

**2021 ICDD Spring Meetings - A Virtual Zoom Event**  
**Non-Ambient Diffraction Subcommittee MINUTES**  
**Thursday, 11 March 2021**  
**9:00 am – 10:00 am**  
**Bryan Wheaton, Chair**

**1. Call to Order: (B. Wheaton)**

Attendance tracked through Zoom.

**2. Appointment of Minutes Secretary**

R. Santangelo appointed.

**3. Review of Mission Statement:**

The Non-Ambient Diffraction Subcommittee of the International Centre for Diffraction Data is organized to facilitate the use of non-ambient diffraction data by the scientific community. It makes recommendations to the ICDD about how diffraction data obtained at non-ambient conditions should be represented in the PDF, and suggests specific research activities that could result in production of non-ambient new patterns for the PDF. It also maintains contact with various research and administrative groups throughout the world to exchange information about new developments in non-ambient diffraction techniques and results.

**4. Approval of Minutes of the 2019 March Meetings**

A. Payzant Moved

T. Fawcett Second

No objections, Motion passes with unanimous consent

**5. Comments from Board of Directors' Liaison (R. Dinnebier)**

No motions, no report.

**6. Old Business**

- Status of review paper on non-ambient diffraction methods and best practices. Initial paper: HTXRD furnace calibration methods. *See PowerPoint by [B. Wheaton], available upon request.*

Discussion on B. Wheaton's PowerPoint presentation on the methods he developed for HTXRD furnace calibration and the importance making this calibration method part of best practices. The calibration method delivered reliable data and was well worth the time it takes to implement. T. Fawcett, S. Misture, P. Whitfield, A. Payzant, M. Suchomel have positive response to the method and corresponding data in the presentation. Brian was encouraged to submit a publication to Powder Diffraction Journal covering non-ambient XRD analysis.

- Task group to identify materials including unstable and reactive materials for which the diffraction data is deemed likely to be highly sensitive to measurement conditions. Update from T. Ely. See Word Doc by [Tom Ely – "Ambient Discussion Outline\_Tom Ely.docx"]

Discussion centered around how to best capture the behaviors of compounds that transform under ambient conditions. T. Fawcett suggested that other subcommittees have handled similar issues by attaching property sheets that documents the stability of phases of interest. S. Kabekkodu suggested using our current practice to add comments to the sensitivity field in the PDF database. A request was made to notify ICDD so data can be flagged within the PDF database if these conditions are known. All agreed this is a broad-based issue. B. Wheaton suggested sending [Tom Ely – “Ambient Discussion Outline\_Tom Ely.docx”] to subcommittees for feedback in future Zoom meeting. T. Blanton named D. Zulli as the person B. Wheaton should contact regarding who should receive this outline for discussion.

## 7. New Business

### Upcoming opportunities at DXC 2021

- Non-Ambient XRD ½ Day Workshop led by Barbara Pühr, Anton Paar GmbH, Austria
- Non-ambient Analysis Session: Covers all aspects of non-ambient analysis and techniques to gain knowledge of the behavior of materials under various conditions. Presentations involving use of non-ambient analysis techniques are encouraged.

Invited Speakers:

Kevin Stone, SLAC National Accelerator Laboratory

Barbara Pühr, Anton Paar GmbH, Austria

Abstract deadline – March 16<sup>th</sup>.

## 8. Adjournment