

**X-ray Diffraction Methods Subcommittee Minutes**  
**Wednesday, 14 March 2018**  
**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 2017

Moved: Jim Kaduk  
Second: Dave Taylor

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

No prior motions; nothing to report.

6. Two short presentations

Clustering soils data, Steve Hillier - presented by Chris Gilmore.

Steve Hillier was unable to attend so Chris presented Steve Hillier's data on clustering soil data (pre-treatment of soils). Questions and discussion followed regarding applications, especially agriculture.

Partial Least Squares - Chris Gilmore

Chris then presented the use of partial least squares as a tool for quantitative analysis. This is a standard procedure in spectroscopy. An example using PXRD cement data with the PLS NIPALS formalism was shown. The method needs a training data set.

7. Discussion

The extensive discussion expressed interest in the PLS method as an alternative to standard search-match procedures and it could have uses with PDF data although it would be an entirely new approach.

**Motion:** The XRD Subcommittee recommends to the Technical Committee that headquarters explore the possibilities given by traditional and advanced machine learning (e.g. partial least squares) for expanding the capabilities of the database software towards quantification.

Proposed: Matteo leoni  
Seconded: Pete Wallace  
Votes for: 10 Passed to Tech Committee

8. Adjournment