

TITLE

LiNiO2 ideal structure

Instrumental And Size Broadening

!Type of Radiation

Radiation X-Ray

! lambda1 lambda2 ratio

Wavelength 1.5406 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

SPGR R-3 m

! a b c alpha beta gamma

Avercell 2.8659 2.8659 14.253 90 90 120.0

! a b c gamma

Cell 2.8659 2.8659 14.253 120.0

11.00 11.00 1.00 0.00

! FullProf Studio commands

FST_CMD SEQ 9 1 2 3 1 2 3 1 2 3

FST_CMD CONN Ni O 0.0 2.3

FST_CMD box -2 2 -2 2 -0.01 1.01

FST_CMD stack_vect 0 0 0.5

!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 0.8 1.0

0.00 0.00 0.00 1.00 0.00

!Atom name number x y z Biso Occ

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

1.00 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