INVESTIGATING THE PRECURSORS OF ETHANOLAMINE, THE SIMPLEST PHOSPHOLIPID IN THE CELLULAR MEMBRANES DISCOVERED IN THE ISM

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Ethanolamine ($NH_2CH_2CH_2OH$, EtA), a key molecular component of phospholipids in cell membranes, has been recently detected in the G+0.693 molecular cloud[1]. This same molecule was detected in the Almahata Sitta meteorite as well. In this case, its formation has been suggested to be due to the unusual thermal conditions that might have caused the decomposition of amino acids[2]. On the other hand, its formation route in the interstellar medium (ISM) is suggested in a work led by Charnley et al. 2002[3]. Due to the addition of a carbon atom to CO, through subsequent hydrogenation and nitrogenation steps of the already detected HCCO radical intermediate, it might be possible to produce EtA. Additionally, a recent study showed the NH_3+CO+C reaction to be a barrier-less process, paving the way to an alternative route to the formation of EtA precursors in the ISM[4]. We herein perform a comprehensive quantum chemical analysis of the isomers involved in the EtA formation pathway. We extend the ensemble of isomers that can take part in this route, and we compute the energy of those that might be acting as crucial actors in the chemical steps. We optimise their molecular geometry and obtained a set of rotational and distortion constants at a high level of theory to assist their spectroscopic characterization for their future interstellar search.

[1]Rivilla, V. M. et al. PNAS, 118, 22 (2021)
[2]Glavin, D.P. et al. 45, 10-11 (2010)
[3]Charnley, S.B., et al. Earth, Moon, and Planets, v. 90, Issue 1, p. 349-360 (2002)
[4]Krasnokutski, S.A. et al. Nat Astron 6, 381–386 (2022)