

**Phase classification**

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

## Refined crystal structure

**Crystallographic data**

<b>Space group</b>	F m -3 m (225)
<b>Crystal system</b>	cubic
<b>Cell parameters</b>	a= 5.4847 Å

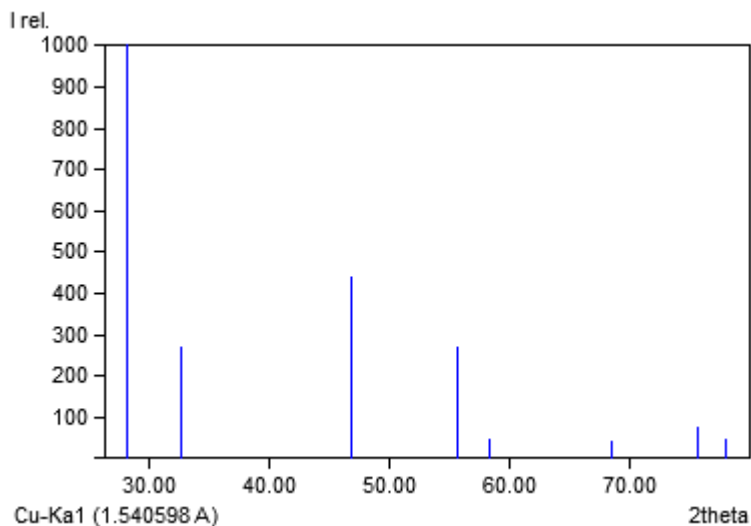
<b>Atom coordinates</b>	<b>Element</b>	<b>Oxid.</b>	<b>x</b>	<b>y</b>	<b>z</b>	<b>Bi</b>	<b>Focc</b>
	Li		0.250	0.250	0.250	5.861537	1.000000
	Li		0.500	0.500	0.500	23.339428	0.310000
	S		0.000	0.000	0.000	0.492002	0.410000
	N		0.000	0.000	0.000	0.492002	0.450000
	Cl		0.000	0.000	0.000	0.492002	0.034000
	Br		0.000	0.000	0.000	0.492002	0.103000

## Refined diffraction data

**Diffraction lines**

<b>d [Å]</b>	<b>Int.</b>	<b>h</b>	<b>k</b>	<b>l</b>	<b>Mult.</b>
3.1666	1000.0	1	1	1	8
3.1666	497.4	1	1	1	8
2.7424	269.9	2	0	0	6
2.7424	134.2	2	0	0	6
1.9391	437.5	2	2	0	12
1.9391	217.5	2	2	0	12
1.6537	271.2	3	1	1	24
1.6537	134.8	3	1	1	24
1.5833	46.5	2	2	2	8
1.5833	23.1	2	2	2	8
1.3712	40.9	4	0	0	6
1.3712	20.3	4	0	0	6
1.2583	75.3	3	3	1	24
1.2583	37.4	3	3	1	24
1.2264	46.5	4	2	0	24
1.2264	22.9	4	2	0	24

## Diffraction pattern graphics



## Rietveld refinement using FullProf

**Refinement results**

<b>Automatic refinement</b>	Yes
<b>Final weighted average Bragg R-factor</b>	7.4
<b>Final reduced <math>\chi^2</math></b>	2.0
<b>FullProf comment</b>	Your refinement could still be improved! => Your refinement could still be improved!

**Refined parameters**

<b>Parameter</b>	<b>Final value</b>
Bck_0_pat1	0.996556
Scale_ph1_pat1	0.0216839
Bover_ph1_pat1	2.0868
U-Cagl_ph1_pat1	2.46771
Cell_A_ph1_pat1	5.48474

**Fixed parameters**

Parameter	Final value
Zero_pat1	-0.191825
SyCos_pat1	-0.215988
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	0.493141
EtaPV_ph1_pat1	0.662494
Cell_B_ph1_pat1	5.48468
Cell_C_ph1_pat1	5.48468
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	5.86154
Occ_Li1_ph1	1
X_Li2_ph1	0.5
Y_Li2_ph1	0.5
Z_Li2_ph1	0.5
Biso_Li2_ph1	23.3394
Occ_Li2_ph1	0.31
X_S3_ph1	0
Y_S3_ph1	0
Z_S3_ph1	0
Biso_S3_ph1	0.492002
Occ_S3_ph1	0.41
X_N4_ph1	0
Y_N4_ph1	0
Z_N4_ph1	0
Biso_N4_ph1	0.492002
Occ_N4_ph1	0.45
X_CI5_ph1	0
Y_CI5_ph1	0
Z_CI5_ph1	0
Biso_CI5_ph1	0.492002
Occ_CI5_ph1	0.034
X_Br6_ph1	0
Y_Br6_ph1	0
Z_Br6_ph1	0
Biso_Br6_ph1	0.492002
Occ_Br6_ph1	0.103