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Database of Raman spectra for REE mineral endmembers and applications to aqueous REE complexation

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Rare earth elements (REE) are critical elements important for society due to their use in the high-tech and green energy industries. They are economically enriched in ore deposits, where they are hosted in phosphate, carbonate, and/or fluoride minerals. Ligands such as chloride and hydroxyl form aqueous complexes with the REE and allow their mobilization in these deposits. However, there is a significant knowledge gap when it comes to understanding the formation conditions and stability of these REE minerals and aqueous species. Here we use a LabRAM HR Evolution confocal Raman microscope equipped with a 532 nm Nd-Yag laser (100mW) and a 266 nm DPSS UV (50mW) laser to measure the spectra of high purity (>99.99%) synthetic solid REE endmembers (monazite, rhabdophane, oxides, hydroxides, and chlorides) and aqueous solutions with variable pH and salinity, and REE concentrations of 0.2 and 2 mol/kg. Solutions are measured at room temperature and using two different hydrothermal cells (i.e., a capillary cell and a hydrothermal diamond anvil).

Lattice vibrations for REE-O generally occur between 87-428 cm^{-1} and 466-1091 cm^{-1} for vibrational PO_4 bending and stretching bands [1] in REE phosphates (Fig. 1). Oxides show the simplest Raman spectra with a dominant band between 320-420 cm^{-1} [2]; the dominant band for NdO is at 431 cm^{-1} in the anhydrous oxide and three main peaks occur at 290, 359 and 475 cm^{-1} in the Nd-hydroxide (Fig. 1). These results indicate that REE-O coordination chemistry affects the position of these vibrational bands. Raman shifts for REE-chlorides occur ~200 cm^{-1}. For REE endmembers with decreasing atomic radii and increasing atomic weights these bands shift systematically from lower to higher wave numbers indicating a high sensitivity for minor changes in bond chemistry. Preliminary data for $NdCl_3$-bearing solutions at room temperature show a REE-O peak band at 296 cm^{-1} overlapping with the peak bands of the Nd-hydroxide solids. Systematic evaluation of REE-bearing solutions at elevated temperature will provide new information on the coordination chemistry of aqueous REE complexes relevant to hydrothermal fluids.

[1] Silva et al. (2006), Opt. Mat., 26, p.224-230.

[2] Ubaldini & Carnasciali (2006), J. Alloys Compd., 454, p.374-378.