Reactions of complex organic molecules at the low temperatures of interstellar media

Researchers:

- Octavio Roncero. Instituto de Física Fundamental, Consejo Superior de Investigaciones Científicas

Language Undefined

Description:

Proyecto asignado a través de la Red Española de Supercomputación (RES [1]).

Quantum simulations of reaction rates of complex organic molecules (COMs), like methanol and formaldehide, with OH, for temperature in the 10-100K range to determine the reaction mechanism and the reaction rates under single collision conditions. Quantum effects will be accounted for by the semi-classical Ring polymer Molecular Dynamic approach based on Path Integrals. These simulations will serve to validate or not the available experimental data, since they may be due to formation of dimers as recently proposed. The rate obtained will be implemented in astrophysical models to determine the abundance of different COMs under the different physical conditions of different astrophysical objects.

Web:

Links

[1] https://www.res.es/