

# 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).

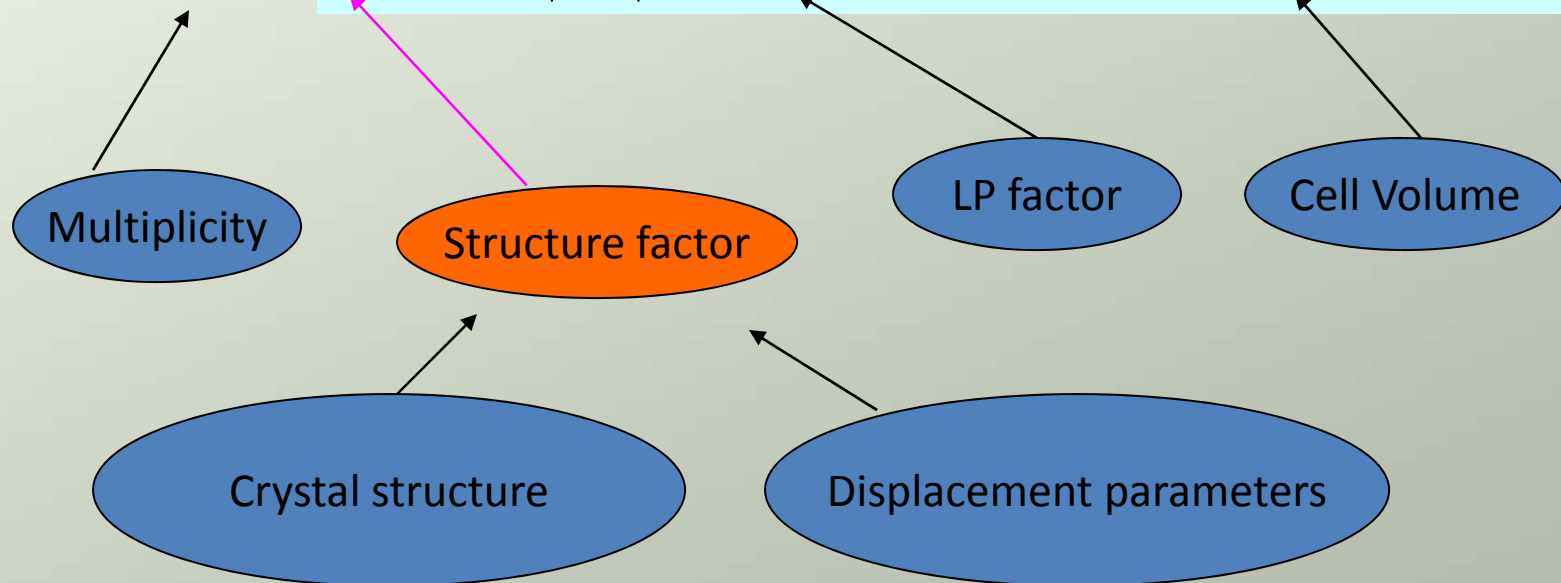
# QM for Experimental Patterns

- **Star** (Well characterized chemically and crystallographically, no unindexed lines,  $\Delta 2\theta \leq 0.03^\circ$ )
- **R** (d values obtained from Rietveld refinement)
- **I** (Well characterized chemically, no unindexed strong lines,  $\Delta 2\theta \leq 0.06^\circ$ )
- **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.

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



## 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
<b>No Warning</b>	*
<b>Minor Warning</b>	I
<b>Significant Warning</b>	B
<b>Assigned structure (Prototype)</b>	P
<b>Hypothetical</b>	H
<b>Major Warning</b>	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.

**Search**

Global Operator   Numeric Input   Help

**Subfiles/Database Filters**   Periodic Table   Elements   Names   References   Structures   Miscellaneous

**Database**

☐ Not ☐ Or

- ICDD (00)
- ICSD-FIZ (01)
- Cambridge (02)
- NIST (03)
- LPF (04)

**Status**

☐ Not ☐ Or

- Primary
- Alternate
- Deleted

**Ambient/Non-ambient**

☐ Not ☐ Or

- Ambient
- Pressure (Non-ambient)
- Temperature (Non-ambient)
- Pressure & Temperature (Non-ambient)

**Quality Mark (QM)**

☐ Not ☒ Or

- Star (S)
- Indexed (I)
- Blank (B)
- Low-Precision (O)
- Calculated (C)
- Prototyping (P)
- Rietveld (R)
- Hypothetical (H)

**Subfile/Subclass**

☐ Not ☐ And ☐ Or

- Battery Material
- Cement Material
- + Ceramics
- Common Phase
- Education
- Excipient
- Explosive
- Forensic
- Giant Magneto Resistance
- Inorganic
- Intercalate
- Ionic Conductor
- Metals & Alloys
- + Mineral Related
- NBS
- Organics
- Pharmaceutical
- Pigment
- Polymer
- + Superconducting Materials

☒ Show Results

# Excluding a Particular QM

**Search**

Global Operator Numeric Input Help

Subfiles/Database Filters Periodic Table Elements Names References Structures Miscellaneous

**Database**

☐ Not ICDD (00) Or ICSD-FIZ (01) Cambridge (02) NIST (03) LPF (04)

**Status**

☐ Not Primary Or Alternate Deleted

**Ambient/Non-ambient**

☐ Not Ambient Or Pressure (Non-ambient) Temperature (Non-ambient) Pressure & Temperature (Non-ambient)

**Quality Mark (QM)**

☒ Not Star (S) Or Indexed (I) Blank (B) Low-Precision (O) Calculated (C) Prototyping (P) Rietveld (R) Hypothetical (H)

**Subfile/Subclass**

☐ Not Battery Material And Cement Material Or Ceramics Common Phase Education Excipient Explosive Forensic Giant Magneto Resistance Inorganic Intercalate Ionic Conductor Metals & Alloys Mineral Related NBS Organics Pharmaceutical Pigment Polymer Superconducting Materials

Search Show Results Undock Page Reset Page Reset All

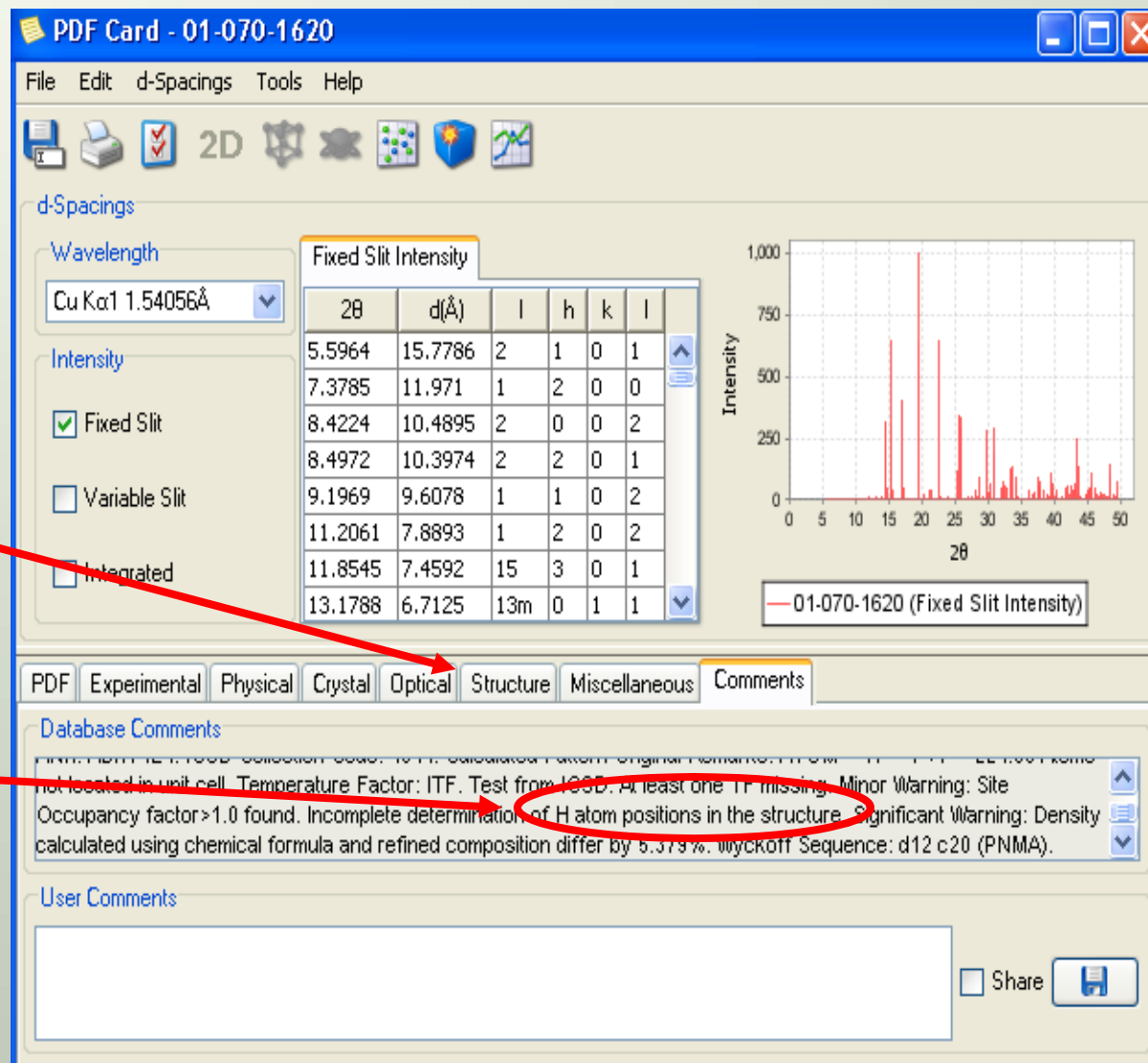
To exclude a particular QM, be sure to check the **Not** box. Here, patterns with O quality marks will not be included in the search results.

# 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](http://www.icdd.com)).



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