PDF Editorial Staff Subcommittee Minutes
Wednesday, 17 March 2010
ICDD Headquarters
Chairman - Suri Kabekkodu

Call to Order

Appointment of Minutes Secretary
Lisa Lanno

Motion 1:
The minutes from the March 2009 PDF Editorial Staff meeting were approved.
Kabekkodu, Wallace
8 Yes, 0 No, 0 Abstain
Motion passed.

Board report (Scott Misture)
The Board approved the motion to define the "R" quality mark as: "The "R" quality mark is used for patterns where it is clear that the d-values are directly the result of whole powder pattern fitting methods such as the Rietveld or decomposition methods. The entry should meet all the requirements of star quality mark."

Editorial Progress Report
Annual routine tasks, such as subfile and quality mark assignments, duplicate reviews, reviewing raw data, cross references, etc. were performed as normal. This year we had some targeted materials, i.e., polymers and amorphous materials that were included in the database.

S. Kabekkodu reported on the details of Release 2010 and the editorial work that went into it. There are a total of 59,510 new entries being published. S. Kabekkodu's report begins on page 3.

A. Roberts helped with a mineral editorial flag clean up. A new flag (NAT – naturally occurring mineral) was created and the non-ambient flag for minerals, because it exists elsewhere, was removed.

Metals and Alloys structure types – about 30,000 were updated by the Metals and Alloys Task Group. Beginning this year, we are reviewing ANX formulas from ICSD. J. Dann worked on this project and reviewed close to 17,000 ANX formulas.

Pattern distribution was also shown. Close to 60,000 entries were removed during the duplicate review.

Summary of Sunday's Editors' Meeting

- Seven new subfiles have been added to the PDF-4/Organics 2010: Alkaloids (ALK); Amino Acids, Peptides & Complexes (APC); Carbohydrate (CAR); Nucleosides & Nucleotides (NUC); Porphyrins, Corrins & Complexes (PCC); Steroids (STE)
- A guide, to assist abstractors and editors, to help standardize physical property comments is being established. Work on this guide is on-going in an attempt to make the list more complete.
- A brief background and introduction of modulated structures was given the importance of them and the work that is being done at ICDD.
- Headquarters is beginning to include non-crystalline materials in the PDF. The first target material is an amorphous cellulose pattern.
- The DataQUACkER program is in use and continues to be modified and tweaked.

Motion 2:
The PDF Editorial Staff Subcommittee recommends to the Technical Committee 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

Kabekkodu, Wallace
14 Yes, 0 No, 1 Abstain
Motion passed.

Motion 3:
The PDF Editorial Staff Subcommittee recommends to the Technical Committee to approve a round robin for amorphous and poorly crystalline materials.

Kabekkodu, Rotella
11 Yes, 0 No, 1 Abstain
Motion passed.

Physical Properties (see Joel's presentation beginning on page 13 for further details)
J. Reid gave a status report on the work being done at Headquarters on physical properties. We have been thinking about what additional types of properties that are in the literature that we would like to capture and how we would like to standardize and express them. We would like to give users key quantities that will help them avoid going back to the original literature. We started by looking at our subfiles and specific related quantities that are widely available within our subfiles and prepared a guide. We would like to get some feedback and suggestions to help us expand the guide.

General Discussion
There was no general discussion or new business.

Adjournment
Motion to adjourn meeting.
Kabekkodu, Wallace
6 Yes, 0 No, 0 Abstain
Motion passed.

Editorial Progress in Release 2010

The editorial task

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

New Entries

Database	Diffraction Patterns	Atomic Coordinates
Experimental	1517	872
ICSD	10219	9205
LPF	13458	13458
CSD	34316	
TOTAL	59510	23535

Processed Vs Published

Database	Processed	Published
LPF	14006	13458
ICSD	17115	10219
CSD	37675	34316
Atomic Coordinates (exp)	1312	872
Raw Data	~1200	936

Mineral Flags

- Introduced a new flag nNAT for the easy identification of naturally occurring minerals
- Removed non-amabient flag for minerals as we already have such flag in the database for all entries

Structure types

- M&A structure type updates (~30,000) based on M&A task group effort
- Introduced ANX formula for LPF entries

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

		PDF-2		PDF-4		
DBStatus	Experimental	ICSD	NIST	ICSD	NIST	LPF
Primary	89035	69311	5856	43363	2568	64470
Alternate	1411	26733	2832	25767	2077	42492
Deteted	12106	2444	1379	1634	478	1
Removed				27724	4944	
Check	*102552*	98488	10067	98488	10067	106963
Total		211107		285402		

		PDF-2		PDF-4		
DBStatus	Experimental	ICSD	NIST	ICSD	NIST	LPF
Primary	90500	72460	5776	39582	2506	74102
Alternate	1440	26876	2912	21116	1564	44711
Deteted	12116	5151	1379	3392	410	1
Removed				40397	5587	
Check	*104056*	104487	10067	104487	10067	118814
Total		218610		291440		

		PDF-2		PDF-4		
DBStatus	Experimental	ICSD	NIST	ICSD	NIST	LPF
Primary	91964	82587	5887	37837	1839	84335
Alternate	1476	26798	2986	19178	1446	47936
Deteted	12133	5321	1194	2787	350	1
Removed				54904	6432	
Check	*105573*	114706	10067	114706	10067	132272
Total		230346		301282		

Physical Properties

Joel Reid

Goals

- Abstract additional information critical to describing the functional properties of technologically important materials.
- Standardize the format and units used for physical properties where possible.

Why add physical properties?

- Provide users with quantitative information for technologically important materials.
- Prevent users from always having to go to the primary literature.
- Increase the value of PDF entries.

Physical Parameters - Subfiles

Ion Conductor
Ion conductivity, σ (S/cm)

Semiconductor
Conductivity, σ (S/cm)
Band gap, E_g (eV)

Superconductor
Transition temperature, T_c (K)
Energy gap, E_g (eV)
Critical magnetic field, H_c (T)

Battery
Gravimetric capacity (mAh/g)
Volumetric capacity (mAh/cm^3)

Ferroelectric (Piezoelectric)
Curie temperature, T_C (K)
Polarization, P (μC/cm^2)

Microwave
Dielectric constant, ε
Temperature coefficient of resonant frequency, TCF (ppm/K)
Quality Factor, Q (none)

Physical Parameters

Mechanical

Young's modulus, E (GPa, MPa)

Shear modulus, G (GPa)

Bulk modulus, K (GPa)

Poisson's ratio, υ

Fracture toughness, K_{1c} (MPa $m^{1/2}$)

Strength (MPa, GPa)

Thermal

Heat capacity, C_p & C_v ($J\ g^{-1}\ K^{-1}$, $J\ mol^{-1}\ K^{-1}$)

Linear thermal expansion coefficient, α (K^{-1})

Thermal conductivity, k ($W\ m^{-1}\ K^{-1}$)

Magnetic

Transition temperature, T_c (K)

Neel temperature, T_N (K)

Weiss temperature, Θ (K)

Effective magnetic moment, μ_{eff} (in Bohr magnetons, μ_B)

Example: Ferroelectrics

Key Quantities:

- Curie temperature (T_C or T#C)
  - Units: Kelvin (K)

- Polarization (P) at a given temperature (K)
  - Units: micro-Coulombs per square centimeter ($\mu C/cm^2$ or $GMC/cm@2)
  - Conversions: $P\ (\mu C/cm^2) = P(esu)/3000$

    $P\ (\mu C/cm^2) = P(C/m^2) \times 100$
  - Notes: Types include saturation polarization (P_s or P#s) and remnant polarization (P_r or P#r)

Ferroelectrics (cont.)

Format for Database Comments:

PP Curie temperature, T#C = 96 (3) K
PP Polarization, P = 5.0 (1) $GMC/cm@2 at 80 K

Feedback

- What physical property information is of most interest to you?