On the Potential Catalytic Role of Small Heterocycles in Interstellar H_2 Formation: A Laboratory Astrochemistry Study on Furan and its Hydrogenated Forms

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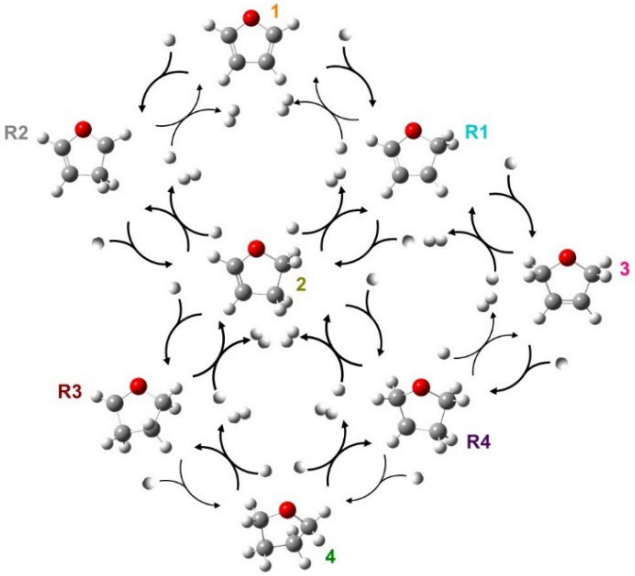
The formation of H_2, the most abundant molecule of the universe in the interstellar medium (ISM), is not fully understood. There are some hypotheses which can explain it. One of these is chemisorption. On the surface of icy grains, some molecules can chemisorb H atoms, then other H atoms can abstract these H atoms, resulting in the formation of an H_2 molecule and the original molecule; therefore, this process can be considered a catalytic cycle. Possible catalysts can be polyaromatic hydrocarbons (PAHs) and small organic molecules. According to recent quantum chemical computations,[1] small heterocycles can be more efficient catalysts than PAHs in the formation of interstellar H_2.

We have studied the reactions of H atoms with small heterocycles, furan (1) and its hydrogenated forms, 2,3-dihydrofuran (2), 2,5-dihydrofuran (3), and tetrahydrofuran (4) in solid *para*-H_2 at 3.1 K.[2] (See structures in the Figure.) The reactions were followed by Fourier transform infrared (FTIR) spectroscopy. To support the experimental results and help the spectral analysis, quantum chemical computations were performed.

By the analysis of spectra, 2-hydrofuran-3-yl (R1), 3-hydrofuran-2-yl (R2), 2,3,4-trihydrofuran-5-yl (R3), and 2,3,5-trihydrofuran-4-yl (R4) radicals were identified among the products. (See Figure.) According to our experiments, furan and tetrahydrofuran can efficiently react with H atoms in an H-atom-addition and an H-atom-abstraction reaction, respectively. In addition, 2,3- and 2,5-dihydrofurans can react with H atoms both in H-atom-addition and abstraction reactions. Since the reactions can take place in every possible direction, in the presence of H atoms, quasi-equilibrium should exist in the ISM between the investigated molecules and the radicals formed during the reactions with H atoms.



[1] Miksch, A. M.; Riffelt, A.; Oliveira, R.; Kästner, J. and Molpeceres, G. Hydrogenation of small aromatic heterocycles at low temperatures. *Monthly Notices Roy. Astron. Soc.* **2021**, *505*, 3157–3164.
[2] Schneiker, A.; Ragupathy, G.; Bazsó, G. and Tarczay, G. Potential Catalytic Role of Small Heterocycles in Interstellar H_2 Formation: A Laboratory Astrochemistry Study on Furan and Its Hydrogenated Forms. *J. Phys. Chem. A* **2022**, *126*, 2832–2844.