Comparisons of sets of electron-neutral scattering cross sections and calculated swarm parameters in H_2

LC Pitchford, S Chowdhury, GJM Hagelaar, S Pancheshnyi, MC Bordage (LAPLACE, CNRS and Univ Toulouse, France);
LL Alves and CM Ferreira (IPFN/IST-UTL, Lisbon, Portugal); SF Biagi (Univ Liverpool, UK) ;
Y Itikawa (Inst of Space and Astronautical Sci, Japan); AV Phelps (JILA, NIST and Univ Colorado, USA)

Introduction

The GEC Plasma Data Exchange Project is an informal effort on the part of the low temperature plasma community to organize the collection, evaluation, and distribution of data both for modeling and for interpretation of experiments. In the context of this project, we present a description of the four independently-compiled sets of electron-neutral scattering cross sections for H_2 presently available on the open-access LXCat site (www.lxcat.net). Three of these sets were derived using the requirement that they be consistent with available experimental swarm data, and the fourth set consists of recommended values from beam experiments and theory. To assess the validity of each of these cross section sets for use in modeling low temperature plasmas, we calculated electron transport and rate coefficients using these cross sections as input and compared with measured values also available on the LXCat site. We also show the influence of rotational temperatures between 77 and 300 K, and again confirm that a two-term Boltzmann solver yields results in very good agreement with Monte Carlo simulations.

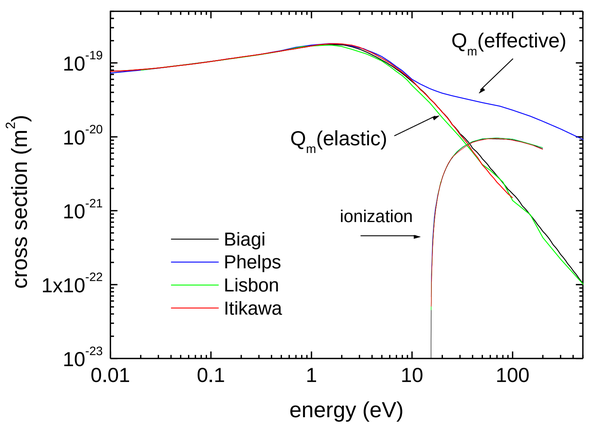
"Complete" sets of cross sections available on LXCat for electron scattering from H_2

Databases containing cross sections sets for H_2 available on LXCat

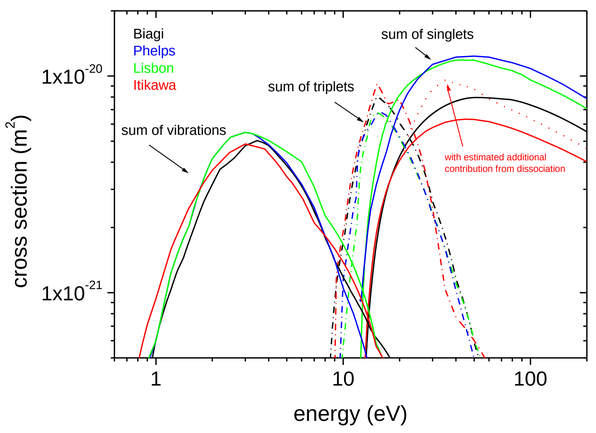
Database	Level of detail for excitation	Comments
Phelps	**2 rotational levels; 3 vibrational levels; 4 triplet levels, 3 singlet levels, dissociation into n=2 and n=3, Rydberg excitation and ionization**	For use in a 2-term Boltzmann solver. The rotational cross sections (j=0-2 and j=1-3) are weighted supposing a thermal distribution of para and ortho hydrogen at 300K. The cross sections for rotational excitation must be rescaled for use with a different gas temperature.
IST-Lisbon	**3 vibrational levels; 4 triplet (dissociative) levels, 3 singlet Rydberg levels (partially dissociative), dissociation into n=2(s or p), 3, 4 and 5, and ionization**	For use with a two-term Boltzmann solver. See L Marques, J Jolly and LL Alves, 2007 J. Appl. Phys. 102 063305 1-14. Rotational cross sections on LXCat are input via additional "species" and the rotational distribution is input through the concentrations of these species. This cross section set is consistent with the assumption that the energy difference between j=0 and j=1 is zero.
Biagi	**4 rotational levels, 3 vibrational levels, multiple electronically excited levels , some with separated vibrational levels for more precise energy loss, and ionization**	Extracted from SF Biagi's Fortran code, Magboltz version 8.9 and intended for use with Monte Carlo or multi-term Boltzmann solver. On LXCat, the rotational cross sections are weighted supposing a thermal distribution at 300K. The cross sections for rotational excitation must be rescaled accordingly for use at a different gas temperature. The label "DIS" on the electronicall excited levels indicates DISSOCIATIVE excitation.
Itikawa	**1 rotational, 1 vibrational level, 3 triplet levels, 3 singlet levels, and ionization.** **Total dissociation , total scattering and total elastic cross sections are also listed but should not to be used in a Boltzmann calculation.**	A compilation of the recommended data from beam experiments and from theory. See J. Yoon et al., J. Phys. Chem. Ref. Data, Vol. 37, 913 (2008). This reference gives cross sections for total dissociation and triplet excitation (which leads to dissociation), but does not propose cross sections for the higher singlet states of H_2 that can lead to dissociation. We have estimated this cross section by subtracting the sum of the triplet cross sections from the measured total dissociation cross section and some results are shown below using this "modified" cross section for dissociation.

The first three sets were developed specifically for input to Boltzmann solvers or Monte Carlo simulations.

The cross sections sets for H_2 in the MORGAN and SIGLO databases on LXCat are the same as in the Phelps database.



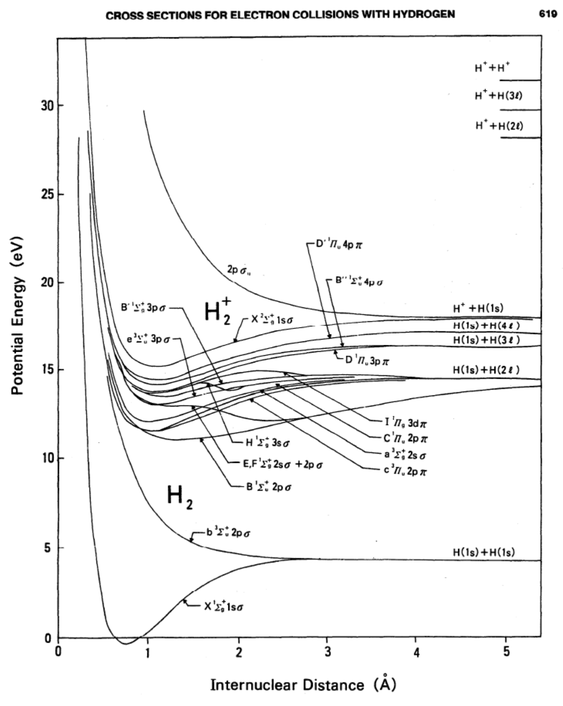
Comparisons of momentum transfer and ionization cross sections from the 4 sets of cross sections



Comparisons of total triplet and singlet excitation cross sections from the 4 sets

$$Q_m(\text{effective}) = Q_m(\text{elastic}) + \Sigma\, Q_k$$

Q_m(effective) is the sum of the elastic momentum transfer cross section and the total cross sections for excitation and ionization. This quantity appears naturally when the angle dependence of the distribution function is expanded in Legendre polynomials.

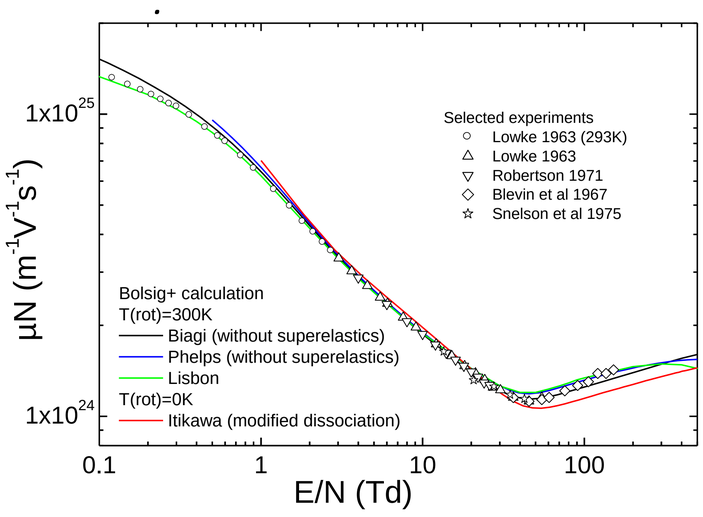


From fig. 1 of Tawara et al, JPCRD, 1990.

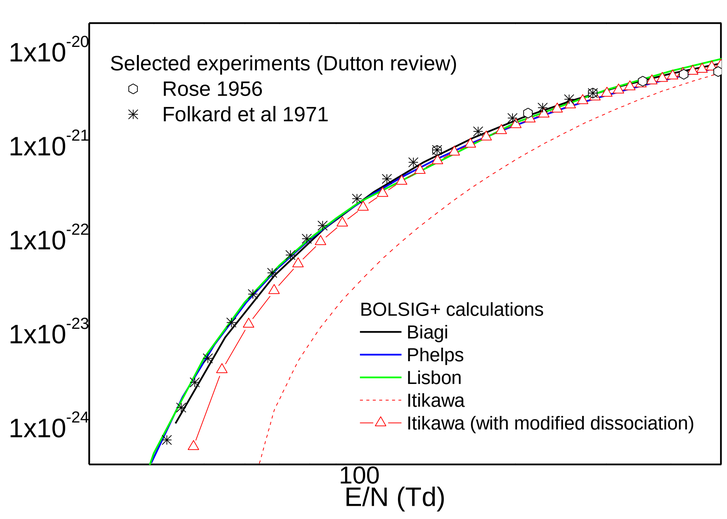
Transport and rate coefficients calculated using LXCat input data and comparisons with experiment

Most of these calculations were performed using BOLSIG+, a 2-term Boltzmann solver.

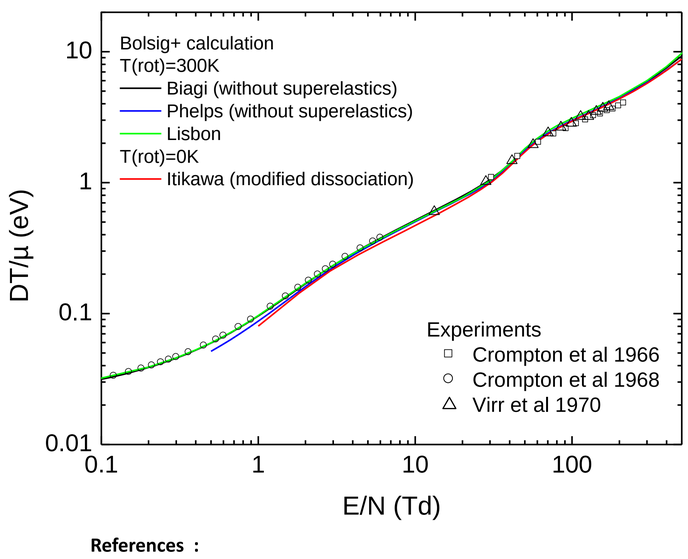
Mobility x neutral gas density vs E/N



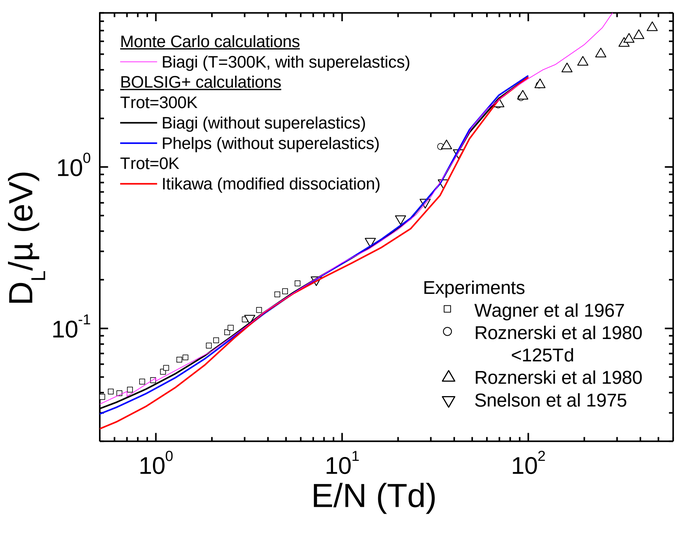
Townsend ionization coefficient normalized to neutral gas density



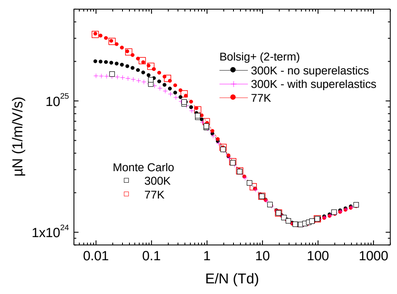
Characteristic energy, D_T/μ, vs E/N

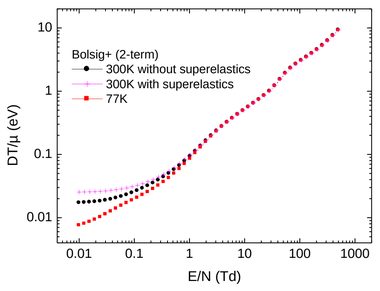


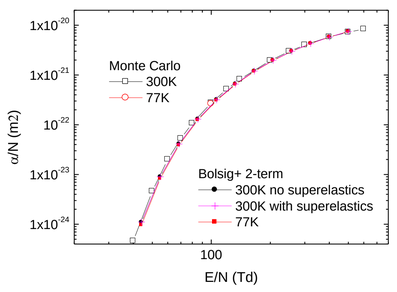
D_L/μ vs E/N

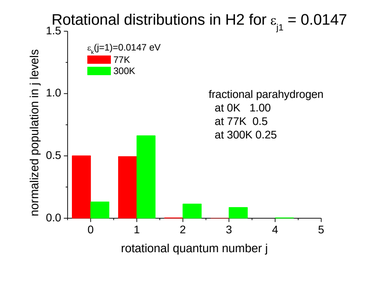


Gas temperature effects and accuracy of two-term approximation (calculations using Biagi cross section set for H_2)









The differences between results at 77K and 300 K without superelastic collisions reflect the temperature dependence of the rotational distributions and the dependence of rotational excitation cross section on the specific state of the target. The influence of T_{gas} is important at low E/N but small differences remain for higher E/N. This is because of the large rotational cross sections in H_2 (as compared to other gases) in the 3 to 6 eV region. The inclusion of superelastic rotational collisions is observable only at low E/N.

Conclusions

The two-term Boltzmann solver BOLSIG+ yields results for μN, D_T/μ, and α/N in good agreement with Monte Carlo simulations over the full range studied.

It is important to take into account the excited state populations of the rotational levels, including deexcitation collisions, when analyzing electrons in H_2 at a gas temperature of 300K.

Transport and reaction coefficients calculated using the cross section data from Yoon et al, labeled Itikawa in the LXcat tables, are still being evaluated. Cross sections for processes leading to dissociation, in particular, merit further attention.

Finally, the LXCat website and interface provides a convenient way to make intercomparisons of available data. New contributors are welcome.

References :
- BOLSIG+ : Hagelaar, 2-term Boltzmann solver (http://www.bolsig.laplace.univ-tlse.fr/download.php)
- Biagi Monte Carlo : Magboltz (http://consult.cern.ch/writeup/magboltz/)
- Experimental data with details of the references are on www.lxcat.net
- Cross sections are available for plotting, downloading or on-line calculations on www.lxcat.net.