Crystal structure of lithium (S)-2-pyrrolidone-5-carboxylate monohydrate, $\text{LiC}_5\text{H}_6\text{NO}_3 \cdot \text{H}_2\text{O}$

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Abstract

$\text{C}_5\text{H}_6\text{LiNO}_4$, orthorhombic, $P2_12_12_1$ (No. 19), $a = 5.275(1) \text{ \AA}$, $b = 8.022(2) \text{ \AA}$, $c = 15.865(3) \text{ \AA}$, $V = 671.3 \text{ \AA}^3$, $Z = 4$, $R_{\text{gt}}(F) = 0.035$, $wR_{\text{ref}}(F^2) = 0.091$, $T = 299 \text{ K}$.

Source of material

Single crystals of several millimeters in diameter were obtained from aqueous solutions of the title compound by slow evaporation at about 295 K.

Table 3. Atomic coordinates and displacement parameters (in $\text{\AA}^2$).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Li	4a	0.4597(5)	0.2888(3)	0.6550(2)	0.031(1)	0.022(1)	0.035(1)	−0.0032(9)	−0.003(1)	0.0006(9)
O(1)	4a	0.2762(2)	0.5236(1)	0.16800(7)	0.0331(5)	0.0182(4)	0.0446(5)	0.0011(4)	0.0048(5)	0.0038(4)
O(2)	4a	0.0497(2)	0.3515(1)	0.24796(7)	0.0413(6)	0.0284(5)	0.0381(5)	0.0052(5)	0.0138(5)	0.0049(4)
O(3)	4a	0.2389(2)	−0.1416(1)	0.08183(6)	0.0450(6)	0.0235(4)	0.0355(5)	−0.0080(5)	0.0098(5)	−0.0035(4)
N	4a	0.2703(3)	0.0841(1)	0.16879(8)	0.0390(7)	0.0198(5)	0.0347(6)	−0.0054(5)	0.0136(6)	−0.0020(4)

Discussion

The structure consists of distorted LiO_4 tetrahedra (the Li—O distances vary between 1.899 $\text{\AA}$ and 1.965 $\text{\AA}$) which are connected via pyroglutamic anions to form bands parallel to [010]. These strong periodic bond chains are connected by hydrogen bonds of the types $\text{N—H}\cdots\text{O}$ and $\text{O—H}\cdots\text{O}$ characterized by donor-acceptor distances of about 2.85 $\text{\AA}$ and D—H $\cdots$ A angles of about 162°.

Table 1. Data collection and handling.

Crystal:	colorless ellipsoid, size $0.20 \times 0.20 \times 0.25 \text{ mm}$
Wavelength:	Mo K_{α} radiation (0.71069 $\text{\AA}$)
μ :	1.28 cm^{-1}
Diffractometer, scan mode:	Nonius CAD4, $\omega/2\theta$
$2\theta_{\text{max}}$:	60°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	2279, 1969
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1718
$N(\text{param})_{\text{refined}}$:	132
Programs:	SHELXS-97 [1], SHELXL-97 [2], ATOMS [3]

Table 2. Atomic coordinates and displacement parameters (in $\text{\AA}^2$).

Atom	Site	x	y	z	U_{iso}
H(1)	4a	0.528(4)	0.232(2)	0.227(1)	0.034(5)
H(2)	4a	0.732(4)	0.296(3)	0.109(1)	0.053(6)
H(3)	4a	0.468(4)	0.331(2)	0.059(1)	0.041(5)
H(4)	4a	0.712(4)	0.014(3)	0.075(1)	0.044(5)
H(5)	4a	0.547(4)	0.066(2)	0.002(2)	0.046(5)
H(6)	4a	0.156(4)	0.044(3)	0.204(1)	0.047(6)
H(1W)	4a	0.905(5)	0.376(3)	0.612(2)	0.062(7)
H(2W)	4a	0.765(4)	0.334(3)	0.544(2)	0.051(6)

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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(1)	4 <i>a</i>	0.2310(3)	0.3832(2)	0.19945(8)	0.0266(6)	0.0204(5)	0.0237(5)	0.0008(5)	−0.0037(5)	−0.0009(4)
C(2)	4 <i>a</i>	0.4105(3)	0.2394(2)	0.17880(9)	0.0266(6)	0.0184(5)	0.0312(6)	0.0003(5)	−0.0003(5)	0.0008(5)
C(3)	4 <i>a</i>	0.5589(3)	0.2525(2)	0.0955(1)	0.0299(6)	0.0231(6)	0.0404(7)	−0.0026(6)	0.0085(6)	−0.0002(5)
C(4)	4 <i>a</i>	0.5584(3)	0.0759(2)	0.0595(1)	0.0335(7)	0.0270(7)	0.0392(8)	−0.0043(6)	0.0117(7)	−0.0031(6)
C(5)	4 <i>a</i>	0.3390(3)	−0.0076(2)	0.10292(9)	0.0293(6)	0.0198(5)	0.0293(6)	0.0000(5)	0.0047(5)	0.0021(5)
O(1W)	4 <i>a</i>	0.7612(2)	0.3476(2)	0.59677(8)	0.0316(6)	0.0441(6)	0.0420(6)	−0.0060(5)	0.0022(5)	0.0031(5)

References

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