

# INDEXING OF POWDER DIFFRACTION PATTERNS BY ITERATIVE USE OF SINGULAR VALUE DECOMPOSITION

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A fast and simple method for indexing powder diffraction patterns has been developed for large and small lattices of all symmetries. The method is relatively insensitive to missing high d-spacing reflections where on simulated data little effect in terms of successful indexing has been observed when one third of the d-spacings are removed. Comparison with two of the most popular indexing programs ITO12 and DICVOL91 have shown that the present method as implemented in the program TOPAS [1] can successfully index simulated data where others fail. Also significant is that the present method performs well on typically noisy d-spacings comprising large diffractometer  $2\theta$  zero errors. Critical to its success the present method uses Singular Value Decomposition in an iterative manner for solving linear equations relating hkl's to d-spacings.

Reference:

- [1] Bruker AXS (2000): TOPAS V2.0: General profile and structure analysis software for powder diffraction data. Bruker AXS, Karlsruhe, Germany.