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= 5.3840 Å

Atom coordinates

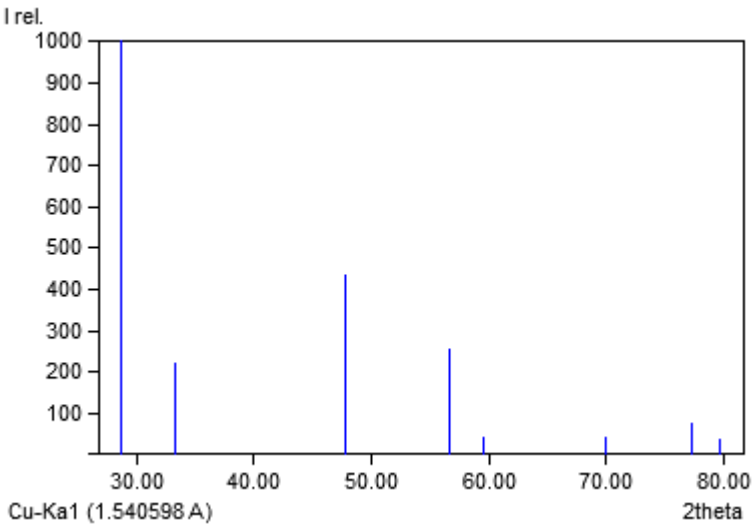
Element	Oxid.	*x*	*y*	*z*	Bi	Focc
Li		0.250	0.250	0.250	5.984046	1.000000
Li		0.500	0.500	0.500	1.000000	0.037500
S		0.000	0.000	0.000	0.724239	0.138000
N		0.000	0.000	0.000	0.724239	0.450000
Cl		0.000	0.000	0.000	0.724239	0.412000

Refined diffraction data

Diffraction lines

d [Å]	Int.	h	k	l	Mult.
3.1085	1000.0	1	1	1	8
3.1085	497.3	1	1	1	8
2.6920	218.5	2	0	0	6
2.6920	108.7	2	0	0	6
1.9035	435.9	2	2	0	12
1.9035	216.7	2	2	0	12
1.6233	256.9	3	1	1	24
1.6233	127.7	3	1	1	24
1.5542	40.5	2	2	2	8
1.5542	20.1	2	2	2	8
1.3460	42.7	4	0	0	6
1.3460	21.2	4	0	0	6
1.2352	74.4	3	3	1	24
1.2352	36.8	3	3	1	24
1.2039	34.2	4	2	0	24
1.2039	14.0	4	2	0	24

Diffraction pattern graphics



Rietveld refinement using FullProf

Refinement results

Automatic refinement	No
Final weighted average Bragg R-factor	6.3
Final reduced chi^2	6.2
FullProf comment	Your refinement could still be improved! => Your refinement could still be improved!

Refined parameters

Parameter	Final value
Biso_S3_ph1	0.724239
Biso_N4_ph1	0.724239
Biso_Cl5_ph1	0.724239

Fixed parameters

Parameter	Final value
Zero_pat1	-0.728586

SyCos_pat1	-0.805811
SySin_pat1	0
Lambda_pat1	1.54187
P0_mabs_pat1	0
Cp_mabs_pat1	0
Tau_mabs_pat1	0.1
Bck_0_pat1	1.00216
Bck_1_pat1	0
Bck_2_pat1	0
Bck_3_pat1	0
Scale_ph1_pat1	0.0305232
Bover_ph1_pat1	1.17118
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	1.61621
V-Cagl_ph1_pat1	0
W-Cagl_ph1_pat1	0.32317
EtaPV_ph1_pat1	0.711928
Cell_A_ph1_pat1	5.384
Cell_B_ph1_pat1	5.384
Cell_C_ph1_pat1	5.384
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	5.98405
Occ_Li1_ph1	1
X_Li2_ph1	0.5
Y_Li2_ph1	0.5
Z_Li2_ph1	0.5
Biso_Li2_ph1	1
Occ_Li2_ph1	0.0375
X_S3_ph1	0
Y_S3_ph1	0
Z_S3_ph1	0
Occ_S3_ph1	0.138
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	0.412