

International Centre for Diffraction Data
X-RAY FLUORESCENCE SUBCOMMITTEE MEETING
Wednesday, 16 March 2016
Mark Rodriguez, Chairman

1. Call to Order and Opening Remarks Mark Rodriguez

2. Roll Call and Attendance
Please see attendance sheet; attached.

3. Approval of the 2015 Minutes
Minor change in mission statement: change of “composition” to “identification.”
Motion to approve minutes by Mark Rodriguez. Seconded by Dave Taylor.
Voted: 5-YES, 0-NO, 0-Abstain

4. Appointment of Minutes Secretary
Stacy Gates-Rector was nominated to record this year’s minutes.

5. Review of Mission Statement
Change was made during review of the minutes to the mission statement. The word “composition” was corrected to “identification.” Noticed that mission statement was not updated on agenda or on website. Request is submitted for mission statement to be updated to the following.

New Mission Statement:

The X-ray Fluorescence Subcommittee will provide recommendations for X-ray Fluorescence to be a complement to both the PDF and ICDD. This entails synergistic interchange between data collected from XRD and XRF:

- Use of chemical identification to support powder diffraction analysis
- Ability to improve chemical composition by use of the powder diffraction data
- To ultimately obtain simulated XRF data as a means of material analysis validation such as refinement of data from multiple analytical methods

In addition, the subcommittee shall develop new educational opportunities for ICDD and offer guidance on addressing elemental composition issues which are of strategic interest to ICDD.

Moved by: Mark Rodriguez

Seconded by: Tim Fawcett

Vote: 5-YES, 0-NO, 0-Abstain

6. BoD Liaison Report Dave Taylor

Phase Identification from XRF data (*response to Motion 1*) – **Tim Fawcett**
2015 Motion 1: The XRF Subcommittee recommends to the Technical Committee that a test of the databased be performed wherein X-ray Fluorescence composition results

from a series of common compounds and/or minerals be processed through the *Composition field* of the *Elements* tab. The test of these known single phase materials (perhaps 50-100 “common phases” in the PDF database) would assess the effectiveness of the database to perform phase identification from XRF results alone. A report would be generated by ICDD to document how well the identification process worked, as well as possible recommendations for improved means of identification. With a request that a report would be completed by the Fall Board 2015 meeting.

- Discussion was carried out by John Anzelmo for clarification on the testing procedure Tim Fawcett used during his analysis.
- Tim Fawcett presented in detail analyses pertaining to NIST SRM 99a Sodium Feldspar.
- Mark Rodriguez pointed out that in order to do successful search match, “three” distinct pieces of information are required.
- Discussion by subcommittee about some additional capabilities of PDF.
- Mark Rodriguez questioned the feasibility of making a tutorial to indicate how this process is done.

Tim Fawcett discussed the possibility of incorporating this process into the PDF as a new feature (right-click option) → Goodness of Merit algorithm/processing for XRF phase identification.

- John Anzelmo questioned who the major user would be for this process. Would it be for XRD community or XRF?

Answer:

(i) Firstly, it would be XRD users who know how to do XRF.

(ii) Secondly, XRF person using it as a screening tool, or someone attempting to provide guidance to the XRD community.

- **Fundamental Parameters Database (*response to Motion 2*) – Mark Rodriguez**
2015 Motion 2: The XRF Subcommittee recommends to the Technical Committee that newly determined (updated) Fundamental Parameters (FP) values be compiled and archived by ICDD for the benefit of XRF experimentalists, equipment manufacturers, and future ICDD projects requiring accurate FP tabulations.
 - Mark Rodriguez pointed out that the major issue with the fundamental parameters is that even though the work is being done, it currently has no place for it to be housed. He showed the current status of the companies involved in the advancement of fundamental parameters.
 - John Anzelmo & Tim Fawcett point out that the major issue for us would not be housing, but editing or identifying the “GOOD” data.
 - Concern was expressed by committee that currently XRF parameters are not complete
 - Dave Taylor expresses that there’s no revenue in it, unless we get good advertisement and a method where users can go to our website and download the values.

7. New Business

Motion 1:

The XRF Subcommittee recommend to the Technical Committee to develop a figure of merit algorithm for XRF data to be used for phase identification.

Moved by: John Anzelmo

Seconded by: Dave Taylor

Vote: 5-YES, 0-NO, 0-Abstain

Motion 2:

The XRF subcommittee recommends to the Technical committee that a Fundamental Parameters (FP) database for XRF analysis be established using the currently existing Elam FP database. This newly created database would serve as a baseline repository to archive and incrementally enhance FP data for the purposes of improving quantification for XRF users, equipment manufacturers, and future ICDD projects requiring accurate FP tabulations.

Moved by: Mark Rodriguez

Seconded by: Stacy Gates-Rector

Vote: 4-YES, 0-NO, 0-Abstain

8. Adjournment