

Theoretical and experimental study of the micro-hydration of an ion-molecule reaction involving the formation of a peptide-type bond

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Previous studies have shown that the presence of explicit water molecules can lower the energy barrier to the formation of a C-N peptide bond between acetic acid and methylamine¹.

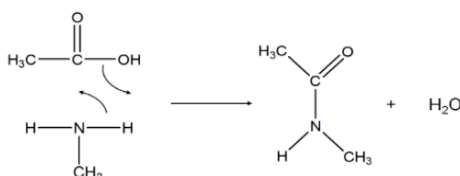


Figure 1: Reaction to form methylacetamide from acetic acid and methylamine.

A dual theoretical/experimental approach was therefore taken to understand the role of non-covalent interactions on reactivity by studying the ion-molecule reactivity between hydrated protonated acetic acid aggregates and methylamine.

The experimental study used a molecular jet coupled to mass spectrometry (CERISES "Collision Et Réactions d'Ions Sélectionnés par Electrons de Seuil") to mass-select hydrated acetic acid aggregates for reaction with methylamine^{2,3}.

The theoretical study was carried out using density functional theory, coupled with interpretative tools from theoretical chemistry such as quantum theory of atoms in the molecule and molecular electrostatic potential, to understand the role of non-covalent interactions on reactivity.

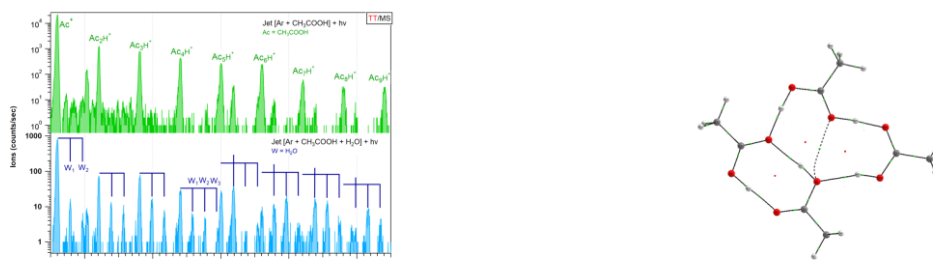


Figure 2: Mass spectra of acetic acid aggregates. QAIM image of an acetic acid aggregate.

Keywords: Mass spectrometry, Micro-hydration, DFT, QAIM, MESP, non-covalent interaction.

¹ I. Derbali, Thèse, Impact de la micro-hydratation sur la réactivité et étude de la photoionisation dissociative de petites molécules organiques d'intérêt prébiotique, 2020.

² B. K. Cunha de Miranda, C. Romanzin, S. Chefdeville, V. Vuitton, J. Zabka, M. Polasek, and C. Alcaraz, J. Phys. Chem. A 119, 6082 (2015).

³ C. Alcaraz, C. Nicolas, R. Thissen, J. Zabka, and O. Dutuit, J. Phys. Chem. A 108, 9998 (2004).