

In 1972, the use of a dichotomy algorithm for indexing powder diffraction patterns was introduced by Louër and Louër¹, in the form of a computer program DICVOL². Over time, updates have been made to expand the program, and optimize its indexing precision and accuracy. In the most recent version, DICVOL14 allows users to investigate all crystal systems for proper indexing (instead of just orthorhombic or higher symmetry). Additionally, the program now has an increased tolerance for large data sets/small step sizes, which has become extremely important with the evolution of X-ray instrumentation (i.e. high resolution data)³. With all the new functionality of DICVOL, a need for better visualization grew, and in 2019, ICDD collaborated with R. Papoular and D. Louër to generate the Premier DICvol Tool (PreDICT)⁴.

PreDICT is a graphical user interface for the powder diffraction pattern indexing program DICVOL14, an updated version of DICVOL04².

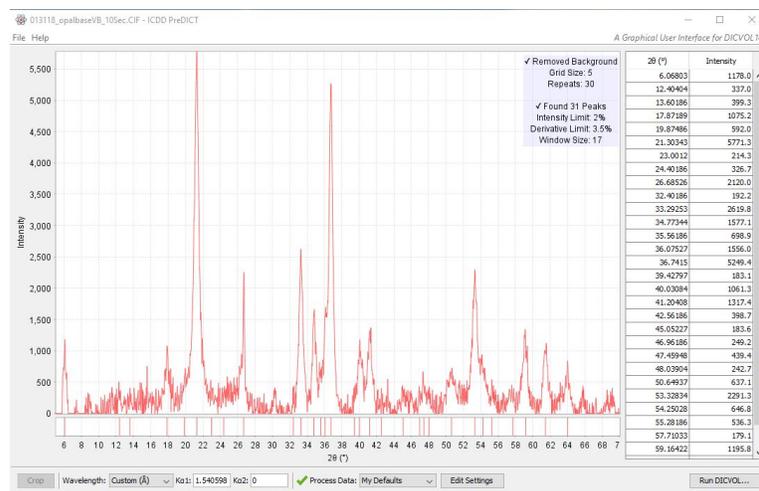


Figure 1: Graphical display of analysis of opal base, using PreDICT.

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DICVOL14 Output
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LOWER BOUND = 2400.00 Å*3    HIGHER BOUND = 2500.00 Å*3
ANGLE RANGE SCANNED : BETA MIN= 90.000 Deg.  BETA MAX= 95.000 Deg.
ANGLE RANGE SCANNED : BETA MIN= 95.000 Deg.  BETA MAX=100.000 Deg.
ANGLE RANGE SCANNED : BETA MIN=100.000 Deg.  BETA MAX=105.000 Deg.
ANGLE RANGE SCANNED : BETA MIN=105.000 Deg.  BETA MAX=110.000 Deg.
ANGLE RANGE SCANNED : BETA MIN=110.000 Deg.  BETA MAX=115.000 Deg.
ANGLE RANGE SCANNED : BETA MIN=115.000 Deg.  BETA MAX=120.000 Deg.
ANGLE RANGE SCANNED : BETA MIN=120.000 Deg.  BETA MAX=125.000 Deg.
ITERATION NUMBER AT EACH DICHO TOMY LEVEL:
3889 11862 24614 26550 27565 24902 28250
--- TIME FOR SEARCH DOWN TO MONOCLINIC SYMMETRY: 74.00 SEC
SEARCH OF TRICLINIC SOLUTION(S)
*****
VOLUME DOMAIN BEING SCANNED :
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Figure 2: Example of DICVOL14 output when using PreDICT.

System Requirements: Windows XP or later, Java Runtime Environment (JRE) 8 or higher.

[1] Louër, D. and Louër, M. (1972). "Méthode d'essais et erreurs pour l'indexation automatique des diagrammes de poudre." J. Appl. Crystallogr. 5, 271-275. [DOI: 10.1107/S0021889872009483]

[2] Louër, D. and Boulif, A. (2014). "Some further considerations in powder diffraction pattern indexing with the dichotomy method." Powder Diffr. 29, Suppl. S2, pp. S7-S12. [DOI: 10.1017/S0885715614000906]

[3] Boulif, A. and Louër, D. (2004). "Powder pattern indexing with the dichotomy method." J. Appl. Crystallogr. 37, 724-731. [DOI: 10.1107/S00218898040148]

[4] Blanton, J., Papoular, R., & Louër, D. (2019). "PreDICT: A graphical user interface to the DICVOL14 indexing software program for powder diffraction data." Powder Diffr., 34(3), 233-241. [DOI:10.1017/S0885715619000514]