Evaluating Data Quality

Quality Mark

What is a Quality Mark?

- **A Quality Mark is a reliability index used in Powder Diffraction File (PDF).**
- Data validation and the assignment of the quality mark are the most important steps in the editorial process.
- **The Powder Diffraction File is the only crystallographic database that categorizes data based on its quality.**

Quality Mark (QM) Types

- Experimental patterns
- Calculated patterns

The criteria for the assignment of the quality marks differ between patterns obtained experimentally and those determined from the crystal structure (calculated patterns).

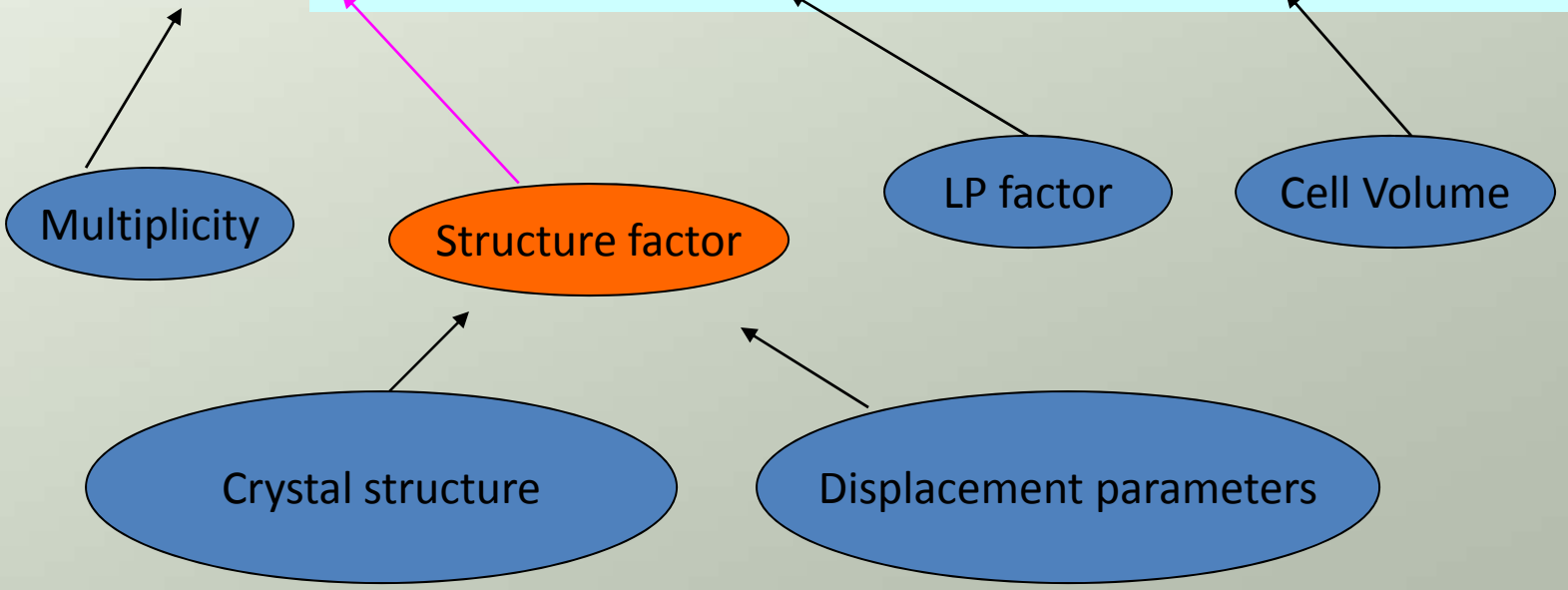
QM for Experimental Patterns

- **Star** (Well characterized chemically and crystallographically, no unindexed lines, $\Delta 2\theta \leq 0.03º$)
- **R** (d values obtained from Rietveld refinement)
- **I** (Well characterized chemically, no unindexed strong lines, $\Delta 2\theta \leq 0.06º$)
- **O** (Poorly characterized, with editorial comment explaining the reason)
- **B** (Does not meet the criteria for *, I, O)
- **C** (Author calculated d values)
- **H** (Hypothetical)

What are Calculated Patterns?

If we know the crystal structure, we can calculate the diffraction pattern using the following equation.

$$I_{hkl} = M_{hkl}\left|F_{hkl}\right|^2\left(1+\cos^2(2\theta)\cos^2(2\theta_m)/\sin^2\theta\cos\theta\right)_{hkl}/V^2$$



NOTE:

It is extremely important to make sure that the crystal structure used for the calculation is correct. In fact, this is the rate-determining step in the editorial process of calculated patterns.

QM for Calculated Patterns

The major step in this method involves several crystallographic and editorial checks by the 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.

Calculated Patterns QM Notations

Category	QM
No Warning	*
Minor Warning	I
Significant Warning	B
Assigned structure (Prototype)	P
Hypothetical	H
Major Warning	O

Quality Mark

Why?

- The Quality Mark plays an important role in interpreting search match results.
- Editorial comments describing the quality of the pattern are extremely useful in evaluating and eventually accepting the search/match results.
- For example, while using RIR in semi-quantitative analysis, editorial comments on incomplete or disordered structures are valuable.

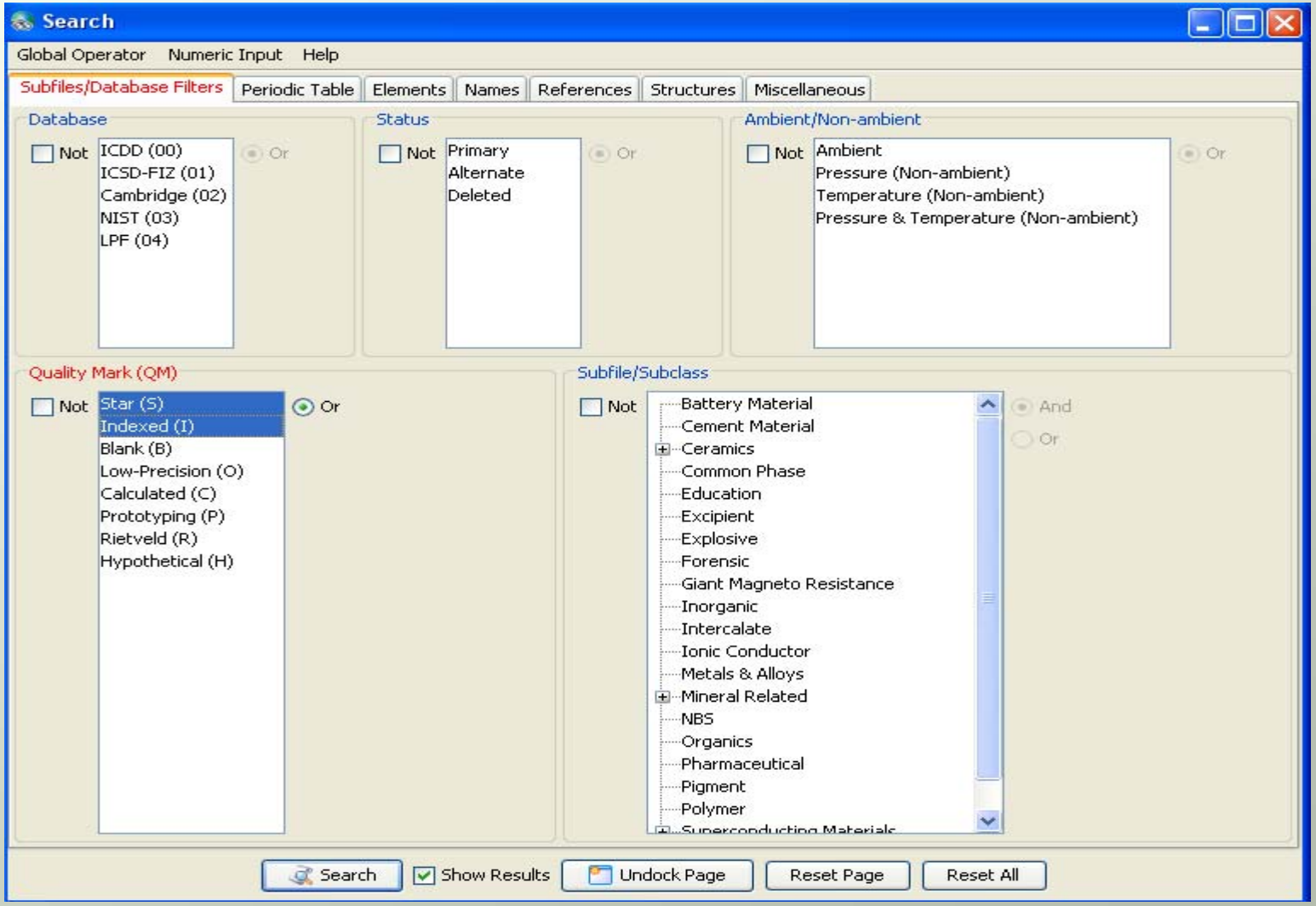
Quality Mark

How?

- Quality mark search is under Subfiles/Database Filters tab.
- Quality mark criteria can be used as a filter.
- Multiple QMs can be chosen by clicking on the QM symbol while holding the Ctrl key.
- Low quality patterns can be excluded by selecting the undesired QM with the Not box checked.

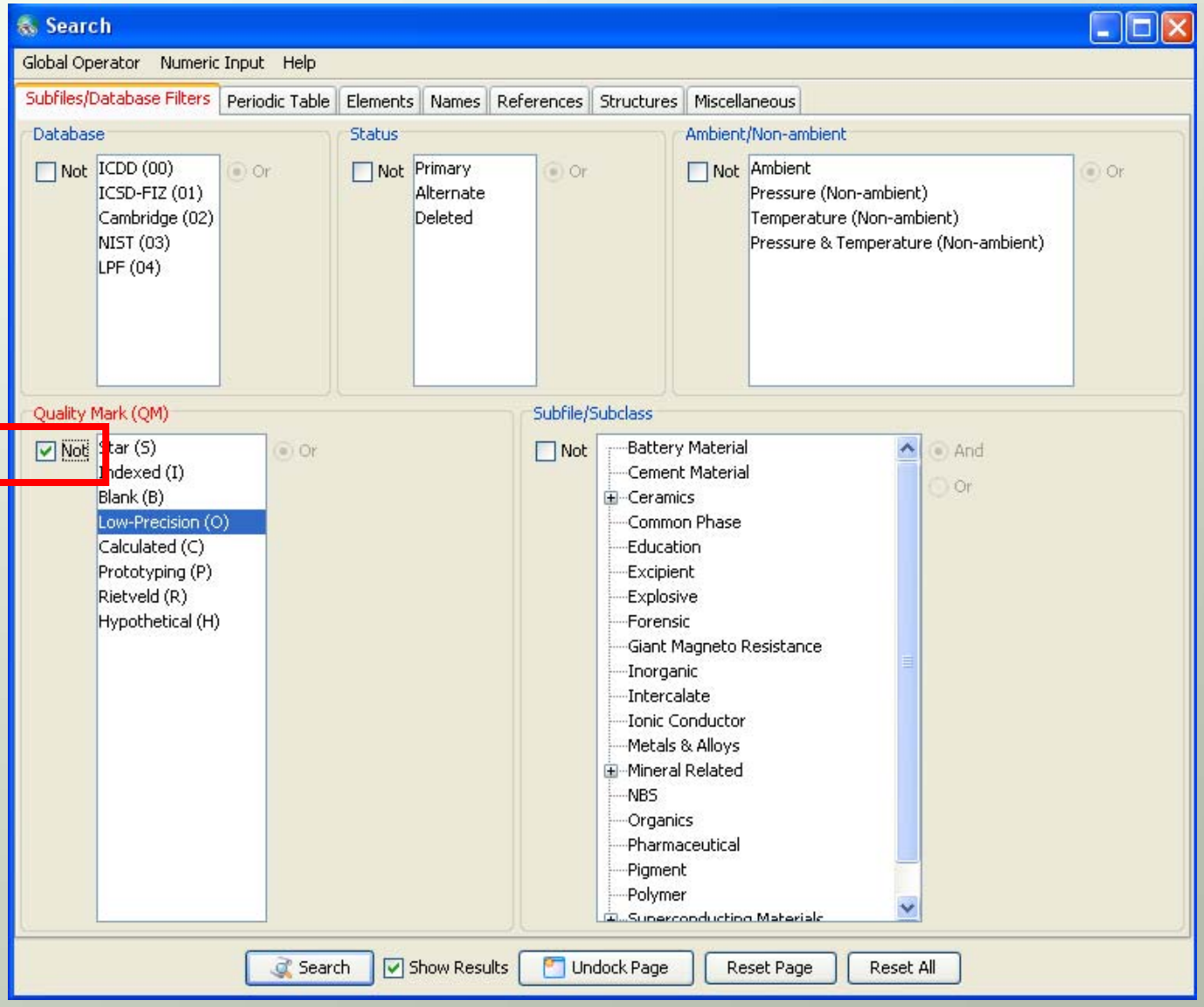
QM: Multiple Selection

In this example, patterns with either S or I quality marks will be returned in the search results.



Excluding a Particular QM

To exclude a particular QM, be sure to check the Not box. Here, patterns with O quality marks will not be included in the search results.

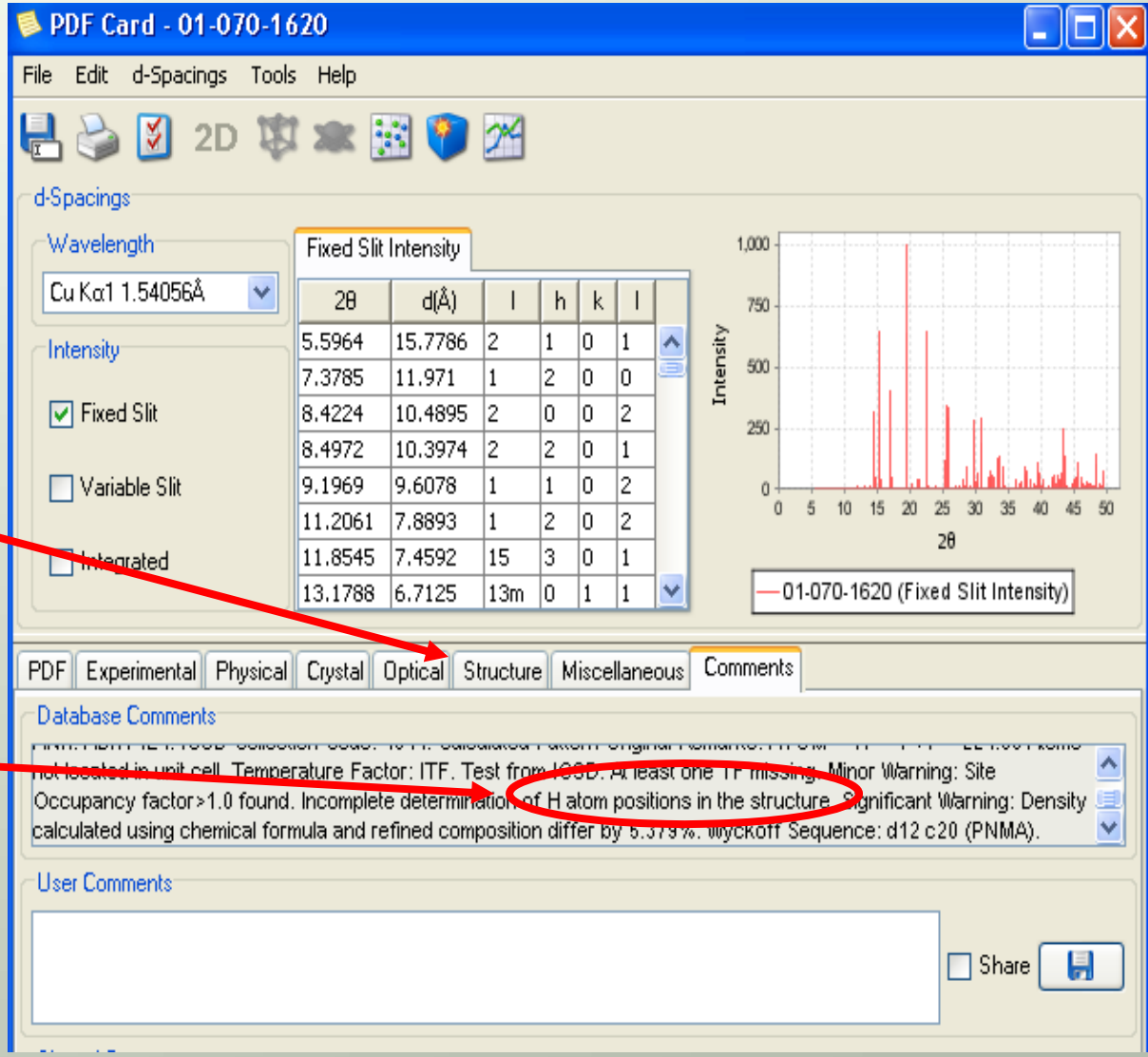


Quality Mark

Example of Editorial Comments

Explanations of a pattern's quality mark can be found in the editorial comments.

This Significant Warning gives this calculated pattern a quality mark of B.



Thank you for viewing our tutorial.
Additional tutorials are available at the ICDD website (www.icdd.com).

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