IST-LISBON database with LXCat: Electron scattering cross sections for oxygen and carbon dioxide

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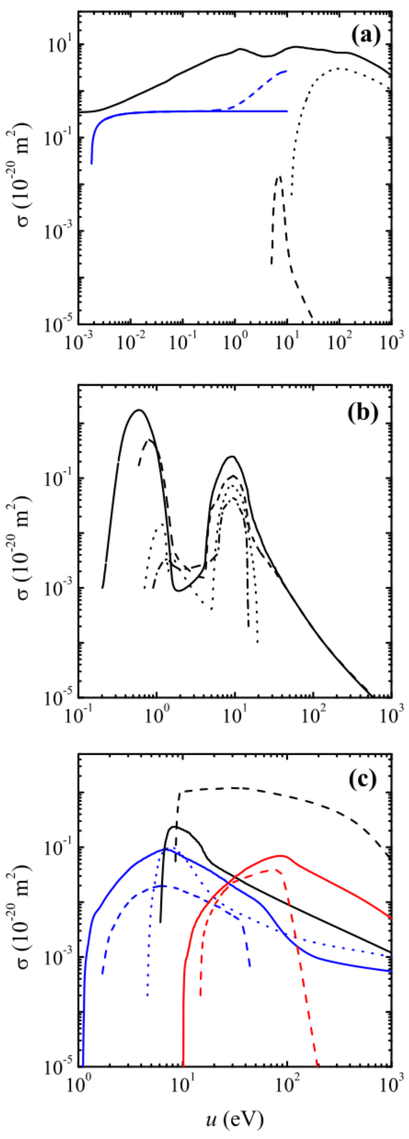
Introduction

Oxygen-containing low-temperature plasmas, often produced in combination with other molecular gases and/or with noble gases, are the focus of a wide-range of interests spanning from fundamental studies to applications in various fields, such as material processing and functionalisation, biomedical purposes and environmental/energy applications. Carbon dioxide is at the heart of environmental issues, usually due to the greenhouse effect and recently because this gas can contribute to facilitate energy storage [2]. Therefore there is need for an accurate description of the electron kinetics by solving the electron Boltzmann equation. This work proposes sets of electron scattering cross sections compiled for kinetic energies up to 1 keV, as part of the IST-LISBON database with LXCat, for both molecular and atomic oxygen and for carbon dioxide. The complete and consistent sets of cross sections for O_2, O and CO_2 are validated using the two-term Boltzmann solver embedded in LoKI (LisbOn KInetics) numerical code to calculate swarm parameters, yielding fairly good agreement with the available experimental data. It is evidenced that the inclusion of rotational transitions in O_2 and superelastic collisions with CO_2(010) molecules is essential to reproduce the experimental values of the swarm parameters for E/N < 1 Td.

Electron cross section for O_2



The IST-LISBON complete set of electron-scattering cross sections with ground-state molecular oxygen includes the following 14 mechanisms [3]:

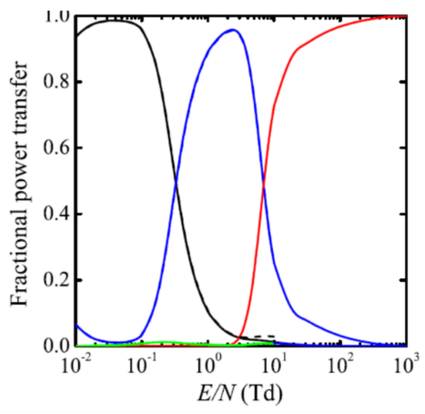
Fig. 1a
- effective momentum-transfer (black solid line)
- dissociative attachment (black dashed)
- ionization (black dotted)
- Rotational excitation $J = 1 \rightarrow J' = 3$ from Gerjuoy and Stein (blue solid) and from Oksyuk (blue dashed)

Fig. 1b
- excitations to 4 vibrational levels
  - v=0 to v=1 (solid line)
  - v=0 to v=2 (dashed)
  - v=0 to v=3 (dotted)
  - v=0 to v=4 (dashed-dotted)

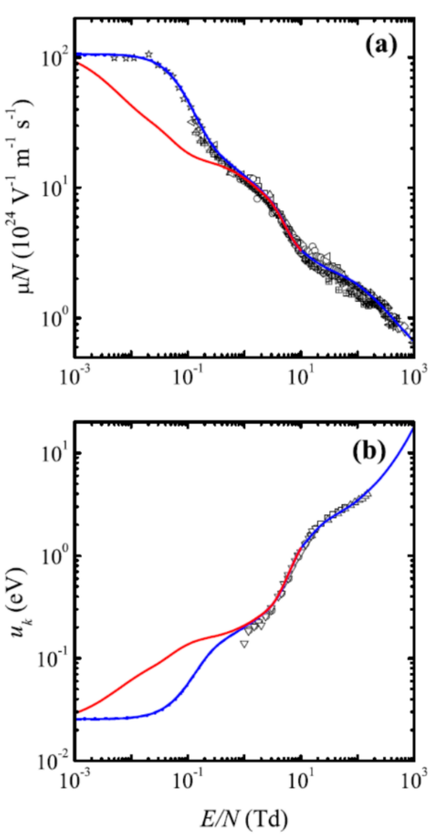
Fig. 1c
- excitations to 7 electronic levels
  - a $1\Delta_g$ (blue solid line)
  - b $^1\Sigma^+_g$ (blue dashed)
  - A $^3\Sigma^+_u$ + C $^3\Delta_u$ + c $^1\Sigma^-_u$ bound (blue dotted)
  - A $^3\Sigma^+_u$ + A' $^3\Delta_u$ + c $^1\Sigma^-_u$ dissociative (black solid)
  - B $^3\Sigma^-_u$ dissociative (black dashed)
- radiative levels with thresholds at 9.97 eV (red solid) and 14.7 eV (red dashed).

Fractional power (relative to the electron power gained from the electric field): elastic (green line), rotational (black), vibrational (blue) and electronic (red). The lines are calculations at Tg = 300 K, using the following approaches and data: for E/N < 10 Td, the discrete collisional operator for rotational transitions up to level J = 30, with the Gerjuoy-Stein [5] (solid lines) or the Oksyuk [6] (dashed) cross sections; for E/N > 10 Td, the CC-CAR operator.

The inclusion of rotational transitions is essential to reproduce the experimental values of the transport parameters for E/N < 1 Td. For this purpose, the rotational collision operator can be written using either a discrete description (e.g. considering the rotational cross sections proposed by Gerjuoy and Stein) or a continuous approximation for rotations, duly corrected by a Chapman-Cowling term proportional to the rotational/gas temperature.



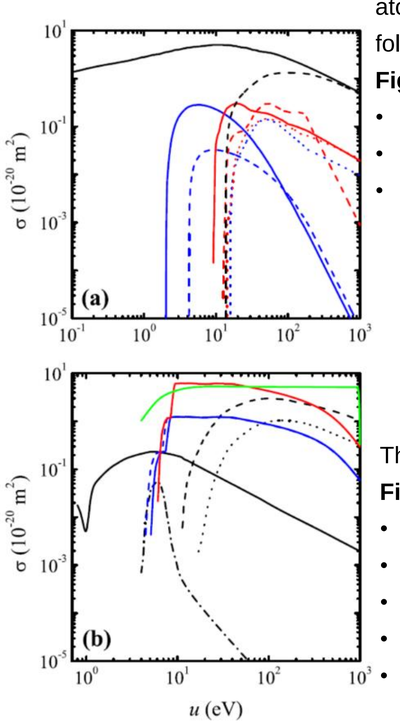
Swarm analysis in O_2



Electron transport parameters in oxygen, as a function of the reduced electric field, for Tg = 300 K. The lines are calculation results obtained using the two-term Boltzmann solver with LoKI. For E/N < 10 Td, calculations include rotational encounters described according to the following approaches:
discrete collisional operator, for rotational transitions up to level J = 30 with the Gerjuoy-Stein [5] (blue solid line) or
the Oksyuk [6] (blue dashed) cross sections;
CC-CAR (blue dotted) with a quadrupole moment constant Q = 1.4; no rotational transitions (red). The points are experimental data, retrieved from the LXCat databases DUTTON (open symbols) and LAPLACE (crossed symbols).

The relative difference between calculations and measurements is below 20% for E/N < 10 Td and between 5–20% for E/N > 10 Td, against 40% dispersion in the experimental data [3].

Electron cross section for O

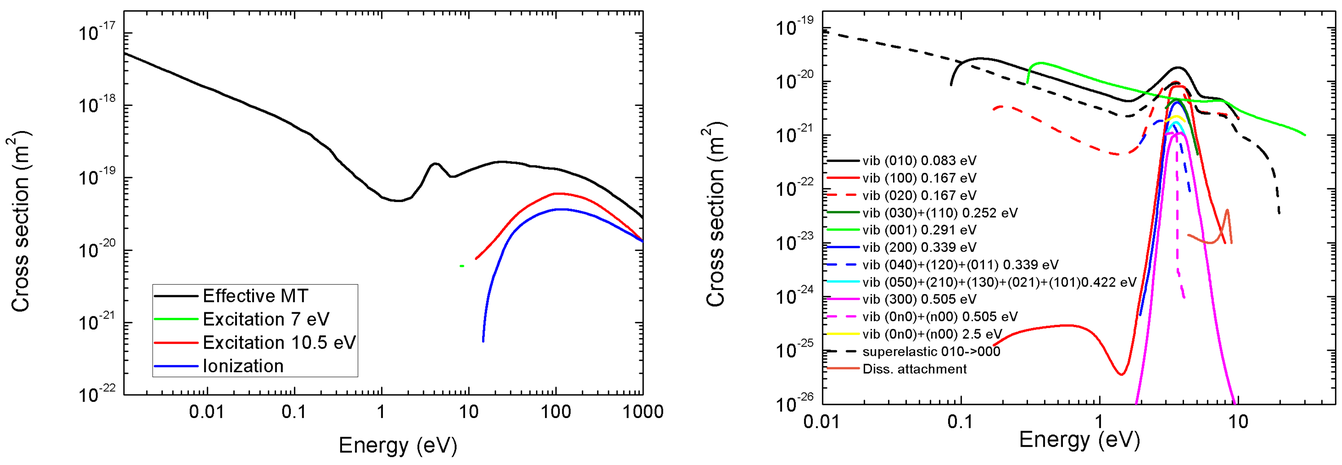


The set of electron-scattering cross sections with ground state atomic oxygen O($2s^2 2p^4\ ^3P$) represented in a more simplified notation as O(^3P) includes the following 8 cross sections [3]:

Fig a:
- elastic momentum-transfer (black solid line);
- ionization (black dashed line)
- excitations to 6 electronic levels:
  - (i) O($2s^2 2p^4\ ^1D$), O($2s^2 2p^4\ ^1S$) and O($2s^2 p^5\ ^3P^0$), represented as O(^1D) (Fig. a) blue solid), O(^1S) (blue dashed) and O($^3P^0$) (blue dotted) , respectively;
  - (ii) the most important Rydberg states: 3s $^5S^0$, 3p ^5P, 4s $^3S^0$, 3d $^3D^0$, 4p ^3P and 4d $^3D^0$ with core $2s^2 2p^3\ ^4S^0$, noted as O(($^4S^0$)*nl*); 3d $^3S^0$, 3d $^3P^0$, 3d $^3D^0$, 4d $^3SPD^0$ and 4s $^3D^0$ with core $2s^2 2p^3\ ^2D^0$, noted as O(($^2D^0$)*nl*); 3s $^3P^0$, 3d $^3P^0$ and 4s $^3P^0$ with core $2s^2 2p^3\ ^2P^0$, noted as O(($^2P^0$)*nl*). In the simplified notation, n < 5 and l = *s, p, d*.

These collisional data are complemented by the electron-impact cross sections represented in **Fig. b**:
- excitation of b 1Σ+g from a $^1\Delta_g$ e + O_2(a) → e + O_2(b) (black solid line)
- ionization e + O_2(a) → 2e + O_2^+(black dashed);
- dissociative ionization e + O_2(a) → 2e + O^+ + O(^3P) (black dotted) and;
- dissociative attachment from a $^1\Delta^g$ e + O_2(a) → O^- + O (black dashed-dotted)
- dissociation from the a $^1\Delta^g$ e+O_2(a) → e + 2O (blue solid), and from the b $^1\Sigma^+_g$ e+O_2(b) → e + 2O (blue dashed),
- dissociation of ozone e + O_3 → e + O_2 + O (red);
- detachment e + O^- → 2e + O(^3P) (green)

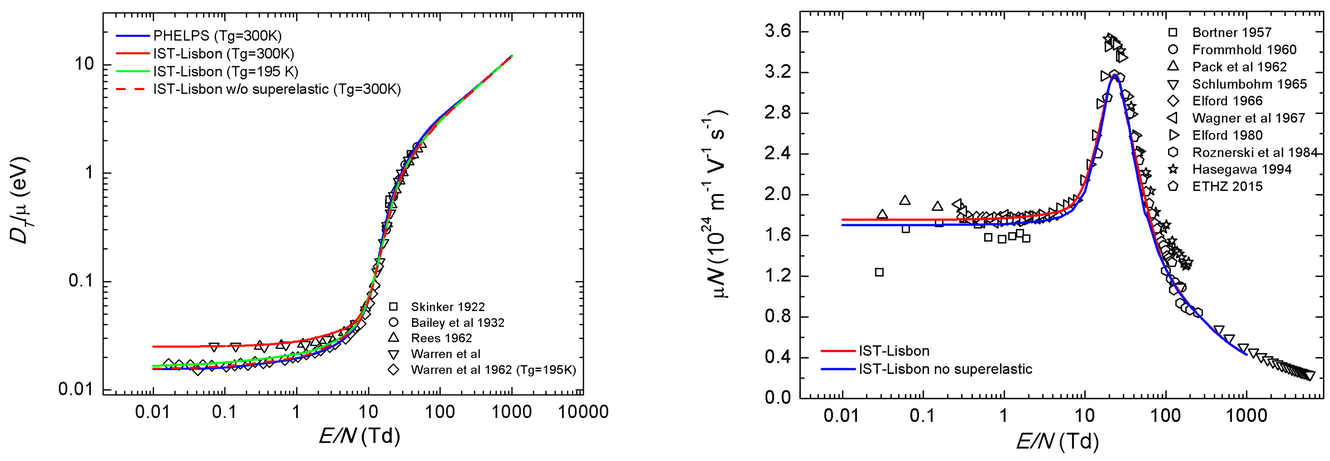
Electron cross section for CO_2



The proposed cross section set, compiled mostly from Phelps CO_2, includes 17 cross sections defined up to 1 keV describing [4]:
- dissociative attachment
- effective momentum transfer
- eleven vibrational excitation energy losses (corresponding to the excitation of either individual levels or groups of vibrational levels)
- superelastic collisions with the CO_2(010) vibrational state
- excitation of two groups of electronic states
- ionization.

The present calculations show that the energy gained in the superelastic process is relevant for low reduced electric fields, while for E/N > 10 Td the electron energy distribution function is not significantly affected by this process.

Swarm analysis in CO_2



The new set yields accurate predictions of the swarm parameters when used as input data to the Boltzmann solver of the LoKI (LisbOn KInetics) numerical code, that solves the electron Boltzmann equation in the usual two-term expansion in spherical harmonics. For instance, the calculated characteristic energy exhibits the correct dependence with the gas temperature, very evident for E/N <10 Td, only possible when superelastic collisions are taken into account. In addition, the proposed cross sections are able to produce reduced electron mobility within 1% of the measurements for the lower values of E/N [4].

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