26.9: Molecular Partition Functions and Related Thermodynamic Data Are Extensively Tabulated

Real molecules can be significantly more complicated than the simple models that we often use to approximate them. To obtain a high degree of accuracy, calculations include complex corrections that can significantly decrease the efficiency of the calculations. For this reason, numerical tables of partition functions and other thermodynamical data are extensively tabulated. By placing these data in tables, they become readily accessible. The tables include experimental data combined with theoretical calculations that represent a collection of thermodynamic properties of substances.

The tabulated thermochemical properties of a substance are often given in JANAF (joint, army, navy, air force) tables. NIST contains are a large database of JANAF tables for many substances. Consider the JANAF table for methane (CH_4). The table contains the constant pressure heat capacity (C_P), standard state entropy (S°), standard state Gibbs energy (G°), standard state enthalpy (H°), standard state enthalpy of formation ($\Delta_f H^\circ$), standard state Gibbs energy of formation ($\Delta_f H^\circ$), equilibrium constant of formation expressed as a log value ($\log(K_f)$). G° and H° are expressed relative to the standard molar enthalpy at 298.15 K, $H^\circ(298.15\ \text{K})$.