Contribution ID: **8** Type: **not specified**

Kinetics in a cavity: the role of dynamical effects

Monday 2 October 2023 15:15 (40 minutes)

The observed modification of thermal chemical rates in Fabry-Perot cavities remains poorly understood. Mounting evidence supported by theory indicates that the cavity has a small effect on the potential energy barrier, suggesting that dynamical corrections may play a prominent role. This is in line with the relatively small modifications of the rate constant usually reported, often not exceeding a factor of 10, at most.

Here we will describe classical atomistic simulations on an ab initio potential of the cis-trans isomerization reaction of nitrous oxide (HONO) in a cavity [1]. Using the flux method to compute the recrossing coefficient, we will examine the conditions under which the cavity induces modifications of the reactive flux leading to modifications of the thermal rate. We will also consider small ensembles of HONO molecules in the gas phase, and thus shed light on the role of collective effects through specific numerical experiments [2].

Switching gears, and if time permits, I will introduce a few hints on the role of molecular symmetry and Jahn-Teller distortions in optical cavities, and how vibronic effects can result in exotic "inverse polarization" states.

References:

[1] Sun, Vendrell; JPCL 13, 4441 (2022)
[2] Sun, Vendrell; JPCL 14, 8397 (2023)
[3] Nandipati, Vendrell; PRA 107, L061101 (2023)

Presenter: VENDRELL, Oriol (University of Heidelberg)

Session Classification: Afternoon session