ENTHALPIES OF FORMATION OF CRYSTALLINE SILICATES CALCULATED WITH THE ICN MODEL

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The newly developed ICN model permits the calculation of enthalpies of forma- tion of crystalline silicates from the oxides out of structural data with ex- perimentally attainable accuracy. The calculated enthalpy of formation is com- bined from a ionic, a covalent and a nonbonded proportion. The ionic propor- tion is based on all bond lengths in the structure. The covalent proportion of the enthalpy is calculated from partial enthalpies of oxygen in special bonding arrangements. Nonbonded proportions are based on the molar volume of the phase, standardized to one oxygen. The model uses 34 phases of the systems SiO2,MgO- SiO2, CaO-SiO2, Na2O-SiO2, K2O-SiO2, Al2O3-SiO2 and CaO-Al2O3 with known en- thalpy and structure as a database. This record contains a broad structural spec- trum: silicon in tetrahedral and octa- hedral coordination, high pressure pha- ses apart from high temperature phases (e.g. stishovite, alite, mullite) and also non-silicates, i.e. pure oxides and calcium aluminates. The average error referring to experimentally determined values from the literature amounts to fewer than 0,5 kJ (per mol of the for- mula unit, standardized to one mole oxy- gen). Using the database derived from binary systems, the enthalpies of for- mation of 8 ternary phases of the sys- tems CaO-MgO-SiO2 and CaO-Al2O3-SiO2 were directly calculated with an average error of fewer than 0,5 kJ/mol oxygen. Enthalpies of formation are always cal- culated for the conditions, under which the structure determination of the phase was executed.