

Determination of Thermodynamic Data for Gaseous Phases using Knudsen Effusion Mass Spectrometry

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Abstract

All materials vaporize, if the temperature is sufficient high however the technically interesting range of use lies in the solid state. Generally, their use is limited by the beginning of the vaporization. On the other hand, thermodynamic data of the condensed phase can be obtained from the partial pressures of the evaporating species. The knowledge of the thermodynamic data of chemical substances is important to understand the chemical and thermochemical behavior of materials like for example the interplay of substances during chemical reactions. The knowledge of the thermodynamic data helps to compute the and simulate the chemical process.

High temperature mass spectrometry is one of the most important methods for the analysis of vapors over condensed phases in order to determine thermodynamic data. One special variant is the Knudsen Effusion Mass Spectrometry (KEMS).

The thermodynamic data result from the measured temperature dependence of the partial pressures for the identified gaseous species. Vaporization studies with temperatures in the range between room temperature and temperatures above 2500K can be carried out by this method. The dissociation energies of a large number of gaseous species were obtained by this method. Investigations by Knudsen effusion mass spectrometry generally mean the study of equilibrium reactions involving neutral molecules and/ or atoms.

A completely new experimental setup up using this method has been constructed and is being build up in our laboratory.

The presentation will give an overview of the new apparatus and also examples of the determination of thermodynamic data like vapor pressures, activities, enthalpies and entropies of formation for various samples and systems which have been investigated. Studies for further developments as well as comparisons between experiments and model calculations complete the presentation.