Instanton Theory: Prediction of Rate Constants for Astrochemical Reactions

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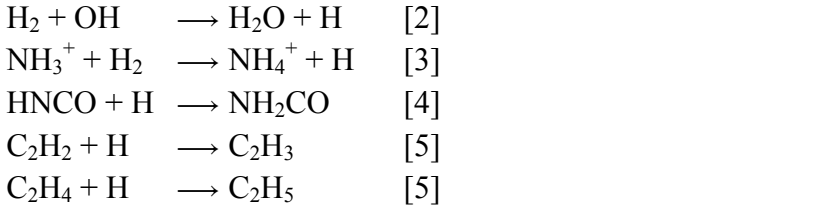
Simulations of reaction rates including quantum tunneling of atoms complement measurements and help to interpret data. An appropriate rate theory must be accurate enough to provide reliable predictions, but efficient enough to allow for computationally intensive electronic structure calculations at large enough structural models. Instanton theory, based on Feynman path integrals, matches these requirements [1]. It provides the dominant tunneling path at a given temperature or energy.

We have used it to calculate rate constants for a number of reactions of astrochemical interest both in the gas phase and on surfaces. Examples are:



$H_2 + OH$	$\longrightarrow H_2O + H$	[2]
$NH_3^+ + H_2$	$\longrightarrow NH_4^+ + H$	[3]
$HNCO + H$	$\longrightarrow NH_2CO$	[4]
$C_2H_2 + H$	$\longrightarrow C_2H_3$	[5]
$C_2H_4 + H$	$\longrightarrow C_2H_5$	[5]

Models of surface reactions need to include the interplay between reactions and diffusion.

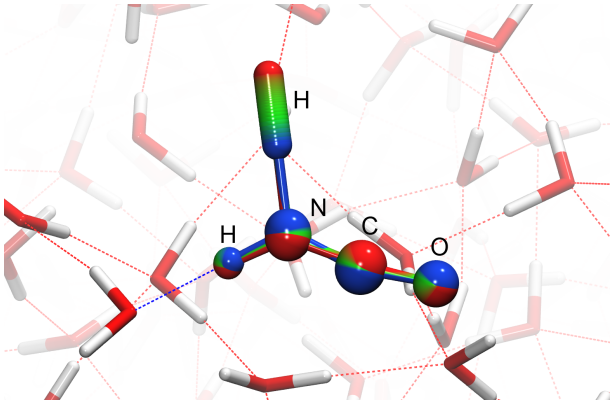


Figure 1: Tunneling path (instanton path) of the reaction HNCO + H $\longrightarrow$ NH_2CO on a surface of amorphous solid water [4]. The path is colored from the reactant side (red) to the product side (blue).

References

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