

**PDF Editorial Staff Subcommittee Meeting Minutes**  
**Wednesday, 13 March 2019**  
**International Centre Headquarters**  
**Conference Room A**  
**9:00 a.m. – 10:00 a.m.**  
**S. Kabekkodu, Chairman**

**Call to Order**

The meeting was called to order at 9:00 a.m.

**Appointment of Minutes Secretary**

Lisa Lanno

**Approval of Minutes from March 2018**

Minutes from the March 14, 2018 PDF Editorial Staff Subcommittee approved.

Approved 8

Opposed 0

Abstain 0

**Review of Mission Statement**

The PDF Editorial Staff shall be responsible for evaluating and recommending improvements in the editorial and bibliographic procedures of the ICDD.

**Board of Directors' Liaison Report**

D. Rafaja nothing to report from Board – no motions.

**Editorial Progress in PDF Release 2020**

New Entries in the Current Release

Experimental	→	1,530
ICSD	→	5,917*
LPF	→	10,404
Modulated	→	0
Total	→	17,851

\*ICSD delivery contained 1200 hypothetical structures, 1430 organometallic entries with no name.

PDF Organics → 8,319 new entries abstracted in-house and 213 from ICSD

**Topological Analysis:** Implementation of topological descriptors in Powder Diffraction File was presented.

**Diffraction Laboratory Activities**

Compounds investigated included minerals, metals pharmaceuticals, pigments, polymers, excipients, etc.  
Data collected for targeted materials which are included in our product  
Top Pharmaceutical Project (screening and sample preparation) – J. Kaduk  
Pharmaceutical analysis methods and materials investigation – T. Fawcett  
Cultural Heritage Studies – Philadelphia Museum of Art – T. Fawcett  
Current studies – T. Blanton

**Possible New Subfiles**

NTE- Negative Thermal Expansion

Definition: Single phase material that shows a contraction of at least one unit cell axis over a minimum temperature range of at least 50K.

SOL- Solar Materials

Definition: Class of semiconductors with bandgaps of 0.50-4.96 eV, which can absorb solar irradiation (Wavelength of 250 nm-2500 nm).

## **MOTION**

PDF Editorial Staff Subcommittee recommends to the Technical Committee that a subfile for Solar Materials to be created.

Definition: Solar materials (SOL) are a class of semiconductors with bandgaps of 0.50 - 4.96 eV, which can absorb solar irradiation (wavelength of 250 nm- 2500 nm).

Subfile reviewer Dr. Lan.

John Faber moved.

Jeff Dann second.

15 yes

0 no

0 abstain

## **Amy Gindhart Experimental Report**

Patterns Published in Experimental Set 69

Grants - 812

Pharmaceuticals Project – 3

Literature “BIBS” – 225

Writes/Contributed – 493

Total – 1530

\*146 were minerals

\*\*Patterns inserted were 1974 however 1530 made the set because of the amount of patterns rejected.

The amount of time spent inserting patterns has decreased because of D. Sagnella’s checks.

## **Diane Sagnella Report**

New DataQuacker Features:

Structure factors are usable.

Duplicate review decreases time for editor review by using DQEd to check for duplicates by parcel and easy visualization of candidates.

Parcel going out review for editors now can pull entire parcel and scroll through patterns to view raw data and reflections, and if comments from editor, the database is updated automatically.

Visual identification of kBeta lines.

New 2D Images and SMILES

This allows user to go from 3D coordinates to a 2D image and SMILES code.

2D Structures can also be “drawn” and SMILES codes derived and user can update the database with the new SMILES strings.

## **New Business**

None

## **Adjournment**

PDF Editorial Staff Subcommittee

Attendance Sheet

Wednesday, 13 March 2019

Time: 9:00 a.m. - 10:00 a.m.

Conference Room A

Soorya Kabekkodu, Chairman

David Rafaja, BoD Liaison

Name of Member	Signature	Name of Member	Signature
Antipov, Evgeny		Myer, George	
Bernstein, Lawrence		Rafaja, David	
Blanton, Justin+++		Roberts, Andrew	
Blanton, Tom		Rodriguez, Mark	
Bosnic, Vesna+++		Rost, Megan	
Bucio, Lauro		Rotella, Frank	
Carr, Michael+++		Sagnella, Diane+++	
Clapp, Rodney		Sarmiento, Janeth (SA)	
Clark, Harlan		Sharma, Yogendra Kumar	
Cockcroft, Jeremy		Singh, Gurvinderjit	
Dann, Jeffrey		Sornadurai, Dhamardoss	
Fawcett, Timothy		Turley, June	
Garvey, Roy		Vithayathil, Rose+++	
Gates-Rector, Stacy+++		Wallace, Peter	
Gindhart, Amy+++		Zavalij, Peter	
Kabekkodu, Soorya			
Kahmer, Theresa			
Lanno, Lisa+++			
Leoni, Matteo			
Mayo, William			

(SA) Student Affiliate, Non-voting

\*\* Associate Member, Non-voting

+++ Staff Consultant - Voting

Guests - Please sign on the next page.

J. N. Gunn  
 ALAN COELHO  
 Janet Grande  
 Jacky Hollencamp  
 Chuck Wexh  
 Joseph Sunzeri

Fred Wireko  
 John Salva  
 Xiaojing Zhu

Guest List  
Attendance Sheet

Name (Please print)                      Signature

JAMES A ICAONX                      *[Signature]*  
NICK ERNST BORIS                      *[Signature]*  
DENISE DELCASALE                      *[Signature]*

Name (Please print)                      Signature