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INTEGRATED DATABASE OF RAMAN SPECTRA, X-RAY DIFFRACTION AND CHEMISTRY DATA FOR MINERALS

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The presentation is an update on a multi-institutional effort to build an integrated database of vibrational spectroscopy, crystal structures and chemical composition of all minerals. Mao influenced one of the members of the project when he told Downs, who was just finishing his post-doc, that Raman spectroscopy had a bright future and could be used to identify and characterize minerals. 'If you can afford a Raman instrument, then go and get one!'

The goal of this database project is to collect a complete set of high quality data from fully characterized minerals, and to develop and adapt technologies on data acquisition and on information storage and sharing. The philosophy of the project is to provide a portal of fully integrated and searchable information that mineralogist, geoscientists, gemologists and general public can easily utilize for identification of unknown minerals, earth and planetary exploration, and broad scientific research, and for examining systematic relationships among structural, chemical and physical properties.

Currently, this database project is completing its first year. Essentially, all technological developments are complete and logistics are refined for complete data acquisition from raw mineral preparation to data collection and analysis. Portability of single crystals with known crystallographic orientation is essential for polarized single crystal Raman spectroscopy, and facilitates alternative studies of oriented crystals such as for other spectroscopic and acoustic measurements. Techniques are developed and fully tested for orientation and consistent transfer of single crystals for analysis and characterization. Database technologies are adapted to ensure consistency of stored data and the web-based interface is designed for the specific type of data in this project. The design allows easy retrieval of desired data sets, and is expandable to include data from alternative analysis and characterization, or documentation and reference.

Currently, the database hosts data for about 900 mineral entries with data from Raman spectroscopy of un-oriented and oriented crystals, X-ray diffraction and electron microprobe analysis. Multiple data sets are collected and stored that represent compositional variations in minerals and multiple examples of a particular mineral from different localities.