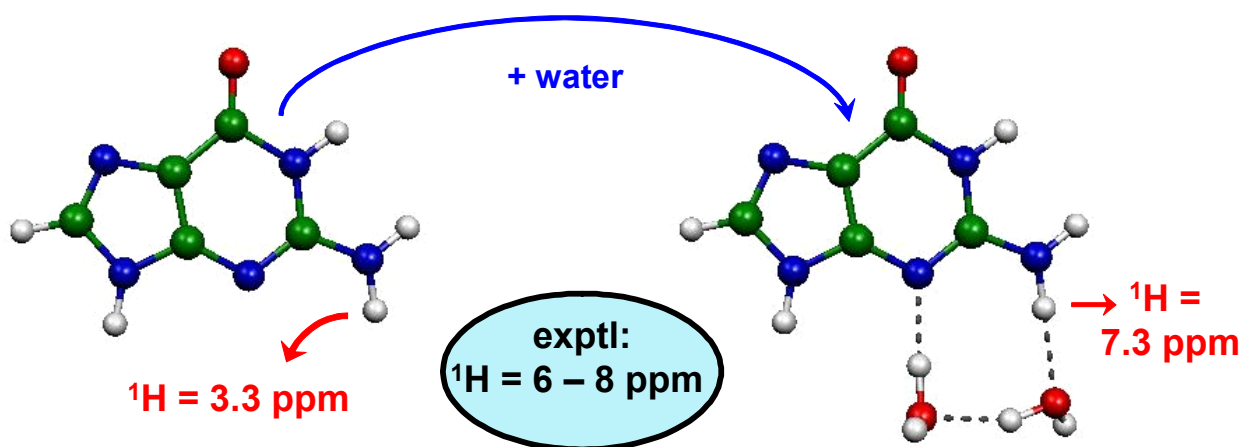




The area of computational quantum chemistry has developed drastically over the last decades, due to both increased computer power and the efficient implementation of quantum chemical methods in readily available computer programs. Because of this, accurate computational techniques can now be applied to much larger systems than before, bringing the area of biochemistry within the scope of electronic structure quantum chemistry (*ab initio* methods and density functional theory). Research in my group focuses on studying molecules of biological interest using accurate quantum chemical methods. Current research areas include the conformation of flexible biomolecules, the calculation of spectroscopic (infrared and nuclear magnetic resonance) properties and solvation effects.



Our research efforts also include the investigation of methodological accuracy, such as the determination of the intrinsic accuracy of methods, basis set convergence, and the elimination of methodological errors.

## SELECTED RECENT PUBLICATIONS

1. V.I. Danilov, T. van Mourik and V.I. Poltev, Modeling of the "hydration shell" of uracil and thymine by DFT and MP2 methods, *Chem. Phys. Lett.* **429**, 255-260 (2006).
2. D. Toroz and T. van Mourik, The structure of the gas-phase tyrosine-glycine dipeptide. *Mol. Phys.* **104**, 559-570 (2006).
3. T. van Mourik, P. Panagiotis and S.L. Price, Molecular conformations and relative stabilities can be as demanding of electronic structure method as intermolecular calculations, *J. Phys. Chem. A* **110**, 8-12 (2006).
4. T. van Mourik and A.J. Dingley, Characterization of the monovalent ion position and hydrogen bond network in guanine quartets by DFT calculations of NMR parameters, *Chem. Eur. J.* **11**, 6064-6079 (2005).
5. T. van Mourik, The shape of neurotransmitters in the gas phase: A theoretical study of adrenaline, pseudo-adrenaline, and hydrated adrenaline, *Phys. Chem. Chem. Phys.* **6**, 2827-2837 (2004).