

FoM proposals for indexing powder diffraction patterns of high-symmetry lattices

O.A. Smirnova

Institute for Chemical Research, Kyoto University, Uji, Kyoto-fu 611-0011, Japan

Indexing is known as a “bottleneck” in structure solution from powder diffraction data and sometimes course a complicated choice among several possible cells. Presently well-known, efficient and popular indexing programs like ITO, TREOR and DICVOL employ figures of merit [1,2] to estimate the best proposed cell. For both cases, the higher FoM, the better solution is considered. However, $M(20)$ and $F(20)$ cannot serve for a final decision, but can only help to chose several best solutions. As it can be observed in the Table 1, the DICVOL program suggest several possible solutions and the correct solution of highest symmetry among them. The repetition of the same lattice described by different cells should be considered as an indication of the correct indexing solution. From the other hand, that might be random and unfruitful indexing solution if the lattice is non-primitive but is not observed among proposed cells with its primitive representation. The extension to indexing algorithms, eliminating lower symmetry cells for the same lattice described by high-symmetry cell, and the corrected figures of merit taking into account the number of equal proposal cells might be drawn as follows:

$$M'(20) = M(20)_h \cdot N_{ep}$$

$$F'(20) = F(20)_h \cdot N_{ep}$$

where $M(20)_h$ and $F(20)_h$ are $M(20)$ and $F(20)$ for the ***h***ighest symmetry cell
 N_{ep} is the number of ***e***qual ***p***roposal cells

Table 1. Three best indexing solutions proposed by DICVOL for the simulated powder pattern of pyrochlore compound $Tl_2Nb_2O_7$.

System	a, Å	b, Å	c, Å	M(20)	F(20)
cubic	10.6224	10.6224	10.6224	386.9	257.4
tetragonal	7.5112	7.5112	10.6224	329.8	215.8
orthorhombic	10.6224	7.5112	2.5037	536.7	341.4

[1] De Wolff, P.M., J. APPL. CRYST. 5, 108-113 (1968).

[2] Smith, G. S. & Snyder, R. L., J. APPL. CRYST. 12, 60-65 (1979).