

ELECTRON SCATTERING BY MOLECULAR RADICALS (NO, CF)

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Low-energy scattering of electrons by radicals is of interest in a wide range of chemical and physical processes. Nitric oxide, for instance, is important in atmospheric processes and plays key functional roles in a variety of physiological systems. It is also used as a plasma gas. Knowledge of collision dynamics with CF is important in plasma etching processes. It is formed within plasmas under electron bombardment of C_2F_4 , which has been proposed as a new feed gas due to its relatively benign impact on the atmosphere. Because of their high reactivity, radicals like CF are difficult to work with experimentally, making theoretical studies of collision processes crucial in the determination of cross sections, transition rates and other quantitative characteristics. Despite the need for *ab initio* results on electron scattering by NO and CF radicals, such calculations are scarce, particularly in the energy region below 2 eV, which is dominated by negative ion resonances. In the case of NO, recent experimental measurements of Allan [1] and of Jelisavcic *et al.* [2] allowed comparison and represented a test to theoretical models that could later be applied to radicals for which experimental data is unavailable, like CF. This prompted us to perform an *ab initio* study of elastic scattering and vibrational excitation of NO by electron impact in the low-energy (0-2 eV) region where the cross sections are dominated by resonance contributions [3]. We employed a non-local treatment of the nuclear dynamics, which was found to remedy the principal deficiencies of the local complex potential model. The complex-valued potential curves were obtained by combining large-scale configuration-interaction calculations for the resonance positions with fixed-nuclei, complex Kohn calculations for determining the resonance lifetimes. The resulting low-energy cross sections are dominated by shape resonance contributions associated with the $^3\Sigma^-$, $^1\Delta$ and, to a lesser extent, $^1\Sigma^+$ states of NO^- and display pronounced, overlapping boomerang structures that give irregularly shaped vibrational excitation cross sections.

We have also studied dissociative electron attachment to NO via the $^3\Sigma^-$ negative ion resonance which gives ground state $N(^4S) + O(^2P)$. Our results show that the dissociative attachment cross sections in this channel that originate from the ground vibrational state of NO are extremely small, as confirmed by several experimental studies. However, the dissociative attachment cross section is predicted by these calculations to increase by several orders of magnitude when the dissociation takes place from vibrational excited states of NO. We investigated the origin of this dramatic enhancement and predict that dissociative attachment cross sections producing ground state atomic products should be measurable starting from vibrational levels above approximately $\nu = 10$.

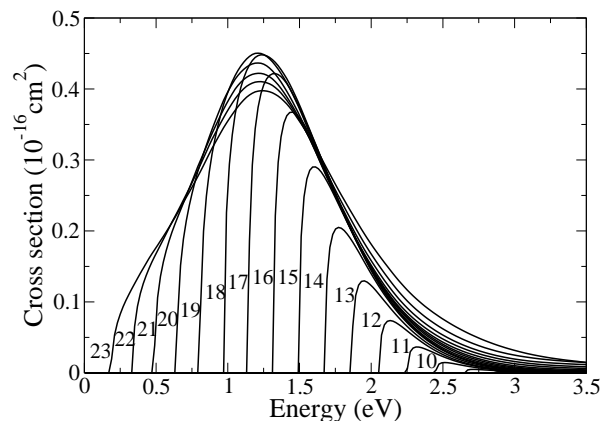


Fig. 1. NO Dissociative attachment cross sections from vibrationally excited states.

Preliminary results of low-energy electron scattering by radical CF, which is isoelectronic with NO, will also be discussed.

References

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