

Technical Committee Meeting Minutes
Thursday, 15 March 2018
International Centre Headquarters
9:30 a.m. – 12:30 p.m.
Conference Room A
Mark Rodriguez, Chairman

1. Call to Order and Opening Remarks Mark Rodriguez
2. Roll Call and Attendance/ Minutes Secretary Linda Shertz
3. Additions and/or Deletions to the Agenda Mark Rodriguez
4. Approval of the 2017 Minutes Mark Rodriguez
The minutes were unanimously approved.
5. Reports/Presentations of Technical Regional Co-Chairs and International Guests (access on Membersonly website.)
 - A. Eastern Pacific Rim Takashi Ida
 - B. European Community Matteo Leoni
 - C. India T.N. Guru Row
 - D. Indian Ocean Rim Vanessa Peterson
 - E. Newly Independent States Evgeny Antipov
 - F. North America Mark Rodriguez
 - G. People's Republic of China Xiaolong Chen
 - H. South America Miguel Delgado
 - I. United Kingdom & Ireland Steve Hillier

6. Subcommittee Reports and Motions

A. Materials

1) Ceramics Winnie Wong-Ng

Motion 1: The Ceramics Subcommittee recommends to the Technical Committee that ICDD Headquarters expand the Battery Materials Subfile, beyond Lithium battery electrode materials.

Wong-Ng moved, Wallace seconded – Motion passed unanimously.

Motion 2: The Ceramics Subcommittee recommends to the Technical Committee that Headquarters secure a list of materials, from Antipov, who found materials that should not be flagged as superconductors.

Discussion: Antipov found that some materials, from unknown editors, are flagged as superconductors when they shouldn't be. Antipov will supply the list of materials.

Wong-Ng moved, Payzant seconded – Motion passed unanimously.

2) Metals and Alloys Pete Wallace

Motion 3: The M&A Subcommittee recommends to the Technical Committee that Headquarters explore five components or higher systems in composition diagram capability. Graphical display within product is not required at this time. A report from headquarters, from TBlanton and JBlanton, will be given in fall 2018.

Discussion: TBlanton said it can be implemented. Wallace: We need a scope before we develop anything. Sagnella: Equimolar list will be small, but if you get variations, how should it be displayed? TBlanton & JBlanton will put together a paper and present it at the Fall Board Meeting.

Wallace's slide:

M&A Subcommittee moves to the Technical Committee that *Prototype Structure Profiles* be made available to PDF users.

Supplemental Information

- M&A *Prototype Structure Profiles* are (a) a useful analytical tool, (b) easily generated, (c) easily toggled from the profile to the list of examples and back, and (d) would be helpful in marketing our product.
- These profiles are based on the Crystal Data cell and contain the value of Z, as well as observed ranges for the:
 - Pearson Symbol Code,
 - Lattice parameters, cell angles, and axial ratios,
 - Atomic volumes, and
 - Calculated densities.

Important Note

- This motion *does not* require *site-specific chemical information for Crystal Data cells* to be a part of these profiles. However, should this data become available, it should be added to these profiles.

Wallace moved, Quick seconded – Motion approved unanimously.

Motion 4: The M&A Subcommittee recommends to the Technical Committee that headquarters explores graphical representation of composition diagram capability for binary and ternary systems.

Wallace moved, Quick seconded – Motion passed unanimously.

Motion 5: The M&A Subcommittee recommends to the Technical Committee that prototype structure profiles be made available to PDF users.

Discussion: TBlanton: Wallace will be the point of contact, and have a discussion in the fall. The extra paragraph is in Wallace's slide which is shown above.

Wallace moved, Misture seconded – Motion passed unanimously.

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| 3) Micro and Meso – No motions | Cyrus Crowder |
| 4) Minerals – No motions | Andy Roberts |
| 5) Organic and Pharmaceutical – No motions | Fred Wireko |
| 6) Polymers – No motions | Lizhi Liu |

B. Characterization Methods and Tools

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| 1) Electron Diffraction – No motions | Bryan Wheaton |
| 2) Non-Ambient Diffraction | Andrew Payzant |

Motion 6: The Non-Ambient Subcommittee recommends to the Technical Committee that Headquarters encourage submission of new non-ambient data that complete details of procedures and conditions and that they be documented in the PDF.

Payzant moved, Delgado seconded – Motion passed unanimously.

Motion 7: The Non-Ambient Subcommittee recommends to the Technical Committee that a task group identify materials (including unstable and reactive materials) for which the diffraction data is deemed likely to be highly sensitive to measurement conditions such as ambient humidity, partial pressure of oxygen, etc. Once such material areas are identified, there is an opportunity to evaluate whether additional warnings need to be recorded in the PDF.

Discussion: Ely will be the point of contact. Ely said first, state the scope of this issue and the rest can come later. TBlanton said this is a task group responsibility.

Payzant moved, Ely seconded – Motion passed unanimously.

Motion 8: The Non-Ambient Subcommittee recommends to the Technical Committee that ICDD provide financial support for a task group meeting at DXC2018 to organize writing of a PDJ review paper on non-ambient diffraction methods and best practices.

Payzant moved, Wallace seconded – Motion passed unanimously.

3) Synchrotron & Neutron Scattering Methods Pamela Whitfield

Motion 9: The Synchrotron and Neutron Scattering Methods Subcommittee recommends to Technical Committee that: Clarification and requirements of information are needed for submission of TOF data. Faber to be point of contact. Also, evaluate the possibility for Genie to be modified to read TOF data.

Whitfield moved, Faber seconded – Motion passed unanimously.

Motion 10: The Synchrotron and Neutron Scattering Methods Subcommittee recommends to the Technical Committee that: Headquarters explore the flagging of elements that pose issues for neutron simulation and known magnetic structure.

Whitfield moved, Peterson seconded – Motion passed unanimously.

Motion 11: The Synchrotron and Neutron Scattering Methods Subcommittee recommends to the Technical Committee that: Pair Distribution Function be generated from the PDF. Point of contact would be Whitfield.

Discussion: TBlanton: We will need more discussion if we implement this.

Whitfield moved, Quick seconded – Motion passed unanimously.

4) X-ray Diffraction Methods Chris Gilmore

Motion 12: 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.

Gilmore moved, Wallace seconded – Motion passed unanimously.

5) X-ray Fluorescence Mark Rodriguez

Motion 13: The XRF Subcommittee recommends to the Technical Committee that Headquarters merge the search match method in SIEve on XRD data with the chemical analysis data read into the database via a *.csv file and report back to the subcommittee in one year concerning the effectiveness of using this multidimensional search procedure. Consider a light element filter for data collected systems that have limited chemical diagnosis (XRF). We desire a multiphase search/match capability for combined XRD/XRF by the release of the 2020 product.

Rodriguez moved, Segre seconded – Motion passed unanimously.

C. ICDD Activities

1) Education Carlo Segre

Motion 14: The Education Subcommittee Chair recommends to the Technical Committee that ICDD Staff effort be assigned to assess the possibility of using the ATeLearning Virtual X-ray Laboratory platform to improve training in the collection of diffraction data and use of the PDF 4+ database.

Discussion: TBlanton stated that the first meeting took place at 7:30 am today.

Segre moved, TBlanton seconded – Motion passed unanimously.

2) PDF Editorial Staff – No motions

Soorya Kabekkodu

7. New Business

Mark Rodriguez

8. Adjournment