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= 5.4871 Å

Atom coordinates

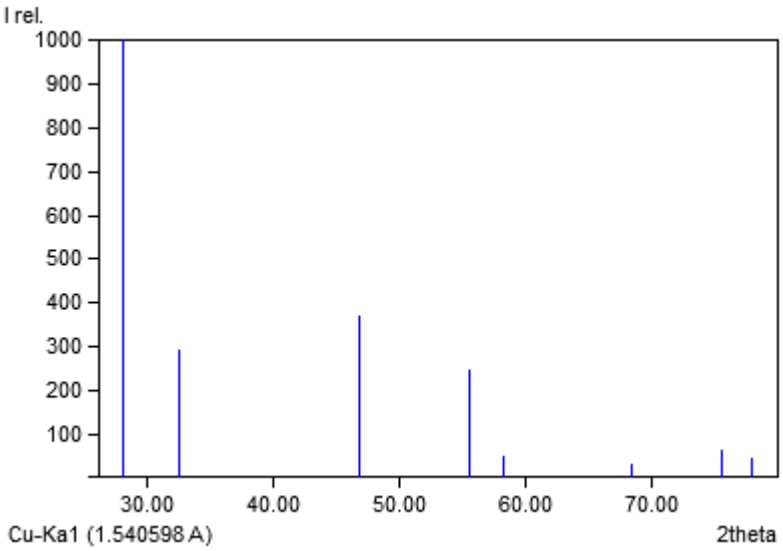
Element	Oxid.	*x*	*y*	*z*	Bi	Focc
Li		0.250	0.250	0.250	8.336306	1.000000
Li		0.500	0.500	0.500	17.400820	0.174900
S		0.000	0.000	0.000	1.121068	0.275000
N		0.000	0.000	0.000	1.121068	0.450000
Cl		0.000	0.000	0.000	1.121068	0.093500
Br		0.000	0.000	0.000	1.121068	0.180000

Refined diffraction data

Diffraction lines

d [Å]	Int.	h	k	l	Mult.
3.1680	1000.0	1	1	1	8
3.1680	497.4	1	1	1	8
2.7436	289.1	2	0	0	6
2.7436	143.8	2	0	0	6
1.9400	371.5	2	2	0	12
1.9400	184.7	2	2	0	12
1.6544	245.5	3	1	1	24
1.6544	122.0	3	1	1	24
1.5840	48.1	2	2	2	8
1.5840	23.9	2	2	2	8
1.3718	31.5	4	0	0	6
1.3718	15.6	4	0	0	6
1.2588	61.1	3	3	1	24
1.2588	30.4	3	3	1	24
1.2270	41.9	4	2	0	24
1.2270	20.6	4	2	0	24

Diffraction pattern graphics



Rietveld refinement using FullProf

Refinement results

Automatic refinement	Yes
Final weighted average Bragg R-factor	9.7
Final reduced chi^2	2.2
FullProf comment	Chi-square is LOW but the HIGH R-Bragg factor can be due to => Chi-square is LOW but the HIGH R-Bragg factor can be due to a bad structural model and/or a rather poor statistic

Refined parameters

Parameter	Final value
Bck_0_pat1	0.991247
Scale_ph1_pat1	0.0195318
Bover_ph1_pat1	2.26151

U-Cagl_ph1_pat1	1.09713
Cell_A_ph1_pat1	5.48711

Fixed parameters

Parameter	Final value
Zero_pat1	-0.169175
SyCos_pat1	-0.196121
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	0.516903
EtaPV_ph1_pat1	1.02785
Cell_B_ph1_pat1	5.48696
Cell_C_ph1_pat1	5.48696
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	8.33631
Occ_Li1_ph1	1
X_Li2_ph1	0.5
Y_Li2_ph1	0.5
Z_Li2_ph1	0.5
Biso_Li2_ph1	17.4008
Occ_Li2_ph1	0.1749
X_S3_ph1	0
Y_S3_ph1	0
Z_S3_ph1	0
Biso_S3_ph1	1.12107
Occ_S3_ph1	0.275
X_N4_ph1	0
Y_N4_ph1	0
Z_N4_ph1	0
Biso_N4_ph1	1.12107
Occ_N4_ph1	0.45
X_Cl5_ph1	0
Y_Cl5_ph1	0
Z_Cl5_ph1	0
Biso_Cl5_ph1	1.12107
Occ_Cl5_ph1	0.0935
X_Br6_ph1	0
Y_Br6_ph1	0
Z_Br6_ph1	0
Biso_Br6_ph1	1.12107
Occ_Br6_ph1	0.18