

## Electrostatics for Exploring Hydration Patterns of Molecules. 3. Uracil

**Shridhar R. Gadre\*** and **K. Babu**

*Department of Chemistry, University of Pune, Pune-411 007, India*

**Alistair P. Rendell**

*Supercomputer Facility, Australian National University, Canberra, ACT 0200, Australia*

*Received: March 28, 2000; In Final Form: July 21, 2000*

A systematic investigation of the stepwise hydration of uracil has been carried out. The rich molecular electrostatic potential (MESP) topographical features of uracil provide clues on the probable water binding sites. The most noteworthy among these are the MESP minima due to carbonyl oxygens where the MESP value is negative as well as those over the uracil ring at which the MESP value is positive. Hydrated structures of uracil have been obtained employing an electrostatics-based model, EPIC (Electrostatic potential for Intermolecular Complexation) followed by *ab initio* optimization at the HF/6-31G(d,p) levels. Further geometry optimizations carried out at the HF/6-31+G(2d,p) and B3LYP/6-31+G(2d,p) levels, for smaller clusters, lead to trends in interaction energies which are in general agreement with those observed at the HF/6-31G(d,p) level. These structures incorporate squares and cubes of water as the dominant building blocks. An analysis of the difference in interaction energies ( $\Delta E_{\text{rel}}$ ) of  $\text{U}\dots n(\text{H}_2\text{O})$  and  $(\text{H}_2\text{O})_n$  clusters is seen to provide valuable information regarding hydration shells. This  $\Delta E_{\text{rel}}$  stabilizes to  $-7$  to  $-8$  kcal mol<sup>-1</sup> for  $n > 8$  and this value of  $n$  may correspond to the number of water molecules that make up the first solvation shell of uracil, based on a criterion of the interaction energy.