

TITLE

LiNiO2 WITH FAULTS

Instrumental And Size Broadening

!Type Of Radiation

Radiation X-Ray

! lambda1 lambda2 ratio

Wavelength 1.5418 0.0 0.0

!instrumental aberrations zero sycos sysin

Aberrations 0.0000 0.0000 0.0000
0.00 0.00 0.00

!instr. broadening u v w x Dg DI

Pseudo-Voigt 0.11 -0.0036 0.009 0.7000 479.26 459.87 Trim
0.00 0.00 0.00 0.00 0.00 0.00

Structural

! a b c gamma

Cell 2.7868 2.7868 14.453 120.0
11.00 11.00 1.00 0.00

!Laue symmetry

Symm unknown

!number of layer types

Nlayers 3

!layer width

Lwidth infinite

Layer 1

!Layer symmetry

LSYM none

!Atom name number x y z Biso Occ

Atom Ni3+ 1 0.000 0.000 0.000 1.0 1.0
0.00 0.00 0.00 0.00 0.00

!Atom name number x y z Biso Occ

Atom O2- 2 1/3 2/3 -0.075 1.0 1.0
0.00 0.00 0.00 0.00 0.00

!Atom name number x y z Biso Occ

Atom O2- 3 2/3 1/3 0.075 1.0 1.0
0.00 0.00 0.00 0.00 0.00

!Atom name number x y z Biso Occ

Atom Li1+ 4 1/3 2/3 0.2667 1.0 1.0
0.00 0.00 0.00 0.00 0.00