Crystal structure of betaine dihydrogen selenite, $C_5H_{13}NO_5Se$

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Table 1. Parameters used for the X-ray data collection

Crystal:	colorless transparent prism, size 0.1 x 0.1 x 0.2 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	40.30 cm ⁻¹
Diffractometer:	Enraf Nonius CAD4
Scan mode:	profile data from $\omega/2\theta$
$T_{\text{measurement}}$:	293 K
$2\theta_{\text{max}}$:	60°
$N(hkl)_{\text{unique}}$:	1756
Criterion for I_o :	$I_o > 2 \sigma(I_o)$
$N(\text{param})_{\text{refined}}$:	114
Program:	SHELXL-93

Source of material: The title compound was synthesized by reaction of 1 mmol of betaine (Aldrich, 98% purity) and SeO_2 (Merck, 98% purity) in a 1:1:1 solution of isopropanol, methanol and water. Crystals were grown from this solution by cooling to 253 K for a few days.

The H_2SeO_3 molecules link the betaine molecules together by hydrogen bonds of 2.626(7) Å between O2 and O4 ($x-1/4, -y+3/4, z+1/4$) and 2.575(6) Å between O3 and O4 ($x-1/4, -y+3/4, z-3/4$). The geometry of the H_2SeO_3 molecule (two large and one short Se–O bonds) show that the protons have not been transferred to the betaine molecule and thus this compound should be classified as an adduct of the dihydrogen selenite acid. Related compounds: betaine trihydrogen phosphate and betaine trihydrogen arsenate (see ref. 7).

$C_5H_{13}NO_5Se$, orthorhombic, $Fdd2$ (No. 43), $a = 28.042(2)$ Å, $b = 21.815(2)$ Å, $c = 6.073(2)$ Å, $V = 3715.1$ Å³, $Z = 16$, $R(F) = 0.036$, $R_w(F^2) = 0.049$.

Table 2. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	x	y	z	U_{iso}
H(2)	16a	0.222(2)	0.3695(9)	0.685(7)	0.078
H(3)	16a	0.251(1)	0.359(2)	0.133(4)	0.070
H(2A)	16a	0.4052(2)	0.4949(2)	0.4959(9)	0.053
H(2B)	16a	0.3781(2)	0.4353(2)	0.5634(9)	0.053
H(3A)	16a	0.386(1)	0.5674(3)	0.910(3)	0.072
H(3B)	16a	0.3405(2)	0.5984(6)	0.812(6)	0.072
H(3C)	16a	0.386(1)	0.5913(7)	0.667(2)	0.072
H(4A)	16a	0.2900(6)	0.544(1)	0.559(2)	0.082
H(4B)	16a	0.307(1)	0.4817(2)	0.458(4)	0.082
H(4C)	16a	0.3335(4)	0.543(1)	0.398(2)	0.082
H(5A)	16a	0.2967(8)	0.5031(8)	0.928(4)	0.076
H(5B)	16a	0.3447(4)	0.474(2)	1.007(3)	0.076
H(5C)	16a	0.313(1)	0.4398(7)	0.832(2)	0.076

Table 3. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Se	16a	0.27337(2)	0.33236(2)	0.45629(8)	0.0354(2)	0.0302(2)	0.0420(2)	−0.0030(2)	−0.0041(3)	0.0011(3)
O(1)	16a	0.3253(1)	0.3511(1)	0.5523(7)	0.037(2)	0.053(2)	0.062(3)	−0.005(1)	−0.020(2)	−0.006(2)
O(2)	16a	0.2354(1)	0.3857(1)	0.5807(8)	0.053(2)	0.046(2)	0.057(3)	0.010(2)	0.008(2)	0.000(2)
O(3)	16a	0.2738(1)	0.3706(1)	0.2087(7)	0.045(2)	0.054(2)	0.042(2)	−0.012(2)	−0.006(3)	0.014(2)
O(4)	16a	0.4629(1)	0.4256(2)	0.688(1)	0.044(2)	0.068(2)	0.045(2)	0.025(2)	−0.002(3)	−0.001(2)
O(5)	16a	0.4297(1)	0.4734(1)	0.9732(8)	0.052(2)	0.052(2)	0.043(3)	0.007(2)	−0.009(3)	−0.006(2)
N	16a	0.3500(1)	0.5116(1)	0.702(1)	0.028(2)	0.029(2)	0.043(2)	0.001(1)	0.004(3)	0.001(2)
C(1)	16a	0.4305(2)	0.4578(2)	0.779(1)	0.039(3)	0.036(3)	0.038(4)	−0.001(2)	−0.001(3)	0.000(2)

Table 3. (Continued)

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
C(2)	16a	0.3910(2)	0.4735(2)	0.6196(9)	0.033(3)	0.034(2)	0.040(3)	−0.001(2)	0.000(3)	−0.001(2)
C(3)	16a	0.3673(2)	0.5726(2)	0.780(1)	0.046(3)	0.029(2)	0.069(5)	−0.002(2)	0.009(3)	−0.010(2)
C(4)	16a	0.3171(2)	0.5208(2)	0.512(1)	0.044(3)	0.053(3)	0.066(6)	0.005(2)	−0.018(3)	−0.002(3)
C(5)	16a	0.3237(2)	0.4791(2)	0.884(1)	0.046(3)	0.047(3)	0.058(5)	−0.005(2)	0.019(3)	0.000(3)

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