Институт физики СО РАН им. Л.В. Киренского, Красноярск

Обзор сетевых ресурсов и примеры их практического применения при исследованиях методом комбинационного рассеяния света

Светлана Крылова

Третий сибирский семинар
«Спектроскопия комбинационного рассеяния света»

Доступная информация

- Базы данных
- Кристаллографический сервер Bilbao
- Web of knowledge:

ü *Web of Science*

ü *Additional resources*

Journal Citation Reports

Researcher ID

Базы данных

Название базы	Описание	Кол.спектров
RUFF http://rruff.info/all/	Объединенная база (США, Франция, Бразилия, Канада, Россия) Raman, IR, X-ray,	>3,055 Bob Downs, Director rdowns@u.arizona.edu
UCL pigment library http://www.chem.ucl.ac.uk/resources/raman/	Спектры синт. и натуральных пигментов (Англия) Черные, синие, зеленые, оранжевые, красные, белые, желтые.	56
Handbook of Minerals Raman Spectra http://www.ens-lyon.fr/LST/Raman/index.php	Спектры минералов, синтетических веществ, стекол. (Франция)	>60 Form for send spectra
University of Parma mineral data base http://www.fis.unipr.it/phevix/ramandb.php	Спектры минералов. (Италия)	>100
Minerals and Chemicals http://wwwobs.univ-bpclermont.fr/sfmc/ramandb2/index.html	Спектры минералов и химические вещества. (Франция)	542
The Goblentz Society Spectral Data Collections http://www.coblentz.org/links/spectral-data-collections **SDBS - Database for Organic Compounds** http://riodb01.ibase.aist.go.jp/sdbs/cgi-bin/cre_index.cgi?lang=end **Mineral Spectroscopy Server** http://minerals.gps.caltech.edu/FILES/Index.html	Органические вещества. (Общ. приклад. спектроскопии) MS, IR, ^{13C}NMR, Raman, ^{1H}NMR, ESR	3573 орган. веществ
RASMIN http://riodb.ibase.aist.go.jp/rasmin/E_index.htm	Спектры минеральных и неорганических материалов. (Япония)	576 минералов 1022 Неор. веществ

RUFF

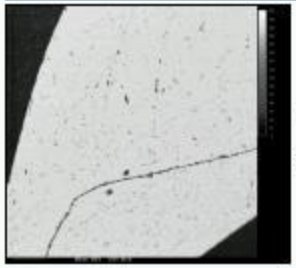
Web | rruff.info/all/

Almandine	R040076	$Fe^{2+}_3Al_2(SiO_4)_3$	University of Arizona Mineral Museum 7976	Barton Garnet mine, Gore Mountain, Warren
Almandine	R040079	$Fe^{2+}_3Al_2(SiO_4)_3$	University of Arizona Mineral Museum 13736	Ontario, Canada
Almandine	R040168	$Fe^{2+}_3Al_2(SiO_4)_3$	University of Arizona Mineral Museum 16323	Pocos Dos Cavatos, Ceara, Brazil
Almandine	R050029	$Fe^{2+}_3Al_2(SiO_4)_3$	University of Arizona Mineral Museum 4307	Barton Garnet mine, Gore Mountain, Warren
Almandine	X050009	$Fe^{2+}_3Al_2(SiO_4)_3$	George R. Rossman GRR-943	Riverside County, California, USA
Almandine	X050010	$Fe^{2+}_3Al_2(SiO_4)_3$	George R. Rossman GRR-1056	Wrangel, Alaska, USA
Almandine	X050011	$Fe^{2+}_3Al_2(SiO_4)_3$	George R. Rossman GRR-43	Rutherford #2 mine, Amelia, Virginia, USA
Almandine	R060099	$Fe^{2+}_3Al_2(SiO_4)_3$	Roland Boehne	Alaska, USA
Almandine	R060450	$Fe^{2+}_3Al_2(SiO_4)_3$	Gemological Institute of America 16606	Canada
Almandine	R070129	$Fe^{2+}_3Al_2(SiO_4)_3$	Michael Scott S100422	Wrangell, Wrangell Island, Wrangell-Petersb
Almandine	R100046	$Fe^{2+}_3Al_2(SiO_4)_3$	William W Pinch	Altai, Xinjiang Province, China
lactose monohydrate	D120008	$C_{12}H_{24}O_{12}$	David Blake	Synthetic from Aldrich
Alstonite	R050483	$BaCa(CO_3)_2$	California Institute of Technology 7890	Minerva #1 mine, Cave-in-Rock, Hardin Coun
Alstonite	R090049	$BaCa(CO_3)_2$	Bob Jenkins	Admiralty flats, Haggs mine, Nentsberry, Cum
Altaite	R060939	PbTe	Michael Scott S100891	870 Level, Mattagami mine, Matagami, Queb
Althausite	R070113	$Mg_4(PO_4)_2(OH,O)(F,\square)$	Bob Jenkins	Tingelstadtjern, Modum, Norway
Alum-(K)	R040134	$KAl(SO_4)_2{\cdot}12H_2O$	University of Arizona Mineral Museum 9391	Alunite mine, Esmeralda County, Nevada, US
Alum-(K)	R060014	$KAl(SO_4)_2{\cdot}12H_2O$	American Museum of Natural History 16802	Tolfa, Italy
Alum-(K)	R060528	$KAl(SO_4)_2{\cdot}12H_2O$	Michael Scott S100782	El Desierto mine fumaroles, Potosí, Bolivia
Alum-(Na)	R110204	$NaAl(SO_4)_2{\cdot}12H_2O$	Gordon W Downs	Flux mine, Arizona
Aluminite	R060691	$Al_2SO_4(OH)_4{\cdot}7H_2O$	Michael Scott S101225	Newhaven, East Sussex, England, United Kin
Aluminium	R070230	Al	Michael Scott S103000	Mud Volcano, Bulla Apsheron penninsula, Cas Azerbaijan
lumohydrocalcite	R061067	$CaAl_2(CO_3)_2(OH)_4{\cdot}3H_2O$	Michael Scott S100395	Lubom'ra, Czech Republic

RUFF

Name: Almandine
RRUFF ID: R040168
Ideal Chemistry: $Fe^{2+}_3Al_2(SiO_4)_3$
Locality: Pocos Dos Cavatos, Ceara, Brazil
Source: University of Arizona Mineral Museum
Owner: RRUFF
Description: Dark red etched single crystal
Status: The identification of this mineral has b

Quick search: [All Almandine samples (11)]



RRUFF ID: R040168.2
Sample Description: Microprobe Fragment
Measured Chemistry: $(Fe^{2+}_{1.48}Mn_{1.47}Ca_{0.0}$
Microprobe Data File: [Download Excel File]

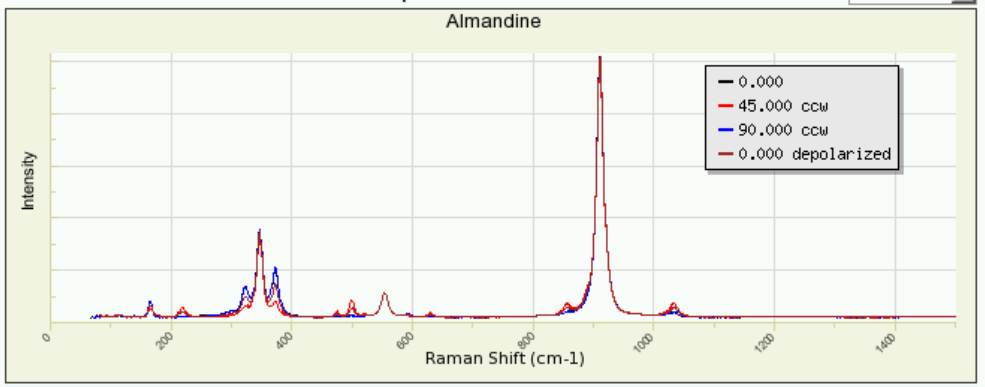
RRUFF ID: R04016
Sample Description: Sample
Pin ID: L00513
Orientation: Laser p

DOWNLOADS:

To download sample data, please select a specific orientation angle.

Raman Mode Analysis

Direction of polarization of laser relative to fiducial mark: all data



X Min: 0 X Max: 1500 X Sort: asc refresh reset

atom	x	y	z	Wyckoff
Fe	0	0.25	0.125	24c
Al	0	0	0	16a
Si	0.375	0	0.25	24d
O	0.03401	0.04901	0.65278	96h

Raman Active Modes

WP	A_{1g}	A_{1u}	A_{2g}	A_{2u}	E_u	E_g	T_{2u}	T_{2g}	T_{1u}	T_{1g}
96h	3	-	-	-	-	6	-	9	-	-
24d	-	-	-	-	-	1	-	3	-	-
24c	-	-	-	-	-	1	-	2	-	-
16a	-	-	-	-	-	-	-	-	-	-

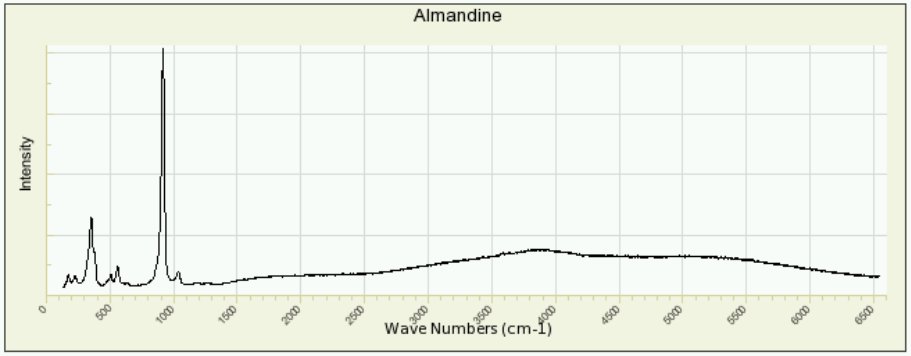
Total number of modes:
$3A_{g_1} + 8E_g + 14T_{2g} = 25$

RUFF

RRUFF ID: R040168
Wavelength: 532 nm
Sample Description: Unoriented
Instrument settings: Thermo Alm

DOWNLOADS:

Raman Data (RAW)
RRUFF File




```
##NAMES=Almandine
##LOCALITY=Pocos Dos Cavatos, Ceara, Brazil
##RRUFFID=R040168
##CHEMISTRY=Fe^2+^_3_Al_2_(SiO_4_)_3_
135.3528, 102.8389
137.2813, 115.8527
139.2097, 129.7559
141.1382, 144.4035
143.0667, 160.7849
144.9951, 177.0289
146.9236, 192.1146
148.8521, 202.1329
150.7805, 215.8496
152.7090, 235.3700
154.6375, 259.4792
156.5659, 283.9028
158.4944, 305.6499
160.4229, 328.7348
162.3513, 358.0035
164.2798, 399.1541
166.2083, 436.6672
168.1367, 468.2595
170.0652, 495.3648
171.9937, 509.0094
```

RRUFF ID: R040168.
Sample Description: Powder
Instrument settings: SensIR Du
Resolution:

DOWNLOADS:

Infrared Data (RAW)
RRUFF File

RUFF

DOWNLOADS:

- Cell Refinement Data
- Cell Refinement Output Data
- DIF File
- X-ray Data (XY - Processed)
  RRUFF File
- X-ray Data (XY - RAW)
  RRUFF File

REFERENCES for Almandin

American Mineralogist Crystal Structure Database Record: [view record]

Anthony J W, Bideaux R A, Bladh K W, and Nichols M C (1990) Handbook of Mineralogy, Mineral Data Publishing, Tucson Arizona, USA, by permission of the Mineralogi

Manning P G (1967) The optical absorption spectra of the garnets almandine-pyrope, pyrope and spessartine and some structural interpretations of mineralogical signi

Novak G A, Gibbs G V (1971) The crystal chemistry of the silicate garnets, American Mineralogist, 56, 791-825 [view file]

Emiliani F, Venturelli G (1972) Sharp compositional zoning in an almandine garnet, The Canadian Mineralogist, 11, 464-472 [view file]

Crawford M L (1977) Calcium zoning in almandine garnet, Wissahickon Formation, Philadelphia, Pennsylvania, The Canadian Mineralogist, 15, 243-249 [view file]

Shimazaki H (1977) Grossular-spessartine-almandine garnets from some Japanese scheelite skarns, The Canadian Mineralogist, 15, 74-80 [view file]

Speer J A (1981) Petrology of cordierite– and almandine–bearing granitoid plutons of the southern Appalachian Piedmont, U.S.A., The Canadian Mineralogist, 19, 35-4

Hofmeister A M, Chopelas A (1991) Vibrational spectroscopy of end-member silicate garnets, Physics and Chemistry of Minerals, 17, 503-526 [link]

Armbruster T, Geiger C A, Lager G A (1992) Single-crystal X-Ray structure study of synthetic pyrope almandine garnets at 100 and 293 K, American Mineralogist, 77,

Griffen D T, Hatch D M, Phillips W R, Kulaksiz S (1992) Crystal chemistry and symmetry of a birefringent tetragonal pyralspite$_{75}$–grandite$_{25}$ garnet, American Mineral

Newton R C, Harlov D E (1993) Standard thermodynamic properties of almandine, The Canadian Mineralogist, 31, 391-399 [view file]

Pinet M, Smith D C (1994) Raman microspectrometry of garnets $X_3Y_2Z_3O_{12}$ 2. The natural aluminium series pyrope-almandine-spessartine, Schweizerische Mineralog

Pilati T, Demartin F, Gramaccioli C M (1996) Atomic displacement parameters for garnets: A lattice-dynamical evaluation, Acta Crystallographica, B52, 239-250

Chmielová M, Martinec P, Weiss Z (1997) Almandine-pyrope-grossular garnets: a method for estimating their composition using X-ray powder diffraction patterns, Eur

Kolesov B A, Geiger C A (1997) Raman scattering in silicate garnets an investigation of their resonance intensities, Journal of Raman Spectroscopy, 28, 659-662 [link

Kolesov B A, Geiger C A (1998) Raman spectra of silicate garnets, Physics and Chemistry of Minerals, 25, 142-151 [link]

Milman V, Winkler B, Nobes R H, Akhmatchaya E V, Pickard C J, White J A (2000) Garnets: structure, compressibility, dynamics, and disorder, Journal of the Minerals,

UCL pigment library

Raman Spectroscopic Library

ACS PUBLICATIONS
Essential Resources for the Chemical Sciences

Introduction to the site

Staff Intranet

Table of Black Pigments

UCL pigment library

Table of Black Pigments

Name	Composition	Band Wavenumbers[a] / cm^{-1} and Relative Intensities[b]	Excitation Wavelength & Power	Notes and Date[c]
ivory black	carbon	961 [illegible] PO_4^{3-} [illegible] 1325vs(br); ~1580vs(br)	632.8 nm [illegible]	Antiquity. Also contains calcium phosphate
lamp black	carbon	~1325vs(br); ~1580vs(br)	632.8 nm [illegible]	Antiquity

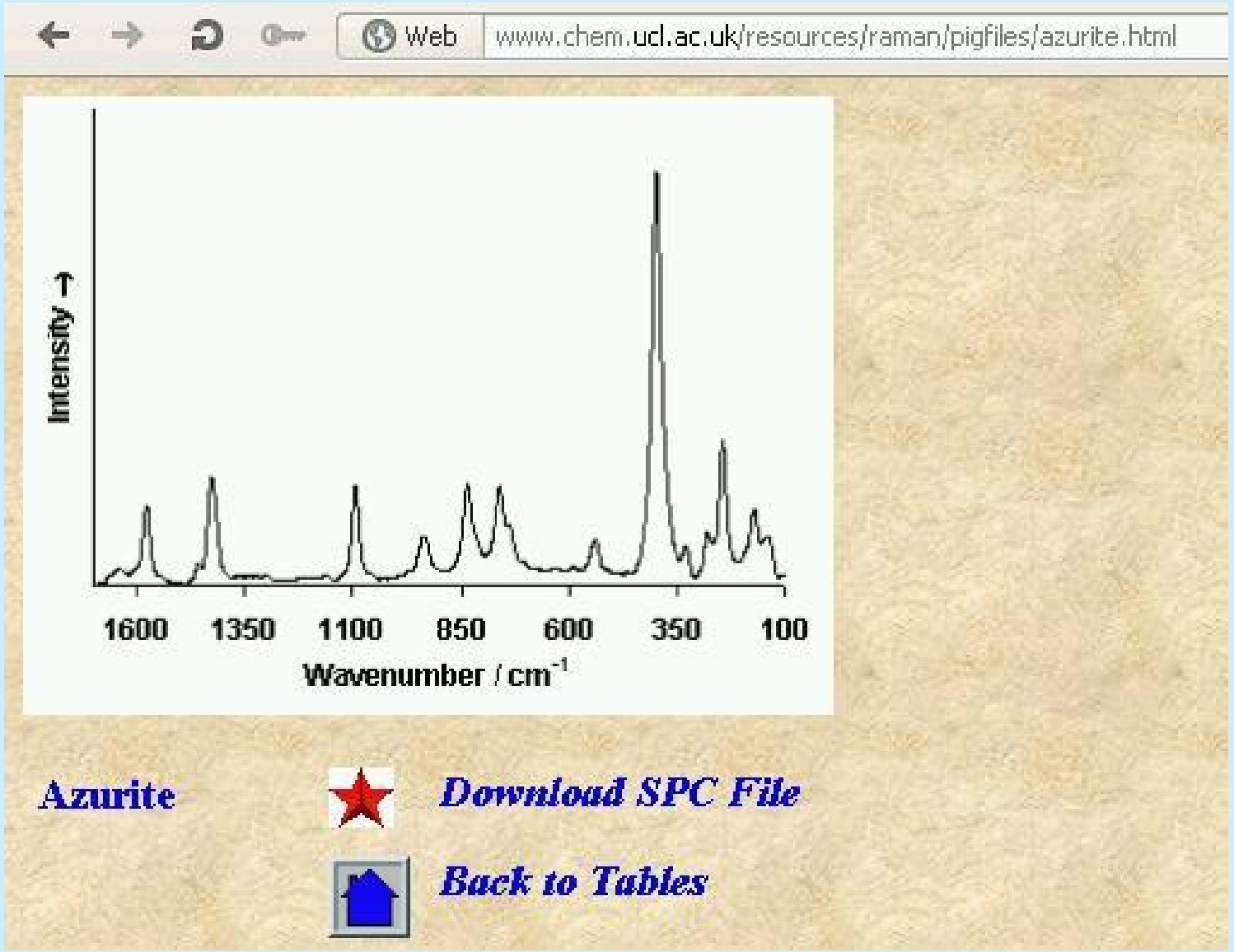
[a] Approximate centres of broad bands in the laser fluorescence spectrum.
[b] s = strong, m = medium, w = weak, v = very, sh = shoulder, br = broad
[c] The pigment is either specified to be a mineral or the date of its first manufacture is listed

Back to Palette   Back to Top

Table of Blue Pigments

Name	Composition	Band Wavenumbers[a] / cm^{-1} and Relative Intensities[b]	Excitation Wavelength and Power	Notes, Raman Literature References and Date[c]
azurite	basic copper(II) carbonate $2CuCO_3.Cu(OH)_2$	[illegible] 940vw; [illegible]	514.5 nm [illegible]	Mineral
cerulean blue	cobalt(II) stannate $CoO.nSnO_2$	[illegible] 674vs	514.5 nm [illegible]	182
cobalt blue	cobalt(II)-doped alumina glass $CoO.Al_2O_3$	203vs; 512vs	514.5 nm [illegible]	1775

UCL pigment library



Handbook of Minerals Raman Spectra

Handbook of Minerals Raman Spectra

ENS DE LYON

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enter phase name or part of the name

[all] [advanced search]

Facilties

raman spectrometers of **Laboratoire de Sciences de la Terre** are national instruments supported by **Institut des Sciences de L Univers** and therefore to work with one of this machine :

- consult the [facilities] booking system
- send us an email [raman@geologie-lyon.fr]

Pressure calculation

- [wavelength in cm^{-1}]
- [wavelength in nm]

To send spectrum

to help us to increase this data base, fill [this form] and send new spectrum file

Links

The Rruff Project website containing an integrated database of Raman spectra, X-ray diffraction and chemistry data for minerals [link]

Raman Mineral Spectroscopy Server (Caltech) [link]

Raman Spectra Minerals (University of Parma) [link]

Raman data base of minerals (SFMC) [link]

Laser spot on a Pyrite sample

Raman spectroscopy can be used to identify, with a minimum of preparation, minerals, glasses and fluids in geological samples [LST]. We therefore present a selection of Raman spectra of minerals representative of some major mineral groups [use search engine]. The spectra provide the main vibrational fingerprints of each main mineral group and related minerals. We report here more recent references and references for Raman studies carried out at high-pressures and high-temperatures are also mentionned. Most of the spectra were recorded on a XY ©DILOR Raman microspectrometer equipped with a CCD detector [Picture]. The spectrometer was used in *backscattering geometry*. The laser beam (488 or 514.5 nm exciting lines of a Spectra Physics® Ar^+ laser) was focussed through microscope objectives (x50) down to a *2 micrometer spot* on sample and the backscattered light was collected through the same objective.

Even though polarization effects are minimized, the intensity of the Raman modes can be sensitive to crystal orientation.

Instruments

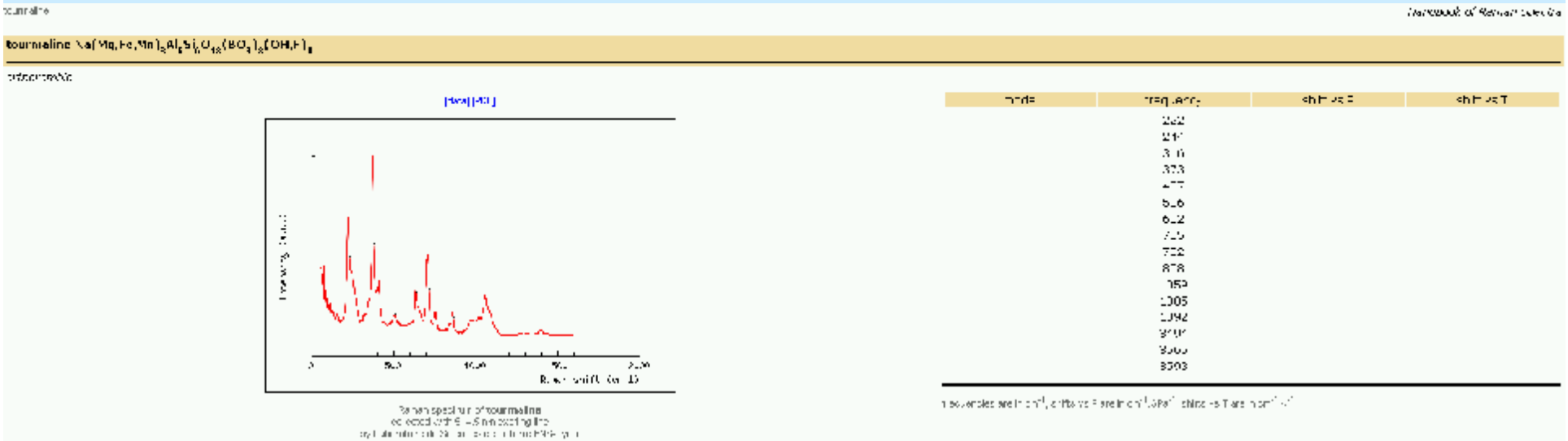
spectrometer	laser source
Labram HR800 vis Jobin Yvon Horiba semi-confocal microscope - mapping stage	Spectra Physics® 2018 Ar^+/Kr^+ 647.1 nm 514.5nm 452.5nm HeNe 632.8nm
Labram HR800 vis Jobin Yvon Horiba confocal microscope and fiber entrance	Spectra Physics® 2017 Ar^+ 514.5nm
Labram HR800 UV Jobin Yvon Horiba	Spectra Physics®Pilas Train 244nm
XY Dilor	Spectra Physics®177G Ar^+ 514.5nm 488nm 452.5nm

[This page is in progress]

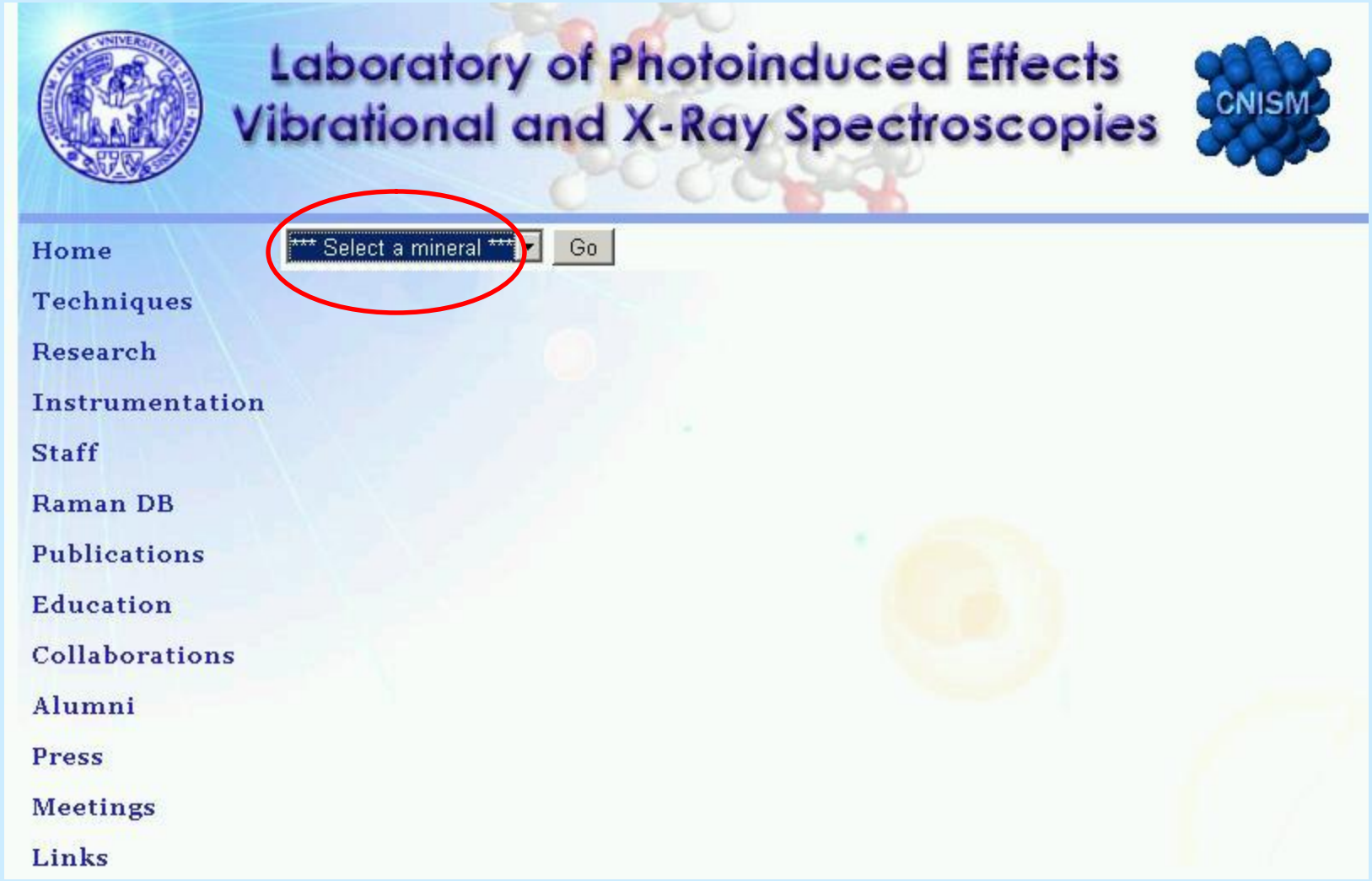
Gilles.Montagnac@ens-lyon.fr

Handbook of Minerals Raman Spectra

Handbook of Minerals Raman Spectra



University of Parma mineral data base



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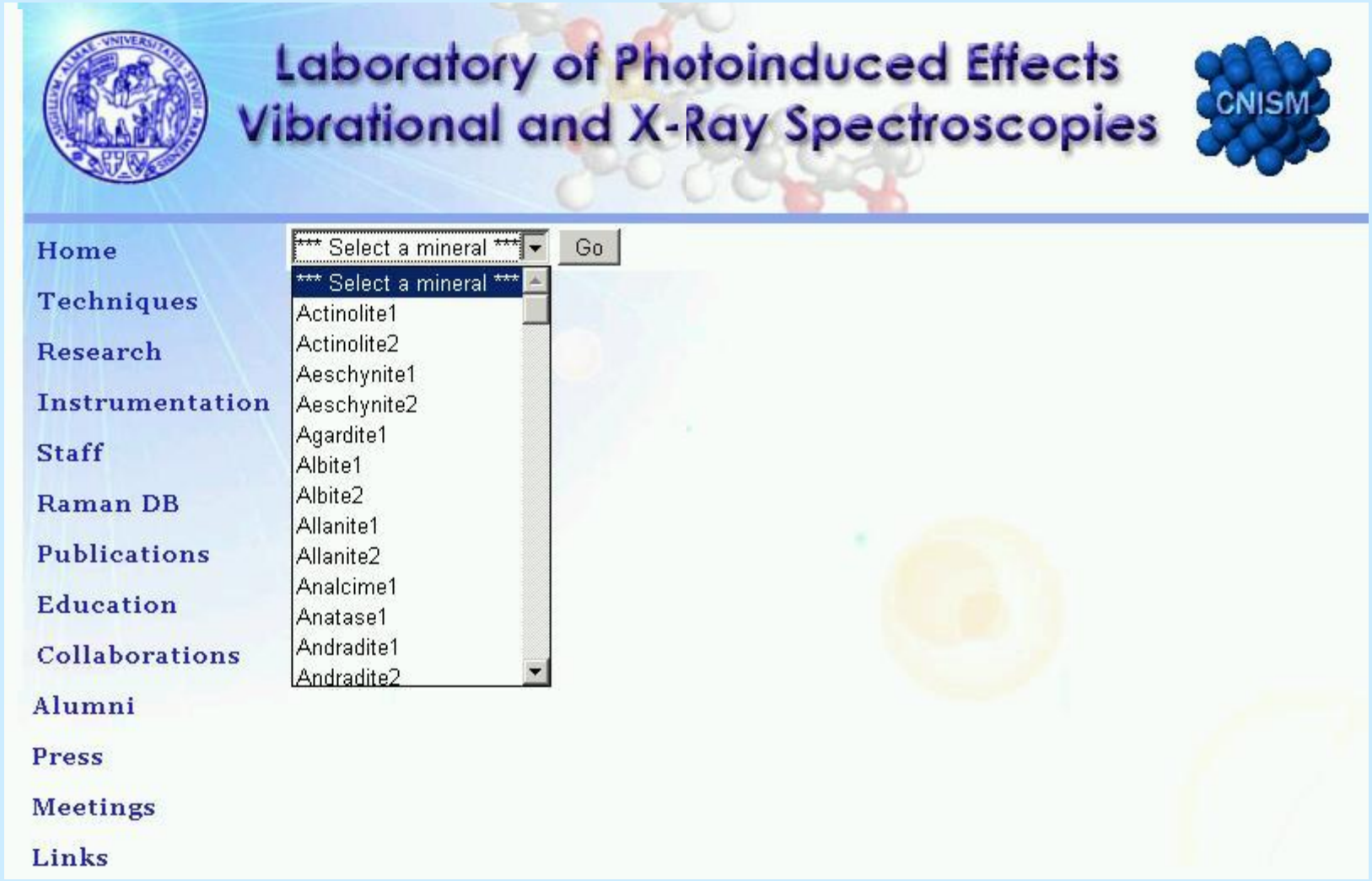

University of Parma mineral data base

Laboratory of Photoinduced Effects
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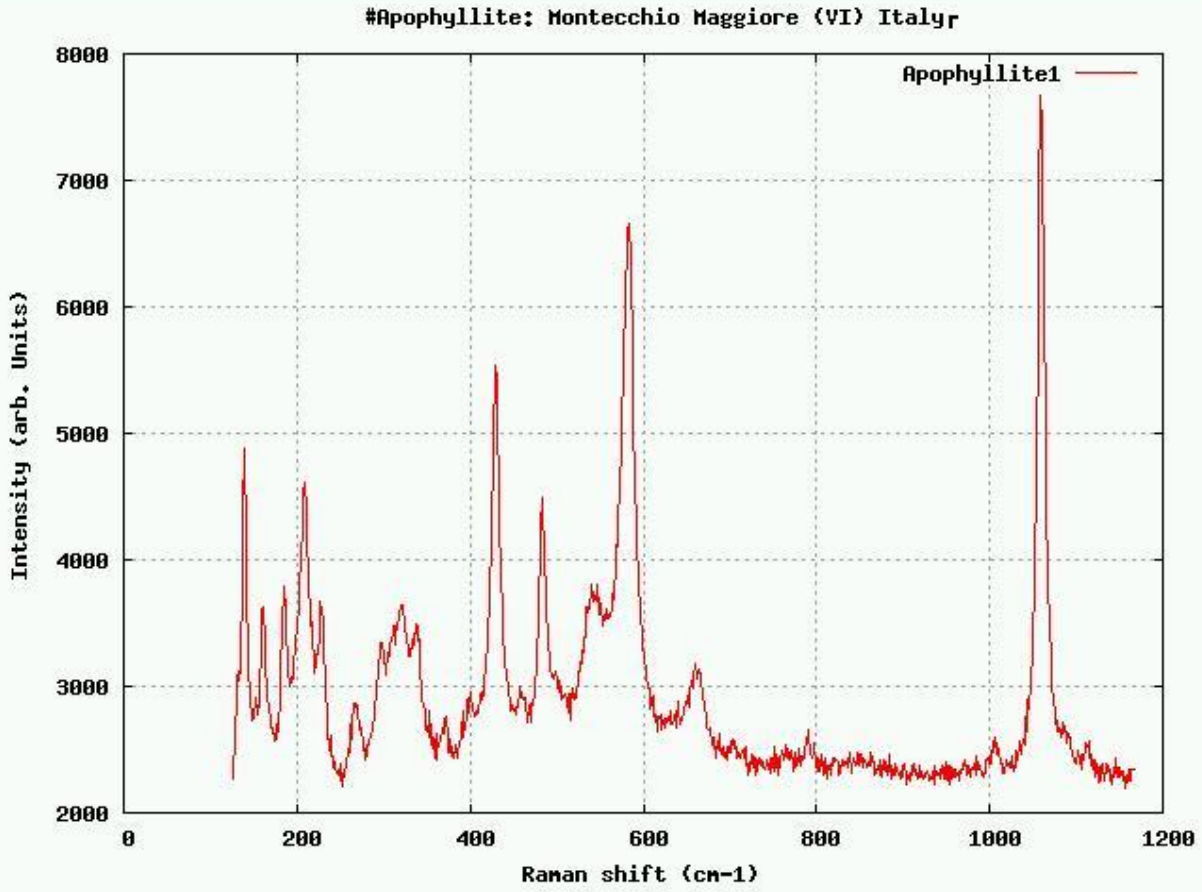

Minerals and Chemicals

Ha…yne	Na3Ca(Si3Al3)O12(SO4)	HAUYN31	HAUYN3.S00	./kyo/lwkyo/HAUYN3.KYO ./s00/HAUYN s00pdf/HAUYN3.pdf
Heavy water	D2O	HEAVYW11	D2O-A.S00	./kyo/dernierskyo/D2O-A.BAA
Hedenbergite	CaFeSi2O6	HEDEN11	HED100.S00	./kyo/akkyo/HED100.BAC ./s00/HED100.S HED100.pdf
Herderite	CaBePO4(OH,F)	HERDE11	HERDEB.S00	./kyo/akkyo/HERDEB.BAB ./s00/HERDEB s00pdf/HERDEB.pdf
Herderite	CaBePO4(OH,F)	HERDE21	HERDED.S00	./kyo/akkyo/HERDED.BAB ./s00/HERDED s00pdf/HERDED.pdf
Heulandite	(Na,K,Ca,Sr,Ba)5(Al9Si29)O72.26H2O	HEULAN11	HEULA1.S00	./kyo/dernierskyo/HEULA1.KYO ./s00/HEU s00pdf/HEULA1.pdf
High albite	NaAlSiO8	HALBIT11	S7015C.S00	./s00/S7015C.S00 ./s00pdf/S7015C.pdf
Hornblende	Ca2(Mg,Fe,Al)8O22(OH)2	HORNB11	HORNB1.S00	./kyo/lwkyo/HORNB1.BAA ./s00/HORNB s00pdf/HORNB1.pdf
Howlite	Ca2B5SiO9(OH)5	HOWLI11	HOWLI2.S00	./kyo/lwkyo/HOWLI2.BAC ./s00/HOWLI2 s00pdf/HOWLI2.pdf
Howlite	Ca2B5SiO9(OH)5	HOWLI21	HOWLI4.S00	./kyo/lwkyo/HOWLI4.BAC ./s00/HOWLI4 s00pdf/HOWLI4.pdf
Hydrocerussite	Pb3(CO3)2(OH)2	HYDPB11	HYDPB1.S00	./kyo/lwkyo/HYDPB1.BAA ./s00/HYDPB1 s00pdf/HYDPB1.pdf
Hydrogen	H2	H211	HCOCOA.S00	
Hydrogen	H2	H221	HCOCOB.S00	
Hydrogen sulfide	H2S	H2SL11	PALL11.S00	
Hydromagnesite	Mg5(CO3)4(OH)2.4H2O	HYMAG11	HYDMG1.S00	./kyo/lwkyo/HYDMG1.BAB ./s00/HYDMG s00pdf/HYDMG1.pdf
Hydroxyapophyllite	KCa4(Si4O10)2(F,OH).8H2O	APOPH11	APOPH2.S00	./kyo/lwkyo/APOPH2.BAC ./s00/APOPH2 s00pdf/APOPH2.pdf
Hydroxyapophyllite	KCa4(Si4O10)2(F,OH).8H2O	APOPH21	APOPH4.S00	./kyo/lwkyo/APOPH4.BAA ./s00/APOPH4 s00pdf/APOPH4.pdf
Intermediate albite	NaAlSi3O8	IALBIT11	O8431C.S00	./s00/O8431C.S00 ./s00pdf/O8431C.pdf

Minerals and Chemicals

AIR 327a pdf index

Author(s): BENY C.
Date: 20 november 90
file name: AIRMA1.S00 pdf
Recording laboratory: Lab. mixte (BRGM-CNRS- Univ. OrlÈans) de spectro
References:
2nd file name:
Structural formula: N2+O2
Name: Air
Family: 327a
Group:
Origin: natural [x] locality: OrlÈans (France) synthetic [_] method: P: T:
Solid: crystal [_] powder [_] glass [_]
Fluid: liquid [_] gas [x]
Preparation: Thick section [_] thin section [_] raw sample [_]
Colour: opaque [_] transparent [_] translucent [_]
Conditions of measurement: room P room T
Polarization setting: PORTO ( ) VV [_]; VH [_]; none [x]
Laser: Ar+ 0 = 514.5 nm;
Sample photosensibility:
Laser power: at laser: 800 mW, at sample:
Raman scattering efficiency: *
Spectral resolution: 5 cm-1
Calibration: Ar+: cm-1
Spectrometer: JOBIN-YVON; model: U1000 macro [x] micro [_] objective:;
scan rate: cm-1/mn
step: 0.5 cm-1
counting time: 2 s

Minerals and Chemicals

U1000
BENY
11/20/90
b:AIRMA1.S00

INT.TIME : 2.000 Sec
INCREMENT : −0.50 Cm−1
NB.SCANS : 4
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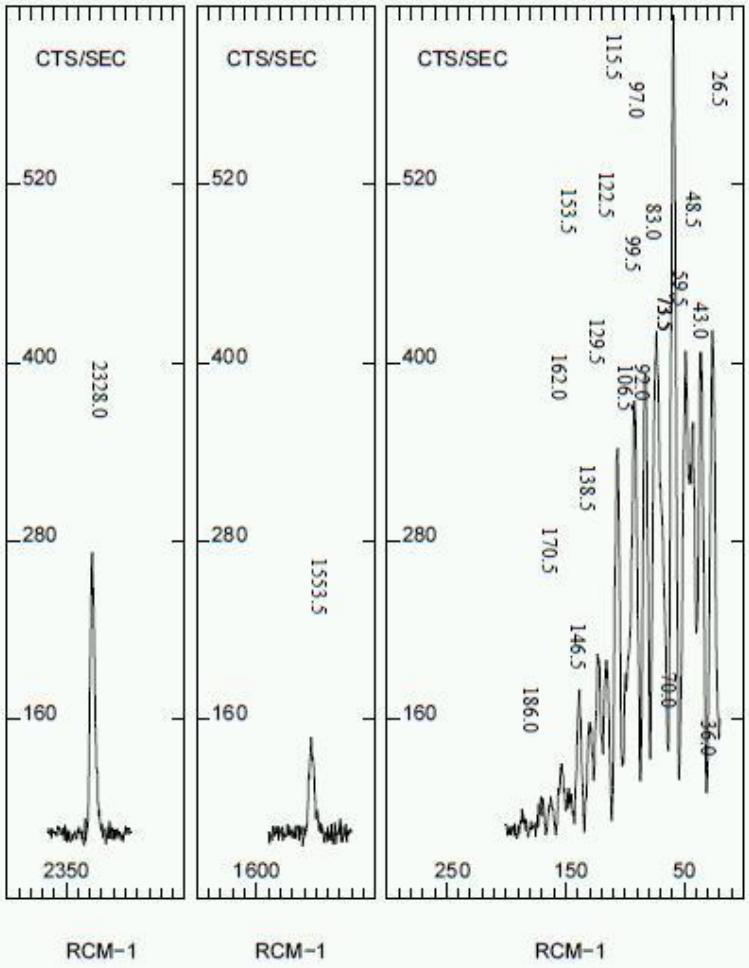
utilisation des 2 miroirs de renvoi de la platine

laser power
slits
objective PM
operator
sample



The Goblentz Society
Spectral Data Collections

Mineral spectroscopy server

Web minerals.gps.caltech.edu/#Data

Mineral Spectroscopy Server

California Institute of Technology

Pasadena, California, USA

This server provides information about mineralogy and is primarily dedicated to providing information about **color in minerals** and access to data on **Mineral Absorption Spectra** in the visible and inf
Caltech mineral spectroscopy labs. Other types of spectroscopic data on minerals are also available.

Visible, near-infrared and infrared absorption spectra are available for a number of minerals. Examples include common rock-forming minerals, gem minerals, and other minerals of particular interest.

Spectroscopic Data | Mineral Spectroscopy References | Causes of Color in Minerals | Representative Data from our lab | Data from our Recent Publications

Special Topics: Ametrine | Manganese Dendrites | Desert Varnish | Silica Polymorphs | Painite | Rossmanite | Tourmaline

---

Spectroscopic Data: hundreds of files and graphs

Have a look at our List of Data Files or Data from Recent Publications

This is the ever growing list of the minerals available on this server. Both data coordinates and images of the spectra are available for selected minerals. Information about the origin of color is available f
lines. Raman, infrared, and reflectance data are available and Mössbauer data are solicited. More details follow.

Extensive references to Optical Spectroscopic data now av

Have a look at our updated List of 722 References

Mineral spectroscopy server

Index to Data Files on the Mineral Spectroscopy Server

Visible Spectra

Our extensive collection of single crystal transmission data in the 300 - 2500 nm range.

External Databases:

- The Edward J. Gübelin Gem Collection: Unpolarized spectra of a wide variety of gemstones in the 350-750 nm range from GIA.

Infrared Spectra (under development - several sections are ready now)

KBr pellet data in the 4000 - 200 cm^{-1} range.

OH-region : single crystal data in the 4000 - 3000 cm^{-1} range.

Far-Infrared : Both ATR and Polyethylene pellet data are available. ATR-Far-IR data for samples that are part of the RRUFF project are available on the RRUFF website.

External Databases

- Interstellar Dust Analogue database from Washington University
- Aerosol particle database from Jena

Reflectance data

- Reflectance data from oriented crystals in the 1800 - 400 cm^{-1} range.
- Our ATR (Attenuated Total Reflectance) data of hundreds of mineral powders on a diamond plate in the 4000 - 450 cm^{-1} range are now incorporated in the RRUFF project.
- An extensive collection of **reflectance spectra** of minerals is available from the USGS Spectroscopy Lab .
- Another collection of **reflectance spectra** is available from the Advanced Spaceborne Thermal Emission Reflectance Radiometer (ASTER) project at JPL.
- A collection of vis-NIR **reflectance spectra** of rocks and minerals is available from the the RELAB Public Spectroscopy Database at Brown University.
- A limited collection of infrared **reflectance spectra** of minerals is available from the the Chemical and Spectroscopy Laboratory at the Astrophysics Institute and University Observatory, Jena.

Thermal Emission Spectra

- Plots of spectra are available from the Arizona State University's Thermal Infrared Mineral Spectroscopy Laboratory
- Sulfate mineral data from Melissa D. Lane of the Planetary Science Institute.

Raman Spectra. Our data are now part of the RRUFF project, a large composite database that combines the American Mineralogist Crystal Structure Database with thousands of Raman spectra obtaine Raman spectra, and, infrared spectra and, ultimately, other types of data in a convenient, single database.

American Mineralogist Crystal Structure Database

This site is an interface to a crystal structure database that includes every structure published in the American Mineralogist, The Canadian Mineralogist, European Journal of Mineralogy and Physics and Chemistry of Minerals, as well as selected datasets from other journals. The database is maintained under the care of the Mineralogical Society of America and the Mineralogical Association of Canada, and financed by the National Science Foundation.

Mineral

Author

Chemistry Search

Cell Parameters and Symmetry

Diffraction Search

General Search

Search Tips

Search Reset

Logic interface ◉ AND ○ OR

Viewing (About File Formats) ◉ amc long form ○ amc short form ○ cif

Download ◉ amc ○ cif ○ diffraction data

People Extra

Number of Files downloaded since Apr 1, 2003: 273011180
Data Last Updated: August 27, 2012
Web Page Last Updated: September 22, 2008
This page has been accessed 1480739 times.

Also see our complete list of minerals and complete list of authors.

Mineral spectroscopy server

rruff.geo.arizona.edu/AMS/all_minerals.php

American Mineralogist Crystal Structure Database

Abenakiite-(Ce)	Abernathyite	Abhurite	Abswurmbachite
Acetamide	Acetylene-hydrate	Achavalite	Actinium
Acuminite	Adamantane	Adamantane-methane-hydrate	Adamite
Adelite	Admontite	Adolfpateraite	Adranosite
Aeniqmatite	Aerinite	Aeruqite	Aeschynite-(La)
Afqhanite	Afmite	Afwillite	Agardite-(Ce)
Agricolaite	Agrinierite	Ahlfeldite	Aikinite
Ajoite	Akaganeite	Akatoreite	Akdalaite
Akhtenskite	Akimotoite	Akrochordite	Aksaite
Alabandite	Alacranite	Alamosite	Alarsite
Albrechtschraufite	Alflarsenite	Alforsite	Alfredstelznerite
Alite	Allaboqdanite	Allactite	Allanite-(Ce)
Allanite-(Nd)	Allanite-subqroup mineral	Allanpringite	Allargentum
Allochalcoselite	Alloclasite	Alloriite	Alluaivite
Almandine	Almarudite	Alpersite	Alsakharovite-Zn
Althausite	Althupite	Altisite	Alum-(K)
Alum-K	Alum-Na	Aluminite	Aluminium
Alumino-magnesiotaramite	Aluminoceladonite	Aluminocerite-(Ce)	Aluminocoquimbite
Aluminotaramite	Aluminum	Alumoklyuchevskite	Alumotantite
Alunoqen	Alvanite	Amakinite	Amarantite

Mineral spectroscopy server

American Mineralogist Crystal Structure Database

3 matching records for this search.

Adamite

Hill R J

American Mineralogist 61 (1976) 979-986

The crystal structure and infrared properties of adamite

_database_code_amcsd 0000532

8.306 8.524 6.043 90 90 90 Pnnm

atom	x	y	z	B(1,1)	B(2,2)	B(3,3)	B(1,2)	B(1,3)	B(2,3
As	.25048	.24394	.5	.00181	.00079	.00286	-.00014	0	0
Zn1	0	0	.24737	.00529	.00260	.00311	-.00159	0	0
Zn2	.13482	.36423	0	.00267	.00128	.00444	-.00001	0	0
O1	.0760	.1447	.5	.0031	.0021	.0024	-.0009	0	0
O2	.1079	.1268	0	.0035	.0011	.0059	.0001	0	0
O3	.3960	.1063	.5	.0033	.0008	.0126	-.0002	0	0
O4	.2685	.3615	.2778	.0041	.0028	.0039	-.0010	-.0006	.001
H	.20	.13	0						

Download AMC data (View Text File)

Download CIF data (View Text File)

Download diffraction data (View Text File)

View JMOL 3-D Structure

Adamite

Hawthorne F C

The Canadian Mineralogist 14 (1976) 143-148

The Goblentz Society
Spectral Data Collections

Welcome to Spectral Database for Organic Compounds, SDBS.

This is a free site organized by National Institute of Advanced Industrial Science and Technology (AIST), Japan.

NMR: *T.Yamaji, T.Saito, K.Hayamizu, M.Yanagisawa and O.Yamamoto*
MS: *N.Wasada*
ESR: *K.Someno*
IR: *S.Kinugasa, K.Tanabe and T.Tamura*
Raman: *K.Tanabe and J.Hiraishi*

What's New

2012.04.04 FAQ was updated.
2012.04.04 New data were updated.(774 Spectra)
2011.09.22 SDBS had a problem in a compound search system. Due to the problem, SDBS had been down between 17 and 20, September. We apologize for

Disclaimer

We are doing our best to compile high quality databases. However, there are no such databases without any errors or mistakes. We make no warranties to those effects and shall not be liable for any damage that may result from errors in the database. When you find errors or mistakes, please inform us using the form which can be accessed from the Contact button shown above.

Access to this database is free of charge. However we request visitors to our database not to download more than 50 spectra and/or compound information in one day. All accesses are recorded. It is prohibited that you use any information of SDBS for profit-making or commercial use without obtaining proper permission from us. If more spectra are required for some specific purpose or commercial use, you should consult us and describe the intended usage or purpose of our SDBS.

I agree the disclaimer and use SDBS.

SDBS Compounds and Spectral Search

Compound Name:
[ ] match partial

Molecular Formula:
[ ]
C, H, then the other elements are alphabetical order, "%,*" for the wild card

Molecular Weight:
[ ] to [ ]
Numbers between left and right columns
Up to the first place of a decimal point

CAS Registry No.:
[ ]
"%,*" for the wild card.

SDBS No.: [ ]
"%,*" for the wild card.

Atoms:

C(Carbon)	[ ]	to	[ ]
H(Hydrogen)	[ ]	to	[ ]
N(Nitrogen)	[ ]	to	[ ]
O(Oxygen)	[ ]	to	[ ]
F(Fluorine)	[ ]	to	[ ]
Cl(Chlorine)	[ ]	to	[ ]
Br(Bromine)	[ ]	to	[ ]
I(Iodine)	[ ]	to	[ ]
S(Sulfur)	[ ]	to	[ ]
P(Phosphorus)	[ ]	to	[ ]
Si(Silicon)	[ ]	to	[ ]

Numbers between left and right columns.

Spectrum:
Check the spectra of your interest.
☐ MS ☐ IR
☐ ^{13}C NMR ☐ Raman
☐ ^{1}H NMR ☐ ESR

IR Peaks(cm^{-1}): Allowance
[ ] ± [10]
"," or space is the separator for multiple peaks.
Use "-", to set a range:. eg. 550-750,1650 3000-
Transmittance < [80] %

^{13}C NMR Shift(ppm): Allowance
[ ] ± [2.0]
"," is the separator for multiple shifts, eg. 129.3,18.4,...
No shift regions: [ ]
Range defined by two numbers separated by a space, eg. 110 78,...

^{1}H NMR Shift(ppm): Allowance
[ ] ± [0.2]
No shift regions: [ ]

MS Peaks and intensities:
[ ]
Mass and its intensity are a set of data separated by a space, eg. 110 22,..

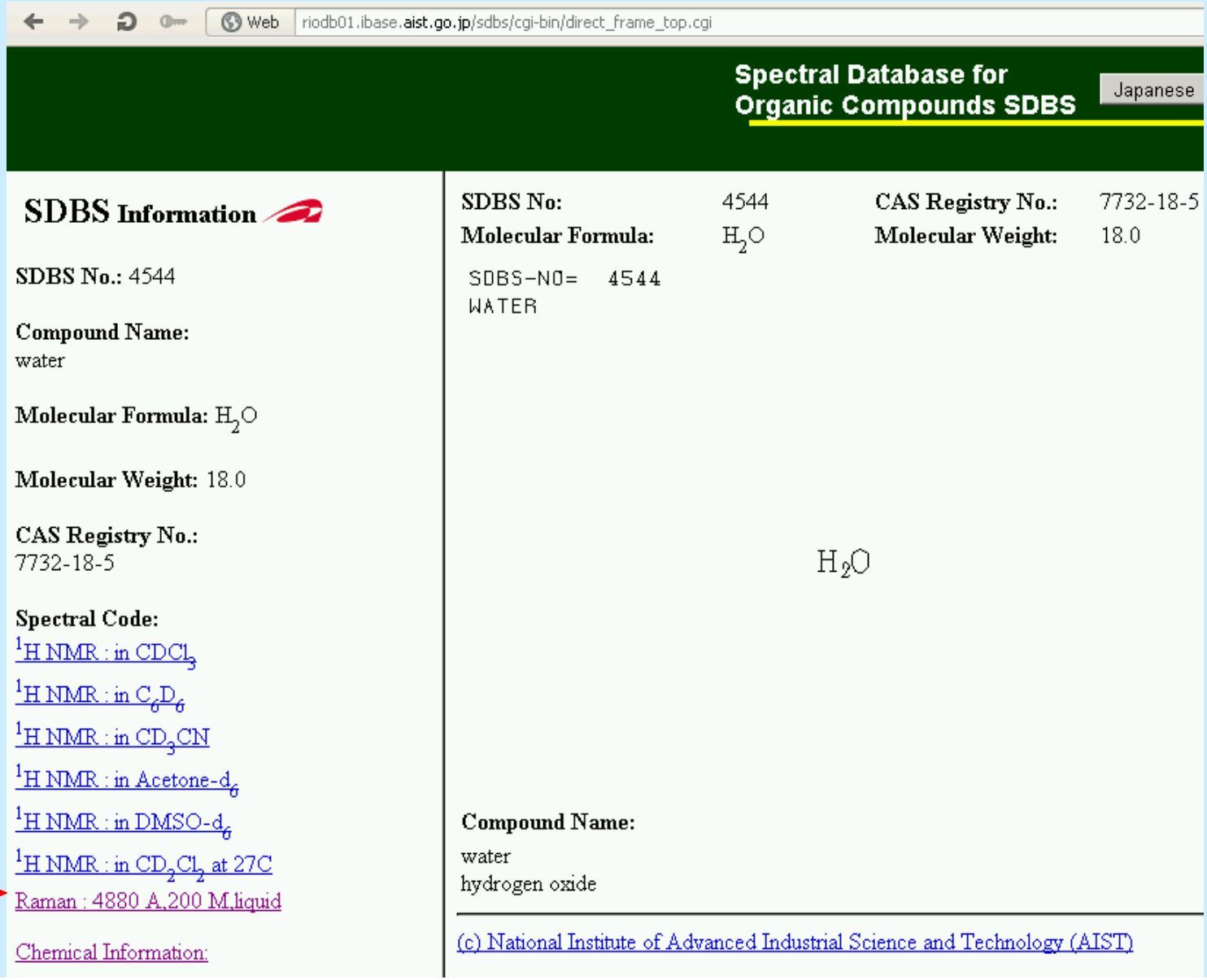
Search | Clear | Hit: [20hit] | Sort by: [Molecular Weight] [Ascending Order]

SDBS Search Results: 1 - 20 out of 3573 hits

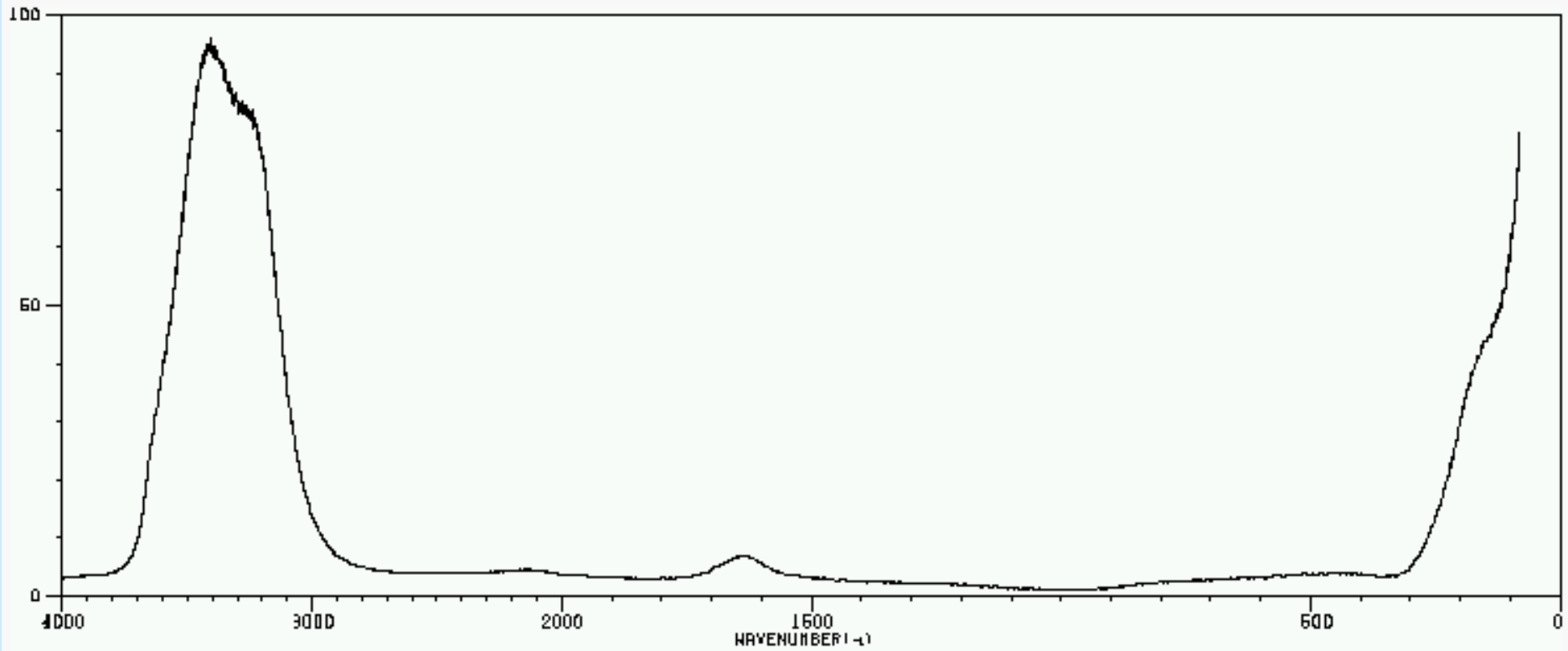
Sort by: Molecular Weight | Ascending Order | Search

SDBS No	Molecular Formula	Molecular Weight	MS	CNMR	HNMR	IR	Raman	ESR	Compound Name
4544	H2O	18.0	N	N	Y	N	Y	N	water
4218	CH5N	31.1	N	N	N	Y	Y	N	methylamine
3302	CH4O	32.0	Y	Y	Y	Y	Y	Y	methanol
2539	H3NO 1/2C2H2O4	33.0	Y	N	N	Y	Y	N	hydroxylamine oxalate
7948	CH3DO	33.0	Y	Y	Y	Y	Y	N	methanol-d
1218	C2H3N	41.1	Y	Y	Y	Y	Y	Y	acetonitrile
3958	CH4N2 HCL	44.1	Y	Y	Y	Y	Y	N	formamidine hydrochloride
931	CH3NO	45.0	Y	N	Y	Y	Y	Y	formamide
12577	C2H7N H3B	45.1	Y	Y	Y	Y	Y	N	borane-dimethylamine com
10523	CH2O2	46.0	Y	Y	Y	Y	Y	N	formic acid
1300		46.1	Y	Y	Y	Y	Y	Y	ethyl alcohol
3946	CH5NO HCL	47.1	Y	Y	Y	Y	Y	N	O-methylhydroxylamine hyc
1283	C3H3N	53.1	Y	Y	Y	Y	Y	N	acrylonitrile
2939	CH3NAO	54.0	N	N	N	Y	Y	N	sodium methoxide
4119	C3H7N	57.1	Y	Y	Y	Y	Y	N	propyleneimine
3657	C2H6N2 HCL	58.1	Y	Y	Y	Y	Y	N	acetamidine hydrochloride
319	C3H6O	58.1	Y	Y	Y	Y	Y	N	acetone
320	C3H6O	58.1	Y	Y	Y	Y	Y	Y	allyl alcohol
2899	C3H6O	58.1	Y	Y	Y	Y	Y	N	propionaldehyde
3599	CH5N3 1/2CH2O3	59.1	Y	Y	N	Y	Y	N	guanidine carbonate

Database for Organic Compounds



Database for Organic Compounds



WATER

SDBSNO = 4544 H_2O RM-01-00034 : 4880A.200M.LIQUID

3439	92
3423	94
3405	95
3396	94
3362	90
3330	88
3309	86
3227	82
3200	77

Raman Spectra Database of Minerals and Inorganic Materials

RASMIN

Introduction Contact

NOTICE

1. We request that when you use the data of our RASMIN in your publication or presentation, a proper acknowledgement be given as follows:

   RASMIN Web: http://riodb.ibase.aist.go.jp/rasmin/
   (National Institute of Advanced Industrial Science and Technology, date of access)

2. We have been providing raw spectral data in TXT format in RASMIN. However, increasing threats of illegal download by malicious users make us halt the service.

3. Access to this database is free of charge. However, all accesses are recorded. It is prohibited that you use any information of RASMIN for profit-making or commercial use without obtaining proper permission from us. If more spectra are required for some specific purpose or commercial use, you should consult us and describe the intended usage or purpose of our RASMIN.

Disclaimer

- We are doing our best to compile high quality databases. However, there are no such databases without any errors or mistakes. We make no warranties to those effects and shall not be liable for any damage that may result from errors in the database. When you find errors or mistakes, please inform us using the form which can be accessed from the Contact button shown above.

I agree the disclaimer and use RASMIN.

RASMIN

Raman Spectra Database of Minerals and Inorganic Materials

RASMIN

Minerals (576 spectra)	Search	List
Inorganic materials (1022 spectra)	Search	List
Literature (100 papers & books)		

List of inorganic chemicals

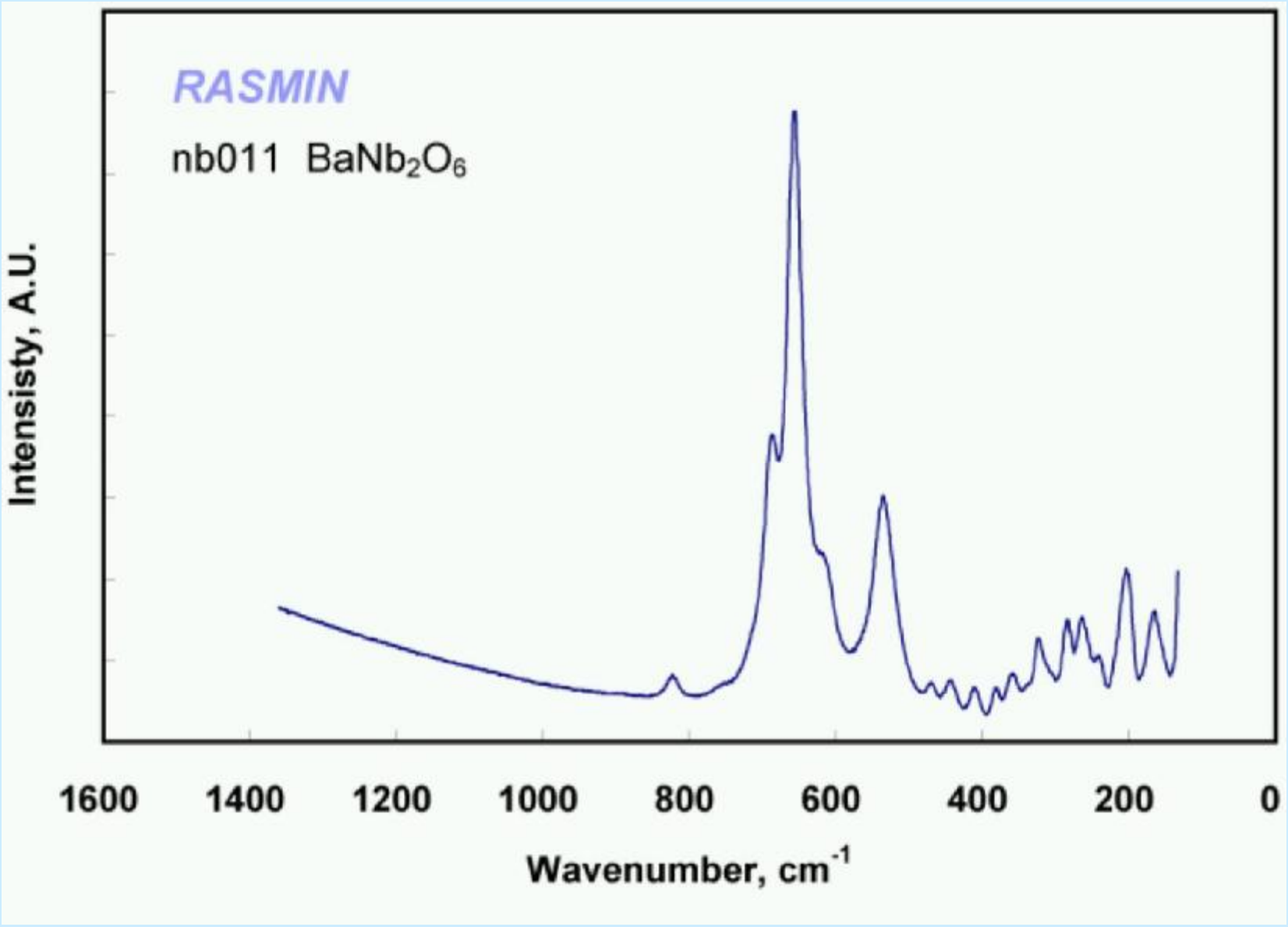
Usage : Click the name (alphabet letters) in the table

Name	#
All	1022
A-B-C-D-E	323
F-G-H-I-J	78
K-L-M-N-O	356
P-Q-R-S-T	184
U-V-W-X-Y-Z	81

RASMIN

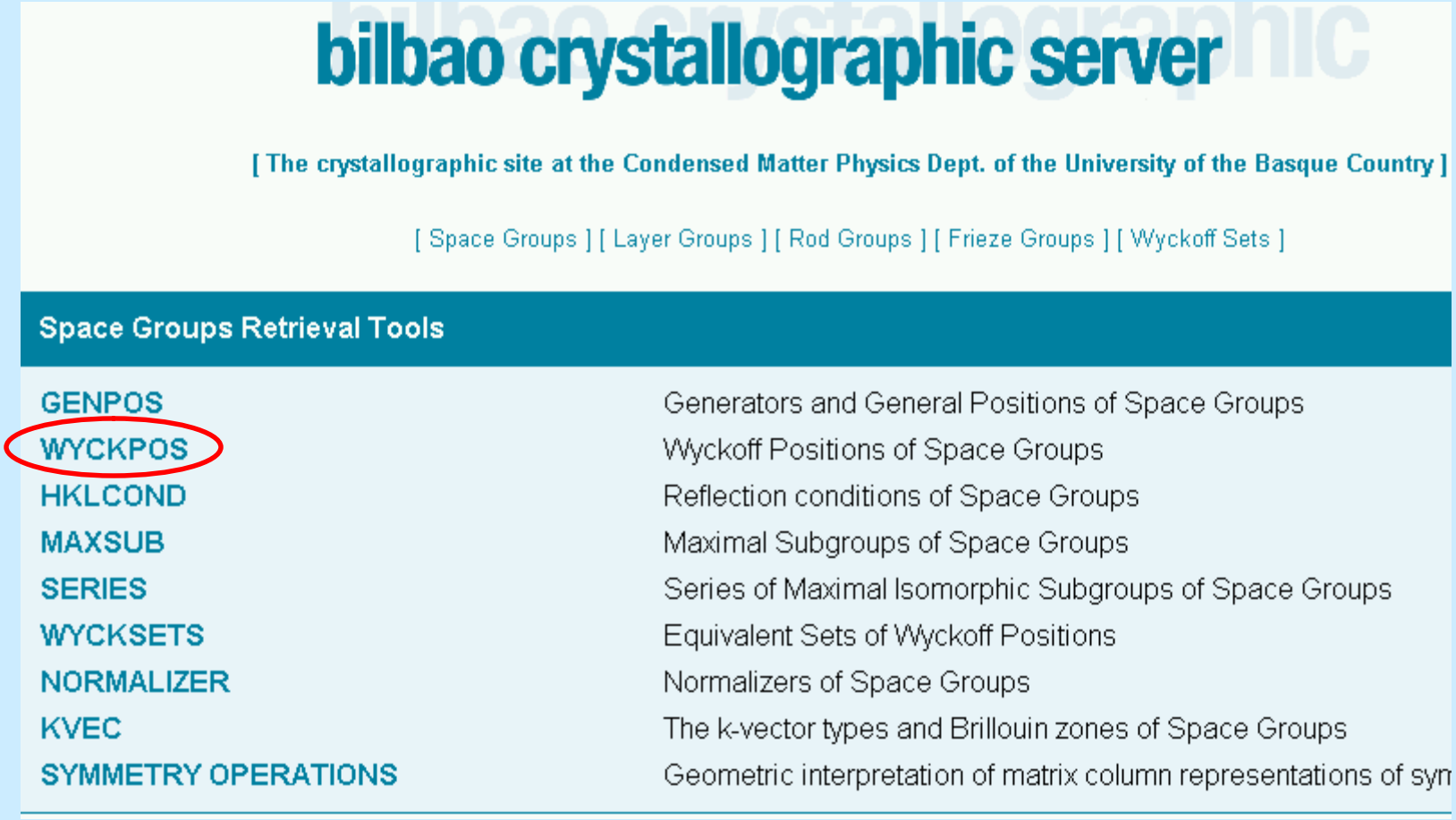
Chemical Formula A B C D E	Name	Spectrum image (PDF)
EDTA 2Na	ethylenediaminetetraacetic acid disodium salt	*
$BaNb_2O_6$	barium niobium oxide	*
$CaNb_2O_6+Ca_2Nb_2O_7$	calcium niobium oxide	*
$Cu(C_2H_5COO)_2H_2O$	copper propionate	**
Cu_2O	copper (I) oxide	**
$Cu_2C_6H_4O_7 \cdot 2.5H_2O$	copper citrate	*
$Cu(ClO_4)_2 \cdot 6H_2O$	copper perchlorate	*
CuI	copper (I) iodide	*
$Cu_2(OH)_3NO_3$	copper nitrate, basic	*
$CuC_2O_4 \cdot 0.5H_2O$	copper oxalate	*
$Cu(C_{17}H_{35}COO)_2$	copper stearate	*
$Cu(C_7H_{15}COO)_2 \cdot H_2O$	copper caprylate	**
$Cu(CH_3CHOHCOO)_2$	copper lactate	*
$CuF_2 \cdot 2H_2O$	copper fluoride	*
$Cu(C_7H_5O_3)_2 \cdot 2H_2O$	copper salicylate	*
$Cu(HCOO)_2 \cdot 4H_2O$	copper formate	*
$CuCl_2 \cdot 2NH_4Cl \cdot 2H_2O$	copper ammonium chloride	*

RASMIN


RASMIN
nb011 $BaNb_2O_6$
Intensisty, A.U.
1600
1400
1200
1000
800
600
400
200
0
Wavenumber, cm^{-1}

Bilbao Crystallographic Server

http://www.cryst.ehu.es/



Bilbao Crystallographic Server

Databases	
B-IncStrDB ⚠	The Bilbao Inconmensurate Crystal Structure Database

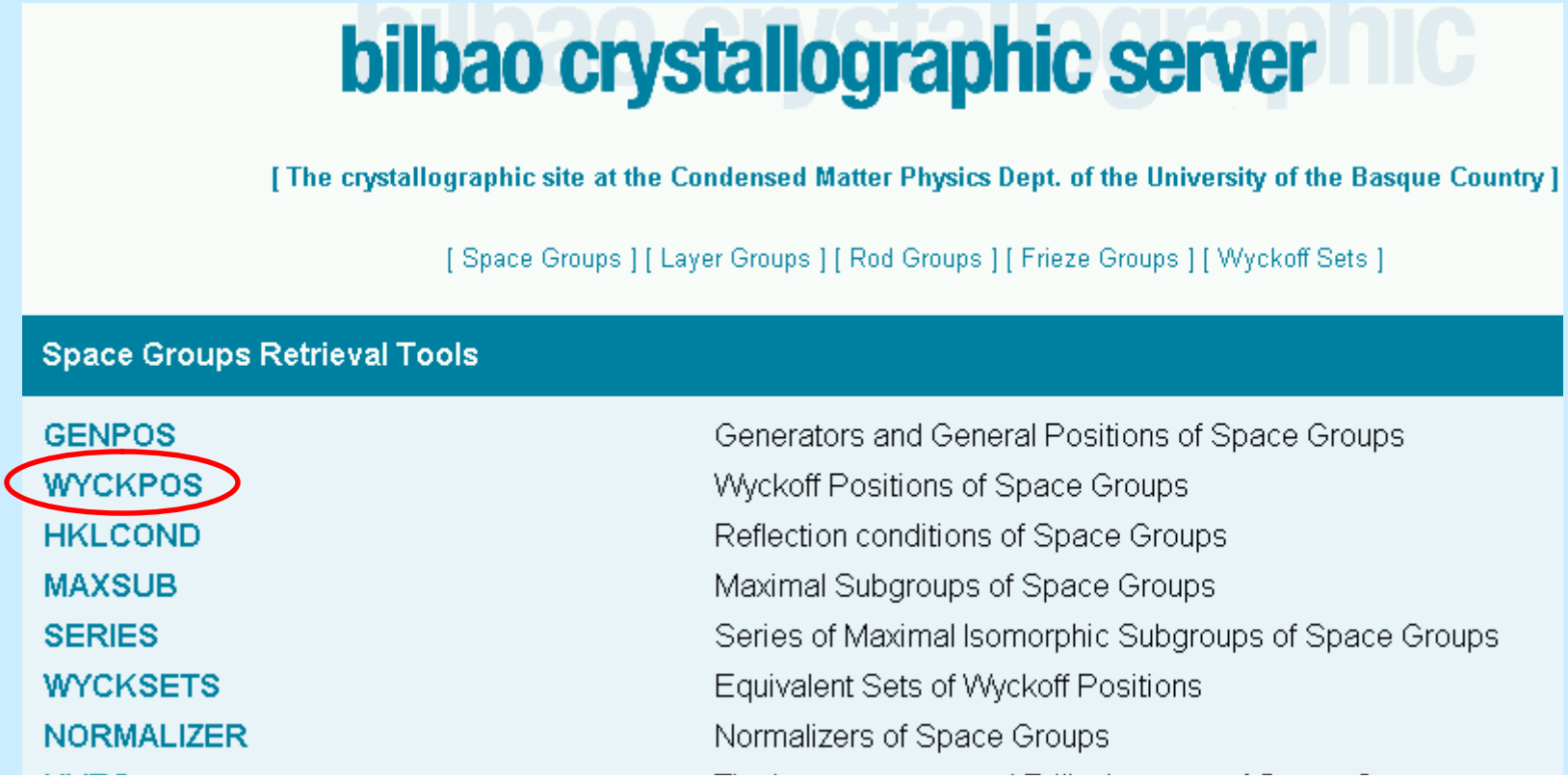
Raman and Hyper-Raman scattering	
SAM	Spectral Active Modes (IR, RAMAN and HYPER-RAMAN Selection Rules).
RAMAN AND HYPER-RAMAN TENSORS	Raman and Hyper-Raman tensors in any orientation
POLARIZATION SELECTION RULES	Polarization Selection Rules for Raman and Hyper-Raman Scattering processes
TWINS TENSORS	Raman or Hyper-Raman Tensors for Different Orientation Domains
CORRELATIONS POINTS	Relation between the symmetry modes in a high and low symmtry phases and their activity.
RAMAN CORRELATIONS SPACE	IR and Raman activity under a symmetry break for a given structures.
MORPHIC EFFECTS	Correlation relations for point groups under the action of an electric or magnetic field

Bilbao Crystallographic Server

$LiTaO_3$

R3C (161), координаты в гексагональных осях

Ta	0,	0,	0
Li	0,	0,	0.279
O	0.5,	0.34,	0.69

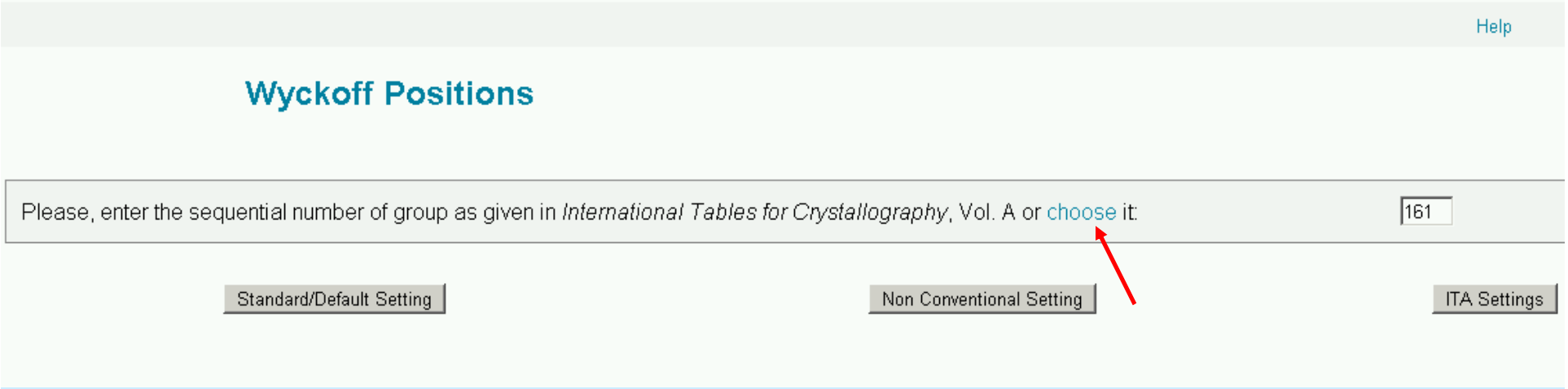


Bilbao Crystallographic Server

$LiTaO_3$

R3C (161), координаты в гексагональных осях

Ta	0,	0,	0
Li	0,	0,	0.279
O	0.5,	0.34,	0.69



Bilbao Crystallographic Server

$LiTaO_3$

R3C (161), координаты в гексагональных осях

Ta	0,	0,	0
Li	0,	0,	0.279
O	0.5,	0.34,	0.69

148	*R*-3:rhombohedral axes *R*-3:hexagonal axes	149	*P*312	150	*P*321
151	$P3_112$	152	$P3_121$	153	$P3_212$
154	$P3_221$	155	*R*32:rhombohedral axes *R*32:hexagonal axes	156	*P*3*m*1
157	*P*31*m*	158	*P*3*c*1	159	*P*31*c*
160	*R*3*m*:rhombohedral axes *R*3*m*:hexagonal axes	161	*R*3*c*:rhombohedral axes *R*3*c*:hexagonal axes	162	*P*-31*m*
163	*P*-31*c*	164	*P*-3*m*1	165	*P*-3*c*1
166	*R*-3*m*:rhombohedral axes *R*-3*m*:hexagonal axes	167	*R*-3*c*:rhombohedral axes *R*-3*c*:hexagonal axes	168	*P*6
169	$P6_1$	170	$P6_5$	171	$P6_2$
172	$P6_4$	173	$P6_3$	174	*P*-6
175	*P*6/*m*	176	$P6_3/m$	177	*P*622
178	$P6_122$	179	$P6_522$	180	$P6_222$
181	$P6_422$	182	$P6_322$	183	*P*6*mm*
184	*P*6*cc*	185	*P*6₃*cm*	186	*P*6₃*mc*

Bilbao Crystallographic Server

$LiTaO_3$

R3C (161), координаты в гексагональных осях

Ta	0,	0,	0
Li	0,	0,	0.279
O	0.5,	0.34,	0.69

Wyckoff Positions of Group 161 (*R3c*) [h axes]

Multiplicity	Wyckoff letter	Site symmetry	Coordinates
			(0,0,0) + (2/3,1/3,1/3) + (1/3,2/3,2/3) +
18	b	1	(x,y,z) (-y,x-y,z) (-x+y,-x,z) (-y,-x,z+1/2) (-x+y,y,z+1/2) (x,x-y,z+1/2)
6	a	3.	(0,0,z) (0,0,z+1/2)

Wyckoff position and site symmetry group of a specific point

Specify the point by its relative coordinates (in fractions or decimals)
Variable parameters (x,y,z) are also accepted

x = 0 y = 0 z = 0

Show

If you want to see the Wyckoff position in other setting, click here

Bilbao Crystallographic Server

$LiTaO_3$

R3C (161), координаты в гексагональных осях

Ta	0,	0,	0
Li	0,	0,	0.279
O	0.5,	0.34,	0.69

Space Group : 161 (*R*3*c*) [hexagonal axes]
Point : (0,0,0)
Wyckoff Position : 6a

Site Symmetry Group 3.

x,y,z	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	1
-y,x-y,z	$\begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	3^+ 0,0,z
-x+y,-x,z	$\begin{pmatrix} -1 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	3^- 0,0,z

Bilbao Crystallographic Server

$LiTaO_3$
R3C (161),

Atom	Coordinates	Wyckoff position
Ta	0, 0, 0	6a
Li	0, 0, 0.279	6a
O	0.5, 0.34, 0.69	18b

Raman and Hyper-Raman scattering

SAM	Spectral Active Modes (IR, RAMAN and HYPER-RAMAN Selection Rules)
RAMAN AND HYPER-RAMAN TENSORS	Raman and Hyper-Raman tensors in any orientation
POLARIZATION SELECTION RULES	Polarization Selection Rules for Raman and Hyper-Raman Scattering proc
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MORPHIC EFFECTS	Correlation relations for point groups under the action of an electric or mag

Bilbao Crystallographic Server

IR Raman and Hyper-Raman Modes

◉ **OPTION 1: Space group**

Enter the sequential number of group as given in *International Tables for Crystallography*, Vol. A or choose it: 161

○ **OPTION 2: Structure**

Structure Data
[in CIF format]

HINT: [The option for a given filename is preferential]

```
# Comments start with #
# Space Group ITA number
167
# Lattice parameters
4.7597 4.7597 12.9935 90 90 120
# Number of independent atoms in the asym
2
# [atom type] [number] [WP] [x] [y] [z]
Al 1 12c 0.0000 0.0000 0.3523
O  1 18e 0.3065 0.0000 0.2500
```

Structure

Show

Bilbao Crystallographic Server

$LiTaO_3$

R3C (161),

Atom	Coordinates	Wyckoff position
Ta	0, 0, 0	6a
Li	0, 0, 0.279	6a
O	0.5, 0.34, 0.69	18b

Choose the Wyckoff Positions of the atoms in your structure for the space group *R*3*c* (No. 161) [hexagonal axes]

Check	WP	Representative
☑	18b	x,y,z
☑	6a	0,0,z

Continue

Bilbao Crystallographic Server

Information of the Point Group C_{3v} (3m)

Character Table[1]

C_{3v}(3m)	#	1	3	m	functions
Mult.	-	1	2	3	·
A_1	Γ_1	1	1	1	z,x^2+y^2,z^2
A_2	Γ_2	1	1	-1	J_z
E	Γ_3	2	-1	0	$(x,y),(xz,yz),(x^2-y^2,xy),(J_x,J_y)$

To get the list of the **irreducible representations in their matrix form** please click **here**.

Raman Tensors

A_1,z			E,x			E,y		
a	·	·	·	c	d	c	·	·
·	a	·	c	·	·	·	-c	d
·	·	b	d	·	·	·	d	·

Hyper-Raman Tensors

A_2			A_1,z			E,x*			E,y		
a	-a	·	·	·	·	3d	d	f	·	·	·
·	·	·	-b	b	·	·	·	·	d	3d	f
·	·	·	c	c	d	·	·	·	e	-e	·

Bilbao Crystallographic Server

Information of the Point Group C_{3v} (3m)

точечная группа

число операций в каждом классе

Character Table[1]

C_{3v}(3m)	#	1	3	m	functions
Mult.	-	1	2	3	.
A_1	Γ_1	1	1	1	z,x^2+y^2,z^2
A_2	Γ_2	1	1	-1	J_z
E	Γ_3	2	-1	0	$(x,y),(xz,yz),(x^2-y^2,xy),(J_x,J_y)$

активные в КР

активные в ИК

вращательные

To get the list of the **irreducible representations in their matrix form** please click **here**.

Raman Tensors

A_1,z			E,x			E,y		
a	·	·	·	c	d	c	·	·
·	a	·	c	·	·	·	-c	d
·	·	b	d	·	·	·	d	·

Hyper-Raman Tensors

A_2			A_1,z			E,x*			E,y		
a	-a	·	·	·	·	3d	d	f	·	·	·
·	·	·	-b	b	·	·	·	·	d	3d	f
·	·	·	c	c	d	·	·	·	e	-e	·

Bilbao Crystallographic Server

- **IR Active Modes: ($\Gamma_{acoustic} = A_1 + E$)**

WP	A_1	A_2	E
18b	3	·	6
6a	1	·	2

- **Raman Active Modes**

WP	A_1	A_2	E
18b	3	·	6
6a	1	·	2

- **Hyper-Raman Active Modes**

WP	A_1	A_2	E
18b	3	3	6
6a	1	1	2

The polarization selection rules for Raman and Hyper-Raman processes.

Modes Activity

This table is a summary of the activity of the different modes of the space group.

-	A_1	A_2	E
Infrared	x	·	x
Raman	x	·	x
Hyper-Raman	x	x	x

Note: x ≡ represents the modes which can be detected.

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Polarization Selection Rules

Back scattering geometry

If you want to know more about this configuration please click here.

	A_1(LO)	A_1(TO)	E(LO)	E(TO)
-X(YY)X	·	x	·	x
-X(YZ)X	·	·	·	x
-X(ZZ)X	·	x	·	·
-Y(XX)Y	·	x	x	·
-Y(XZ)Y	·	·	·	x
-Y(ZZ)Y	·	x	·	·
-Z(XX)Z	x	·	·	x
-Z(XY)Z	·	·	·	x
-Z(YY)Z	x	·	·	x

Note: x ≡ represents the modes that can be observed in each one of the directions
In the first column the experimental configuration in **Porto's notation** is given.

Right angle scattering geometry

If you want to know more about this configuration please click here

	A_1(LO+TO)	A_1(TO)	E(LO+TO)	E(TO)
X(YY)Z	x	·	·	x
X(YZ)Y	·	·	x	·
X(ZZ)Y	·	x	·	·
Y(XX)Z	x	·	x	·
Y(XY)X	·	·	x	·
Y(XY)Z	·	·	·	x
Y(XZ)X	·	·	x	·
Y(ZZ)X	·	x	·	·
Z(XX)Y	x	·	x	·
Z(XY)X	·	·	x	·
Z(XZ)X	·	·	x	·
Z(XZ)Y	·	·	·	x
Z(YY)X	x	·	·	x
Z(YZ)X	·	·	·	x
Z(YZ)Y	·	·	x	·

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More information: show hide

Permutational Representation

The permutational representation represents

WP	A_1	A_2	E
18b	1	1	2
6a	1	1	·

Mechanical Representation

The mechanical representation is defined as

WP	A_1	A_2	E	Modes
18b	3	3	6	Show
6a	1	1	2	Show

Note: Click in the *Show* option to obtain the sym

Irreps decompositions

In the following table one can find the decom

C_{3v} (3m)	A_1	A_2	E
V	1	·	1
A	·	1	1
$[V^2]$	2	·	2
$[V^2] \times V$	4	2	6

Information about second order processes: show hide

Second Order IR Activity

In the next table one can find the information the second order IR active modes:

⊗	A_1	A_2	E
A_1	**A_1**	A_2	**E**
A_2	·	**A_1**	**E**
E	·	·	**$A_1 + A_2 + E$**

Active Inactive **bold** IR active modes

Second Order Raman Activity

In the next table one can find the information the second order Raman active modes:

⊗	A_1	A_2	E
A_1	**A_1**	A_2	**E**
A_2	·	**A_1**	**E**
E	·	·	**$A_1 + A_2 + E$**

Active Inactive **bold** Raman active modes

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Правила отбора:

Atom R3C 161	Coordinates (hexagonal axes)	Wyckoff position	G-point phonon modes	
Ta	0,0,0	6a	$\mathbf{A}_1+2\mathbf{E}+A_2$	
Li	0,0,0.279	6a	$\mathbf{A}_1+2\mathbf{E}+A_2$	
O	0.5, 0.34, 0.69	18b	$3\mathbf{A}_1+6\mathbf{E}+3A_2$	
Modes classification				
$\Gamma_{raman}=5A_1+10E$	$\Gamma_{ir}=5A_1+10E$	$\Gamma_{ac}=A_1+E$		$\Gamma_{meh}=5A_1+5A_2+10E$
Raman tensors				
A_1, z $\begin{bmatrix} a & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & b \end{bmatrix}$	E,x $\begin{bmatrix} c & 0 & 0 \\ 0 & -c & d \\ 0 & d & 0 \end{bmatrix}$		E,y $\begin{bmatrix} 0 & c & d \\ c & 0 & 0 \\ d & 0 & 0 \end{bmatrix}$	

Моды, ожидаемые в спектре КР $4A_1+9E$

Моды, ожидаемые в спектре гипер КР $4A_1+9E+5A_2$

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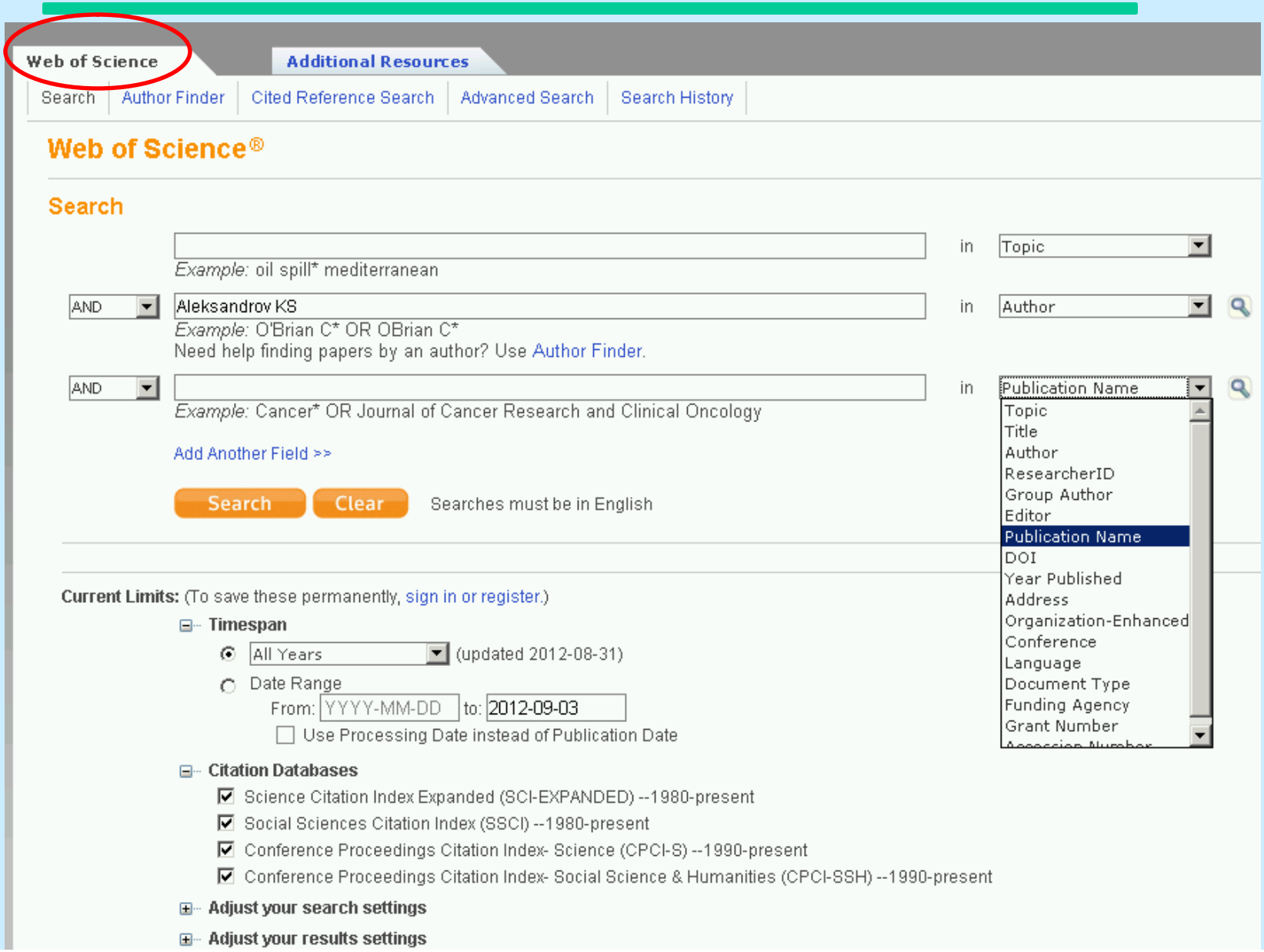

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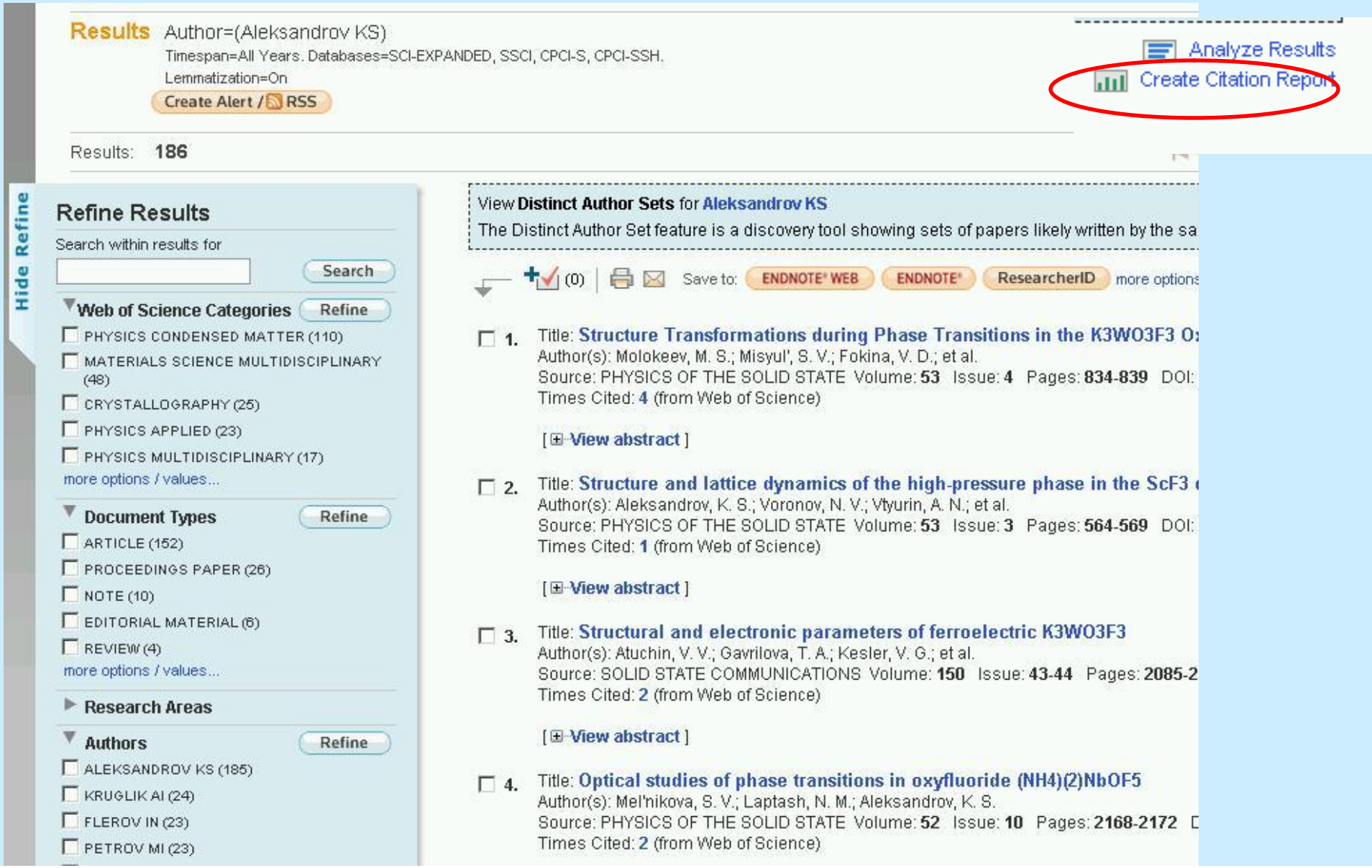

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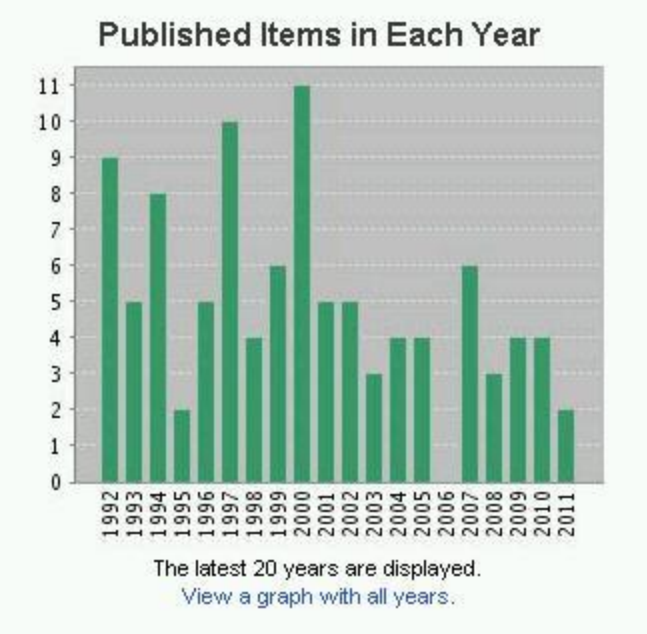

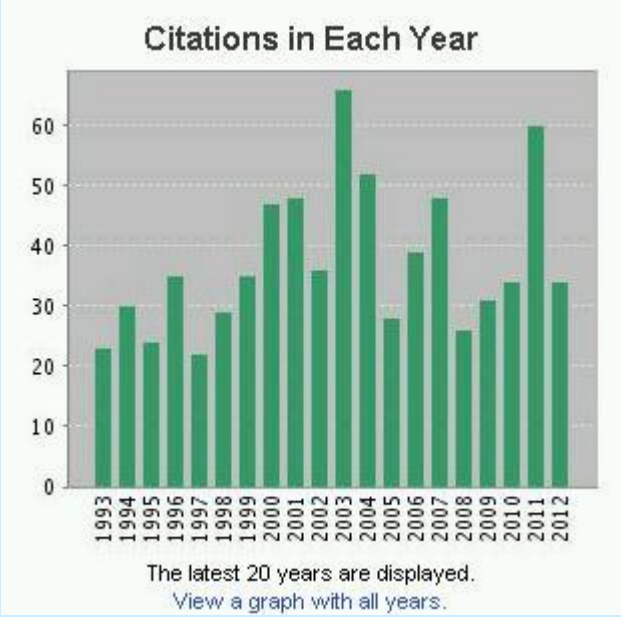

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2. Title: **PHASE-TRANSITIONS IN THE PEROVSKITE-LIKE A2BX4 STRUCTURE** Author(s): HATCH, DM; STOKES, HT; ALEKSANDROV, KS; et al. Source: PHYSICAL REVIEW B Volume: **39** Issue: **13** Pages: **9282-9288** DOI: **10.11**	1	2	1	2	2	39	1.62
3. Title: **Influence of static electric field, mechanical pressure and temperatur** Author(s): Sorokin, BP; Turchin, PP; Burkov, SI; et al. Book Group Author(s): IEEE Conference: **1996 IEEE International Frequency Control Symposium** Location: **HONOL** Sponsor(s): **IEEE, Ultrason Ferroelect & Frequency Control Soc** Source: PROCEEDINGS OF THE 1996 IEEE INTERNATIONAL FREQUENCY CONTRO	1	4	3	5	1	35	2.06
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Phase transitions in elpasolites (ordered perovskites)

Author(s): Flerov, IN (Flerov, IN); Gorev, MV (Gorev, MV); Aleksandrov, KS (Aleksandrov,

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the possibility of describing these transitions in the framework of the thermodynamic L
temperature of phase transitions. The hypothesis of bond stresses is able to predict th
phase transitions in elpasolites and related compounds has also been considered. O
with monoatomic cations. On the other hand, for instance, in cryolites with ammonium

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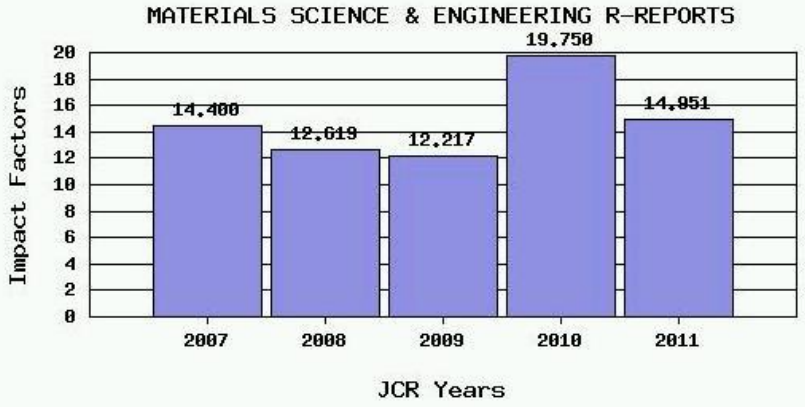

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Cites in 2011 to articles published in:	2010 = 256	Number of articles published in:	2010 = 29
	2009 = 357		2009 = 12
	Sum: 613		Sum: 41

Calculation: Cites to recent articles 613 = **14.951**
Number of recent articles 41

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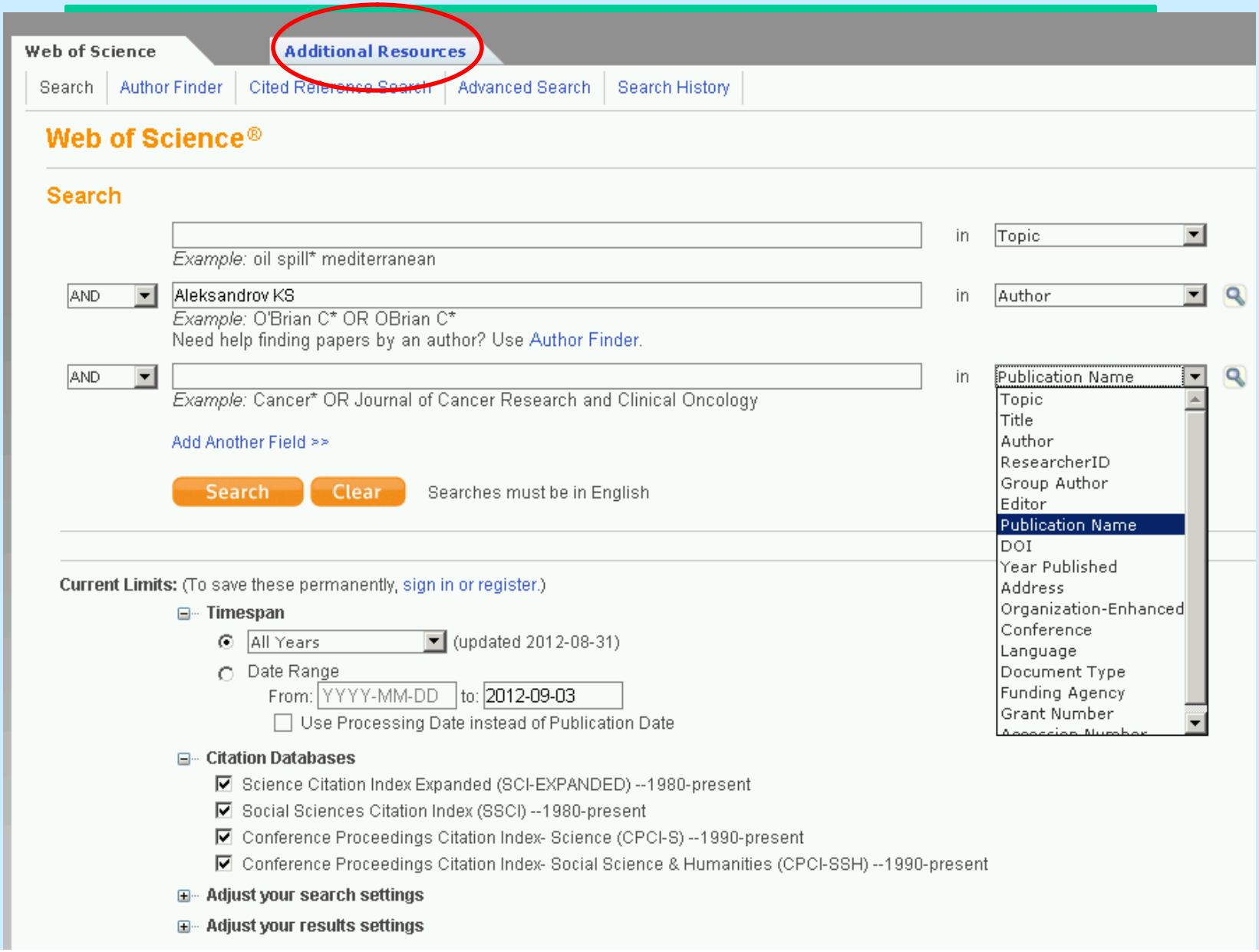

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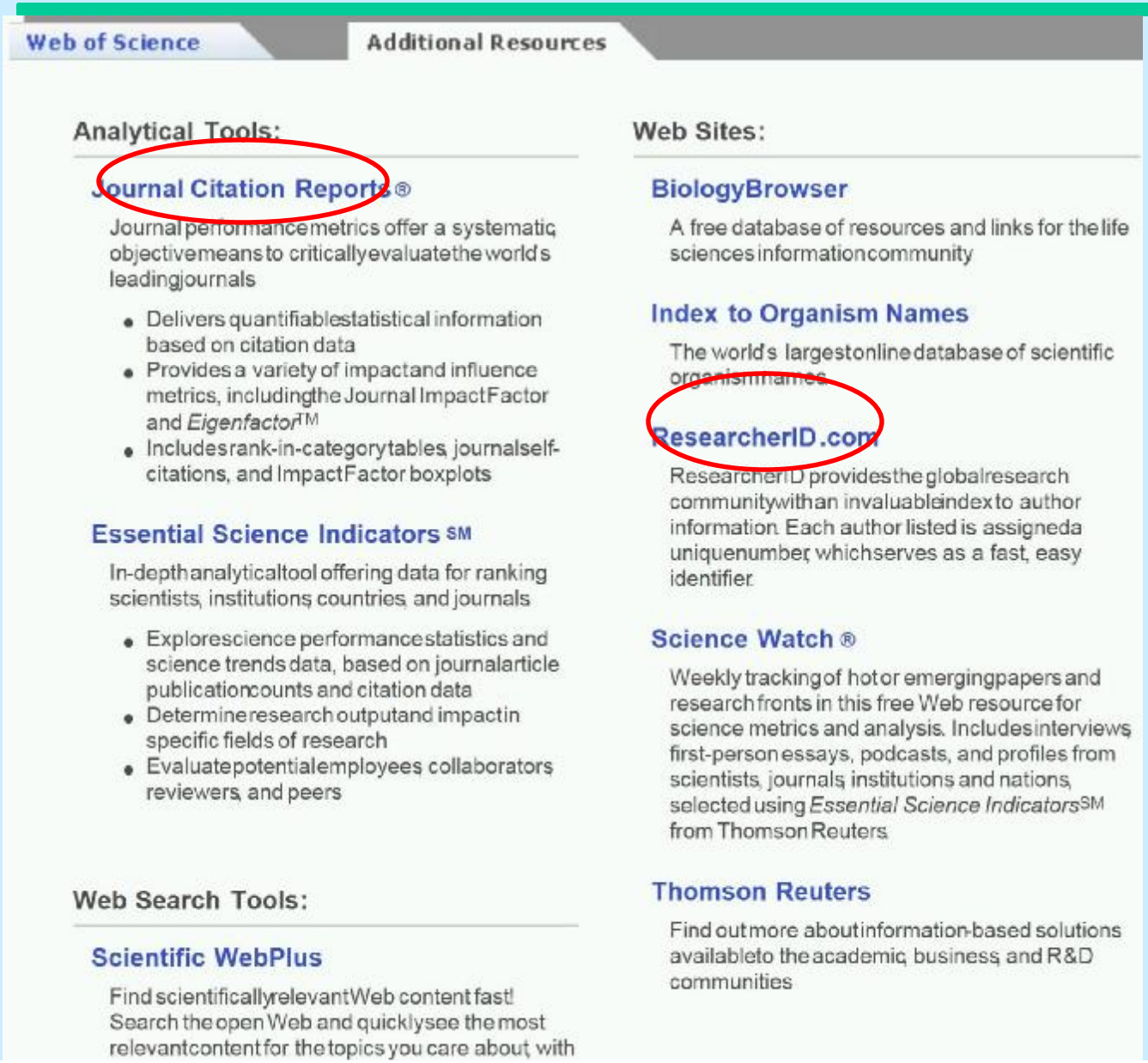

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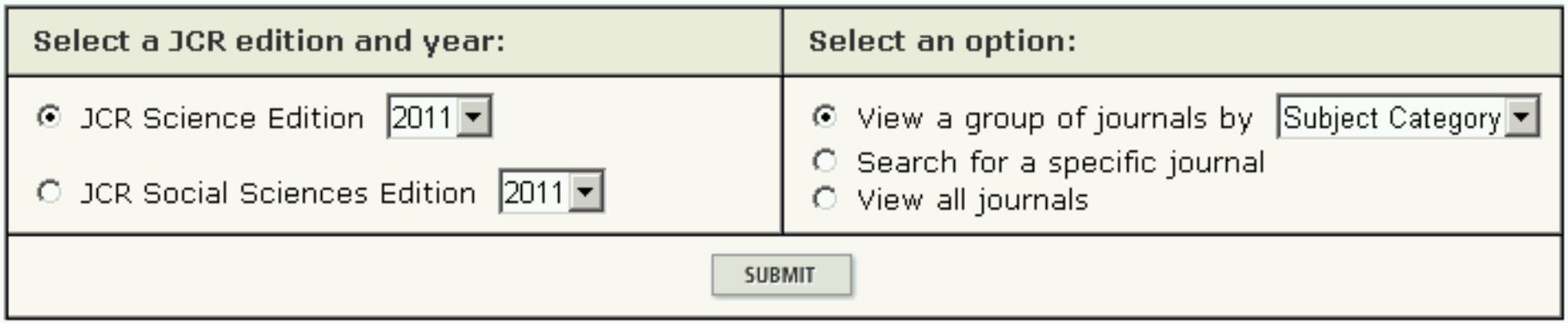

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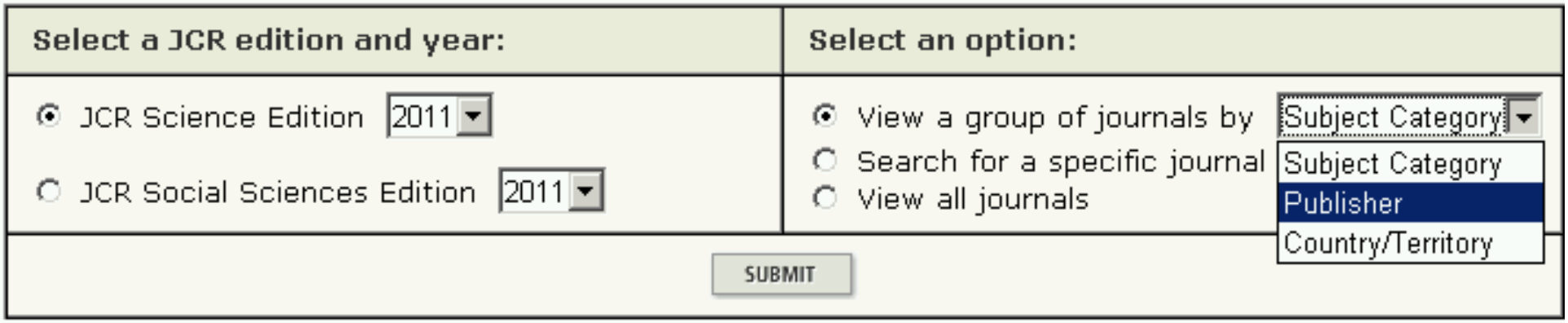

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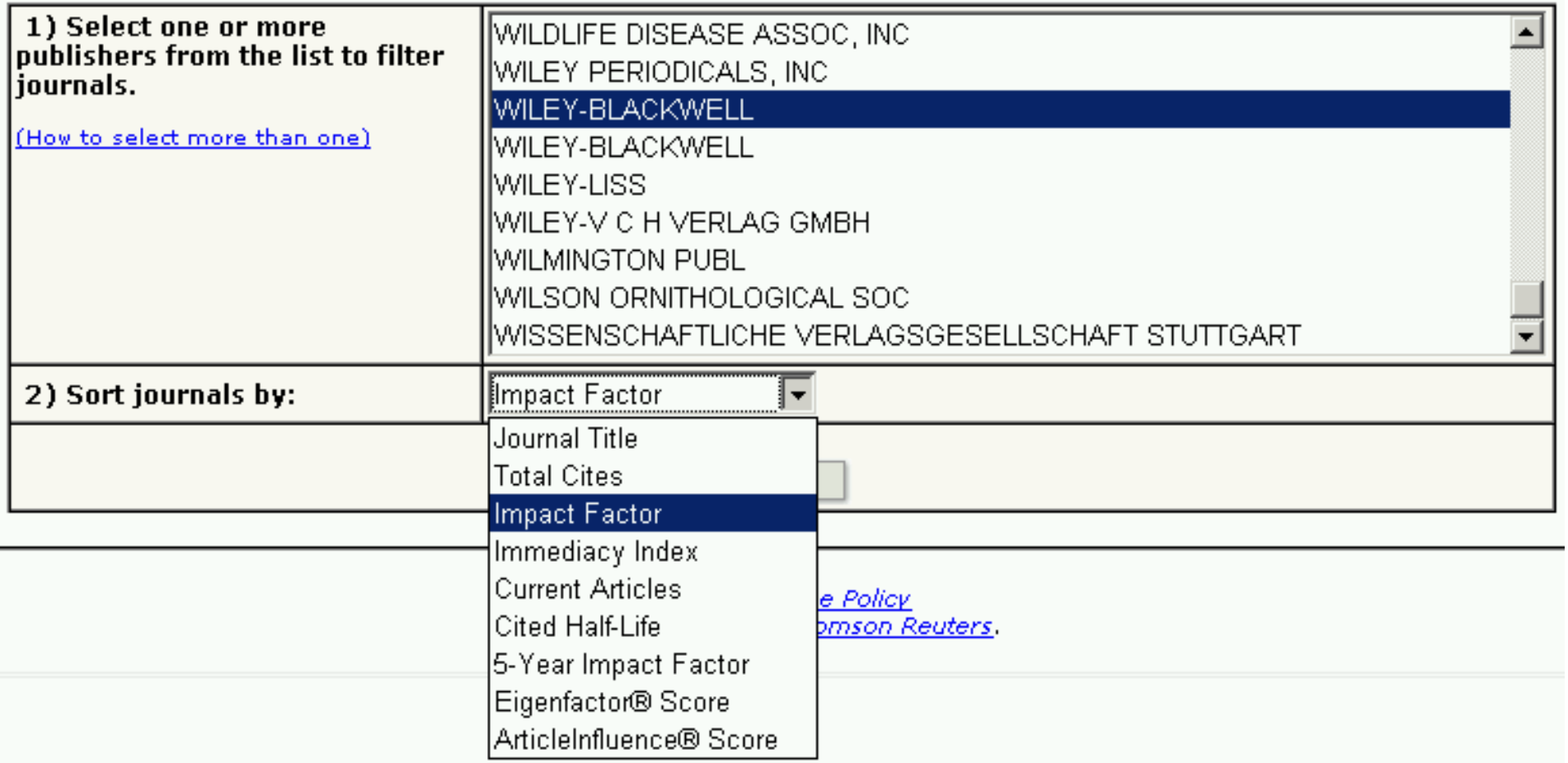

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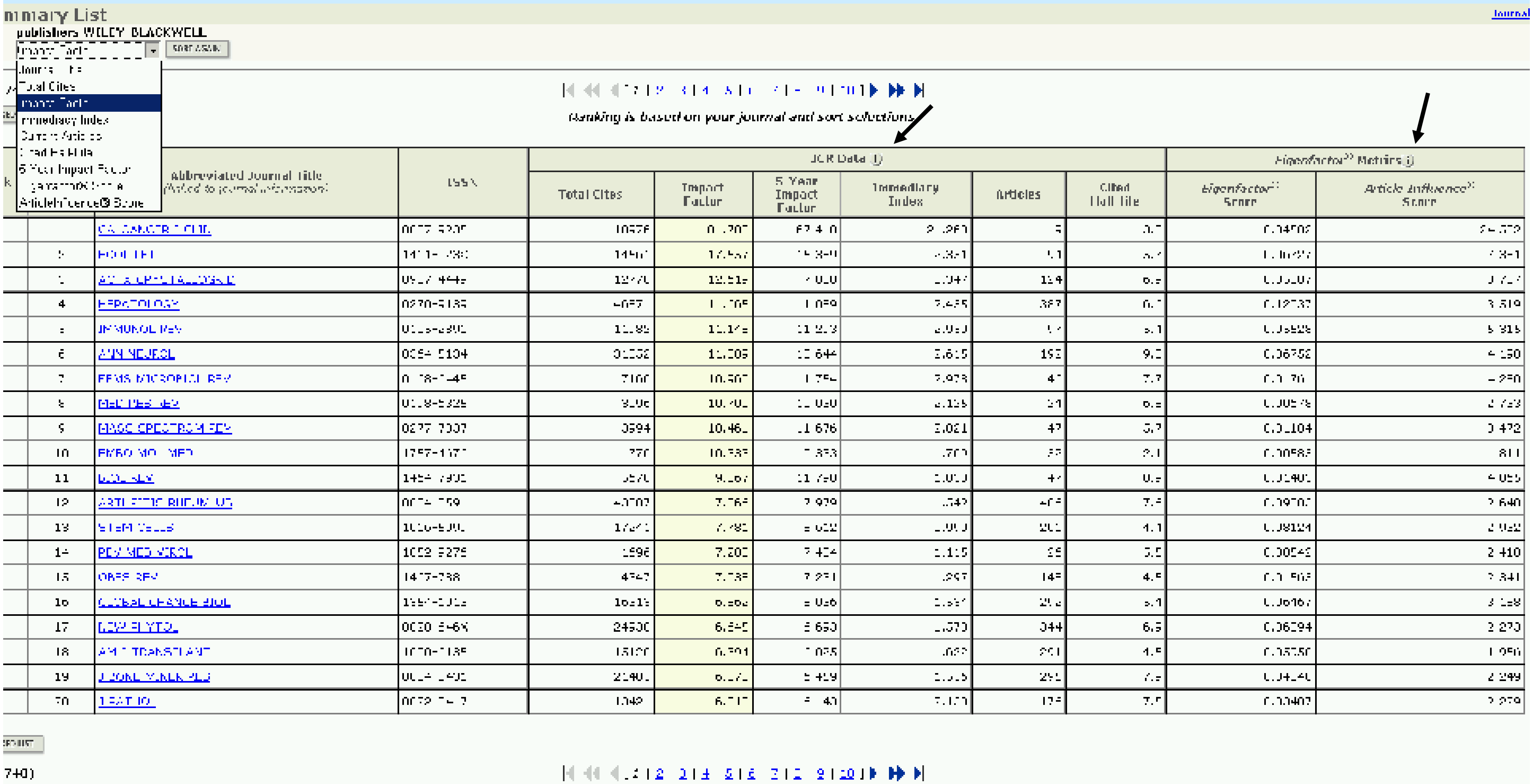

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10	EMBO MOL MED	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	811
11	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
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16	GLOBAL CHANGE BIOL	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
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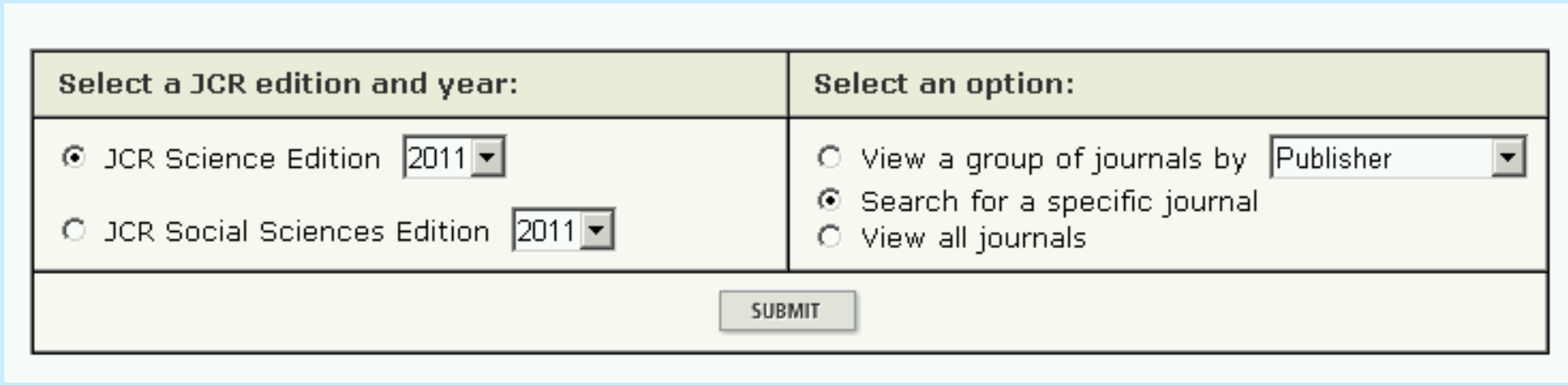

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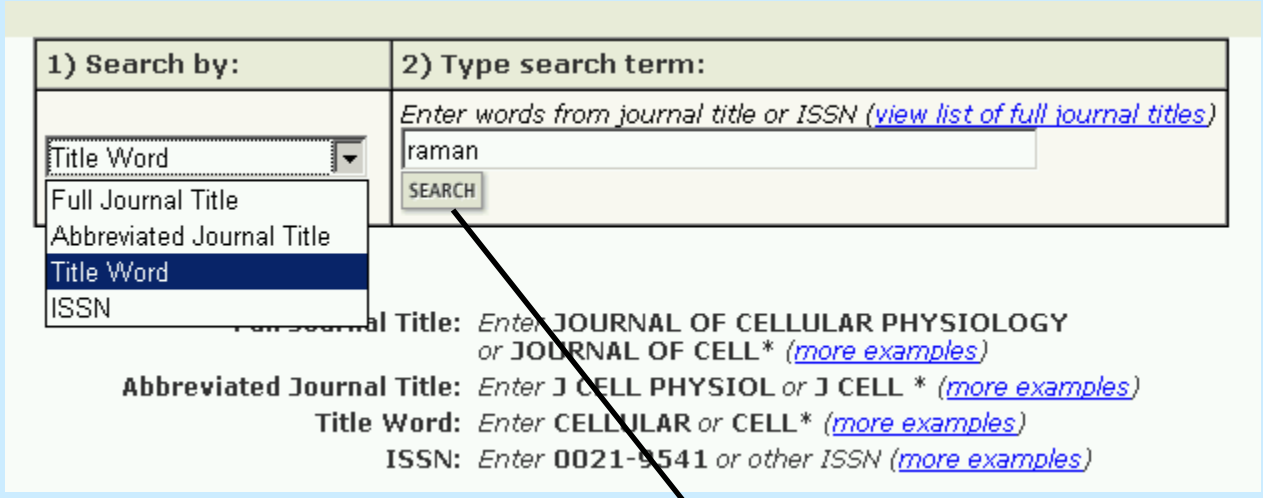

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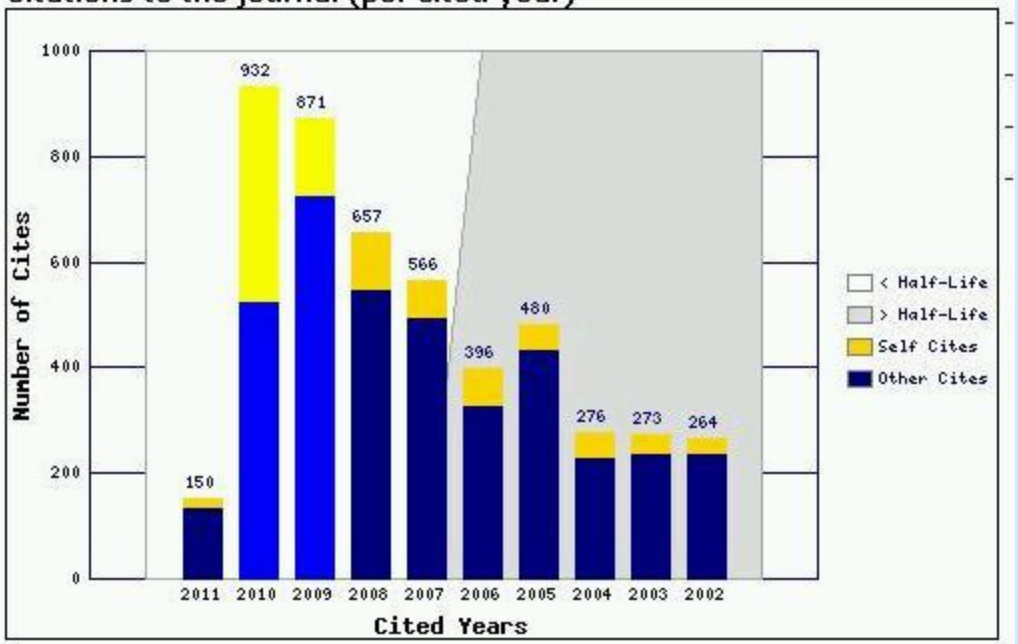

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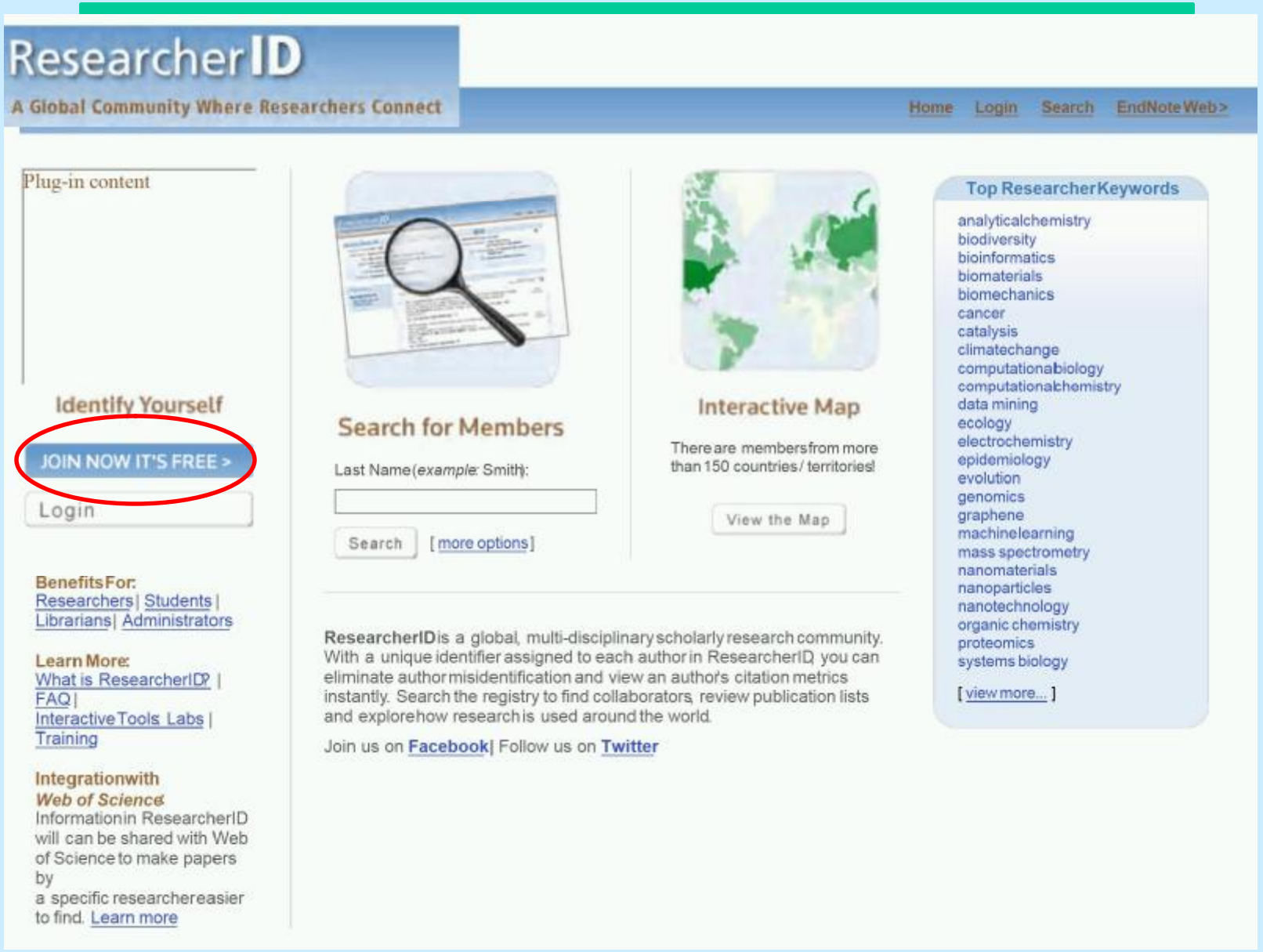

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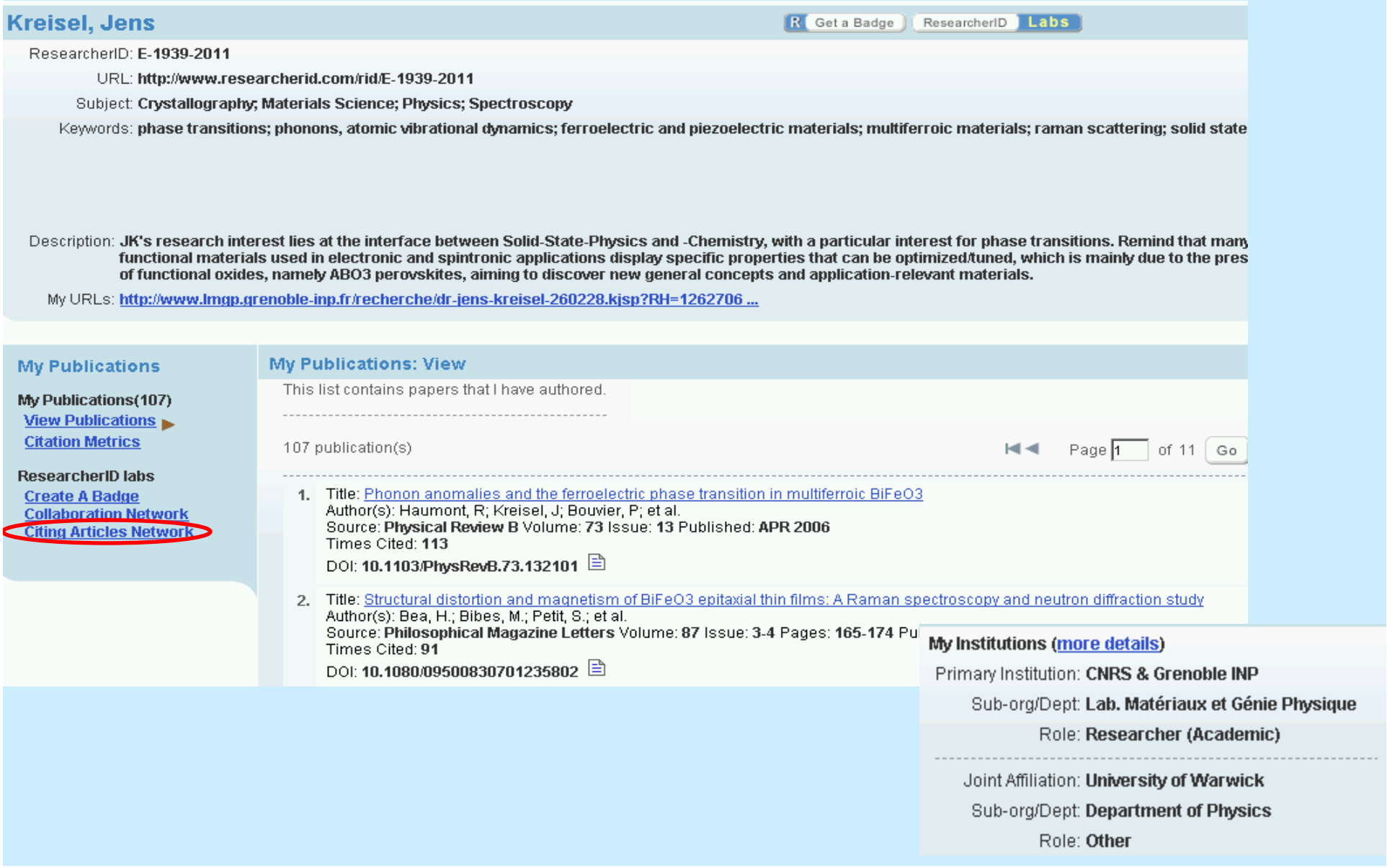

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Description: **JK's research interest lies at the interface between Solid-State-Physics and -Chemistry, with a particular interest for phase transitions. Remind that many functional materials used in electronic and spintronic applications display specific properties that can be optimized/tuned, which is mainly due to the pres of functional oxides, namely ABO3 perovskites, aiming to discover new general concepts and application-relevant materials.**

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Times Cited: **113**
DOI: **10.1103/PhysRevB.73.132101**

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Source: **Philosophical Magazine Letters** Volume: **87** Issue: **3-4** Pages: **165-174** Pu
Times Cited: **91**
DOI: **10.1080/09500830701235802**

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Primary Institution: **CNRS & Grenoble INP**
Sub-org/Dept: **Lab. Matériaux et Génie Physique**
Role: **Researcher (Academic)**

Joint Affiliation: **University of Warwick**
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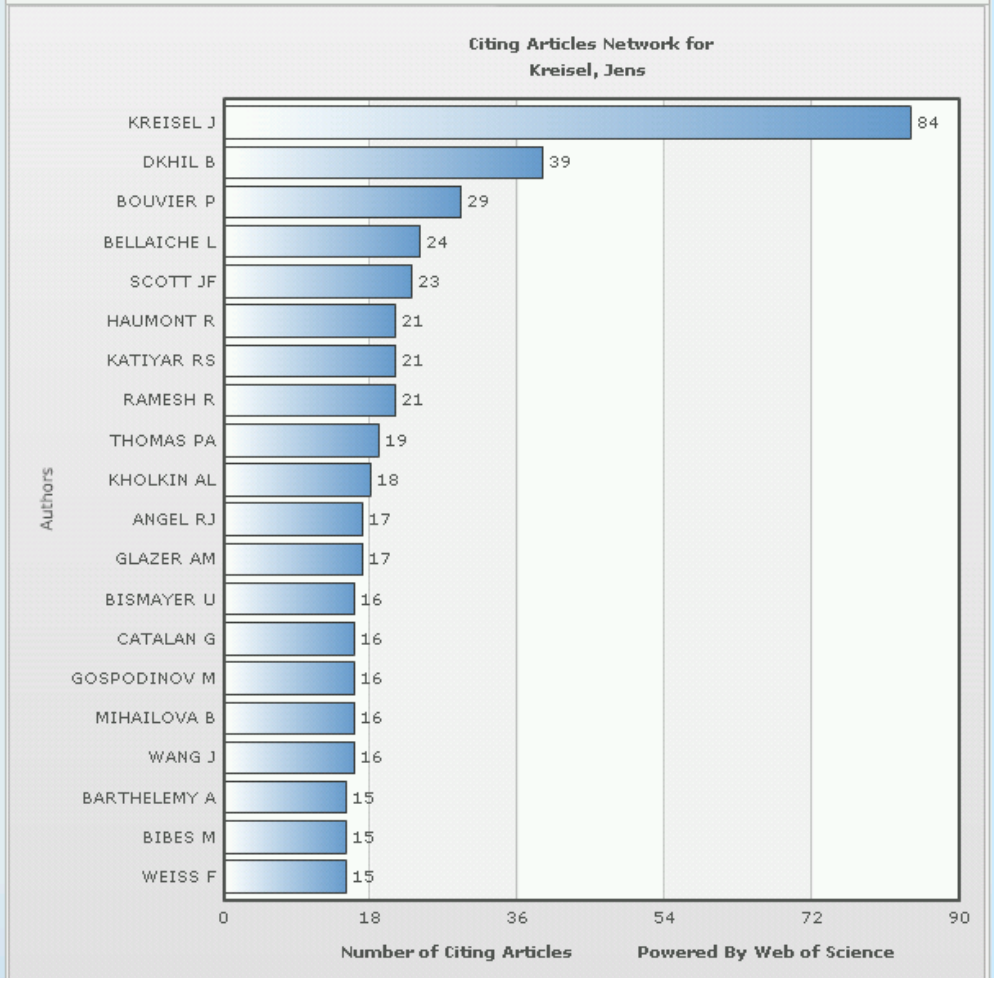
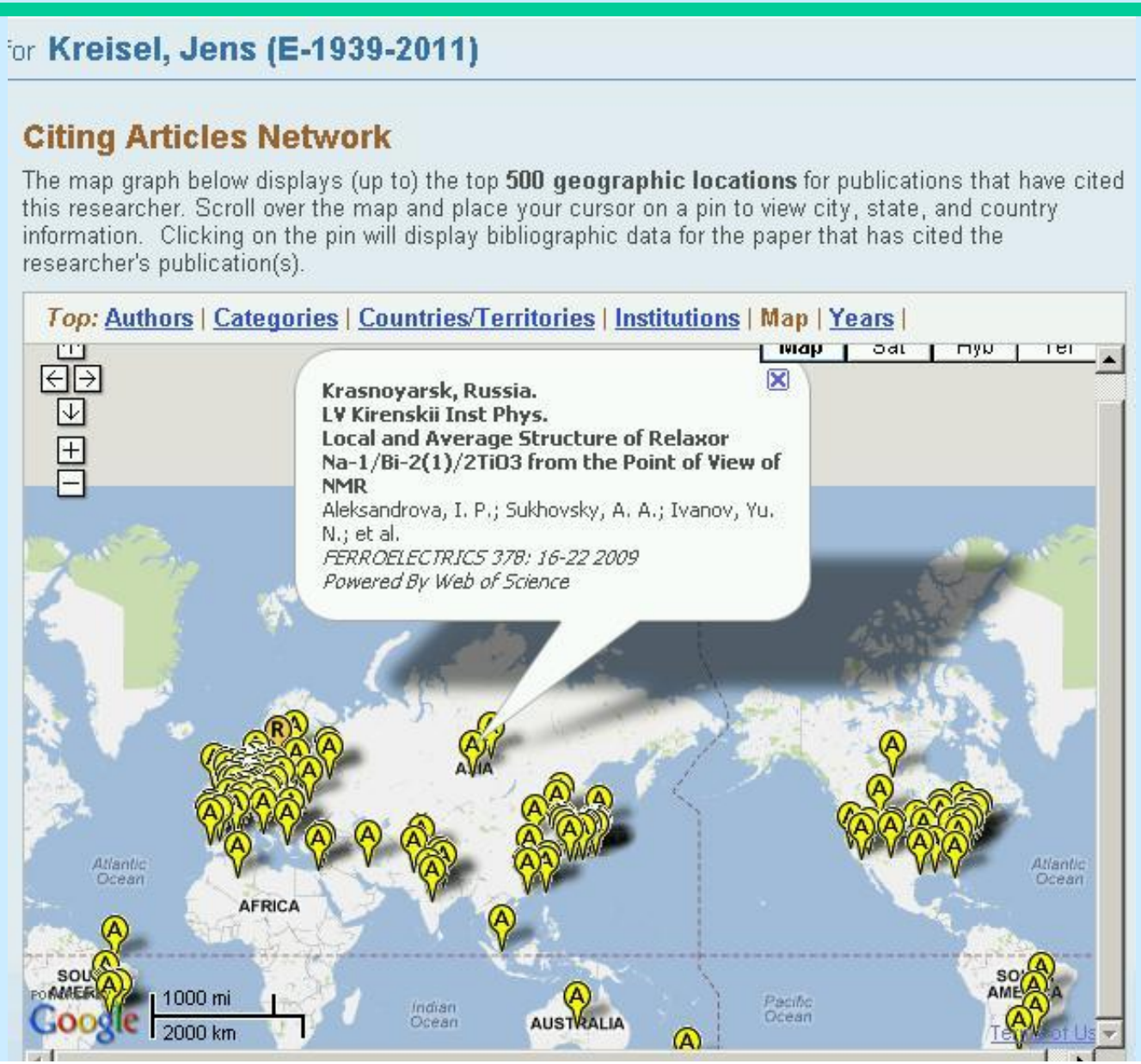


Researcher ID



Спасибо за внимание!