

PDF Editorial Staff Subcommittee
Wednesday, 21 March 2007
ICDD Headquarters
Chairman - Suri Kabekkodu

Minutes Approved

The minutes from the March 2006 PDF Editorial Staff meeting were approved.

Editorial Progress in PDF Release 2007

One special project this year was abstraction of atomic coordinates.

New diffraction entries this year totaling 20,418 and 9,344 atomic coordinates.

Database Status

All patterns were classified into primary/alternate using composition, quality mark and temperature/pressure of data collection.

Subfiles

~34,000 entries have been populated with subfiles using an automated procedure in-house (chemistry and crystallographic parameters matched a very strict criteria this year).

Subfile list is found on page 3 and 4.

Summary of Sunday's Editors' Meeting

- Duals
- Naming conventions (compound name inconsistencies)
- Wavelengths (way off from standard wavelengths in literature – need some standard wavelength)
- New policy is to abstract atomic coordinates as well as the powder pattern.
- Properties under the ceramic subfile should be moved to another property class. Ceramic Subcommittee will discuss and give the feedback back to headquarters.
- Graph codes – headquarters has a scanner in-house to digitize a pattern.
- Use Kelvin instead of Celsius for temperatures.

General Discussion

C. Crowder stated that 90% or more of the patents get rejected, and maybe we shouldn't waste time abstracting. J. Kaduk said more and more patents have complete powder pattern. D. Smith is still having trouble determining the composition when he is abstracting patterns. M. Bennett said data more than 10 years old is useless from patents. F. Rotella noticed that most of the patents are pharmaceuticals and is useful to have in the File. D. Rendle said it is difficult making a decision with the patents. If not sure, he would like to take them out. S. Quick suggested when it is difficult to make a decision, it should be forwarded to the Task Group to review. S. Kabekkodu said possibly the patents should be sent to the Zeolite Task Group for pre-review. The guidelines for the bibliographers will be to search on patents that are not over 10 years old and a list of patent numbers will be sent out for pre-review to the various Task Groups. Volunteers for this review will be David Rendle and Frank Rotella for the organic patents and Cyrus Crowder volunteered for the zeolite patents.

New Business

J. Kaduk quantitative phase analysis using I/I corundum.

Looking into I/I corundum distributions of like compositions. Headquarters wants to start database analysis and discuss next year.

Adjournment

Releases 2005 - 2007

Subfile:

2005:

2006:

2007:

<i>Battery Materials</i>	300	434	720
<i>Bioceramics</i>	96	123	233
<i>Cements</i>	414	418	1,048
<i>Ceramics</i>	4,075	4,566	8,674
<i>Excipients</i>	961	1,699	2,023
<i>Explosives</i>	700	754	1,006
<i>Ferroelectrics</i>	669	735	1,623
<i>Forensics</i>	3,778	3,782	9,961
<i>Intercalates</i>	320	336	394
<i>Ionic Conductors</i>	308	410	929
<i>Metals & Alloys</i>	82,096	106,281	113,989
<i>Microwaves</i>	499	604	973
<i>Mineral Related</i>	18,529	20,430	27,650
<i>Minerals</i>	18,529	20,227	20,738

<i>Gems</i>	0	0	86
<i>Nonambients</i>	0	641	2,788
<i>Synthetics</i>	0	5,889	10,366
<i>Perovskites</i>	1,779	1,947	3,624
<i>Pharmaceuticals</i>	2,360	3,628	4,157
<i>Pigments</i>	372	416	1,245
<i>Polymers</i>	895	933	1,042
<i>Semiconductors</i>	400	508	1,650
<i>Superconducting Materials</i>	2,631	2,749	6,996
<i>Superconductor Conventional</i>	227	227	237
<i>Superconductor High Tc</i>	160	160	160
<i>Superconductor Reaction Products</i>	298	296	296
<i>Superconductor Related Materials</i>	492	492	498
<i>Zeolites</i>	2,190	2,284	3,178