

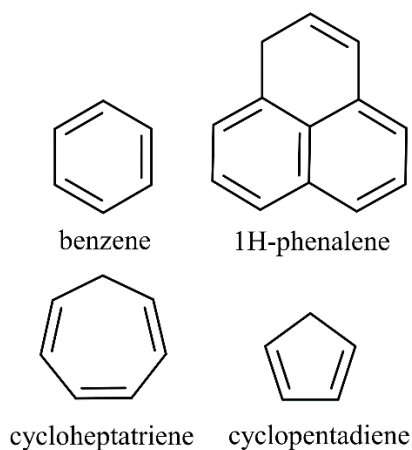
Polyaromatic Hydrocarbons with an Imperfect Aromatic System as Catalysts in Interstellar H₂ Formation

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Although H₂ is the smallest and the most abundant molecule of the interstellar medium (ISM), its formation in the present Universe is still not fully understood. Due to the low-pressure conditions in the ISM, and the lack of dipole moment of H₂, its gas-phase formation rate from H atoms both by three-body collision and by radiative association mechanisms is practically zero. It is now well accepted in astrochemistry that H₂ can form on the surface of icy grains. The models considering simple physisorption do not provide a satisfactory solution for the interstellar H₂ formation problem. A possible solution can be chemisorption. In the proposed mechanism, first, a molecule can chemisorb an H atom, and in the second step, another H atom can abstract this H atom, resulting in the formation of an H₂ molecule and the reformation of the original molecule. Therefore, this process can be considered a catalytic cycle. Possible catalysts can be for example polyaromatic hydrocarbons (PAHs).

Computations have revealed that, in contrast to graphene or graphite, the H-atom-addition to benzene and pyrene by tunneling mechanism has non-negligible reaction rates at low temperatures. From the experimental side, it was shown that atomic and molecular hydrogen reacts with benzene and small PAHs for example coronene¹. Schneiker et al.² have suggested that in the case of PAHs with an imperfect aromatic system, such as phenalene the barrier of the reaction with an H atom can be smaller and therefore, can be better catalysts than PAHs with a perfect aromatic system.

In the present study computations were performed for the H-atom-abstraction and H-atom-addition reactions. Heights of reaction barriers and reaction rates were determined for benzene, cyclopentadiene (identified in the ISM in 2021³), and cycloheptatriene with density functional theory. For each molecule, the reaction path and the tunneling reaction rates were determined at different temperatures using ring-polymer instanton theory.⁴ Furthermore, the reactions of these molecules with H atoms were investigated experimentally by *para*-H₂ matrix isolation method.

¹ Menella, V.; Hornekær, L.; Thrower, J.; Accolla, M. The Catalytic Role of Coronene for Molecular Hydrogen Formation. *Astrophys. J. Lett.* **2012**, *745*, L2.

² Schneiker, A.; Csonka, I. P.; Tarczay, G. Hydrogenation and Dehydrogenation Reactions of the Phenalenyl Radical/1H-Phenalene System at low Temperatures *Chem. Phys. Lett.* **2020**, *743*, 137183.

³ Cernicharo, J.; Agúndez, M.; Cabezas, C.; Tercero, B.; Marcelino, N.; Pardo, J. R. and de Vicente, P. Pure hydrocarbon cycles in TMC-1: Discovery of ethynyl cyclopropenylidene, cyclopentadiene and indene. *A&A* **2021**, *649*, L15.

⁴ Richardson, J. O. Ring-polymer instanton theory. *Int. Rev. Phys. Chem.* **2018**, *37.2*, 171.