

Gibbs–Helmholtz Equation: Practical Applications in Thermochemistry

S. P. Verevkin

Department of Physical Chemistry, University of Rostock, Rostock, Germany

The thermodynamic feasibility of a chemical process is determined by the sign of the Gibbs reaction energy. The Gibbs-Helmholtz equation applied to thermochemistry is clearly represented by the enthalpic and entropic contributions to the Gibbs energy. Various thermochemical methods useful to derive these contributions from experiment and theory are collected and analyzed. The concept of the “in-silico” based Gibbs-Helmholtz equation was proposed. The application of the “in-silico” procedure to modern areas of chemistry such as hydrogen storage and ionic liquids was demonstrated.

Acknowledgments: This research work was supported by the Government of Russian Federation (decree №220 of 9 April 2009), agreement №14.Z50.31.0038.