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Bis[μ-2-(1*H*-imidazol-2-yl)phenolato]-bis[chloromethanolcopper(II)]

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.036
wR factor = 0.084
Data-to-parameter ratio = 16.5

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

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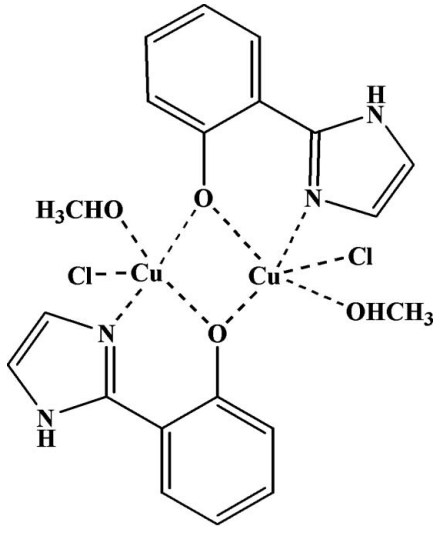
In the title complex, $[Cu_2(C_9H_7N_2O)_2Cl_2(CH_4O)_2]$, the two copper(II) ions are bridged by phenolate O atoms. Each Cu is further coordinated by one imidazole N atom, one chloride ion and a methanol molecule. The metal ions adopt a distorted square-pyramidal geometry. A crystallographic twofold rotation axis passes through the mid-point of the Cu···Cu vector.

Comment

The phenolate anion is one of the strong bridging ligands for the building of dinuclear transition metal complexes (Gavrilova *et al.*, 2004). Modification of the phenolate anion in its *ortho* position(s) with a secondary coordinating atom can lead to the formation of stable dinuclear complexes through chelation. Copper complexes of pyridyl-modified phenolate ligands have been characterized (Otter *et al.*, 1997).



(I)

In the title compound, (I), two phenolate anions hold the two Cu^{II} ions together with O as the bridging atom. Each Cu^{II} ion is further coordinated by one imidazole N atom, one O atom from methanol and one chloride ion. Each Cu adopts an approximately square-pyramidal geometry. A crystallographic twofold rotation axis passes through the mid-point of the Cu···Cu vector. The angle between the least-squares planes of the phenol and the imidazole rings is 14.9 (3)°. One 2-(1*H*-imidazol-2-yl)phenolate ligand is almost perpendicular to the other within the same complex. The distance between the two Cu^{II} ions is 3.0176 (10) Å, which is shorter than the sum of the covalent radii of two Cu^{II} ions (3.04 Å), indicating that there is a weak interaction between the two Cu^{II} ions.

Experimental

Equimolar quantities of 2-(1*H*-imidazol-2-yl)phenol, prepared according to the literature method of Bishop *et al.* (2002), and anhydrous copper chloride were dissolved separately in methanol (10 ml). The solutions were mixed and stirred for 1 h. Dark-brown crystals were obtained after 3 d by slow evaporation of the solution at room temperature.

Crystal data

$[Cu_2(C_9H_7N_2O)_2Cl_2(CH_4O)_2]$
M_r = 580.40
Monoclinic, $C2/c$
a = 20.574 (4) Å
b = 8.4773 (17) Å
c = 16.859 (3) Å
β = 127.12 (3)°
V = 2344.6 (12) Å^3
Z = 4
D_x = 1.644 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 2.08 mm^{-1}
T = 293 (2) K
Prism, dark brown
0.20 × 0.20 × 0.10 mm

Data collection

Bruker SMART 1K CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
T_{min} = 0.682, T_{max} = 0.819
17383 measured reflections
2539 independent reflections
1483 reflections with $I > 2\sigma(I)$
R_{int} = 0.088
θ_{max} = 27.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.084
S = 1.00
2539 reflections
154 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0222P)^2 + 5.6781P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.54 e Å^{-3}

H atoms on N2 and O2 were refined [refined distances: H—N = 0.76 (4), H—O = 0.70 (4) Å], while the other H atoms were geometrically constrained and refined in riding mode as follows: methyl C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C); aromatic C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT-Plus* (Bruker, 1998); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

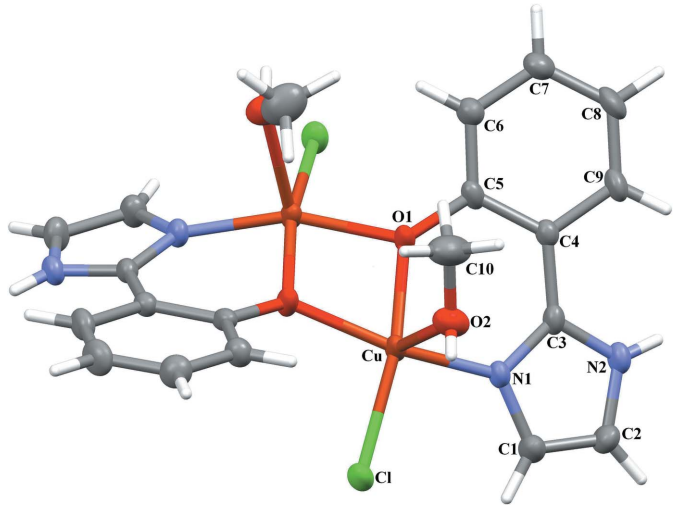


Figure 1
Diagram of (I), with displacement ellipsoids drawn at the 30% probability level and H atoms drawn as spheres of arbitrary radii.

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