



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



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

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«Спектроскопия комбинационного рассеяния света»

# Доступная информация

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

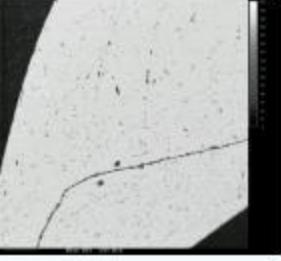
# RUFF

Almandine	R040076	$Fe^{2+} _3 Al_2 (SiO_4)_3$	University of Arizona Mineral Museum 7976	Barton Garnet mine, Gore Mountain, Warren	
Almandine	R040079	$Fe^{2+} _3 Al_2 (SiO_4)_3$	University of Arizona Mineral Museum 13736	Ontario, Canada	
Almandine	R040168	$Fe^{2+} _3 Al_2 (SiO_4)_3$	University of Arizona Mineral Museum 16323	Pocos Dos Cavatos, Ceara, Brazil	
Almandine	R050029	$Fe^{2+} _3 Al_2 (SiO_4)_3$	University of Arizona Mineral Museum 4307	Barton Garnet mine, Gore Mountain, Warren	
Almandine	X050009	$Fe^{2+} _3 Al_2 (SiO_4)_3$	George R. Rossman GRR-943	Riverside County, California, USA	
Almandine	X050010	$Fe^{2+} _3 Al_2 (SiO_4)_3$	George R. Rossman GRR-1056	Wrangel, Alaska, USA	
Almandine	X050011	$Fe^{2+} _3 Al_2 (SiO_4)_3$	George R. Rossman GRR-43	Rutherford #2 mine, Amelia, Virginia, USA	
Almandine	R060099	$Fe^{2+} _3 Al_2 (SiO_4)_3$	Roland Boehne	Alaska, USA	
Almandine	R060450	$Fe^{2+} _3 Al_2 (SiO_4)_3$	Gemological Institute of America 16606	Canada	
Almandine	R070129	$Fe^{2+} _3 Al_2 (SiO_4)_3$	Michael Scott S100422	Wrangell, Wrangell Island, Wrangell-Petersb	
Almandine	R100046	$Fe^{2+} _3 Al_2 (SiO_4)_3$	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, Cur	
Altaite	R060939	PbTe	Michael Scott S100891	870 Level, Mattagami mine, Matagami, Quebec	
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 Apsheren peninsula, Caspian Sea, Azerbaijan	
Lumohydrocalcite	R061067	$CaAl_2(CO_3)_2(OH)_4 \cdot 3H_2O$	Michael Scott S100395	Lubom'ra, Czech Republic	

# RUFF

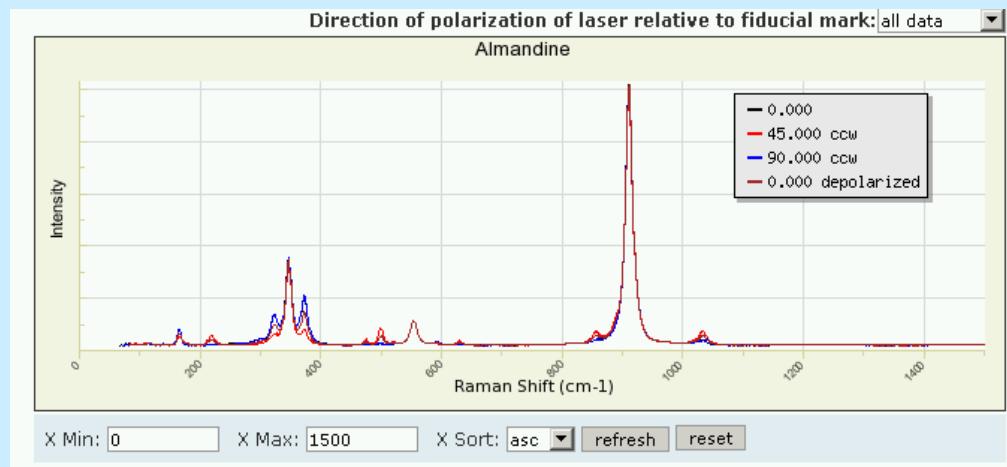
 Name: Almandine  
RRUFF ID: R040168  
Ideal Chemistry:  $\text{Fe}^{2+} \text{Al}_3(\text{SiO}_4)_3$   
Locality: Pocos Dos Cavatos, Ceara, Brazil  
Source: University of Arizona Mineral Museum  
Owner: RRUFF  
Description: Dark red etched single crystal  
Status: The identification of this mineral has been confirmed by Raman spectroscopy

Quick search: [ All Almandine samples (11) ]

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

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

 Raman Mode Analysis



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 <sub>1g</sub>	A <sub>1u</sub>	A <sub>2g</sub>	A <sub>2u</sub>	E <sub>u</sub>	E <sub>g</sub>	T <sub>2u</sub>	T <sub>2g</sub>	T <sub>1u</sub>	T <sub>1g</sub>
96h	3	-	-	-	-	6	-	9	-	-
24d	-	-	-	-	-	1	-	3	-	-
24c	-	-	-	-	-	1	-	2	-	-
16a	-	-	-	-	-	-	-	-	-	-

Total number of modes:  
 $3\text{A}_{1g} + 8\text{E}_g + 14\text{T}_{2g} = 25$

# RUFF

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

**DOWNLOADS:**

- Raman Data (RAW)
- RRUFF File

Almandine

Intensity

Wave Numbers (cm<sup>-1</sup>)

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

**DOWNLOADS:**

- Infrared Data (RAW)
- RRUFF File

```
##NAMES=Almandine
##LOCALITY=Pocos Dos Cavatos, Ceara, Brazil
##RRUFFID=R040168
##CHEMISTRY=Fe2+2+_3_Al2(SiO4)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
```

# 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 Mineralogical Society of America
- Manning P G (1967) The optical absorption spectra of the garnets almandine-pyrope, pyrope and spessartine and some structural interpretations of mineralogical significance, American Mineralogist, 52, 100-110 [\[view file\]](#)
- 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, 35-45
- 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, 100-106
- Griffen D T, Hatch D M, Phillips W R, Kulaksiz S (1992) Crystal chemistry and symmetry of a birefringent tetragonal pyralspite<sub>75</sub>-grandite<sub>25</sub> garnet, American Mineralogist, 79, 100-106
- 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 Mineralogische und Petrographische Zeitschrift, 72, 100-106
- Pilati T, Demartin F, Gramaccioli C M (1996) Atomic displacement parameters for garnets: A lattice-dynamical evaluation, Acta Crystallographica, B52, 239-250
- Chmielevá M, Martinec P, Weiss Z (1997) Almandine-pyrope-grossular garnets: a method for estimating their composition using X-ray powder diffraction patterns, European Journal of Mineralogy, 9, 100-106
- 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, Metals and Materials Society, 52, 100-106

# UCL pigment library

SEARCH SEARCH ADVANCED SEARCH

Records: 60

Raman Spectroscopic Library of UCL Black Pigments

10 authors' research in this field was reported in the 2008 edition of the *New Science* magazine, and one of their research papers has been selected as a 'Hot Article' for February 1, 2009 by the American Chemical Society.

Click on the logo to access the relevant ACS publications.

**Introduction to the site**

Raman microscopy is now established as the technique that is most specific, sensitive, rapidly refined and immune to interference for the non-destructive, in-situ analysis of pigmented objects. To complement the increasing use of the technique, this is the Raman spectra of eleven common organic and natural dyes, known to have been in use before 1850 AD, have been studied by Raman microscopy. Fifty pigments have a cited bibliographic history and these have been added to this library with their corresponding Raman spectra for reference purposes.

The spectra have been measured by Raman spectrometers which can be assessed according to the relevant literature. The spectra are available online. The only pigments that failed to give adequate spectra at either of the excitation wavelengths are indicated in a separate table. The spectra may be viewed by clicking on the name of the entries.

Spectral information in SPC format may be obtained via the spectra pages. They may be viewed in many spectroscopic software packages including QMol (Chem3D) (<http://www.cambridgeSoft.com/chem3d.html>), A free viewer for SPC files, eSpectra, may be down loaded from the Galactic Technologies page (<http://www.galactic.com>).

**Warning:**  
Before you proceed, please note that the wavenumbers quoted in the tables were obtained from spectra recorded with Neurite 100. The wavenumbers are available to  $\pm 1\text{ cm}^{-1}$ . A caption header marked as 'estimated' on the other side of the table. However, the SPC files have not yet been corrected and the band positions in the downloadable spectra may differ from those in the table.

**SERS NOTE:**  
Some users have experienced trouble with the downloadable SPC files. The uncorrected spectra have a gross non-linear distortion of the x-axis, which is owing to error with the uncorrected band position (see above statement). The SPC has now been released and are now reading correctly colour and, if you use it you will further problems, please contact the Webmaster. Thank you.

22nd May 2008

Some Raman libraries referred to the pigments have been provided and clicking the 'link' on the numbers in the table can access these. To reference the authors' publications in the hole of the Raman library click here.

Table of Black Pigments

# UCL pigment library

Table of Black Pigments

Name	Composition	Band Wavenumbers <sup>a</sup> / cm <sup>-1</sup> and Relative Intensities <sup>b</sup>	Excitation Wavelength & Power	Notes, References and Date <sup>c</sup>
iron black	carbon	951(w); 1011(s); PO <sub>2</sub> (s) > 1225vs(br) > 1300vs(br)	322.8 nm 5 mW	An quarry. Also contains Fe(II) in phosphate
iron oxide	carbon	> 1025vs(sh); > 1500vs(sh)	502.0 nm 5 mW	An quarry

<sup>a</sup> Approximate centres of broad bands in the laser fluorescence spectrum.

<sup>b</sup> s = strong, m = medium, w = weak, v = very, br = shoulder, b = broad

<sup>c</sup> The pigment is either assigned to be a mineral or the date of first manufacture is listed

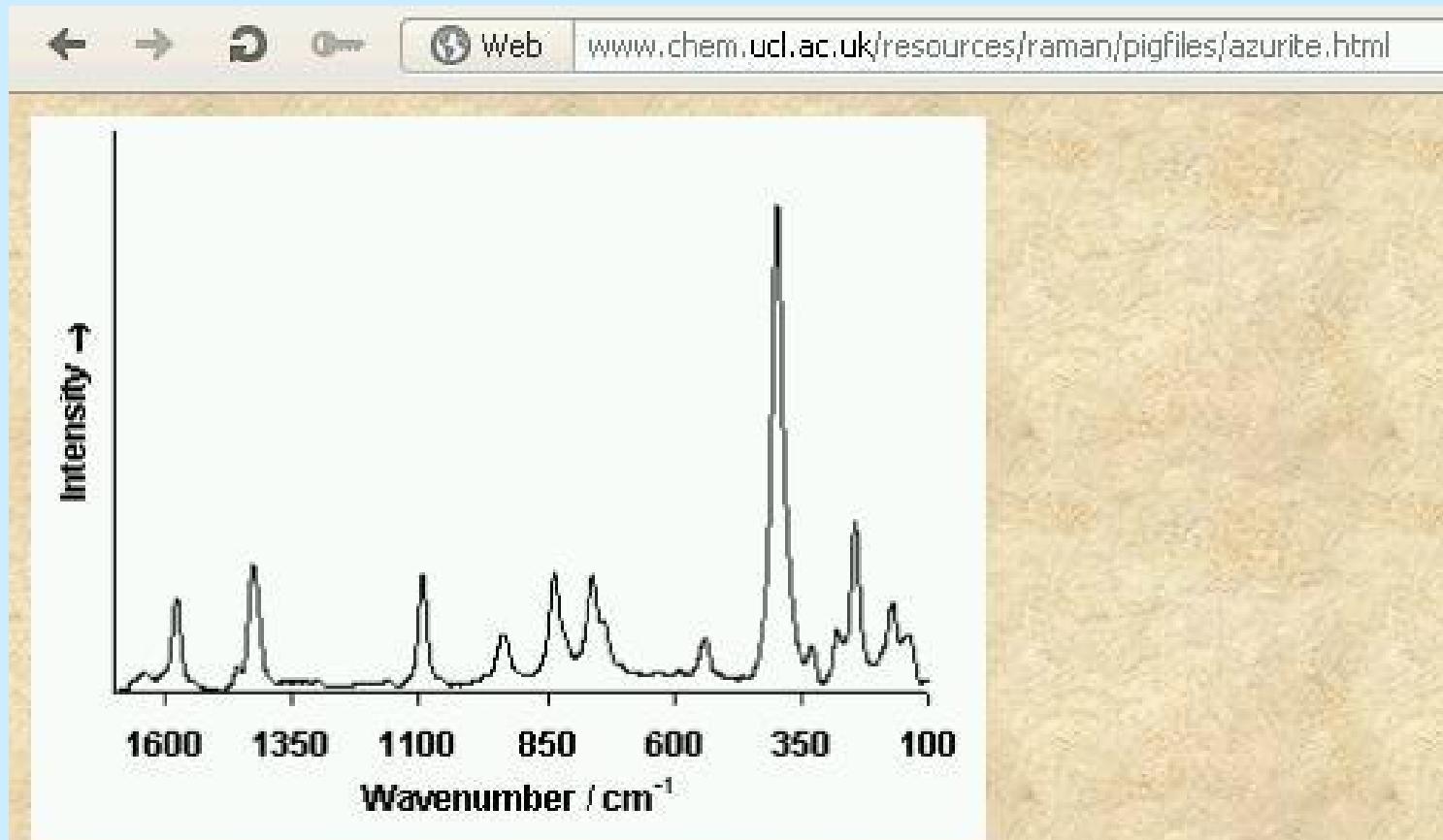
 [Open in Palette](#)

 [Back to Top](#)

Table of Blue Pigments

Name	Composition	Band Wavenumbers <sup>a</sup> / cm <sup>-1</sup> and Relative Intensities <sup>b</sup>	Excitation Wavelength and Power	Notes, References and Date <sup>c</sup>
<u>azurite</u>	basic copper(II) carbonate Cu <sub>2</sub> (OH) <sub>2</sub> CO <sub>3</sub>	470s; 570s; 770m; 274w; 325w; 413w; 561b; 720s; (sh); 777m; 830m; 940vs; 1150m; 1160w; 1381m; 1725w;	344.7 nm 2 mW	2004
cerulean blue	corundum alumina Al <sub>2</sub> O <sub>3</sub>	457m(s); 557s; 624w	344.7 nm 2 mW	182
cobalt blue	cobalt(II)-oxide, alumina - glass Co <sub>3</sub> O <sub>4</sub> .Al <sub>2</sub> O <sub>3</sub>	200vs; 312vs	514.5 nm 2 mW	1775

# UCL pigment library



Azurite



*Download SPC File*



*Back to Tables*

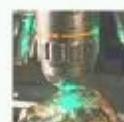
# Handbook of Minerals Raman Spectra

**Facilities**  
Raman microscopes 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 [mnmin@geologie-lyon.fr](mailto:mnmin@geologie-lyon.fr)

**Pressure calculation**  
- [wavelength in cm<sup>-1</sup>]  
- [wavelength in nm]

**To send spectrum**  
To help us to increase this data base, [\[fill the form\]](#) and send new spectra file.

**Links**  
The Ruff 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 Perma) [\[link\]](#)  
Raman data base of minerals (SPMC) [\[link\]](#)



Laser spot on a Pyrite sample

## Handbook of Minerals Raman Spectra



Search engine  
Enter phase name or part of the name  
[all] [advanced search]

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 isolated minerals. We report here more recent references and references for Raman studies carried out at high-pressure and high-temperatures are also mentioned. Most of the spectra were recorded on a XY DOLCOR 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<sup>+</sup> 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

#### Apachimaster

Librarie HR800 vis John Yvon Horiba  
internal-confocal microscope - mapping stage

Librarie HR800 vis John Yvon Horiba  
confocal microscope and fiber entrance

Librarie HR800 UV John Yvon Horiba

KV Dilar

#### laser source

Spectra Physics® 2018 Ar<sup>+</sup>/Kr<sup>+</sup> 847.1 nm 514.5 nm 457.9 nm  
HeNe 632.8 nm

Spectra Physics® 2017 Ar<sup>+</sup> 514.5 nm

Spectra Physics® WaveTrain 24-nm

Spectra Physics® 1730 Ar<sup>+</sup> 514.5 nm, 488nm, 457.9 nm

[This page is in progress]  
Gilles Montagnac@ens-lyon.fr

# Handbook of Minerals Raman Spectra

All spectra *Handbook of Raman Spectra*

[actinote] [akimotoite (synthetic ilmenite type)] [albite] [albite glass] [almandine] [anatase] [andalusite]  
[andradite] [anglesite] [anhydrite] [anorthite (Val di Fassa)] [anorthite glass] [antigorite] [apatite]  
[aragonite] [barite] [berlinite] [biotite] [brucite] [calcite] [CAS] [clinochlore] [coesite] [cordierite] [corundum]  
[cotunnite] [cristobalite] [diamond] [diamond in an ureilite meteorite] [diopside] [dolomite] [forsterite]  
[geikielite] [glaucophane] [graphite (desordered)] [graphite (ordered)] [grossular] [gypsum] [hematite]  
[hollandite (high pressure feldspar)] [jadeite] [kyanite (disthene)] [lawsonite] [magnesite] [majorite  
(synthetic)] [obsidienne] [olivine of San Carlos] [orthenstatite] [orthoclase] [perovskite (calcic)] [perovskite  
(high pressure phase)] [pyrite (anisotropic)] [pyrope] [quartz (powder)] [rhodesite] [ringwoodite (in shoked  
meteorite)] [rutile] [siderite] [siderite Mn Mg Ca rich] [silica glass] [sillimanite] [spinel] [staurolite]  
[stishovite] [strontianite] [talc] [tourmaline] [tridymite] [wadsleyite beta-phase] [whitlockite (merrilite)]  
[xenotime] [zircon] [zoisite]

Free database 2000-2012 [Laboratoire de Sciences de la Terre ENS-Lyon France](#)

[www.ens-lyon.fr/LST/Raman](http://www.ens-lyon.fr/LST/Raman) *Handbook of Raman Spectra*

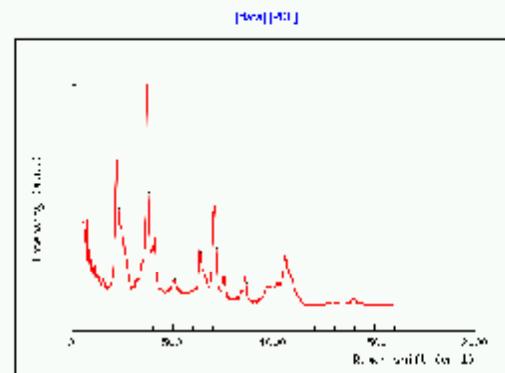
# Handbook of Minerals Raman Spectra

Tourmaline

Handbook of Raman spectra

Tourmaline:  $\text{Na}(\text{Mg},\text{Fe},\text{Mn})_3\text{Al}_5\text{Si}_6\text{O}_{18}(\text{BO}_3)_3(\text{OH,F})_4$

Incident: 514 nm



Raman spectrum of tourmaline  
excited with 514 nm exciting line  
detected with 514 nm detection line

Wavenum	freq. (cm⁻¹)	shift (cm⁻¹)	shift (ppm)
	2262		
	2147		
	3116		
	3733		
	477		
	516		
	612		
	715		
	722		
	878		
	1052		
	1095		
	1192		
	9719		
	9863		
	9903		

Intensity (a.u.), wavenum (cm⁻¹), shift (cm⁻¹), ppm =  $(\text{shift} - \text{freq.}) / \text{freq.}$

References:

B. Chatterjee, B. Mukherjee, and I. Chatterjee, Eur. J. Mineral., 5, 537-540 (1993).

Ring silicates

Incident: 1064 nm

# University of Parma mineral data base

The screenshot shows the homepage of the University of Parma mineral data base. At the top left is the university's seal. To its right, the text "Laboratory of Photoinduced Effects Vibrational and X-Ray Spectroscopies" is displayed in blue, with a molecular model graphic in the background. On the far right is the logo for CNISM, featuring a cluster of blue spheres and the acronym. A red circle highlights the search bar, which contains the text "\*\*\* Select a mineral \*\*\*". Below the search bar is a "Go" button. To the left of the search bar is a vertical menu with links: Home, Techniques, Research, Instrumentation, Staff, Raman DB, Publications, Education, Collaborations, Alumni, Press, Meetings, and Links.

- [Home](#)
- [Techniques](#)
- [Research](#)
- [Instrumentation](#)
- [Staff](#)
- [Raman DB](#)
- [Publications](#)
- [Education](#)
- [Collaborations](#)
- [Alumni](#)
- [Press](#)
- [Meetings](#)
- [Links](#)

\*\*\* Select a mineral \*\*\*

# University of Parma mineral data base

The screenshot shows the homepage of the University of Parma mineral data base. The header features the university's crest, the text "Laboratory of Photoinduced Effects Vibrational and X-Ray Spectroscopies", and the CNISM logo. A navigation menu on the left includes links for Home, Techniques, Research, Instrumentation, Staff, Raman DB, Publications, Education, Collaborations, Alumni, Press, Meetings, and Links. A dropdown menu titled "Select a mineral" lists various mineral names, such as Actinolite1, Actinolite2, Aeschynite1, Aeschynite2, Agardite1, Albite1, Albite2, Allanite1, Allanite2, Analcime1, Anatase1, Andradite1, and Andradite2.

- [Home](#)
- [Techniques](#)
- [Research](#)
- [Instrumentation](#)
- [Staff](#)
- [Raman DB](#)
- [Publications](#)
- [Education](#)
- [Collaborations](#)
- [Alumni](#)
- [Press](#)
- [Meetings](#)
- [Links](#)

\*\*\* Select a mineral \*\*\*

- Actinolite1
- Actinolite2
- Aeschynite1
- Aeschynite2
- Agardite1
- Albite1
- Albite2
- Allanite1
- Allanite2
- Analcime1
- Anatase1
- Andradite1
- Andradite2

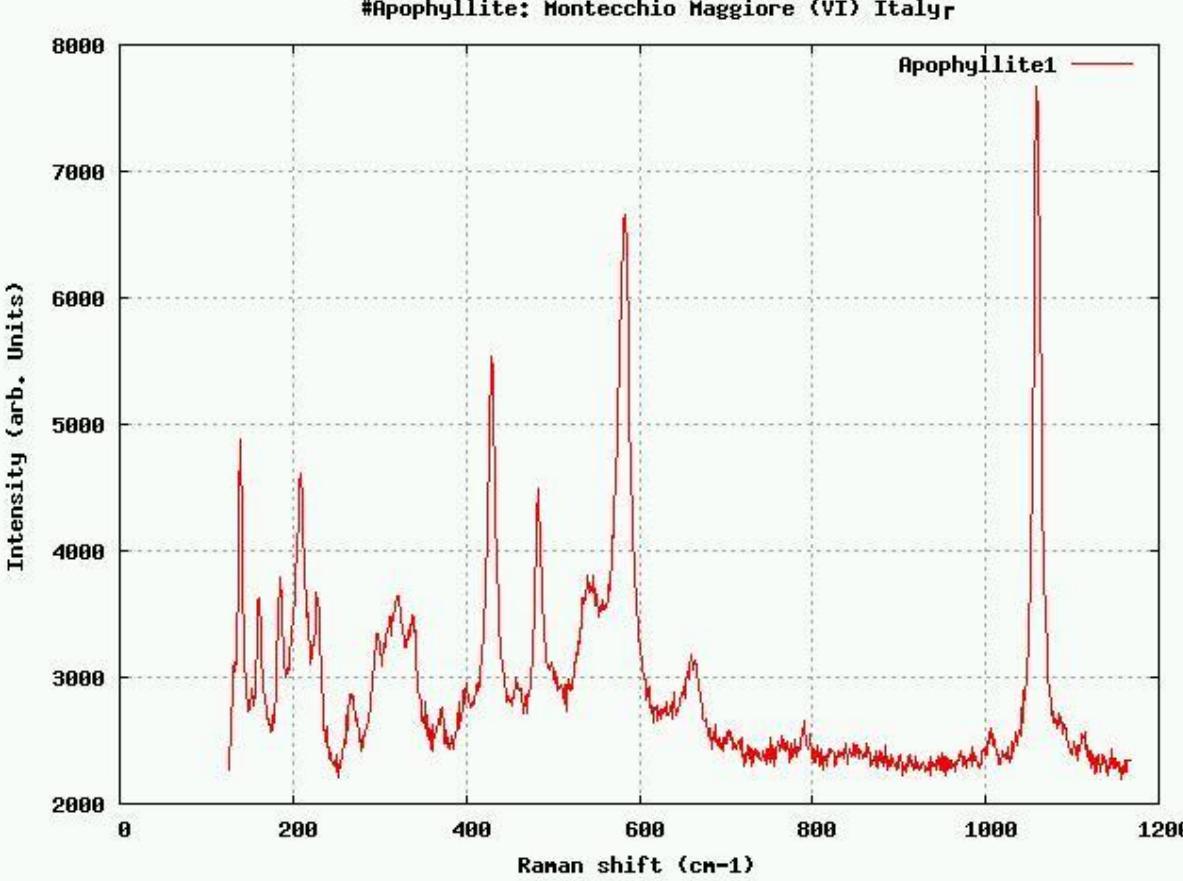
# University of Parma mineral data base

 **Laboratory of Photoinduced Effects  
Vibrational and X-Ray Spectroscopies** 

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[Research](#)  
[Instrumentation](#)  
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[Alumni](#)  
[Press](#)  
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[Google™](#)

#Apophyllite: Montecchio Maggiore (VI) Italy



# Minerals and Chemicals

<a href="#">Ha...yne</a>	Na3Ca(Si3Al3)O12(SO4)	HAUYN31	HAUYN3.S00	<a href="#">/kyo/lwkyo/HAUYN3.KYO</a> <a href="#">./s00/HAUYN3.pdf</a> <a href="#">/kyo/dernierskyo/HAUYN3.pdf</a>
<a href="#">Heavy water</a>	D2O	HEAVYW11	D2O-A.S00	<a href="#">/kyo/dernierskyo/D2O-A.BAA</a> <a href="#">/kyo/akkyo/HED100.BAC</a> <a href="#">./s00/HED100.pdf</a>
<a href="#">Hedenbergite</a>	CaFeSi2O6	HEDEN11	HED100.S00	<a href="#">/kyo/akkyo/HED100.BAC</a> <a href="#">./s00/HED100.pdf</a>
<a href="#">Herderite</a>	CaBePO4(OH,F)	HERDE11	HERDEB.S00	<a href="#">/kyo/akkyo/HERDEB.BAB</a> <a href="#">./s00/HERDEB.pdf</a>
<a href="#">Herderite</a>	CaBePO4(OH,F)	HERDE21	HERDED.S00	<a href="#">/kyo/akkyo/HERDED.BAB</a> <a href="#">./s00/HERDED.pdf</a>
<a href="#">Heulandite</a>	(Na,K,Ca,Sr,Ba)5(Al19Si29)O72.26H2O	HEULAN11	HEULA1.S00	<a href="#">/kyo/dernierskyo/HEULA1.KYO</a> <a href="#">./s00/HEULA1.pdf</a>
<a href="#">High albite</a>	NaAlSiO8	HALBIT11	S7015C.S00	<a href="#">./s00/S7015C.S00</a> <a href="#">./s00pdf/S7015C.pdf</a>
<a href="#">Hornblende</a>	Ca2(Mg,Fe,Al)8O22(OH)2	HORNB11	HORNB1.S00	<a href="#">/kyo/lwkyo/HORNB1.BAA</a> <a href="#">./s00/HORNB1.pdf</a>
<a href="#">Howlite</a>	Ca2B5SiO9(OH)5	HOWLI11	HOWLI2.S00	<a href="#">/kyo/lwkyo/HOWLI2.BAC</a> <a href="#">./s00/HOWLI2.pdf</a>
<a href="#">Howlite</a>	Ca2B5SiO9(OH)5	HOWLI21	HOWLI4.S00	<a href="#">/kyo/lwkyo/HOWLI4.BAC</a> <a href="#">./s00/HOWLI4.pdf</a>
<a href="#">Hydrocerussite</a>	Pb3(CO3)2(OH)2	HYDPB11	HYDPB1.S00	<a href="#">/kyo/lwkyo/HYDPB1.BAA</a> <a href="#">./s00/HYDPB1.pdf</a>
<a href="#">Hydrogen</a>	H2	H211	HCOCOA.S00	
<a href="#">Hydrogen</a>	H2	H221	HCOCOB.S00	
<a href="#">Hydrogen sulfide</a>	H2S	H2SL11	PALL11.S00	
<a href="#">Hydromagnesite</a>	Mg5(CO3)4(OH)2.4H2O	HYMAG11	HYDMG1.S00	<a href="#">/kyo/lwkyo/HYDMG1.BAB</a> <a href="#">./s00/HYDMG1.pdf</a>
<a href="#">Hydroxyapophyllite</a>	KCa4(Si4O10)2(F,OH).8H2O	APOPH11	APOPH2.S00	<a href="#">/kyo/lwkyo/APOPH2.BAC</a> <a href="#">./s00/APOPH2.pdf</a>
<a href="#">Hydroxyapophyllite</a>	KCa4(Si4O10)2(F,OH).8H2O	APOPH21	APOPH4.S00	<a href="#">/kyo/lwkyo/APOPH4.BAA</a> <a href="#">./s00/APOPH4.pdf</a>
<a href="#">Intermediate albite</a>	NaAlSi3O8	IALBIT11	O8431C.S00	<a href="#">./s00/O8431C.S00</a> <a href="#">./s00pdf/O8431C.pdf</a>

# Minerals and Chemicals

**AIR 327a** [pdf](#) [index](#)

**Author(s):** BENY C.

**Date:** 20 novembre 90

**file name:** AIRMA1.S00 [pdf](#)

**Recording laboratory:** Lab. mixte (BRGM-CNRS- Univ. Orléans) de spectroscopie de l'air

**References:**

**2nd file name:**

**Structural formula:** N<sub>2</sub>+O<sub>2</sub>

**Name:** Air

**Family:** 327a

**Group:**

**Origin:** natural [x] locality: Orléans (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 photosensitivity:**

**Laser power:** at laser: 800 mW, at sample:

**Raman scattering efficiency:** \*

**Spectral resolution:** 5 cm<sup>-1</sup>

**Calibration:** Ar+ cm<sup>-1</sup>

**Spectrometer:** JOBIN-YVON; model: U1000 macro [x] micro [ ] objective:;

**scan rate:** cm<sup>-1</sup>/mn

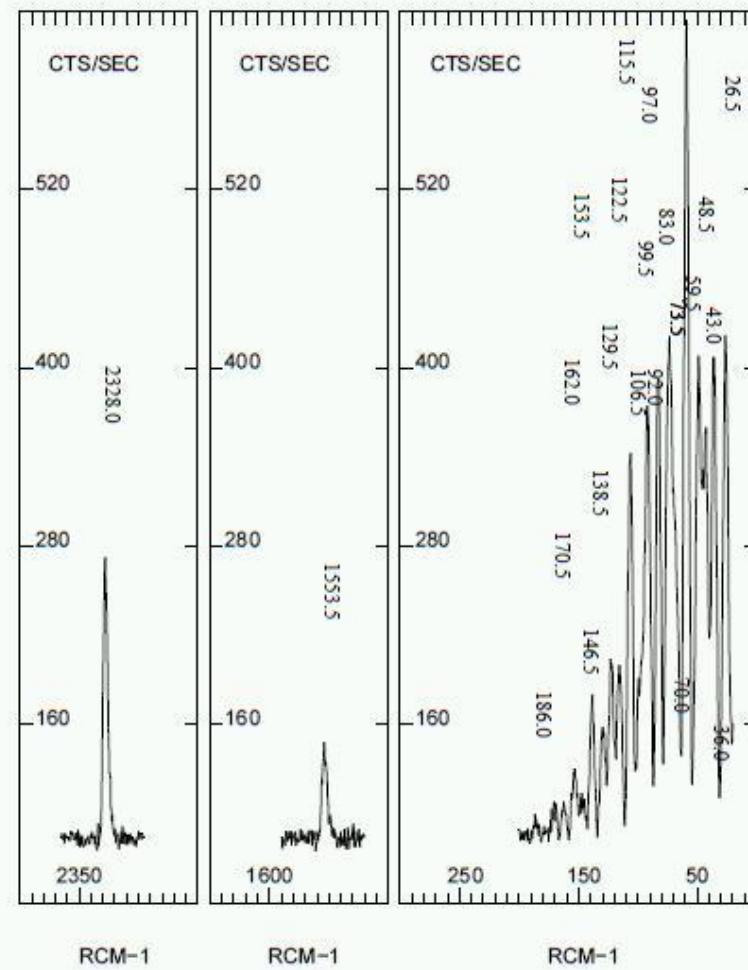
**step:** 0.5 cm<sup>-1</sup>

**counting time:** 2 s

# Minerals and Chemicals

U1000            INT.TIME :        2.000 Sec  
BENY            INCREMENT :     -0.50 Cm<sup>-1</sup>  
11/20/90        NB.SCANS :        4  
b:AIRMA1.S00    air seul  
filtre ouvert au max  
utilisation des 2 miroirs de renvoi de la platine

laser power  
slits      objective PM  
operator  
sample



# The Goblenz Society Spectral Data Collections

Web [www.coblentz.org/links/spectral-data-collections](http://www.coblentz.org/links/spectral-data-collections)



**The Coblenz Society**

**Links >**

## Spectral Data Collections

- [AEDC-EPA Spectral Database](#)
- [jcampdx.html at wwwchem.uwimona](#)
- • [Mineral Spectroscopy Server](#)
- • [SDBS Database for Organic Compounds](#)
- [SPECARB Database on Raman Spectra of Carbohydrates](#)
- [SpecInfo](#)
- [USGS Spectroscopy Lab - Spectral Library](#)

# 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 infrared spectra. 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 for many minerals. Raman, infrared, and reflectance data are available and Mössbauer data are solicited. More details follow.

**Extensive references to Optical Spectroscopic data now available**

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<sup>-1</sup> range.

[OH-region](#) : single crystal data in the 4000 - 3000 cm<sup>-1</sup> 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<sup>-1</sup> range.
- Our ATR (Attenuated Total Reflectance) data of hundreds of [mineral powders](#) on a diamond plate in the 4000 - 450 cm<sup>-1</sup> 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 obtained from 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.

<input type="text"/>	<a href="#">Mineral</a>
<input type="text"/>	<a href="#">Author</a>
<input type="text"/>	<a href="#">Chemistry Search</a>
<input type="text"/>	<a href="#">Cell Parameters and Symmetry</a>
<input type="text"/>	<a href="#">Diffraction Search</a>
<input type="text"/>	<a href="#">General Search</a> <a href="#">Search Tips</a>
<input type="button" value="Search"/> <input type="button" value="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	Abswurmbackite
Acetamide	Acetylene-hydrate	Achavalite	Actinium
Acuminitite	Adamantane	Adamantane-methane-hydrate	Adamite
Adelite	Admontite	Adolfpaterite	Adranosite
Aenigmatite	Aerinite	Aerugite	Aeschynite-(La)
Afghanite	Afmite	Afwillite	Agardite-(Ce)
Agricolaite	Agrinierite	Ahlfeldite	Aikinite
Ajoite	Akaaganeite	Akatoreite	Akdaleite
Akhtenskite	Akimotoite	Akrochordite	Aksaite
Alabandite	Alacranite	Alamosite	Alarsite
Albrechtschraufite	Alflarsenite	Alforsite	Alfredstelznerite
Alite	Allabogdanite	Allactite	Allanite-(Ce)
Allanite-(Nd)	Allanite-subgroup mineral	Allanpringite	Allargentum
Allohalcoselite	Allocasite	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
Alunogen	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

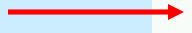
The crystal structure and infrared properties of adamite  
\_database\_code\_amcsd 0000532

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	.0011
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 Goblenz Society Spectral Data Collections

Web [www.coblentz.org/links/spectral-data-collections](http://www.coblentz.org/links/spectral-data-collections)



## The Coblenz Society

**Links >**

### Spectral Data Collections

- [AEDC-EPA Spectral Database](#)
- [jcampdx.html at wwwchem.uwimona](#)
- [Mineral Spectroscopy Server](#)
- [SDBS Database for Organic Compounds](#)
- [SPECARB Database on Raman Spectra of Carbohydrates](#)
- [SpecInfo](#)
- [USGS Spectroscopy Lab - Spectral Library](#)

## 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:** **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  $^{13}\text{C}$  NMR Raman  $^1\text{H}$  NMR ESR**IR Peaks(cm<sup>-1</sup>):**

Allowance

 ±10

"," or space is the separator for multiple  
peaks.

Use "-", to set a range: eg. 550-750,1650  
3000-

Transmittance <  %

 **$^{13}\text{C}$  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,...

 **$^1\text{H}$  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,...

Hit: 20hit

Sort by: Molecular Weight

Ascending Order

**Spectral Database for  
Organic Compounds SDBS**

Japanese

Introduction

Disc

**SDBS Search Results:** 1 - 20 out of 3573 hits   Sort by: Molecular Weight ▾ Ascending Order ▾ 

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

# Database for Organic Compounds

← → ⌂ ⌃ Web riodb01.ibase.aist.go.jp/sdbs/cgi-bin/direct\_frame\_top.cgi

Spectral Database for  
Organic Compounds SDBS Japanese

**SDBS Information**

SDBS No.: 4544  
Compound Name:  
water  
Molecular Formula: H<sub>2</sub>O  
Molecular Weight: 18.0  
CAS Registry No.:  
7732-18-5  
Spectral Code:  
[¹H NMR : in CDCl<sub>3</sub>](#)  
[¹H NMR : in C<sub>6</sub>D<sub>6</sub>](#)  
[¹H NMR : in CD<sub>3</sub>CN](#)  
[¹H NMR : in Acetone-d<sub>6</sub>](#)  
[¹H NMR : in DMSO-d<sub>6</sub>](#)  
[¹H NMR : in CD<sub>2</sub>Cl<sub>2</sub> at 27C](#)  
[Raman : 4880 Å, 200 M, liquid](#)  
[Chemical Information](#)

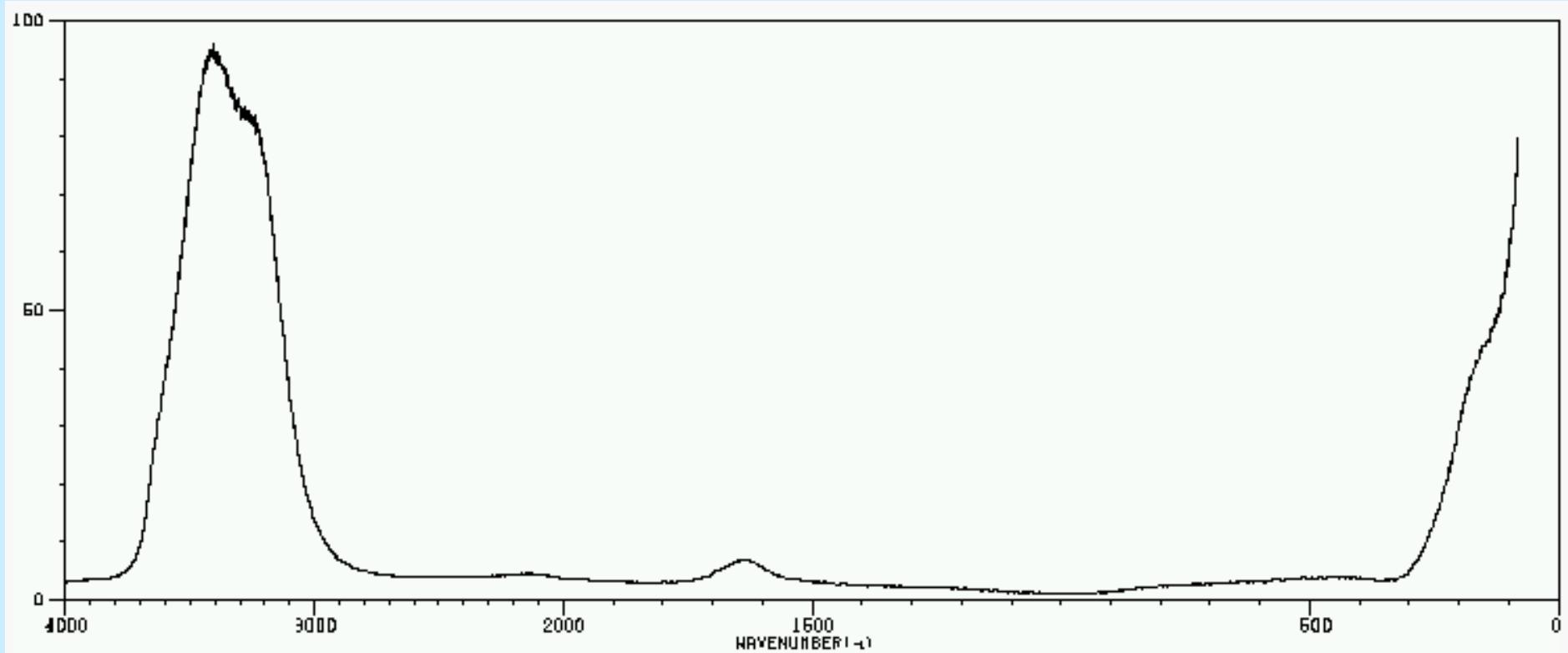
SDBS No: 4544  
Molecular Formula: H<sub>2</sub>O  
SDBS-NO= 4544  
WATER  
CAS Registry No.: 7732-18-5  
Molecular Weight: 18.0  
H<sub>2</sub>O

Compound Name:  
water  
hydrogen oxide

(c) National Institute of Advanced Industrial Science and Technology (AIST)

# Database for Organic Compounds

---



WATER

SDBSNO = 4544

H<sub>2</sub>O

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)

Inorganic materials (1022 spectra)

Literature (100 papers & books)

Search    List

Search    List

## List of inorganic chemicals

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

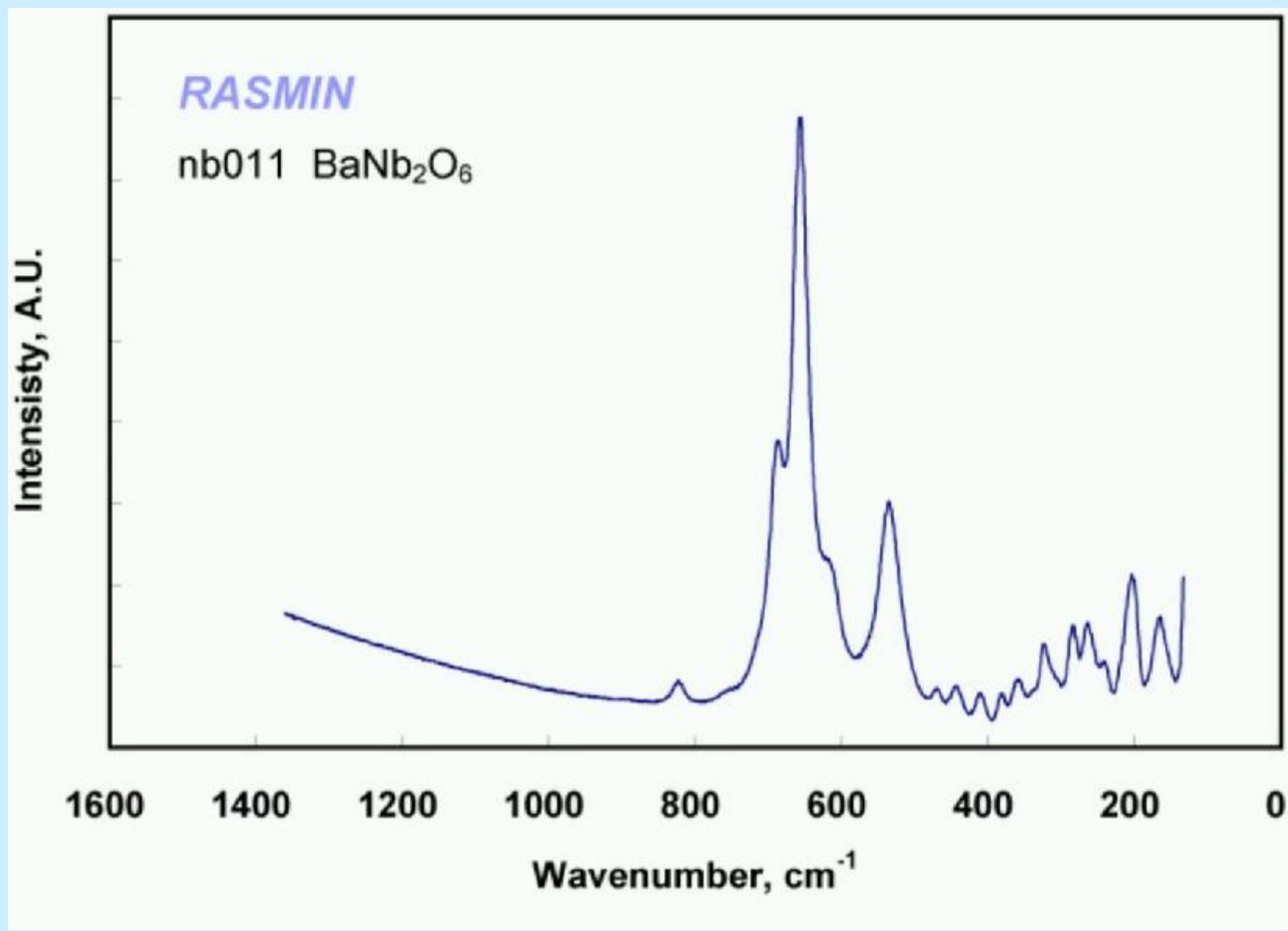
Name	#
All	1 0 2 2
A - B - C - D - E	3 2 3
F - G - H - I - J	7 8
K - L - M - N - O	3 5 6
P - Q - R - S - T	1 8 4
U - V - W - X - Y - Z	8 1

# RASMIN

Chemical Formula A B C D E	Name	Spectrum image (PDF)
EDTA.2Na	ethylenediaminetetraacetic acid disodium salt	+
BaBaO <sub>6</sub>	barium monobasic oxide	++
C <sub>6</sub> NH <sub>2</sub> C <sub>6</sub> -Ca <sub>2</sub> Ti <sub>2</sub> O <sub>7</sub>	calcium titanate oxide	+
Cu(C <sub>2</sub> H <sub>5</sub> COO) <sub>2</sub> .H <sub>2</sub> O	copper propionate	++
Cu <sub>2</sub> O	copper (I) oxide	++
Cu <sub>2</sub> O <sub>3</sub> =Cu <sub>2</sub> O.5=2O	copper nitrate	+
Cu(C <sub>2</sub> O <sub>4</sub> ) <sub>2</sub> .H <sub>2</sub> O	copper perchlorate	+
CuI	copper (I) iodide	++
Cu <sub>2</sub> (OEt) <sub>3</sub> NO <sub>3</sub>	copper nitrate, basic	+
Cu <sub>2</sub> O <sub>4</sub> O.5Li <sub>2</sub> O	copper oxalate	+
Cu(C <sub>17</sub> F <sub>35</sub> OOC) <sub>2</sub>	copper oleate	++
Cu(C <sub>2</sub> H <sub>5</sub> COO) <sub>2</sub> .H <sub>2</sub> O	copper propionate	++
Cu(CH <sub>2</sub> CH(OH)COO) <sub>2</sub>	copper lactate	+
CuF <sub>2</sub> .2H <sub>2</sub> O	copper fluoride	+
Cu(C <sub>2</sub> H <sub>5</sub> O) <sub>2</sub> .2H <sub>2</sub> O	copper salicylate	+
Cu(HOO) <sub>2</sub> .4Li <sub>2</sub> O	copper formate	+
CuCl <sub>2</sub> .LiPF <sub>6</sub> .CH <sub>2</sub> Cl <sub>2</sub> O	copper formate solvates	+

# RASMIN

---



# Bilbao Crystallographic Server

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

**bilbao crystallographic server**

[ The crystallographic site at the Condensed Matter Physics Dept. of the University of the Basque Country ]

[ Space Groups ] [ Layer Groups ] [ Rod Groups ] [ Frieze Groups ] [ Wyckoff Sets ]

**Space Groups Retrieval Tools**

<b>GENPOS</b>	Generators and General Positions of Space Groups
<b>WYCKPOS</b>	Wyckoff Positions of Space Groups
<b>HKLCOND</b>	Reflection conditions of Space Groups
<b>MAXSUB</b>	Maximal Subgroups of Space Groups
<b>SERIES</b>	Series of Maximal Isomorphic Subgroups of Space Groups
<b>WYCKSETS</b>	Equivalent Sets of Wyckoff Positions
<b>NORMALIZER</b>	Normalizers of Space Groups
<b>KVEC</b>	The k-vector types and Brillouin zones of Space Groups
<b>SYMMETRY OPERATIONS</b>	Geometric interpretation of matrix column representations of syn

# Bilbao Crystallographic Server

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## Databases

B-IncStrDB 

The Bilbao Incommensurate 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

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CORRELATIONS POINTS

Relation between the symmetry modes in a high and low symmetry 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

$\text{LiTaO}_3$

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**

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**Space Groups Retrieval Tools**

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Ta	0,	0,	0
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O	0.5,	0.34,	0.69

Help

## Wyckoff Positions

Please, enter the sequential number of group as given in *International Tables for Crystallography*, Vol. A or [choose it](#):

161

Standard/Default Setting

Non Conventional Setting

ITA Settings



# Bilbao Crystallographic Server

$\text{LiTaO}_3$

R3C (161), координаты в гексагональных осях

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

148	<i>R</i> -3:rhombohedral axes <i>R</i> -3:hexagonal axes	149	<i>P</i> 312	150	<i>P</i> 321
151	<i>P</i> 3 <sub>1</sub> 12	152	<i>P</i> 3 <sub>1</sub> 21	153	<i>P</i> 3 <sub>2</sub> 12
154	<i>P</i> 3 <sub>2</sub> 21	155	<i>R</i> 32:rhombohedral axes <i>R</i> 32:hexagonal axes	156	<i>P</i> 3m1
157	<i>P</i> 31m	158	<i>P</i> 3c1	159	<i>P</i> 31c
160	<i>R</i> 3m:rhombohedral axes <i>R</i> 3m:hexagonal axes	161	<i>R</i> 3c:rhombohedral axes <i>R</i> 3c:hexagonal axes	162	<i>P</i> -31m
163	<i>P</i> -31c	164	<i>P</i> -3m1	165	<i>P</i> -3c1
166	<i>R</i> -3m:rhombohedral axes <i>R</i> -3m:hexagonal axes	167	<i>R</i> -3c:rhombohedral axes <i>R</i> -3c:hexagonal axes	168	<i>P</i> 6
169	<i>P</i> 6 <sub>1</sub>	170	<i>P</i> 6 <sub>5</sub>	171	<i>P</i> 6 <sub>2</sub>
172	<i>P</i> 6 <sub>4</sub>	173	<i>P</i> 6 <sub>3</sub>	174	<i>P</i> -6
175	<i>P</i> 6/m	176	<i>P</i> 6 <sub>3</sub> /m	177	<i>P</i> 622
178	<i>P</i> 6 <sub>1</sub> 22	179	<i>P</i> 6 <sub>5</sub> 22	180	<i>P</i> 6 <sub>2</sub> 22
181	<i>P</i> 6 <sub>4</sub> 22	182	<i>P</i> 6 <sub>3</sub> 22	183	<i>P</i> 6mm
184	<i>P</i> 6cc	185	<i>P</i> 6~cm	186	<i>P</i> 6~mc

# Bilbao Crystallographic Server

$\text{LiTaO}_3$

R3C (161), координаты в гексагональных осях

Ta	0,	0,	0
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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 =  y =  z =

Show

If you want to see the Wyckoff position in other setting, click [here](#)

# Bilbao Crystallographic Server



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 (R3c) [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

---

$\text{LiTaO}_3$

R3C (161),

Atom Coordinates

Ta 0, 0, 0

Li 0, 0, 0.279

O 0.5, 0.34, 0.69

Wyckoff position

6a

6a

18b

## Raman and Hyper-Raman scattering

### SAM

RAMAN AND HYPER-RAMAN TENSORS

POLARIZATION SELECTION RULES

TWINS TENSORS

CORRELATIONS POINTS

RAMAN CORRELATIONS SPACE

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IR and Raman activity under a symmetry break for a given structures.

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]

Structure

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 asymm
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
```

Show

# Bilbao Crystallographic Server

---

$\text{LiTaO}_3$

R3C (161),

Atom Coordinates

Ta 0, 0, 0

Li 0, 0, 0.279

O 0.5, 0.34, 0.69

Wyckoff position

6a

6a

18b

Choose the Wyckoff Positions of the atoms in your structure for the space group *R3c* (No. 161) [hexagonal axes]:

Check	WP	Representative
<input checked="" type="checkbox"/>	18b	x,y,z
<input checked="" type="checkbox"/>	6a	0,0,z

Continue

# Bilbao Crystallographic Server

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

### Character Table<sup>1</sup>

$C_{3v}$ (3m)	#	1	3	m	functions
Mult.	-	1	2	3	
$A_1$	$\Gamma_1$	1	1	1	$z, x^2+y^2, z^2$
$A_2$	$\Gamma_2$	1	1	-1	$J_z$
$E$	$\Gamma_3$	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

точечная группа

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

Character Table<sup>1</sup>

$C_{3v}$ (3m)	#	1	3	m	functions
Mult.	-	1	2	3	
$A_1$	$\Gamma_1$	1	1	1	$zx^2+y^2, z^2$
$A_2$	$\Gamma_2$	1	1	-1	$J_z$
$E$	$\Gamma_3$	2	-1	0	$(x,y), (xz,yz), (x^2-y^2, xy), (J_x, J_y)$

число операций  
в каждом классе

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
	a		c		
		b	d		

Hyper-Raman Tensors

$A_2$		$A_1, z$		$E, x^*$		$E, y$	
a	-a					3d	d
			-b	b			f
			c	c	d		

# Bilbao Crystallographic Server

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

WP	A <sub>1</sub>	A <sub>2</sub>	E
18b	3	.	6
6a	1	.	2

- Hyper-Raman Active Modes

WP	A <sub>1</sub>	A <sub>2</sub>	E
18b	3	3	6
6a	1	1	2

- Raman Active Modes

WP	A <sub>1</sub>	A <sub>2</sub>	E
18b	3	.	6
6a	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 <sub>1</sub>	A <sub>2</sub>	E
Infrared	x	.	x
Raman	x	.	x
Hyper-Raman	x	x	x

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

# Bilbao Crystallographic Server

## Polarization Selection Rules

### Back scattering geometry

If you want to know more about this configuration please click [here](#).

	A <sub>1</sub> (LO)	A <sub>1</sub> (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 <sub>1</sub> (LO+TO)	A <sub>1</sub> (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	.

# Bilbao Crystallographic Server

More information: [show](#) [hide](#)

## Permutational Representation

The permutational representation represents

WP	A <sub>1</sub>	A <sub>2</sub>	E
18b	1	1	2
6a	1	1	.

## Mechanical Representation

The mechanical representation is defined as

WP	A <sub>1</sub>	A <sub>2</sub>	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 decompo

C <sub>3v</sub> (3m)	A <sub>1</sub>	A <sub>2</sub>	E
V	1	.	1
A	.	1	1
[V <sup>2</sup> ]	2	.	2
[V <sup>2</sup> ] x 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 <sub>1</sub>	A <sub>2</sub>	E
A <sub>1</sub>	<b>A<sub>1</sub></b>	A <sub>2</sub>	E
A <sub>2</sub>	.	<b>A<sub>1</sub></b>	E
E	.	.	<b>A<sub>1</sub> + A<sub>2</sub> + E</b>

 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 <sub>1</sub>	A <sub>2</sub>	E
A <sub>1</sub>	<b>A<sub>1</sub></b>	A <sub>2</sub>	E
A <sub>2</sub>	.	<b>A<sub>1</sub></b>	E
E	.	.	<b>A<sub>1</sub> + A<sub>2</sub> + E</b>

 Active    Inactive   **bold** Raman active modes

# Bilbao Crystallographic Server

## Правила отбора:

Atom R3C 161	Coordinates (hexagonal axes)	Wyckoff position	G-point phonon modes
Ta	0,0,0	6a	$\mathbf{A}_1+2\mathbf{E}+\mathbf{A}_2$
Li	0,0,0.279	6a	$\mathbf{A}_1+2\mathbf{E}+\mathbf{A}_2$
O	0.5, 0.34, 0.69	18b	$3\mathbf{A}_1+6\mathbf{E}+3\mathbf{A}_2$
Modes classification			
$\Gamma_{\text{raman}}=5\mathbf{A}_1+10\mathbf{E}$	$\Gamma_{\text{ir}}=5\mathbf{A}_1+10\mathbf{E}$	$\Gamma_{\text{ac}}=\mathbf{A}_1+\mathbf{E}$	$\Gamma_{\text{meh}}=5\mathbf{A}_1+5\mathbf{A}_2+10\mathbf{E}$
Raman tensors			
$\mathbf{A}_1, z$ $\begin{bmatrix} a & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & b \end{bmatrix}$	$\mathbf{E}, x$ $\begin{bmatrix} c & 0 & 0 \\ 0 & -c & d \\ 0 & d & 0 \end{bmatrix}$	$\mathbf{E}, y$ $\begin{bmatrix} 0 & c & d \\ c & 0 & 0 \\ d & 0 & 0 \end{bmatrix}$	

Моды, ожидаемые в спектре КР

4 $\mathbf{A}_1+9\mathbf{E}$

Моды, ожидаемые в спектре гипер КР

4 $\mathbf{A}_1+9\mathbf{E}+5\mathbf{A}_2$

# Web of knowledge

<http://apps.webofknowledge.com>

The screenshot shows the Web of Science search interface. At the top, there's a navigation bar with tabs for "Web of Science" (which is circled in red), "Additional Resources", and links for "Search", "Author Finder", "Cited Reference Search", "Advanced Search", and "Search History".

The main search area is titled "Web of Science®" and has a "Search" section. It includes a search bar with the placeholder "Example: oil spill\* mediterranean", a dropdown for "in Topic", and a search button. Below this, there are two search fields separated by "AND": one for "Aleksandrov KS" (in Author) and another for "Publication Name" (with a dropdown menu listing various options like Topic, Title, Author, ResearcherID, etc.). There's also a link to "Add Another Field >>".

At the bottom of the search section are "Search" and "Clear" buttons, and a note that "Searches must be in English".

Below the search area, there's a "Current Limits" section with "Timespan" and "Citation Databases" settings. Under "Timespan", the "All Years" option is selected (updated 2012-08-31). Under "Citation Databases", several boxes are checked: "Science Citation Index Expanded (SCI-EXPANDED) --1980-present", "Social Sciences Citation Index (SSCI) --1980-present", "Conference Proceedings Citation Index- Science (CPCI-S) --1990-present", and "Conference Proceedings Citation Index- Social Science & Humanities (CPCI-SSH) --1990-present".

At the very bottom, there are links for "Adjust your search settings" and "Adjust your results settings".

# Web of science

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Timespan=All Years. Databases=SCI-EXPANDED, SSCI, CPCI-S, CPCI-SSH.  
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Results: 186

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**Authors** [Refine](#)

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- FLEROV IN (23)
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Author(s): Molokeev, M. S.; Misyl', S. V.; Fokina, V. D.; et al.  
Source: PHYSICS OF THE SOLID STATE Volume: 53 Issue: 4 Pages: 834-839 DOI:  
Times Cited: 4 (from Web of Science)  
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Author(s): Aleksandrov, K. S.; Voronov, N. V.; Vtyurin, A. N.; et al.  
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3. Title: **Structural and electronic parameters of ferroelectric K<sub>3</sub>WO<sub>3</sub>F<sub>3</sub>**  
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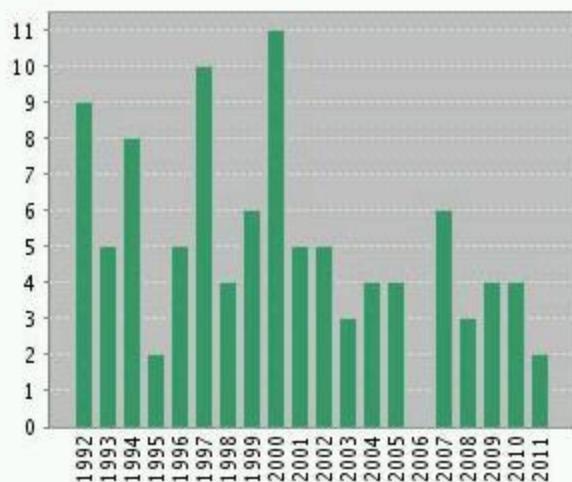
4. Title: **Optical studies of phase transitions in oxyfluoride (NH<sub>4</sub>)<sub>2</sub>NbOF<sub>5</sub>**  
Author(s): Mel'nikova, S. V.; Laptash, N. M.; Aleksandrov, K. S.  
Source: PHYSICS OF THE SOLID STATE Volume: 52 Issue: 10 Pages: 2168-2172 DOI:  
Times Cited: 2 (from Web of Science)

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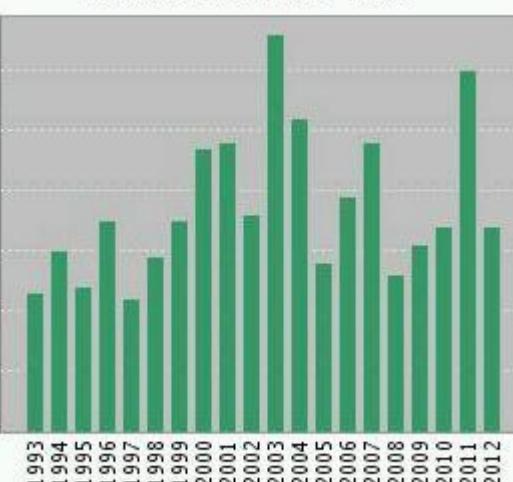
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# Web of science

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<input type="checkbox"/>	1. Title: <a href="#">Phase transitions in elpasolites (ordered perovskites)</a> Author(s): Flerov, IN; Gorev, MV; Aleksandrov, KS; et al. Source: MATERIALS SCIENCE & ENGINEERING R-REPORTS Volume: 24 Issue: 3	26	31	34	60	34	989	29.97
<input type="checkbox"/>	2. Title: <a href="#">PHASE-TRANSITIONS IN THE PEROVSKITE-LIKE A2BX4 STRUCTURE</a> Author(s): HATCH, DM; STOKES, HT; ALEKSANDROV, KS; et al. Source: PHYSICAL REVIEW B Volume: 39 Issue: 13 Pages: 9282-9288 DOI: 10.1103/PhysRevB.39.9282	5	7	8	9	5	89	5.93
<input type="checkbox"/>	3. Title: <a href="#">Influence of static electric field, mechanical pressure and temperature on the phase transitions in the A2BX4 perovskite-like crystals</a> Author(s): Sorokin, BP; Turchin, PP; Burkov, SI; et al. Book Group Author(s): IEEE Conference: <b>1996 IEEE International Frequency Control Symposium</b> Location: HONOLULU, HI, USA Sponsor(s): IEEE, Ultrason Ferroelect & Frequency Control Soc Source: PROCEEDINGS OF THE 1996 IEEE INTERNATIONAL FREQUENCY CONTROL SYMPOSIUM Volume: 1996-1996	1	2	1	2	2	39	1.62
<input type="checkbox"/>	4. Title: <a href="#">PHASE-TRANSITIONS IN CS2CDI4 SINGLE-CRYSTALS</a> Author(s): ALEKSANDROV, KS; MELNIKOVA, SV; FLEROV, IN; et al. Source: PHYSICA STATUS SOLIDI A-APPLIED RESEARCH Volume: 105 Issue: 2 Pages: 231-234	1	4	3	5	1	35	2.06
<input type="checkbox"/>	5. Title: <a href="#">OCTAHEDRAL TILT PHASES IN PEROVSKITE-LIKE CRYSTALS WITH SINGLY CHARGED ANIONIC SUBSTITUTION</a> Author(s): ALEKSANDROV, KS; BARTOLOME, J Source: JOURNAL OF PHYSICS-CONDENSED MATTER Volume: 6 Issue: 40 Pages: 7953-7960	1	0	2	1	0	33	1.32

# Web of science

## Phase transitions in elpasolites (ordered perovskites)

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

**Source:** MATERIALS SCIENCE & ENGINEERING R-REPORTS **Volume:** 24 **Issue:** 3

**Times Cited:** 89 (from Web of Science)

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**Abstract:** Many compounds with general chemical formula A(2)BBX-6 and with tolerance Bridgman technique is the most suitable method of growing single crystals of halogen connected with octahedral rotations and displacements of ions. Experimental observation 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 the phase transitions in elpasolites and related compounds has also been considered. OI with monoatomic cations. On the other hand, for instance, in cryolites with ammonium I

**Accession Number:** WOS:000078300200001

**Document Type:** Review

**Language:** English

**KeyWords Plus:** ELASTIC NEUTRON-DIFFRACTION; MII = CO; RAMAN-SCATTERING; FORM; HIGH-RESOLUTION

**Reprint Address:** Flerov, IN (reprint author), LV Kirensky Phys Inst, Krasnoyarsk 660031

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Volkov, N. V. Temperature-dependent features of Pb<sub>3</sub>Mn<sub>7</sub>O<sub>15</sub> crystal structure. PHYSICA B-CONDENSED MATTER, FEB 15 2012.

Ma, Guanxiang. Phase-controlled synthesis and gas-sensing properties of zinc stannate (Zn<sub>2</sub>SnO<sub>3</sub> and Zn<sub>2</sub>SnO<sub>4</sub>) faceted solid and hollow microcrystals. CRYSTENGCOMM, 2012.

Fedorov, P. P. Fluoride laser nanoceramics. IV NANOTECHNOLOGY INTERNATIONAL FORUM (RUSNANOTECH 2011), 2012.

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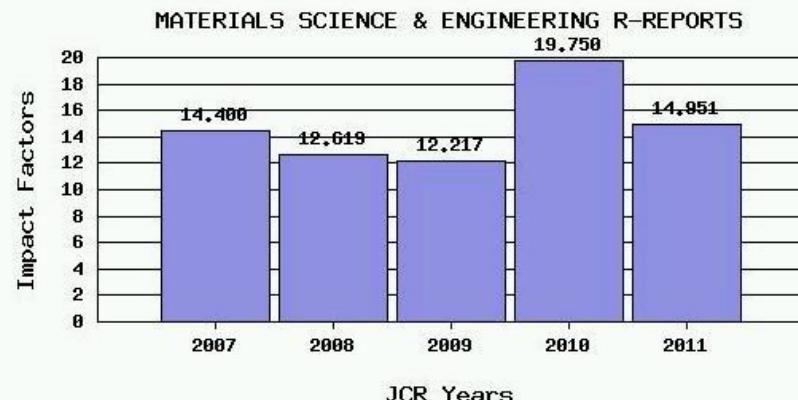
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2009 = 357

2009 = 12

Sum: 613

Sum: 41

Calculation: Cites to recent articles 613 = **14.951**

Number of recent articles 41

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**Journal Part**

**Total Cites**

**Impact Factor**

**Immediacy Index**

**Cited Half-life**

**5-Year Impact Factor**

**Eigenfactor® Score**

**Article Influence® Score**

**Sort Order**

**Ranking is based on your journal and sort selections.**

**JCR Data (1)**

**Eigenfactor® Metrics (2)**

Abbreviated Journal Title (linked to journal information)	ISSN	JCR Data (1)						Eigenfactor® Metrics (2)	
		Total Cites	Impact Factor	5 Year Impact Factor	Immediacy Index	Articles	Cited Half-life	Eigenfactor® Score	Article Influence® Score
<a href="#">CA CANCER J CLIN</a>	0002-238X	10576	0.707	62.40	2.261	5	3.7	0.14707	24.579
<a href="#">CANCER</a>	0008-543X	14497	1.745	14.84	2.321	11	3.7	1.16927	43.1
<a href="#">CARCINOGENESIS</a>	0898-2603	12470	12.515	20.0	2.047	114	6.5	0.13207	37.7
<a href="#">HEPATOLOGY</a>	0270-5318	4677	1.706	1.00	2.425	387	6.7	0.12737	3.519
<a href="#">IMMUNOL REV</a>	0161-4535	11.85	11.175	11.23	0.933	1	3.1	0.13828	5.915
<a href="#">ANN NEUROL</a>	0003-4510	9133	11.205	11.64	1.615	192	9.2	0.06752	4.150
<a href="#">FEMS MICROBIOL REV</a>	0167-7055	7107	10.507	1.75	2.978	47	7.7	0.11761	-2.0
<a href="#">EUR J PEDIATR</a>	0170-4328	9.95	10.701	11.00	0.155	24	6.5	0.05578	2.723
<a href="#">ENZYMES</a>	0277-7307	3594	10.461	11.676	1.021	47	5.7	0.01104	0.472
<a href="#">EMBO J MOL MED</a>	1435-9351	777	10.785	7.353	0.701	35	2.1	0.00583	8.11
<a href="#">EUROPEAN</a>	1454-7801	2570	9.267	11.70	1.013	47	6.5	0.11401	4.025
<a href="#">ARTERIOSCLEROTIC HYPERTENS</a>	0004-3550	40703	7.765	7.979	0.549	464	7.5	0.10707	2.640
<a href="#">STEM CELLS</a>	1016-5100	17271	7.482	8.021	1.013	201	4.1	0.08124	2.022
<a href="#">REV MEDICAL</a>	1002-9275	1596	7.201	7.424	1.115	25	5.5	0.00245	2.410
<a href="#">OBST REV</a>	1477-7888	4547	7.135	7.251	0.857	145	4.5	0.11502	2.841
<a href="#">GLOBAL CHANGE BOL</a>	1957-1212	1615	6.564	6.056	1.551	214	5.1	0.06167	3.128
<a href="#">TOP ELYTO</a>	0020-246X	24500	6.545	6.653	1.070	344	6.5	0.06294	2.270
<a href="#">AM J TRANSPLANT</a>	1070-1188	15127	6.701	7.055	0.623	201	4.5	0.15750	1.956
<a href="#">JOURNAL OF KINETICS</a>	0161-4402	2140	6.171	5.19	0.935	251	7.5	0.04440	2.249
<a href="#">EAT JG</a>	0029-6707	1049	6.717	6.40	0.101	124	7.5	0.03403	2.970

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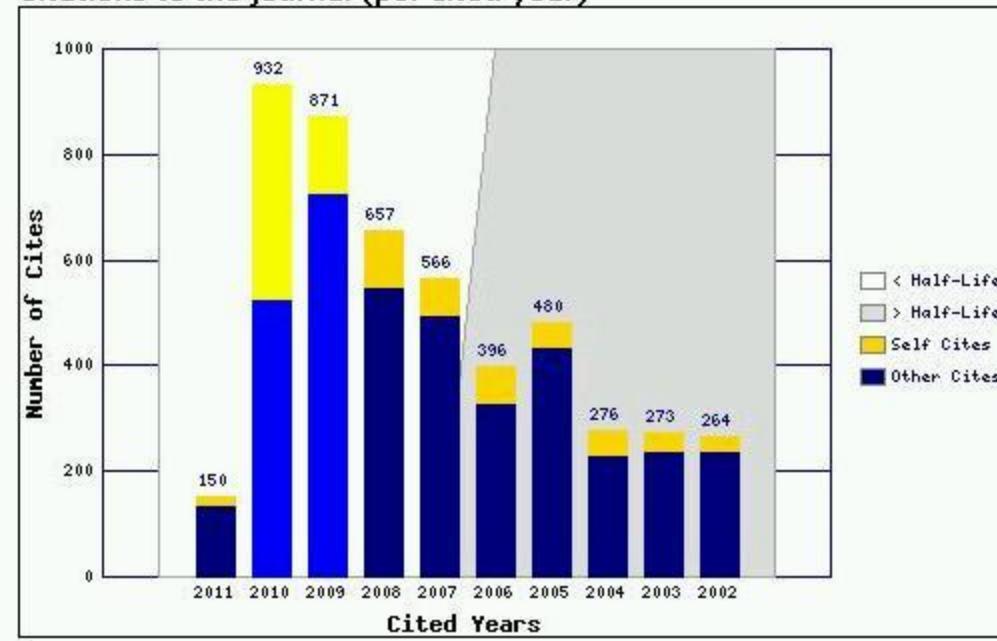


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Kreisel, Jens

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Subject: Crystallography; Materials Science; Physics; Spectroscopy

Keywords: phase transitions; phonons, atomic vibrational dynamics; ferroelectric and piezoelectric materials; multiferroic materials; raman scattering; solid state

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 presence of functional oxides, namely ABO<sub>3</sub> perovskites, aiming to discover new general concepts and application-relevant materials.

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Source: **Physical Review B** Volume: 73 Issue: 13 Published: APR 2006  
Times Cited: 113  
DOI: [10.1103/PhysRevB.73.132101](https://doi.org/10.1103/PhysRevB.73.132101)
2. Title: [Structural distortion and magnetism of BiFeO<sub>3</sub> epitaxial thin films: A Raman spectroscopy and neutron diffraction study](#)  
Author(s): Bea, H.; Bibes, M.; Petit, S.; et al.  
Source: **Philosophical Magazine Letters** Volume: 87 Issue: 3-4 Pages: 165-174 Published: APR 2007  
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## My Institutions ([more details](#))

Primary Institution: CNRS & Grenoble INP

Sub-org/Dept: Lab. Matériaux et Génie Physique

Role: Researcher (Academic)

Joint Affiliation: University of Warwick

Sub-org/Dept: Department of Physics

Role: Other

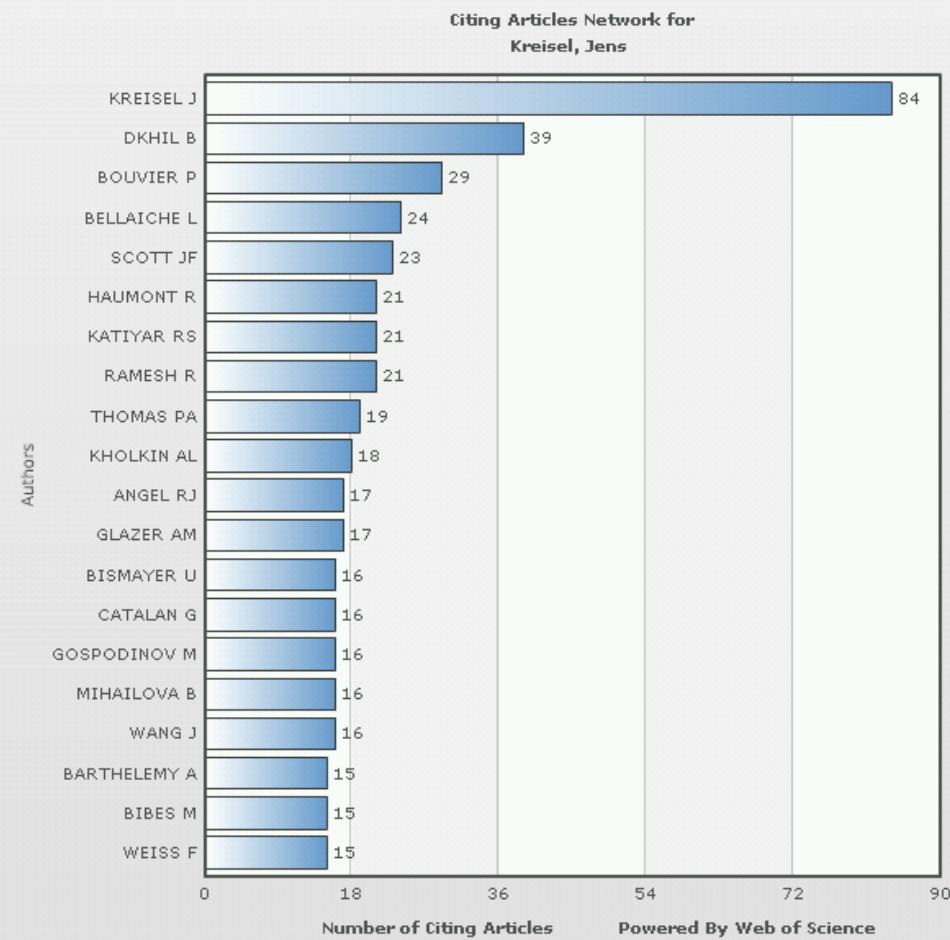
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