

### Phase classification

Formula
$I/I_c$

Refined crystal structure

### Crystallographic data

### Space group

### Crystal system

## Cell parameters

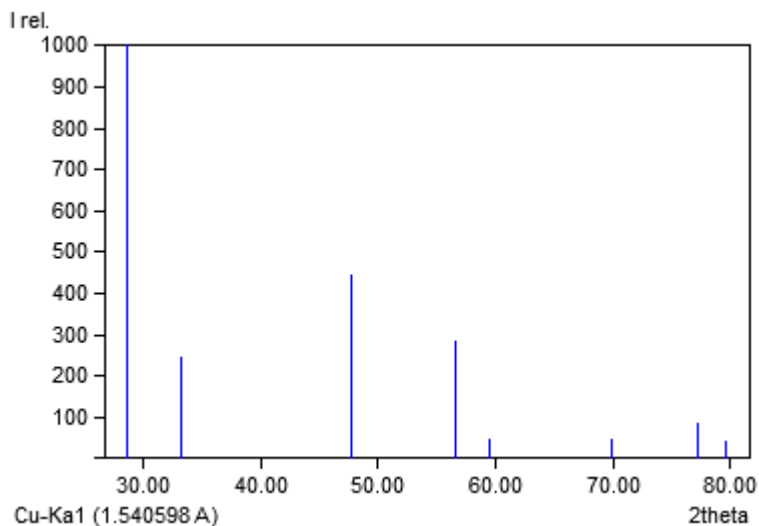
## Atom coordinates

## Refined diffraction data

### Diffraction lines

d [Å]	Int.	h	k	l	Mult.
3.1118	1000.0	1	1	1	8
3.1118	497.3	1	1	1	8
2.6949	243.7	2	0	0	6
2.6949	121.2	2	0	0	6
1.9056	443.4	2	2	0	12
1.9056	220.4	2	2	0	12
1.6251	284.9	3	1	1	24
1.6251	141.6	3	1	1	24
1.5559	47.4	2	2	2	8
1.5559	23.6	2	2	2	8
1.3475	47.6	4	0	0	6
1.3475	23.6	4	0	0	6
1.2365	86.5	3	3	1	24
1.2365	42.8	3	3	1	24
1.2052	42.4	4	2	0	24
1.2052	18.0	4	2	0	24

## Diffraction pattern graphics



## Rietveld refinement using FullProf

### Refinement results

## Automatic refinement

**Final weighted average Bragg R-factor**

**Final reduced chi<sup>2</sup>**

<b>FullProf comment</b>	Your refinement seems to be very good! => Your refinement seems to be very good!
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### Refined parameters

Parameter	Final value
Biso_S3_ph1	0.789155
Biso_N4_ph1	0.789155
Biso_C15_ph1	0.789155
Biso_Br6_ph1	0.789155

### Fixed parameters

Parameter	Final value
Zero_pat1	-0.768648
SyCos_pat1	-0.85839
SySin_pat1	0
Lambda_pat1	1.54187
P0_mabs_pat1	0
Cp_mabs_pat1	0
Tau_mabs_pat1	0.1
Bck_0_pat1	0.99473
Bck_1_pat1	0
Bck_2_pat1	0
Bck_3_pat1	0
Scale_ph1_pat1	0.0233358
Bover_ph1_pat1	0.836904
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	1.3241
V-Cagl_ph1_pat1	0
W-Cagl_ph1_pat1	0.32317
EtaPV_ph1_pat1	0.842665
Cell_A_ph1_pat1	5.38983
Cell_B_ph1_pat1	5.38983
Cell_C_ph1_pat1	5.38983
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	5.2433
Occ_Li1_ph1	1
X_Li2_ph1	0.5
Y_Li2_ph1	0.5
Z_Li2_ph1	0.5
Biso_Li2_ph1	1
Occ_Li2_ph1	0.03
X_S3_ph1	0
Y_S3_ph1	0
Z_S3_ph1	0
Occ_S3_ph1	0.1375
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	0.3
X_Br6_ph1	0
Y_Br6_ph1	0
Z_Br6_ph1	0
Occ_Br6_ph1	0.103