A wide utilization of zeolites of different composition owing to their high porosity, propensity to the cation exchange, and processes of hydration and re-hydration results in an increasing interest to their study. Zeolites of the chabasite and phillipsite groups show the largest sizes of cavities in the net-work. Therefore, they are used more widely in diverse specific technological processes, such as catalysis, ion exchange, molecular screens, ecological problems, agriculture, etc.

Thermodynamic properties of zeolites are necessary for estimation of fields of their stability, in study of dehydration processes, and application of sorptive and catalytic properties of dehydrated zeolites. There are some data on low-temperature heat capacity of chabasite [1], erionite [2], and phillipsite [3] and data on enthalpies of formation and dehydration of synthetic calcic chabasites of diverse composition [4]. Thermodynamic data on gmelinite and harmotome are unknown so far. We studied natural samples of chabasite (Trans-Baikal, Russia) and harmotome (Khibiny, Russia) to study the hydration and dehydration of these zeolites. As a result, the following values of enhalpy of the complete dehydration were obtained: \( \Delta H_{\text{dehyd}}^0 = 1116 \text{ kJ/mol for harmotome in the interval 40-440°C} \) and \( \Delta H_{\text{dehyd}}^0 = 991 \text{ kJ/mol for phillipsite in the interval 50-500°C} \). Enthalpies of dehydration of chabasite, gmelinite, and harmotome were calculated from the experimental (microcalorimeter Kalve) data. The necessary values of \( H_{\text{f, ox}}^0(298.15 \text{ K}) \) for the corresponding oxides [5], the values of standard enthalpies of formation of these values on the basis of the enthalpy increment for number of dehydrated zeolites, measured previously, is shown. For all dehydrated zeolites, we calculated the \( H_{\text{f, ox}}^0(298.15 \text{ K}) = 353.4 \pm 13.6 \text{ kJ/mol (erionite)} \), \( 671 \pm 75 \text{ kJ/mol (gmelinite)} \), and \( 382 \pm 47 \text{ kJ/mol (chabasite)} \). The values involve all thermal effects of all processes, which accompany the zeolite dehydration, including the compaction of the Al-Si net-work.

The values of Gibbs free energies of formation of the studied zeolites were calculated: \( \Delta G_{\text{f, ox}}^0(298.15 \text{ K}) = -13466.3 \pm 33 \text{ kJ/mol (chabasite)} \), \( -39492.1 \pm 106 \text{ kJ/mol (erionite)} \), \( -28575.8 \pm 89 \text{ kJ/mol (gmelinite)} \), \( -18200 \pm 34 \text{ kJ/mol (phillipsite)} \), and \( -18082 \pm 42 \text{ kJ/mol (harmotome)} \). The study is supported by the Russian Foundation for Basic Research (project no. 00-05-64548).

References:

5. Robie R.A., Hamingway B.S. Thermodynamic properties of minerals and related substances at 298.15 K and
1 bar (105 Pascal) pressure and at high temperatures //