

Reply to “Comments on ‘Theoretical Estimations of the 298 K Gas-Phase Acidities of the Pyrimidine-Based Nucleobases Uracil, Thymine and Cytosine’”

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Received: October 22, 2003

We recently published a paper¹ on the gas-phase acidities of all the possible proton donor sites of the most stable tautomers of uracil, thymine, and cytosine (at the B3LYP/aug-cc-pVTZ//B3LYP/6-31+G(d) level). This study was inspired by the lack of a comprehensive investigation covering *all* the possible acidic sites (and not just the most acidic sites) in *all* the pyrimidine bases. Our intention was to begin the paper by summarizing all

the literature that has appeared on the experimental and computational studies of the acidities of the pyrimidine bases, such as Zeegers-Huyskens et al. examination of the acidities of the two most acidic sites (the N–H bonds) in uracil.² Unfortunately, we failed to be comprehensive in our literature discussion and did not directly reference the same authors' nice studies on the acidities of the N–H bonds (most acidic sites) in cytosine and in thymine.^{3,4} We deeply regret this mistake. Fortunately, a careful reader is still able to find these publications via the other references given in our publication.

References and Notes

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- (2) Nguyen, M. T.; Chandra, A. K.; Zeegers-Huyskens, T. *J. Chem. Soc., Faraday Trans.* **1998**, *94*, 1277.
- (3) Chandra, A. K.; Nguyen, M. T.; Zeegers-Huyskens, T. *J. Phys. Chem. A* **1998**, *102*, 6010.
- (4) Chandra, A. K.; Nguyen, M. T.; Zeegers-Huyskens, T. *J. Mol. Struct.* **2000**, *519*, 1.