Crystal structure of sodium 2-(*N'*-n-dodecylureido) ethanesulfonate, $C_{15}H_{31}N_2O_4SNa$

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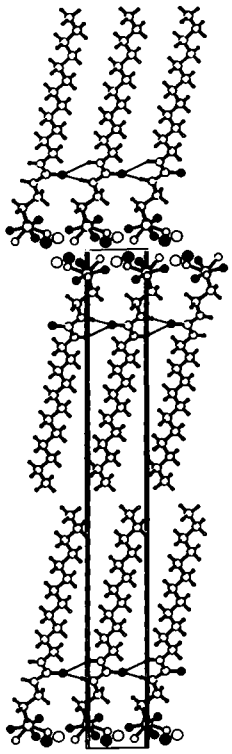

Source of material: 62.5 g (0.5 mol) taurine was dissolved in 500 ml 1 molar aqueous solution of sodium hydroxide. Under vigorous stirring 105.5 g (0.5 mol) n-dodecylisocyanate was added dropwise within 10 minutes to this mixture at 333 K. During this procedure the temperature increased short-time about 5 K – 8 K. Then the mixture was stirred for four hours at 333 K. *N,N'*- di-n-dodecyl urea formed as minor product was removed by filtration at high temperatures. At slow cooling down to room temperature the substance crystallizes quantitatively. Long plate shaped crystals were obtained by twice slow recrystallisation from water.

The sulfonate oxygen atoms and the sodium cation were found to be disordered. For each of them two positions and population parameters were refined.

$C_{15}H_{31}N_2NaO_4S$, triclinic, $P\bar{1}$ (No. 2), a =4.658(2) Å, b =5.467(2) Å, c =37.62(2) Å, α =91.19(3)°, β =90.47(4)°, γ =105.52(3)°, V =922.8 Å^3, Z =2, $R(F)$ =0.076, $R_w(F^2)$ =0.207.

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

Crystal:	colorless plate, size 0.01 x 0.30 x 0.42 mm
Wavelength:	Cu K_α radiation (1.54180 Å)
μ:	19.59 cm^{-1}
Diffractometer:	Enraf-Nonius CAD4
Scan mode:	$\theta/2\theta$
$T_{measurement}$:	298 K
$2\theta_{max}$:	91.65°
$N(hkl)_{unique}$:	1713
Criterion for I_o:	$I_o > 2\,\sigma(I_o)$
$N(param)_{refined}$:	245
Programs:	MolEN, SHELXS-86, SHELXL-93, SCHAKAL-92

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

Atom	Site	x	y	z	U_{iso}
H(21A)	2*i*	1.153(2)	2.064(1)	0.0774(2)	0.088
H(21B)	2*i*	1.204(2)	2.317(1)	0.0999(2)	0.088
H(22A)	2*i*	0.725(1)	2.206(1)	0.1184(2)	0.066
H(22B)	2*i*	0.646(1)	1.967(1)	0.0927(2)	0.066
H(1)	2*i*	1.071(1)	1.943(1)	0.1399(1)	0.062
H(2)	2*i*	0.968(1)	1.615(1)	0.1755(2)	0.070
H(1A)	2*i*	0.452(1)	1.283(1)	0.1782(2)	0.072
H(1B)	2*i*	0.447(1)	1.486(1)	0.2080(2)	0.072
H(2A)	2*i*	0.866(2)	1.403(1)	0.2349(2)	0.072
H(2B)	2*i*	0.860(2)	1.194(1)	0.2055(2)	0.072
H(3A)	2*i*	0.400(1)	0.958(1)	0.2254(2)	0.069
H(3B)	2*i*	0.399(1)	1.169(1)	0.2542(2)	0.069
H(4A)	2*i*	0.794(1)	0.860(1)	0.2547(2)	0.073
H(4B)	2*i*	0.803(1)	1.075(1)	0.2831(2)	0.073
H(5A)	2*i*	0.333(2)	0.635(1)	0.2749(2)	0.074
H(5B)	2*i*	0.338(2)	0.851(1)	0.3030(2)	0.074
H(6A)	2*i*	0.734(2)	0.756(1)	0.3325(2)	0.075
H(6B)	2*i*	0.726(2)	0.539(1)	0.3046(2)	0.075
H(7A)	2*i*	0.265(2)	0.534(1)	0.3521(2)	0.079
H(7B)	2*i*	0.262(2)	0.316(1)	0.3244(2)	0.079
H(8A)	2*i*	0.661(2)	0.444(1)	0.3822(2)	0.084
H(8B)	2*i*	0.654(2)	0.224(1)	0.3547(2)	0.084
H(9A)	2*i*	0.188(2)	0.222(1)	0.4020(2)	0.088
H(9B)	2*i*	0.185(2)	0.001(1)	0.3748(2)	0.088
H(10A)	2*i*	0.576(2)	–0.090(1)	0.4059(2)	0.094
H(10B)	2*i*	0.582(2)	0.133(1)	0.4329(2)	0.094
H(11A)	2*i*	0.101(2)	–0.299(2)	0.4255(2)	0.126
H(11B)	2*i*	0.122(2)	–0.080(2)	0.4536(2)	0.126
H(12A)	2*i*	0.221(2)	–0.424(2)	0.4806(3)	0.149
H(12B)	2*i*	0.507(2)	–0.194(2)	0.4829(3)	0.149
H(12C)	2*i*	0.485(2)	–0.414(2)	0.4547(3)	0.149

Table 3. Final atomic coordinates and displacement parameters (in $Å^2$)

Atom	Site	Occ.	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Na(1A)	2*i*	0.55(1)	0.318(2)	1.2388(9)	–0.0155(2)	0.067(6)	0.038(3)	0.056(5)	0.015(3)	–0.013(4)	–0.014(3)
Na(1B)	2*i*	0.45	0.520(2)	1.269(1)	–0.0244(2)	0.033(5)	0.026(4)	0.050(4)	0.009(4)	0.001(4)	–0.015(3)
S(1)	2*i*		0.9643(4)	1.3479(6)	0.04772(7)	0.040(1)	0.092(2)	0.064(2)	0.022(1)	0.008(1)	0.033(2)
O(1A)	2*i*	0.55(1)	0.774(3)	1.527(2)	0.0613(3)	0.042(7)	0.034(5)	0.070(7)	0.016(5)	–0.007(6)	–0.021(4)
O(2A)	2*i*	0.55(1)	1.258(2)	1.553(2)	0.0406(2)	0.039(6)	0.076(7)	0.070(7)	0.001(6)	–0.006(5)	0.010(6)
O(3A)	2*i*	0.55(1)	0.844(4)	1.191(2)	0.0248(3)	0.11(2)	0.053(6)	0.036(7)	0.040(8)	–0.023(8)	–0.026(5)
O(1B)	2*i*	0.45	0.967(3)	1.567(2)	0.0540(3)	0.023(8)	0.036(8)	0.041(7)	0.002(6)	–0.022(6)	–0.001(5)
O(2B)	2*i*	0.45	1.180(2)	1.295(2)	0.0180(2)	0.034(6)	0.033(6)	0.029(7)	0.017(4)	–0.001(5)	–0.023(4)
O(3B)	2*i*	0.45	0.642(3)	1.163(2)	0.0334(3)	0.021(6)	0.041(6)	0.048(7)	0.011(5)	–0.004(6)	–0.006(5)
C(21)	2*i*		1.059(2)	2.193(1)	0.0854(2)	0.056(5)	0.085(5)	0.059(5)	0.014(4)	0.006(4)	0.029(5)
C(22)	2*i*		0.802(1)	2.075(1)	0.1076(2)	0.056(4)	0.055(4)	0.042(4)	0.019(3)	–0.004(4)	–0.007(4)
N(1)	2*i*		0.885(1)	1.925(1)	0.1350(1)	0.047(3)	0.053(3)	0.042(4)	0.012(3)	–0.006(3)	0.007(3)
C(23)	2*i*		0.680(2)	1.759(1)	0.1530(2)	0.045(5)	0.051(4)	0.033(4)	0.008(4)	–0.003(4)	–0.006(4)
O(23)	2*i*		0.409(1)	1.7512(8)	0.1511(1)	0.047(3)	0.062(3)	0.060(3)	0.015(2)	0.002(2)	0.009(2)
N(2)	2*i*		0.780(1)	1.601(1)	0.1741(2)	0.051(3)	0.056(4)	0.051(4)	0.006(3)	0.001(3)	0.013(3)
C(1)	2*i*		0.576(1)	1.408(1)	0.1944(2)	0.061(4)	0.054(4)	0.047(4)	0.009(4)	–0.005(4)	0.002(4)
C(2)	2*i*		0.736(2)	1.277(1)	0.2192(2)	0.068(5)	0.049(4)	0.045(4)	0.009(4)	–0.005(4)	–0.002(4)
C(3)	2*i*		0.527(1)	1.084(1)	0.2413(2)	0.065(4)	0.049(4)	0.044(4)	0.015(4)	0.000(4)	–0.001(4)
C(4)	2*i*		0.672(1)	0.949(1)	0.2676(2)	0.066(4)	0.047(4)	0.054(5)	0.012(4)	–0.002(4)	–0.004(4)
C(5)	2*i*		0.462(2)	0.762(1)	0.2904(2)	0.065(5)	0.050(4)	0.052(5)	0.009(4)	–0.003(4)	0.002(4)
C(6)	2*i*		0.603(2)	0.629(1)	0.3171(2)	0.071(5)	0.051(4)	0.051(5)	0.015(4)	–0.007(4)	–0.002(4)
C(7)	2*i*		0.390(2)	0.445(1)	0.3398(2)	0.078(5)	0.051(4)	0.050(5)	0.010(4)	–0.001(4)	0.006(4)
C(8)	2*i*		0.531(2)	0.315(1)	0.3669(2)	0.074(5)	0.058(4)	0.056(5)	0.009(4)	–0.003(4)	0.009(4)
C(9)	2*i*		0.313(2)	0.131(1)	0.3901(2)	0.081(5)	0.055(4)	0.066(5)	0.017(4)	–0.003(4)	0.006(4)
C(10)	2*i*		0.453(2)	0.003(1)	0.4178(2)	0.084(5)	0.065(5)	0.067(5)	0.019(4)	0.001(5)	0.013(5)
C(11)	2*i*		0.238(2)	–0.175(2)	0.4407(2)	0.110(7)	0.097(6)	0.079(6)	0.019(5)	0.003(6)	0.038(6)
C(12)	2*i*		0.375(2)	–0.315(2)	0.4671(3)	0.135(8)	0.116(7)	0.100(8)	0.041(6)	0.016(6)	0.051(7)

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