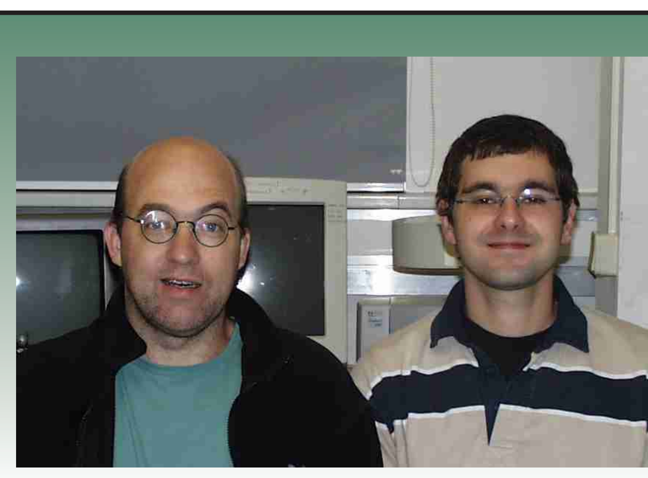
Development of a high quality Raman spectral library for minerals and fluids

Ronald J. Bakker, Christoph J. Piribauer, Verena Strauß

Mineralogy & Petrology, Department of Applied Geosciences & Geophysics, University of Leoben, Austria

www.unileoben.ac.at



Introduction

Raman Spectroscopy has become a standard analytical technique within geological sciences. The obtained spectra of unknown minerals or fluids must be compared to standard raman spectra to identify the phases. Commercial raman libraries mainly consist of organic materials. Libraries for Raman spectra of minerals and fluids are mainly available on the internet. The list of shortcomings of these online libraries include (1) to few spectra displayed; (2) no indication of accuracy, standards, deviation, relationship to crystallography or measurement conditions; (3) poor presentation of spectra; (4) bad quality of spectra; (5) relatively high cut off wavenumber; (6) absence of a search engine for spectra of unknown minerals; and (7) carelessly designed website.

The aim of this study is to address these deficiencies and to present a large series of high quality Raman spectra of all mineral groups and fluids, including an interactive search engine for unknown mineral/fluid-spectra in a well designet website.

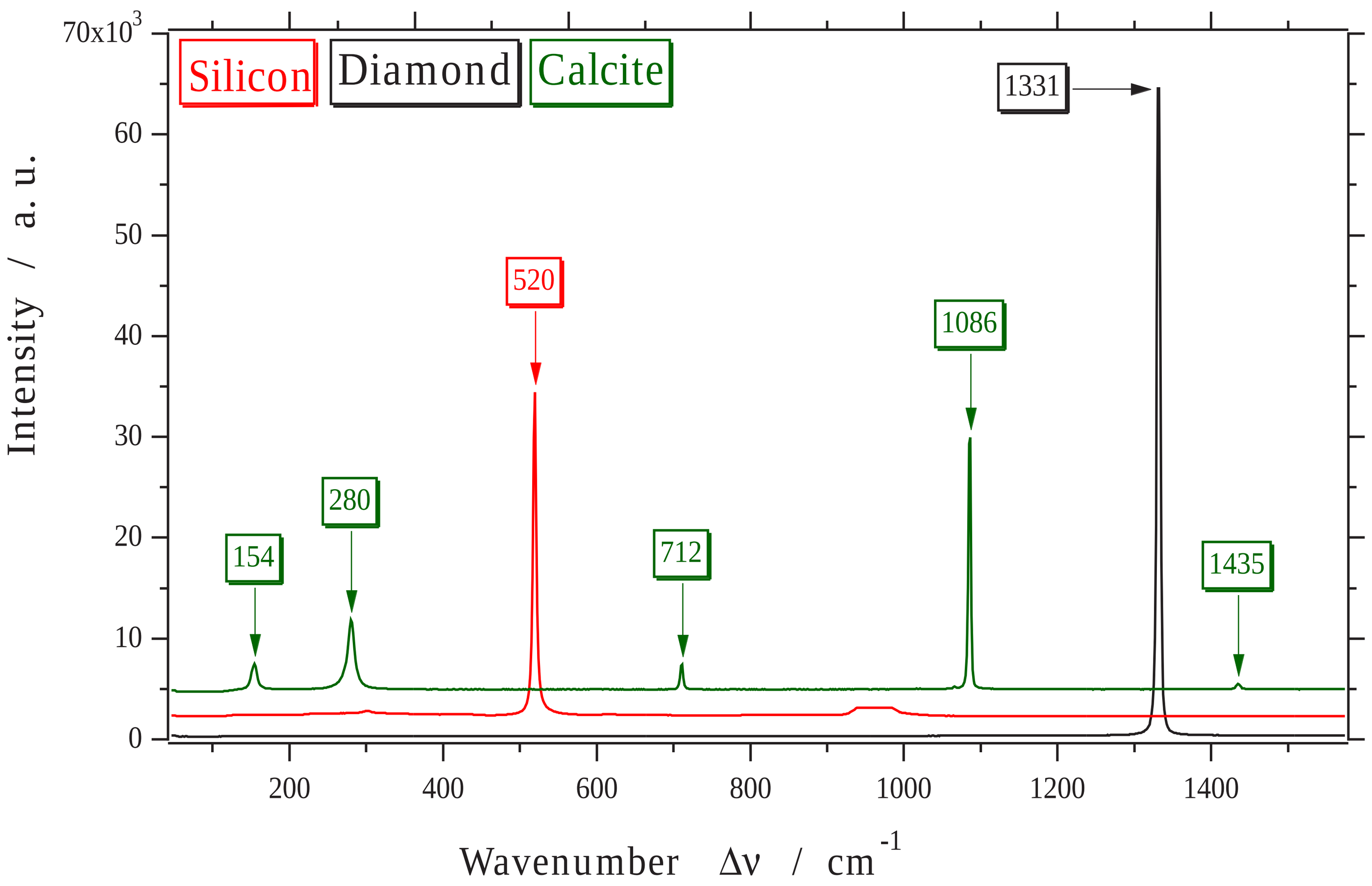
Theory

Raman spectroscopy provides information about vibration and rotation modes of molecules. The Raman effect results from interaction between electromagnetic waves (laser light) and electron clouds of molecules.

Raman spectroscopic measurements were done with a LABRAM (ISA Jobin Yvon) instrument. The laser beam is focussed through an Olympus BX 90 microscope onto the object of interest, either mineral or fluid, using 40x or 100x magnification combined with a confocal optical arrangement, enabling a spatial resolution in the order of a cubic micrometre. The apparatus has a 100 mW frequency-doubled Nd-YAG laser with a 532 nm wavelength (green), which is reduced to 38 mW at the measured object. A portion of the scattered light is collected through the microscope and focused onto a diffraction grating. The grating selects the desired region of the raman spectrum and reflects this onto a Peltier-cooled, CCD matrix detector.

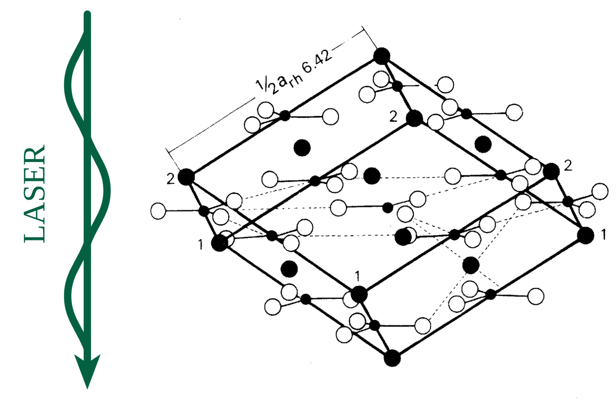
Standards

Calibration of a spectrum is obtained from comparison to silicon, diamond and calcite standard, in addition to poly-ethylene and neon-light.



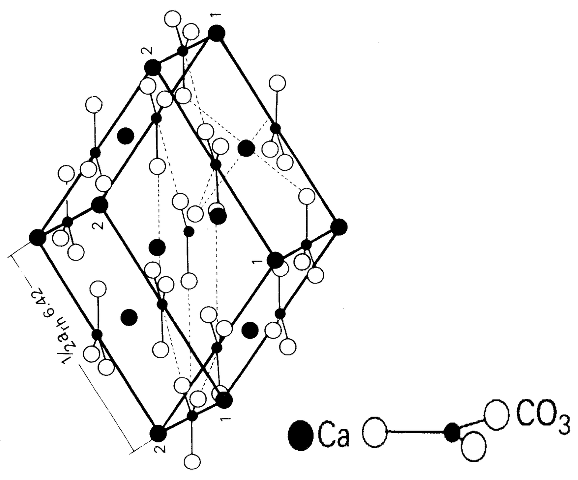
Crystal Orientation

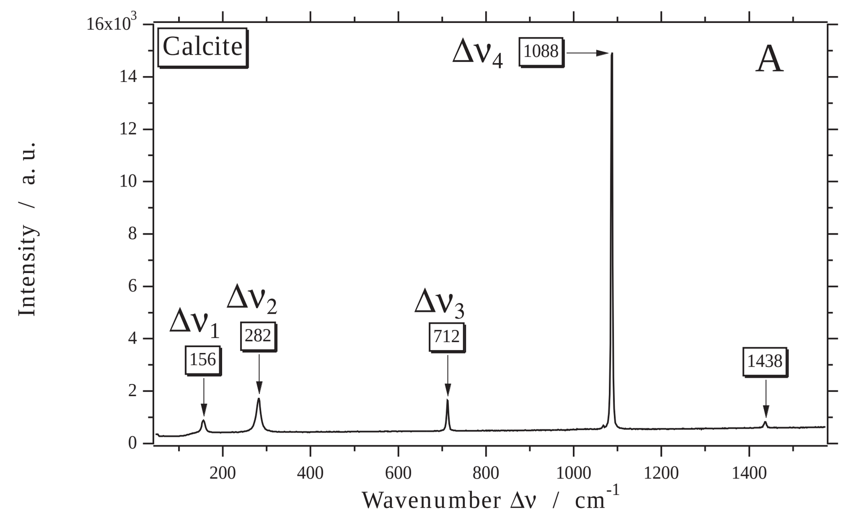
Example calcite

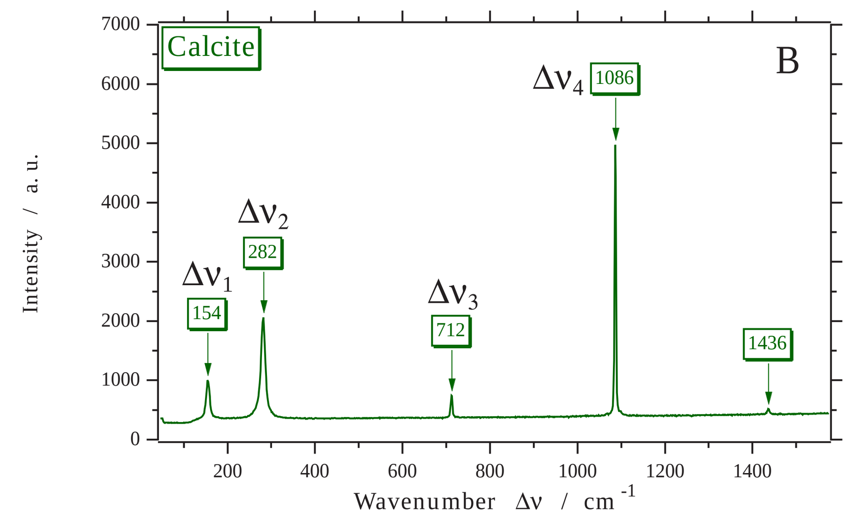


intensity ratios

	A	B
$\Delta\nu_1/\Delta\nu_4$	0.059	0.20
$\Delta\nu_2/\Delta\nu_4$	0.12	0.41
$\Delta\nu_3/\Delta\nu_4$	0.11	0.15



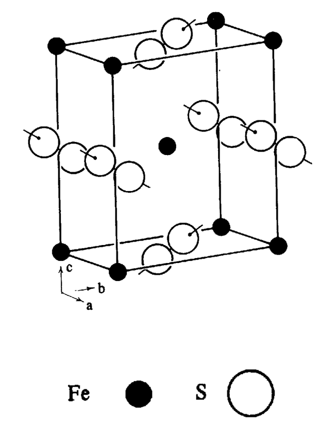




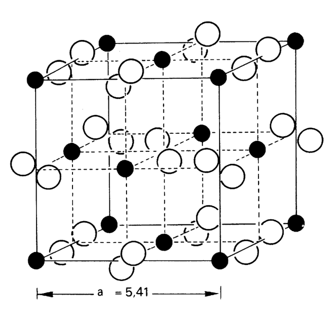
Polymorphy

Example Marcasite & Pyrite

Marcasite

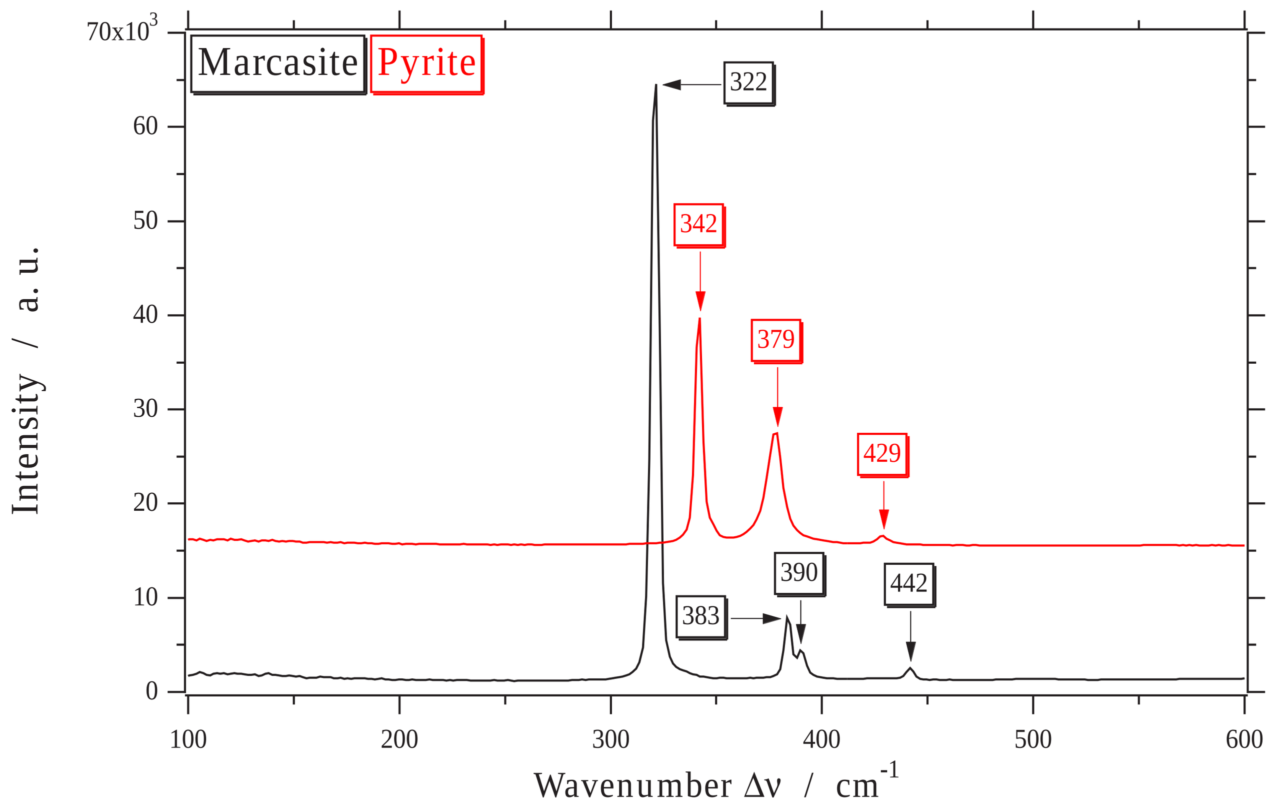


Pyrite



Pyrite

Marcasite

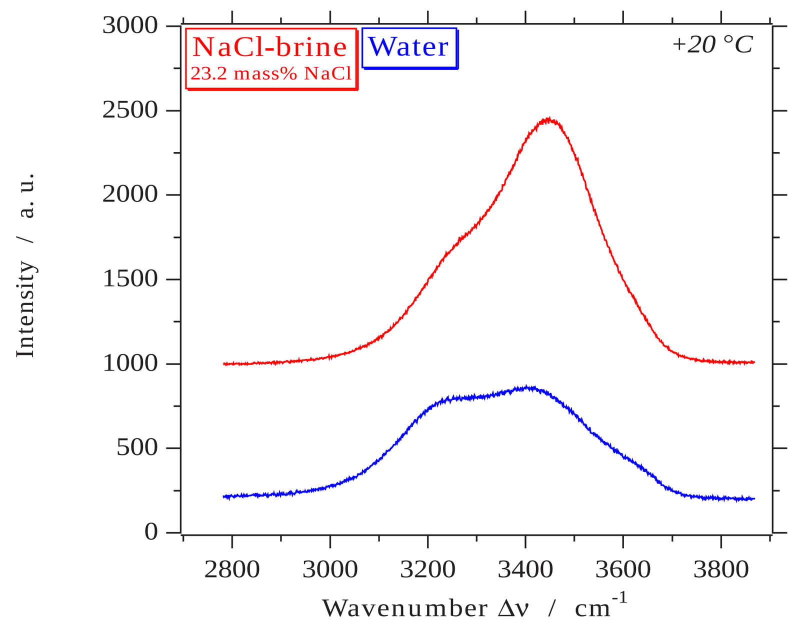


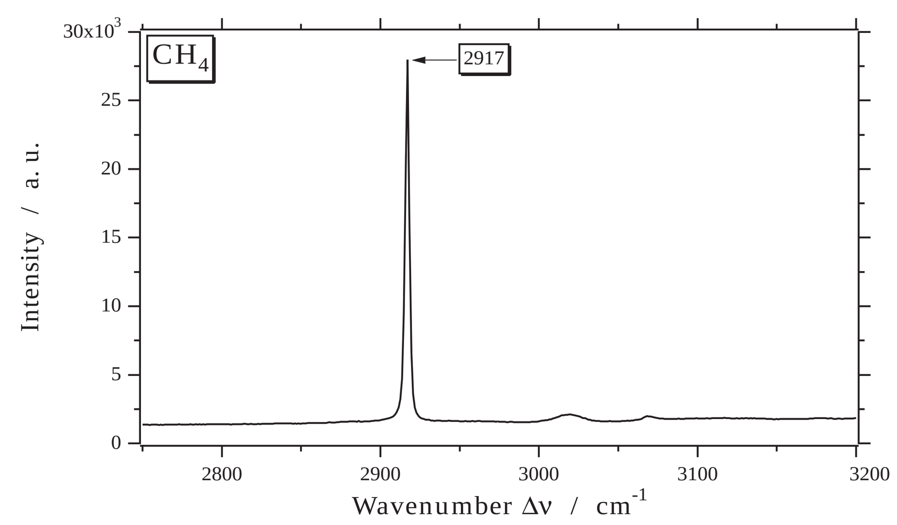
Fluids and gases

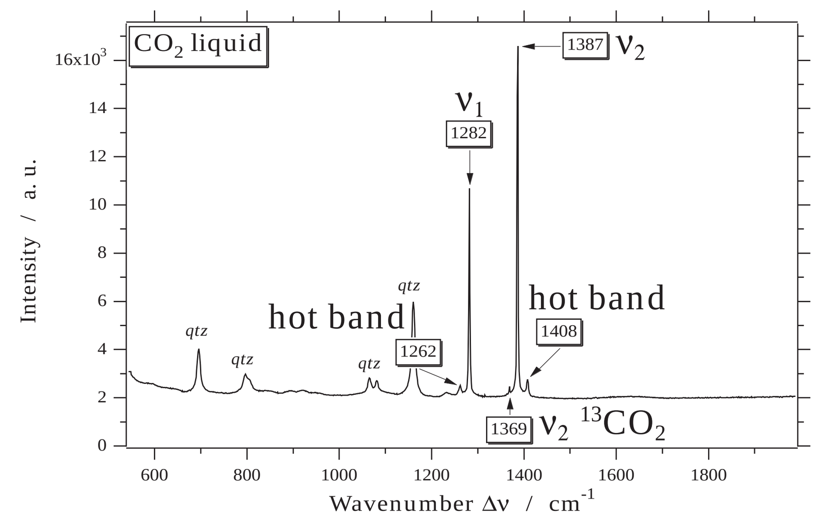
Fluid inclusions:

saline, liquid-rich

vapour-rich







Excel

How the data is stored:

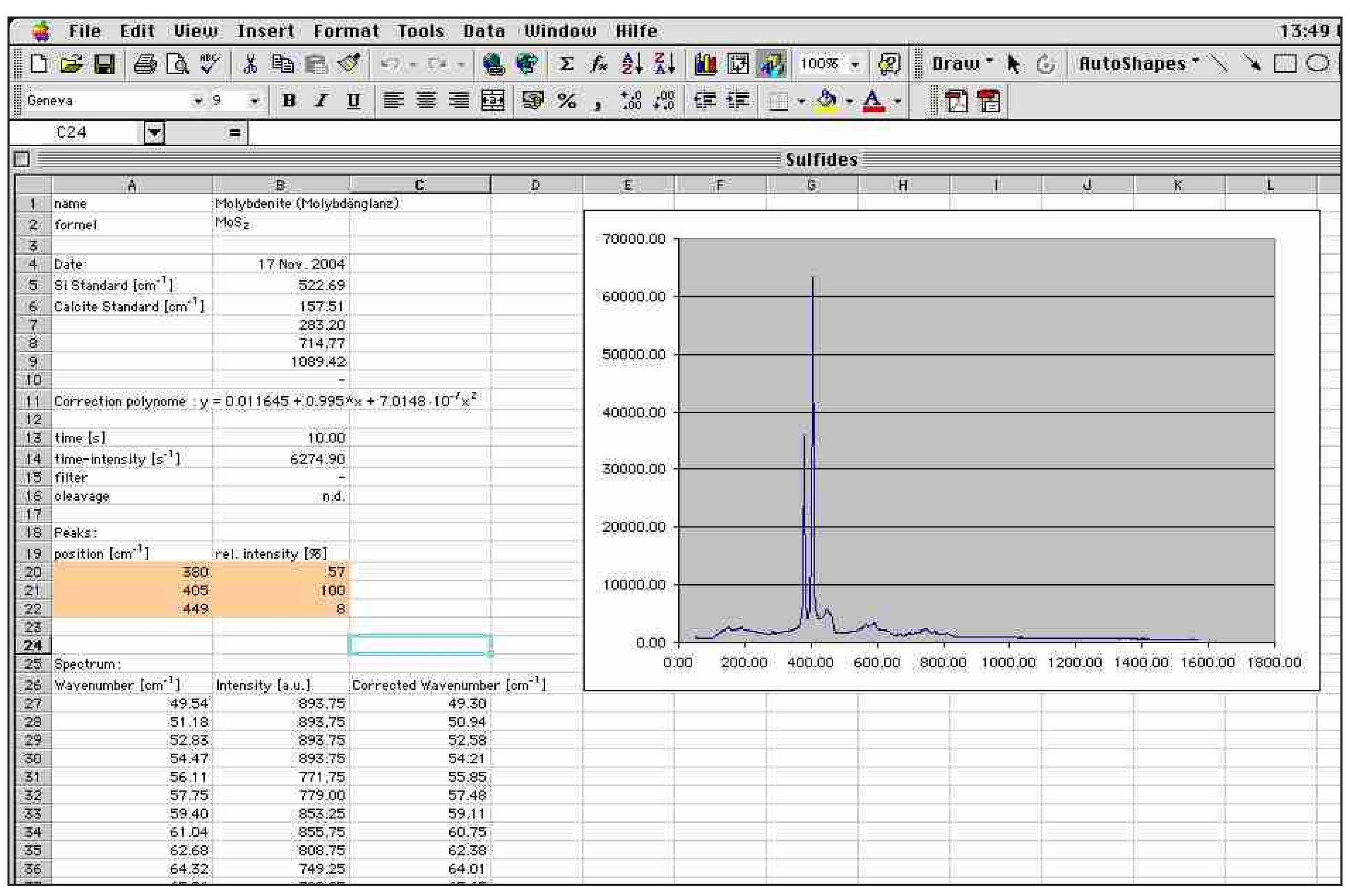
mineral

standards

conditions

peaks

spectrum



Future

A complete data set off all mineral groups will be gathered. Each mineral that is measured with Raman spectroscopy will be chemically characterised with a microprobe to establish a semi-qualitative Raman analysis.

An interactive search-machine will be designed in a web-page, with the ability to search according to complete spectra, parts of spectra, mineral names, and chemical composition.

Temperature dependent variation of Raman spectra of fluids and gases will be documented and modelled. The user can select a temperature to visualize a specific spectra (especially aqueous solutions), that is produced in a cooling/heating run of fluid inclusions.

The data set will be expanded with chemical substances, including metal alloys, oxides, hydrocarbons, ceramics, plastics, composite materials, polymeric materials.