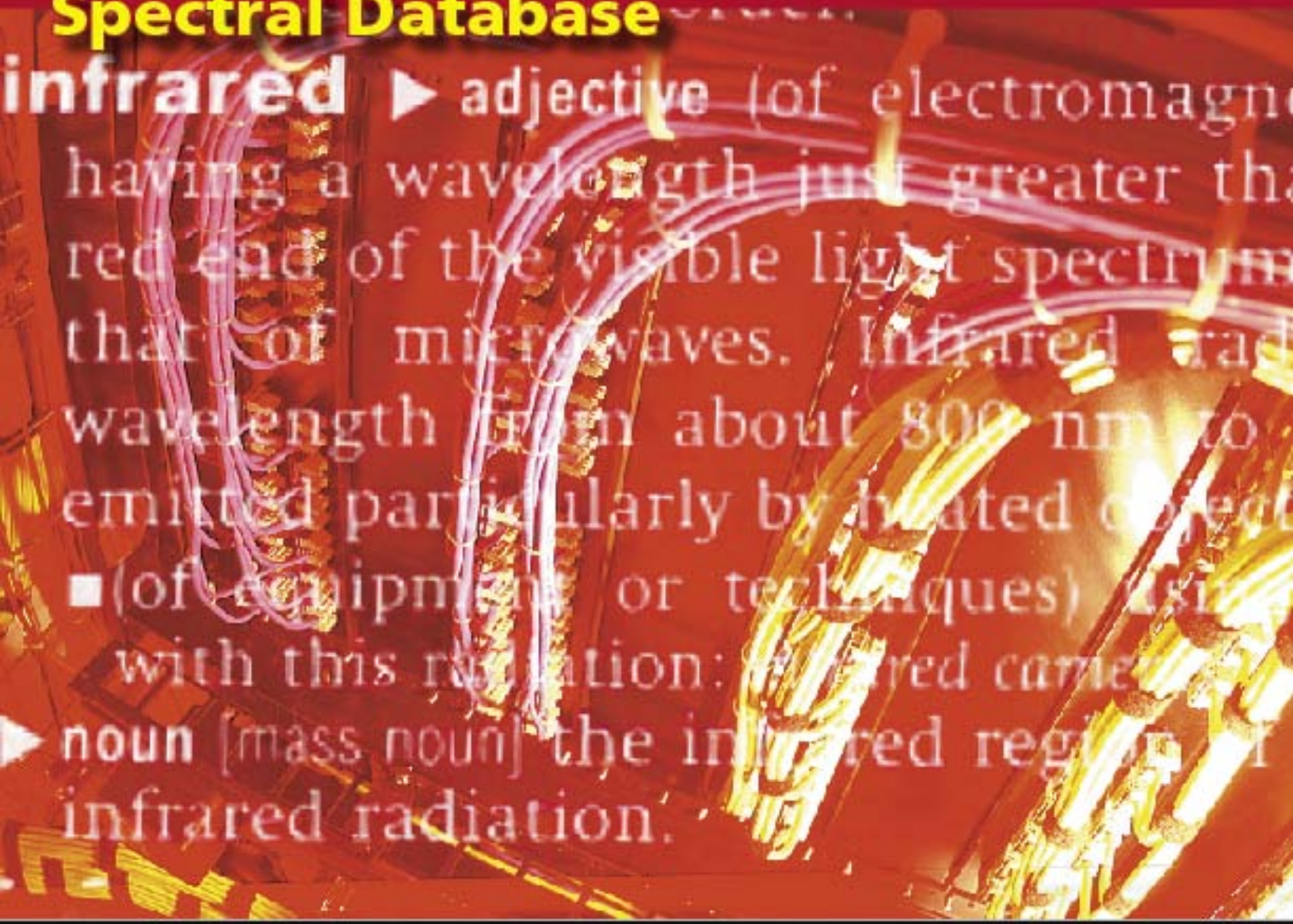
Materials Research Series

2003-03

Development and Implementation of the Internet Accessible Infrared and Raman Users Group (IRUG) Spectral Database



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APPENDIX

Table of Contents

I. Home

II. About Us

- A. Mission
- B. History
- C. Conferences
- D. Board
- E. Participation

III. Spectral Database

- A. About the Database
- B. Search Edition 2000
  1. Search Engine
  2. Search Results
  3. Spectrum Graphics Page
  4. "How to Read the Title Line" Key
- C. Edition 2000 Common Name Index
- D. Contributing Individuals
- E. Contributing Institutions
- F. JCAMP Paper
- G. Database Feedback

IV. Bibliography

- A. About the Bibliography

B. Search the Bibliography

C. Bibliography Feedback

V. Credits

A. Current Review Committee

B. Contributing Individuals

C. Contributing Institutions

D. Support

VI. Site Services – IRUG Login

A. How to Submit a Spectrum

1. Begin New

2. Check and Send Submissions

3. Check Submission Status

B. Review Committee Software

1. Review and Evaluate New and Undecided Submissions

2. List Decided Submissions Sent to Sr. Editors

C. Senior Editor Software

1. Check Review Decisions and Vote

2. Return Submissions

3. Make Final Approvals

4. Senior Editor Discussion Forum

D. View Approved Submissions

E. Online Bibliography

1. Submit New Citation from Book

2. Submit New Citation from Periodical

3. Submit New Citation from An Electronic Publication
4. List Non-Approved Citations
5. List Approved Citations
6. List All Citations

F. Get Database Updates

G. IRUG Community: IRUG Discussion Forum

H. Spectral Database Info

1. Search Edition 2000: See Section 3B
2. JCAMP Information: See Section 3F

I. On-Line Help

J. Manage My Information

1. Edit My Profile
2. Reset My Password

VII. Links

VIII. Site Info

A. Frequently Asked Questions (FAQ)

B. Website Feedback

C. Privacy Statement

D. Technical Requirements

E. Site Map

I. Home

I

Infrared and Raman Users Group

A collaboration to encourage the exchange of information, develop IR and Raman spectral standards, and distribute comparative spectral data for the study of works of art, architecture, and archeological materials.

Current News

Get Ready for IRUG 6 Conference!

- **Date:** 29 March - 1 April 2004
- **Location:** Florence. Italy
- **Host:** Institute for Applied Physics "Nello Carrara" (IFAC) of the Italian National Research Council (CNR)
- **Abstract Submission Deadline:** 30 September 2003
  Abstract must be sent as attached file (RTF or DOC) to: m.picollo@ifac.cnr.it
- For late registration please contact Marcello Picollo, m.picollo@ifac.cnr.it

Edition 2000 Spectral Database

Click Here To Search Now

Want to get involved?

Click Here to Request More Info.

Support Provided By:

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KRESS

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PHILADELPHIA MUSEUM OF ART

Philadelphia Museum of Art

Technical Requirements
This web site is designed for use by Microsoft Internet Explorer version 4.0 and newer and Netscape Navigator versions 4.77 and newer and is best viewed at 1024 x 768.
Cookies are required to use Account Services

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II. About Us

II A

Mission

The international Infrared and Raman Users' Group (IRUG) is dedicated to the professional development of its members by providing a forum for the exchange of infrared (IR) and Raman spectroscopic information, reference spectra and materials. IRUG is composed primarily of individuals within the art conservation and historic preservation fields who use IR and Raman spectroscopy to study the world's cultural heritage.

At biennial meetings, the IRUG initiative is sustained by members and invited speakers who present papers on a range of topics. A primary goal of IRUG is to improve and expand the data generated and shared by its members. Toward this end, a cooperative database of IR and Raman spectra relevant to cultural materials has been undertaken.

Web site by Digital Bridgeway, Inc.

II B

History of IRUG and the Spectral Database

IRUG is an independent not-for-profit corporation of individuals who use infrared and Raman spectroscopy for the study of the world's cultural heritage. Originating in the United States in 1993, the Group facilitates the development and distribution of reliable reference spectra and spectral standards for the art conservation and historic preservation communities. IRUG also encourages the professional development of it participants through biennial conferences where spectroscopic information is exchanged and papers presented.

The first formal meeting of IRUG was held at the Philadelphia Museum of Art, in 1994. Subsequently, conferences took place at the Victoria and Albert Museum, London (1995); Winterthur Museum, Garden and Library, Winterthur, Delaware (1998); Bonnefanten Museum, Maastricht (2000); and Getty Conservation Institute, Los Angeles (2002). Over the years, participation in IRUG has grown. Accordingly, in 1998, the Group adopted a committee-based structure with regional chairs. In 1999, IRUG broadened its scope and thus changed its name from the Infrared Users Group to the Infrared and Raman Users Group. In 2001, it incorporated as a not-for-profit in the State of Pennsylvania with a governing Board of Directors.

A major focus of IRUG throughout its history has been the development of its collaborative Database of spectra of artists' and related materials. Early compilations were distributed in 1993 and 1995. Later, a reliable, customized spectral file format using the standardized protocol, JCAMP-DX was developed. In 1999, a review committee met at the Istituto di Ricerca Sulle Onde Elettromagnetiche (IROE-CNR) in Florence, Italy to evaluate spectra using uniform criteria for quality and accuracy of material identification. The reviewed spectra were then formatted and compiled as the Infrared and Raman Users Group Spectral Database - Edition 2000, which was distributed in 2001.

Today, IRUG has an Internet presence, which you are currently visiting. The web site includes a publicly viewable and searchable version of Edition 2000 - the continuing collaborative collection of high quality reference spectra, an on-line bibliography of spectroscopic and related literature, a discussion forum. The success of IRUG and its Database has been due in large part to the support of a community that represents conservation and historic preservation endeavors on an international scale, beyond the interests of any single institution or organization. Its growth and accomplishments are the product of the collaborative efforts of the larger scientific community in conservation, which it is intended to serve.

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II C

IRUG Conferences: Past, Present and Future

IRUG conferences, which are held every two years, encourage professional development and enhance a sense of community.

Institute for Applied Physics "Nello Carrara", Florence, Italy

29 March - 1 April 2004

- Abstract Submission Deadline: 30 September 2003
- For late registration please contact Marcello Picollo, m.picollo@ifac.cnr.it

.

Fifth International Infrared and Raman Users Group Conference

February 2002
Getty Conservation Institute, Los Angeles, CA, US

IRUG5 Program

IRUG4: The Fourth Infrared Users' Group Meeting in Conservation Science

February 2000
Bonnefantenmuseum, Maastricht, The Netherlands

IRUG4 Program

Editing Committee Meeting: Infrared and Raman Users Group Spectral Database©

May 1999
Istituto di Ricerca Sulle Onde Elettromagnetiche
Florence, Italy

IRUG3

May 1998
Winterthur Museum, Gardens and Library, Winterthur, DE, US

Program

IRUG2

September 1995
Victoria and Albert Museum, London, UK

View on line or download IRUG2 Postprints

IRUG1

March 1994
Philadelphia Museum of Art, Philadelphia, PA, US

Infrared User's Group (IRUG) for the Analysis of Artistic and Historic Materials

View Meeting Program on line

Web site by Digital Bridgeway, Inc.

II D

Board of Directors

- **Janice Carlson,** Winterthur Museum, Winterthur, DE, US
- **Kate Duffy,** Williamstown Art Conservation Center, Williamstown, MA, US
- **Herant Khanjian,** Getty Conservation Institute, Los Angeles, CA, US
- **Suzanne Quillen Lomax,** National Gallery of Art, Washington, DC, US
- **Richard Newman,** Museum of Fine Arts, Boston, MA, US
- **Marcello Picollo,** Institute for Applied Physics "Nello Carrara", CNR, Firenze, IT
- **Boris Pretzel,** Victoria and Albert Museum, London, UK
- **Beth Price,** Philadelphia Museum of Art, Philadelphia, PA, US
- **Masanori Sato,** Nara Cultural Research Institute, Nara JP
- **Manfred Schreiner,** Academy of Fine Arts, Institute of Chemistry, Vienna, AU
- **Raymond White,** National Gallery of Art, London, UK

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II E

Sign In

Welcome Guest!

Participation in IRUG

Participation in IRUG is open to all individuals who actively use and maintain a serious interest in infrared or Raman spectroscopy for the technical analysis of cultural property. Most participants are conservation scientists, but the group also includes several conservators and conservation students as well as individuals from academia and industry. Applications for membership are reviewed by the Directors. Contact the appropriate chairperson for your region for information. Members may may update their user profiles in Site Services.

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III. Spectral Database

III A

The IRUG Database - A Collaborative FTIR Library

The Infrared and Raman Users Group (IRUG) Spectral Database© is an ongoing, collaborative compilation of peer-reviewed spectra of artists' and related materials for the study of the world's cultural heritage. Currently, the Database contains over 1250 spectra of oils, waxes, natural and synthetic resins, dyes, pigments, proteins, gums, and minerals. Scientists and other professionals from the art conservation, historic preservation, and academic communities have generously contributed their spectra to the Database (Individuals, Institutions).

Early draft versions of the Database, containing "as-contributed" JCAMP-DX spectra, were issued in June 1993 and June 1995. To enhance spectral quality and accuracy of sample identification, peer review was implemented in 1999 (Review Committee). A customized IRUG-JCAMP-DX format (JCAMP paper) was also developed to ensure file uniformity and to incorporate both numerical data and descriptive text (sample, instrument, and analysis conditions) into the spectral files. Important details such as sample age, color, source, mw, formula, detector limits, sample preparation, etc. make the IRUG files independent, complete data records. Utilizing these protocols, the latest database version - IRUG Spectral Database, Edition 2000 - was compiled and distributed in printed and digitized formats in 2001.

Edition 2000 was made publicly viewable and keyword searchable via the IRUG website, in 2002. The JCAMP-DX files are currently available to not-for-profit institutions and/or individuals in return for contributions of 10 or more accepted spectra or standards. Contributors license accepted spectra to IRUG for compilation and distribution while retaining the copyright on their own submitted data. IRUG continues to solicit spectra and materials, especially those that are not well represented in the Database (Common Name Index). Spectral files may be submitted via the IRUG web site (Site Services). Contact your regional chairperson to learn how to participate. (Regional Chairs)

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III B1

Sign In

Welcome Guest!

IRUG Spectral Database Edition 2000 Search Engine

☑ I have read and accept the Terms of Use and Legal Conditions

Common name keyword search:

glue

To search the IRUG Edition 2000 Database, enter search terms and click the Search button below.

- (•) Match At Least One Keyword
- ( ) Match *Every* Keyword

- (•) Match Keywords Loosely (e.g. "carbon" matches "carbonate")
- ( ) Match Keywords Exactly (e.g. "carbon" *will not* match "carbonate")

Click Here To Begin Search

Prepared by

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Philadelphia Museum of Art

Boris Pretzel
Victoria & Albert Museum

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New York, NY, US

Masahiko Tsukada
The National Museum of Western Art
Tokyo, JP

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III B2

IRUG Spectral Database Edition 2000 Search Results

Results 1 to 10 of (11)

Search Terms: "*glue*"

Begin New Search Modify Search

Next >> Last >>

IMX00020.DX Indigo in rabbit skin glue	(Mixtures) Straus Conservation Center (Fogg), Harvard University Art Museums
IPR00001.DX Glue, animal, Shirish atha	(Proteinaceous Materials) M.H. De Young Museum
IPR00002.DX Glue, animal, pearl	(Proteinaceous Materials) British Museum
IPR00010.DX Glue	(Proteinaceous Materials) Philadelphia Museum of Art
IPR00016.DX Glue, hide, German	(Proteinaceous Materials) Williamstown Art Conservation Center
IPR00017.DX Glue, rabbit skin, unbleached	(Proteinaceous Materials) Philadelphia Museum of Art
IPR00019.DX Glue, hide	(Proteinaceous Materials) Philadelphia Museum of Art
IPR00020.DX Glue, hide, German	(Proteinaceous Materials) Philadelphia Museum of Art
IPR00036.DX Glue, deer, Russian	(Proteinaceous Materials) Grabar Art Conservation Center (Russian Scientific Conservation Center named after Grabar)
IPR00037.DX Glue, hare, Russian	(Proteinaceous Materials) Grabar Art Conservation Center (Russian Scientific Conservation Center named after Grabar)

Results 1 to 10 of (11)

Begin New Search Modify Search

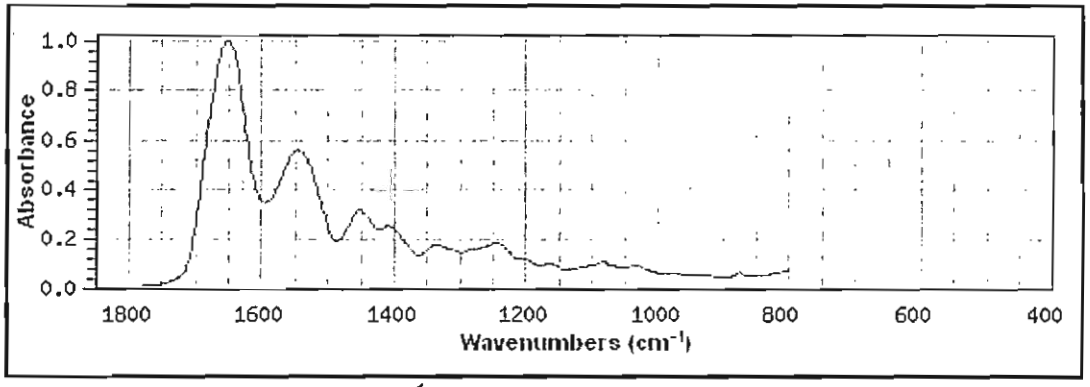
Next >> Last >>

Web site by Digital Bridgeway, Inc.

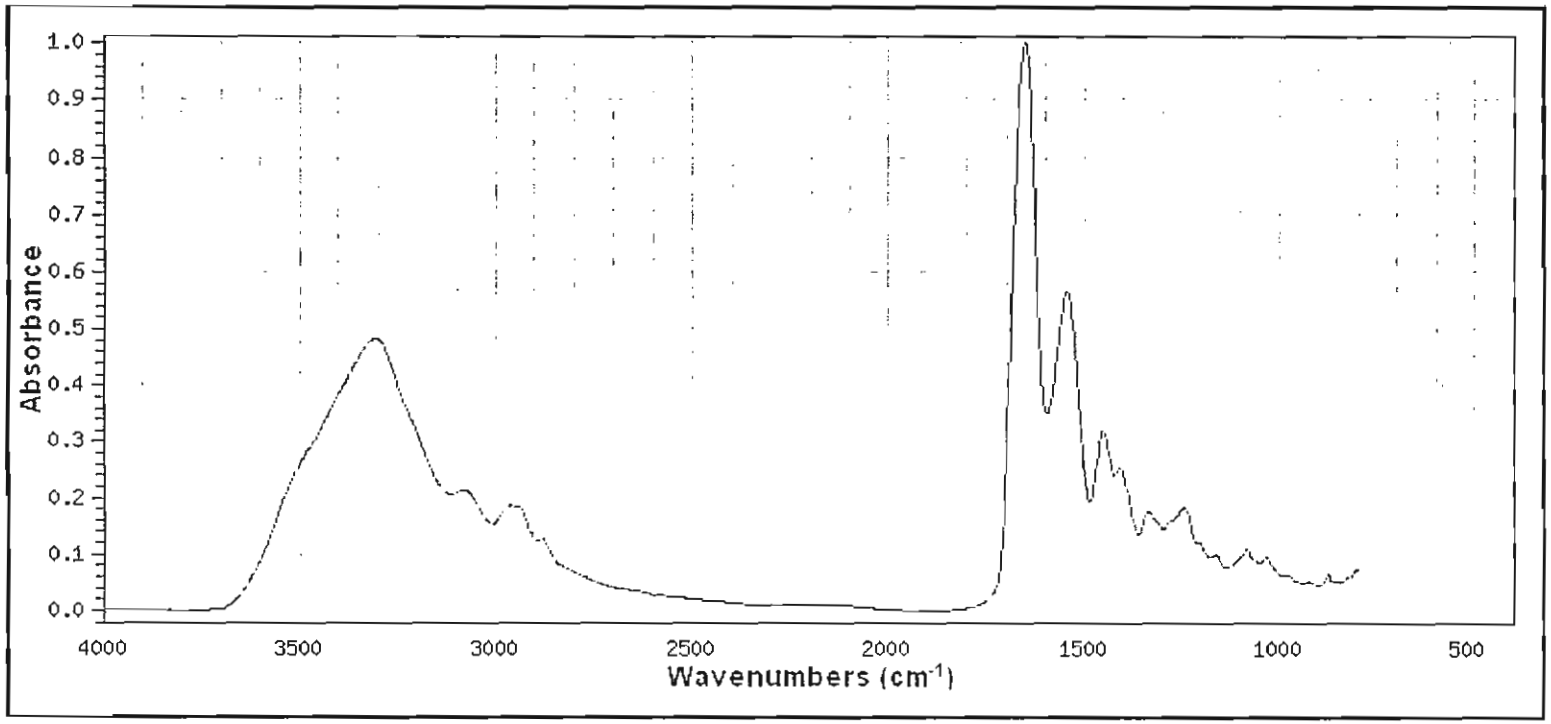
IRUG DATABASE

EDITION 2000

www.irug.org



Expanded region: 1850-400 cm $^{-1}$



IPR00001 Glue, animal, Shirish atha, SAM Monowar Jahan, deYNG, tran

Section 11 **Proteinaceous Materials** **Page 1**

(Title Line Key)

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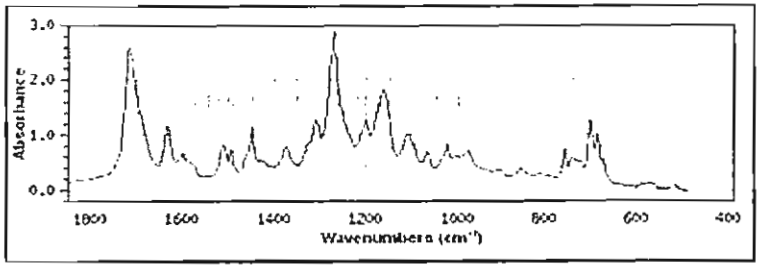
III B3

How to Read an IRUG Spectrum Title Line

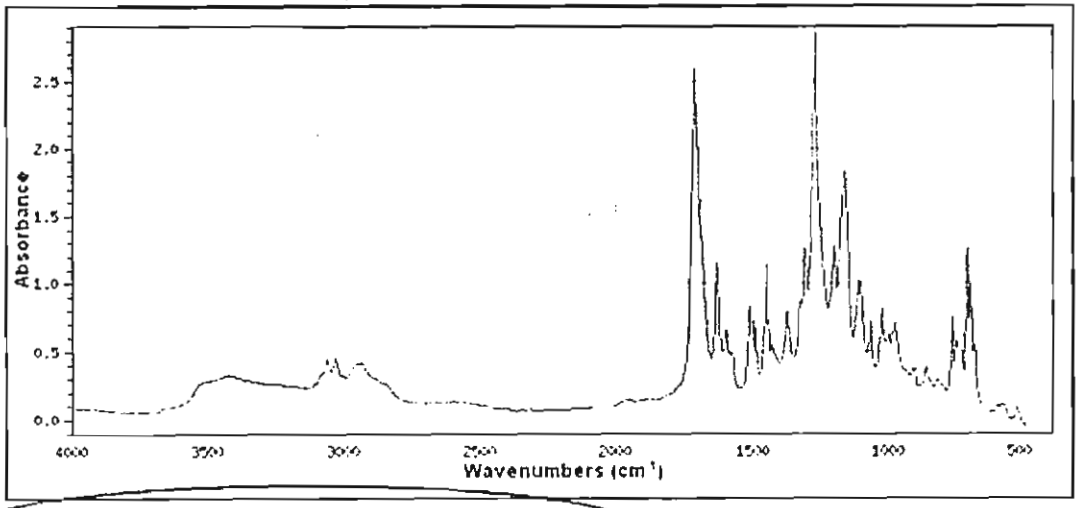
IRUG DATABASE

EDITION 2000

www.irug.org



Expanded region: 1850-400 cm⁻¹



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INR00118 Peruvian balsam, HNM, R/57, HNM, tran

Section 8 Natural Resins Page 118

INR00118 Peruvian balsam, HNM, R/57, HNM, tran

INR00118 = filename

[*I* = infrared, *NR* = material class (natural resins), *00118* = sequential number]

Peruvian balsam = common / material name

HNM = material source

R/57 = sample identifier

HNM =originating institution acronym (Hungarian National Museum)

tran = collection mode (transmission)

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III B4

III C

IRUG Common Name Index

(Material Class Code Key) (Institution Acronym Index) (How to Read an IRUG Title Line)

A B C D E F G H I J K L M N O P Q R S T U V W X Y Z Bottom of page

Common Name	Filename	Material Class	Institution
Abies spectabillis resin	INR00191.DX	NR	VA
Acacetin, 5,7-dihydroxy-4'-methoxyflavone	IOD00139.DX	OD	GCI
Acacia gum	ICB00018.DX	CB	deYNG
Acacia gum, from Acacia species	ICB00042.DX	CB	VA
Acetate "silk", cellulose acetate	ISR00062.DX	SR	PMA
Acrocryl 63822	ISR00022.DX	SR	GCI
Acrocryl 63943	ISR00023.DX	SR	GCI
Acryloid B-48N	ISR00032.DX	SR	GCI
Acryloid B-67 film, aged	ISR00057.DX	SR	PMA
Acryloid B-67, poly(iso-butyl methacryate)	ISR00074.DX	SR	NGA
Acryloid B-72, aged	ISR00056.DX	SR	PMA
Acrylonitrile / butadiene / styrene resin	ISR00095.DX	SR	WM
Agateen 27	ISR00050.DX	SR	WACC
Agateen 2B, nitrocellulose	ISR00001.DX	SR	GCI
Agua-aceite, VanGogh Phthalo Blue 570	IMX00013.DX	MX	MNRS
Agua-aceite, VanGogh Zinc White 104	IMX00012.DX	MX	MNRS
Albite	IMP00171.DX	MP	PMA
Albite	IMP00172.DX	MP	PMA
Albite	IMP00257.DX	MP	PMA
Albumin	IPR00007.DX	PR	GCI
Albumin, chicken egg	IPR00023.DX	PR	PMA
Alginic acid, sodium salt	ISR00093.DX	SR	WM
Alizarin	IOD00103.DX	OD	GCI
Alizarin crimson, light	IOD00205.DX	OD	GCI
Alizarin red PS, mordant dye	IOD00063.DX	OD	GCI
Alizarin red S	IOD00062.DX	OD	GCI
Alizarin red SS	IOD00064.DX	OD	GCI
Alizarin Yellow GGN, CI Mordant Yellow 1	IOD00211.DX	OD	GCI
Alizarin, 1,2 dihydroxyanthraquinone	IOD00192.DX	OD	PMA
Alizarin, 97% pure	IOD00214.DX	OD	SCC
Alkanet, aldanet, CI Natural Red 20	IOD00095.DX	OD	GCI
Alkannin	IOD00135.DX	OD	GCI
Alkyd French ultramarine, with CO3	IMX00006.DX	MX	MNRS
Alkyd London Yellow	IMX00004.DX	MX	MNRS
Alkyd Prussian Blue, with carbonate	IMX00003.DX	MX	MNRS

Alkyd Titanium White, with carbonate	IMX00002.DX	MX	MNRS
Alkyd Viridian	IMX00005.DX	MX	MNRS
Almond gum, garden prince, with some kaolinite	ICB00014.DX	CB	GCI
Alstonite	IMP00267.DX	MP	PMA
Alstonite	IMP00286.DX	MP	PMA
Alum	IMP00262.DX	MP	SCC
Alumina hydrate	IMP00290.DX	MP	SCC
Amaranth, CI Acid Red 27	IOD00022.DX	OD	GCI
Amber resin	INR00076.DX	NR	BM
Amber varnish B, aged	INR00088.DX	NR	PMA
Amber, Baltic	INR00035.DX	NR	BM
Amber, Baltic Sea	INR00103.DX	NR	PMA
Amber, Baltic, succinite	INR00214.DX	NR	VA
Amber, Baltic, succinite	INR00215.DX	NR	VA
Amber, Baltic, succinite, aged	INR00211.DX	NR	VA
Amber, Baltic, succinite, from Denmark	INR00212.DX	NR	VA
Amber, Baltic, succinite, from Denmark	INR00213.DX	NR	VA
Amber, non-Baltic	INR00066.DX	NR	BM
Amesite	IMP00195.DX	MP	PMA
Amesite	IMP00282.DX	MP	PMA
Amido Black 10B, CI Acid Black 1	IOD00032.DX	OD	GCI
Amido Naphthol Red G, CI Acid Red 1	IOD00028.DX	OD	GCI
Ammoniacum gum, from Dorema ammoniacum	ICB00048.DX	CB	VA
Ammonial gum	ICB00035.DX	CB	CIA
Amphibole	IMP00150.DX	MP	PMA
Anatase	IMP00229.DX	MP	PMA
Anglesite	IMP00194.DX	MP	PMA
Anglesite	IMP00231.DX	MP	PMA
Anhydrite	IMP00116.DX	MP	PMA
Anhydrite	IMP00173.DX	MP	PMA
Anhydrite, gypsum impurity	IMP00228.DX	MP	PMA
Aniseed oil	IOF00019.DX	OF	deYNG
Ankerite	IMP00190.DX	MP	PMA
Ankerite	IMP00283.DX	MP	PMA
Annatto, CI Natural Orange 4	IOD00086.DX	OD	GCI
Anorthite	IMP00197.DX	MP	PMA
Anorthite	IMP00270.DX	MP	PMA
Anorthite	IMP00284.DX	MP	PMA
Anorthoclase	IMP00271.DX	MP	PMA
Anthraflavin acid, 2,6-dihydroxyanthraquinone	IOD00114.DX	OD	GCI
Anthragallol	IOD00118.DX	OD	GCI
Anthrapurpurin	IOD00124.DX	OD	GCI
Anthrarufin, 1,5-dihydroxyanthraquinone	IOD00108.DX	OD	GCI
Antigorite	IMP00184.DX	MP	PMA
Antiquax, natural	IWX00079.DX	WX	PMA
Antlerite	IMP00196.DX	MP	PMA
Antlerite	IMP00232.DX	MP	PMA
Antlerite	IMP00291.DX	MP	SCC
Apatite	IMP00051.DX	MP	MMA
Apatite	IMP00259.DX	MP	PMA
Apigenin	IOD00141.DX	OD	GCI
Apricot tree resin, darian, Egyptian	ICB00027.DX	CB	deYNG
Aquacryl, Azure Blue 842	IMX00010.DX	MX	MNRS

Aquacryl, Lascaux Green 850	IMX00011.DX	MX	MNRS
Aquacryl, Permanent Orange 820	IMX00008.DX	MX	MNRS
Aquacryl, Permanent Yellow 812	IMX00007.DX	MX	MNRS
Aquacryl, Transparent White 881	IMX00009.DX	MX	MNRS
Aquadhere, poly(vinyl acetate)	ISR00027.DX	SR	GCI
Aquazol 50, poly(2-ethyl-2-oxazoline)	ISR00054.DX	SR	PMA
Aquazol 500, poly(2-ethyl-2-oxazoline)	ISR00053.DX	SR	PMA
Arabic gum	ICB00001.DX	CB	GCI
Arabic gum	ICB00012.DX	CB	PMA
Arabic gum, from Acacia spp.	ICB00040.DX	CB	VA
Arabic gum, from Acacia spp.	ICB00046.DX	CB	VA
Aragonite	IMP00251.DX	MP	PMA
Aragonite	IMP00285.DX	MP	PMA
Aragonite, from shell, with some CH stretches	IMP00292.DX	MP	SCC
Araldite Rapid standard	ISR00034.DX	SR	TG
Araucaria columnaris resin	ICB00052.DX	CB	VA
Araucaria columnaris resin	ICB00053.DX	CB	VA
Archil Red, CI Acid Red 74	IOD00210.DX	OD	GCI
Arrowroot, Thai	ICB00059.DX	CB	PMA
Artinite	IMP00264.DX	MP	PMA
Artinite	IMP00288.DX	MP	PMA
Asphalt	INR00133.DX	NR	VA
Asphalt, Camborne, UK	INR00155.DX	NR	VA
Asphalt, lake, admix., Trinidad, with kaolinite and quartz	INR00004.DX	NR	BM
Asphalt, lake, Trinidad, with kaolinite and quartz	INR00145.DX	NR	VA
Asphalt, rock, Syrian, mainly calcite phase	INR00144.DX	NR	VA
Asphalt/bitumen, France	INR00151.DX	NR	VA
Asphaltite	INR00207.DX	NR	VA
Asphaltite, aged	INR00131.DX	NR	VA
Asphaltite-gilsonite, American	INR00002.DX	NR	BM
Asphaltum	INR00109.DX	NR	SCC
Asphaltum	INR00206.DX	NR	VA
Asphaltum	INR00260.DX	NR	SCC
Asphaltum, aged	INR00130.DX	NR	VA
Asphaltum, chocdolomite, Slovakia	INR00149.DX	NR	VA
Asphaltum, Dead Sea, Palestine	INR00154.DX	NR	VA
Asphaltum, Longmynd beds, UK	INR00156.DX	NR	VA
Asphaltum, manjac, Trinidad	INR00148.DX	NR	VA
Atacamite	IMP00248.DX	MP	PMA
Atacamite	IMP00293.DX	MP	SCC
Atacamite, natural	IMP00198.DX	MP	PMA
Atacamite, paratacamite mixture	IMP00062.DX	MP	FGA
Atacamite, synthetic	IMP00162.DX	MP	PMA
Attapulgite	IMP00140.DX	MP	PMA
Augite	IMP00052.DX	MP	MMA
Augite	IMP00272.DX	MP	PMA
Auramine, CI Acid Yellow 2	IOD00039.DX	OD	GCI
Aurichalcite	IMP00289.DX	MP	PMA
Azo Flavine 3R, CI Acid Orange 1	IOD00078.DX	OD	GCI
Azo Fuchsine 6B, CI Acid Violet 7	IOD00029.DX	OD	GCI
Azurite	IMP00001.DX	MP	SCC
Azurite	IMP00094.DX	MP	PMA
Azurite	IMP00099.DX	MP	PMA

Azurite	IMP00200.DX	MP	PMA
Azurite	IMP00275.DX	MP	PMA
Azurite	IMP00276.DX	MP	PMA
Azurite	IMP00277.DX	MP	PMA
Azurite	IMP00294.DX	MP	SCC

Top of Page
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III D

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Museum Applied Science Center for Archaeology, University of Pennsylvania, Philadelphia, US
Museum of Fine Arts Boston, Boston, US
Museum of Modern Art, New York, US
National Archives and Records Administration, Washington, US
National Center for Preservation Technology and Training , Natchitoches, US
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III F

JCAMP-DX Spectral File Format for Submissions to the Infrared & Raman Users Group (IRUG) Database

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Abstract *(Updated 25 February 2002)*

This paper presents guidelines for the submission of spectra in the JCAMP-DX format to the IRUG (Infrared and Raman Users Group) Database. JCAMP-DX was chosen as the file format as it is platform independent and will allow error-free transfer of spectral information between various instruments and users. IRUG will use the JCAMP-DX files as the principal source of information for submitted spectra. All information pertaining to the sample and spectrum (as outlined on the IRUG Spectrum Submission Form) is incorporated into the JCAMP-DX file in a consistent format to create a complete data record. This format, consisting of both JCAMP-DX 4.24 and user (IRUG) defined labelled data-records (LDRs), is described. The LDRs for IRUG have been kept to a minimum to facilitate automatic transfer of the information when the IRUG JCAMP-DX files are imported into the users' infrared software packages.

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JCAMP-DX Spectral File Format for Submissions to the Infrared & Raman Users Group (IRUG) Database

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updated 25 February 2002

Abstract. This paper presents guidelines for the submission of spectra in the JCAMP-DX format to the IRUG (*Infrared and Raman Users Group*) Database. JCAMP-DX was chosen as the file format as it is platform independent and will allow error-free transfer of spectral information between various instruments and users. IRUG will use the JCAMP-DX files as the principal source of information for submitted spectra. All information pertaining to the sample and spectrum (as outlined on the IRUG Spectrum Submission Form) is incorporated into the JCAMP-DX file in a consistent format to create a complete data record. This format, consisting of both JCAMP-DX 4.24 and user (IRUG) defined Labelled-data-records (LDRs), is described. The LDRs for IRUG have been kept to a minimum to facilitate automatic transfer of the information when the IRUG JCAMP-DX files are imported into the users' infrared software packages.

1. Introduction

JCAMP-DX files are non-proprietary ASCII text files, developed by the *Joint Committee on Atomic and Molecular Physical Data* [1] to allow transfer of spectral information between different instruments and different users. The files can be read and edited using standard text editors (such as WordPad® or Notepad®) and are compatible to varying degrees with most commercial IR software packages. JCAMP-DX files consist of descriptive information (title, JCAMP version, data type, origin of data, instrument, sampling, sample details, etc.) in addition to the spectral data. JCAMP-DX was chosen as the file format for submission of spectra to the ***Infrared and Raman Users Group (IRUG) Database*** as it is platform independent and should allow error-free transfer of spectral information between various instruments and users. IRUG will use the JCAMP-DX files as the primary information source for all spectra in the database. All information pertaining to the sample and spectrum must be incorporated into the JCAMP-DX file in a consistent format. This paper details how descriptive information is directly inserted into the JCAMP-DX file using both JCAMP-DX 4.24 and a limited number of user (IRUG) defined *labelled-data-records* to assemble a complete IRUG formatted JCAMP-DX file for each spectrum.

2. Background: the JCAMP-DX Format for IRUG Submissions

The **IRUG Spectrum Submission Form** and **Numerical Key** (pages 6 and 7) list the information to accompany spectra submitted to the IRUG database. Acronyms for institutions are listed in **Institution Acronym Key** (pages 16 and 17). Most of this information is not automatically inserted into a native (proprietary) spectral file when it is acquired using commercial instrument IR software. To insert / restore the missing information, the user must manually edit the JCAMP-DX file after it has been created.

Format and Content

A JCAMP-DX file consists of a series of linked *labelled-data records (fields)* known as *LDRs*. Each LDR is one or more lines in an ASCII file beginning with a *data label name (label)* followed by corresponding information and data [1].

Column A of the **IRUG Guidelines for JCAMP-DX Files** (pages 8 - 13) lists the labels required by IRUG. There are two types of labels: *JCAMP-DX 4.24* and *IRUG*. The JCAMP labels are recognized in a file by the prefix ## and are defined by JCAMP. Many are automatically inserted into the native file during conversion but must be edited when storing additional information from the IRUG submission form. ##TITLE= is an example of a JCAMP defined label. IRUG labels are denoted by the prefix ##$. These are known as "user" defined labels and were developed by IRUG to store information for which there is no pre-existing JCAMP label. Since IRUG labels are not automatically generated, these must be both inserted and edited by the user. There are a total of eight IRUG labels: ##$Material Source=, ##$Source Location=, ##$Sample Identifier=, ##$Colour=, ##$Age=, ##$Institution File Name=, ##$IRUG Material Class=, and ##$License=.

Column C of the **Guidelines** lists the corresponding information/data required for each label as defined by JCAMP [2]. These JCAMP requirements have been modified by IRUG and resulting IRUG definitions are listed in Column B. To simplify the creation of IRUG formatted JCAMP files, the **General Format for IRUG Infrared JCAMP-DX Files** and the **General Format for IRUG Raman JCAMP-DX Files**, have been developed as user templates (pages 14 and 15) and examples of spectral files in the **General Format** are found on pages 18 to 20.

Order of LDRs

For a JCAMP file to function properly, the first three LDRs must always be in the order of ##TITLE=, ##JCAMP-DX=, ##DATA TYPE=. It is also necessary for the final LDR to be ##END=. The order of the remaining LDRs is not critical and various JCAMP converters may order the LDRs differently (compare examples on pages 18 to 20). For convenience, IRUG has grouped the LDRs as follows: compulsory (title, JCAMP version, data type), submitting institution details, instrument details, sampling details, sample details, additional IRUG sample details, and spectral information.

Characters per Line Limit
Lines in the JCAMP file must not exceed a total of 80 characters (including the label). This ensures that lines are not truncated when data are imported and that the file will open properly. Where necessary, entries for labels (except the first label, ##TITLE=) can be split over multiple lines by continuing the entry on the next line (see page 19, Example 2B, ##SAMPLING PROCEDURE). Since 17 spaces in the first or title line are reserved for the label and IRUG file name, a maximum of 63 characters remain for file description.

Appearance and consistency
For consistency in appearance, the format for the title should be: the filename followed by a space, then the material name with an initial capital letter. The remaining entries on the title line should be lower case, except for proper names and the institution acronym, and should be separated by comas. To minimize compatibility issues between different spectral software, infrared files should be converted to absorbance. Apart from title entries, multiple data entries in a single field should be separated by semicolons.

Optional LDRs
Some LDRs are optional; data for these labels may not be available or applicable (see page 19, Example 2B, ##PATHLENGTH, ##PRESSURE, ##TEMPERATURE, etc). If there is no information to enter, the square brackets enclosing generic text should remain as shown in the **General Format for IRUG JCAMP-DX Files** on pages 14 and 15)

Duplicate Information
In some cases, information is entered in more than one LDR to satisfy the JCAMP definitions (see page 19, Example 2B, ##SAMPLE DESCRIPTION= and ##SAMPLING PROCEDURE=).

3. How to Edit the JCAMP-DX file

The general procedure for creating a complete IRUG formatted JCAMP-DX 4.24 file from a native infrared file is as follows:

1. Convert the native infrared file (Perkin Elmer, Nicolet, Analect, etc. format) in **absorbance** using a JCAMP converter (spectrometer manufacturer's software, GRAMS32®, or other software) to JCAMP-DX format.

2. Open the converted JCAMP-DX file in a text editor such as WordPad or Notepad. The converted file will resemble Examples 1A - 3A shown on pages 18 to 20.

3. Edit the JCAMP-DX file following the **General Format for IRUG JCAMP-DX Files** (page 14 or 15):
   Insert any missing JCAMP-DX labels and the eight IRUG defined labels (##$License=, ##$Institution File Name=, ##$Material Source=, ##$Source

Location=, ##$Sample Identifier=, ##$Colour=, ##$Age=, and ##$IRUG Material Class=) before ##XUNITS=.

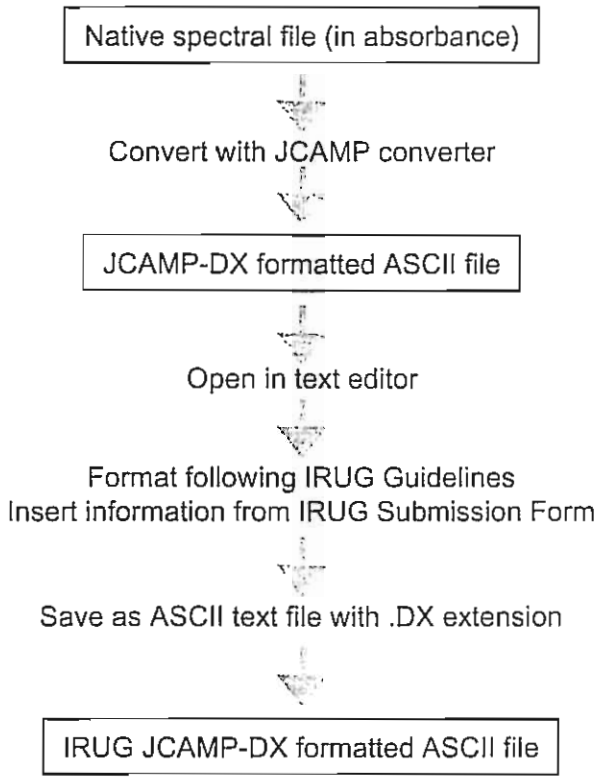
Insert the information listed on the IRUG Spectral Submission Form after the appropriate labels. Complete as many the LDR fields as possible. Be mindful of 80-character line limit; continue entries in excess of 80 characters on consecutive lines. The edited file should resemble Examples 1B - 3B shown pages 18 to 20.

4. Save the new JCAMP-DX file as an **ASCII text file** with the DX extension (NAME.DX). Check that the new file will open in your spectrometer's software.

5. **CAUTION: do not overwrite** the newly edited JCAMP-DX files with files from the original manufacturer's operating software (or JCAMP-DX converter software) as the changes/additions made in WordPad or Notepad will be overwritten and lost.

IRUG formatted Raman files are edited in a similar manner but the ordinate axis units should be **relative intensity**.

Editing procedure summary



4. Summary

A uniform, platform-independent format based on JCAMP-DX has been adopted for spectra submitted to the **Infrared and Raman Users Group (IRUG) Database**. The format uses combined JCAMP-DX 4.24 and IRUG defined labels for labelled-data-records (LDRs) that will accommodate the information requested for spectral submissions to the **IRUG Database**. The use of all labels, insofar as possible, will ensure that all pertinent information is contained within the JCAMP-DX file, creating a complete data record for each spectrum. The result is data of improved quality, and an **IRUG Database** that may be treated as a primary reference.

5. References

1 HTTP://members.aol.com/rmcdjcamp/dxlabels.htm
2 HTTP://members.aol.com/rmcdjcamp/defines.htm

IRUG Spectrum Submission Form

The information requested for submissions is listed below. Terms are defined on the **Numerical Key** on the next page. The **Submission Form** is also available on the **IRUG web site: *www.irug.org***. If possible, provide the information in digital format.

IRUG File Name (0): (8 characters assigned by IRUG editors)
Institution (1):
Institution acronym (2):
Address (3):
Analyst (4):
Telephone (5):
Fax (6):
E-mail (7):

Data Description

Institution file name (8) and date/time of acquisition (9):
Format (10):

Sample Description

Common/trade name (11):
Chemical name (12):
Material class (13):
Physical state (14):
Form (15):
Colour/color (16):
Age (17):

Origin

Material source (18):
Source location (19):
Sample identifier (20):

Instrument Parameters

Instrument + software (21):
Spectral range (22):
Resolution (23):
Scans (24):
Apodization (25):
Instrument purge (26): (purge: Y/N)

Technique

Mode (27): (tran/refl/scat)
Accessory (28):
Sample support (29):
Sample preparation (30):

Data Processing History

CO_2 correction (31): (CO2: Y/N)
Baseline Correction (32): (baseline corr.: Y/N)
Other data processing (33)

Supplemental Analytical Data

Other analytical methods (34):
Additional Information (44 – 57):

Raman Specific Data

Monochromator (35)
Source (36)
Power (37)
Detector (38)
Detector parameters (39)
Collecting lens (40)
Angle (41)
Polarisation (42)
Filters (43)

Numerical Key

0 IRUG filename: 8 character filename, beginning "I" for infrared or "R" for Raman, followed by 2 letter IRUG materials class acronym, and a five digit No. assigned and inserted by IRUG editing committee after receipt of the file, e.g., filename: inr00603.dx.
1 Originating institution name: full name
2 Originating institution acronym: see institution acronym list
3 Address: full address of institution
4 Analyst: name of analyst who acquired the spectrum
5 Telephone: contact telephone # of analyst +/or analytical lab +/or conservation dept., etc
6 Fax: contact fax # of analyst +/or analytical lab +/or conservation dept., etc
7 Email: contact fax # of analyst +/or analytical lab +/or conservation dept., etc
8 Institution filename: 8-character name for spectral file as assigned in originating institution
9 Date/time of acquisition: date + time spectrum was acquired
10 Format: JCAMP + version number
11 Common/trade name: e.g. gypsum, Paraloid B-72
12 Chemical name: e.g. calcium sulfate dihydrate, poly(methyl acrylate-ethyl methacrylate) copolymer
13 Material Class: ***organic***: carbohydrate-gum/sugar (CB), organic pigments and dyes (OD), natural resin (NR), oil/fat (OF), protein (PR), synthetic resin (SR), wax (WX); ***inorganic***: minerals, pigments, and corrosion product (MP), glass (GL); ***other***: mixtures (MX), unclassified (UC)
14 Physical state: solid (s), liquid (l), gas (g)
15 Form: chunk, emulsion, flake, fibre/fiber, paste, powder, sheet, etc
16 Color /colour: colour of sample material
17 Age: approximate age of material, aging history, if known
18 Material source: (of sample) manufacturer, supplier, collector, etc
19 Source location: country, region, state, city/town, site
20 Sample identifier: catalog/catalogue #, CI #, collection #, or any other unique institutional #, e.g. Forbes pigment #, Sigma catalogue/catalog #, etc
21 Instrument + software: manufacturer, model, software version
22 Spectral range: e.g. 4000 - 650 cm^{-1}
23 Resolution: (of spectrum as measured, not of JCAMP file) 4 or 8 cm^{-1} minimum recommended
24 Scans: number of scans
25 Apodization: boxcar (B), Happ-Genzel (HG), Norton-Beer -weak, medium, strong (NB-w, m, s), triangular (T), etc.
26 Instrument purge: Y or N
27 Mode: transmission (tran), reflectance (refl), scatter (scat – for Raman)
28 Accessory (ies): attenuated total reflectance (atr), beam condenser (bc), diffuse reflectance (drift), fibreoptic (fo), grazing angle (ga), microscope (micr), spectral reflectance (sr), etc
29 Sample support(s): AgCl, AgBr, BaF_2, CaF_2, CdTe, CsI, diamond, Ge, KBr, KRS5, NaCl, Nujol (nj), Si, SiC, ZnS, ZnSe, etc
30 Sample preparation: neat, CH_2Cl_2 extract, sample ground with KBr, sample and KBr ground separately and mixed, etc
31 CO_2 correction: Y or N
32 Baseline correction: Y or N
33 Other data processing details: spectral subtraction, transformations etc.
34 Analytical methods, other (cross-reference): VLM, FLM, PLM, SEM, EDS, EPMA, XRF, AA, ICP, ICP-MS, GC, GC-MS, GC-IR, FT-Raman, RP-HPLC, PAGE, TLC, etc
44- Additional information: pathlength, cm (44), pressure (45), temperature °C (46), CAS name (47), molecular formula (48), CAS reg. No (49), Wiswesser line notation (50), Beilstein Lawson No (51), melting point, °C (52), boiling point, °C (53), refractive index (at 20°C for NaD) (54), density g/cm^3 (55), molecular weight (56), concentration (57), etc.

Raman Specific Data:

35 Monochromator: dispersive or interferometric
36 Source: excitation source wavelength in nm
37 Power: power incident on sample, in mW
38 Detector: detector type; CCD, PMT, PDA, etc.
39 Detector parameters: integration time, number of accumulations
40 Collecting lens: magnification (eg 100x), numerical aperture
41 Angle: collecting angle of scattered radiation, in degrees
42 Polarisation: polarisation of excitation radiation
43 Filters: details of any Notch or interference filters, analyser, etc

IRUG Guidelines for JCAMP-DX Files

(Superscripts [1, 2...] refer to location of information on **IRUG Sample Submission Form and Numerical Key**)

A	B	C
Labels	**IRUG** **Definition of entries**	**JCAMP** **Definition of entries**
##TITLE=	*insert:* IRUG filename [0] Common name [11], material source [18], sample identifier [20], institution acronym [2], mode [27]	##TITLE= should contain a concise description of the contents, suitable as a title for a data plot. ##TITLE= is required as the first LDR of each JCAMP-DX FILE or BLOCK.
##JCAMP-DX=	JCAMP version [10] (4.24)	Required immediately after each ##TITLE= to show Version number of JCAMP-DX. Version of software which generates a JCAMP-DX file should be added as a comment after the Version Number.
##DATA TYPE=	INFRARED SPECTRUM or RAMAN SPECTRUM	##DATA TYPE= defines the data technique for the current JCAMP-DX BLOCK.
Submitting Institution Details		
##ORIGIN=	*insert:* originating institution name [1]; address [3]; analyst's name [4]; telephone [5]; fax [6]; e-mail [7] NB use abbreviations (Tel:, Fax:, Email:) and leave missing data sections blank (e.g.: ... Victoria & Albert Museum, London SW7 2RL, Tel:; Fax: +44 (0)207...)	Name of organization, address, telephone number, FAX number, E-mail address, name of individual contributor, etc., as appropriate. This information is not optional; the originator of a JCAMP-DX file should always see that it is included. The instrument manufacturer cannot be responsible for this information. NOTE: Omission of this information is not necessarily a valid reason for software to refuse to process a JCAMP-DX file. Under no circumstances should a file be retransmitted without this information.
##OWNER=	*insert:* originating institution name [1] OR COPYRIGHT © (year) by originating institution name [1]. (Copyright statement is optional)	Name of owner of proprietary data. The organization or person named under ##ORIGIN= is responsible for accuracy of this field. If the data are copyrighted, this line should read "COPYRIGHT © (year) by (name)." This information is not optional; the originator of a JCAMP-DX file should always see that it is included. If ##OWNER= contains "PUBLIC DOMAIN", the implication is that the data may be copied without permission on the authority of whoever is names under ##ORIGIN=. Absence of ##OWNER= does not imply permission to copy.
##$License=	*insert:* 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.	IRUG defined data label - no JCAMP definition.

A	B	C
Labels	**IRUG** **Definition of entries**	**JCAMP** **Definition of entries**
##$Institution File Name=	*insert:* originating institution's file name [8]	IRUG defined data label – no JCAMP definition.
##DATE=	YY/MM/DD date of spectrum acquisition [9]	Date when data was measured, in the form: YY/MM/DD (note order).
##TIME=	HR/MIN/SEC time of spectrum acquisition [9]	Time when data was measured, in the form: HR/MIN/SEC (24-hour clock).
Instrument Details		
##SPECTROMETER/ DATA SYSTEM=	*insert:* instrument and software [21] For Raman, *include:* monochromator [35]; detector [38]	This field contains manufacturer's name, model of the instrument, software system, and release number, as appropriate, in the form used by the manufacturer.
##INSTRUMENT PARAMETERS=	*Insert:* apodization [25]; No of scans [24]; instrument purge [26]; spectral range [22] For Raman, *include:* source [36]; power [37]; detector parameters [39]	This optional field is a list of pertinent instrument settings using standard notation when available, otherwise using the notation of the manufacturer. Only settings which are essential for applications should be included.
##RESOLUTION=	*insert:* resolution [23] - of acquired spectrum (not of data in DX file)	Nominal resolution in units specified by ##XUNITS=, as a single number for spectra at constant resolution throughout, or as pairs of the form :R1,X1,...,Rn,Xn, where R stands for Resolution at abscissa X.
##DATA PROCESSING=	*insert:* entries for CO2 correction [31]; baseline correction [32]; and any other data processing performed [33]	Description of background correction, smoothing, subtraction, deconvolution procedures, apodization function, zero-fill, or other data processing, together with reference to original spectra used for subtractions.
Sampling Details		
##SAMPLE DESCRIPTION=	*insert:* mode [27]; accessory [28]; sample support [29] For Raman, *include:* collecting lens [40]; angel [41]; polarisation [42]; filters [43]	First entry in this field should be MODE of observation (transmission, specular reflection, PAS, matrix isolation, etc., for spectra, or column type, etc., for chromatograms, or ionization parameters, etc. for mass spectra, or appropriate information for any other techniques or applications. Name and model of appropriate accessories, cell thickness, and window material for fixed liquid cells, ATR plate material, angle and cone of incidence, and effective number of reflections for ATR measurements, polarization, and special modulation techniques, as discussed by Grasselli, Griffiths, and Hannah, Appl.Spectroscopy, 1982, 36, 87, etc., are appropriate for other types of measurement. (For V5.0, this information should be under ##APPLICATION=.)
##SAMPLING PROCEDURE=	*insert:* mode [27]; and sample preparation [30]	First entry in this field should be MODE of observation (transmission, specular reflection). Use enough space to describe the procedure. Give a citation to a description of a standard procedure.
##PATH LENGTH=	*insert*: pathlength [44], where applicable	Path length in cm.
##PRESSURE=	*insert*: pressure [45], where significantly different from atmospheric	Sample pressure in appropriate units if significantly different from atmospheric.

A	B	C
Labels	**IRUG** **Definition of entries**	**JCAMP** **Definition of entries**
##TEMPERATURE=	*insert*: temperature [46], where significantly different from room temperature	Sample temperature in degrees C if significantly different from room temperature.
	Sample Details	
##CAS NAME=	*insert*: CAS name [47], where available	Name according to Chemical Abstracts naming conventions as described in Appendix IV of the 1985 CAS Index Guide. Examples can be found in Chemical Abstracts indices or the Merck Index. Greek Letters are spelled out, and standard ASCII capitals are used for small capitals. Sup/Superscripts are indicated by prefixes / and ^, respectively. Example, alpha-D-glucopyranose, 1-(dihydrogen phosphate).
##NAMES=	*insert:* common/trade name [11], chemical name [12] etc. Multiple names placed on separate lines	Common, trade, or other names. Multiple names are placed on separate lines.
##MOLFORM=	*insert*: molecular formula [48], where available	Molecular formula. Elemental symbols are arranged with carbon first, followed by hydrogen, and then remaining element symbols in alphabetic order. The first letter of each elemental symbol is capitalised. The second letter, if required, is in lower case. One-letter symbols must be separated from adjacent symbols by a blank or digit. Sub/super scripts are terminated by the next non-digit. Slash may be omitted for subscripts. For readability, each atomic symbol may be separated from its predecessor by a space. For substances which are represented by dot-disconnected formulas (hydrates, etc.), each fragment is represented in the above order, and the dot is represented by *. Isotopic mass is specified by a leading superscript. D and T may be used for deuterium and tritium, respectively. Examples: C2H4O2 or C2 H4 O2 (Acetic acid) C6 H9 Cr O6 * H2 O (Chromic acetate monohydrate) H2^17O (water, mass 17 oxygen)
##CAS REGISTRY No=	*insert*: CAS registry number [49], where available	CAS Registry Numbers for many compounds can be found in Chemical Abstracts indices, Merck Index, or CAS ON-LINE.
##WISWESSER=	*insert*: Wiswesser line notation [50], where available	The Wiswesser line notation is a precise and concise means of expressing structural formulas as character strings. The basic idea is to use letter symbols to denote functional groups and numbers to express the lengths of chains and the sizes of rings. Wiswesser notation is described I detail by Smith, "The Wiswesser-Line Formula Chemical Notation", McGraw-Hill, New York, 1968), 2nd Ed; and Chemical Information Management, Inc., 3rd Ed, 1975.

A	B	C
Labels	**IRUG** **Definition of entries**	**JCAMP** **Definition of entries**
##BEILSTEIN LAWSON No=	*insert*: Beilstein Lawson Number [51], where available	The Beilstein Lawson Number is a structural formula clustering code based on the Beilstein System. It is used for locating information in Beilstein databases, including the STN on-line database. The code contains only structural information and can be generated locally on microcomputers from connection table data alone. A simple description of the algorithm has be published by Lawson, "Structure Graphics" in Pointers to Beilstein Out, ACS Symposium 341, Graphics for Chemical Structures - Integration of Text and Data, 1987, pp 80-87.
##MP=	*insert*: melting point [52], where available	Melting Point in degrees C.
##BP=	*insert*: boiling point [53], where available	Boiling Point in degrees C followed by pressure in mm Hg if other than one atmosphere.
##REFRACTIVE INDEX=	*insert*: refractive index [54], where available	In the form: ND = 1542^20 (index at 20 degrees C for NaD line).
##DENSITY=	*insert*: density [55], where available	Density in g/cc.
##MW=	*insert*: molecular weight [56], where available	Molecular weight.
##CONCENTRATIONS=	*insert*: concentration [57],where available. Include known impurities	List of known components and impurities and their concentrations in the following form, where N stands for name (enclosed in angle brackets if more than one word); C, for concentration; and U, for units of concentration: EXAMPLE: ##CONCENTRATIONS= (NCU) (N1, C1, U1), (N2, C2, U2), etc. The group for each component is enclosed in parentheses. Each group starts a new line and may continue on the following lines.
##STATE=	*insert:* physical state [14] and form [15] (For IRUG, sample prep is under ##Sampling Procedure)	Solid, liquid, gas, solution, KBr pellet, powder, nujol mull, etc.
##CROSS REFERENCE=	*insert:* all supplemental/other analytical methods [34]	Cross references refer to additional data on the same sample, i.e., different thickness, mulling agent, polarisation, temperature, time, etc., or serve to link a peak table or interferogram with a spectrum, etc.
Additional IRUG sample details		
##$Material Source	*insert:* material source [18]	IRUG defined data label – no JCAMP definition.
##$Source location	*insert:* source location [19]	IRUG defined data label – no JCAMP definition.
##$Sample Identifier	*insert:* sample identifier [20]	IRUG defined data label – no JCAMP definition.
##$Colour=	*insert:* color/colour [16]	IRUG defined data label – no JCAMP definition.

A	B	C
Labels	**IRUG** **Definition of entries**	**JCAMP** **Definition of entries**
##$Age=	*insert:* age [17]	IRUG defined data label – no JCAMP definition.
##$IRUG Material Class=	*insert:* materials class [13]	IRUG defined data label - no JCAMP definition.
##=	*insert:* any additional information	Comments may be introduced by a DATA-LABEL-FLAG (##) plus a DATA-LABEL-TERMINATOR (=), with null DATA-LABEL-NAME. Such comments may continue for more than one line, terminating at the next DATA-LABEL-FLAG. Sub-headings (not JCAMP-DX Labels) may be used within such comments at the discretion of the end-user. As many such comments as needed may be included between ##TITLE= and ##END=.
Spectral Information		
##DELTAX=	Automatically inserted by commercial software converter	This LDR gives the nominal spacing between points for informing the user. Actual X-values should be calculated from (##LASTX= minus ##FIRSTX=)/(##NPOINTS= - 1).
##XUNITS=	Automatically inserted by commercial software converter, 1/cm preferred	##XUNITS= gives the abscissa units for the current DATA TYPE. Any standard unit is acceptable. For infrared spectra, the following units are appropriate: 1/CM (representing wavenumber), MICROMETERS, NANOMETERS, SECONDS, ARBITRARY UNITS
##YUNITS=	Automatically inserted by commercial software converter: absorbance / transmittance /arbitrary units... **For maximum compatibility, IR spectra for submission to IRUG should be in ABSORBANCE.** For Raman, this should be **RELATIVE INTENSITY**.	Gives the ordinate units for the current DATA TYPE. Any standard units are acceptable. For infrared spectra, the following units are appropriate: TRANSMITTANCE, REFLECTANCE, ABSORBANCE, KUBELKA-MONK, ARBITRARY UNITS
##XFACTOR=	Automatically inserted by commercial software converter	##XFACTOR= and ##YFACTOR= ,respectively, are factors by which components of tabulated abscissa and ordinate values should be multiplied to obtain actual values. For ASCII representation, these factors should be chosen to convert tabulated values to integers, clipping off all but about 1 digit of noise on the average.
##YFACTOR=	Automatically inserted by commercial software converter	
##FIRSTX=	Automatically inserted by commercial software converter	##FIRSTX= and ##LASTX= are the first and last ACTUAL abscissa values for current DATA TYPE, as appropriate. First tabulated abscissa time ##XFACTOR= should equal ##FIRSTX=. Spectral data are tabulated in order of EITHER increasing or decreasing abscissa values. ##FIRSTX= specifies the abscissa corresponding to the first value listed under the current DATA TYPE, not the smallest abscissa.
##LASTX=	Automatically inserted by commercial software converter	
##NPOINTS=	Automatically inserted by commercial software converter	##NPOINTS= is the number of components of a ##DATACLASS= like ##XYDATA=.

A	B	C
Labels	**IRUG** **Definition of entries**	**JCAMP** **Definition of entries**
##FIRSTY=	Automatically inserted by commercial software converter	##FIRSTY= is the actual Y-value corresponding to ##FIRSTX=. ##FIRSTY= should equal ##YFACTOR= times the first Y-value in the current ##DATACLASS=. NOTE: If the ordinate value corresponding to ##FIRSTX= is undefined, i.e., represented by ?, then ##FIRSTY= also is represented by ?. This is the reason for recommending the different way of checking data scaling which is outlined under ##MAXX=, etc.
##MAXY= ##MAXX=	Automatically inserted by commercial software converter	These attributes of the data array were listed as OPTIONAL in V4.24. It is currently recommended that ##MAXY= and ##MINY= be required for ##XYDATA=. It is now recommended that the difference ##MAXY= minus ##MINY= be compared to the difference between converted values to check Ordinate scaling rather than comparing ##FIRSTY= to the product of ##YFACTOR= and the first converted ordinate as recommended in V4.24. See NOTE under ##FIRSTY=
##MINY= ##MINX=	Automatically inserted by commercial software converter	
##XYDATA=	Automatically inserted by commercial software converter	##XYDATA= is the heading for a data array which consists of a list or ordinates at equal X-intervals, as specified by the following Data Labels: ##XUNITS=, ##YUNITS=, ##XFACTOR=, ##YFACTOR=, ##FIRSTX=, ##LASTX=, ##MAXY=, ##MINY=, ##NPOINTS=, ##FIRSTY=. The tabular form of the ##XYDATA= is a series of lines organized as follows: X1 Y1 Y2 Y3 Y4 Y5 ... YN. This form of data is represented symbolically by a VARIABLE LIST, as follows: ##XYDATA= (X++(Y..Y)), - where X++ indicates that the first item in a line is an X-value, ++ indicates that X is incremented for each following Y-value and (Y..Y) indicates that the initial X-value is followed by a succession of Y-values
...	Automatically inserted by commercial software converter, data...	
##End=		##END= indicates the end of a JCAMP-DX FILE or BLOCK. There must be one ##END= for each ##TITLE= in a COMPOUND JCAMP-DX file.

General Format for IRUG Infrared JCAMP-DX Files

(Numbers in brackets refer to location of the information on the IRUG Sample Submission Form and Numerical Key)

##TITLE=[IRUG filename (0)] [Common/trade name (11)], [sample source (19)], [sample identifier (20)], [INSTITUTION ACRONYM (2)], [mode (27)]
##JCAMP-DX=4.24
##DATA TYPE=INFRARED SPECTRUM
##ORIGIN=[originating institution (1)]; [address (3)]; [analyst (4)]; tel: [telephone (5)]; fax: [fax (6)]; email: [e-mail (7)]
##OWNER=COPYRIGHT © [year] by [institution name (1) or acronym (2)]
##$LICENSE=By accepting this database user agrees to be bound by the terms of
the IRUG user's license. Any reference written/oral made to this file must
include accreditation to BOTH the originating individual/institution and IRUG.
Contributor agrees to be bound by the terms of the IRUG contributor's license.
##$INSTITUTION FILE NAME=[institution filename (8)]
##DATE=[date/time of acquisition (9)]
##TIME=[date/time of acquisition (9)]
##SPECTROMETER/DATA SYSTEM=[instrument and software (21)]
##INSTRUMENT PARAMETERS= apodization: [apodization (25)]; scans: [No of scans (24)]; purge: [instrument purge Y/N (26)]; range: [spectral range (22)]
##RESOLUTION=[resolution (23)]
##DATA PROCESSING= CO2 corr.: [CO2 correction Y/N (31)]; baseline corr.: [baseline correction Y/N (32)]; [other data processing (33)]; further data processing information may automatically be inserted by JCAMP converter
##SAMPLE DESCRIPTION= [mode (27)]; accessories: [accessory (28)]; support: [sample support (29)]
##SAMPLING PROCEDURE=[mode (27)]; prep: [sample preparation (30)]
##PATHLENGTH=[pathlength (44)]
##PRESSURE=[pressure (45)]
##TEMPERATURE=[temperature (46)]
##CAS NAME=[CAS name (47)]
##NAMES=[common/trade name (11)]
[chemical name (12)]
##MOLFORM=[molecular formula (48)]
##CAS REGISTRY NUMBER=[CAS registry number (49)]
##WISWESSER=[Wiswesser line notation (50)]
##BEILSTEIN LAWSON No=[Beilstein Lawson number (51)]
##MP=[melting point (52)]
##BP=[boling point (53)]
##REFRACTIVE INDEX=[refractive index (54)]
##DENSITY=[density (55)]
##MW=[molecular weight (56)]
##CONCENTRATIONS=[concentrations (57)]
##STATE=[physical state (14)]; [form (15)]
##CROSS REFERENCE=[other analytical methods (34)]
##$MATERIAL SOURCE=[source of sample(18)]
##$SOURCE LOCATION=[source location (19)]
##$SAMPLE IDENTIFIER=[sample identifier (20)]
##$COLOUR=[color/colour (16)]
##$AGE=[age (17)]
##$IRUG MATERIALS CLASS=[material class (13)]
##DELTAX=[automatically inserted]
##XUNITS=[automatically inserted]
##YUNITS=[automatically inserted]
##FIRSTX=[automatically inserted]
##LASTX=[automatically inserted]
##FIRSTY=[automatically inserted]
##MAXX=[automatically inserted]
##MINX=[automatically inserted]
##MAXY=[automatically inserted]
##MINY=[automatically inserted]
##XFACTOR=[automatically inserted]
##YFACTOR=[automatically inserted]
##NPOINTS=[automatically inserted]
##XYDATA=[automatically inserted] 624.823 .....
##END=[automatically inserted]

General Format for IRUG Raman JCAMP-DX Files

(Numbers in brackets refer to location of the information on the IRUG Sample Submission Form and Numerical Key)

##TITLE=[IRUG filename (0)] [Common/trade name (11)], [sample source (19)], [sample identifier (20)], [INSTITUTION ACRONYM (2)], scat (27)
##JCAMP-DX=4.24
##DATA TYPE=RAMAN SPECTRUM
##ORIGIN=[originating institution (1)]; [address (3)]; [analyst (4)]; tel: [telephone (5)]; fax: [fax (6)]; email: [e-mail (7)]
##OWNER=COPYRIGHT © [year] by [institution name (1) or acronym (2)]
##$LICENSE=By accepting this database user agrees to be bound by the terms of
the IRUG user's license. Any reference written/oral made to this file must
include accreditation to BOTH the originating individual/institution and IRUG.
Contributor agrees to be bound by the terms of the IRUG contributor's license.
##$INSTITUTION FILE NAME=[institution filename (8)]
##DATE=[date/time of acquisition (9)]
##TIME=[date/time of acquisition (9)]
##SPECTROMETER/DATA SYSTEM=[instrument and software (21)]; monochromator: [dispersive / interferometric monochromator (35)]; detector: [detector type (38)]
##INSTRUMENT PARAMETERS= apodization: [apodization (25)]; scans: [No of scans (24)]; purge: [instrument purge Y/N (26)]; range: [spectral range (22)]; source: [source (36)]; power: [power (37)]; detector parameters: [detector parameters (39)]
##RESOLUTION=[resolution (23)]
##DATA PROCESSING= CO2 corr.: [CO2 correction Y/N (31)]; baseline corr.: [baseline correction Y/N (32)]; [other data processing (33)]; further data processing information may automatically be inserted by JCAMP converter
##SAMPLE DESCRIPTION= scat; accessories: [accessory (28)]; support: [sample support (29)]; objective: [collecting lens (40)]; angle: [angle (41)]; polarisation: [polarisation (42)]; filters: [filters (43)]
##SAMPLING PROCEDURE=scat; prep: [sample preparation (30)]
##PATHLENGTH=[pathlength (44)]
##PRESSURE=[pressure (45)]
##TEMPERATURE=[temperature (46)]
##CAS NAME=[CAS name (47)]
##NAMES=[common/trade name (11)]
[chemical name (12)]
##MOLFORM=[molecular formula (48)]
##CAS REGISTRY NUMBER=[CAS registry number (49)]
##WISWESSER=[Wiswesser line notation (50)]
##BEILSTEIN LAWSON No=[Beilstein Lawson number (51)]
##MP=[melting point (52)]
##BP=[boling point (53)]
##REFRACTIVE INDEX=[refractive index (54)]
##DENSITY=[density (55)]
##MW=[molecular weight (56)]
##CONCENTRATIONS=[concentrations (57)]
##STATE=[physical state (14)]; [form (15)]
##CROSS REFERENCE=[other analytical methods (34)]
##$MATERIAL SOURCE=[source of sample(18)]
##$SOURCE LOCATION=[source location (19)]
##$SAMPLE IDENTIFIER=[sample identifier (20)]
##$COLOUR=[color/colour (16)]
##$AGE=[age (17)]
##$IRUG MATERIALS CLASS=[material class (13)]
##DELTAX=[automatically inserted]
##XUNITS=[automatically inserted]
##YUNITS=Relative intensity
##FIRSTX=[automatically inserted]
##LASTX=[automatically inserted]
##FIRSTY=[automatically inserted]
...
...
##XFACTOR=[automatically inserted]
##YFACTOR=[automatically inserted]
##NPOINTS=[automatically inserted]
##XYDATA=[automatically inserted] 624.823 .....
##END=[automatically inserted]

Institution Acronym Key for Database Contributors as of July 2000

ADSL	Archaeological Department, Colombo, Sri Lanka, LK
AFA-V	Academy of Fine Arts, Institute of Chemistry, Vienna, AU
AIC	Art Institute of Chicago, Chicago, IL, US
AMNH	American Museum of Natural History, New York, NY, US
BM	British Museum, London, GB
BSU	Ball State University, Muncie, IN, US
CCI	Canadian Conservation Institute, Ottawa, CA
CIA	Courtauld Institute of Art, University of London, GB
COA-CNR	Centro Opere D'Arte, Consiglio Nazionale delle Ricerche, Firenze, IT
CU	Cardiff University, School of History and Archaeology, Cardiff, Wales, GB
deYNG	M.H. De Young Museum, San Francisco, CA, US
FAUK	Department of Fine Arts, University of Kelaniya, Kelaniya, Sri Lanka, LK
FGA	Freer Gallery of Art, Smithsonian Institution, Washington, DC, US
FU	CECOR – Escola de Bela Artes, Federal University of Minas Gerais, BR
GACC	Garbar Art Conservation Center (Russian Scientific Conservation Center named after Grabar), Moscow, RU
GCI	Getty Conservation Institute, Los Angeles, CA, US
HKI	Hamilton Kerr Institute, Cambridge, GB
HNM	Hungarian National Museum, Budapest, HU
IROE-CNR	Instituto di Ricerca Sulle Onde Elettromagnetiche, Consiglio Nazionale delle Ricerche, Firenze, IT
LMU	Loyola Marymount University, Los Angeles, CA, US
MASCA	Museum Applied Science Center for Archaeology, University of Pennsylvania, Philadelphia, PA, US
McC	McCrone Research Institute, Chicago, IL, US
MFA-B	Museum of Fine Arts Boston, Boston, MA, US
MMA	Metropolitan Museum of Art, New York, NY, US
MNRS	Museo Nacional Reina Sofia, Madrid, ES
MOMA	Museum of Modern Art, New York, NY, US
MU	Miami University, Oxford, OH, US
NARA	National Archives and Records Administration, Washington, DC, US
NG	National Gallery, London, GB

NGA	National Gallery of Art, Washington, DC, US
NMGM	National Museums and Galleries on Merseyside, Liverpool, GB
NMWA	National Museum of Western Art, Tokyo, JP
NSC	National School of Conservation, Mexico City, MX
OADC	Ormylia Art Diagnosis Centre, Ormylia, GR
PMA	Philadelphia Museum of Art, Philadelphia, PA, US
RFL	Rathgen –Forschungslabor, Staatliche Museen Preußischer Kulturbesitz, Berlin, DE
SC	School of Conservation, Det Kongelige Danske Kunstakademi, Copenhagen, DK
SCC	Straus Conservation Center (Fogg), Harvard University Art Museums, Cambridge, MA, US
TG	Tate Gallery, London, GB
UF	University of Florence, Firenze, IT
UI	University of Iceland, Reykjavik, IS
UM	Micro-analytical Research Centre, School of Physics, University of Melbourne, VIC 3010, AU
VA	Victoria and Albert Museum, London, GB
WACC	Williamstown Art Conservation Center, Williamstown MA, US
WM	Winterthur Museum, Garden and Library, Winterthur, DE, US

Example 1A

JCAMP-DX file as generated by Nicolet converter.

```
##TITLE=PMAI2037 SEEDLAC NO. 4858 AF SUTER & CO LTD
##JCAMP-DX=4.24  $$ Nicolet v. 410
##DATA TYPE=INFRARED SPECTRUM
##ORIGIN=PMA Conservation Dept.
##OWNER=Nicolet
##DATE=98/06/30
##TIME=13:45:06
##DATA PROCESSING=
Ratio against background
%Transmittance->Absorbance
Straight Line generate
Truncated
##XUNITS=1/CM
##YUNITS=ABSORBANCE
##FIRSTX=624.823181
##LASTX=3999.639893
##FIRSTY=0.029192
##MAXX=3999.639893
##MINX=624.823181
##MAXY=0.981087
##MINY=-0.001622
##XFACTOR=1.000000
##YFACTOR=1.000000E-009
##NPOINTS=1751
##DELTAX=1.928467
##XYDATA=(X++(Y..Y))
624.823 ...
...

##END=
```

Example 1B

Same JCAMP-DX file edited to meet IRUG guidelines.

```
##TITLE=INR00610 Seedlac, AF Suter, #4858, PMA, tran
##JCAMP-DX=4.24  $$ Nicolet v. 410
##DATA TYPE=INFRARED SPECTRUM
##ORIGIN=Philadelphia Museum of Art; Box 7646, Philadelphia, PA 19101, USA; Beth
Price; tel:+1 215 684 7552; fax: +1 215 684 7550; email: bprice@phillamuseum.org
##OWNER=COPYRIGHT © 98 by Philadelphia Museum of Art, Cons Dept Analytical Lab
##$LICENSE=By accepting this database user agrees to be bound by the terms of
the IRUG user's license. ...
##$INSTITUTION FILE NAME=PMAI2037
##DATE=98/06/30
##TIME=13:45:06
##SPECTROMETER/DATA SYSTEM=Nicolet 510P bench w/ NIC-Plan micr; OMNIC v2.1
##INSTRUMENT PARAMETERS=apodization: HG; scans: 200; purge: dry air; range: 4000
-625 cm-1
##RESOLUTION=4 cm-1
##DATA PROCESSING=CO2 corr.:Y; baseline corr.:Y; Multiplied by a scalar,
Converted from OMNIC, Ratio against background, Straight Line gen., Truncated
##SAMPLE DESCRIPTION=tran; accessories: micr; support: dia
##SAMPLING PROCEDURE=tran; prep: scraping
##PATHLENGTH=[pathlength (44)]
##PRESSURE=[pressure (45)]
##TEMPERATURE=[temperature (46)]
##CAS NAME=[CAS name (47)]
##NAMES=seedlac
[chemical name (12)]
##MOLFORM=[molecular formula (48)]
##CAS REGISTRY NUMBER=[CAS registry No (49)]
##WISWESSER=[Wiswesser line notation (50)]
##BEILSTEIN LAWSON No=[Beilstein Lawson No (51)]
##MP=[melting pont (52)]
##BP=[boiling point (53)]
##REFRACTIVE INDEX=[refractive index (54)]
##DENSITY=[density (55)]
##MW=[molecular weight (56)]
##CONCENTRATIONS=[concentration (57)]
##STATE=solid; bulk
##CROSS REFERENCE=GC-MS
##$MATERIAL SOURCE=AF Suter & Co, Ltd
##$SOURCE LOCATION=London, England, UK
##$SAMPLE IDENTIFIER=AF Suter #4858
##$COLOR=orange-brown
##$AGE=unknown, purchased 1996
##$IRUG MATERIALS CLASS=NR
##XUNITS=1/CM
##YUNITS=ABSORBANCE
##FIRSTX=624.823181
##LASTX=3999.639893
...
.##XYDATA=(X++(Y..Y))
624.823  . ...
##END=
```

Example 2A

JCAMP-DX file as generated by Perkin-Elmer converter.

```
##TITLE= Cellulose nitrate by SiC. Millipore SC 8micron. GLM
##JCAMP-DX= 4.24
##DATA TYPE= INFRARED SPECTRUM
##ORIGIN= Exported PE Spectrum Data File
##OWNER=
##DATE= 94/05/04
##TIME= 14:31:19.00
##SPECTROMETER/DATA SYSTEM= PERKIN-ELMER Not Specified IR
##INSTRUMENT PARAMETERS=
  APODIZATION=Not Specified
  DETECTOR=Not Specified
##RESOLUTION= 1.000000
##DELTAX= -1.000000
##XUNITS= 1/CM
##YUNITS= TRANSMITTANCE
##XFACTOR= 1.00
##YFACTOR= 0.00000023841857910156
##FIRSTX= 4000.00
##LASTX= 400.00
##NPOINTS= 3601
##FIRSTY= 55.46
##MAXY= 9.209990
##MINY= 163.83
##XYDATA= (X++(Y..Y))
4000.000000  687173699  687173699 ...
  ...
##END=
```

Example 2B

Same JCAMP-DX file edited to meet IRUG guidelines.

```
##TITLE=ISR05000 Cellulose nitrate, VA, refl
##JCAMP-DX= 4.24
##DATA TYPE= INFRARED SPECTRUM
##ORIGIN= Victoria & Albert Museum; South Kensington; GB London SW7 2RL; Boris
Pretzel; tel:+44 (0)20 7942 2116; fax:+44 (0)20  942 2092; email:
boris.pretzel@vam.ac.uk
##OWNER=COPYRIGHT © 1989 by Victoria & Albert Museum
##$LICENSE=By accepting this database user agrees to be bound by the terms of
the IRUG user's license. Any reference...
##$INSTITUTION FILE NAME=DR0008
##DATE=89/05/04
##TIME=13:45:06
##SPECTROMETER/DATA SYSTEM= PERKIN-ELMER 1730
##INSTRUMENT PARAMETERS=apodization: NB(weak); scans: 250; purge: N;
range: 4000-400
##RESOLUTION=8 cm-1
##DATA PROCESSING=CO2 corr.: N; baseline corr: N
##SAMPLE DESCRIPTION= refl; accessories: drift, Barnes Diffuse Reflectance;
support: SiC
##SAMPLING PROCEDURE= refl; prep: surface sampled with Millipore SiC 8 microns.
Direct from SiC, ratioed to blank SiC (background)
##PATHLENGTH=[pathlength (44)
##PRESSURE=[pressure (45)]
##TEMPERATURE=[temperature (46)]
##CAS NAME=[CAS name (47)]
##NAMES= cellulose nitrate
[chemical name (12)]
##MOLFORM=(C6H10O5)x(ONO2)y
##CAS REGISTRY NUMBER=[CAS registry No (49)]
##WISWESSER=[Wiswesser line notation (50)]
##BEILSTEIN LAWSON No=[Beilstein Lawson No (51)]
##MP=[melting pont (52)]
##BP=[boiling point (53)]
##REFRACTIVE INDEX=[refractive index (54)]
##DENSITY=[density (55)]
##MW=[molecular weight (56)]
##CONCENTRATIONS=[concentration (57)]
##STATE=solid; FILM
##CROSS REFERENCE=GC-MS
##$MATERIAL SOURCE=British Museum
##$SOURCE LOCATION=London WC1B 3DG, England, UK
##$SAMPLE IDENTIFIER=
##$COLOUR=transparent
##$AGE=50 years
##$IRUG MATERIALS CLASS=SR
##DELTAX= -1.000000
...
...
##END=
```

Example 3A

JCAMP-DX file as generated by Analect converter.

```
##TITLE=Yellow  refined beeswax , Ross Wax Co.
##JCAMP-DX=4.24
##DATA TYPE=INFRARED SPECTRUM
##ORIGIN=.Winterthur
##OWNER=Winterthur
##SAMPLING DESCRIPTION=Winterthur Museum Analytical Laboratory
##Spectrometer/Data System=Analect Instruments. Analect DS-20
##RESOLUTION=4.0
##DATE=97/07/09
##TIME=10:18:30
##XUNITS=1/CM
##YUNITS=ABSORBANCE
##FIRSTX=4400.762
##LASTX=698.01
##FIRSTY=0.1153
##XFACTOR=1.000000
##YFACTOR=0.000091553
##NPOINTS=2075
##DELTAX=1.92846702
##XYDATA=(X++(Y..Y))
4400.762 1356337920 .....

##END=
```

Example 3B

Same JCAMP-DX file edited to meet IRUG guidelines.

```
##TITLE=IWX05000 Beeswax, refined, yellow, Ross Wax, WM,  tran
##JCAMP-DX=4.24
##DATA TYPE=INFRARED SPECTRUM
##ORIGIN=Winterthur Museum; Winterthur, DE 19735. USA; Janice Carlson; tel:
+1 302 888 4732; fax: +1 302 888 4838; email: jcarls@winterthur.org
##OWNER=COPYRIGHT© 97 by Winterthur Museum
##$LICENSE=By accepting this database user agrees to be bound by the terms of
the IRUG user's license. Any reference...
##$INSTITUTION FILE NAME=WMwax1
##DATE=97/0709
##TIME=10:18:30
##SPECTROMETER/DATA SYSTEM=Analect RFX-65 bench with XAD microscope; DS-20
##INSTRUMENT PARAMETERS=apodization: HG; scans: 200; purge: Y dry air;
range: 4400-700
##RESOLUTION=4 cm-1
##DATA PROCESSING=CO2 corr: N; baseline corr: N; converted from Analect
##SAMPLE DESCRIPTION=tran; accessories: micr; support: dia
##SAMPLING PROCEDURE=tran; prep: scraping
##PATHLENGTH=[pathlength (44]
##PRESSURE=[pressure (45)]
##TEMPERATURE=[temperature (46)]
##CAS NAME=[CAS name (47)]
##NAMES=beeswax, yellow refined
[chemical name (12)]
##MOLFORM=[molecular formula (48)]
##CAS REGISTRY NUMBER=[CAS registry No (49)]
##WISWESSER=[Wiswesser line notation (50)]
##BEILSTEIN LAWSON No=[Beilstein Lawson No (51)]
##MP=[melting pont (52)]
##BP=[boiling point (53)]
##REFRACTIVE INDEX=[refractive index (54)]
##DENSITY=[density (55)]
##MW=[molecular weight (56)]
##CONCENTRATIONS=[concentration (57)]
##STATE=solid; bulk
##CROSS REFERENCE=[additional information (33)]
##$MATERIAL SOURCE=Ross Wax Co.
##$SOURCE LOCATION=New York, USA
##$SAMPLE IDENTIFIER=unknown
##$COLOUR=yellow, pale
##$AGE=unknown
##$IRUG MATERIALS CLASS=WX
##XUNITS=1/CM
##YUNITS=ABSORBANCE
##FIRSTX=4400.762
##LASTX=698.01
...
##END=
```

III G

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IV A

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- Janice Carlson, Winterthur Museum, Gardens and Library, Winterthur, DE, US
- Janet Douglas, Freer Gallery of Art, Smithsonian Institution, Washington, DC, US
- Kate Duffy, Williamstown Art Conservation Center, Williamstown, MA, US
- Kate Helwig, Canadian Conservation Institute, Ottawa, CA
- Herant Khanjian, Getty Conservation Institute, Los Angeles, CA, US
- Susan Lake, Hirshhorn Museum and Sculpture Garden, Smithsonian Institution, Washington, DC, US
- Suzanne Quillen Lomax, National Gallery of Art, Washington, DC, US
- Mitura Mimura, Nara Cultural Research Institute, Nara, JP
- Jennifer Mass, Winterthur Museum, Gardens and Library, Winterthur, DE, US
- Alison Murray, Queens University, Kingston, ONT, CA
- Richard Newman, Museum of Fine Arts, Boston, MA, US
- Mark Ormsby, National Archives and Records, Washington, DC, US
- Marcello Picollo, Institute for Applied Physics "Nello Carrara", CNR, Firenze, IT
- Boris Pretzel, Victoria and Albert Museum, London, UK
- Beth Price, Philadelphia Museum of Art, Philadelphia, PA, US
- Masanori Sato, Nara Cultural Research Institute, Nara, JP
- Renee Stein, Michael C. Carlos Museum, Emory University, Atlanta, GA
- Ken Sutherland, Philadelphia Museum of Art, Philadelphia, PA, US
- David Thickett, English Heritage, London, UK
- Manfred Schreiner, Academy of Fine Arts, Institute of Chemistry, Vienna, AU
- Masahiko Tsukada, National Museum of Western Art, Tokyo, JP
- Siobhan Watts, National Museums and Galleries on Merseyside, Whitechapel, UK
- Raymond White, National Gallery of Art, London, UK
- Scott Williams, Canadian Conservation Institute, Ottawa, CA
- Boris Zhadanov, Grabar Art Conservation Center (Russian Scientific Conservation Center named after Grabar), Moscow, RU

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School of Conservation, Det Kongelige Danske Kunstakademi, Copenhagen, DK
Straus Conservation Center (Fogg), Harvard University Art Museums, Cambridge, US
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VI

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VI A

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Welcome Andrew Lins!

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Please fill in details, attach JCAMP file, check license box, and click "Upload".
Spectral files must be in JCAMP format (.dx or *.jdx)*

* = required field ? = online help

Spectral Analyst Information

Analyst name * ?

Email * ?

Telephone * ?

Fax ?

Choose institution * ?

-- Not Listed --

If institution is not listed

Sample Description

Common/trade name(s) * ?
(place each on separate line)

Chemical name(s) ?
(place each on separate line)

Material class * ?

Select material class...

Color ?

Form * ?

Select...

Physical state * ?

Select...

Other, insert in space below

Additional Info

Material source ? Unknown

Source location ? Unknown

Sample identifier ? Unknown

Sample Age ? Unknown

Concentrations ? (name, concentration, unit)
(place each group on separate line)

Other information

Origin

Spectrometer and detector *
(manufacturer and model) ?

Software * ?
(name and version)

Spectral Range * ?
(in wavenumbers)

to cm^{-1}

Number of scans ?

Apodization ?

Select...

Resolution * ? [ ] cm^{-1} Other, insert in space below [ ]

Instrument purge ? ○ Yes ◉ No

IR Technique

Mode * ? [Select Mode...] Datatype * ? [Infrared]

Accessories, e.g., microscope, fiberoptic ?
(manufacturer, model, and detector, if applicable)

[ ]

Sample support * ?

- ☐ AgCl
- ☐ AgBr
- ☐ BaF2
- ☐ CaF2
- ☐ CdTe
- ☐ CsI
- ☐ Diamond
- ☐ Ge
- ☐ KBr
- ☐ KRS5
- ☐ NaCl
- ☐ Nujol
- ☐ Si
- ☐ SiC
- ☐ ZnS
- ☐ ZnSe
- ☐ Other, insert in space below [ ]

Sample Preparation * ?

- ☐ Extracted
- ☐ Filtered
- ☐ Ground/powdered
- ☐ Mixed w/support matrix
- ☐ Pressed pellet
- ☐ Thin sectioned
- ☐ None (bulk)
- ☐ None (neat)
- ☐ Other... [ ]

Data Processing History

Baseline correction * ? ○ Yes ○ No CO_2 correction * ? ○ Yes ○ No

Other processing details ?
(normalization, background correction,etc.) [ ]

Other Analytical Methods Used ?

- None
- Visible light microscopy
- Fluorescence light microscopy
- Polarized light microscopy
- Scanning electron microscopy
- Energy dispersive spectroscopy
- Wavelength dispersive spectroscopy

(To select multiple items on Windows, ctrl+click, on Mac, cmd-click)

☐ Other, insert in space below [ ]

Sample Details

Molecular weight ? [ ]

Molecular formula ? [ ]

Melting point ? [ ] °C

Boiling point ? [ ] °C

Refractive index ? [ ] 20° C, NaD

Density ? [ ] (g/cm^3)

Path length ? [ ]

Pressure ?
(if different from room conditions) [ ] (include units)

Temperature ?
(if different from room conditions) [ ] °C

CAS name ? [ ]

CAS registry number ? [ ]

Wiswesser line notation ? [ ]

Beilstein Lawson number ? [ ]

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Select JCAMP file from your computer [ ] Browse...

Spectral files must be in JCAMP format (.dx or *.jdx)*

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Files 1 to 10 of (23) Next>> Last>>

Use this page to view, edit, delete, or send submissions to the Review Committee.

Common Name	Filename/ Upload Date	Desired Action
CI Pigment Red 202 XX017732 Pigment Red 202	PMAI4295.JDX Thu, 23 Oct 2003	View Edit Delete Thumbnail... Submit to Review Committee
Heliogen Blau, 27490 Pigment Blue 16	PMAI4344a.jdx Thu, 22 Jan 2004	View Edit Delete Thumbnail... Submit to Review Committee
Heliogen Blau, 27490 Pigment Blue 16	PMAI4344b.jdx Thu, 22 Jan 2004	View Edit Delete Thumbnail... Submit to Review Committee
Cromophthal Violet Pigment Violet 23	PMAI4343a.jdx Thu, 22 Jan 2004	View Edit Delete Thumbnail... Submit to Review Committee
Cromophthal Violet Pigment Violet 23	PMAI4343b.jdx Thu, 22 Jan 2004	View Edit Delete Thumbnail... Submit to Review Committee
Chromophtol Pink FT Pigment Red 122	PMAI4346a.JDX Thu, 22 Jan 2004	View Edit Delete Thumbnail... Submit to Review Committee

Check Submission Status

Submissions 1 to 10 of (35) Next>> Last>>

Common Name	Filename/ Submission Date	Submission Status
CI Pigment Red 202 XX017732 Pigment Red 202 (View Detail) (View Thumbnail...)	PMAI4294.JDX Fri, 23 Jan 2004	Under Review
Chromophtol Pink FT Pigment Red 122 (View Detail) (View Thumbnail...)	PMAI4346a.JDX Fri, 23 Jan 2004	Not Yet Sent to Review Committee
Chromophtol Pink FT Pigment Red 122 (View Detail) (View Thumbnail...)	PMAI4346b.jdx Fri, 23 Jan 2004	Not Yet Sent to Review Committee
CI Pigment Red 202 XX017732 Pigment Red 202 (View Detail) (View Thumbnail...)	PMAI4295.JDX Fri, 23 Jan 2004	Not Yet Sent to Review Committee
Cinquasia Violet Pigment Violet 19 (View Detail) (View Thumbnail...)	PMAI4351a.jdx Fri, 23 Jan 2004	Not Yet Sent to Review Committee
Cinquasia Violet Pigment Violet 19 (View Detail) (View Thumbnail...)	PMAI4351b.jdx Fri, 23 Jan 2004	Not Yet Sent to Review Committee
Cromophthal Violet Pigment Violet 23 (View Detail) (View Thumbnail...)	PMAI4343a.jdx Fri, 23 Jan 2004	Not Yet Sent to Review Committee
Cromophthal Violet Pigment Violet 23 (View Detail) (View Thumbnail...)	PMAI4343b.jdx Fri, 23 Jan 2004	Not Yet Sent to Review Committee

Submission Details

Return to List

Spectral Analyst Information

Name Beth Price Email bprice@philamuseum.org
Telephone 215-684-7552 Fax 215-684-7550
Institution PMA: Philadelphia Museum of Art, Philadelphia, PA, US

Original JCAMP filename: PMAI4294.JDX

Sample Description

Common name	CI Pigment Red 202 XX017732 Pigment Red 202	Chemical name	2,9 Dichloroquinacridone
Material class	OD	Color	Red
Physical state	Solid	Form	Powder

Sample Description

Material source	Bayer
Source location	Tate gallery, London
Sample identifier	CI 73907
Sample age	Unknown
Concentrations	
Other info	

Origin

Instrument	Thermo Nicolet Nexus 670 Spectrometer DTGS	Software	Omnic 6.0a
Spectral range	4000 to 600	Number of scans	200
Resolution	4	Apodization	Happ-Genzel
Instrument purge	1		

IR Technique

Submission Details

Mode	tran	Datatype	INFRARED SPECTRUM
Accessories	Microscope Thermo Nicolet Continuum MCTA		
Sample support	Diamond		
Sample preparation	OtherFlattened with roller tool		

Data Processing History

Baseline correction	○ Yes ◉ No
CO_2 correction	○ Yes ◉ No
Other processing details	

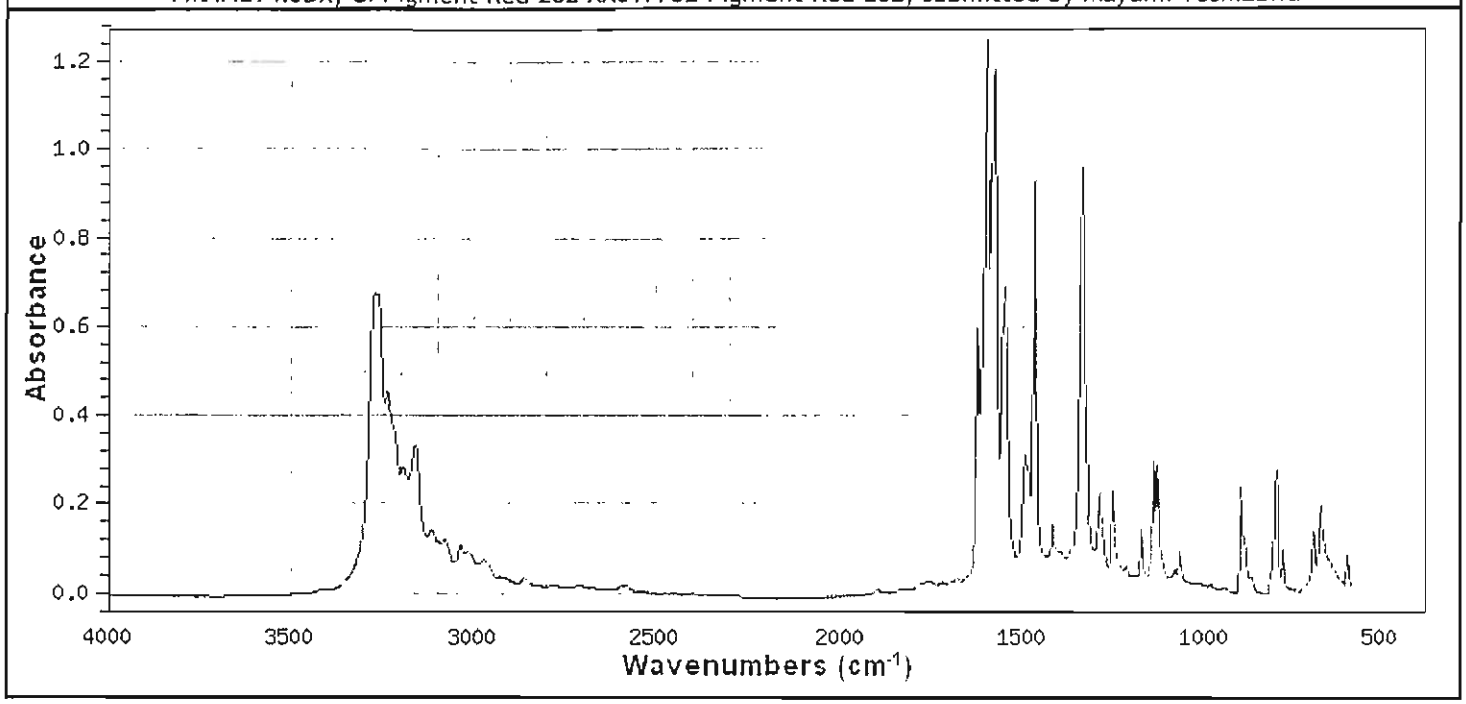
Other Analytical Methods Used

Sample Details

Molecular weight	381.2172	Pressure	
Molecular formula	C20H10Cl2N2O2	Temperature	
Melting point		CAS name	
Boiling point		CAS registry number	3089-17-6
Refractive index		Wisswesser line notation	
Density		Beilstein Lawson number	
Path length			

Return to List

Spectrum Thumbnail
PMAI4294.JDX, CI Pigment Red 202 XX017732 Pigment Red 202, submitted by Mayumi Yoshizawa



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Submission Count
10 NEW!
2 Undecided
0 Decided (Sent to Senior Editors)

Step 1: Review and Evaluate Pending Decisions
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Final Status

View Approved/Returned Submissions 4

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Submissions 1 to 10 of (12) next>> last>>

Sort by: [Common Name] [Submitter Name] [Submitter Institution] [Analyst Institution] [Submit Date]

Organic Dyes, Pigments

Common Name: Sunfast Blue Pigment Blue 15:0
Analyst: Beth Price (PMA)
Submitter/Date: Mayumi Yoshizawa (PMA) Fri, 23 Jan 2004 (Email)
Original Filename: PMAI4271A.JDX

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Common Name: Sunfast Blue Pigment Blue 15:0 NEW!
Analyst: Beth Price (PMA)
Submitter/Date: Mayumi Yoshizawa (PMA) Fri, 23 Jan 2004 (Email)
Original Filename: PMAI4272A.JDX

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Common Name: Sunfast Blue Pigment Blue 15:0 NEW!
Analyst: Beth Price (PMA)
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Common Name: Irgalite Blue PG Pigment Blue 15:3 NEW!
Analyst: Beth Price (PMA)
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Original Filename: PMAI4277.JDX

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Common Name: Irgalite Blue GLVO Pigment Blue 15:4 NEW!
Analyst: Beth Price (PMA)
Submitter/Date: Mayumi Yoshizawa (PMA) Fri, 23 Jan 2004 (Email)
Original Filename: PMAI4268B.JDX

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Analyst: Beth Price (PMA)
Submitter/Date: Mayumi Yoshizawa (PMA) Fri, 23 Jan 2004 (Email)
Original Filename: PMAI4269B.JDX

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Common Name: Irgalite Blue GLVO Pigment Blue 15:4 NEW!
Analyst: Beth Price (PMA)
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Original Filename: PMAI4267A.JDX

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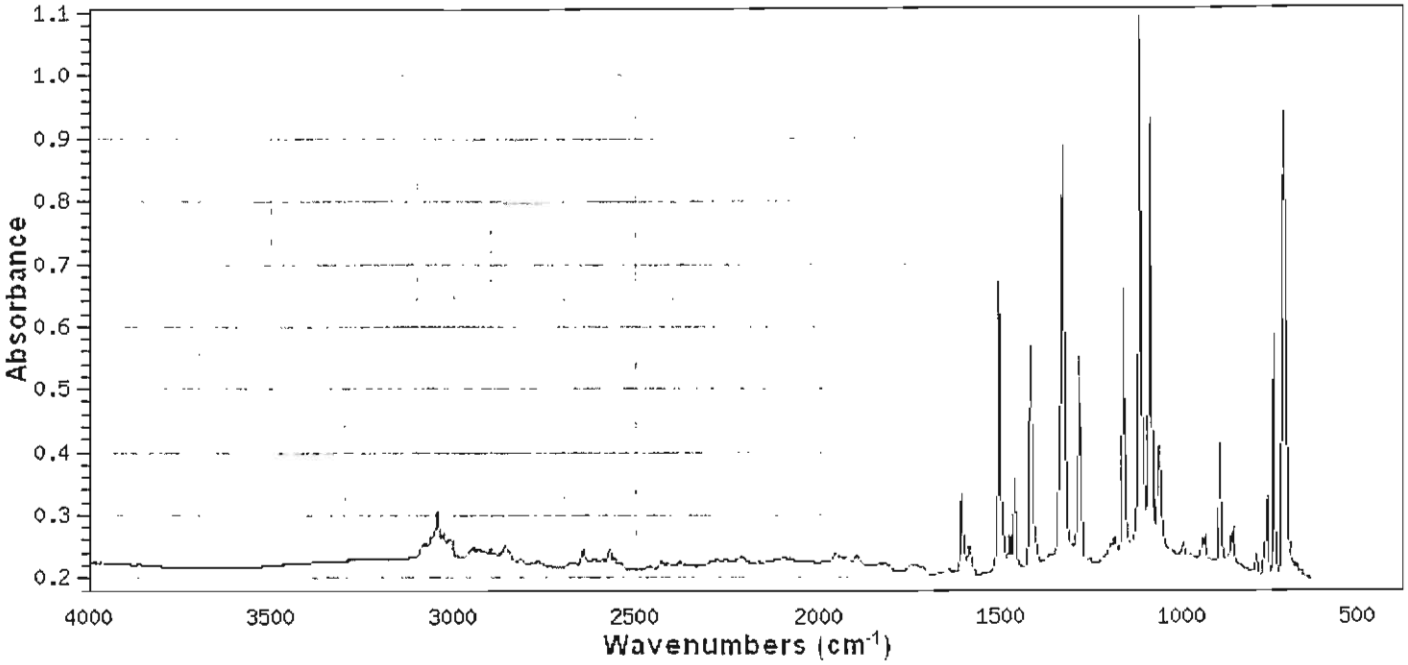
Absorbance
1.1
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
4000
3500
3000
2500
2000
1500
1000
500
Wavenumbers (cm-1)

Review & Evaluate Submissions

Submissions 1 to 10 of (12) next>> last>>

Sort by: [Common Name] [Submitter Name] [Submitter Institution] [Analyst Institution] [Submit Date]

Organic Dyes, Pigments

Common Name: Sunfast Blue Pigment Blue 15:0
Analyst: Beth Price (PMA)
Submitter/Date: Mayumi Yoshizawa (PMA) Fri, 23 Jan 2004 (Email)
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Common Name: Irgalite Blue PG Pigment Blue 15:3 NEW!
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Common Name: Irgalite Blue GLVO Pigment Blue 15:4 NEW!
Analyst: Beth Price (PMA)
Submitter/Date: Mayumi Yoshizawa (PMA) Fri, 23 Jan 2004 (Email)
Original Filename: PMAI4269B.JDX

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Common Name: Irgalite Blue GLVO Pigment Blue 15:4 NEW!
Analyst: Beth Price (PMA)
Submitter/Date: Mayumi Yoshizawa (PMA) Fri, 23 Jan 2004 (Email)
Original Filename: PMAI4267A.JDX

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Raw JCAMP-DX
Filename: PMAI4271A.JDX
Submitted by: Mayumi Yoshizawa
Download this file...

```
##TITLE=PMAI4271 Sunfast Blue PB 15:0 Sun blue powder on dc, MCTA det
##JCAMP-DX=4.24  $$ Nicolet v. 1
##DATATYPE=INFRARED SPECTRUM
##ORIGIN=Philadelphia Museum of Art
##OWNER=Nicolet
##DATE=103/07/28
##TIME=14:24:04
##DATA PROCESSING=
Ratio against background
%Transmittance->Absorbance
Truncated
ElementMultiply or ElementDivide
##XUNITS=1/CM
##YUNITS=ABSORBANCE
##FIRSTX=649.903992
##LASTX=3999.705811
##FIRSTY=0.198269
##MAXX=3999.705811
##MINX=649.903992
##MAXY=1.095191
##MINY=0.197945
##XFACTOR=1.000000
##YFACTOR=1.000000E-008
##NPOINTS=1738
##DELTAX=1.928499
##XYDATA=(X++(Y..Y))
649.904 19826894 19794508 19872556 19900218 19968312 20027800 20104660
663.404 20123514 20230332 20277946 20395124 20421460 20511310 20652590
676.903 20932460 21077626 21043904 20975738 21260770 21822338 22264364
690.403 22017812 21746978 21747542 21981824 22204668 22396270 22561138
703.903 22888804 23250816 23863370 24760146 26499096 29455260 34845432
717.402 46704372 69445416 89955656 94143304 89378672 78399064 63128144
730.902 47798308 34600428 26061544 22002626 20644486 20592044 21292452
744.402 22400962 23895914 25416428 29057190 41626736 58811760 44323188
757.902 26372606 21257350 20859172 21445576 22983432 27328706 32991060
771.401 31677106 27240354 25878906 25481820 24503114 23340982 22232158
784.901 21224870 20729566 20499340 20486438 20522882 20643600 20889216
798.401 21685554 22925394 23568014 22801818 21662838 21074892 20924086
811.900 20892490 20913818 20970964 21014468 21047234 21122854 21177386
825.400 21238630 21315164 21384502 21418216 21445178 21516574 21627006
838.900 21704768 21752938 21829118 21895782 21974504 22042506 22146920
852.399 22253426 22352220 22443882 22681014 23547406 26225644 27994218
865.899 26367360 25646096 26624442 26569768 24906952 23869166 23566366
879.399 23447556 23184652 22980056 22881488 22881440 22985456 23275788
892.898 23931984 25412410 28856928 35885776 41172788 34902476 26949040
906.398 23863850 23037836 22816734 22712206 22684274 22652488 22677068
919.898 22681498 22688540 22689130 22738930 22787906 22832426 22847120
933.398 22901772 22997786 23420604 25062088 26712012 25853136 25124008
946.897 25533494 26178756 25912708 24805310 23979966 23540848 23278478
960.397 23135022 23037080 22998150 22998334 23075092 23240192 23369010
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Organic Dyes, Pigments

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Analyst: Beth Price (PMA)
Submitter/Date: Mayumi Yoshizawa (PMA) Fri, 23 Jan 2004 (Email)
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Common Name: Sunfast Blue Pigment Blue 15:0 NEW!
Analyst: Beth Price (PMA)
Submitter/Date: Mayumi Yoshizawa (PMA) Fri, 23 Jan 2004 (Email)
Original Filename: PMAI4272A.JDX

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Common Name: Sunfast Blue Pigment Blue 15:0 NEW!
Analyst: Beth Price (PMA)
Submitter/Date: Mayumi Yoshizawa (PMA) Fri, 23 Jan 2004 (Email)
Original Filename: PMAI4273B.JDX

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Common Name: Irgalite Blue PG Pigment Blue 15:3 NEW!
Analyst: Beth Price (PMA)
Submitter/Date: Mayumi Yoshizawa (PMA) Fri, 23 Jan 2004 (Email)
Original Filename: PMA'4277.JDX

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Common Name: Irgalite Blue GLVO Pigment Blue 15:4 NEW!
Analyst: Beth Price (PMA)
Submitter/Date: Mayumi Yoshizawa (PMA) Fri, 23 Jan 2004 (Email)
Original Filename: PMAI4268B.JDX

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Common Name: Irgalite Blue GLVO Pigment Blue 15:4 NEW!
Analyst: Beth Price (PMA)
Submitter/Date: Mayumi Yoshizawa (PMA) Fri, 23 Jan 2004 (Email)
Original Filename: PMAI4269B.JDX

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Common Name: Irgalite Blue GLVO Pigment Blue 15:4 NEW!
Analyst: Beth Price (PMA)
Submitter/Date: Mayumi Yoshizawa (PMA) Fri, 23 Jan 2004 (Email)
Original Filename: PMAI4267A.JDX

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Title | Institution | Instrument | Sampling Details | Sample Details | Spectral Information | Summary

Title Details: Sunfast Blue Pigment Blue 15:0 (id: 1121)

Submission Status: *Under Review*

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Raw JCAMP:

##TITLE = PMAI4271 Sunfast Blue PB 15:0 Sun blue powder on dc, MCTA det

Submitter Input

Common/trade name(s)

Sunfast Blue Pigment Blue 15:0

Material source

Sun

Sample identifier

CI 74160

Institution

(PMA)

Raw JCAMP:

##DATATYPE = *LDR contained no data or was not present.*

##$IRUG_Material_Class = *LDR contained no data or was not present.*

Submitter Input

Datatype:

INFRARED SPECTRUM

Material class:

OD

Raw JCAMP:

##JCAMP-DX = 4.24 $$ Nicolet v. 1

Next ▷

Title | Institution | Instrument | Sampling Details | Sample Details | Spectral Information | Summary

Institution Details: Sunfast Blue Pigment Blue 15:0 (id: 1121)

Submission Status: *Under Review*

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Raw JCAMP:
##ORIGIN = Philadelphia Museum of Art
##OWNER = Nicolet
##$Institution File Name = *LDR contained no data or was not present.*

Submitter Input

Anaylyst name
Beth Price
Email
bprice@philamuseum.org
Telephone
215-684-7552
Fax
215-684-7550
Institution filename
PMAI4271A.JDX

Raw JCAMP:
##DATE = 103/07/28 ##TIME = 14:24:04

Previous | Next

Title | Institution | Instrument | Sampling Details | Sample Details | Spectral Information | Summary

Instrument Details: Sunfast Blue Pigment Blue 15:0 (id: 1121)

Submission Status: *Under Review*

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Raw JCAMP:
##SPECROMETER/DATA SYSTEM = *LDR contained no data or was not present.*

Submitter Input

Instrument and detector:
Thermo Nicolet Nexus 670 Spectrometer DTGS

Software:
Omnic 6.0a

Raw JCAMP:
##INSTRUMENT PARAMETERS = *LDR contained no data or was not present.*
##RESOLUTION =

Submitter Input

Apodization
Happ-Genzel

Number of scans:
200

Instrument purge:
1

Spectral range:
From:4000 to: 600cm^{-1}

Resolution:
4

Raw JCAMP:
##DATA PROCESSING= Ratio against background %Transmittance->Absorbance Truncated ElementMultiply or ElementDivide

Submitter Input

Baseline correction
No

CO2 correction
No

Other processing details
Submitter did not supply

◁ Previous | Next ▷

Title | Institution | Instrument | Sampling Details | Sample Details | Spectral Information | Summary

Sampling Details: Sunfast Blue Pigment Blue 15:0 (id: 1121)

Submission Status: *Under Review*

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Raw JCAMP:
##SAMPLE DESCRIPTION= *LDR contained no data or was not present.*

Submitter Input

Accessories (and detector, if applicable): Microscope Thermo Nicolet Continuum MCTA

Sample support: Diamond

Raw JCAMP:
##SAMPLING PROCEDURE= *LDR contained no data or was not present.*
##PATH LENGTH = *LDR contained no data or was not present.*
##PRESSURE = *LDR contained no data or was not present.*
##TEMPERATURE = *LDR contained no data or was not present.*

Submitter Input

Path length: *Submitter did not supply*

Pressure: *Submitter did not supply*

Temperature: *Submitter did not supply*

Mode: tran

Sample preparation: Other, Flattened with roller tool

Previous | Next

Title | Institution | Instrument | Sampling Details | Sample Details | Spectral Information | Summary

Sample Details: Sunfast Blue Pigment Blue 15:0 (id: 1121)

Submission Status: *Under Review*

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Raw JCAMP:
##NAMES = *LDR contained no data or was not present.*
##CAS NAME = *LDR contained no data or was not present.*
##CAS REGISTRY No = *LDR contained no data or was not present.*

Submitter Input

Common/trade name(s)
Sunfast Blue Pigment Blue 15:0

CAS name(s)
Submitter did not supply

Chemical name(s)
Copper Phthalocyanine

CAS registry number
Submitter did not supply

Raw JCAMP:
##MOLFORM = *LDR contained no data or was not present.*
##MW = *LDR contained no data or was not present.*
##WISWESSER = *LDR contained no data or was not present.*
##BEILSTEIN LAWSON = *LDR contained no data or was not present.*

Submitter Input

Molecular formula
C32H16CuN8

Molecular weight
576.07

Wiswesser line notation
Submitter did not supply

Beilstein Lawson number
Submitter did not supply

Raw JCAMP:
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##BP = *LDR contained no data or was not present.*
##DENSITY = *LDR contained no data or was not present.*
##REFRACTIVE INDEX = *LDR contained no data or was not present.*
##$Age =
##$Color =
##STATE =

Submitter Input

Melting point
Submitter did not supply

Boiling point
Submitter did not supply

Density
1.6

Refractive index
1.38

Age
Unknown

Color
Blue

Physical state
Solid

Form
Powder, Powder

Raw JCAMP:
##CONCENTRATIONS = *LDR contained no data or was not present.*
##CROSS REFERENCE =

Submitter Input
Concentrations
Submitter did not supply
Other analytical methods used
Submitter did not supply

Raw JCAMP:
##$Material Source =
##$Source Location =
##$Sample Identifier =

Submitter Input
Material source
Sun
Source location
Tate Gallery, London
Sample identifier
CI 74160

Previous | Next

Title | Institution | Instrument | Sampling Details | Sample Details | Spectral Information | Summary

Spectral Details: Sunfast Blue Pigment Blue 15:0 (id: 1121)

Submission Status: *Under Review*

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Raw JCAMP:

##DELTAX =1.928499
##XFACTOR = 1.000000
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##LASTX = *LDR contained no data or was not present.*
##MINX = 649.903992
##MAXX = *LDR contained no data or was not present.*
##NPOINTS =1738
##YFACTOR = 1.000000E-008
##FIRSTY = 0.198269
##MINY = *LDR contained no data or was not present.*
##MAXY = *LDR contained no data or was not present.*

Raw JCAMP:

##XYDATA =

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663.404 20123514 20230332 20277946 20295124 20421460 20511310 20652590
676.903 20932460 21077626 21043904 20975738 21260770 21822338 22264364
690.403 22017812 21746978 21747542 21981824 22204668 22396270 22561138
703.903 22889804 23250816 23863370 24760146 26499096 29455260 34845432
717.402 46704372 69445416 89955656 94143304 89378672 78399064 63128144
730.902 47798308 34600428 26061544 22002626 20644480 20592044 21292452
744.402 22400962 23895914 25416428 29057190 41626730 59811760 44323188
757.902 26372606 21257350 20859172 21445576 22983432 27328706 32991060
771.401 31677106 27240354 25878906 25481820 24503114 23240982 22232158
784.901 21224870 20729566 20499340 20486428 20522842 20642600 20889216
798.401 21685554 22325394 23568014 22601818 21662838 21074892 20924086
811.900 20892490 20913818 20970964 21014468 21047234 21122854 21177386
825.400 21238630 21315164 21384502 21418216 21445178 21516574 21627006
838.900 21704768 21752928 21829118 21895782 21974504 22042506 22146920
852.399 22253426 22352220 22443882 22681014 22547406 26225644 27994218
865.899 26367360 25646096 26624442 26569768 24906952 23869166 23566366
879.399 23447556 23184652 22980056 22881488 22881440 22985456 23275798
892.898 23931984 25412410 28456928 35885776 41172788 34902476 26949040
906.398 23863850 23037826 22816734 22712206 22684274 22652489 22677068
919.898 22681498 22688540 22689130 22738930 22787906 22832426 22847120
933.398 22901772 22997786 23420604 25062088 26712012 25853136 25124008
946.897 25532494 26178756 25912706 24805310 23979906 23540848 23278478
960.397 23125022 23037080 22998150 22998334 23075092 23240192 23369010
973.897 23360074 23279056 23471164 23621356 23681784 23592828 23451572
987.396 23379066 23370462 23391830 23455768 23673214 24101242 24788836
1000.896 25382248 25269166 24654914 24170082 23930434 23798224 23683310
1014.396 23605804 23576192 23590694 23627508 23712304 23810324 23883934
1027.895 23956976 24077228 24211464 24293722 24332472 24396724 24468392
1041.395 24507574 24558754 24618142 24724048 24999378 25393414 25900754
1054.894 26550472 27353260 28410844 29955086 32256678 35324316 39674216
1068.394 40851064 40386592 37580372 33958288 30877626 29028952 28422646
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1108.891	32843796	35989268	41001056	49671216	66282092	92633224	109519056
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1135.889	27088892	26400850	26052398	25807610	25585920	25424424	25374314
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1702.859	20601984	20700246	20830628	20977898	21154362	21322584	21379062
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1986.343	22541432	22568308	22579994	22530644	22473410	22421102	22420054
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2310.326	22153612	22094990	22063204	22037252	22012798	22009230	22012282
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2350.823	21976916	21976650	21940900	21907916	21885154	21900084	21930782
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2566.812	23039176	23331762	23665154	24336752	24430476	24148210	23641128
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2620.809	23016028	22916046	22777670	22713170	22722760	22765836	22713040
2634.308	22751654	22750648	22739892	22850960	22851120	22898730	22812474
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2661.307	22225854	22161290	22136302	22149786	22183520	22254490	22324644
2674.806	22408698	22451598	22426448	22398426	22401088	22413916	22401424
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2701.804	21764960	21726814	21686808	21642270	21592370	21562756	21571054
2715.304	21587864	21594406	21577030	21557676	21550350	21563836	21586592
2728.803	21621204	21649138	21696056	21760560	21865178	21910282	21911246
2742.302	21881798	21835368	21811300	21820844	21854878	21915560	22001480
2755.802	22080960	22161138	22245748	22317036	22390250	22465960	22553768
2769.301	22685186	22774250	22754110	22657142	22556284	22484724	22423830

2782.600	22374808	22377110	22293720	22259002	22240582	22248880	22267974
2796.299	22285790	22305864	22313402	22317592	22343836	22378396	22415220
2809.799	22473712	22536880	22736418	22852498	22939670	22944278	22905194
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2836.797	22700918	22801114	22914614	23077336	23306546	23616060	23939494
2850.296	24168792	24251592	24211944	24449644	24692454	24966996	25107480
2863.796	25094968	24787120	24541398	24373884	24228492	24104148	23950468
2877.295	23804178	23697362	23627066	23621454	23673710	23766822	23866812
2890.794	23908060	23904872	23892620	23920514	24031446	24228678	24405644
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2917.793	24208448	24277450	24201442	24308328	24316602	24358060	24444148
2931.292	24561830	24651792	24622872	24464982	24295684	24233292	24323794
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3025.787	26244992	26925160	27084360	26883110	26536368	26347268	26421022
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3052.785	27908250	27071756	26685298	26587078	26570294	26502668	26204526
3066.285	25995738	25633178	25329402	25156486	25121808	25171196	25268474
3079.784	25395420	25467146	25433118	25312766	25174568	25005054	24735900
3093.283	24397360	24066074	23794410	23605194	23163792	23351438	23251746
3106.782	23188976	23185154	23176740	23140916	23126886	23145698	23141088
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3133.781	23092372	23072596	23064936	23065070	23062066	23045384	23046870
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3160.780	23067098	23072516	23074984	23063034	23070380	23095410	23091204
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3282.273	22809090	22823118	22794098	22756238	22773386	22802224	22783638
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3309.271	22768784	22752992	22717310	22698716	22716952	22758352	22749736
3322.771	22706664	22692404	22701092	22720746	22717594	22681458	22646312
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3430.765	22332020	22307862	22298818	22302580	22291584	22278544	22277976
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3606.255	21661270	21625412	21594596	21603356	21615342	21640194	21655590
3619.755	21665474	21689386	21679000	21652334	21612350	21627476	21648224

3633.254	21611298	21602244	21616142	21629680	21645806	21630836	21616164
3646.753	21616854	21614658	21650288	21681068	21630266	21628008	21666502
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3754.747	21660510	21667074	21682456	21709264	21747472	21740008	21762096
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3943.737	22344698	22363556	22372642	22377148	22398094	22426670	22440362
3957.236	22442434	22463582	22455462	22470068	22487860	22466940	22445042
3970.736	22438642	22437876	22455726	22448896	22424508	22457394	22492176
3984.235	22483726	22469002	22465542	22462130	22460440	22471242	22515524
3997.734	22513626	22491416					

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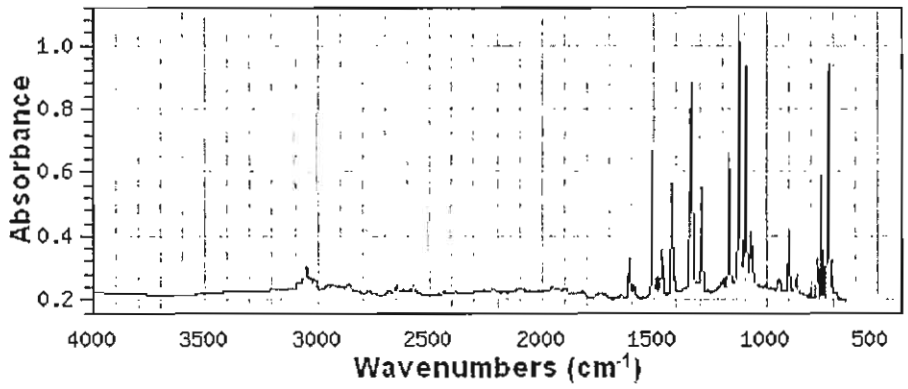
Title | Institution | Instrument | Sampling Details | Sample Details | Spectral Information | Summary

Summary Details: Sunfast Blue Pigment Blue 15:0 (id: 1121)

Submission Status: *Under Review*

Spectrum Thumbnail



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My Comments267

My Decision

- Accept as is
- Accept with minor revision
- Return for revision/resubmission

Reason:

Register My Decision

I have NOT decided yet.

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0 Decided (Sent to Senior Editors)

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3 Undecided
6 Decided (Sent to Senior Editors)

Step 1: Review and Evaluate Pending Decisions
Step 2: List Decided Submissions Sent to Senior Editor

Senior Editor Software

Submission Count
22 NEW!
0 Undecided
9 Decided

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Reviewer Decisions

<<First <<Previous Submissions 11 to 20 of (22) Next>> Last>>
Page: 2 3 4
Sort by: [Common Name] [Submitter Name] [Submitter Institution] [Analyst Institution] [Submit Date]

Organic Dyes, Pigments

Common Name: Irgalite Blue BSNF Pigment Blue 15:2 NEW!
Analyst: Beth Price (PMA)
Submitter: Mayumi Yoshizawa (PMA) Fri, 23 Jan 2004 (Email)
Original Filename: PMAI4274b.JDX
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Common Name: Irgalite Blue BSNF Pigment Blue 15:2 NEW!
Analyst: Beth Price (PMA)
Submitter: Mayumi Yoshizawa (PMA) Fri, 23 Jan 2004 (Email)
Original Filename: PMAI4275b.JDX
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Common Name: Irgalite Blue BSNF Pigment Blue 15:2 NEW!
Analyst: Beth Price (PMA)
Submitter: Mayumi Yoshizawa (PMA) Fri, 23 Jan 2004 (Email)
Original Filename: PMAI4276a.JDX
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Common Name: Irgalite Blue GLVO Pigment Blue 15:4 NEW!
Analyst: Beth Price (PMA)
Submitter: Mayumi Yoshizawa (PMA) Fri, 23 Jan 2004 (Email)
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Common Name: Irgalite Blue GLVO Pigment Blue 15:4 NEW!
Analyst: Beth Price (PMA)
Submitter: Mayumi Yoshizawa (PMA) Fri, 23 Jan 2004 (Email)
Original Filename: PMAI4268B.JDX
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Common Name: Irgalite Blue GLVO Pigment Blue 15:4 NEW!
Analyst: Beth Price (PMA)
Submitter: Mayumi Yoshizawa (PMA) Fri, 23 Jan 2004 (Email)
Original Filename: PMAI4269B.JDX
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Common Name: Irgalite Blue PG Pigment Blue 15:3 NEW!
Analyst: Beth Price (PMA)
Submitter: Mayumi Yoshizawa (PMA) Fri, 23 Jan 2004 (Email)
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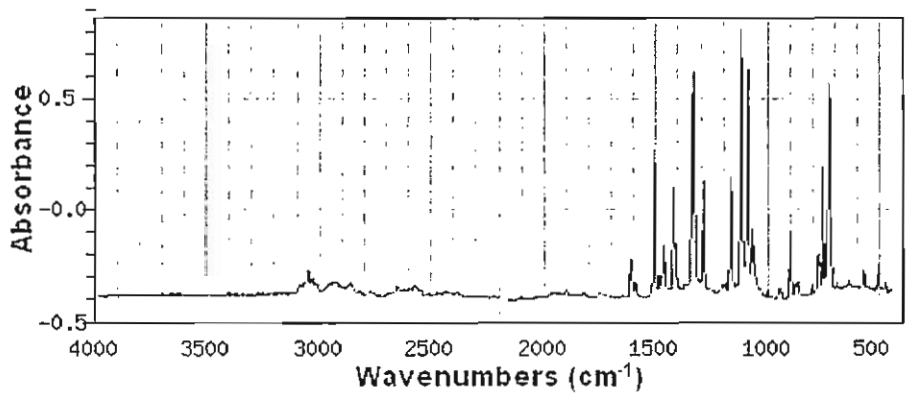
Spectrum Thumbnail



Common/Trade Name(s): Irgalite Blue BSNF Pigment Blue 15:2
Material Class: Organic Dyes, Pigments
Filename: PMAI4274b.JDX
Submitted by: Mayumi Yoshizawa

My Decision

- Accept as is
- Accept with minor revision
- Return for revision/resubmission

Register My Decision

I have NOT decided yet.

Reason:

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Decisions	Field Comments
By: Boris Pretzel Vote: Return for revision/resubmission Duped	No editor has given comment on this spectrum.

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Submissions 1 to 6 of (6)

Sort by: [Common Name] [Submitter Name] [Submitter Institution] [Analyst Institution] [**Submit Date**]

Carbohydrates

Common Name: ad Returned
Analyst: malcolm price (PMA)
Submitter/Date: malcolm price (PMA) Fri, 7 Nov 2003 (Email)
Original Filename: PMAI1078.JDX

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Common Name: dfs Returned
Analyst: malcolm price (XXX)
Submitter/Date: malcolm price (PMA) Thu, 6 Nov 2003 (Email)
Original Filename: animalglue.JDX

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Common Name: asfd Returned
Analyst: malcolm price (XXX)
Submitter/Date: malcolm price (PMA) Thu, 6 Nov 2003 (Email)
Original Filename: ABSORB.JDX

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Common Name: gummi6 Returned
Analyst: Janice Carlson (WM)
Submitter/Date: Janice Carlson (XXX) Mon, 13 Oct 2003 (Email)
Original Filename: #10 Resin Acacia Pycnantha Benth.-2.DX

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Common Name: ONE MO' TIME Returned
Analyst: ONE MO' TIME (UI)

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- RE: institution name (11/10/2003 9:26:52 AM)
  - RE: (11/10/2003 9:27:22 AM)
- RE: This spectrum (10/10/2003 8:10:51 AM)
- RE: (10/9/2003 11:15:00 PM)

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Approved Spectra 1 to 4 of 4

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Carbohydrates

Common Name: gummi gum3
Analyst: Janice Carlson (WM)
Submitter/Date: Janice Carlson (XXX) Mon, 13 Oct 2003 (Email)
Original Filename: #2 Acacia dealbata.DX

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Common Name: gummi gum 4
Analyst: Janice Carlson (WM)
Submitter/Date: Janice Carlson (XXX) Mon, 13 Oct 2003 (Email)
Original Filename: #4 Acacia ferruginea Dc.DX

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Natural Resins

Common Name: gummi gum 5
Analyst: Janice Carlson (WM)
Submitter/Date: Beth Price (PMA) Mon, 13 Oct 2003 (Email)
Original Filename: #26 Butea frondosa.DX

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Unclassifed

Common Name: sdg
Analyst: Beth Price (PMA)
Submitter/Date: Ken Ehrman (PMA) Thu, 2 Oct 2003 (Email)
Original Filename: PMAI4269B.JDX

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- ☐ Synthetic Resins
- Glass
- Unclassified

- [ ] Minerals, Inorganic Pigments
- [ ] Mixtures
- [ ] Natural Resins
- [ ] Oils, Fats
- [ ] Organic Dyes, Organic Pigments
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- ☐ Glass
- ☐ Minerals, Inorganic Pigments
- ☐ Mixtures
- ☐ Natural Resins
- ☐ Oils, Fats
- ☐ Organic Dyes, Organic Pigments
- ☐ Synthetic Resins
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- Synthetic Resins
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Book Title: Infrared Analysis of Essential Oils
Page number(s) 147; Spec. 203-214
Author(s): Juana Bellanato, Antonio Hidalgo
Publisher: Heyden & Sons Ltd.
Place of publication: London
Year of publication: 1971

Subject matter: Oils, Fats
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Author(s): C. J. Pouchert
Edition: 3rd
Publisher: Aldrich Chemical Company
Place of publication: Milwaukee
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Article title: Analysis of Aged Paint Binders by FTIR Spectroscopy
Journal Title: Studies in Conservation
Page number(s) 33-51
Author(s): Raymond J. Meilunas, James G. Bentson, Arthur Steinberg
Issue number: 35
Year of publication: 1990

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Page number(s) 204-243
Author(s): David N. Kendall

Subject matter: Synthetic Resins, Natural Resins
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Editor(s): Donatas Satas
Edition: 2nd
Publisher: Van Nostrand Reinhold
Place of publication: New York
Year of publication: 1989

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Article title: **Application of FTIR Microspectroscopy to the Identification of Naturally Occurring Minerals in Works of Art**
Book Title: **Art '96**
Conference title **5th International Conference on Non-Destructive Testing, Microanalytical Methods and Environmental Evaluation for Study and Conservation of Works of Art**
Page number(s) 513-532
Author(s): Beth A. Price, Janice H. Carlson, Richard Newman, et al.
Publisher: Hungarian Chemical Society
Place of publication: Budapest
Year of publication: 1996

Subject matter:
Minerals, Inorganic Pigments
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Book Title: Infrared Analysis of Essential Oils
Page number(s) 147; Spec. 203-214
Author(s): Juana Bellanato, Antonio Hidalgo
Publisher: Heyden & Sons Ltd.
Place of publication: London
Year of publication: 1971

Subject matter: Oils, Fats
Citation type: Article in book
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Book Title: Aldrich Library of Infrared Spectra, The
Author(s): C. J. Pouchert
Edition: 3rd
Publisher: Aldrich Chemical Company
Place of publication: Milwaukee
Year of publication: 1981

Subject matter: General Materials
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Search Edition 2000
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On-Line Help
List All Online Help

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Prepared by

Beth Price
Philadelphia Museum of Art

Boris Pretzel
Victoria & Albert Museum

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Richard Newman

JCAMP-DX Spectral File Format for Submissions to the Infrared & Raman Users Group (IRUG) Database

Boris Pretzel, Victoria & Albert Museum
Beth Price, Philadelphia Museum of Art
Janice Carlson, Winterthur Museum, Garden & Library

Abstract *(Updated 25 February 2002)*

This paper presents guidelines for the submission of spectra in the JCAMP-DX format to the IRUG (Infrared and Raman Users Group) Database. JCAMP-DX was chosen as the file format as it is platform independent and will allow error-free transfer of spectral information between various instruments and users. IRUG will use the JCAMP-DX files as the principal source of information for submitted spectra. All information pertaining to the sample and spectrum (as outlined on the IRUG Spectrum Submission Form) is incorporated into the JCAMP-DX file in a consistent format to create a complete data record. This format, consisting of both JCAMP-DX 4.24 and user (IRUG) defined labelled data-records (LDRs), is described. The LDRs for IRUG have been kept to a minimum to facilitate automatic transfer of the information when the IRUG JCAMP-DX files are imported into the users' infrared software packages.

Click here to read the full paper

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VII

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12559: ## CAS REGISTRY No

12739: ##$Age

12727: ##$Color

12319: ##$Institution Filename

12751: ##$IRUG Material Class

12307: ##$License

12691: ##$Material Source

12715: ##$Sample Identifier

12703: ##$Source Location

12583: ##BEILSTEIN LAWSON NO

---

1 to 10 of 131 Next >> Last

Page: [1] 2 3 4 5 6 7 8 9 10 11 12 13 14

On-Line Help Article Detail

Welcome Beth Price!

Title: (id=12403) Labeled-data records (LDR)

Article Text:

JCAMP-DX files consist of a series of linked labeled-data records (or fields) known as LDRs. Each LDR is one or more lines in an ASCII file beginning with a data label name (label) followed by corresponding information and data (each line has an 80 character limit).

For JCAMP files to function properly, the first three LDRs must be in this order: ##TITLE=, ##JCAMP-DX=, ##DATA TYPE=, and the final LDR must be ##END=. The order of all other LDRs is not critical and various JCAMP converters may order LDRs differently.

In IRUG spectral files LDRs are grouped as follows: compulsory (title, JCAMP version, data type), submitting institution details, instrument details, sampling details, sample details, additional IRUG sample details, and spectral information.

Article Location:

Edit this Article | Return to List

On-Line Help Article Detail

Welcome Beth Price!

Title: (id=12127)	Temperature
Article Text:	Sample temperature during acquisition of data in degrees Celsius (°C) if significantly different from room temperature.
Article Location:	Upload New Spectral File, Editor

Edit this Article | Return to List

On-Line Help Article Detail

Welcome Beth Price!

Title: (id=11647)	Chemical name (11)
Article Text:	Scientific name that clearly identifies a material. Examples: calcium sulfate dihydrate, poly (methyl acrylate-ethyl methacrylate) copolymer. Multiple chemical names must be entered on separate lines. Example: methyl palmitate palmitic acid methyl ester hexdecanoic methyl ester
Article Location:	Upload New Spectral File, Editor

Edit this Article | Return to List

VI J

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Step 1: Begin New Submission
Step 2: Check and Send Submissions to Review Comittee
Step 3: Check Submission Status

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Username:
bprice

First Name: Beth *

Last Name: Price *

Email: bprice@philamuseum.org *

Institution: Philadelphia Museum of Art... *

Job Title: Senior Scientist *

Address:
Conservation Department
Box 7646 *

City/Town/Village: Philadelphia *

State/Province: PA *

Postal Code: 19101 *

Country: US: UNITED STATES *

Telephone: +1 215 684 7552 *

Fax: +1 215 684 7550

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New Password

Re-type Password

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-contain only letters and numbers, and
-contain at least one number.

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VII

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- Infrared and Raman Users Group (IRUG) Spectral Database - Edition 2000

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- About Us
  - Mission
  - History
  - Conferences
  - Board
  - Participation
- Spectral Database
  - About the Database
  - Search Edition 2000
  - Edition 2000 Index
  - Contributing Individuals
  - Contributing Institutions
  - JCAMP Paper
  - Feedback
- Bibliography
  - About the Bibliography
  - Search the Bibliography
  - Feedback
- Credits
  - Current Review Committee
  - Contributing Individuals
  - Contributing Institutions
  - Support
- Site Services
- Links
- Site Info
  - Frequently Asked Questions (FAQ)
  - Feedback
  - Privacy
  - Technical Requirements
  - Site Map

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- Home
- About Us
  - Mission
  - History
  - Conferences
  - Board
  - Participation
- Spectral Database
  - About the Database
  - Search Edition 2000
  - Edition 2000 Index
  - Contributing Individuals
  - Contributing Institutions
  - JCAMP Paper
  - Feedback
- Bibliography
  - About the Bibliography
  - Search the Bibliography
  - Feedback
- Credits
  - Current Review Committee
  - Contributing Individuals
  - Contributing Institutions
  - Support
- Site Services
- Links
- Site Info
  - Frequently Asked Questions (FAQ)
  - Feedback
  - Privacy
  - Technical Requirements
  - Site Map