

Phase classification

Formula	LiSCIN
I/Ic	3.530000

Refined crystal structure

Crystallographic data

Space group	F m -3 m (225)
Crystal system	cubic
Cell parameters	a= 5.4972 Å

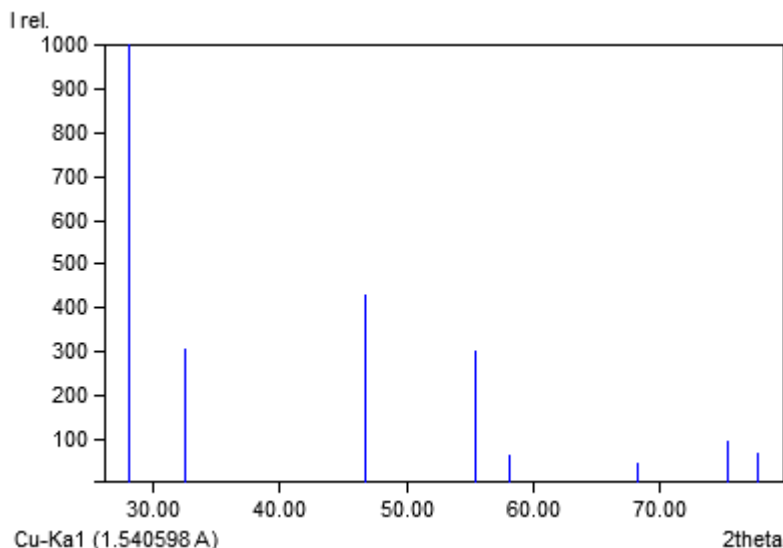
Atom coordinates	Element	Oxid.	x	y	z	Bi	Focc
	Li		0.250	0.250	0.250	7.637094	1.000000
	Li		0.500	0.500	0.500	10.000000	0.174900
	S		0.000	0.000	0.000	0.583831	0.275000
	N		0.000	0.000	0.000	0.583831	0.450000
	Cl		0.000	0.000	0.000	0.583831	0.068500
	Br		0.000	0.000	0.000	0.583831	0.206000

Refined diffraction data

Diffraction lines

d [Å]	Int.	h	k	l	Mult.
3.1738	1000.0	1	1	1	8
3.1738	497.3	1	1	1	8
2.7486	306.2	2	0	0	6
2.7486	152.3	2	0	0	6
1.9436	426.6	2	2	0	12
1.9436	212.1	2	2	0	12
1.6575	301.2	3	1	1	24
1.6575	149.7	3	1	1	24
1.5869	62.4	2	2	2	8
1.5869	31.0	2	2	2	8
1.3743	44.5	4	0	0	6
1.3743	22.1	4	0	0	6
1.2612	92.1	3	3	1	24
1.2612	45.7	3	3	1	24
1.2292	66.5	4	2	0	24
1.2292	32.9	4	2	0	24

Diffraction pattern graphics



Rietveld refinement using FullProf

Refinement results

Automatic refinement	No
Final weighted average Bragg R-factor	5.3
Final reduced χ^2	1.8
FullProf comment	Your refinement could still be improved! => Your refinement could still be improved!

Refined parameters

Parameter	Final value
Biso_S3_ph1	0.583831
Biso_N4_ph1	0.583831
Biso_Cl5_ph1	0.583831
Biso_Br6_ph1	0.583831

Fixed parameters

Parameter	Final value
Zero_pat1	-0.0163514
SyCos_pat1	-0.130356
SySin_pat1	0
Lambda_pat1	1.54187
P0_mabs_pat1	0
Cp_mabs_pat1	0
Tau_mabs_pat1	0.1
Bck_0_pat1	0.997212
Bck_1_pat1	0
Bck_2_pat1	0
Bck_3_pat1	0
Scale_ph1_pat1	0.0143462
Bover_ph1_pat1	1.31313
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	2.30258
V-Cagl_ph1_pat1	0
W-Cagl_ph1_pat1	0.493141
EtaPV_ph1_pat1	0.755847
Cell_A_ph1_pat1	5.49723
Cell_B_ph1_pat1	5.49723
Cell_C_ph1_pat1	5.49723
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	7.63709
Occ_Li1_ph1	1
X_Li2_ph1	0.5
Y_Li2_ph1	0.5
Z_Li2_ph1	0.5
Biso_Li2_ph1	10
Occ_Li2_ph1	0.1749
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_CI5_ph1	0
Y_CI5_ph1	0
Z_CI5_ph1	0
Occ_CI5_ph1	0.0685
X_Br6_ph1	0
Y_Br6_ph1	0
Z_Br6_ph1	0
Occ_Br6_ph1	0.206