

Table M24-i-001. Li(N₂H₅)SO₄. Crystal structure [74And]. Fractional coordinates and temperature parameters. U_{ij} [Å²] is defined by Eq. (d) in Introduction and given for non-hydrogen atoms. U is related with B in Eq. (e) in Introduction by $U = B/(8\pi^2)$ and given for hydrogen atoms.

	x	y	z	U or U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Li	0.3312 (3)	0.4333 (3)	0.2533 (12)	0.021 (1)	0.019 (1)	0.018 (1)	−0.001 (1)	−0.001 (2)	−0.002 (2)
S	0.1580 (1)	0.1285 (1)	0.2500	0.0110 (1)	0.0124 (1)	0.0117 (1)	−0.0014 (1)	−0.0009 (2)	0.0001 (2)
O (1)	0.1909 (2)	0.1052 (2)	0.5271 (3)	0.0266 (7)	0.0243 (7)	0.0127 (6)	−0.0025 (5)	−0.0053 (5)	0.0022 (5)
O (2)	0.0115 (1)	0.1540 (2)	0.2282 (5)	0.0115 (4)	0.0317 (7)	0.0281 (8)	−0.0005 (4)	−0.0013 (7)	0.0061 (8)
O (3)	0.2299 (1)	0.2593 (2)	0.1533 (4)	0.0219 (6)	0.0202 (7)	0.0242 (7)	−0.0089 (5)	0.0022 (6)	0.0039 (6)
O (4)	0.3040 (2)	0.4957 (2)	0.6023 (3)	0.0320 (7)	0.0194 (7)	0.0220 (7)	−0.0062 (6)	0.0048 (6)	−0.0087 (6)
N (1)	0.0235 (2)	0.4157 (2)	0.7488 (7)	0.0308 (8)	0.0276 (8)	0.0353 (9)	−0.0086 (6)	−0.0010 (13)	0.0035 (13)
N (2)	0.4400 (2)	0.2136 (2)	0.7381 (6)	0.0221 (6)	0.0235 (6)	0.0218 (7)	0.0016 (5)	0.0015 (10)	−0.0001 (10)
H (1)	0.103 (4)	0.392 (4)	0.776 (9)	0.016 (9)					
H (2)	0.026 (7)	0.445 (6)	0.582 (15)	0.065 (20)					
H (3)	0.358 (4)	0.192 (6)	0.680 (11)	0.040					
H (4)	0.446 (6)	0.234 (8)	0.895 (17)	0.069 (26)					
H (5)	0.462 (3)	0.282 (4)	0.616 (8)	0.008 (8)					

Table M24-i-002. Li(N₂H₅)SO₄. Interatomic distances and bond angles [74And]. *T* = RT.

LiO ₄ tetrahedron			
Li–O(1)	1.950(5) Å	O(1)–Li–O(2)	112.3(2)°
Li–O(2)	1.959(3)	O(1)–Li–O(3)	114.9(3)
Li–O(3)	1.928(4)	O(1)–Li–O(4)	108.7(2)
Li–O(4)	1.912(6)	O(2)–Li–O(3)	97.8(2)
		O(2)–Li–O(4)	108.0(3)
		O(3)–Li–O(4)	114.7(2)
SO ₄ tetrahedron			
S–O(1)	1.487(2) Å	O(1)–S–O(2)	108.2(1)°
S–O(2)	1.477(1)	O(1)–S–O(3)	109.7(1)
S–O(3)	1.462(2)	O(1)–S–O(4)	109.5(1)
S–O(4)	1.465(2)	O(2)–S–O(3)	109.3(1)
		O(2)–S–O(4)	109.8(1)
		O(3)–S–O(4)	110.4(1)
(N ₂ H ₅) ion			
N(1)–N(2)	1.427(3) Å	N(2)–N(1)–H(1)	111(2)°
N(1)–H(1)	0.83(4)	N(2)–N(1)–H(2)	102(4)
N(1)–H(2)	0.91(8)	N(2)–N(1)–H(2')	111(2)
N(1)–H(2')	2.18(7)	H(1)–N(1)–H(2)	102(5)
		H(1)–N(1)–H(2')	103(4)
		H(2)–N(1)–H(2')	126(4)
N(2)–H(3)	0.89(5)	N(1)–N(2)–H(3)	111(4)
N(2)–H(4)	0.84(9)	N(1)–N(2)–H(4)	96(5)
N(2)–H(5)	0.91(4)	N(1)–N(2)–H(5)	116(2)
		H(3)–N(2)–H(4)	116(6)
		H(3)–N(2)–H(5)	98(4)
		H(4)–N(2)–H(5)	121(6)

Table M24-i-003. Li(N₂H₅)SO₄. Hydrogen bond distances and bond angles [74And]. *T* = RT.

<i>D</i> –H... <i>A</i>	<i>D</i> –H	H... <i>A</i>	<i>D</i> – <i>A</i>	∠ <i>D</i> –H... <i>A</i>
N(1)–H(1)...O(4)	0.83(4) Å	2.38(4) Å	2.975(3) Å	129(3)°
N(1)–H(2)...N(1')	0.91(8)	2.18(7)	3.043(3)	156(5)
N(2)–H(3)...O(1)	0.89(5)	2.00(7)	2.874(3)	169(5)
N(2)–H(4)...O(2)	0.84(9)	2.10(8)	2.892(4)	158(7)
N(2)–H(5)...O(2)		2.15(5)	2.982(4)	153(3)
N(2)–H(5)...O(4)	0.91(4)	2.48(4)	2.954(3)	113(3)

Table M24-i-004. Li(N₂H₅)SO₄. Refractive indices at RT [77Bud].

λ [nm]	<i>n_a</i>	<i>n_b</i>	<i>n_c</i>
436	1.5485	1.5435	1.5500
546	1.5378	1.5354	1.5416
590	1.5343	1.5318	1.5380