WURM

Use WURM in research and teaching to:

- view crystal structures of minerals
- assess the idea of dynamical atomic charges
- visualize Raman spectra
- apprehend vibrational spectra
- see atoms vibrating

Hosted by

ÉCOLE NORMALE SUPÉRIEURE DE LYON

Computed with:

abinit.org

Want to help us?

- Donate money
- Donate computing time
- Ask for interesting spectra to compute
- Verify our theoretical predictions
- Read and cite our papers
- Add links to our website

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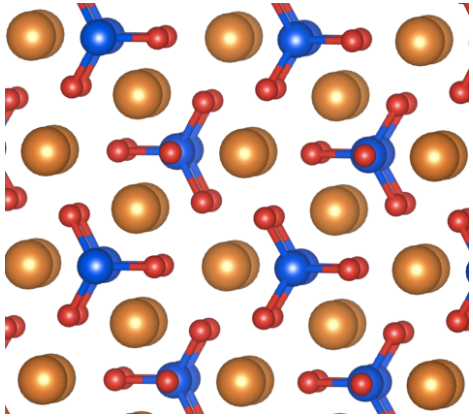
We thank Michael Scott for his long-standing generous support!

- The WURM project is a database of computed Raman and infrared spectra and other physical properties for minerals.
- All values are computed using quantum mechanics



- You will find common minerals as well as rare minerals, synthetic compounds, pure phases and solid solutions, stable, unstable, and theoretical structures
- Systematic studies under pressure, under stress, and with varying compositions
- Designed for teaching, research, and as a complement for mineral identification in the field
- User friendly, interactive

COMPUTATIONAL MINERALOGY

WURM project

We help you see the atoms as they are in crystals:

V I B R A T I N G

visit us at:
http://wurm.info

WURM

WHAT YOU WILL FIND INSIDE?

List of spectra

List of minerals

CRYSTAL STRUCTURE

Symmetry (theoretical):

Space group:	58	Pnnm	
Lattice parameters (Å):	7.8276	7.8980	5.5308
Angles (°):	90.0	90.0	90.0

Atomic positions (theoretical):

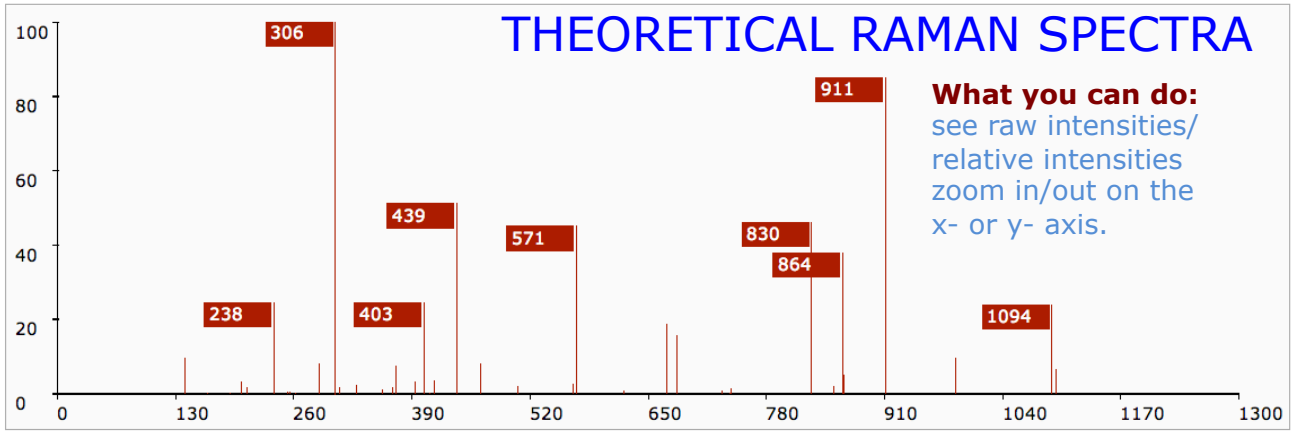
Atom type	X	Y	Z
Al:	0.0000	0.0000	0.2419
Al:	0.3716	0.1395	0.5000
Si:	0.2449	0.2541	0.0000
O:	0.4277	0.3626	0.5000
O:	0.4210	0.3674	0.0000
O:	0.1019	0.4013	0.0000
O:	0.2319	0.1368	0.2406
Al:	0.6284	0.8605	0.5000
Si:	0.7551	0.7459	0.0000
O:	0.5723	0.6374	0.5000
O:	0.5790	0.6326	0.0000
O:	0.8981	0.5987	0.0000
O:	0.7681	0.8632	0.2406

TECHNICAL DETAILS OF THE CALCULATIONS

DIELECTRIC TENSORS

Refractive index (N):	1.5488	0.0000	0.0000
	0.0000	1.5478	0.0000
	0.0000	0.0000	1.5482
Eig. Value:	**1.5488**	**1.5478**	**1.5482**

THEORETICAL RAMAN SPECTRA



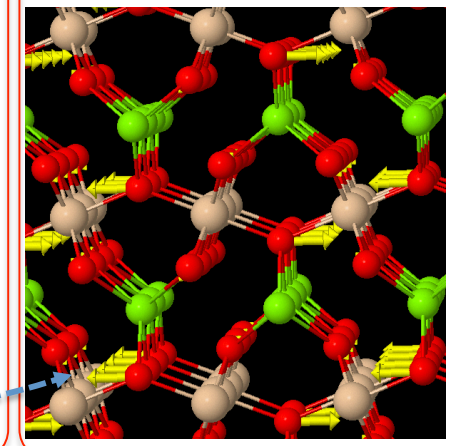
What you can do:
see raw intensities/ relative intensities
zoom in/out on the x- or y- axis.

VIBRATIONAL MODES

No.	Char.	ω TO	ω LOx	ω LOy	ω LOz
55	B2g	631	633	631	631
56	B1u	633	634	633	633
57	B3u	973	973	973	973
58	B1u	974	974	974	974
59	B2g	976	976	976	976
60	A1g	977	977	977	977
61	B2u	1056	1056	1057	1056
62	Au	1057	1057	1072	1057
63	B1g	1072	1072	1080	1072
64	B3g	1080	1080	1090	1080
65	B1u	1090	1090	1100	1100

What you can do:
click to see atoms vibrating

VIBRATIONAL PATTERN



Embedded jmol applets allow direct visualization of vibrational modes.

What you can do:
Pick fragment size, zoom in, zoom out, rotate and spin, change colors, etc.