

## INVESTIGATING PREBIOTIC CHEMISTRY WITH CRYOGENIC ACTION SPECTROSCOPY - GAS-PHASE GLYCOLALDEHYDE FORMATION VIA A CATIONIC "FORMOSE" REACTION

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Many complex organic molecules (iCOMs) ranging from diatoms to molecules containing up to 70 atoms, including formaldehyde, protonated formaldehyde, and glycolaldehyde<sup>a</sup> have been detected in space using astronomical observations. To understand the synthetic pathways of such potential prebiotic species in space, it is crucial to investigate their formation in the laboratory. In this work, we present results relevant to the synthesis of the simplest "sugar", glycolaldehyde, using a cryogenic 22-pole ion trap stationed at the infrared free-electron laser laboratory FELIX.<sup>b</sup> We investigate the ion-neutral gas-phase formation of (protonated) glycolaldehyde starting from neutral formaldehyde and its cationic forms,  $[\text{H}_2\text{CO}]^+$  and  $[\text{H}_3\text{CO}]^+$ . Gas-phase vibrational spectra of the reactant  $[\text{H}_3\text{CO}]^+$  and the mass-spectroscopically identified products  $[\text{H}_5\text{C}_2\text{O}]^+$  and  $[\text{H}_5\text{C}_2\text{O}_2]^+$  were recorded using cryogenic IR action spectroscopy in the frequency range 650-1900  $\text{cm}^{-1}$ , and are compared to results of quantum chemical calculations for structural characterization between different isomers. First insights into potential reaction pathways will be presented based on this combined approach, and they will be complemented with a Markov state model of the reaction mechanisms based on molecular dynamics simulations<sup>c,d</sup> to identify efficient pathways for forming glycolaldehyde and other iCOMs under low-temperature astrophysical conditions.

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<sup>a</sup>L.E. Snyder, D. Buhl, B. Zuckerman, P. Palmer, *Phys. Rev. Lett.* 22 (1969) 679–681.; M. Ohishi, S.I. Ishikawa, T. Amano, H. Oka, W.M. Irvine, J.E. Dickens, L.M. Ziurys, A.J. Apponi, *Astrophys. J.* 471 (1996) L61–L64.; J.M. Hollis, F.J. Lovas, P.R. Jewell, *Astrophys. J.* 540 (2000) L107–L110.

<sup>b</sup>D.B. Rap, J.G.M. Schrauwen, A.N. Marimuthu, B. Redlich, S. Brünken, *Nat. Astron.* 6 (2022) 1059–1067.

<sup>c</sup>W. Wang, X. Liu, J. Pérez-Ríos, *J. Phys. Chem. A.* 125 (2021) 5670–5680.

<sup>d</sup>X. Liu, W. Wang, S.C. Wright, M. Doppelbauer, G. Meijer, S. Truppe, J. Pérez-Ríos, *J. Chem. Phys.* 157 (2022) 074305.