Quasi-classical study of the photodissociation dynamics of the methyl radical.

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The photodissociation dynamics of the methyl radical from selected vibrational levels of the 3s and 3pz Rydberg states has been studied using the trajectory surface hopping method. One-dimensional ab initio potential energy surfaces along the carbon-hydrogen dissociative coordinate have been used. Lifetimes and the distribution over the dissociation channels have been reported for all the studied vibrational levels and compared with previous theoretical and experimental works. The obtained lifetimes show a decreasing trend as vibrational excitation in the symmetric stretch and bending umbrella modes increases. The results have been compared with recent experiments [1] showing very good accordance for the lowest energy levels.

References

[1] Balerdi et al., Phys. Chem. Chem. Phys., 18 (2016) 110

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