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Theoretical study of vibrational excitation and dissociative electron attachment of NO_2 by an electron impact

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Synopsis Cross sections for vibrational excitation and dissociative electron attachment (DEA) of the nitrogen dioxide (NO_2) molecule in collisions with low-energy electrons are determined theoretically. The thermally-averaged rate coefficients of vibrational excitation are presented for the temperatures from 10 K to 10000 K. The obtained DEA cross section for NO_2 agrees well with experimental data.

NO_2 is a common atmospheric pollutant which can cause health hazards. Electron scattering from this molecule has attracted great attention due to its increasing concentration. Notably, the processes of vibrational excitation and dissociative electron attachment play a crucial role in depollution. However, the theoretical description of these two processes for this open-shell molecule is still an extremely challenging task to date.

In this study, electron-impact vibrational excitation cross sections of NO_2 are calculated by a theoretical approach that combines the normal modes approximation for the vibrational states of the target molecule, fixed-nuclei R-matrix formalism [1] to determine the e-NO_2 scattering matrices, and the vibrational frame transformation [2] employed to evaluate the scattering matrix for vibrational transition. Corresponding thermally-averaged rate coefficients for vibrational excitation in ground electronic state of NO_2 are presented for the temperatures region 10 K-10000 K for each normal mode.

The cross sections for DEA to NO_2 are estimated through a simplified approach that following the Bardsley [3] and O'Malley [4] theory proposed for diatomic targets. We extends the formalism of resonant scattering which has already satisfactorily applied to diatomic molecules to polyatomic molecules relies on a generalized dissociation coordinate. The calculated DEA cross section is compared with the experimental data of Rangwala S A *et al.* [5]. An excellent agreement could be seen in figure 1, especially for the first peak at about 1.46 eV.

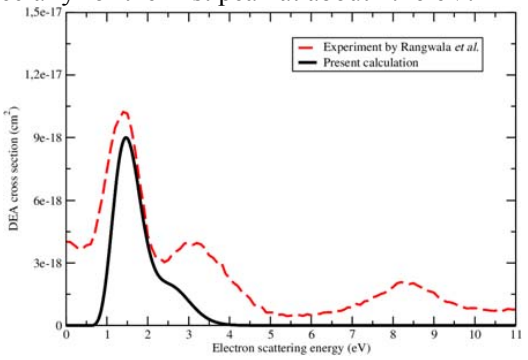

Figure 1. Calculated DEA cross section (black solid line) compared with experimental data (red dashed line) of Rangwala S A *et al.* [1].

We expect that the currently obtained e-NO_2 collisions deduced vibrational excitation and DEA data could be used as the fundamental input quantities for the kinetic modeling of the diffused low-temperature NO_2-containing plasma. Moreover, investigation of applying our model for other triatomic molecules by electron impact will be carried out in the further work.

References

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