114.21 (15)
O1—Cu1—O4^{i}	89.71 (5)	C5—C6—C7	122.52 (15)
O1—Cu1—O5^{i}	92.56 (6)	O5—C9—N1	125.16 (17)
O4—Cu1—O5	87.33 (5)	C1—C2—H2	119.38
O1^{i}—Cu1—O4	89.71 (5)	C3—C2—H2	119.39
O4—Cu1—O4^{i}	180.00	C6—C7—H7A	109.52
O4—Cu1—O5^{i}	92.67 (5)	C6—C7—H7B	109.45
O1^{i}—Cu1—O5	92.56 (6)	C6—C7—H7C	109.46
O4^{i}—Cu1—O5	92.67 (5)	H7A—C7—H7B	109.47
O5—Cu1—O5^{i}	180.00	H7A—C7—H7C	109.50
O1^{i}—Cu1—O4^{i}	90.29 (5)	H7B—C7—H7C	109.42
O1^{i}—Cu1—O5^{i}	87.44 (6)	C3—C8—H8A	109.43
O4^{i}—Cu1—O5^{i}	87.33 (5)	C3—C8—H8B	109.48
Cu1—O1—C1	126.09 (11)	C3—C8—H8C	109.46
C3—O2—C4	122.47 (13)	H8A—C8—H8B	109.47
Cu1—O4—C6	128.72 (11)	H8A—C8—H8C	109.43
Cu1—O5—C9	120.37 (13)	H8B—C8—H8C	109.55
C9—N1—C10	121.90 (17)	O5—C9—H9	117.39
C9—N1—C11	120.71 (18)	N1—C9—H9	117.45
C10—N1—C11	117.35 (18)	N1—C10—H10A	109.46
O1—C1—C2	116.55 (14)	N1—C10—H10B	109.52
O1—C1—C5	125.50 (14)	N1—C10—H10C	109.50
C2—C1—C5	117.94 (14)	H10A—C10—H10B	109.46
C1—C2—C3	121.23 (15)	H10A—C10—H10C	109.40
O2—C3—C2	121.52 (15)	H10B—C10—H10C	109.48
O2—C3—C8	111.62 (15)	N1—C11—H11A	109.47
C2—C3—C8	126.86 (16)	N1—C11—H11B	109.47
O2—C4—O3	113.66 (15)	N1—C11—H11C	109.50
O2—C4—C5	117.70 (14)	H11A—C11—H11B	109.48
O3—C4—C5	128.63 (16)	H11A—C11—H11C	109.43
C1—C5—C4	119.01 (14)	H11B—C11—H11C	109.47
C1—C5—C6	121.40 (14)		

O4—Cu1—O1—C1	−22.49 (15)	C2—C1—C5—C6	−174.68 (16)
O4^{xvi}—Cu1—O1—C1	157.51 (15)	O1—C1—C5—C4	−178.35 (16)
O1—Cu1—O4—C6	19.61 (16)	C2—C1—C5—C4	2.3 (2)
O1^{xvi}—Cu1—O4—C6	−160.39 (16)	O3—C4—C5—C6	−3.7 (3)
Cu1—O1—C1—C5	15.0 (2)	O2—C4—C5—C6	177.92 (15)
Cu1—O1—C1—C2	−165.66 (12)	O3—C4—C5—C1	179.2 (2)
O1—C1—C2—C3	176.54 (17)	O2—C4—C5—C1	0.8 (2)
C5—C1—C2—C3	−4.1 (3)	Cu1—O4—C6—C5	−8.1 (3)
C1—C2—C3—O2	2.5 (3)	Cu1—O4—C6—C7	172.88 (13)
C1—C2—C3—C8	−177.56 (19)	C1—C5—C6—O4	−8.3 (3)
C4—O2—C3—C2	1.0 (3)	C4—C5—C6—O4	174.68 (16)
C4—O2—C3—C8	−178.96 (18)	C1—C5—C6—C7	170.61 (18)
C3—O2—C4—O3	178.73 (17)	C4—C5—C6—C7	−6.4 (3)
C3—O2—C4—C5	−2.6 (3)	C10—N1—C9—O5	179.3 (2)
O1—C1—C5—C6	4.6 (3)	C11—N1—C9—O5	1.8 (3)

Symmetry codes: (i) −*x*, −*y*, −*z*; (ii) *x*, *y*+1, *z*; (iii) −*x*, −*y*−1, −*z*; (iv) *x*−1, *y*, *z*; (v) *x*, *y*, *z*+1; (vi) −*x*+1, −*y*−1, −*z*; (vii) *x*+1, *y*, *z*; (viii) −*x*+1, −*y*, −*z*+1; (ix) −*x*, −*y*, −*z*+1; (x) *x*, *y*, *z*−1; (xi) *x*, *y*−1, *z*; (xii) −*x*, −*y*−1, −*z*+1; (xiii) −*x*+1, −*y*, −*z*; (xiv) *x*−1, *y*, *z*+1; (xv) *x*+1, *y*, *z*−1; (xvi) −*x*, −*y*, −*z*.

Fig. 1

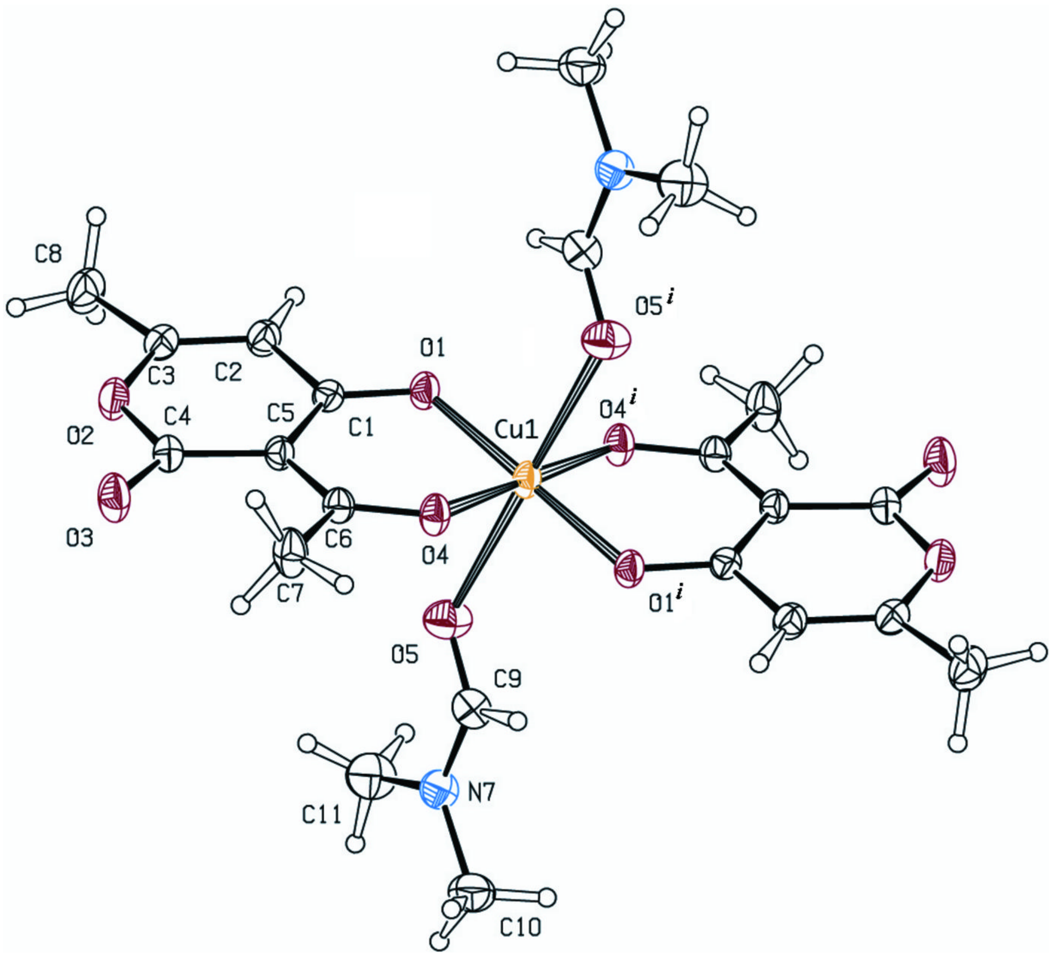

Fig. 2