

## Resonant vibration excitation cross sections and rate coefficients for electron–CO and CO<sub>2</sub> scattering

V. Laporta<sup>(\*)1</sup>, J. Tennyson<sup>1</sup>, R. Celiberto<sup>2</sup>

<sup>1</sup> *Department of Physics and Astronomy, University College London, London WC1E 6BT, UK*

<sup>2</sup> *Department of Water Engineering and Chemistry, Polytechnic of Bari, 70125 Bari, Italy*

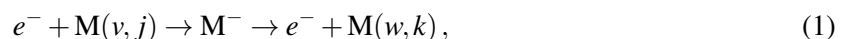
<sup>(\*)</sup> [v.laporta@ucl.ac.uk](mailto:v.laporta@ucl.ac.uk)

Vibrational excitation cross sections and rate coefficients for resonant electron–CO and –CO<sub>2</sub> scattering, in the energy range of 0–10 eV, are presented. Static exchange plus polarization calculations have been performed by using the R-matrix method to estimate resonance positions and widths. The nuclear motion is treated in the local complex potential model. Some examples are shown.

When a spacecraft enters the atmosphere of a planet at a speed exceeding the local speed of sound, a shock wave front is formed behind it and its kinetic energy is transformed into heat. The energy delivered to the gas in this process promotes the excitation of the molecular internal degrees of freedom (rotational, vibrational and electronic) as well as chemical reactions, including dissociation and ionization. The hot reacting and radiating gas, generally in non-equilibrium conditions, gives rise to complex interactions both in gas-phase and with the vehicle surface.

At low electron energies, molecular vibrational excitation induced by electron scattering is the dominant energy-transfer process. In this condition an appropriate simulation of the system requires the so-called state-to-state kinetic approach. According to this approach the molecules, in a given excited state, are considered as independent chemical species; consequently, a theoretical model requires complete sets of cross sections and rate coefficients for all the electron-impact induced transitions among all the possible quantum states of the molecules.

Direct ro-vibrational excitation by inelastic electron-impact is, in general, an inefficient process, due to the small electron-to-molecule mass ratio, and is effective for the excitation of the first few levels only. However, if resonant scattering occurs, i.e. if the incident electron is temporarily trapped by the molecule and re-emitted, high vibrational levels can be excited. A resonant scattering can be represented as:



where  $(v, j)$  and  $(w, k)$  are the initial and final molecular ro-vibrational state respectively.

In this contribution, we present new theoretical cross sections and rate coefficients for resonant scattering of electrons by carbon mono- and di-oxide molecules, aimed to the production of the basic input information for the modeling of the planetary atmospheres in re-entry conditions [1, 2]. In process (1) M stands alternatively for CO( $X^1\Sigma^+$ ) and CO<sub>2</sub>, the main components of Mars and Venus atmospheres. For the CO case the resonant contribution is around 2 eV and comes from the  $^2\Pi$  shape resonance, whereas vibrational excitation in CO<sub>2</sub> has two distinct region: a  $^2\Pi$  shape resonant at 3.8 eV and a threshold enhancement below 2 eV due to a virtual state.

The R-matrix method [3] has been used to obtain the complex potential energy curves for the resonant states. Slater Type Orbitals were employed to represent the molecular target and numerical functions for the continuum. The model includes polarization effects, accounted for by promoting a single target electron into an unoccupied orbital and placing the scattering electron into a virtual orbital. The nuclear motion is described in the framework of the local complex potential where the nuclear resonant wave function,  $\xi(R)$ , for diatomic molecule is a solution of the following equation:

$$\left( T_j + V^- - \frac{i}{2}\Gamma - E \right) \xi(R) = -\mathcal{V} \chi_v(R), \quad (2)$$

where  $T_j$  is the kinetic energy operator,  $V^- - \frac{i}{2}\Gamma$  the complex resonant potential curve,  $\chi_v(R)$  the neutral eigenfunction and  $\mathcal{V}$  the discrete–continuum coupling. This approach has already used to study electron scattering by hydrogen [4] and NO [5] molecules. For the case of polyatomic molecule a multidimensional extension of Eq.(2) is needed. Below some preliminary results, for electron–CO [6] and –CO<sub>2</sub> scattering, are shown.

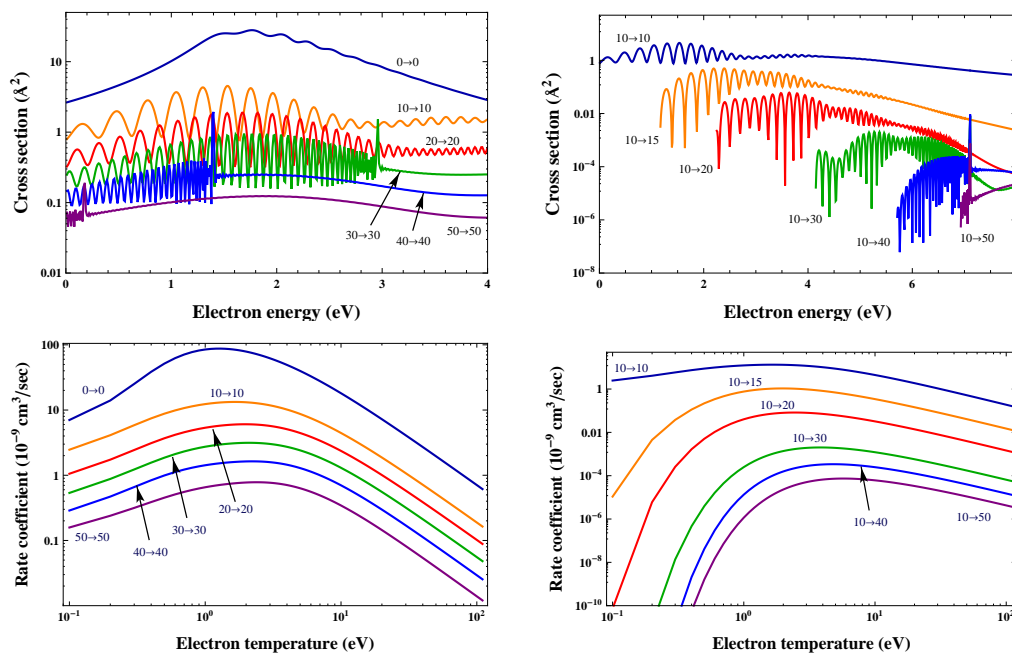


Fig. 1: Resonant electron–CO scattering. Top: elastic cross sections (left) and some examples of vibrational excitation processes (right). Bottom: rate coefficients

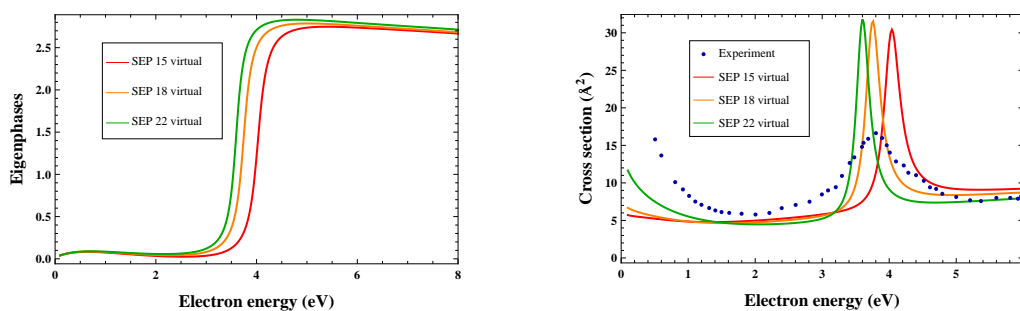


Fig. 2: Eigenphases sum and total cross section for electron–CO<sub>2</sub> scattering. The different curves represent the number of virtual orbital included in the calculation.

## References

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