EXPERIMENTAL THERMOCHEMISTRY OF GAS PHASE CYTOSINE TAUTOMERS

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Enthalpies of interconversion are measured for the three lowest energy tautomers of isolated cytosine. The equilibrium distribution of tautomers near 600 K is frozen upon the capture of the gas phase species by low temperature helium nanodroplets. The temperature dependence of the gas phase cytosine tautomer populations is determined with infrared laser spectroscopy of the helium solvated species. The interconverison enthalpies obtained from the van't Hoff relation are 1.14 ± 0.21 and 1.63 ± 0.12 for the **C31** $\rightleftharpoons$ **C32** and **C31** $\rightleftharpoons$ **C1** equilibria, respectively. **C31** and **C32** are rotamers of an enol tautomer, and **C1** is a keto tautomer. The interconversion enthalpies are compared to recent CCSD(T) thermochemistry calculations of cytosine tautomers.