From quantum chemistry to dissociation kinetics: what we need to know

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Dissociation and association reactions play a central role in combustion, atmospheric and interstellar chemistry. The energy levels of the species involved generally are well characterized from spectroscopy and quantumchemistry. In spite of this, rate theories are far from being satisfactory. What is lacking? This talk gives an overview of the state of the art, both experimentally and theoretically. Reaction systems like

$CH_4 \rightarrow CH_3 + H$,

$C_2F_4 \rightarrow 2CF_2$,

$H_2CO \rightarrow [H_2 + CO, H + HCO]$,

$HO + NO_2 \rightarrow [HONO_2, HOONO]$,

$H + O_2 \rightarrow HO_2$,

$O + O_2 \rightarrow O_3$,

$C + OH \rightarrow COH$,

$SF_6^- \rightarrow [SF_5^- + F, SF_6 + e^-]$,

and $CF_3^- \rightarrow [CF_2 + F^-, CF_3 + e^-]$

are considered.