Entry # 99-900-0017 (refined structure)

Phase classification

Formula	LiSClN
I/Ic	3.530000

Refined crystal structure

Crystallographic data

Space group	F m -3 m (225)
Crystal system	cubic
Cell parameters	a= 5.4566 Å

Atom coordinates

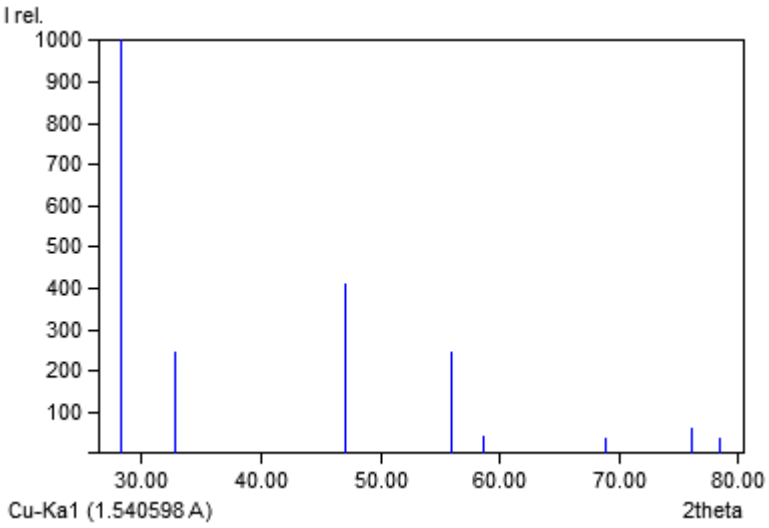
Element	Oxid.	*x*	*y*	*z*	Bi	Focc
Li		0.250	0.250	0.250	6.985016	1.000000
Li		0.500	0.500	0.500	34.458477	0.310000
S		0.000	0.000	0.000	0.814529	0.412000
N		0.000	0.000	0.000	0.814529	0.450000
Cl		0.000	0.000	0.000	0.814529	0.103000
Br		0.000	0.000	0.000	0.814529	0.034000

Refined diffraction data

Diffraction lines

d [Å]	Int.	h	k	l	Mult.
3.1504	1000.0	1	1	1	8
3.1504	497.3	1	1	1	8
2.7283	243.2	2	0	0	6
2.7283	120.9	2	0	0	6
1.9292	408.5	2	2	0	12
1.9292	203.1	2	2	0	12
1.6452	243.3	3	1	1	24
1.6452	120.9	3	1	1	24
1.5752	39.8	2	2	2	8
1.5752	19.8	2	2	2	8
1.3641	34.7	4	0	0	6
1.3641	17.3	4	0	0	6
1.2518	62.2	3	3	1	24
1.2518	30.9	3	3	1	24
1.2201	37.2	4	2	0	24
1.2201	18.2	4	2	0	24

Diffraction pattern graphics



Rietveld refinement using FullProf

Refinement results

Automatic refinement	No
Final weighted average Bragg R-factor	5.8
Final reduced chi^2	2.0
FullProf comment	Your refinement could still be improved! => Your refinement could still be improved!

Refined parameters

Parameter	Final value
Biso_Li1_ph1	6.98502
Biso_Li2_ph1	34.4585

Fixed parameters

Parameter	Final value
Zero_pat1	-0.368632

SyCos_pat1	-0.420195
SySin_pat1	0
Lambda_pat1	1.54187
P0_mabs_pat1	0
Cp_mabs_pat1	0
Tau_mabs_pat1	0.1
Bck_0_pat1	0.989692
Bck_1_pat1	0
Bck_2_pat1	0
Bck_3_pat1	0
Scale_ph1_pat1	0.0259575
Bover_ph1_pat1	2.21978
Strain1_ph1_pat1	0
Strain2_ph1_pat1	0
Strain3_ph1_pat1	0
G-Size_ph1_pat1	0
L-Size_ph1_pat1	0
Y-cos_ph1_pat1	0
EtaRght0_ph1_pat1	0
X-tan_ph1_pat1	0
U-Cagl_ph1_pat1	1.39338
V-Cagl_ph1_pat1	0
W-Cagl_ph1_pat1	0.425208
EtaPV_ph1_pat1	0.933657
Cell_A_ph1_pat1	5.4566
Cell_B_ph1_pat1	5.4566
Cell_C_ph1_pat1	5.4566
Cell_D_ph1_pat1	90
Cell_E_ph1_pat1	90
Cell_F_ph1_pat1	90
Or1_ph1_pat1	0
Or2_ph1_pat1	0
Asym1_ph1_pat1	0
Asym2_ph1_pat1	0
Asym3_ph1_pat1	0
Asym4_ph1_pat1	0
X_Li1_ph1	0.25
Y_Li1_ph1	0.25
Z_Li1_ph1	0.25
Occ_Li1_ph1	1
X_Li2_ph1	0.5
Y_Li2_ph1	0.5
Z_Li2_ph1	0.5
Occ_Li2_ph1	0.31
X_S3_ph1	0
Y_S3_ph1	0
Z_S3_ph1	0
Biso_S3_ph1	0.814529
Occ_S3_ph1	0.412
X_N4_ph1	0
Y_N4_ph1	0
Z_N4_ph1	0
Biso_N4_ph1	0.814529
Occ_N4_ph1	0.45
X_Cl5_ph1	0
Y_Cl5_ph1	0
Z_Cl5_ph1	0
Biso_Cl5_ph1	0.814529
Occ_Cl5_ph1	0.103
X_Br6_ph1	0
Y_Br6_ph1	0
Z_Br6_ph1	0
Biso_Br6_ph1	0.814529
Occ_Br6_ph1	0.034