THEORETICAL INVESTIGATION OF THE FORMATION OF H₂CO IN THEINTERSTELLAR MEDIUM: A WATER ASSISTED REACTION

P. Peters¹, D. Duflot¹, L. Wiesenfeld², C. Toubin¹

¹Laboratoire de Physique des Lasers, Atomes et Molecules, (PhLAM), UMR CNRS 8523, Université Lille 1 ²Laboratoire d'Astrophysique de Grenoble, (LAOG), UMR CNRS 5571, Université Joseph Fourier

It is believed that Formaldehyde is formed on dust grains coated with ice within Molecular Clouds.[1]With this in mind there have been several studies into the hydrogenation of CO to Formaldehyde (H₂CO) reported within the literature.[2-5] These studies all consider the reaction scheme:

$2H+CO \rightarrow HCO + H \rightarrow H_2CO$

However, it is equally plausible that the second Hydrogen may add to the Oxygen of the Formyl radical to generate *trans*-HCOH. This is of importance in the interstellar medium as the gas phase barrier to isomerisation is large, and therefore will be unfavourable at low temperatures. Schreiner et al [6] showed that even with such a high activation barrier that HCOH does indeed isomerise at low temperatures to H_2CO . They propose a tunneling mechanism for the reaction, as it is evident that at 10 K the barrier is insurmountable. They did not however look at the role that water may play within this isomerisation, our work, based on quantum chemistry calculations, focuses on the role that water may play in this reaction.

- (1) A. G. G. M Tielens, W. Hagen, Astronomy and Astrophysics, 114, 245, (1982)
- (2) N. Watanabe, A. Kouchi, Progress in surface Science, 83, 439-489, (2008)
- (3) D. E. Woon, The Astrophysical Journal, 569, 541-548, (2002)
- (4) N. Watanabe, Proceedings IAU Symposium, 231, (2005)
- (5) T.P.M Goumans, C- Richard, A. Catlow, W. A. Brown, J. Chem. Phys., **128**, 134709, (2008)
- (6) P.R. Schreiner, H.P. Reisenauer, F.C. Pickard IV, A.C. Simmonett, W.D. Allen, E. Matyus, A.G. Csaszar, *Nature*, **453**, 906-911, (2008).