Improvements to the Magboltz and Degrad databases

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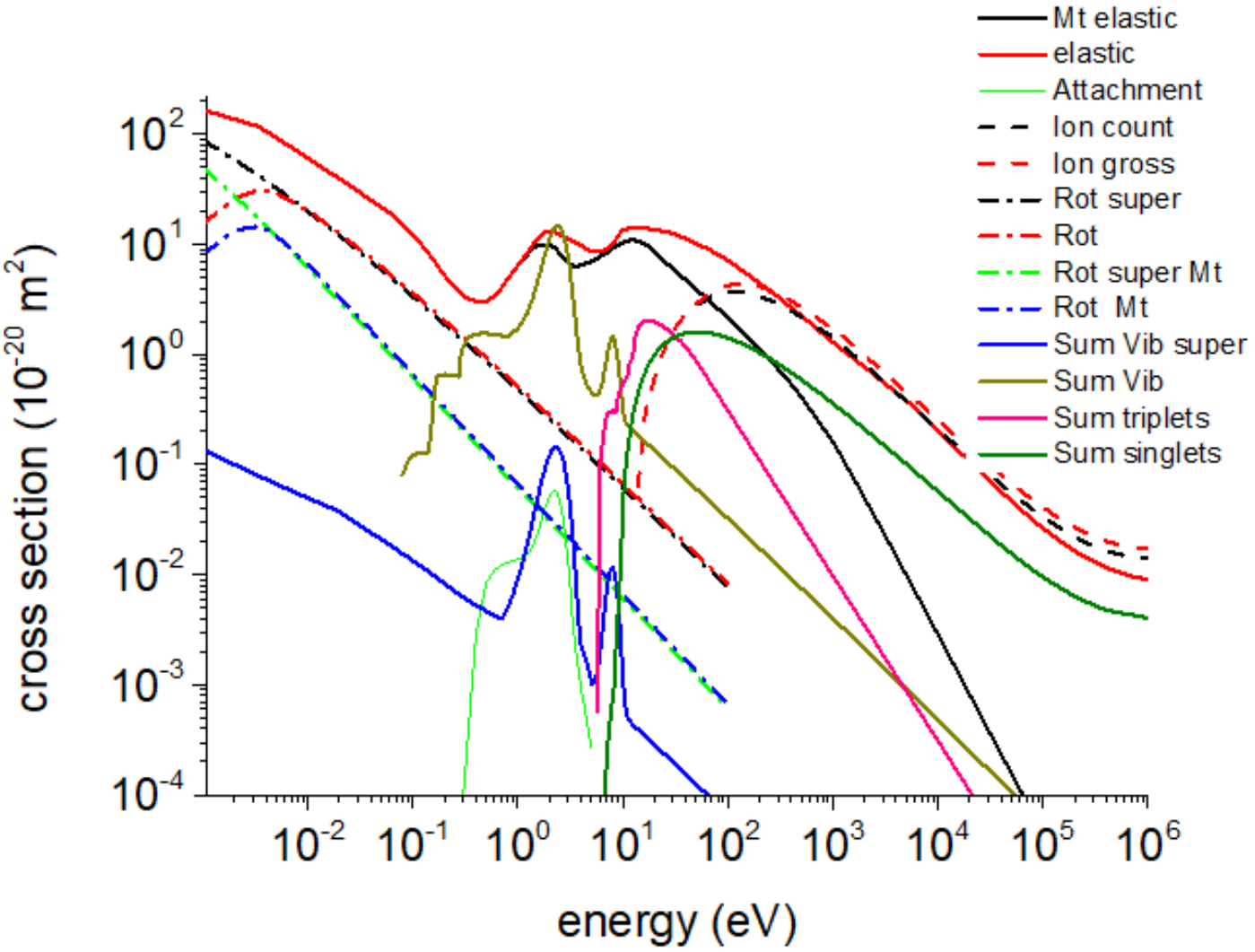
Update of N_2O cross-sections

- The gas is slightly attaching even in mixtures (at low E field).
- Its possible uses are:
  - radiation hard gas;
  - dark matter or double beta decay where the drift of the negative ions give the approximate z position in TPCs.
- (= nitrous oxide, laughing gas, $300 \times CO_2$)

N_2O cross sections



- [Courtesy Leanne Pitchford]

Ionisation

- References:
  - D. Rapp and P. Englander-Golden
    [J. Chem. Phys. **43** (1965) 1464]
  - B. G. Lindsay, R. Rejoub, and R. F. Stebbings
    [J. Chem. Phys. **118** (2003) 5894; doi; 10.1063/1.1556613]
  - Natalie A. Love and Stephen D. Price
    [Phys. Chem. Chem. Phys., **6** (2004) 4558-4565, doi: 10.1039/B408853K]

Ionisation

- Love & Price: goal was to observe the large double ionisation expected in large molecules (Stephen Price, private communication 2018). Confirmed.

- Cross section derived from the combined data is in agreement within experimental error bars, but deviate from the REG gross ionisation data. Normalisation in question.

Attachment

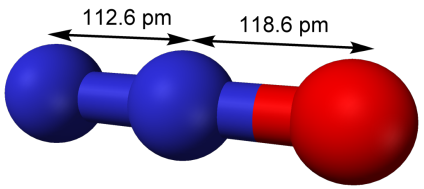
- Low-energy shoulder seems to vary with temperature, while the main peak does not. Accuracy not yet sufficient to warrant a temperature dependent shoulder.
- Possibility of O^- detachment before stabilisation.
- Need for a normalisation factor of 0.67 on the attachment cross section, to account for de-attachment.

Vibrations

- Data of M. Allan and T. Skalický [J Phys B 36 (2003) 3397] are superior. Used to derive cross sections from threshold to 12 eV.
- Resonance at 2.3 eV has a large amplifying effect on the higher vibrational states as seen in CO_2.
- Previous cross-section derivations did not take account of this large enhancement and did not obtain consistency with the experimental measurements of total cross section in the resonance region at 2.3 eV.
- The derived cross-section set sums up to a good fit to the total cross section, within experimental errors.

Rotations

- The rotations are treated using the dipole formula and summed over 60 levels.
- The rotations are only weakly excited in N_2O because the dipole moment is small unlike the case of water where it is large.
- The 2-term approximation to the rotations could be used here instead since the effects are small on the transport parameters.



Excitations

- Dipole-allowed excitation cross-sections are derived using the BEF formalism (binary encounter). Oscillator strength data: average of Shaw et al. and Brion et al.
- Shaw et al. also measured the ionisation efficiency allowing the neutral dissociation to be derived above the ionisation energy.
- The oscillator strength data was piecewise integrated in short energy ranges which also coincide with the structure in the oscillator strength. The accuracy of the data is good and the dipole cross-sections are expected to be accurate to between 2 and 3 %.

Excitations

- The remaining excitations are non-dipole coupled and were split into 4 triplet states which each comprise the sum of many levels.
- The shape of the excitation function of the triplet states is described by a fast rise and a fall at high energy with $1/E^2$ or $1/E^{1.5}$.
- The normalisation of the magnitude of the triplet cross-sections was taken by fitting the amplitudes to the experimental Townsend gain coefficient.

Elastic scattering

- The momentum transfer elastic x-section was obtained in conjunction with the inelastic vibrational cross-section by fitting to transport coefficients in pure N_2 and Ar/N_2O mixtures.

- The final elastic cross-section was obtained by subtracting the inelastic cross-sections from the experimentally measured total cross-section. The derived elastic cross-section shows a smooth behaviour over the resonance region at 2.3 eV unlike previous analyses.

Elastic scattering

- The elastic x-section could not be derived below 1 eV due to the lack of accurate total cross-section measurements so the elastic cross-section was joined smoothly to the momentum transfer cross-section below 1 eV.

- The effect of this is only to force isotropic elastic scattering below 1 eV when using the anisotropic scattering data set.

Plans

- The next gas I will be working on is a small change in the CO_2 vibrational cross-section to bring it into agreement with the CMS measurement
  (low by 0.6 % of the drift velocity at the moment);

- then I will update the NH_3 and after that

- I will try to find a set for the new eco friendly gases such as 1,3,3,3-tetrafluoropropene (HFO-1234ze).