Nonadiabatic Reactions
on Three Coupled PESs of CH_2 and ON_2

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We present the nonadiabatic collision dynamics and gas kinetics of the combustion and atmospheric reactions $C(^1D) + H_2(X\,^1\Sigma_g^+) \rightarrow C(^3P) + H_2(X\,^1\Sigma_g^+)$ / $CH(X\,^2\Pi) + H(^2S)$ and $O(^1D) + N_2(X\,^1\Sigma_g^+) \rightarrow O(^3P) + N_2(X\,^1\Sigma_g^+)$. We use our quantum theory of nonadiabatic effects in triatomics (1,2), the quantum real wavepacket method (3,4), and configuration-interaction PESs, Renner-Teller (RT), and spin-orbit (SO) couplings between the three lowest electronic states of CH_2 and ON_2. We discuss the effects of permutation-inversion symmetry rules and of Coriolis, RT, and SO couplings on reaction probabilities, cross sections, and rate constants. As an example, the figure presents the $O(^1D) + N_2(X\,^1\Sigma_g^+)$ SO+RT cross sections versus the collision energy, resolved on two N_2 rotational states. We see a resonance-dominated barrierless collision, reflecting the $\tilde{X}\,^1A'$ deep potential well, and rotational and Coriolis reactivity enhancements, both due to symmetry selection rules. The nonadiabatic interactions play different roles on the quenching dynamics, because the singlet-triplet SO effects are by far more important than the RT triplet ones.

References

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