Theoretical studies of interstellar isomerism: formic acid and beyond

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In recent years, astrochemistry has entered what can truly be described as a golden era, driven by an unprecedented number of new molecular detections. A defining feature of these discoveries, compared with earlier ones, is the remarkable increase in molecular complexity. For instance, the detection of large polycyclic aromatic hydrocarbons (PAHs) [e.g., 1, 2] and complex organic molecules (COMs) [3, 4] has introduced significant challenges for interpreting their chemistry, both from theoretical and experimental perspectives. A natural consequence of this greater molecular complexity is the emergence of a large variety of isomers, species that share the same chemical formula but differ in their spatial arrangement. In this talk, I will discuss our recent efforts to address interstellar isomerism, focusing on one of the most studied cases: formic acid (HC(O)OH; Figure 1), a molecule on which we have carried out extensive work [5]. I will also introduce our new protocol designed to tackle the challenges posed by the increasing structural diversity of interstellar molecules. This approach combines automated exploration of the reactive landscapes of different isomers with the development of isomer-inclusive astrochemical models, paving the way toward a more comprehensive understanding of interstellar chemistry.

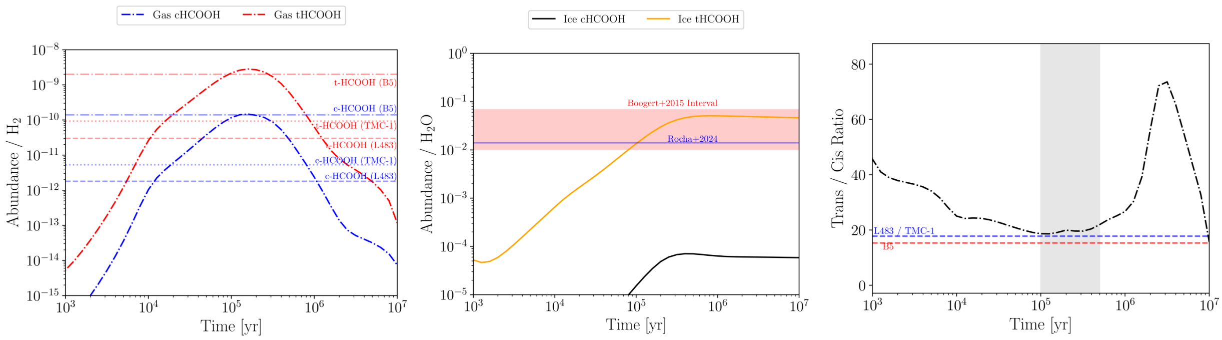

Figure 1: Isomer inclusive astrochemical models for the *cis* and *trans* formic acid. Left- Gas phase abundances compared with the abundances found in B5 [6], L483 [7] and TMC-1 [5]. Middle- Ice abundances in comparison with the literature [8,9]. Right- Gas phase *trans/cis* ratios.

References

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