

Experimental Determinations of Thermochemical Properties

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Abstract

The key for establishing model calculations using ΔG minimization tools like FactSage is the knowledge of the thermodynamic data of molecules and compounds. This includes the partial pressures of gaseous species, the standard enthalpies and entropies of formation of gaseous and condensed phases as well as their enthalpies and entropies of mixing and the knowledge of phases and chemical compounds which are formed upon reactions.

Knudsen effusion - mass spectrometry provides definition of the species present above condensed phases and their partial pressures up to total pressures of ~ 200 Pa. Static vapour pressure measurements provide pressures above condensed phases from ~ 50 to $100,000$ Pa but do not allow individual partial pressures to be determined. The transpiration technique, in conjunction with total pressure measurements, provides monomer - dimer equilibria for single component systems and relative elemental abundances for gas phase species above mixtures.

Differential thermal analysis (DTA) can be used to determine enthalpies and temperatures for fusion, mixing and phase transitions. Differential scanning calorimetry (DSC) can also be used to for these parameters and also to measure heat capacities. Calorimetry is employed to determine enthalpies of formation and mixing.

In this contribution an insight will be given how basic thermodynamic data are derived with the above mentioned methods for the incorporation into thermodynamic databases.