

Table 44A-1-001. $\text{NaNH}_4\text{SO}_4 \cdot 2\text{H}_2\text{O}$ (lecontite). Crystal structure of phase I [94Arz]. Fractional coordinates and mean square displacements [\AA^2]. $T = 295(2)$ K. $\overline{u^2}$ is estimated by $(U_{11} + U_{22} + U_{33})/3$ for non-hydrogen atoms. $\overline{u^2}$ and U_{ij} are defined by Eq. (e) and (d) in Introduction, respectively.

Atom	z	x	y	$\overline{u^2}$
S	0.3729(2)	0.0841(1)	0.1283(1)	0.0237(6)
Na	0.9112(3)	0.2652(2)	0.4848(1)	0.028(1)
O(1)	0.1884(5)	0.0674(5)	0.1990(3)	0.043(3)
O(2)	0.5732(6)	0.0652(5)	0.1882(3)	0.046(3)
O(3)	0.3674(7)	0.2453(4)	0.0805(2)	0.049(3)
O(4)	0.1399(6)	0.0402(3)	0.5468(2)	0.030(2)
O(5)	0.6896(5)	0.2118(5)	0.6352(3)	0.034(2)
O(6)	0.6590(7)	0.0791(5)	0.4040(2)	0.035(2)
N	0.3696(9)	0.1729(6)	0.8553(4)	0.038(3)
H(1)	0.789(9)	0.889(7)	0.160(3)	0.045(6)
H(2)	0.85(1)	0.729(7)	0.172(4)	0.045(6)
H(3)	0.392(9)	0.600(8)	0.142(3)	0.045(6)
H(4)	0.38(1)	0.486(6)	0.080(4)	0.045(6)
H(5)	0.85(1)	0.38(1)	0.189(6)	0.10(1)
H(6)	0.78(1)	0.329(9)	0.101(6)	0.10(1)
H(7)	0.94(1)	0.24(1)	0.136(5)	0.10(1)
H(8)	0.75(1)	0.26(1)	0.171(5)	0.10(1)

Table 44A-1-002. $\text{NaNH}_4\text{SO}_4 \cdot 2\text{H}_2\text{O}$ (lecontite). Crystal structure of phase I [94Arz]. Anisotropic temperature parameters [\AA^2]. $T = 295(2)$ K. U_{ij} is defined by Eq. (d) in Introduction.

Atom	U_{33}	U_{11}	U_{22}	U_{12}	U_{23}	U_{13}
S	0.0297(6)	0.0199(4)	0.0215(5)	−0.0031(6)	0.0007(6)	0.0008(6)
Na	0.0229(9)	0.031(1)	0.0290(9)	−0.0003(8)	0.0020(8)	0.0025(9)
O(1)	0.042(2)	0.050(3)	0.037(2)	−0.005(2)	0.014(2)	−0.005(2)
O(2)	0.041(2)	0.051(2)	0.038(2)	−0.018(2)	−0.016(2)	0.006(2)
O(3)	0.081(3)	0.021(2)	0.042(2)	0.001(2)	0.000(2)	0.000(3)
O(4)	0.035(2)	0.026(2)	0.031(2)	0.012(1)	0.009(2)	−0.001(2)
O(5)	0.038(2)	0.035(2)	0.028(2)	−0.004(2)	−0.003(2)	0.003(2)
O(6)	0.055(3)	0.024(2)	0.031(2)	0.001(2)	−0.010(2)	−0.002(2)
N	0.040(3)	0.044(2)	0.031(3)	−0.003(2)	−0.002(3)	0.002(3)

Table 44A-1-003. $\text{NaNH}_4\text{SO}_4 \cdot 2\text{H}_2\text{O}$ (lecontite). Crystal structure of phase I [67Cor]. Interatomic distances and angles at RT.

Distances	Å	Distances	Å	Angles	deg
Na–O (4)	2.453(10)	S–O (1)	1.483(14)	O (4'')–NH ₄ –O (3')	46.8 (2)
Na–O (5)	2.404(8)	S–O (2)	1.492(14)	O (4'')–NH ₄ –O (3)	85.6 (4)
Na–O (6)	2.468(9)	S–O (3)	1.452(8)	O (4'')–NH ₄ –O (3'')	84.3 (4)
Na–O (4')	2.382(11)	S–O (4)	1.466(7)	O (4'')–NH ₄ –O (1)	127.3 (5)
Na–O (5')	2.341(9)			O (4'')–NH ₄ –O (2)	125.7 (5)
Na–O (6')	2.419(9)	Angles	deg	O (4'')–NH ₄ –O (1')	99.7 (3)
Angles	deg	O (1)–S–O (2)	107.8 (6)	O (3')–NH ₄ –O (3)	72.8 (7)
O (4)–Na–O (5)	85.9 (3)	O (1)–S–O (3)	109.4 (6)	O (3')–NH ₄ –O (3'')	73.5 (7)
O (4)–Na–O (6)	81.3 (3)	O (1)–S–O (4)	110.9 (6)	O (3')–NH ₄ –O (1)	94.5 (4)
O (4)–Na–O (4')	166.7 (7)	O (2)–S–O (3)	109.8 (7)	O (3')–NH ₄ –O (2)	92.4 (3)
O (4)–Na–O (5')	81.0 (3)	O (2)–S–O (4)	109.8 (6)	O (3')–NH ₄ –O (1')	146.1 (4)
O (4)–Na–O (6')	91.6 (3)	O (3)–S–O (4)	109.1 (4)	O (3)–NH ₄ –O (3'')	141.7 (5)
O (5)–Na–O (6)	89.1 (3)	Distances	Å	O (3)–NH ₄ –O (1)	44.2 (3)
O (5)–Na–O (4')	81.2 (3)	NH ₄ –O (4'')	3.009(9)	O (3)–NH ₄ –O (2)	119.3 (4)
O (5)–Na–O (5')	165.3 (6)	NH ₄ –O (3')	2.973(9)	O (3)–NH ₄ –O (1')	116.1 (6)
O (5)–Na–O (6')	82.2 (3)	NH ₄ –O (3)	3.322(20)	O (3'')–NH ₄ –O (1)	122.7 (4)
O (6)–Na–O (4')	101.4 (3)	NH ₄ –O (3'')	3.274(20)	O (3'')–NH ₄ –O (2)	45.4 (4)
O (6)–Na–O (5')	82.4 (3)	NH ₄ –O (1)	3.004(16)	O (3'')–NH ₄ –O (1')	102.0 (5)
O (6)–Na–O (6')	169.1 (4)	NH ₄ –O (2)	2.908(16)	O (1)–NH ₄ –O (2)	80.9 (4)
O (4')–Na–O (5')	112.2 (3)	NH ₄ –O (1')	2.821(10)	O (1)–NH ₄ –O (1')	114.7 (7)
O (4')–Na–O (6')	83.7 (3)			O (2)–NH ₄ –O (1')	108.3 (5)
O (5')–Na–O (6')	104.7 (3)				

Table 44A-1-004. $\text{NaNd}_4\text{SO}_4 \cdot 2\text{D}_2\text{O}$ (deuterated lecontite). Nuclear quadrupole coupling tensors $|eQ\phi_{ii}/h|$ of deuterons and their orientations [69Gen]. $\theta_{x,y,z}$ and $\phi_{x,y,z}$ are spherical coordinates representing the orientations of three principal components (x, y, z) of nuclear quadrupole coupling tensors with respect to crystallographic c and a axes, respectively.

T K	Type	$ eQ\phi_{zz}/h (\theta_z, \phi_z)$	$ eQ\phi_{yy}/h (\theta_y, \phi_y)$	$ eQ\phi_{xx}/h (\theta_x, \phi_x)$
		kHz		
298	$\beta\text{-D}_2\text{O}$	125 (149°, –131°)	112 (103°, –17°)	13 (63°, –100°)
97	ND ₄ ⁺ equatorial deuterons	58 (90°, 53°)	29 (90°, –37°)	29 (0°, ...)
	ND ₄ ⁺ axial deuterons	176 (90°, 53°)	88 (90°, –37°)	88 (0°, ...)