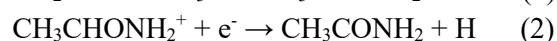


## Theoretical study on the formation of acetamide in the cold halo region of Sagittarius B2(N)

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Acetamide can represent the connection between amino acids and nucleobases which was discovered by J.M.Hollis <sup>1)</sup>. D.Quan suggested that acetamide could be synthesized through radiative association reactions and the following reactions (1) & (2) with formamide and CH<sub>3</sub><sup>+</sup> were suggested <sup>2)</sup>.



For these reactions, different electronic states can be considered. In this study, the reaction between excited triplet state NH<sub>2</sub>CHO(<sup>3</sup>A') and CH<sub>3</sub><sup>+</sup>(<sup>1</sup>A') ground state is studied.

All geometry optimizations were performed using the CCSD method with the aug-cc-pVDZ basis set. The reaction energetics were refined by performing CCSD(T)/aug-cc-pVTZ single-point energy calculations on the optimized structures. Intrinsic reaction coordinates (IRC) calculations were also performed on the B3LYP level of theory using the aug-cc-pVDZ basis set. All the calculations were performed with the Gaussian 16 quantum-chemical software. Reaction pathways are shown in Fig.1. The triplet state NH<sub>2</sub>CHO(<sup>3</sup>A') and CH<sub>3</sub><sup>+</sup>(<sup>1</sup>A') are the starting point for the reactions. Gibbs free energy (ΔG<sup>0</sup>) of reaction pathways (1) & (2) are -0.44 kcal/mol, thus, the reactions are likely to be exothermic.

From reaction (1), TS1a has the highest energy of -70.6 kcal/mol; from reaction 2, TS2 has the highest energy of -74.3 kcal/mol. The carbon atom of the formamide in the TS3 has a more positive charge compared to the TS1a and is energetically more stable. Therefore, hydrogen atom transfers and electron transfers occurred to make the carbon-carbon transition easier.

1) Detection of acetamide: The largest interstellar molecule with a peptide bond.

J.M. Hollis, *The Astrophysical Journal*, **2006**, 643, L25-L28.

2) Possible gas-phase syntheses for seven neutral molecules studied recently with the Green Bank Telescope. D. Quan, E. Herbst, *Astronomy&Astrophysics*, **2007**, 474,521-527.

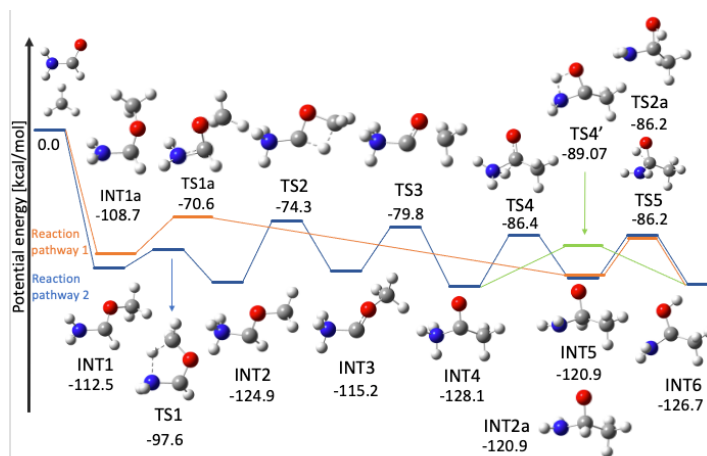


Figure 1. Energy diagram of the acetamide formation reaction