

PDF Editorial Staff Subcommittee
Wednesday, 16 March 2011
ICDD Headquarters
Chairman - Suri Kabekkodu

Call to Order

Appointment of Minutes Secretary

Lisa Lanno

Minutes Approved

The minutes from the March 2010 PDF Editorial Staff Meeting were approved.

Dann, Wallace

5 Yes, 0 No, 0 Abstain

Board Report (Scott Misture)

The Board approved the motion that headquarters use two (2) new Quality Marks for non-crystalline materials. The proposed quality marks are: good (G) and minimal acceptable (M), and defined as:

1. Good (G) patterns should have chemical analysis, characterization of local structure (either by pair distribution function or spectroscopy) & good signal/noise
2. Minimal acceptable (M) patterns should have good signal/noise & chemical analysis

The motion for a round robin for amorphous and poorly crystalline materials was also approved.

Editorial Progress

In the past three years, we have implemented our primary and alternate codes to experimental patterns (93,348 coded as primary; 1,504 are coded as alternates). We now have 12,145 deleted patterns. Unless there is a very good reason (exact duplicate or something crystallographically wrong with a pattern), we do not delete patterns. J. Faber questioned if removal is clearly better option. S. Kabekkodu responded that the criteria are: same unit cell parameters, same reference and structurally identical, then the subfiles are transferred to cross referenced patterns.

New this year is the cross reference related phase. 13,436 ICSD primary patterns are cross referenced to related phases in the LPF (1% on reduced cell volume, 5% on weight difference). This cross reference table is kept separate from the regular cross reference table.

Population of new editorial comments describing quality which include minor warning, significant warning, major warning (these are entries with major warnings which are editorially on hold) can be found on page 9 within the PowerPoint attached.

The thermoelectric materials subfile has been approved and implemented for publication in Release 2011.

The following codes were added in response to a motion from the Micro and Mesoporous Material Subcommittee (MMM): Zeolites 3,185; MOF 69; Clathrates 5,832; no subclass. These entries are coded only in the editorial system and not the product since they are not yet well populated.

The subfile populations show significant increases in polymers, pharmaceuticals (6,500) and thermoelectric materials. Metals and Alloys is a large subfile classification.

Please link to the pages in the attached PowerPoint for the numbers of:

New Entries – page 5

Processed Vs. Published – page 6

Quality mark distribution of newly added LPF entries – page 10

Quality mark distribution of newly added ICSD entries – page 11

Quality mark distribution of newly added CSD entries – page 12

Quality mark distribution of newly added experimental entries – page 13

General discussion

People are needed to abstract Modulated Structures and asked to e-mail S. Kabekkodu, if interested.

P. Wallace noticed Physical Properties are in papers but not in entry – S. Kabekkodu said editors should look for this information and add to comments if missed during abstraction.

P. Wallace mentioned the new method of prototype structures. S. Kabekkodu clarified that in previous years there were only 2 fields for the structure types; one being LPF and the other from the Metals and Alloys. Now it has been expanded, like our compound fields, to allow the specification of the source of the structure type and what structure type it is, which can be very useful in mapping it.

Motion to adjourn meeting

S. Kabekkodu

The background features a dark blue field with several overlapping circles and lines. Three prominent circles are arranged in a triangular pattern, each containing a smaller dotted circle. A vertical line and two diagonal lines intersect these circles, creating a complex geometric pattern.

Editorial Progress in Release 2011

The editorial task

- New EXP data
- New LPF and CSD data
- New ICSD entries (and updates)
- Modulated structures
- Abstracted Atomic coordinates
- Editorial and Duplicate review
- Assigning Calculated pattern QM
- Raw Data
- Target Materials (Polymer)
- Cross Referencing
- Subfile population

New Entries

Database	Diffraction Patterns	Atomic Coordinates
Experimental	1416	324
Modulated	54*	8
ICSD	12141	827
LPF	13092	13092
CSD	28631	
<i>TOTAL</i>	55288	14251

*46 are already published experimental entries now expressed in superspace

Processed Vs Published

Database	Processed	Published
LPF	13793	13092
ICSD	14595	12141
Modulated Structures	74	54
Atomic Coordinates (exp)	726	332
Raw Data	~1200	912
CSD	32811	28631

DBStatus

- All the patterns were classified into Primary/Alternate using Composition, QM and Temp/Pressure of data collection
- DBStatus Distribution in PDF-2 and PDF-4

Cross Referencing Related Phase

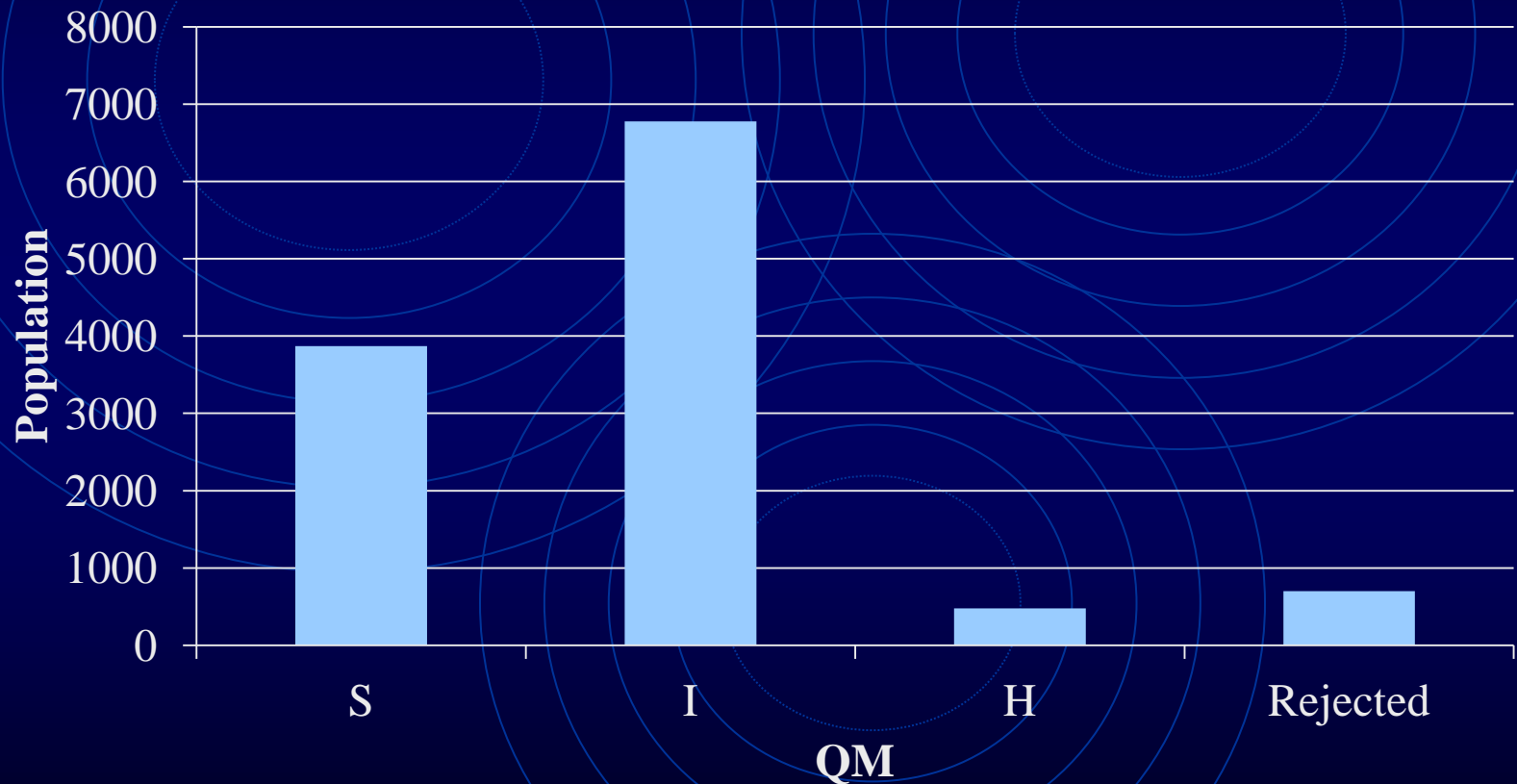
- 13436 ICSD primary patterns are cross referenced to related phase in LPF (1% on reduced cell volume, 5% on weight difference)
- This cross reference table is kept separate from the regular cross reference table.

Population of new editorial comments describing quality

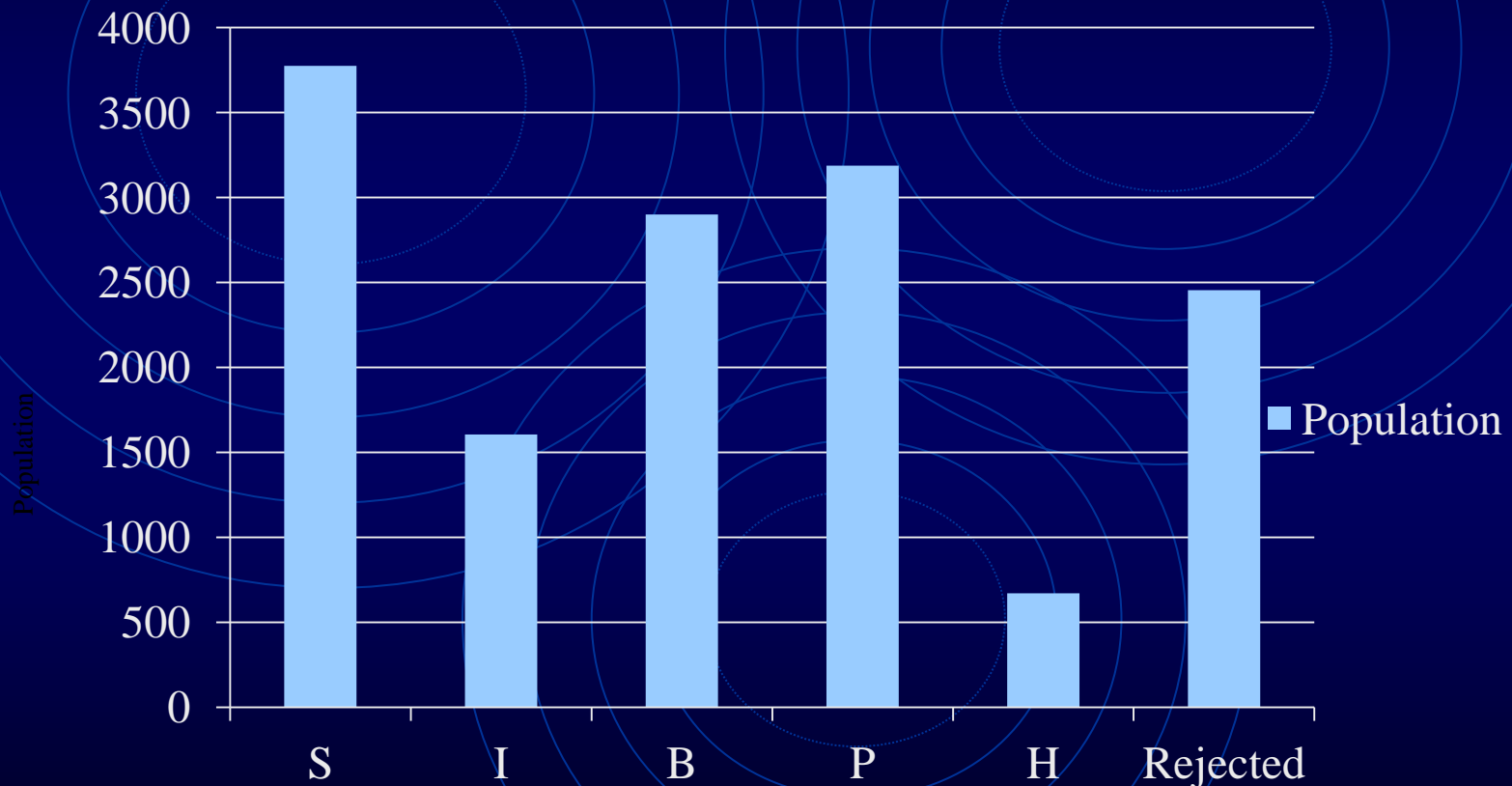
Database	Minor Warning	Significant Warning	Major Warning*	Total
ICSD	11847	7237	367	19451
LPF	17788	2427	37	20252
CSD	5808	4779	2417	13004
Total				52707

**Entries with major warnings are editorially on hold*

Quality mark distribution of newly added LPF entries

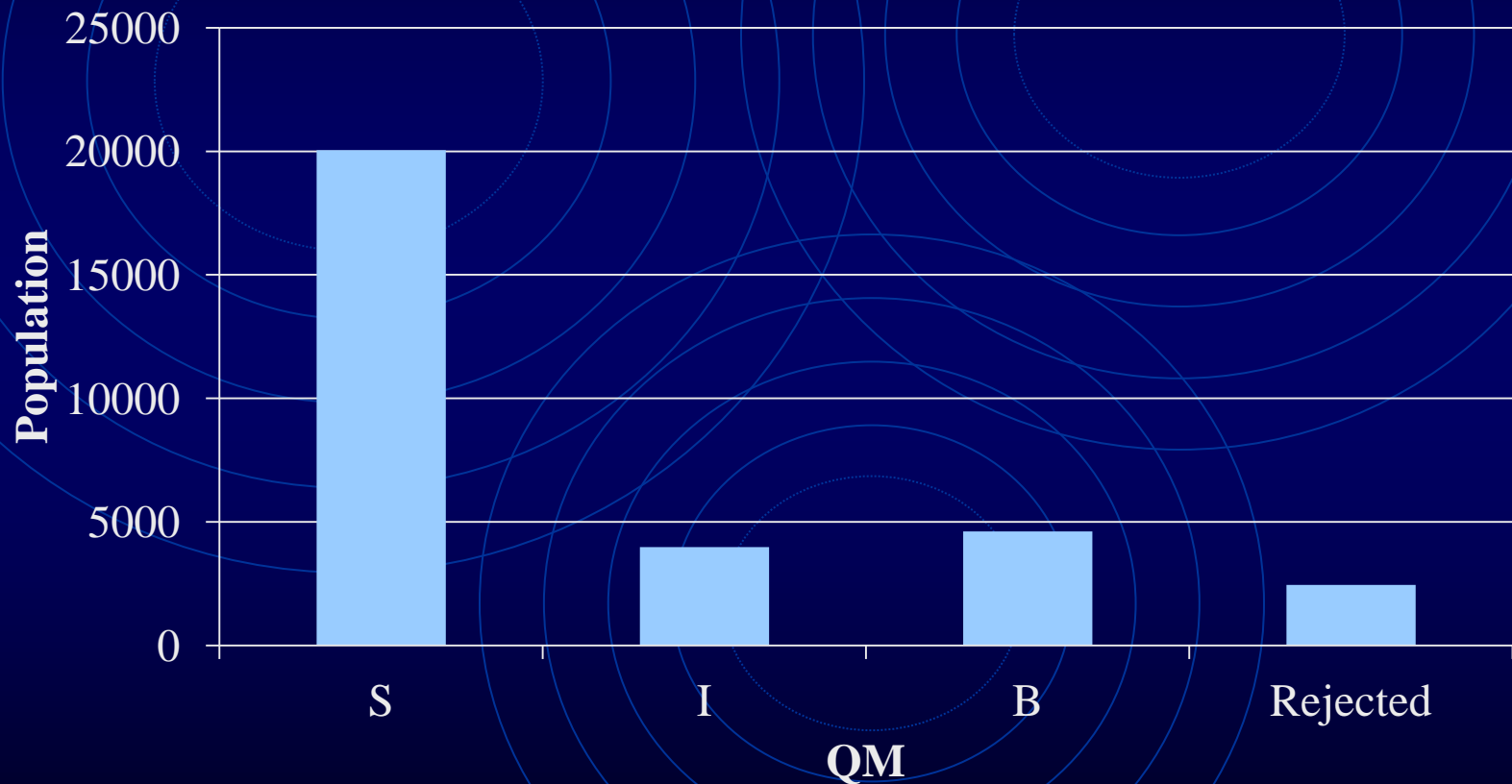


Quality mark distribution of newly added ICSD entries

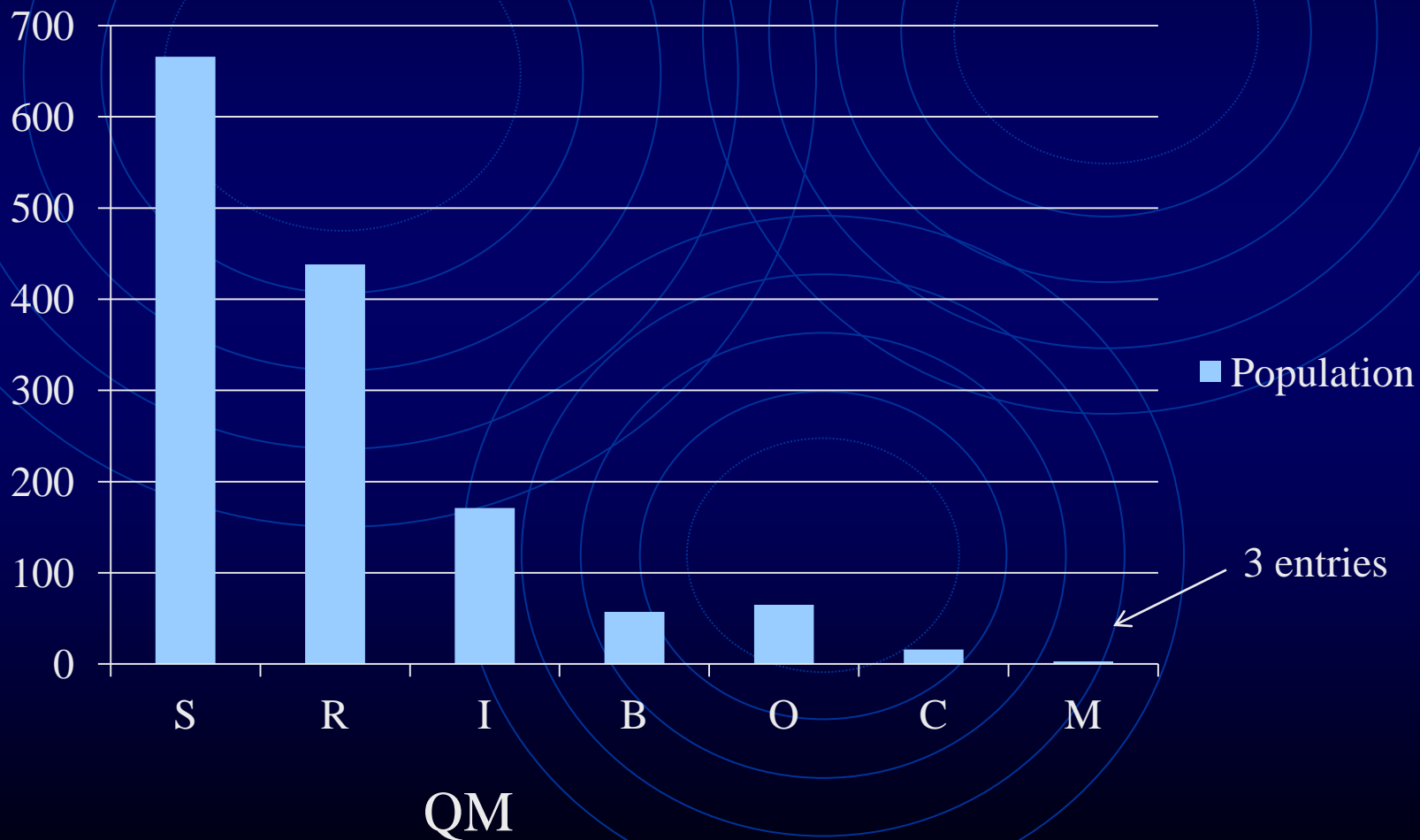


Higher number of rejected entries is on account of ICSD's addition of NIST data

Quality mark distribution of newly added CSD entries



Quality mark distribution of newly added experimental entries



Thermoelectric subfile

- Thermoelectric subfile is now recommended for publication in release 2011

Micro and Mesoporous materials

MMM

Zeolite
(3185)

MOF
(69)

Clathrate
(5832)

No Subclass
(307)