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Di-μ-glutarato-bis[(*N*,*N*,*N*′,*N*′-tetraethylethylenediamine)copper(II)]

BY AARNE PAJUNEN AND SEIJA PAJUNEN

Department of Inorganic Chemistry, University of Helsinki, Vuorikatu 20, *SF*-00100 *Helsinki* 10, *Finland*

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Abstract. $[Cu(C_{10}H_{24}N_2)(C_5H_6O_4)]_2$, $(C_{15}H_{30}CuN_2O_4)_2$, monoclinic, $P2_1/n$, a = 9·365 (4), b = 15·211 (15), c = 12·738 (11) Å, β = 105·33 (5)°, Z = 2, D_m = 1·39, D_c = 1·39 Mg m^{-3}. The structure was refined to R = 0·059 for 1752 observed reflections. The structure is dimeric. Cu is coordinated to the N atoms of the diamine and to four O atoms of two different glutarate ions.

Introduction. Blue crystals of the title compound were prepared from $CuCO_3$, glutaric acid and *N*,*N*,*N*′,*N*′-tetraethylethylenediamine (Pajunen & Näsäkkälä, 1977) and recrystallized from ethanol. The space group was determined as $P2_1/n$ from systematic absences. The cell parameters and intensities of 3410 reflections up to 2θ = 50° were measured on a Syntex $P2_1$ four-circle diffractometer with monochromatized Mo $K\alpha$ radiation (λ = 0·7107 Å). Of these, 1752 were above the 2σ significance level. The structure was solved by direct methods with XRAY 76 (Stewart, Machin, Dickinson, Ammon, Heck & Flack, 1976) and refined by block-diagonal least squares. Anisotropic refinement of the nonhydrogen atoms converged at R = 0·104. The H atoms were located from a difference map and included in the refinement with a fixed U = 0·06 Å^2. Further refinement converged at R = 0·059. Scattering factors for H were those of Stewart, Davidson & Simpson (1965) and for other atoms those of Cromer & Mann (1968). Real and imaginary anomalous-dispersion terms were included for Cu. The final positional parameters are given in Table 1.* The molecular structure is shown in Fig. 1 and bond lengths and angles are listed in Table 2.

Discussion. The structure is dimeric (Fig. 1). The carboxylate groups of the glutarate ions are coordinated to different Cu atoms, so that the glutarate ions and Cu form 16-membered rings. The coordination of the ligands is similar to that in adipato(*N*,*N*-diethylethylenediamine)copper(II) (Pajunen & Näsäkkälä, 1977), but differs from that in glutarato(*N*,*N*,*N*′,*N*′-tetramethylethylenediamine)copper(II) (Pajunen & Pa-

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 33995 (12 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

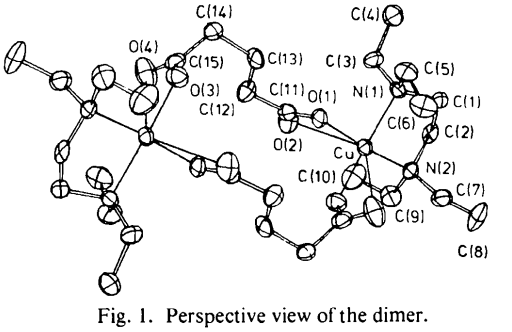

Fig. 1. Perspective view of the dimer.

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Table 1. *Fractional coordinates* ($\times 10^4$, *for* H $\times 10^3$)

	x	y	z		x	y	z
Cu	3933 (1)	6317 (1)	2297 (1)	C(5)	1245 (13)	5291 (8)	1433 (10)
O(1)	3549 (8)	5643 (5)	3517 (5)	C(6)	2274 (14)	4668 (8)	1078 (11)
O(2)	3751 (10)	6992 (5)	4229 (7)	C(7)	4773 (12)	6520 (8)	272 (9)
O(3)	3958 (8)	3709 (5)	7020 (6)	C(8)	4978 (17)	6982 (9)	−737 (10)
O(4)	3955 (11)	4991 (6)	7845 (7)	C(9)	5120 (14)	7848 (8)	1405 (10)
N(1)	1701 (8)	6227 (5)	1498 (6)	C(10)	4796 (18)	8348 (9)	2352 (12)
N(2)	4129 (9)	7084 (5)	1010 (6)	C(11)	3601 (11)	6186 (6)	4301 (8)
C(1)	1524 (11)	6603 (8)	374 (8)	C(12)	3393 (13)	5787 (7)	5347 (9)
C(2)	2611 (12)	7365 (7)	478 (8)	C(13)	2381 (12)	4984 (7)	5168 (8)
C(3)	834 (12)	6779 (8)	2080 (9)	C(14)	1994 (11)	4696 (7)	6227 (8)
C(4)	−837 (13)	6743 (9)	1615 (10)	C(15)	3388 (12)	4466 (7)	7114 (9)
H(C1)	43 (13)	687 (8)	23 (9)	H′(C7)	571 (13)	643 (8)	69 (9)
H′(C1)	173 (13)	618 (7)	−4 (10)	H(C8)	409 (13)	726 (8)	−102 (9)
H(C2)	237 (13)	769 (8)	−31 (9)	H′(C8)	596 (13)	745 (8)	−52 (10)
H′(C2)	224 (13)	776 (8)	93 (9)	H″(C8)	503 (13)	678 (8)	−126 (9)
H(C3)	108 (12)	653 (8)	282 (9)	H(C9)	511 (13)	835 (8)	92 (9)
H′(C3)	100 (13)	736 (8)	213 (9)	H′(C9)	626 (12)	769 (8)	164 (9)
H(C4)	−133 (13)	721 (8)	181 (10)	H(C10)	566 (13)	866 (8)	257 (9)
H′(C4)	−133 (13)	691 (8)	75 (9)	H′(C10)	449 (13)	796 (8)	275 (9)
H″(C4)	−109 (13)	621 (7)	168 (10)	H″(C10)	393 (13)	872 (7)	204 (9)
H(C5)	117 (13)	516 (8)	213 (9)	H(C12)	305 (13)	612 (7)	562 (10)
H′(C5)	38 (13)	519 (8)	122 (9)	H′(C12)	445 (13)	557 (8)	577 (9)
H(C6)	209 (13)	415 (8)	128 (9)	H(C13)	269 (13)	449 (8)	479 (9)
H′(C6)	250 (13)	485 (8)	19 (9)	H′(C13)	149 (13)	511 (9)	466 (9)
H″(C6)	319 (13)	464 (8)	162 (9)	H(C14)	135 (13)	401 (8)	606 (9)
H(C7)	426 (13)	597 (8)	15 (9)	H′(C14)	142 (13)	517 (8)	643 (9)

Table 2. *Bond lengths* (Å) *and angles* (°)

Cu–N(1)	2·073 (7)	C(13)–C(14)	1·550 (16)
Cu–N(2)	2·059 (9)	C(14)–C(15)	1·524 (13)
Cu–O(1)	1·973 (7)	C(11)–O(1)	1·286 (13)
Cu–O(2)	2·714 (9)	C(11)–O(2)	1·241 (13)
Cu–O(3)^{i}	1·937 (7)	C(15)–O(3)	1·288 (14)
Cu–O(4)^{i}	2·845 (10)	C(15)–O(4)	1·235 (14)
C(1)–C(2)	1·525 (15)	N(1)–C(1)	1·509 (13)
C(3)–C(4)	1·520 (15)	N(1)–C(3)	1·495 (15)
C(5)–C(6)	1·504 (19)	N(1)–C(5)	1·483 (14)
C(7)–C(8)	1·521 (19)	N(2)–C(2)	1·467 (13)
C(9)–C(10)	1·524 (21)	N(2)–C(7)	1·512 (15)
C(11)–C(12)	1·523 (16)	N(2)–C(9)	1·489 (14)
C(12)–C(13)	1·527 (15)		
N(1)–Cu–N(2)	86·4 (3)	C(1)–N(1)–C(3)	108·7 (8)
N(1)–Cu–O(1)	89·0 (3)	C(1)–N(1)–C(5)	110·7 (8)
N(1)–Cu–O(2)	100·0 (3)	C(3)–N(1)–C(5)	112·3 (9)
N(1)–Cu–O(4)^{i}	123·4 (3)	C(2)–N(2)–C(7)	112·0 (7)
N(2)–Cu–O(2)	123·2 (3)	C(2)–N(2)–C(9)	111·7 (8)
N(2)–Cu–O(3)^{i}	94·3 (3)	C(7)–N(2)–C(9)	109·7 (9)
N(2)–Cu–O(4)^{i}	97·8 (3)	N(1)–C(1)–C(2)	107·6 (7)
O(1)–Cu–O(2)	54·1 (3)	N(2)–C(2)–C(1)	111·2 (8)
O(1)–Cu–O(3)^{i}	90·6 (3)	N(1)–C(3)–C(4)	115·1 (9)
O(1)–Cu–O(4)^{i}	87·8 (3)	N(1)–C(5)–C(6)	115·0 (10)
O(2)–Cu–O(3)^{i}	84·3 (3)	N(2)–C(7)–C(8)	115·1 (10)
O(2)–Cu–O(4)^{i}	122·2 (2)	N(2)–C(9)–C(10)	114·8 (11)
O(3)^{i}–Cu–O(4)^{i}	51·0 (3)	O(1)–C(11)–O(2)	124·0 (10)
Cu–N(1)–C(1)	106·5 (6)	O(1)–C(11)–C(12)	115·9 (9)
Cu–N(1)–C(3)	109·2 (6)	O(2)–C(11)–C(12)	120·1 (10)
Cu–N(1)–C(5)	109·2 (6)	C(11)–C(12)–C(13)	113·9 (8)
Cu–N(2)–C(2)	104·7 (6)	C(12)–C(13)–C(14)	112·0 (8)
Cu–N(2)–C(7)	107·9 (6)	C(13)–C(14)–C(15)	111·0 (9)
Cu–N(2)–C(9)	110·6 (6)	C(14)–C(15)–O(3)	115·5 (9)
Cu–O(1)–C(11)	107·5 (6)	C(14)–C(15)–O(4)	121·5 (10)
Cu–O(3)^{i}–C(15)^{i}	112·0 (6)	O(3)–C(15)–O(4)	122·8 (9)

Symmetry code

(i) $1-x, 1-y, 1-z$

junen, 1977). The Cu atom is joined by four short bonds to two N atoms of the diamine and two O atoms of different glutarate ions. The coordination is nearly planar, as Cu is displaced only 0·019 Å from the mean plane of N(1), N(2), O(1) and O(3)^{i} [(i) $1-x$, $1-y$, $1-z$]. The diamine coordination plane Cu, N(1), N(2) forms an angle of 6·6° with the Cu, O(1), O(3)^{i} plane. The other O atoms of the carboxylate groups complete the coordination at longer distances.

Bond lengths and angles of the diamine and glutarate ions have the expected values. The C–O bonds of the strongly coordinated O(1) and O(3) are somewhat longer than those of the weakly coordinated O(2) and O(4). Within the crystal the dimers are held together only by normal van der Waals forces.

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