
Contribution of excited electronic states to low temperature rate constants of radical reactions

Juergen Troe^{*1}, Anatol Maergoiz^{†1}, and Evgeny Nikitin^{‡2}

¹University of Goettingen – Tammannstrasse 6 D-37077 Goettingen, Allemagne

²Max-Planck-Institute for Biophysical Chemistry – Am Fassberg 11 D-37077 Goettingen, Allemagne

Résumé

When radicals collide with molecules, the open electronic shell character of the radicals may lead to a passage through a multitude of electronic states of the reaction complex and the Born-Oppenheimer approximation of the potential will break down. The contribution of this effect to the rate constant so far has been taken into account only for very few examples. It is difficult to calculate, but it is of large relevance for all radical reactions under astrochemical conditions. This talk reports on recent theoretical results (refs1 and 2) for the reactions of HO radicals with C and N atoms. Tentative conclusions on the reaction of HO with O atoms are also discussed.

1. A.I. Maergoiz, E.E. Nikitin and J. Troe, Electronic nonadiabatic effects in low temperature radical-radical reactions I. C + OH, J. Chem. Phys. 141, 044302 (2014)

2. A.I. Maergoiz, E.E. Nikitin and J. Troe, Electronic nonadiabatic effects in low temperature radical-radical reactions II. N + OH, in preparation (2015)

*Intervenant

†Auteur correspondant: amaevgo@gwdg.de

‡Auteur correspondant: enikiti@gwdg.de