

Complete and consistent set of electron-neutral scattering cross sections for carbon monoxide

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This work proposes a complete and consistent set of cross sections for electron collisions with carbon monoxide (CO) molecules to be published in the IST-Lisbon database with LXCat. The set is validated by comparing swarm parameters, calculated using a two-term Boltzmann solver, with available experimental data. It is shown that for low values of the reduced electric field ($E/N < 2$ Td) both rotational excitations and de-excitations mechanisms, as well as superelastic collisions with the first vibrational excited level, have to be taken into account in order to accurately predict the electron energy distribution function and the corresponding swarm parameters. The role in the calculations of the effective / elastic momentum-transfer cross section is also discussed.

1. Introduction

Carbon monoxide (CO) is one of the main constituents of Venus and Mars atmospheres [1]; it is the most abundant molecule observed in the interstellar space after hydrogen; and it is relevant in laboratory gas discharges for the production of syngas and the reforming of CO₂.

The study of the electron kinetics is essential to understand how the energy gained by the electrons from the applied field is transferred to the different heavy-particles. This work presents a complete and consistent set of electron-neutral scattering cross sections for carbon monoxide, to be soon included in the IST-Lisbon database with LXCat.

2. Description of the cross section set

The current set includes the elastic cross section, the cross sections for the excitation of 16 rotational states, 10 vibrational states and 7 electronic states, as well as the cross sections for dissociation, dissociative attachment and ionization. The cross sections are defined up to 1000 eV kinetic energy.

The elastic cross section is built in two steps: the mid- and high-energy regions are taken from [2], with small modifications; the low-energy region was re-calculated from an effective cross section in order to ensure consistency when rotational excitations are explicitly accounted for. Special attention is given to rotational excitation and de-excitation mechanisms, which can be very important at low reduced electric fields. Rotational cross sections are taken from [3]. Vibrational and electronic excitation cross sections are essentially taken from [2,4]; vibrational excitation is currently under revision, based in [5]. Finally, the dissociation, dissociative attachment and ionization cross sections are the same as in [4].

3. Results and discussion

The current set reproduces very well the available experimental swarm data. For example, figure 1 depicts the reduced Townsend ionisation coefficient.

Further results (not shown) reveal that it is essential to consider rotational excitation and de-excitation mechanisms, as well as superelastic collisions with the first vibrational level, to correctly describe the low field region ($E/N < 2$ Td) at gas temperatures $T_g \leq 300$ K.

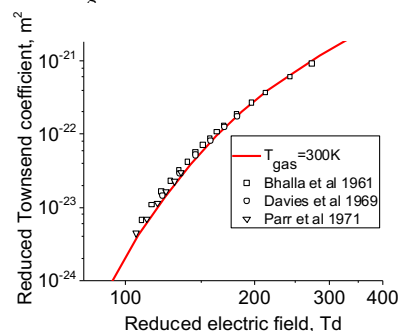


Figure 1. Comparison between calculated and measured reduced Townsend coefficient.

4. References

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Acknowledgements: This work was partially supported by the Portuguese FCT, under Projects UID/FIS/50010/2013 and PTDC/FIS-PLA/1420/2014 (PREMiERE), and grant PD/BD/114398/2016 (PD-F APPLAuSE).