

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= 5.4728 Å
Atom coordinates	

Element	Oxid.	x	y	z	Bi	Focc
Li		0.250	0.250	0.250	8.514675	1.000000
Li		0.500	0.500	0.500	23.395912	0.310000
S		0.000	0.000	0.000	0.894136	0.412000
N		0.000	0.000	0.000	0.894136	0.450000
Cl		0.000	0.000	0.000	0.894136	0.068200
Br		0.000	0.000	0.000	0.894136	0.068200

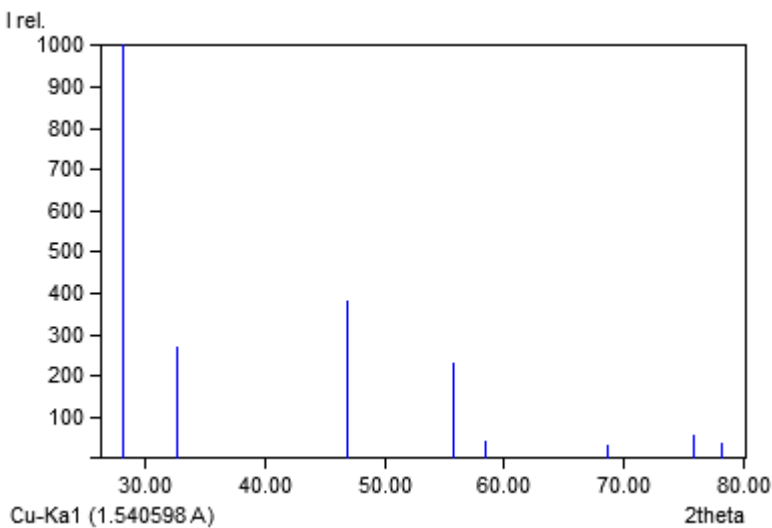
Refined diffraction data

Diffraction lines



d [Å]	Int.	h	k	l	Mult.
3.1597	1000.0	1	1	1	8
3.1597	497.4	1	1	1	8
2.7364	271.5	2	0	0	6
2.7364	135.0	2	0	0	6
1.9349	382.1	2	2	0	12
1.9349	190.0	2	2	0	12
1.6501	231.6	3	1	1	24
1.6501	115.1	3	1	1	24
1.5799	42.6	2	2	2	8
1.5799	21.2	2	2	2	8
1.3682	29.8	4	0	0	6
1.3682	14.8	4	0	0	6
1.2555	55.5	3	3	1	24
1.2555	27.6	3	3	1	24
1.2238	36.6	4	2	0	24
1.2238	18.0	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 chi <sup>2</sup>	2.0
FullProf comment	Your refinement could still be improved! => Your refinement could still be improved!

Refined parameters

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Parameter	Final value
Biso_Li2_ph1	23.3959

Fixed parameters

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Parameter	Final value
Zero_pat1	-0.342714
SyCos_pat1	-0.30122

SySin_pat1	0
Lambda_pat1	1.54187
P0_mabs_pat1	0
Cp_mabs_pat1	0
Tau_mabs_pat1	0.1
Bck_0_pat1	0.999736
Bck_1_pat1	0
Bck_2_pat1	0
Bck_3_pat1	0
Scale_ph1_pat1	0.0254291
Bover_ph1_pat1	2.72185
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	1.78424
V-Cagl_ph1_pat1	0
W-Cagl_ph1_pat1	0.493141
EtaPV_ph1_pat1	0.834886
Cell_A_ph1_pat1	5.47281
Cell_B_ph1_pat1	5.47281
Cell_C_ph1_pat1	5.47281
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	8.51468
Occ_Li1_ph1	1
X_Li2_ph1	0.5
Y_Li2_ph1	0.5
Z_Li2_ph1	0.5
Occ_Li2_ph1	0.31
X_S3_ph1	0
Y_S3_ph1	0
Z_S3_ph1	0
Biso_S3_ph1	0.894136
Occ_S3_ph1	0.412
X_N4_ph1	0
Y_N4_ph1	0
Z_N4_ph1	0
Biso_N4_ph1	0.894136
Occ_N4_ph1	0.45
X_CI5_ph1	0
Y_CI5_ph1	0
Z_CI5_ph1	0
Biso_CI5_ph1	0.894136
Occ_CI5_ph1	0.0682
X_Br6_ph1	0
Y_Br6_ph1	0
Z_Br6_ph1	0
Biso_Br6_ph1	0.894136
Occ_Br6_ph1	0.0682