Ab initio calculations of the H_2CO+H_2O reaction

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Interactions of formaldehyde (H_2CO) with water are of a fundamental interest to understand the origin and fate of formaldehyde in the atmosphere as well as in astrochemistry. In order to understand these interactions between formaldehyde and water in the gas phase and the liquid phase, we performed *ab initio* and DFT calculations with the Gaussian03 and Gaussian09 software packages.

We studied the hydration mechanism of formaldehyde with water to form methanediol ($CH_2(OH)_2$) catalysed by up to 5 water molecules. Reactants, molecular complexes, products and transition state structures were fully optimized at DFT (B3LYP), MP2 and wB97XD levels of theory using the Pople-style 6-311++G** and the larger 6-311++G(3df,2p) basis sets. Two mechanisms have been investigated, in the gas phase and with an implicit solvent, which allows to simulate long range interactions, in order to determine the influence of the presence of the solvent on the reaction.

These *ab initio* calculations will allow us to calculate the rate constants using the bimolecular transition state theory. These rate constants will be compared with experimental data.

Ab initio molecular dynamics simulations have also been performed in the NVE ensemble with Car-Parrinello Moldecular Dynamics (CPMD) software package on systems mimicking 0.01 and 0.05 mol. Frac. formaldehyde solutions at 300 K, for which we have experimental data. These dynamical calculations will provide further information about solvation shell of water around the solute ($CH_2(OH)_2$ and $H(CH_2O)_2OH$).