Crystal structure of zinc suberate, $C_8H_{12}O_4Zn$

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Abstract

$C_8H_{12}O_4Zn$, monoclinic, $P12/c1$ (No. 13), $a = 21.242(2)$ Å, $b = 4.755(1)$ Å, $c = 9.366(1)$ Å, $\beta = 93.132(1)^\circ$, $V = 944.6$ Å³, $Z = 4$, $R_{gt}(F) = 0.046$, $wR_{ref}(F^2) = 0.116$, $T = 293$ K.

Source of material

The compound was synthesized from the reaction of 0.50 g (2.87 mmol) suberic acid with an excess of freshly prepared $ZnCO_3$ in 15 ml double-distilled water. Unreacted $ZnCO_3$ was removed and the filtrate was maintained at room temperature. Colorless plate-like crystals were grown by slow evaporation for several weeks.

Discussion

The Zn atoms are tetrahedrally coordinated (as in zinc succinate [1] and zinc glutarate [2]) by four carboxyl O atoms of different suberate ligands which bis-bidentately bridge four Zn atoms to a 3D network $\frac{1}{4}[Zn(C_8H_{12}O_4)_4]$. The ZnO_4 tetrahedra are slightly distorted with $d(Zn-O) = 1.948$ Å– 1.962 Å and $\angle O-Zn-O = 100.9^\circ$ – 116.6° . Two crystallographically independent suberate ligands have $\bar{1}$ symmetry with the middle C—C bonds centered at $2a$ and $2d$ positions, respectively, and all C and O atoms in the suberate groups are nearly coplanar. The C—O bond lengths vary from 1.251 Å to 1.268 Å and $\angle O-C-O$ are averaged at $120.9(3)^\circ$. The mean C—C bond length is about 1.518 Å with the shortest C—C bonds at the ends and the $\angle C-C-C$ bond angles range over 112.2° – 116.3° . Suberate ligands in the title compound bridge Zn atoms in different fashion from that in the diaquasubercobalt(II), $Co(C_8H_{12}O_4)(H_2O)_2$, where one terminal carboxyl group bridges two metal atoms and the other one chelates the third metal atom [3].

Table 1. Data collection and handling.

Crystal:	colorless thin plate, size $0.033 \times 0.178 \times 0.189$ mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ :	25.79 cm^{-1}
Diffractometer, scan mode:	Bruker P4, $\theta/2\theta$
$2\theta_{\max}$:	55°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	2959, 2079
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1499
$N(\text{param})_{\text{refined}}$:	120
Programs:	SHELXS-97 [4], SHELXL-97 [5]

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U_{iso}
H(2A)	4c	0.8376	0.9118	0.0582	0.05
H(2B)	4c	0.8664	0.6026	0.0908	0.05
H(3A)	4c	0.9333	0.6738	−0.1213	0.05
H(3B)	4c	0.9051	0.9845	−0.1350	0.05
H(4A)	4c	0.9879	0.7695	0.0984	0.05
H(4B)	4c	0.9615	1.1225	0.1115	0.05
H(6A)	4c	0.6017	0.7617	0.2553	0.05
H(6B)	4c	0.6486	0.7760	0.4001	0.05
H(7A)	4c	0.5992	1.1935	0.4796	0.05
H(7B)	4c	0.5589	1.2321	0.3230	0.05
H(8A)	4c	0.5476	0.8352	0.5458	0.05
H(8B)	4c	0.4999	0.7845	0.3739	0.05

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Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
Zn	4c	0.73993(2)	0.5345(1)	0.18452(5)	0.0240(3)	0.0249(3)	0.0294(3)	0.0014(2)	0.0090(2)	0.0028(2)
O(1)	4c	0.7623(2)	0.5126(7)	−0.0156(3)	0.032(2)	0.043(2)	0.028(2)	−0.012(2)	0.007(1)	−0.002(2)
O(2)	4c	0.8163(1)	0.5844(7)	−0.2048(3)	0.030(2)	0.049(2)	0.024(2)	−0.007(2)	0.009(1)	−0.004(2)
O(3)	4c	0.7185(1)	0.9335(6)	0.1993(4)	0.030(2)	0.023(2)	0.054(2)	0.003(1)	0.024(2)	0.004(2)
O(4)	4c	0.6647(1)	1.3211(6)	0.2252(4)	0.028(2)	0.023(2)	0.049(2)	0.000(1)	0.013(1)	0.002(2)
C(1)	4c	0.8100(2)	0.6066(9)	−0.0723(4)	0.033(2)	0.027(2)	0.025(2)	−0.002(2)	0.004(2)	0.002(2)
C(2)	4c	0.8618(2)	0.747(1)	0.0169(5)	0.039(3)	0.075(4)	0.027(2)	−0.024(3)	0.013(2)	−0.008(3)
C(3)	4c	0.9185(2)	0.839(1)	−0.0605(5)	0.041(3)	0.083(4)	0.029(2)	−0.027(3)	0.011(2)	−0.003(3)
C(4)	4c	0.9708(2)	0.958(1)	0.0400(6)	0.037(3)	0.082(4)	0.040(3)	−0.026(3)	0.004(2)	−0.003(3)
C(5)	4c	0.6719(2)	1.0592(9)	0.2455(5)	0.025(2)	0.023(2)	0.031(2)	−0.000(2)	0.004(2)	−0.000(2)
C(6)	4c	0.6237(2)	0.9041(9)	0.3265(5)	0.033(2)	0.026(2)	0.042(3)	0.003(2)	0.018(2)	0.008(2)
C(7)	4c	0.5745(2)	1.086(1)	0.3937(5)	0.031(2)	0.030(2)	0.039(3)	−0.001(2)	0.016(2)	0.003(2)
C(8)	4c	0.5250(2)	0.910(1)	0.4660(5)	0.033(2)	0.032(3)	0.043(3)	0.001(2)	0.020(2)	0.004(2)

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