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THE IRUG RAMAN SPECTRAL WEB DATABASE: OBJECTIVES, PROGRESS AND PLANS

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NOTE

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Abstract

The use of Raman spectroscopy in the study of cultural heritage has increased in recent years. However, its implementation has not been realized fully due in part to a lack of a readily-accessible Raman database of relevant, high-quality reference data. To address this need, the Philadelphia Museum of Art (PMA) and the Infrared and Raman Users Group (IRUG) have partnered to create a centralized Raman spectral database, supported by an Institute of Museum and Library Services (IMLS) National Leadership Grant for Advancing Digital Resources. The database is being built with open source technologies on a re-structured IRUG website (www.irug.org). The project is the second of its type undertaken by IRUG, which previously developed and distributed several infrared spectral compilations online. This paper provides an introduction to the Raman database project, describes the customized JCAMP-DX (Joint Committee on Atomic and Molecular Physical Data Exchange) file format for the spectral data, and outlines the protocol for the collection, evaluation and distribution of the data. A summary of the status of the project is given.

1 Introduction

Raman spectroscopy is a powerful technique for the analysis of cultural heritage materials.[1,2] An unknown sample can be characterized with a high level of confidence when its Raman data matches that of a known substance. Accordingly, its use in the art conservation field has grown substantially in recent years, especially as a convenient alternative to x-ray diffraction analysis of pigments, minerals and corrosion products. The number of Raman systems installed in museum laboratories reflects the growing popularity of the technique. Despite this progress, there remains a lack of readily-accessible, relevant, peer-reviewed reference data on known substances to serve as comparisons for samples taken from works of art and archaeological artifacts.

To help meet this need, the Philadelphia Museum of Art (PMA) and the Infrared and Raman Users Group (IRUG) have partnered to create a Raman spectral database to be housed on the IRUG website at www.irug.org. This project is supported by a National Leadership Grant for Advancing Digital Resources awarded by the Institute of Museum and Library Services (IMLS) in 2009.[I] It is the second of its type to be undertaken by IRUG, which previously developed and distributed infrared (IR) compilations, including the most recent Edition 2007.[3] The latter IR library, containing 2,100 peer-reviewed reference spectra of carbohydrates, minerals and pigments, oils and fats, natural and synthetic resins, and waxes is used routinely by many conservation scientists, conservators, educators, and students engaged in the study and preservation of the world's cultural heritage. When completed, the Raman spectral database is expected to become a similar fundamental resource and will complement the existing IR database.

One of the objectives for the database is to build a web interface for online submission, peer-review, editing, formatting, and distribution of spectra.

The web interface will allow users to upload spectra into the non-proprietary JCAMP-DX (ASCII text) format.[II] The system will merge these "raw" JCAMP-DX files with supporting descriptive information provided by submitters. The merged files then will be forwarded to a committee for a multi-step peer-review process. Accepted spectra will be converted automatically by the system into fully formatted IRUG compliant JCAMP-DX files and published in the Raman database. If a spectrum is not accepted, it will be returned with the reviewers' comments to the submitter, who may revise and resubmit it for reconsideration.

Another objective is the development of an online interface for keyword and spectral searching of the Raman database and for printing of search results and spectra. In addition, a searchable Raman bibliography with a peer-reviewed library of open source papers and a glossary of chemical structures and terms will be included. Users will be able to perform searches of the bibliography, export citation results in the MLA (Modern Language Association) style and download open source papers in PDF format.

The redesigned database will handle the new Raman data, as well as customary infrared data. The database will be built with MySQL®, an open-source database management system; the upgraded design is intended to meet industry best practices and security standards.

2 Formation of Raman Review Committee

A Raman review committee has been formed to oversee the collection and quality control of contributed Raman data. It comprises expert scientists from the museum and academic communities. These experts have agreed to serve as submitters of spectra as well as reviewers in their specific areas of expertise.

3 Development of Customized JCAMP-DX Format

The IRUG standardized Raman file format, based on the JCAMP-DX (ASCII) protocol, has been developed by the Review Committee. A sample file, opened with the text editor Notepad®, is shown in Appendix 1. The file comprises a series of labeled data records, known as LDR's, which are limited to 80 characters per line. Each LDR line includes a label that is followed by a sequence of text fields. The labels follow ## (or ##$) and are written in upper case. The various fields store important descriptive text information regarding a spectrum's title, JCAMP-DX version, data type, origin of data, as well as details about the instrument, sample, and sampling, followed by the x, y spectral data. The Raman format was adapted from the previously defined JCAMP-DX format used by IRUG for IR files, but was broadened by adding twenty-two new Raman specific fields. Full definitions for all LDR's and fields can be found on the IRUG website (www.irug.org) in the white paper, Revised JCAMP-DX Spectral File Format for Submissions to the Infrared & Raman Users Group (IRUG) Spectral Database, Revised May 1, 2012.[III]

Once the LDR's and corresponding fields have been assembled by the IRUG file formatting software and the data have met the QC standards, the spectral file is a discrete (self-contained), universal, electronic data record that can be opened and viewed in any text editor, or in any instrument software equipped with a JCAMP-DX translator. In addition, the file can be transferred between various instruments and users and incorporated into searchable libraries created on local computers.

4 Collection of Pre-build Raman Spectra

Raman spectra have been collected to form the foundation of the Raman database. These initial ("pre-build") spectra help to establish the quality and estimate the quantity of the Raman data that will be received once the new website is launched. They also are aids in the development of the software that must be built to accommodate the variations in the raw JCAMP-DX files generated on the different instruments used by submitters. Files from an assortment of instruments, including Bruker Optics®, Renishaw, Perkin Elmer®, and Thermo Scientific®, have been examined. Thus far, over 600 Raman spectra have been collected from various contributors worldwide.

5 Discovery and Technical Assessment

A discovery and technical assessment phase of the project was completed in August 2011. During this phase, a Systems Requirements Document was produced in collaboration with R2integrated, a digital marketing and technology firm, located in Baltimore, MD, US. The detailed document describes the software functional and nonfunctional requirements for the database and website. It also contains a data dictionary and data model, as well as workflow diagrams or "blueprints". The workflow diagrams specify how a Raman spectral file progresses though the IRUG system from upload and submission as a raw JCAMP-DX file through the evaluation by reviewers and senior editors, editing, approval, and publication in the Raman database as an IRUG compliant JCAMP-DX file. The Systems Requirements Document also contains specifications for the bibliography, glossary of chemical structures and terms, and feedback functionalities. The requirements document contains forty-six pages of specifications as a guide for constructing and implementing the website database and software.

6 Future Work— Website Development and Raman Spectroscopy Workshop

After the discovery and technical assessment phase described above, the project partners engaged Endertech, a Los Angeles based web design and software development company, to build and implement the new database and associated functionalities.[IV] Based on the Systems Requirements Document, Endertech has developed wireframe schematics, representing the skeletal frame of the website, functionality, and behavior and priority of content, and has begun building the website database and software. A functional prototype for JCAMP-DX file upload and review has been built for design testing and refinement. The target date for the launch of the new database is the end of September 2012.

A Raman spectroscopy workshop was held on September 27-29, 2012 at the Philadelphia Museum of Art. The first two days of the workshop, which were open to the public, included lectures on the history of Raman as applied to cultural heritage; theory and instrumentation; as well as applications to the analysis of inorganic and organic colorants, minerals, gems, glass, polymers/plastics, paint and cross-sections; in-situ museum and field methods; and surface enhanced Raman spectroscopy. In addition, the new Raman database was introduced. Peer reviewers attended the third day of the workshop, where they learned how to submit and evaluate spectra with the new software. The workshop was funded by a grant from the National Center for Preservation Training and Technology (NCPTT) with additional support from the PMA, The Dow Chemical Company and Bruker Optics.[V]

7 Conclusion

An online database of Raman reference spectra and associated literature is being built by the PMA and IRUG that will facilitate Raman spectroscopic study of the world's cultural heritage. The database and associated software will reside on the IRUG website (www.irug.org) and be used to collect, evaluate, centrally archive, and disseminate the reference spectra. The data will be formatted in an IRUG customized JCAMP-DX (ASCII text) file format that is both self-contained and platform independent, and all published spectra will be peer-reviewed by trained Raman scientists.

The IRUG database project is a broad collaborative effort across many institutions in the field. It is distinctive from other spectral database endeavors because the IRUG website interactive software architecture fully integrates all spectra submission, review and management processes on a single website. The project is ongoing and relies on the mutual sharing of spectra and other Raman information by individuals in the international museum and academic communities.[VI] The outcome will benefit generations of scientists, conservators, and students, as well as the public interest in preservation of our cultural heritage.

Individuals interested in participating should contact their respective IRUG Regional Chair: Beth Price (bprice@philamuseum.org), Americas; Marcello Picollo (m.picollo@ifac.cnr.it), Asia and Australia; Boris Pretzel (boris.pretzel@vam.ac.uk), Europe and Africa; or the IRUG Raman Committee Chair, Suzanne Lomax, (slomax@nga.gov).

8 Acknowledgements

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National Center for Preservation Training & Technology; The Dow Chemical Company, Advanced Materials and Corporate Information Technology Divisions; Philadelphia Museum of Art; National Gallery of Art, Washington; Victoria and Albert Museum; and Institute of Applied Physics "Nello Carrara" - National Research Council. The authors also recognize Abigail Teller, Lauren Klein, Tara Huber, and Heather Brown for their important contributions to the database project.

9 References

1. G. Smith, R. Clark, *Raman Microscopy in Archeological Science*, J. Archaeol. Sci, 2004, **31**, 1137-1160

2. G. Smith, R. Clark, *Raman Microscopy in art history and conservation science*, Rev. Conserv., 2001, **2**, 92-106.

3. B. Price, B. Pretzel, Eds., *Infrared and Raman Users Group Spectral Database*, Edition 2007, Infrared and Raman Users Group, Philadelphia, 2009.

10 Endnotes

I. The IMLS is the primary source of federal support in the United States for libraries and museums. Its mission is to create strong libraries and museums that connect people to information and ideas; to sustain heritage, culture, and knowledge; to enhance learning and innovation; and to support professional development. For more information, see http://www.imls.gov (accessed 05/03/2012).

II. JCAMP-DX (Joint Committee on Atomic and Molecular Physical Data Exchange) is a file specification. For details, see: R. S., McDonald, P. Wilks, Jr., *JCAMP-DX: A Standard Form for Exchange of Infrared Spectra in Computer Readable Form*, Appl. Spectrosc., 1988, **42**, 151-162; J. G. Grasselli, *JCAMP-DX, A Standard Format for Exchange of Infrared Spectra in Computer Readable Form (IUPAC Recommendations 1991)*, Pure Appl. Chem., 1991, **63**, 1781-1792; and P. Lampen, et al., *An Extension to the JCAMP-DX Standard File Format*, JCAMP-DX V.5.01 (IUPAC Recommendations 1999), Pure Appl. Chem., 1999, **71**, 1549-1556.

III. For full information on the IRUG JCAMP-DX protocol, see B. A. Price, B. Pretzel, S. Q. Lomax, C. Davis, J. Carlson, *Revised JCAMP-DX Spectral File Format for Submissions to the Infrared & Raman Users Group (IRUG) Spectral Database*, http://www.irug.org/ed2k/jcamp.asp (accessed 05/03/2012).

IV. Endertech is a web development company specializing in building advanced web sites with open source technologies. For more information, see: www.endertech.com (accessed 05/03/2012). To implement the IRUG project, Endertech has employed MySQL® (My Sequel) for the database development and management, SymfonyTM for the web application framework, PHP (PHP Hypertext Preprocessor) for the server side scripting language, HTML (HyperText Markup Language) to display the web pages and other information in web browsers, CSS (Cascading Style Sheets) to define the page layouts and formatting, and jQuery® JavaScript library for scripting the HTML.

V. The NCPTT is part of the United States National Park Service and was created under the Historic Preservation Act Amendments of 1992. Its mission is to advance the application of science and technology to historic preservation. The NCPTT accomplishes this mission through training, education, research, technology transfer and partnerships within the fields of archeology, architecture, landscape architecture, and materials conservation. For more information, see http://ncptt.nps.gov (accessed 05/03/2012).

VI. Please note that by submitting spectral files to IRUG, a contributor explicitly accepts the terms of the IRUG Contributor's License Agreement. The copyright to any contributed spectral file remains with the contributor and the originating institution. The contributor grants IRUG a free, indefinite and perpetual right to compile and distribute submitted spectral files as part of the IRUG Spectral Database under the direction of the IRUG Board of Directors.

Appendix 1: Example IRUG JCAMP-DX Raman spectral file

##TITLE=RMP00002 Aragonite; Morro Bay, San Luis Obispo; MMHU; 116189; MFAB; scat

##JCAMP-DX=5.01

##DATA TYPE=RAMAN SPECTRUM

##APPLICATION=Raman microspectroscopy (RM)

##ORIGIN=institution: Museum of Fine Arts, Boston; address: 465 Huntington

Avenue, Boston, MA, 02115, US; analyst(s): Richard Newman, Michele Derrick;

tel: 1 617 267 9300; fax: 1 617 369 3182; email: rnewman@mfa.org;

mderrick@mfa.org; submitter: Beth Price, Philadelphia Museum of Art;

tel: 1 215 684 7552; fax: 1 215 684 7540; email: bprice@philamuseum.org

##OWNER=COPYRIGHT (C) 2008 BY Museum of Fine Arts, Boston

DATABASE COPYRIGHT (C) 2012 BY Infrared and Raman Users Group (IRUG)

##$LICENSE=By accepting this database user agrees to be bound by the terms of

the IRUG user's license. Any reference written/oral made to this file must

include accreditation to BOTH the originating individual/institution and IRUG.

Contributor agrees to be bound by the terms of the IRUG contributor's license.

##$INSTITUTION FILE NAME=Aragonite (HU Min. Museum 116189), 50X, 785 nm.1.dx

##DATE=08/07/29

##LONGDATE=2008/07/29 12:55:37

##TIME=12:55:37

##SPECTROMETER/DATA SYSTEM=spectrometer: Bruker Optics Senterra RMS;

software: Bruker Opus 6.5; detector: CCD; class: dispersive

##INSTRUMENT PARAMETERS=apodization: Happ-Genzel (HG); accumulations: 1; purge:

N; range: 70-1550 1/cm; source: 785 nm; power: 9.4 mW; calibration: multiband

Neon; data collection: static; integration time: 30 sec

##RESOLUTION=3-5 1/cm

##DATA PROCESSING=baseline corr.: N; fluorescence corr.: N; cosmic ray removal:

N; detector binning: Y; other data processing: none

##SAMPLE DESCRIPTION=mode: scat; accessories: Senterra microscope; support:

glass slide; objective magnification: 50x; numerical aperture: 0.75; working

distance: 0.38 mm; spot size: 2 microns; confocal: N; angle: 180 degrees

backscattered; polarization: N, N; filters: Rayleigh, dielectric; cut-off freq:

89 1/cm; grating type: holographic; grating density: 1200 lines/mm; laser

defocus: N

##SAMPLING PROCEDURE=mode: scat; prep: bulk

##PATHLENGTH=

##PRESSURE=

##TEMPERATURE=

##CAS NAME=aragonite

##NAMES=aragonite

calcium carbonate

##MOLFORM=C Ca O3

##$STRUCTFORM=CaCO3

##CAS REGISTRY NUMBER=14791-73-2

##WISWESSER=

##BEILSTEIN LAWSON No=

##MP=transitions to calcite 520 degrees Celsius (literature, Weast, Robert C.,

ed. CRC Handbook of Chemistry and Physics: A Ready-reference Book of Chemical

and Physical Data. 59th ed. Cleveland, OH: CRC, 1978. B-87.)

##BP=

##REFRACTIVE INDEX=1.530, 1.682, 1.686 (literature, cameo.mfa.org)

##DENSITY=2.930 (literature, Weast, Robert C., ed. CRC Handbook as cited above)

##MW=100.09 (literature, Weast, Robert C., ed. CRC Handbook as cited above)

##CONCENTRATIONS=

##STATE=state: solid; form: powder

##CROSS REFERENCE=IRUG spectrum IMP00292.DX

##$LITERATURE REFERENCE=Edwards, H., S. Villar, J. Jehlicka, and T. Munshi. "FT–

Raman Spectroscopic Study of Calcium-rich and Magnesium-rich Carbonate

Minerals." Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy

61.10 (2005): 2273-280.

##$OTHER ANALYTICAL METHODS=Fourier transform infrared spectroscopy (FTIR),

scanning electron microscopy (SEM), energy dispersive spectrometry (EDS)

##$SAMPLE SOURCE 1= Morro Bay

##$SOURCE LOCATION 1=San Luis Obispo County, CA, US

##$SAMPLE IDENTIFIER 1=

##$SAMPLE SOURCE 2=Mineralogical Museum Harvard University (MMHU)

##$SOURCE LOCATION 2=24 Oxford Street, Cambridge, MA, 02138, US

##$SAMPLE IDENTIFIER 2=MMHU# 116189

##$SAMPLE SOURCE 3=Museum of Fine Arts, Boston

##$SOURCE LOCATION 3=465 Huntington Avenue, Boston, MA, 02115, US

##$SAMPLE IDENTIFIER 3=MFA# 116189

##$COLOR=white

##$AGE=

##$IRUG MATERIALS CLASS=MP (minerals and pigments)

##$OTHER=sample type: reference material

##DELTAX=0.5

##XUNITS=1/CM

##YUNITS=RELATIVE INTENSITY

##FIRSTX=70

##LASTX=1550

##FIRSTY=8123.4546

##MAXY=29326.285

##MINY=689.02875

##XFACTOR=1

##YFACTOR=2.7312231e-005

##NPOINTS=2961

##XYDATA=(X++(Y..Y))

70.00...

##END=