

X-ray Diffraction Methods Subcommittee Meeting Minutes
Wednesday, 13 March 2017
International Centre Headquarters
Conference Room A
10-11 a.m.
Chris Gilmore, Chairman

1. Call to Order C. Gilmore
2. Appointment of Minutes Secretary N. Ernst Boris
3. Approval of Minutes from 2016
 - a. Moved by Jim Kaduk
 - b. Seconded by Jeffrey Deschamps
 - c. Approved 8-0

4. Review of Mission Statement

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.

5. Directors' Liaison Report T. Ida
6. Short presentations
 - a. Summary of the results of clustering a subset of the metals and alloys database by Chris Gilmore.
 - b. Topological information in crystallography and crystal chemistry: a route to knowledge databases presentation by Vladislav A. Blatov.
 - c. A brief discussion of the use of 2-D diffraction data by Jim Kaduk.

7. Discussion

Cluster analysis was discussed in relation to Metals and Alloys data using a subset of data selected by Peter Wallace and processed into cif files by Suri Kabekkodu. Chris Gilmore discussed cluster analysis as it relates to this data. There were 359 files representing 6 different structure types, but these did not cluster into 6 groups. This was not unexpected, and it needs further investigation. The cluster analysis modules in EVA software were the primary tool. Further detail on re-clustering as needed and modifying the dendrogram cut line was also presented. The general conclusion was this could be useful. Jim Kaduk and Cam Hubbard then discussed atomic arrangements and radii. Further discussion involved 2D and 3D images and what could be analyzed and clustered. Jim Kaduk asked what our goal was and it was agreed to be pattern matching. Peter Wallace asked could this help with assigning prototypes. Chris Gilmore suggested he look at this further. Also discussed was the wording "Phase Diagram/Prototype" and "ordering" and a question was raised, what does that mean/how does it relate to the clustering analysis. Vladislav A. Blatov then overviewed his plenary discussion which discussed the need to make crystallographic databases knowledge databases. Some software in that direction exists, but more is needed. The meeting was adjourned with no motions.

8. Adjournment