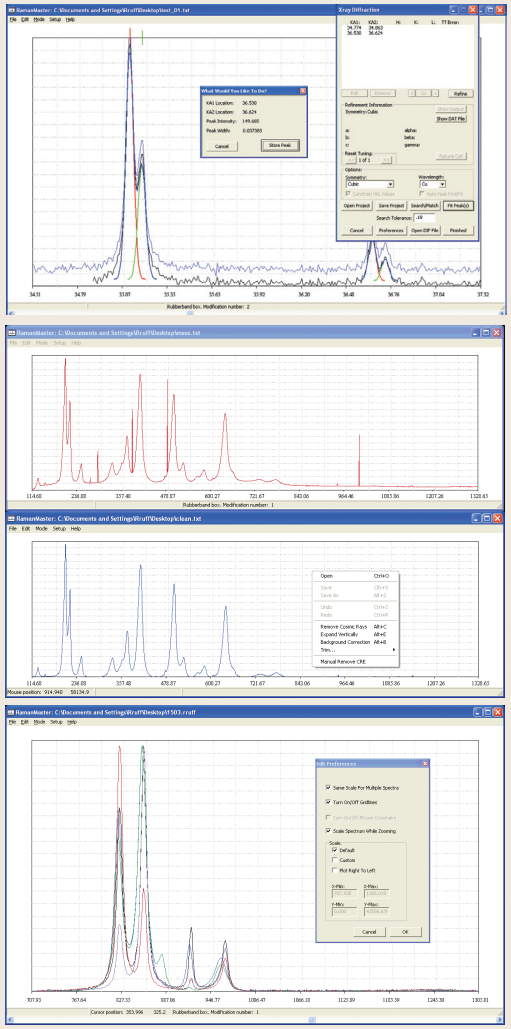
## Software Development

Another task of the project is to develop better software tools for processing and comparing the various data sets. Our software is capable of analyzing and manipulating both Raman and powder diffraction data sets. Utilizing robust routines, we remove background noise and cosmic ray events from patterns with a convenient interface that also permits comparison of multiple spectra. We can automatically locate and store peak positions, refine the unit cell from powder diffraction patterns, as well as search/match by referencing peak positions against the online database. This dynamic utility offers a user definable environment to maximize individual productivity.



The RRUFF™ project includes the research groups of Dr Robert T Downs (Geosciences, Arizona), Dr M Bonner Denton (Chemistry, Arizona), and Dr George R Rossman (Geological and Planetary Science, Caltech).

Our dedicated team of experienced professionals and enthusiastic students works tirelessly to build the premier mineral characterization database. We hope you will find each visit rewarding.

http://rruff.geo.arizona.edu/

**A note to gem and mineral collectors, dealers, and enthusiasts:**

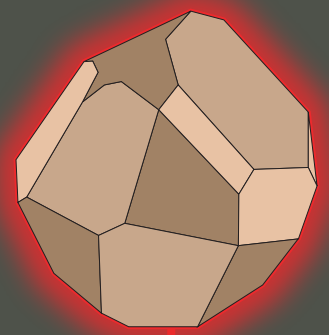
*You can help! We need thumbnail samples of very rare minerals to complete the RRUFF™ library. If you are interested in getting involved with the project or donating samples, please contact :*


Dr. Robert T Downs
email: downs@geo.arizona.edu
phone: 520-621-4938
post: Dept of Geosciences
University of Arizona
1040 E 4th, 85721-0077



*We thank our generous sponsor Michael Scott, and the many individuals & corporations who have donated samples to the project.*



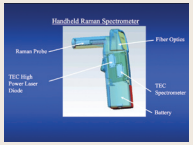
# RRUFF™ Project

## About the project

The RRUFF™ Project is creating a complete set of high quality spectral data from well characterized minerals and is developing the technology to share this information with the world. Our collected data will set the standard for mineralogists, geoscientists, gemologists and the general public for the identification of minerals both on earth and for planetary exploration.

## Spectroscopy Miniaturization

Lab instruments are intrinsically both large and expensive. Miniaturization addresses these problems and makes personal spectroscopy feasible. At the forefront of this effort are the hand-held Raman instruments constructed from "off-the-shelf parts" including the same class 2 lasers used in laser pointers.




## Closer look at the Database

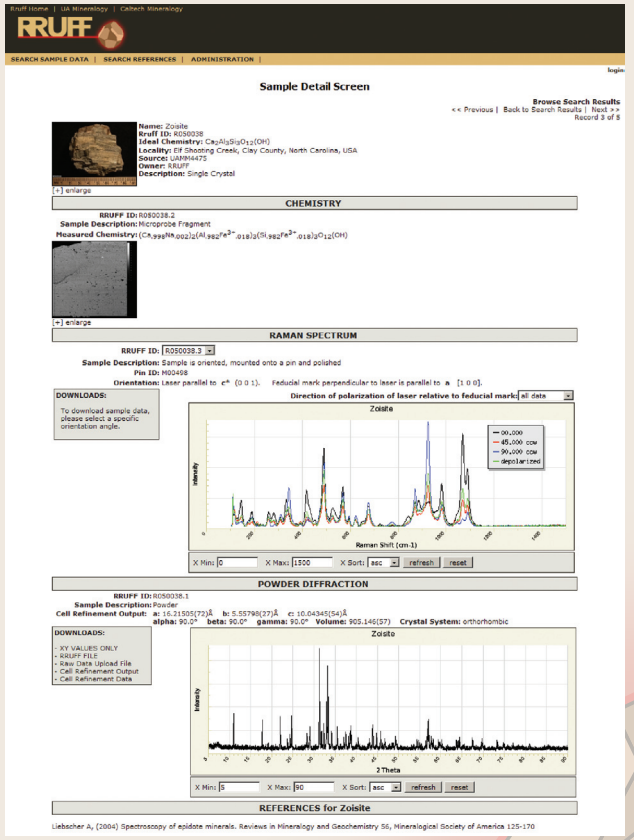
To use the vibrational spectrum as an identification tool, one must reference against a previously established database. The RRUFF™ Project is developing such a database, accessible at:

*http://rruff.geo.arizona.edu*

Anyone with as much as incidental experience in the field of gems and minerals has probably encountered a sample that was mislabeled. The cause of this misidentification may be accidental or unscrupulous, but regardless, mineral misidentification is a common occurrence.
To ensure accurate identification of the many mineral samples used in the database, the RRUFF™ research group determines the identity of minerals using X-ray diffraction and Electron Microprobe analysis. Raman spectra are then recorded on polished, oriented samples.

## Sample Detail

The largest database of it's kind, RRUFF™ contains thousands of mineral spectra. The project welcomes new samples including minerals not present in the database as well as repeated mineral species from different localities.




Advantages to the database design include:

- easy retrieval of multiple data sets for a given sample
- expansibility to include data from alternative analysis and characterization
- linked documentation and references

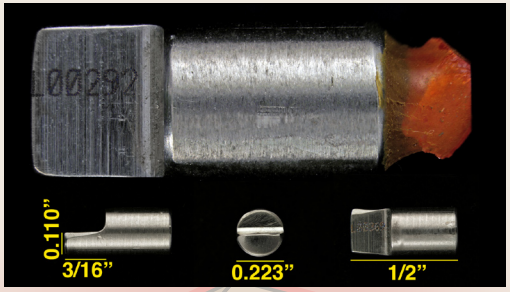
## Equipment

### X-ray Powder Diffraction

For X-ray Powder diffraction, the RRUFF™ project uses the Bruker D8 Advance. A powdered sample is examined from 5° to 90° 2-theta at 2.0 seconds per 0.010° step. The data is matched against the ICDD, and the unit cell is refined using (h k l) values from the American Mineralogist Crystal Structure Database.

### Single Crystal CCD Diffractometer

Crystal orientations are determined using a Bruker Apex X8 single crystal diffractometer. Analysis of diffraction spots from the X8 produces 3x3 matrices that describe the orientation of each crystal. The crystal can then be fixed on a pin in a chosen orientation for use with oriented experiments.




This pin is specially designed with a flat edge in order to unambiguously define two perpendicular crystallographic directions.

### Raman Spectroscopy

Several Raman spectrometers are used for the RRUFF™ Project. The Downs group has both a custom-designed unit with a 514 nm laser and a commercial Thermo Almega XR with 532 and 785 nm lasers. To obtain spectra from oriented samples we built a high-precision translation and rotation stage and goniometer for the optical bench. Denton's group has a 785 nm system that was the prototype of the Thermo instrument. Rossman's lab at Caltech has a Kaiser Optical Systems HoloProbe 785 and a Renshaw microRaman system for work at 514.5 and 780 nm.

### Electron Microprobe

Electron Microprobe Analysis is used to determine the chemical composition of the minerals. We use the UA's modified CAMECA SX50. The operator selects twenty points in the smoothest area of a polished sample for qualitative and quantitative WDS analysis. The experimentally determined elemental compositions provide the chemical formula.