

**Phase classification**

<b>Formula</b>	LiSCIN
<b>I/Ic</b>	3.530000

## Refined crystal structure

**Crystallographic data**

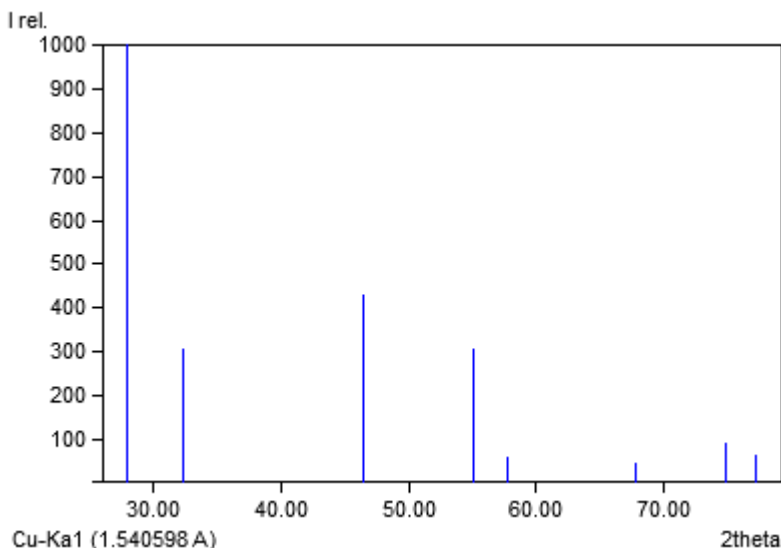
Space group	F m -3 m (225)					
Crystal system	cubic					
Cell parameters	a= 5.5273 Å					
Atom coordinates	Element	Oxid.	x	y	z	Bi
	Li		0.250	0.250	0.250	6.054820
	Li		0.500	0.500	0.500	21.858242
	S		0.000	0.000	0.000	1.052154
	N		0.000	0.000	0.000	1.052154
	Cl		0.000	0.000	0.000	1.052154
	Br		0.000	0.000	0.000	1.052154

## Refined diffraction data

**Diffraction lines**

d [Å]	Int.	h	k	l	Mult.
3.1912	1000.0	1	1	1	8
3.1912	497.3	1	1	1	8
2.7637	305.3	2	0	0	6
2.7637	151.9	2	0	0	6
1.9542	429.4	2	2	0	12
1.9542	213.5	2	2	0	12
1.6666	304.6	3	1	1	24
1.6666	151.5	3	1	1	24
1.5956	58.3	2	2	2	8
1.5956	29.0	2	2	2	8
1.3818	45.4	4	0	0	6
1.3818	22.6	4	0	0	6
1.2681	91.2	3	3	1	24
1.2681	45.3	3	3	1	24
1.2360	61.0	4	2	0	24
1.2360	30.2	4	2	0	24

## Diffraction pattern graphics



## Rietveld refinement using FullProf

**Refinement results**

<b>Automatic refinement</b>	No
<b>Final weighted average Bragg R-factor</b>	10.4
<b>Final reduced <math>\chi^2</math></b>	1.9
<b>FullProf comment</b>	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
Biso_S3_ph1	1.05215
Biso_N4_ph1	1.05215
Biso_Cl5_ph1	1.05215

	Biso_Br6_ph1	1.05215
Fixed parameters	Parameter	Final value
	Zero_pat1	0.223106
	SyCos_pat1	0.0783511
	SySin_pat1	0
	Lambda_pat1	1.54187
	P0_mabs_pat1	0
	Cp_mabs_pat1	0
	Tau_mabs_pat1	0.1
	Bck_0_pat1	1.00047
	Bck_1_pat1	0
	Bck_2_pat1	0
	Bck_3_pat1	0
	Scale_ph1_pat1	0.00917719
	Bover_ph1_pat1	1.06741
	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	2.47096
	V-Cagl_ph1_pat1	0
	W-Cagl_ph1_pat1	0.516903
	EtaPV_ph1_pat1	0.694923
	Cell_A_ph1_pat1	5.52735
	Cell_B_ph1_pat1	5.52735
	Cell_C_ph1_pat1	5.52735
	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	6.05482
	Occ_Li1_ph1	1
	X_Li2_ph1	0.5
	Y_Li2_ph1	0.5
	Z_Li2_ph1	0.5
	Biso_Li2_ph1	21.8582
	Occ_Li2_ph1	0.225
	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
	X_Br6_ph1	0
	Y_Br6_ph1	0
	Z_Br6_ph1	0
	Occ_Br6_ph1	0.275