Entry # 99-400-0006 (refined structure)

Phase classification

Formula	$Cl_{0.60}Li_{1.80}N_{0.40}$
I/Ic	3.170000

References

Publication of original data

Bibliography	Sattlegger H., Hahn H., "Uber Versuche zur Umsetzung von Li~3~N mit Lithiumhalogeniden'", Naturwissenschaften **51**, 534-535 (1964)

Origin of original data

Source of original entry	PCD (Pearson's Crystal Data)
Source reference	P. Villars, K. Cenzual, "Pearson's Crystal Data: Crystal Structure Database for Inorganic Compounds (on CD-ROM)", ASM International™, Materials Park, Ohio, U.S.A.
Publisher	ASM International™
Publisher address	Materials Park, Ohio 44073, U.S.A.
Orig. entry no.	PCD 1713275

Refined crystal structure

Crystallographic data

Space group	F m -3 m (225)
Crystal system	cubic
Cell parameters	a= 5.3542 Å

Atom coordinates

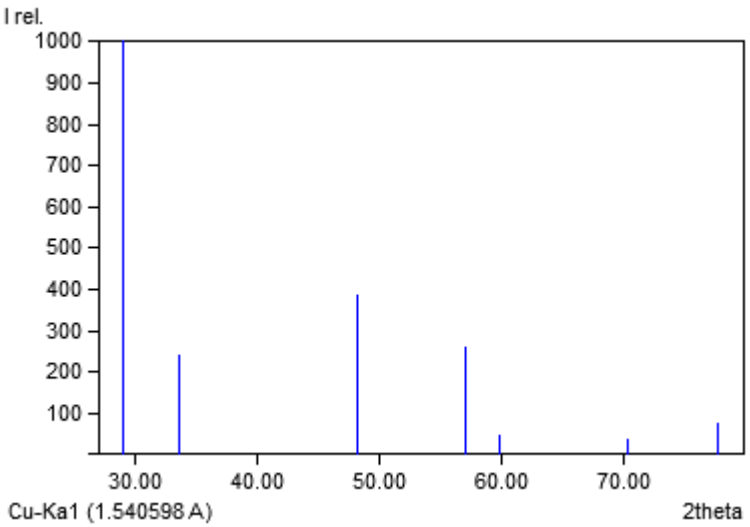
Element	Oxid.	*x*	*y*	*z*	Bi	Focc
Li		0.250	0.250	0.250	8.459057	0.950000
Cl		0.000	0.000	0.000	1.000000	0.550000
N		0.000	0.000	0.000	1.000000	0.450000

Refined diffraction data

Diffraction lines

d [Å]	Int.	h	k	l	Mult.
3.0913	1000.0	1	1	1	8
3.0913	497.4	1	1	1	8
2.6771	239.3	2	0	0	6
2.6771	119.0	2	0	0	6
1.8930	387.0	2	2	0	12
1.8930	192.4	2	2	0	12
1.6144	257.7	3	1	1	24
1.6144	128.1	3	1	1	24
1.5456	46.5	2	2	2	8
1.5456	23.1	2	2	2	8
1.3386	37.3	4	0	0	6
1.3386	18.5	4	0	0	6
1.2283	74.0	3	3	1	24
1.2283	36.6	3	3	1	24

Diffraction pattern graphics



Rietveld refinement using FullProf

Refinement results

Automatic refinement	Yes
Final weighted average Bragg R-factor	4.8

Final reduced chi^2	2.7
FullProf comment	Your refinement seems to be very good! => Your refinement seems to be very good!

Refined parameters

Parameter	Final value
Bck_0_pat1	0.987971
Scale_ph1_pat1	0.0260752
Bover_ph1_pat1	0.794649
U-Cagl_ph1_pat1	0.981392
Cell_A_ph1_pat1	5.35424

Fixed parameters

Parameter	Final value
Zero_pat1	-0.417915
SyCos_pat1	-0.388196
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	0.268656
EtaPV_ph1_pat1	0.953699
Cell_B_ph1_pat1	5.3543
Cell_C_ph1_pat1	5.3543
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	8.45906
Occ_Li1_ph1	0.95
X_Cl2_ph1	0
Y_Cl2_ph1	0
Z_Cl2_ph1	0
Biso_Cl2_ph1	1
Occ_Cl2_ph1	0.55
X_N3_ph1	0
Y_N3_ph1	0
Z_N3_ph1	0
Biso_N3_ph1	1
Occ_N3_ph1	0.45