

Implementation of Calculated Patterns Quality Marks in the Powder Diffraction File

Soorya Kabekkodu, *International Centre for Diffraction Data*
Newtown Square, PA 19073, U.S.A. E-mail: suri@icdd.com

Quality mark assignments for the calculated patterns are becoming a necessity considering their growing population in the Powder Diffraction File™ (PDF®). An estimate of the number of calculated diffraction patterns in the Release 2005 is about 400,000. The focus of the quality mark is to determine the confidence level of the structural model used and its impact on the calculated pattern from the phase identification point of view. The major step in the adopted method involves several crystallographic and editorial checks by the International Centre for Diffraction Data (ICDD), followed by the extraction and flagging of the structural database warnings/comments. Resulting calculated patterns will be classified into various categories based on the significance and nature of the warnings/comments. In the final step, a quality mark (QM) will be assigned to a calculated pattern based on its category.

A database analysis of approximately 400,000 calculated diffraction patterns will be presented with special emphasis on phase identification using some case studies. The prime crystallographic checks implemented in the editorial process will be discussed in detail.

Keywords: phase identification, powder diffraction analysis, data checking