

X-ray Diffraction Methods Subcommittee Minutes
Wednesday March 16th, 2016
Chris Gilmore, Chairman

Call to Order by Chris Gilmore.

Appointment of Minutes Secretary – Amy Gindhart
Approval of the minutes from 2015- moved by Scott Misture, Winnie Wong-Ng seconded.
Approved by room.

The Mission Statement was reviewed. There are no proposed changes as of now, but it may be reviewed in the future. The current statement reads:

The X-ray Methods Subcommittee will provide recommendations for data to be included in the PDF by considering instrument configurations, data collection, and powder pattern calculations, with particular focus on the state-of-the-art methods.

Directors' Liaison Report by Jordi Rius: There were no motions from last year.

Presentation 1:

Jim Kaduk provided a short presentation entitled “An Example of Data Mining in the PDF”.

He showed an example of a pattern search in PDF-4+ 2015 with a graphical representation of cell volume vs atomic percent generated manually after searching elements and space group number.

Jim Kaduk talked about ICDD software and how it should be capable of computing results for solid solution series regression lines automatically. There was a discussion led by Cyrus Crowder and Suri Kabekkodu concerning the difficulties associated with databases and the associated software knowing exactly what the user will want to calculate and display. Jim mentioned that he does regression fits all the time so he is looking for ease of use with associated interactive graphics. Chris mentioned the use of robust regressions to deal in an unbiased way with outliers.

It will be possible to remove quality marks and ambient situations from the graph according to Justin in the 2016 product. Chris wanted to start a dialogue about future data mining in the PDF products. Should there be tools to make true data mining easier and straight-forward in the products?

Allowing an export to Excel was mentioned by Cam Hubbard as one possibility or should we make it available within the ICDD product? Tom Blanton mentioned we restrict the export from the database by design. He mentioned if something was desired ICDD would embed it directly into the software.

Chris mentioned investing time into cluster analysis and porting these methods into the database. He believes that cluster analysis can be used as part of data mining. Tom Blanton mentioned that

the Metals and Alloys subcommittee is working on populating data to be able to do this in one form or another. Tom Blanton proposed a motion for Chris to work with the Metals and Alloys task group and the product to look at cluster analysis options.

Presentation 2:

Jim Kaduk presented information on Volume H: Powder Diffraction.

He went through the parts of the book and the authors of the individual sections and mentioned that if any new sections are needed they are already talking about a second addition. The release of Volume H is scheduled for the Fall 2016.

Motion #1:

The X-ray Diffraction Methods Subcommittee moves that Chris Gilmore is given a license for the PDF-4+ database so that he can work with the Metals and Alloys Task Group to implement cluster analysis with a report to be presented at the March 2017 meeting.

Motion: Tom Blanton

Seconded: Scott Misture

Yes: 19

No: 0

Abstain by Name: Chris Gilmore

Motion #2:

The X-ray Diffraction Methods Subcommittee moves that user-definable equations and robust regressions be implemented in PDF-4 products.

Motion: John Faber

Seconded: Scott Misture

Yes: 24

No: 0

Abstain: 0