

**X-ray Diffraction Methods Subcommittee  
International Centre for Diffraction Data  
Minutes of the Meeting of 21 March 2012**

Attending: List of attendees has been generated separately

The meeting was called to order at 10:00 am by Dr. R. Papoular

I. MINUTES OF PREVIOUS MEETING:

The minutes of the meeting of March, 2011 were approved.

II. OTHER ACTION ITEMS:

1. Dr. V. Petkov was appointed as acting scribe

III. DISCUSSION ITEMS:

1. Dr. Papoular updated the attendees on the mission of the XRD Methods Subcommittee
2. The following topics relevant to PDF2/PDF4 databases were discussed:
  - Extracting reference patterns from Rietveld refinements – extracted single phases vs. full diffraction pattern reporting in the database. How to report the chemistry of the sample – by composition of the individual phases or by composition/chemistry of the full XRD pattern? Unfortunately, no definitive recommendation was agreed upon.
  - How to associate best XRD patterns from the database with structure models? Ideas were discussed, no recommendation made.
  - How to handle XRD patterns of materials that change during data collection. Example – organics. Ideas from the attendees included using supplementary neutron data, repeating scans and saving/reporting all scans so that changes in the material studied can be followed up, using fast scans (strip detectors at synchrotrons) to monitor eventual changes.
  - Including of simulated patterns from known crystal structures. The shared opinion was that those are important pieces of information.
  - How to handle theoretically predicted, and never experimentally confirmed, structures and XRD patterns computed from them given the fact that those are millions? The prevailing opinion was that including them all will clutter the PDF2/PDF4 database though some predicted structures of “important” materials may be a good exception. It was left to the editors of the database to decide which materials are important. It was also emphasized the need to develop “quality marks” for predicted structures.

The meeting was adjourned at 11:00 AM.

Respectfully submitted – V. Petkov