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Thermochemical properties of formamide revisited: New experiment and quantum mechanical calculations

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Abstract

Formamide is one of the key compounds in organic chemistry. Surprisingly, the experimental thermochemical data for this compound are scarce. In this work, the standard molar enthalpy of formation in the gaseous state of formamide ΔfHm°(g, 298.15 K) = (-188.6 ± 0.4) kJ·mol-1 has been derived from enthalpy of formation ΔfHm°(l, 298.15 K) = (-571.4 ± 0.3) kJ·mol-1 (measured calorimetrically) and the molar enthalpy of vaporization Δ1gHm = (62.2 ± 0.3) kJ·mol-1 obtained from the vapor pressure measurements. To verify the experimental data, first-principles calculations have been performed using density functional theory (DFT), MPn, W1U, CBS-n, and Gn methods. © 2011 American Chemical Society.

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