Journal of Physical Chemistry A 2015 vol.119 N37, pages 9680-9691

Benchmark Thermochemistry for Biologically Relevant Adenine and Cytosine. A Combined Experimental and Theoretical Study

Emel'yanenko V., Zaitsau D., Shoifet E., Meurer F., Verevkin S., Schick C., Held C.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

© 2015 American Chemical Society. The thermochemical properties available in the literature for adenine and cytosine are in disarray. A new condensed phase standard (p° = 0.1 MPa) molar enthalpy of formation at T = 298.15 K was measured by using combustion calorimetry. New molar enthalpies of sublimation were derived from the temperature dependence of vapor pressure measured by transpiration and by the quarz-crystal microbalance technique. The heat capacities of crystalline adenine and cytosine were measured by temperature-modulated DSC. Thermodynamic data on adenine and cytosine available in the literature were collected, evaluated, and combined with our experimental results. Thus, the evaluated collection of data together with the new experimental results reported here has helped to resolve contradictions in the available enthalpies of formation. A set of reliable thermochemical data is recommended for adenine and cytosine for further thermochemical calculations. Quantum-chemical calculations of the gas phase molar enthalpies of formation of adenine and cytosine have been performed by using the G4 method and results were in excellent agreement with the recommended experimental data. The standard molar entropies of formation and the standard molar Gibbs functions of formation in crystal and gas state have been calculated. Experimental vapor-pressure data measured in this work were used to estimate pure-component PC-SAFT parameters. This allowed modeling solubility of adenine and cytosine in water over the temperature interval 278-310 K.

http://dx.doi.org/10.1021/acs.jpca.5b04753