Hessisches Kompetenzzentrum
für Hochleistungsrechnen

# *Gas-Phase Sugar Formation Using Hydroxymethylene as the Reactive Formaldehyde Isomer*



## Introduction

Carbohydrates "$(CH_2O)_n$" or sugars are the formal adducts of carbon (atoms) to water with a repeating unit that structurally resembles "H–C–OH" (hydroxymethylene, **3a**). Although hydroxymethylene has been suggested as a viable building block for sugar formation, it is a reactive species that had escaped its detection until recently.[1]

## Results

Here we demonstrate that formaldehyde (**2a**) reacts with its constitutional isomer hydroxymethylene to give glycolaldehyde (**1a**) in a nearly barrierless reaction.[2] This carbonyl-ene-type transformation operates in the absence of base and solvent at cryogenic temperatures similar to those found in extraterrestrial environments or interstellar molecular clouds. Hydroxymethylene acts as a building block for an iterative sugar synthesis as we demonstrate through the formation of the triose glyceraldehyde (**5a**). The results, therefore, provide a link between the well-known formose (Butlerow) reaction and sugar formation under non-aqueous conditions.[3-4] High-level *ab initio* coupled cluster computations confirm our proposed nearly barrierless carbonyl-ene-type reaction.

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