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= 5.4455 Å

Atom coordinates

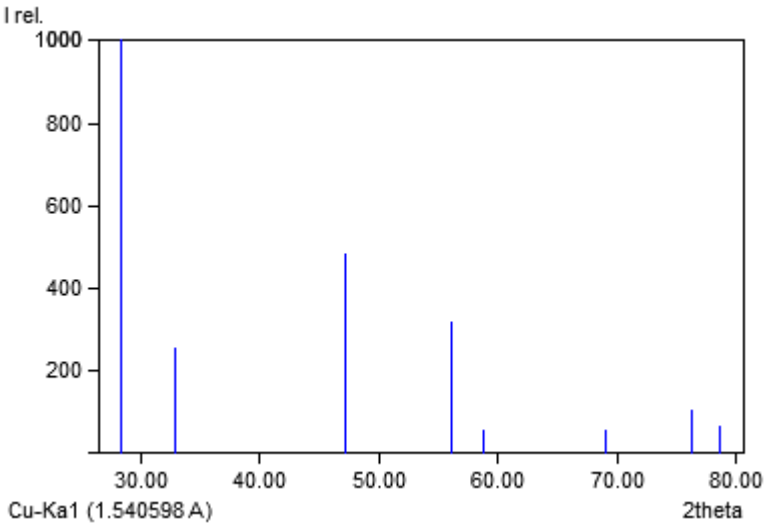
Element	Oxid.	*x*	*y*	*z*	Bi	Focc
Li		0.250	0.250	0.250	6.102110	1.000000
Li		0.500	0.500	0.500	17.997387	0.174900
S		0.000	0.000	0.000	0.758736	0.275000
N		0.000	0.000	0.000	0.758736	0.450000
Cl		0.000	0.000	0.000	0.758736	0.206000
Br		0.000	0.000	0.000	0.758736	0.068000

Refined diffraction data

Diffraction lines

d [Å]	Int.	h	k	l	Mult.
3.1439	1000.0	1	1	1	8
3.1439	497.4	1	1	1	8
2.7227	257.0	2	0	0	6
2.7227	127.8	2	0	0	6
1.9253	482.4	2	2	0	12
1.9253	239.8	2	2	0	12
1.6419	315.6	3	1	1	24
1.6419	156.9	3	1	1	24
1.5720	54.0	2	2	2	8
1.5720	26.9	2	2	2	8
1.3614	54.4	4	0	0	6
1.3614	27.1	4	0	0	6
1.2493	105.7	3	3	1	24
1.2493	52.5	3	3	1	24
1.2176	64.3	4	2	0	24
1.2176	31.3	4	2	0	24

Diffraction pattern graphics



Rietveld refinement using FullProf

Refinement results

Automatic refinement	Yes
Final weighted average Bragg R-factor	7.9
Final reduced chi^2	1.6
FullProf comment	Your refinement could still be improved! => Your refinement could still be improved!

Refined parameters

Parameter	Final value
Bck_0_pat1	1.00045
Scale_ph1_pat1	0.0128275
Bover_ph1_pat1	0.293515
U-Cagl_ph1_pat1	2.32702
Cell_A_ph1_pat1	5.44548

Fixed parameters

Parameter	Final value
Zero_pat1	-0.419944
SyCos_pat1	-0.478471
SySin_pat1	0
Lambda_pat1	1.54187
P0_mabs_pat1	0
Cp_mabs_pat1	0
Tau_mabs_pat1	0.1
Bck_1_pat1	0
Bck_2_pat1	0
Bck_3_pat1	0
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
V-Cagl_ph1_pat1	0
W-Cagl_ph1_pat1	0.362308
EtaPV_ph1_pat1	0.703782
Cell_B_ph1_pat1	5.44551
Cell_C_ph1_pat1	5.44551
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
Biso_Li1_ph1	6.10211
Occ_Li1_ph1	1
X_Li2_ph1	0.5
Y_Li2_ph1	0.5
Z_Li2_ph1	0.5
Biso_Li2_ph1	17.9974
Occ_Li2_ph1	0.1749
X_S3_ph1	0
Y_S3_ph1	0
Z_S3_ph1	0
Biso_S3_ph1	0.758736
Occ_S3_ph1	0.275
X_N4_ph1	0
Y_N4_ph1	0
Z_N4_ph1	0
Biso_N4_ph1	0.758736
Occ_N4_ph1	0.45
X_Cl5_ph1	0
Y_Cl5_ph1	0
Z_Cl5_ph1	0
Biso_Cl5_ph1	0.758736
Occ_Cl5_ph1	0.206
X_Br6_ph1	0
Y_Br6_ph1	0
Z_Br6_ph1	0
Biso_Br6_ph1	0.758736
Occ_Br6_ph1	0.068