Crystal structure of dilithium ethylenediammonium bis[sulfate], $(C_2N_2H_{10})Li_2(SO_4)_2$

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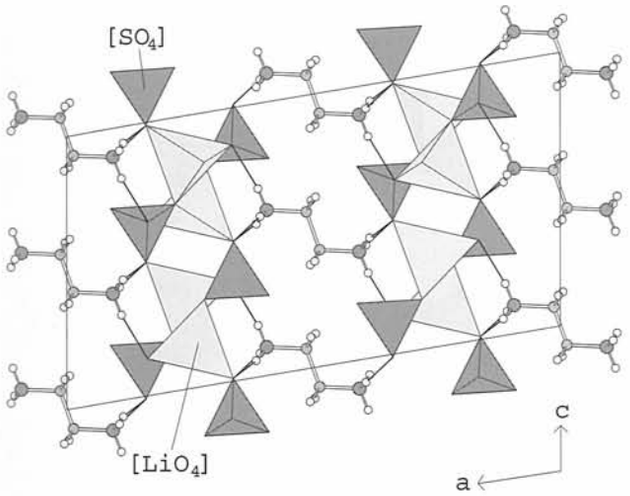

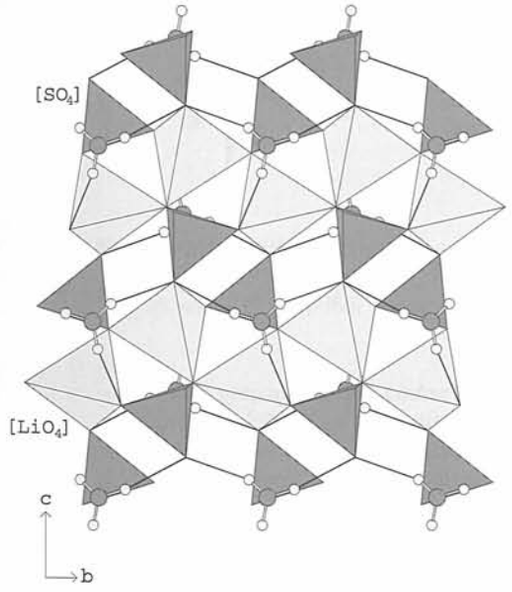

Abstract

$C_2H_{10}Li_2N_2O_8S_2$, monoclinic, $C12/c1$ (No. 15), $a = 18.590(1)$ Å, $b = 4.9035(4)$ Å, $c = 10.1666(4)$ Å, $\beta = 99.599(4)°$, $V = 913.8$ Å^3, $Z = 4$, $R_{gt}(F) = 0.031$, $wR_{ref}(F^2) = 0.087$, $T = 293$ K.

Source of material

The title compound was prepared in the course of systematic search for new "double salts" of ethylenediammonium and monovalent cations of various inorganic acids. It crystallizes from aqueous solution containing lithium sulfate and ethylenediammonium sulfate in stoichiometric ratio by slow evaporation at room temperature in form of colourless, plate-like crystals with dimensions up to 5 mm.

Discussion

The crystal consists of SO_4^{2-} anions, $C_2N_2H_{10}^{2+}$ and Li^+ cations. The structure is built up from 5.8 Å thick tetrahedra layers, interconnected by ethylenediammonium groups (see figure, top). The layers (see figure, bottom) are orientated parallel to the *bc*-plane and composed of (almost ideal) sulfate tetrahedra. Li cations occupy the interstices and are surrounded by four oxygen atoms of four different sulfate groups forming a slightly distorted tetrahedron with usual distances. The basic unit of the layer is a $[SO_4]$-$[LiO_4]$ tetrahedra pair, which shares one common oxygen atom. A centre of symmetry couples two pairs to a circular O-edge-linked group. All double units are edge-linked, whereat only 3 out of 4 oxygen atoms of the $[SO_4]$ are involved in the connections. Therefore the $[LiO_4]$ groups are arranged in a wave-like chain, while the sulfate groups are isolated from themselves. The ethylenediammonium groups show no deviation from the usual conformation. The orientation of the C—N bonds of the $C_2N_2H_{10}^{2+}$ groups are nearly perpendicular to the layers. The oxygen atoms of the ring (O2, O4, O2′, O4′) are connected via H-bridges to 6 different ethylenediammonium groups. The $C_2N_2H_{10}^{2+}$ groups brace the layers like stanchions.

Table 1. Data collection and handling.

Crystal:	colourless parallelepiped, size 0.28 × 0.29 × 0.31 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	6.12 cm^{-1}
Diffractometer, scan mode:	Nonius MACH3, $\omega/2\theta$
$2\theta_{max}$:	60.82°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	4173, 1381
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1200
$N(param)_{refined}$:	94
Programs:	MolEN [1], SHELXL-97 [2], ATOMS [3]

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

Atom	Site	x	y	z	U_{iso}
H(1A)	8*f*	0.496(2)	0.206(7)	0.887(4)	0.07(1)
H(1B)	8*f*	0.506(2)	–0.167(7)	0.877(3)	0.07(1)
H(1)	8*f*	0.393(2)	–0.176(7)	0.914(3)	0.048(8)
H(2)	8*f*	0.389(2)	0.014(6)	0.812(3)	0.053(9)
H(3)	8*f*	0.385(2)	0.091(7)	0.939(3)	0.048(8)

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

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
S(1)	8*f*	0.34232(2)	0.45370(7)	0.63012(3)	0.0132(2)	0.0141(2)	0.0120(2)	0.0003(1)	0.0032(1)	0.0005(1)
O(1)	8*f*	0.27997(6)	0.5772(2)	0.6827(1)	0.0237(5)	0.0192(5)	0.0240(5)	0.0064(4)	0.0132(4)	0.0039(4)
O(2)	8*f*	0.33508(6)	0.1531(2)	0.6354(1)	0.0221(5)	0.0136(5)	0.0273(6)	0.0005(4)	0.0076(4)	0.0013(4)
O(3)	8*f*	0.41143(7)	0.5369(3)	0.7086(1)	0.0192(5)	0.0332(7)	0.0256(6)	–0.0041(5)	–0.0035(4)	–0.0056(5)
O(4)	8*f*	0.33859(6)	0.5355(2)	0.4889(1)	0.0233(5)	0.0284(6)	0.0130(5)	0.0000(4)	0.0051(4)	0.0045(4)
N(1)	8*f*	0.40640(8)	–0.0176(3)	0.8955(2)	0.0186(6)	0.0248(7)	0.0182(6)	0.0007(5)	0.0013(5)	0.0006(5)
C(1)	8*f*	0.4865(1)	0.0153(5)	0.9264(2)	0.0209(7)	0.048(1)	0.0226(8)	–0.0005(7)	0.0033(6)	0.0037(7)
Li(1)	8*f*	0.2522(2)	0.4517(5)	0.8515(3)	0.019(1)	0.019(1)	0.020(1)	0.000(1)	0.005(1)	–0.000(1)

References

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3. Dowty, E.: ATOMS V 3.5. Kingsport, Tennessee, USA 1996.