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catena-Poly[[bis(2-amino-1,3-benzothiazole-κN^3)-copper(II)]-μ-adipato-$\kappa^4 O,O':O'',O'''$]

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In the title polymeric complex, $[Cu(C_6H_8O_4)_2(C_7H_6N_2S)_2]_n$, the Cu^{II} centres are bridged by the dicarboxylate ions in a bis-bidentate fashion, forming polymeric chains. The Cu atoms and dicarboxylate bridges both lie on inversion centres. Interchain N—H$\cdots$O hydrogen bonds connect the chains into two-dimensional layers.

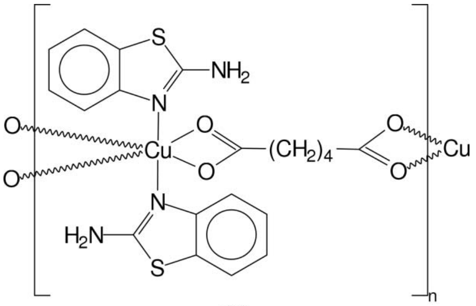
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
Disorder in main residue
R factor = 0.022
wR factor = 0.061
Data-to-parameter ratio = 12.0

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

Comment

The Cu^{II} complexes of dicarboxylic acids are of interest because of their rich variety of structural features and their interesting magnetic properties. A knowledge of the structure is needed to allow an interpretation of the magnetic properties of polynuclear complexes with paramagnetic centres. It has been shown that two paramagnetic centres could interact through extended bridging ligands, even if these centres are relatively far away from each other (Verdaguer *et al.*, 1984). This work forms part of a continuing study of Cu^{II} complexes with dicarboxylate anions and 2-aminobenzothiazole (Sieroń & Bukowska-Strzyżewska, 2000) and benzimidazole (Sieroń & Bukowska-Strzyżewska, 1999; Sieroń, *et al.*, 2002).



(I)

In the title structure, (I), each Cu^{II} atom and each adipate dianion is located on an inversion centre. The Cu^{II} atoms are connected by bridging of the bis-bidentate dicarboxylate ions to form polymeric chains (Fig. 1), $[Cu(C_6H_8O_4)_2(C_7H_6N_2S)_2]_\infty$, extending along the *b* axis. Neighbouring chains are held together *via* N–H$\cdots$O hydrogen bonds (Table 2), leading to the two-dimensional association illustrated in Fig. 2. Atom H21 of the NH$_2$ group does not contribute to the hydrogen-bonding network.

The equatorial plane of the Cu^{II} atom is formed by two short Cu—O and two short Cu—N bonds [Cu—O = 1.9433 (13) and Cu—N = 2.0244 (15) Å]. The carboxylate groups form four-membered unsymmetrical chelate rings and complete the Cu^{II} coordination to sixfold (4+2) by long Cu—O bonds of length 2.6079 (14) Å.

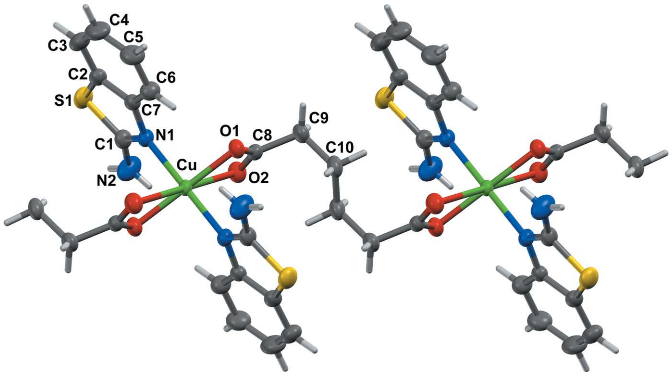


Figure 1
A fragment of the polymeric structure of (I). Displacement ellipsoids are drawn at the 50% probability level. The minor component of the disordered adipate chain has been omitted for clarity. Unlabelled atoms in the ligands attached to Cu are related to labelled atoms by $-x, 1-y, 1-z$ and atoms in the right half are related to those in the left by $-x, 2-y, 1-z$.

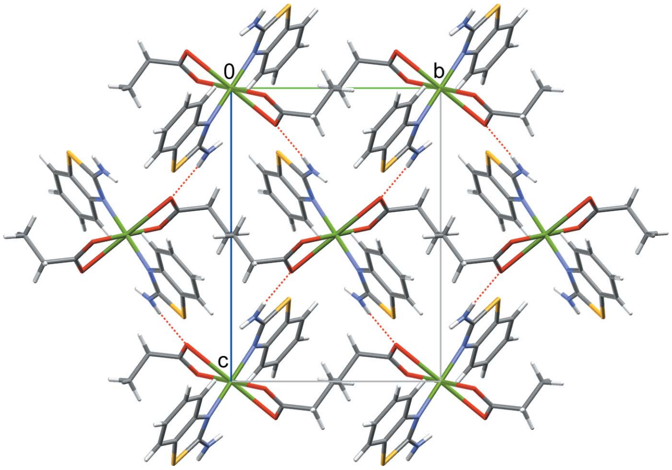


Figure 2
The two-dimensional association of polymeric chains in the structure of (I), formed *via* N—H···O hydrogen bonds (dashed lines).

According to Brown (1994), the correlation between bond length and bond valence represents a measure of the strength of a bond that is independent of the atomic size. The valence-sum rule states that the sum of the valences of the bond formed by an atom is equal to the valence (formal oxidation state) of the atom ($V_i = \Sigma \nu_{ij}$). The bond valences were computed according to Brown (1992, 1997) and O'Keeffe & Brese (1991) as $\nu_{ij} = \exp[(R_{ij} - d_{ij})/0.37]$, where R_{ij} is the bond-valence parameter (formally, it is the single-bond length between the i and j atoms) and d_{ij} is the observed bond length. The application of this correlation allows the comparison of the relative importance of the Cu—O and Cu—N bonds of the Cu polyhedra, and to check the valence-sum rule for the Cu^{II} atom (Brown, 2002). R_{Cu-O} and R_{Cu-N} were taken as 1.679 and 1.713 Å (Sieroń & Bukowska-Strzyżewska, 1999). The computed bond valences of the Cu^{II} atom of (I) show that the Cu—O bonds are distinctly stronger than the Cu—N bonds (ν_{Cu-O1} = 0.490 v.u. and ν_{Cu-N1} = 0.431 v.u.). The longer axial Cu—O2 bonds are very weak, with a bond valence ν_{Cu-O2} = 0.081 v.u. Thus, the computed valence of the Cu^{II} atom (V_{Cu}) is 2.004 v.u.

A similar coordination around the Cu atom was observed in the complexes *catena*-poly[bis(benzimidazole-N^3)copper(II)-μ-suberato-$O,O':O'',O'''$] and *catena*-poly[bis(benzimidazole-N^3)copper(II)-μ-sebacato-$O,O':O'',O'''$] dihydrate (Sieroń & Bukowska-Strzyżewska, 1999).

The intrachain Cu···Cu distance of 9.3336 (2) Å is longer than the shortest interchain Cu···Cu distance of 8.5169 (2) Å.

Experimental

The title complex was prepared by dissolving equimolar quantities (1 mmol) of 2-aminobenzothiazole ($C_7H_6N_2S$), adipic acid ($C_6H_{10}O_4$) and copper(II) chloride dihydrate ($CuCl_2 \cdot 2H_2O$) in water (100 ml). After heating to boiling, the solution was filtered and allowed to cool. Crystals of (I) suitable for X-ray diffraction formed after several days.

Crystal data

$[Cu(C_6H_8O_4)_2(C_7H_6N_2S)_2]$
M_r = 508.09
Monoclinic, $P2_1/n$
a = 8.6406 (2) Å
b = 9.3336 (2) Å
c = 13.3911 (3) Å
β = 102.719 (2)°
V = 1053.46 (4) Å^3
Z = 2
D_x = 1.602 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.27 mm^{-1}
T = 295 K
Prism, violet
0.30 × 0.20 × 0.15 mm

Data collection

Kuma KM4 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2006)
T_{min} = 0.702, T_{max} = 0.832
10766 measured reflections
1852 independent reflections
1665 reflections with $I > 2\sigma(I)$
R_{int} = 0.016
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.061
S = 1.10
1852 reflections
154 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.028P)^2 + 0.6815P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ < 0.001
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu—O1	1.9433 (13)	O1—C8	1.274 (2)
Cu—O2	2.6079 (14)	O2—C8	1.249 (2)
Cu—N1	2.0244 (15)	N1—C1	1.313 (2)
S1—C1	1.7492 (19)	N1—C7	1.402 (2)
S1—C2	1.7451 (19)	N2—C1	1.332 (3)
O1—Cu—O2	55.85 (5)	Cu—O2—C8	75.52 (10)
O1—Cu—N1	91.74 (6)	Cu—N1—C1	123.92 (12)
O2—Cu—N1	88.49 (5)	Cu—N1—C7	124.04 (11)
C1—S1—C2	89.23 (9)	C1—N1—C7	111.01 (15)
Cu—O1—C8	105.61 (11)		

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

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
N2—H22⋯O2^{i}	0.82 (3)	2.05 (3)	2.859 (3)	171 (3)
C5—H5⋯O1^{ii}	0.93	2.58	3.429 (3)	152

Symmetry codes: (i) $-x-\frac{1}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x+1, -y+1, -z+1$.

Atom C10/C10′, together with attached H atoms, in the adipate ion chain is disordered over two positions, with site occupancies of 0.88 and 0.12. This site occupancy was determined by constraining the two sites to sum to 1.0 while refining an overall isotropic displacement parameter. Once the site occupancies had been determined, they were fixed and not further refined. In the final stage of the refinement, atom C10 was refined anisotropically and atom C10′ isotropically. The geometry of the disordered chain was restrained to reasonable values. The aromatic and methylene H atoms were positioned with idealized geometry, with C—H = 0.93 and 0.97 Å, respectively, and refined with fixed isotropic displacement parameters using a riding model, with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C). The amine H atoms were located in a difference Fourier synthesis and their positions and isotropic displacement parameters were refined freely.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2003); program(s) used to refine structure: *SHELXTL*; molecular graphics: *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *PLATON* (Spek, 2003).

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