

!layer 3 to layer 1

LT 0.858000 2/3 1/3 1/3
0.000000 0.000000 0.000000 0.000000
FW 0.00 0.00 0.00 0.00 0.00 0.00
0.00 0.00 0.00 0.00 0.00 0.00

!layer 3 to layer 2

LT 0.000000 0.000000 0.000000 0.000000
0.000000 0.000000 0.000000 0.000000
FW 0.00 0.00 0.00 0.00 0.00 0.00
0.00 0.00 0.00 0.00 0.00 0.00

!layer 3 to layer 3

LT 0.142000 0.000000 0.000000 1/3
0.000000 0.000000 0.000000 0.000000
FW 0.00 0.00 0.00 0.00 0.00 0.00
0.00 0.00 0.00 0.00 0.00 0.00

Calculation

Lmq

Corrmax 30

Maxfun 2400

Tol 0.100000E-04

Nprint 0

Experimental

!Filename Scale factor code

FILE LiNiO2_def_sim6.dat 1.0 0.00

Excluded_Regions 0

FFORMAT free

!Linear interpolation

Bgrinter sim.bgr

!Polynomial Number of coefficients

Bgrcheb 2

!Polynomial coefficients

1.00000 0.20000

0.0 0.0

!number of pattern backgrounds

Bgrnum 1

!Pattern file Filename Scale factor code

Bgrpatt cerusite1.sub 0.026000 1.00 cerusite.hkl