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Kinetic study on dehydration reactions of $Ca(OH)_2$and $Ca(OD)_2$by Thermo Gravimetry measurements

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Hydrous minerals are expected to be present in the downgoing slabs and the uppermost earth's mantle. Knowledge of the physical properties of hydrous minerals, especially, mechanism of dehydration process is important to understand the source of water in the mantle. Portlandite, $Ca(OH)_2$, has a CdI_2type structure (trigonal, space group P-3m1) and one of the most simple hydrous minerals. $Ca(OD)_2$is often used for neutron scattering experiments instead of $Ca(OH)_2$because of the incoherent cross section of H. However, it is not so clear whether $Ca(OD)_2$is good analogous with $Ca(OH)_2$in terms of some physical properties.
In order to understand kinetics of dehydration reactions of $Ca(OH)_2$and $Ca(OD)_2$, we performed Thermo Gravimetry (TG) measurements s at several different rate of elevating temperature (1, 5, 10 and 20 K/min) and determined activation energies of dehydration reactions by the Ozawa method (e.g., Ozawa, 2005). During TG measurements Ar gas was introduced in to the TG furnace to avoid the reaction between the samples and CO_2. We obtained activation energies of 16.6 and 15.2 kcal/mol for $Ca(OH)_2$and $Ca(OD)_2$, respectively. When the activation energy of dehydration reaction reflects the bonding energy of O-H(D), the activation energy for $Ca(OD)_2$is expected to be significantly larger than that for $Ca(OH)_2$.Therefore, the activation process during the dehydration reaction should be different from the breaking of O-H(D) bonding.
We also measured the FT-IR spectra of $Ca(OH)_2$and $Ca(OD)_2$at elevated temperatures. The positions of OH- and OD-stretching bands are shifted to lower wavenumbers with elevating temperature. The temperature coefficients for those bands are -0.28(4) and -0.43(3) cm^{-1}/K, respectively. It is interesting that both of those bands disappear at about 543 K which is more than 100 K below the onset temperature of dehydration.

Keywords: hydrous mineral, dehydration, Thermo Gravimetry, kinetics, $Ca(OH)_2$, $Ca(OD)_2$