

Phase classification

Formula	LiSCIN
I/Ic	3.530000

Refined crystal structure

Crystallographic data

Space group
Crystal system
Cell parameters
Atom coordinates

F m -3 m (225)
cubic
a= 5.4203 Å

Element	Oxid.	x	y	z	Bi	Focc
Li		0.250	0.250	0.250	6.980861	1.000000
Li		0.500	0.500	0.500	14.076056	0.174000
S		0.000	0.000	0.000	0.555006	0.275000
N		0.000	0.000	0.000	0.555006	0.450000
Cl		0.000	0.000	0.000	0.555006	0.275000
Br		0.000	0.000	0.000	0.555006	0.000000

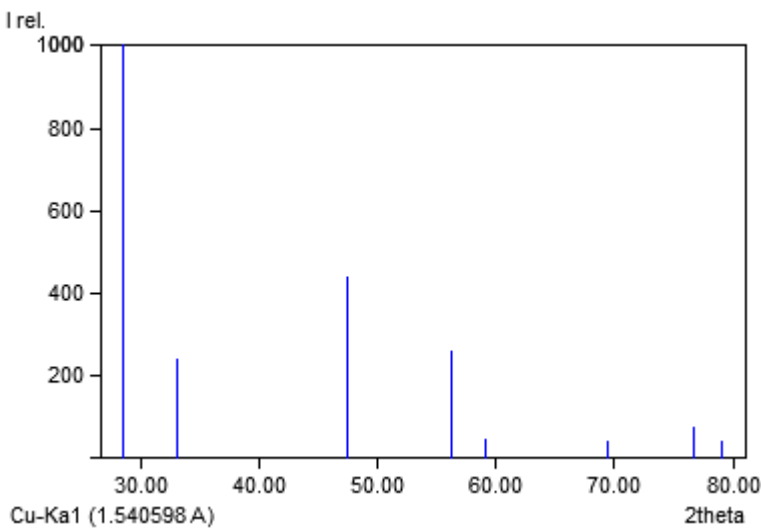
Refined diffraction data

Diffraction lines



d [Å]	Int.	h	k	l	Mult.
3.1294	1000.0	1	1	1	8
3.1294	497.3	1	1	1	8
2.7102	240.7	2	0	0	6
2.7102	119.7	2	0	0	6
1.9164	439.2	2	2	0	12
1.9164	218.4	2	2	0	12
1.6343	260.2	3	1	1	24
1.6343	129.4	3	1	1	24
1.5647	44.2	2	2	2	8
1.5647	22.0	2	2	2	8
1.3551	40.8	4	0	0	6
1.3551	20.3	4	0	0	6
1.2435	74.5	3	3	1	24
1.2435	36.9	3	3	1	24
1.2120	43.6	4	2	0	24
1.2120	20.7	4	2	0	24

Diffraction pattern graphics



Rietveld refinement using FullProf

Refinement results

Automatic refinement
Final weighted average Bragg R-factor
Final reduced chi ²
FullProf comment

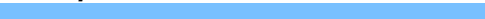
No
3.7
2.2
Your refinement seems to be very good! => Your refinement seems to be very good!

Refined parameters



Parameter	Final value
Biso_S3_ph1	0.555006
Biso_N4_ph1	0.555006
Biso_Cl5_ph1	0.555006
Biso_Br6_ph1	0.555006

Fixed parameters



Parameter	Final value
Zero_pat1	-0.594568
SyCos_pat1	-0.6508
SySin_pat1	0
Lambda_pat1	1.54187
P0_mabs_pat1	0
Cp_mabs_pat1	0
Tau_mabs_pat1	0.1
Bck_0_pat1	0.994642
Bck_1_pat1	0
Bck_2_pat1	0
Bck_3_pat1	0
Scale_ph1_pat1	0.0218531
Bover_ph1_pat1	1.56144
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	1.41413
V-Cagl_ph1_pat1	0
W-Cagl_ph1_pat1	0.362308
EtaPV_ph1_pat1	0.913865
Cell_A_ph1_pat1	5.42034
Cell_B_ph1_pat1	5.42034
Cell_C_ph1_pat1	5.42034
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	6.98086
Occ_Li1_ph1	1
X_Li2_ph1	0.5
Y_Li2_ph1	0.5
Z_Li2_ph1	0.5
Biso_Li2_ph1	14.0761
Occ_Li2_ph1	0.174
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	0.275
X_Br6_ph1	0
Y_Br6_ph1	0
Z_Br6_ph1	0
Occ_Br6_ph1	0