Crystal structure of sodium 2-(*N'*-n-decylureido) ethanesulfonate, $C_{13}H_{27}N_2O_4SNa$

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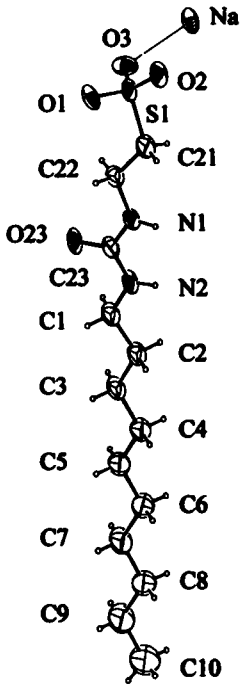

Source of material: 62.5 g (0.5 mol) taurine was dissolved in 500 ml 1 molar aqueous solution of sodium hydroxide. Under vigorous stirring 60.8 g (0.4 mol) n-decylisocyanate was added dropwise within 10 minutes to this mixture at 333 K. During this procedure the temperature increased short-time about 5 K – 8 K. Then the mixture was stirred for four hours at 333 K. After cooling down to room temperature the solution of the final product was filtered to remove *N,N'*-di-n-decyl urea formed as minor product. Finally the solvent was removed under vacuum. For purification from residual *N,N'*-di-n-decyl urea the product was extracted with aceton. The white solid was recrystallised three times with a methanol/water (9:1 v/v) mixture. Long plate shaped crystals were obtained by slow crystallisation.
The sulfonate oxygen atoms and the sodium cation were found to be disordered. For each of these atoms two positions and population parameters were refined.

$C_{13}H_{27}N_2NaO_4S$, triclinic, $P\bar{1}$ (No. 2), a =4.653(1) Å, b =5.470(1) Å, c =33.993(8) Å, α =94.81(2)°, β =88.50(2)°, γ=105.59(2)°, V=830.4 Å^3, Z =2, $R(F)$ =0.090, $R_w(F^2)$ =0.245.

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

Crystal:	colorless plate, size 0.01 x 0.25 x 0.50 mm
Wavelength:	Cu K_α radiation (1.54180 Å)
μ:	21.34 cm^{-1}
Diffractometer:	Enraf-Nonius CAD4
Scan mode:	θ/2θ
$T_{measurement}$:	300 K
$2\theta_{max}$:	99.94°
$N(hkl)_{unique}$:	1711
Criterion for I_o:	$I_o > 2\,\sigma(I_o)$
$N(param)_{refined}$:	227
Programs:	MolEN, SHELXS-86, SHELXL-93

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

Atom	Site	x	y	z	U_{iso}
H(21A)	2*i*	1.140(1)	1.100(1)	0.0860(2)	0.102
H(21B)	2*i*	1.183(1)	1.361(1)	0.1109(2)	0.102
H(22A)	2*i*	0.703(1)	1.251(1)	0.1316(2)	0.077
H(22B)	2*i*	0.631(1)	1.003(1)	0.1029(2)	0.077
H(1)	2*i*	1.051(1)	1.0003(8)	0.1550(1)	0.062
H(2)	2*i*	0.9382(9)	0.6850(8)	0.1947(1)	0.066
H(1A)	2*i*	0.419(1)	0.356(1)	0.1977(2)	0.080
H(1B)	2*i*	0.412(1)	0.572(1)	0.2308(2)	0.080
H(2A)	2*i*	0.827(1)	0.499(1)	0.2606(2)	0.079
H(2B)	2*i*	0.824(1)	0.278(1)	0.2280(2)	0.079
H(3A)	2*i*	0.356(1)	0.271(1)	0.2825(2)	0.081
H(3B)	2*i*	0.360(1)	0.049(1)	0.2505(2)	0.081
H(4A)	2*i*	0.749(1)	−0.038(1)	0.2828(2)	0.084
H(4B)	2*i*	0.757(1)	0.190(1)	0.3142(2)	0.084
H(5A)	2*i*	0.282(1)	−0.251(1)	0.3057(2)	0.087
H(5B)	2*i*	0.287(1)	−0.023(1)	0.3367(2)	0.087
H(6A)	2*i*	0.670(1)	−0.339(1)	0.3384(2)	0.096
H(6B)	2*i*	0.682(1)	−0.107(1)	0.3691(2)	0.096
H(7A)	2*i*	0.199(1)	−0.544(1)	0.3615(2)	0.107
H(7B)	2*i*	0.210(1)	−0.312(1)	0.3921(2)	0.107
H(8A)	2*i*	0.582(1)	−0.639(1)	0.3945(2)	0.106
H(8B)	2*i*	0.602(1)	−0.402(1)	0.4247(2)	0.106
H(9A)	2*i*	0.104(2)	−0.827(2)	0.4182(3)	0.147
H(9B)	2*i*	0.134(2)	−0.593(2)	0.4492(3)	0.147
H(10A)	2*i*	0.223(2)	−0.930(2)	0.4790(3)	0.172
H(10B)	2*i*	0.514(2)	−0.704(2)	0.4804(3)	0.172
H(10C)	2*i*	0.484(2)	−0.938(2)	0.4493(3)	0.172

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*	0.52(1)	0.314(2)	1.2301(7)	–0.0165(2)	0.050(4)	0.031(3)	0.059(3)	0.006(2)	0.002(3)	–0.008(2)
Na(1B)	2*i*	0.48	0.518(2)	1.2603(8)	–0.0270(1)	0.049(5)	0.023(3)	0.046(3)	0.008(3)	–0.002(3)	–0.011(2)
S(1)	2*i*		0.9577(3)	1.3672(5)	0.05309(7)	0.049(1)	0.094(2)	0.065(2)	0.026(1)	0.014(1)	0.035(2)
O(1A)	2*i*	0.52(1)	0.753(3)	1.546(2)	0.0687(2)	0.059(6)	0.036(5)	0.049(5)	0.010(5)	0.015(5)	–0.002(4)
O(2A)	2*i*	0.52(1)	1.247(2)	1.566(1)	0.0442(2)	0.043(5)	0.046(5)	0.069(6)	–0.003(4)	–0.005(4)	0.000(4)
O(3A)	2*i*	0.52(1)	0.843(4)	1.206(2)	0.0270(3)	0.12(1)	0.036(5)	0.030(5)	0.033(7)	–0.001(6)	–0.009(5)
O(1B)	2*i*	0.48	0.950(2)	1.592(2)	0.0593(2)	0.047(7)	0.038(6)	0.026(5)	0.008(5)	–0.016(4)	–0.006(4)
O(2B)	2*i*	0.48	1.172(1)	1.306(1)	0.0198(2)	0.039(4)	0.032(5)	0.050(5)	0.008(3)	0.011(4)	–0.015(4)
O(3B)	2*i*	0.48	0.643(2)	1.174(2)	0.0372(3)	0.045(5)	0.031(5)	0.057(6)	0.001(4)	0.017(5)	0.006(4)
C(21)	2*i*		1.042(1)	1.231(1)	0.0947(2)	0.054(3)	0.084(5)	0.070(5)	0.020(3)	0.011(3)	0.028(4)
C(22)	2*i*		0.784(1)	1.118(1)	0.1194(2)	0.061(3)	0.052(4)	0.046(4)	0.025(3)	0.002(3)	0.002(3)
N(1)	2*i*		0.865(1)	0.9795(8)	0.1497(1)	0.053(3)	0.045(3)	0.042(3)	0.010(2)	0.004(2)	0.000(2)
C(23)	2*i*		0.655(1)	0.819(1)	0.1700(2)	0.055(4)	0.039(3)	0.042(4)	0.013(3)	0.007(3)	–0.005(3)
O(23)	2*i*		0.3860(8)	0.8120(8)	0.1677(1)	0.047(2)	0.068(3)	0.073(3)	0.014(2)	0.011(2)	0.015(2)
N(2)	2*i*		0.7502(9)	0.6710(8)	0.1932(1)	0.048(3)	0.047(3)	0.059(3)	0.013(2)	0.011(2)	0.016(3)
C(1)	2*i*		0.542(1)	0.488(1)	0.2157(2)	0.060(3)	0.046(4)	0.052(4)	0.010(3)	0.003(3)	0.001(3)
C(2)	2*i*		0.699(1)	0.367(1)	0.2433(2)	0.060(3)	0.045(4)	0.049(4)	0.011(3)	0.002(3)	0.001(3)
C(3)	2*i*		0.485(1)	0.182(1)	0.2681(2)	0.057(3)	0.044(3)	0.057(4)	0.009(3)	0.007(3)	0.002(3)
C(4)	2*i*		0.626(1)	0.058(1)	0.2972(2)	0.066(4)	0.046(4)	0.053(4)	0.010(3)	–0.002(3)	0.003(3)
C(5)	2*i*		0.411(1)	–0.118(1)	0.3227(2)	0.070(4)	0.048(4)	0.052(4)	0.012(3)	–0.001(3)	0.002(3)
C(6)	2*i*		0.549(1)	–0.240(1)	0.3524(2)	0.073(4)	0.058(4)	0.060(4)	0.014(3)	–0.004(3)	0.009(4)
C(7)	2*i*		0.332(1)	–0.411(1)	0.3783(2)	0.075(4)	0.062(4)	0.075(5)	0.013(4)	0.009(4)	0.015(4)
C(8)	2*i*		0.466(1)	–0.535(1)	0.4083(2)	0.082(4)	0.065(4)	0.066(4)	0.018(4)	–0.006(4)	0.015(4)
C(9)	2*i*		0.244(2)	–0.698(2)	0.4346(3)	0.094(5)	0.100(6)	0.101(6)	0.018(5)	0.013(5)	0.047(5)
C(10)	2*i*		0.379(2)	–0.829(2)	0.4634(3)	0.129(7)	0.117(7)	0.105(7)	0.033(6)	0.014(6)	0.055(6)

References

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