Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis(cinnamato-κO)bis[2-(dimethylamino)ethanol-$\kappa^2 N,O$]copper(II)

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Received 9 March 2007
Accepted 20 March 2007

Key indicators

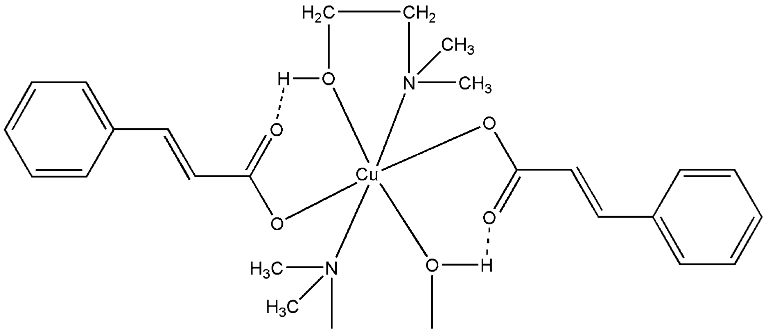
Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.003 Å
Disorder in main residue
R factor = 0.038
wR factor = 0.108
Data-to-parameter ratio = 16.4

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The Cu atom in the title complex, $[Cu(C_9H_7O_2)(C_4H_{11}NO)_2]$, lies on an inversion centre in an octahedral geometry and is coordinated by two bidentate chelating 2-(dimethylamino)ethanol groups and two monodentate cinnamate groups which are mutually *trans* to each other. The non-coordinated O atoms of the cinnamate ligands form intramolecular hydrogen bonds to the OH groups of the 2-(dimethylamino)ethanol ligands, generating six-membered rings.

Comment

There has been considerable interest in the development of chemical routes for the deposition of copper, copper(II) oxide and complex oxides containing copper, which have a number of important industrial applications. For instance, copper oxide is a component of high T_c superconductors (Catania *et al.* 1990) and, because of its excellent electrical conductivity and good resistance to eletromigration, copper metal is used as an alternative to aluminium alloys for multi-level metallization applications in Ultra Large Scale Integration (ULSI) technology (Torres *et al.*, 1996; Li *et al.*, 1994)



(I)

The solid-state structures of octahedral complexes of the type $M(OAc)_2(dmaeH)_2$ {OAc is acetate ($OCOCH_3$) and dmaeH is 2-(dimethylamino)ethanol [$(CH_3)_2NCH_2CH_2OH$]} have recently been reported for Co^{II} (Tahir *et al.*, 2006), Ni^{II} (Williams *et al.*, 2001) and Cu^{II} (Mazhar *et al.*, 2006). Such complexes are potential precursors for chemical vapor deposition to form ceramic oxides used in ceramic material applications.

We report here the structure of an analogous dmaeH/cinnamate complex, (I) (Fig. 1 and Table 1). The copper ion lies on an inversion centre in an octahedral geometry. The coordination environment contains two bidentate chelating 2-(dimethylamino)ethanol groups and two monodentate cinnamate groups. The N atoms are in mutually *trans* positions.

The Cu—O1 bond length of 1.966 (12) Å is significantly shorter than Cu—O3 [2.360 (12) Å] and is comparable to the distances in $[Cu(dmae)(OCOCH_3)(H_2O)]_2$ (Mazhar *et al.*, 2006). The Cu—N [2.124 (14) Å] bond lengths are comparable to those in other copper complexes containing aminoalcohol ligands, such as $Cu(OCHMeCH_2NMe_2)_2$ [Cu—N = 2.052 (3) Å; Goel *et al.*, 1990] and $[Cu(OCMe_2CH_2NMe_2)_2]$ [Cu—N = 2.052 (3) Å; Park *et al.* 2004]. The bite angle of the dmaeH ligand, O—Cu—N, is significantly less than 90° [81.27 (5)°], but is closely comparable to the angle in its cobalt counterpart $[Co(CH_3CO_2)_2(dmaeH)_2]$ [81.67 (5)°; Tahir *et al.*, 2006]. Two intramolecular hydrogen bonds link the hydroxyl function of each dmaeH group with the non-coordinated O atoms of the cinnamate groups (Table 2).

Experimental

2-(Dimethylamino)ethanol (0.1 ml, 1.0 mmol) was added to a stirred solution of $Cu(cinnamate)_2 \cdot 2H_2O$ (0.281 g, 1.0 mmol) in 20 ml toluene. Two hours of continuous stirring at room temperature followed by removal of all volatiles *in vacuo* gave a dry powder of (I). Blue block-shaped crystals suitable for single-crystal X-ray analysis were obtained from a concentrated solution in toluene at room temperature after 2 d.

Crystal data

$[Cu(C_9H_7O_2)(C_4H_{11}NO)_2]$
$M_r = 536.11$
Orthorhombic, *Pbca*
$a = 10.4570$ (1) Å
$b = 10.4520$ (1) Å
$c = 23.2770$ (4) Å
$V = 2544.10$ (6) Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 0.90$ mm^{-1}
$T = 150$ (2) K
0.25 × 0.20 × 0.20 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
$T_{min} = 0.763$, $T_{max} = 0.835$
34803 measured reflections
2913 independent reflections
2210 reflections with $I > 2\sigma(I)$
$R_{int} = 0.053$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.108$
$S = 1.15$
2913 reflections
178 parameters
9 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max} = 0.42$ e Å^{-3}
$\Delta\rho_{min} = -0.39$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.9666 (12)	Cu1—N1^i	2.1246 (14)
Cu1—O1^i	1.9667 (12)	Cu1—O3^i	2.3605 (14)
Cu1—N1	2.1246 (14)	Cu1—O3	2.3605 (14)
O1—Cu1—O1^i	180.0	O1^i—Cu1—O3^i	87.50 (5)
O1—Cu1—N1	89.68 (5)	N1—Cu1—O3^i	98.80 (6)
O1—Cu1—N1^i	90.32 (5)	N1—Cu1—O3	81.20 (6)
N1—Cu1—N1^i	180.0	O3^i—Cu1—O3	179.998 (1)
O1—Cu1—O3^i	92.50 (5)		

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

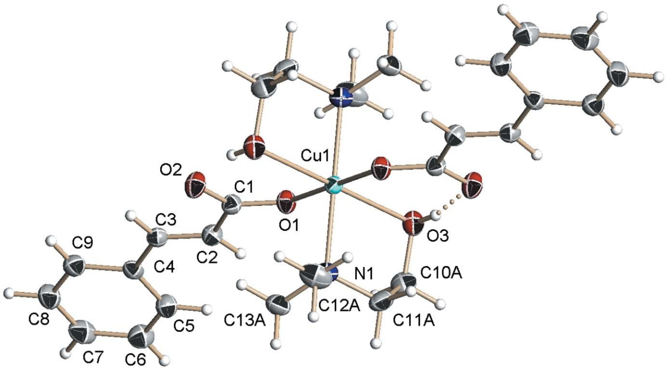


Figure 1
The molecular structure of the title complex, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Atoms of the minor disorder component are omitted for clarity and the intramolecular hydrogen bond is shown as a dashed line. Labelled atoms are related to unlabelled ones by the symmetry operation $(1 - x, -y, 1 - z)$.

Table 2
Hydrogen-bond geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O3—H3$A\cdots$O2^i	0.797 (16)	1.886 (17)	2.6650 (18)	166 (2)

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

The dmae ligand was found to be disordered over two positions with refined occupancy factors of 0.876 (2) and 0.124 (2). Equivalent bonding distances within both ligands were restrained to be the same within a standard deviation of 0.02 Å and the anisotropic displacement parameters of equivalent atoms were set to be identical. The hydroxyl H atom was located in a difference density Fourier map and was refined with an isotropic diplacement parameter 1.5 times U_{eq} of the O atom. The O—H distance was restrained to be 0.84 (2) Å. All other H atoms were placed in calculated positions, with C—H = 0.98, 0.99 and 0.95 Å for methyl, methylene and alkene H atoms, respectively, and were refined with isotropic displacement parameters 1.5 (methyl and hydroxyl) or 1.2 (methylene and alkene) times U_{eq} of the parent C atom. Methyl H atoms were allowed to rotate to best fit the experimental electron density.

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The Higher Education Commission of Pakistan is acknowledged for funding through the 200 merit scholarship scheme.

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