

## Reaction Dynamics in Extreme Environments: Matrix Isolation of Impossible Molecules

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Ice coated interstellar nanoparticles have materialized as molecular factories in the synthesis of complex, often biorelevant organics in cold molecular clouds and star-forming regions. An intimate understanding of the fundamental reaction mechanisms leading to these organics in deep space requires new knowledge on the processing of low temperature ices by (non)ionizing radiation present even deep inside cold molecular clouds. This talk provides an overview on recent surface science and matrix isolation of particular importance in deciphering the underlying reaction dynamics and kinetics leading to complex organics in deep space, many of which should not exist according to classical textbook knowledge. In detail, this talk reports on the preparation and identification of the highly ring-strained oxirene molecule (*c*-C<sub>2</sub>H<sub>2</sub>O) via resonant energy transfer of the internal energy of oxirene to the vibrational modes of the matrix molecules,<sup>[1]</sup> on the synthesis of the homologues series of disubstituted methane molecules [methanediamine (CH<sub>2</sub>(NH<sub>2</sub>)<sub>2</sub>),<sup>[2]</sup> aminomethanol (NH<sub>2</sub>CH<sub>2</sub>OH),<sup>[3]</sup> methanediol (CH<sub>2</sub>(OH)<sub>2</sub>)<sup>[4]</sup>], and the previously elusive methanetriol (CH(OH)<sub>3</sub>) — the simplest orthocarboxylic acid — along with its isomers hydroxyperoxymethane (CH<sub>3</sub>OOOH) and hydroxyperoxymethanol (CH<sub>2</sub>(OH)OOH). Supported by electronic structure calculations, these molecules were identified in the gas-phase upon sublimation from the icy matrices via isomer-selective photoionization reflectron time-of-flight mass spectrometry combined with isotopic substitution studies and detection of photoionization fragments.<sup>[5]</sup>

[<sup>1</sup>] J. Wang, J. H. Marks, A. M. Turner, A. M. Mebel, A. K. Eckhardt, R. I. Kaiser, Gas-Phase Detection of Oxirene, *Sci. Adv.*, 9, eadg1134 (2023).

[<sup>2</sup>] J. H. Marks, J. Wang, R. C. Fortenberry, R. I. Kaiser, Preparation of methanediamine (CH<sub>2</sub>(NH<sub>2</sub>)<sub>2</sub>) - A precursor to nucleobases in the interstellar medium, *Proceedings of the National Academy of Sciences USA*, 119, e2217329119 (2022).

[<sup>3</sup>] S. K. Singh, C. Zhu, J. L. Jeunesse, R. C. Fortenberry, R. I. Kaiser, Experimental Identification of Aminomethanol (NH<sub>2</sub>CH<sub>2</sub>OH) – The Key Intermediate in the Strecker Synthesis, *Nat. Commun.* 13, 375 (2022).

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[<sup>5</sup>] A. M. Turner, R. I. Kaiser, Exploiting Photoionization Reflectron Time-of-Flight Mass Spectrometry to Explore Molecular Mass Growth Processes to Complex Organic Molecules in Interstellar and Solar System Ice Analogs, *Acc. Chem. Res.*, 53, 2791-2805 (2020).