Entry # 99-900-0016 (refined structure)

Phase classification

Formula	LiSClN
I/Ic	3.210000

Refined crystal structure

Crystallographic data

Space group	F m -3 m (225)
Crystal system	cubic
Cell parameters	a= 5.4144 Å

Atom coordinates

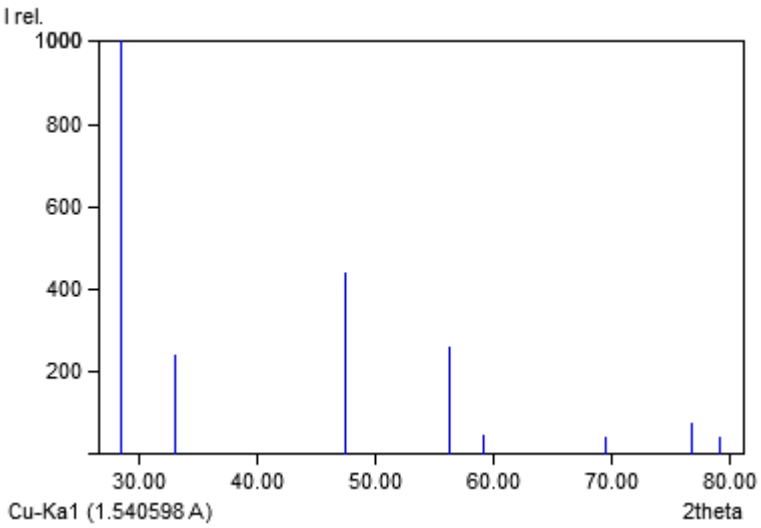
Element	Oxid.	*x*	*y*	*z*	Bi	Focc
Li		0.250	0.250	0.250	7.371166	1.000000
Li		0.500	0.500	0.500	12.441203	0.150000
S		0.000	0.000	0.000	0.955694	0.275000
N		0.000	0.000	0.000	0.955694	0.450000
Cl		0.000	0.000	0.000	0.955694	0.275000

Refined diffraction data

Diffraction lines

d [Å]	Int.	h	k	l	Mult.
3.1260	1000.0	1	1	1	8
3.1260	497.3	1	1	1	8
2.7072	238.6	2	0	0	6
2.7072	118.6	2	0	0	6
1.9143	438.7	2	2	0	12
1.9143	218.1	2	2	0	12
1.6325	260.4	3	1	1	24
1.6325	129.4	3	1	1	24
1.5630	44.3	2	2	2	8
1.5630	22.1	2	2	2	8
1.3536	41.1	4	0	0	6
1.3536	20.4	4	0	0	6
1.2421	75.1	3	3	1	24
1.2421	37.2	3	3	1	24
1.2107	43.7	4	2	0	24
1.2107	20.4	4	2	0	24

Diffraction pattern graphics



Rietveld refinement using FullProf

Refinement results

Automatic refinement	No
Final weighted average Bragg R-factor	3.8
Final reduced chi^2	3.2
FullProf comment	Your refinement seems to be rather good! => Your refinement seems to be rather good!

Refined parameters

Parameter	Final value
Biso_S3_ph1	0.955694
Biso_N4_ph1	0.955694
Biso_Cl5_ph1	0.955694

Fixed parameters

Parameter	Final value
Zero_pat1	-0.536391

SyCos_pat1	-0.574282
SySin_pat1	0
Lambda_pat1	1.54187
P0_mabs_pat1	0
Cp_mabs_pat1	0
Tau_mabs_pat1	0.1
Bck_0_pat1	1.00176
Bck_1_pat1	0
Bck_2_pat1	0
Bck_3_pat1	0
Scale_ph1_pat1	0.0206948
Bover_ph1_pat1	1.10748
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	2.11998
V-Cagl_ph1_pat1	0
W-Cagl_ph1_pat1	0.362308
EtaPV_ph1_pat1	0.719447
Cell_A_ph1_pat1	5.41435
Cell_B_ph1_pat1	5.41435
Cell_C_ph1_pat1	5.41435
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	7.37117
Occ_Li1_ph1	1
X_Li2_ph1	0.5
Y_Li2_ph1	0.5
Z_Li2_ph1	0.5
Biso_Li2_ph1	12.4412
Occ_Li2_ph1	0.15
X_S3_ph1	0
Y_S3_ph1	0
Z_S3_ph1	0
Occ_S3_ph1	0.275
X_N4_ph1	0
Y_N4_ph1	0
Z_N4_ph1	0
Occ_N4_ph1	0.45
X_Cl5_ph1	0
Y_Cl5_ph1	0
Z_Cl5_ph1	0
Occ_Cl5_ph1	0.275