Improvements to the Magboltz and Degrad data bases

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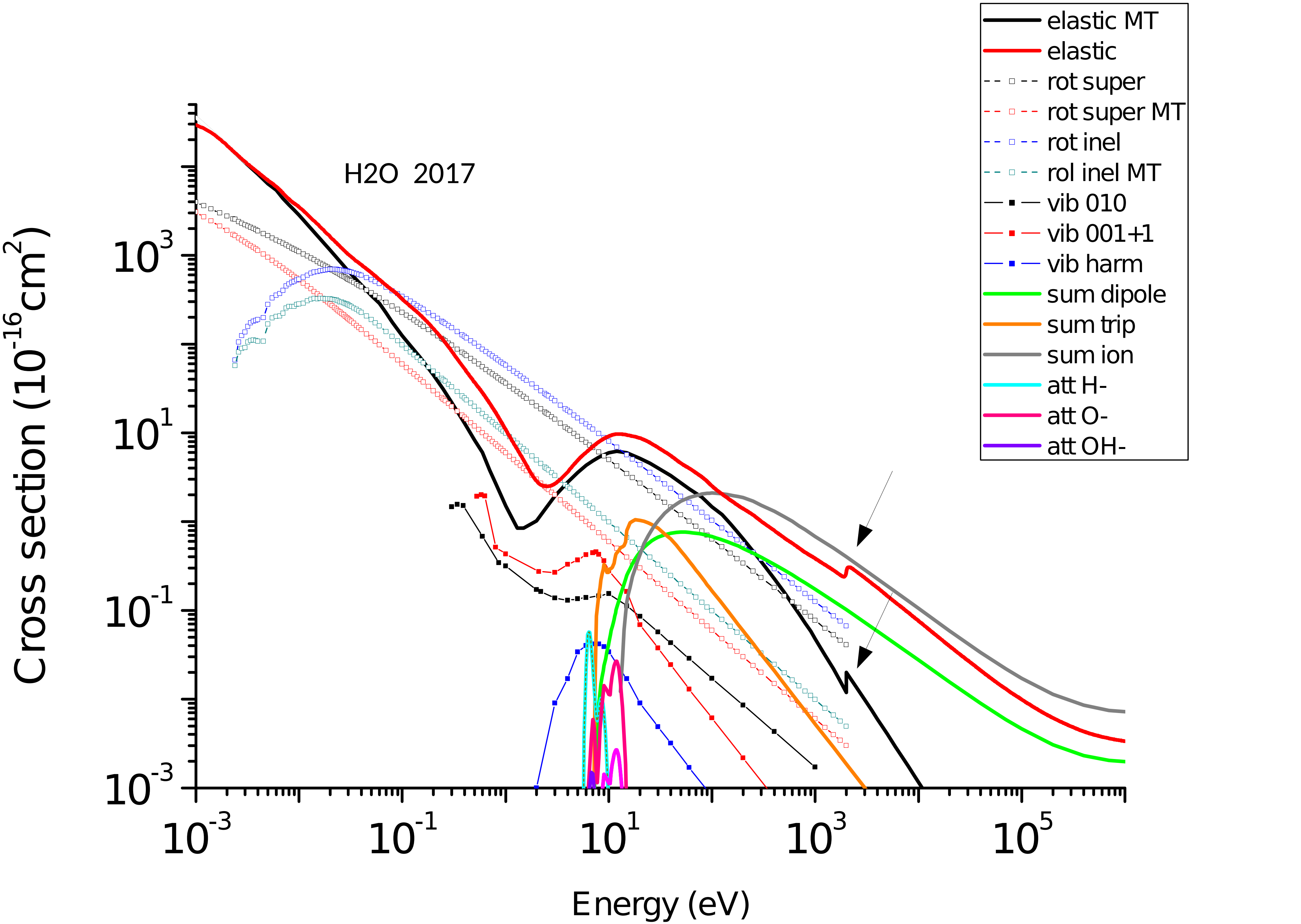
Update of water cross-sections

- The improved set gives good agreement in the mixtures:
  - Ar / CH_4 / H_2O,
  - C_2H_4 / H_2O,
  - Ar / H_2O and
  - He / H_2O.
- Transport parameters such as drift velocity and diffusion are within experimental measurement errors.

Condensed graph of cross-section set:

- sum of 210 rotational cross-sections,
- 3 vibrational transitions,
- 3 dissociative attachments,
- sum of 9 dissociative ionisations,
- sum of 36 dipole dissociative excitations and
- sum of 4 nondipole dissociative excitations.



elastic MT
elastic
rot super
rot super MT
rot inel
rol inel MT
vib 010
vib 001+1
vib harm
sum dipole
sum trip
sum ion
att H-
att O-
att OH-
H2O 2017
Cross section (10^{-16} cm^2)
Energy (eV)
10^{3}
10^{1}
10^{-1}
10^{-3}
10^{5}

The 2 keV glitch

- The glitch at 2 keV in the elastic total and elastic momentum transfer cross-sections are due to the rotational transitions being terminated at 2 keV and added to the elastic cross-section.

- This approximation has less than 0.1% effect on transport parameters and saves computing time.

H2O 2004 vs the new H2O 2017

- Detail of improvements:

  - Rotational states now have angular momentum L=1 and integration of the Born approximation for this term over angle gives the momentum transfer cross-section. [Same formula as Ness and Robson Phys Rev A38 (1988) 1446] Before: forward-backward asymmetrical scattering treatment.
  - The vibrational states were reduced by about 10% to fit better to the drift velocity in the mixtures.
  - The dissociative excitations above ionisation energy were included.
  - Dissociative ionisation was included.
  - The elastic and rotational cross-sections could be derived separately.

- These upgrades improve the deviations between accurate experimental measurements and calculation to the 1% level from the 2 or 3% level of the old data set.

$H2O$ 2004 vs the new $H2O$ 2017

- Detail of improvements (continued)
  - New measurements of the Townsend coefficient at high field deviated from older measurements. The newer Townsend measurements are well fit with the new data set.
  - The cross-sections are now also included in Degrad and the following slide gives some predictions for the energy loss around minimum ionising energy.

H_2O dE/dx and primary cluster density

Energy Mev	0.15	0.3	0.6	1.3	2.6	5.2	10	20	100
Beta*Gamma	0.825	1.24	1.944	3.427	6.057	11.23	20.74	40.52	198.6
Np 1/cm	33.13	23.53	19.27	18.03	18.6	19.93	21.49	23.29	26.93
De/Dx elastic	0.198	0.146	0.126	0.126	0.133	0.14	0.145	0.148	0.144
De/Dx exc	112.2	80	65.8	61.9	64.2	69.1	74.8	81.4	94.6
De/Dx ion	2400	1786	1526	1491	1593	1760	1947	2158	2600
De/Dx brem	3.72	4.7	6.36	12.46	27.42	61.82	135.7	304.6	1818
De/Dx tot	2516	1871	1599	1566	1685	1891	2158	2544	4513
De/Dx cut(9kev)	2095	1490	1221	1144	1182	1268	1369	1485	1723
% pass cut	99.95	99.94	99.94	99.92	99.94	99.94	99.94	99.94	99.94

$\beta\gamma_{mip} \approx 3$

- All calculations for 20 ºC and 1 atmosphere;
- asymptotic W value = 28.8 eV, ICRU 31 value = 29.15 eV;
- minimum ionising energy loss (without bremsstrahlung):
  - Estar = 1417, Don Groom (PDG) = 1552, Degrad = 1554 [eV/cm].

Applications

- The data set also includes some null collisions which are included to allow the calculation of light emission from OH(A-X) and Hα and Hydrogen Balmer emission. Also the total dissociation is calculated by null collision.

- The data set may have application in the calculation of accurate radiation damage dosage due to ionising radiation in biological tissue.

- Water is a very good thermalising gas and may have application in doping dark matter and double β decay detectors to improve spatial resolution by reducing diffusion.

- The OH(A-X) transition may also be of use to derive an S1 signal.

[OH(A-X): 310 nm, Balmer: 656, 486, 434 … nm, Hα : 656.28 nm]