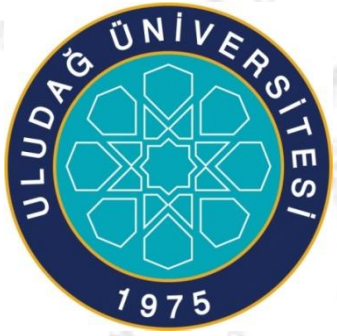

Magboltz Updates on N_2O, CO_2, NH_3, Alcohols and HFOs

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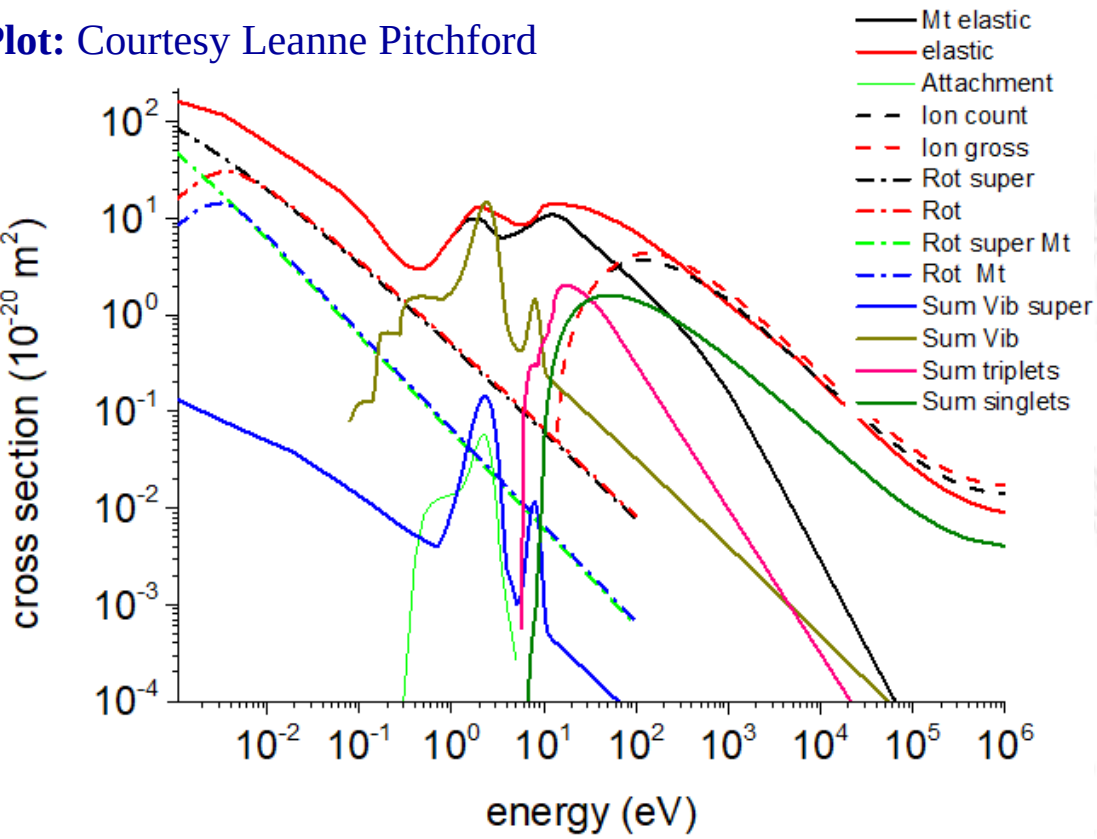
N_2O Update (Magboltz 11.4)

Plot: Courtesy Leanne Pitchford



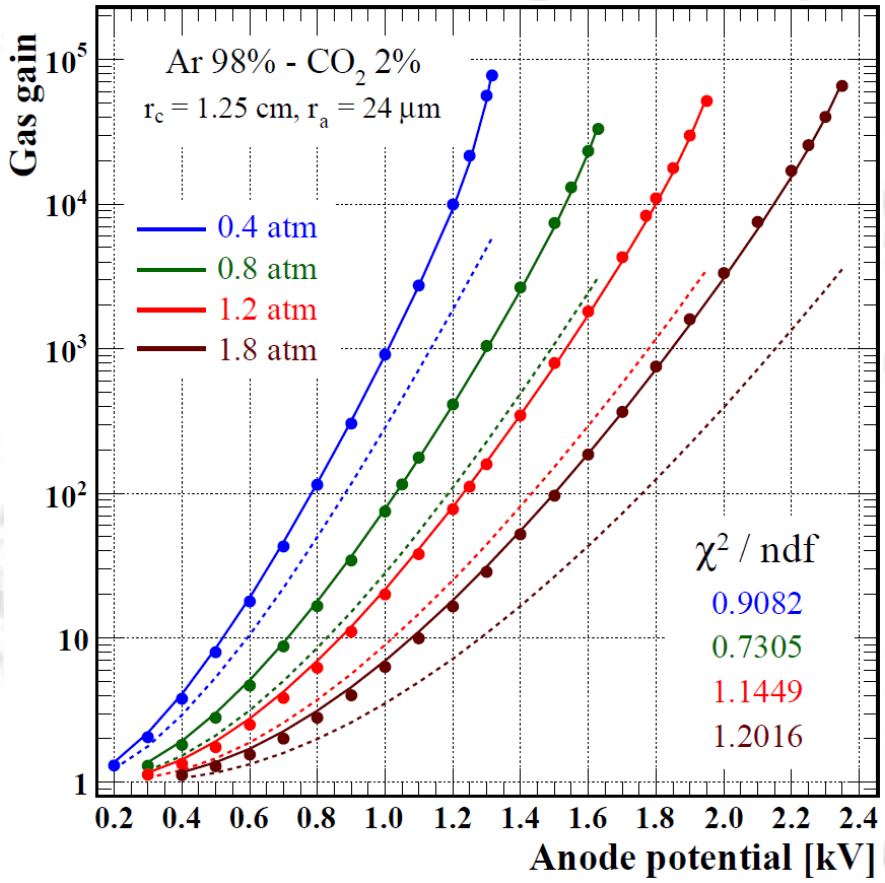
- Ionisations
- Attachments
- Vibrations
- Rotations
- Excitations
- Elastic

- The gas is slightly attaching even in mixtures (at low E field).
- Possible uses
  - Radiation hard gas;
  - dark matter or double beta decay where the drift of the negative ions give the approximate z position in TPCs.

CO_2 Update (Magboltz 11.5)

- Small change in the CO_2 **vibrational** cross section to get agreement with the **CMS** drift veolocity data measured in Ar/CO_2 85/15 mixture used in muon chamber
  - Magboltz prediction was low by 0.6 % of the drift velocity
  - V(001) vibration x-section scaled by a factor of 0.975 (2.5%)
  - Now, increase for Magboltz drift veolocity by 0.5 %,
    - Error in experimental data was ± 0.25 %
- Such a small change is not expected to effect on the agreement with other transport parameters
  - Best way to check with systematic gas gain fits
    - Townsend coefficients,
    - Ionisations,
    - Excitations

Gain measurements and fits in Ar-CO2



- Dashed lines: **without** corrections
- Points: experimental gas gains,
- Thick lines: final fits **with** Penning and feedback corrections.

- **Penning correction**

$$G = e^{\int \alpha_{Pen}(E(r))\,dr}$$

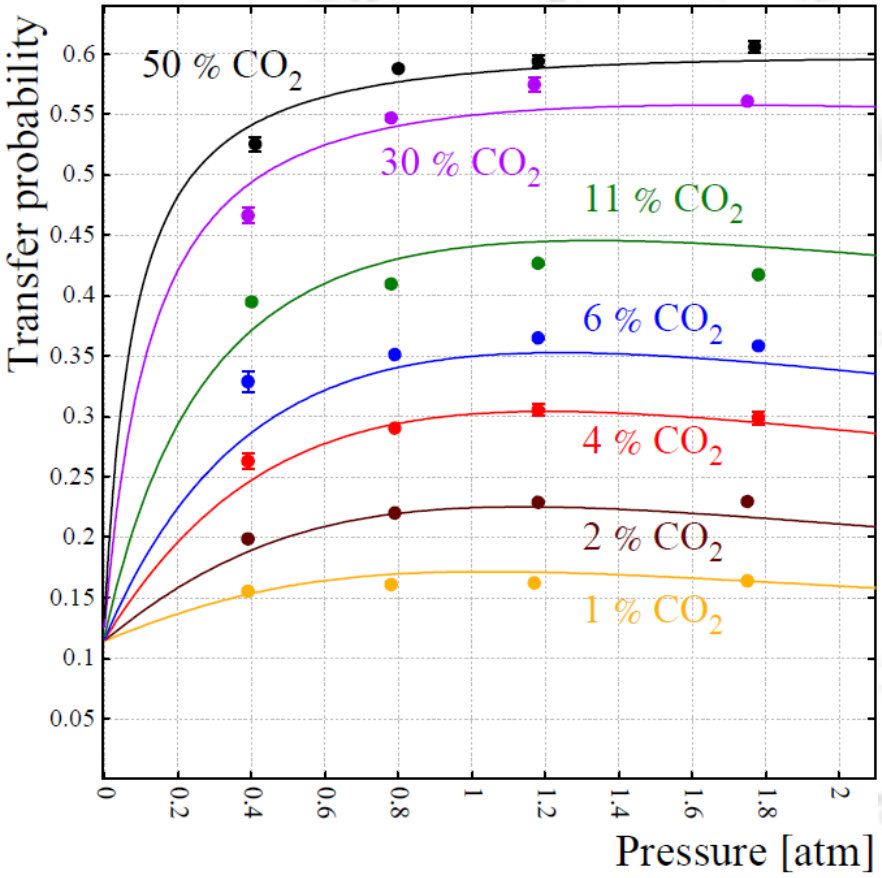
- $Ar^* + CO_2 \rightarrow Ar + CO_2^+ + e^-$
- Ar^* $3p^5 3d$ (13.8 eV) and higher level excitations can ionise CO_2 (13.77 eV)

$$\alpha_{Pen} = \alpha\left(1 + r_{Pen}\frac{f_{Ar}^{exc}}{f_{mix}^{ion}}\right)$$

- **Feedback correction** for the over-exponential increases in gas gain

$$G_{total} = G/(1-\beta G)$$

Energy transfer probabilities (Magboltz 9.01)



- **Numerator: increase the ionizations**
- **Denominator: excitation loses**

$$r_{Pen}(p,c)=\frac{a_5 p^2(1-c)^2 + a_1 pc + a_4 c + a_3}{a_6 p^2(1-c)^2 + pc + a_2}$$

Ar_2^* - CO_2 **Ar^* - CO_2** **Ar^* - γ**

1) **Excimers**
2) **Collosional ionizations**
3) **Radiative energy transfers**

Plot and calculations (Magboltz 9.01):

Ö. Şahin, T.Z. Kowalski, *A comprehensive model of Penning energy transfers in Ar− CO_2 mixtures*, *JINST* **12** C01035 (2017).

Energy transfer mechanisms

- **a_1: collisional ionization efficiency**

$$Ar^* + CO_2 \rightarrow Ar + CO_2^+ + e^-$$

- **a_2: decay by emitting photons**

$$Ar^* \rightarrow Ar + \gamma$$

- **a_3: photo-ionization**

$$\gamma + CO_2 \rightarrow CO_2^+ + e^-$$

- **a_3/a_2 = 0.114 ± 0.043** radiative transfer efficiency

- **a_4:** concentration dependence of the radiative transfer efficiency

- **a_5: ionization with argon excimers:**

$$Ar_2^+ + Ar^* \rightarrow Ar_2^+ + Ar + e^-$$

$$Ar_2^+ + Ar_2^+ \rightarrow Ar_2^+ + Ar + Ar + e^-$$

$$Ar_2^+ + Ar \rightarrow 2Ar + Ar^+ + e^-$$

- **a_6: excimer formation probability in Ar* - Ar – Ar collisions**

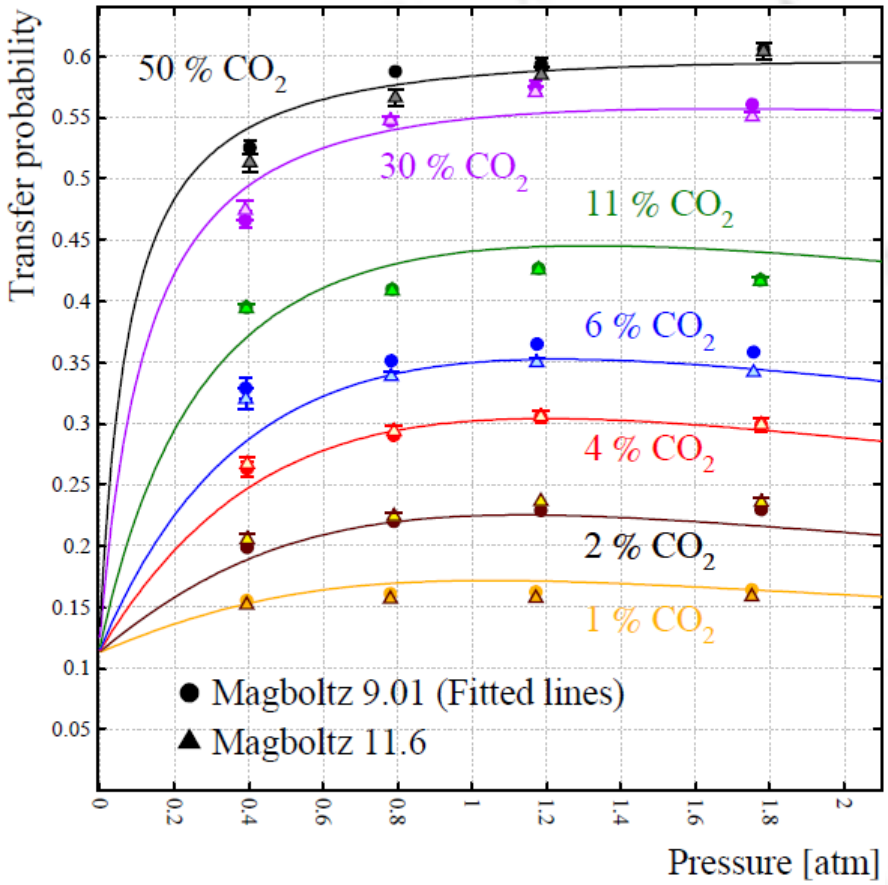
$$Ar^* + Ar + Ar \rightarrow Ar_2^* + Ar$$

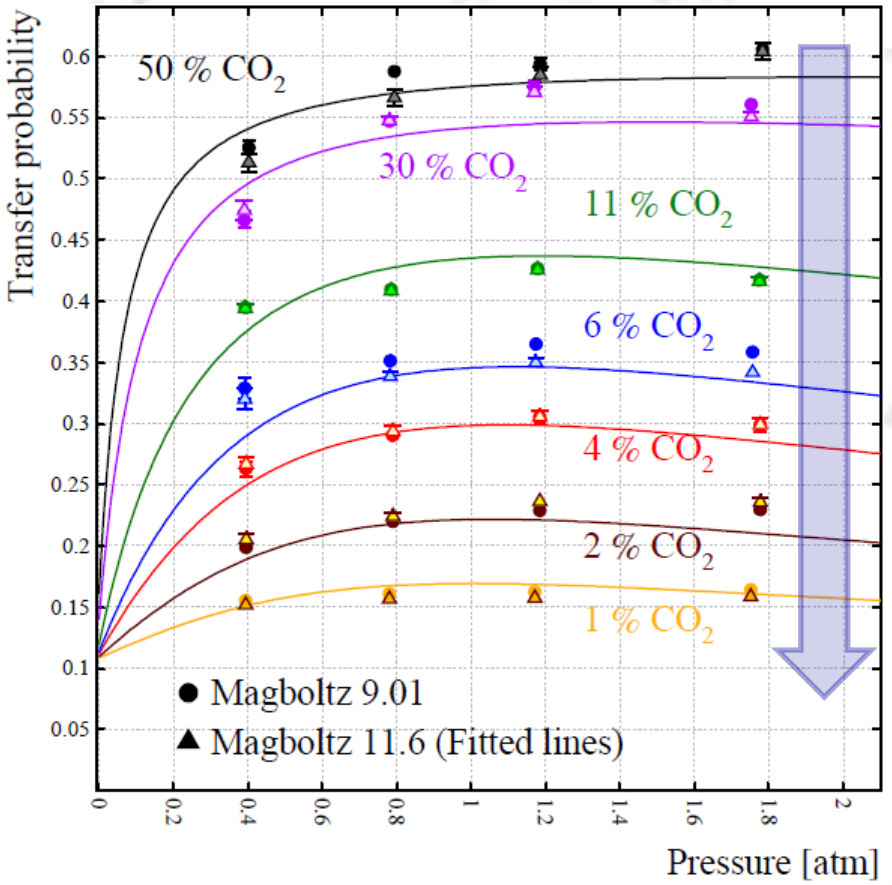
- **$a_5/a_6 \approx$ 9 % of the created excimers contribute to the total ionizations**

!!! No evidence for the Hornbeck-Molnar ionisations !!!

$$Ar^* + Ar \rightarrow Ar_2^+ + e^-$$

Magboltz 9.01 and 11.6 Calculations: Transfer rates





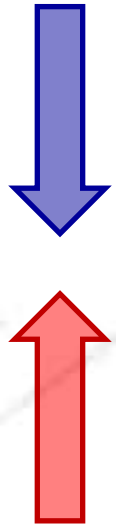
- Magboltz 11.6 gives almost same transfer rates in 1 %, 4 % and 11 % CO_2 mixtures
- Higher rates in 2% CO_2 with Magboltz 11.6
- Lower rates in 6 %, 30 %, and 50 % CO_2

!!! No systematic decreases or increases !!!

- **Modelling:** Transfer rates derived from the latest version lead to bigger drops at the highest pressures

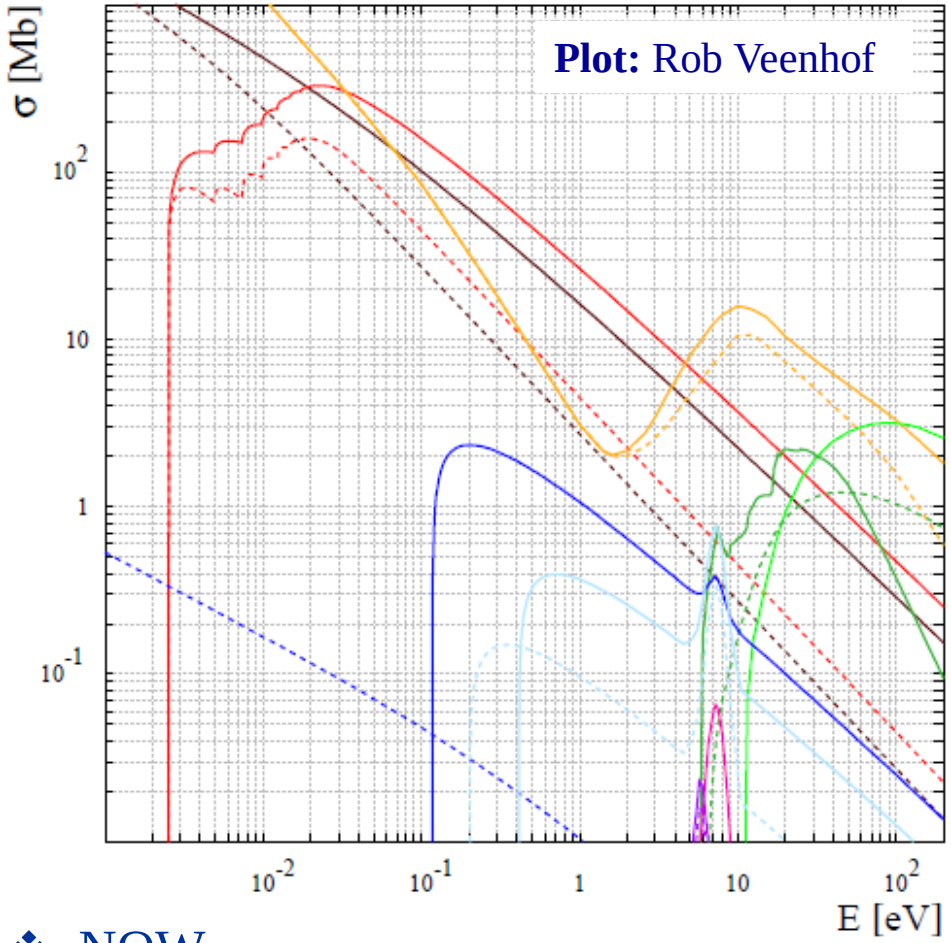
Comparision of the model parameters

Parameter	Magboltz 9.01	Magboltz 11.6
a_1	0.627898 ± 0.018083	0.613603 ± 0.020611
a_2	0.041394 ± 0.008297	0.036893 ± 0.008424
a_3	0.004716 ± 0.001512	0.003960 ± 0.001457
a_4	0.001562 ± 0.017566	0.003924 ± 0.020341
a_5	0.002422 ± 0.001171	0.002942 ± 0.001272
a_6	0.027115 ± 0.005836	0.030677 ± 0.006837



- Decrease on first 3 parameters,
- All the new parameters (derived from Magboltz 11.6) are in the range of errors found for Magboltz 9.01, **except parameter a_2**
- No particular change is seen in the transfer rates by using Magboltz 11.6
  - Confirms that transport parameters is not affected with a small update in one of the vibrational x-section (V001)

NH_3 Update (Magboltz 11.6)



- The gas is slightly attaching,
- Has very small diffusion
- 2004 cross section data fitted
- V. Lisovskiy et. al, *Electron drift velocity in NH_3 in strong electric fields determined from rf breakdown curves*, J. PHYS. D **38** (2005) 872.

- NOW
  - Includes dissociation above ionisation energy
  - improved angular distribution for rotational states (120 rotational levels)
  - angular distribution for dipole excitation

Next

- Alcohols:
  - Methanol (CH_3OH), 1999 3*
    - Almost finished
    - Very small diffusion and almost no attachment
      - Can be used in high accuracy drift chambers
  - Ethanol (C_2H_5OH), 1999 3*
  - Propanol (C_3H_7OH), 1999 3*
- Hydrofluoroolefins (HFOs), eco friendly gas
  - There is little electron scattering data,
  - Any attempt will likely have large errors since only scaling from similar molecules will probably be the only way to proceed.