INTERMOLECULAR INTERACTIONS BETWEEN URACIL AND REACTIVE SPECIES

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We have investigated intermolecular interactions between uracil (U) and each of the fluoride ion, superoxide anion, and the hydroxyl radical. Computational study of these new systems presents several challenges, most importantly is the choice of the proper level of theory and the appropriate size of the basis set. Our investigations on the U-F^- complex showed that the MP2 and density functional method (DFT) with aug-cc-pVDZ and aug-cc-pVTZ basis sets provide results that are consistent with those obtained with highly correlated methods for H_2O-F^-. This suggests that these levels of calculations are suitable for exploring the structures and the potential energy surfaces of the U-$O_2{}^-$ and U-OH complexes. Our preliminary results show that each of the F^- and the superoxide ions forms a very strong hydrogen bond with a specific hydrogen atom in the uracil ring. Also, results suggest that proton transfer occurs between the bonding site in uracil and each of the F^- and $O_2{}^-$ ions. On the other hand, preliminary results show that the OH radical chemically reacts with the uracil molecule. Discussion of details of calculations and results will be presented.