Comparisons of sets of electron-neutral scattering cross sections and calculated swarm parameters in N_2 and O_2

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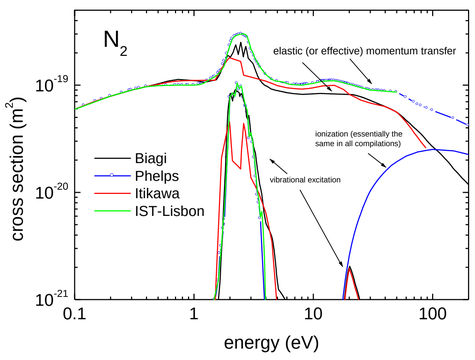
Introduction

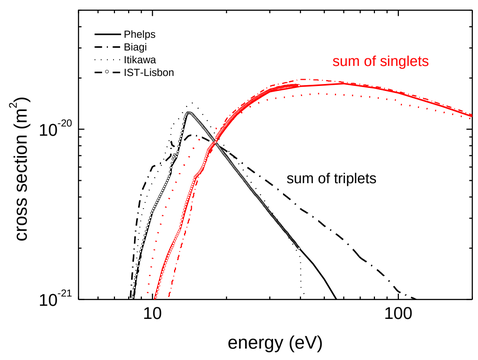
We present a description of the sets of electron-neutral scattering cross sections for N_2 (4 sets) and for O_2 (4 sets) presently available on the open-access LXCat site (www.lxcat.net). Three of these sets are complete in that the main momentum and energy loss processes are taken into account, if we can neglect internal excitation in the gas, and were derived using the requirement that they be consistent with available experimental swarm data. The fourth set consists of recommended values from beam experiments and theory. We describe these cross section sets and show, for each, comparisons of calculated swarm parameters with selected experimental data.

Sets of cross sections available on LXCat for N_2

Database	Level of detail for excitation	Comments
Phelps	**1 rotational level (single level approximation for rotation), 8 vibrational levels, 6 triplet levels, 5 singlet levels, 2 ionization levels.**	Based on Phelps and Pitchford, Phys. Rev. 31, 2932 (1985) as tabulated in the JILA Information Center Report No. 26. Since then, we recommend rescaling the $C^3\Pi_u$ excitation by 0.67, and some minor errors have been corrected. In addition, the ionization cross section has been divided into two parts so as to facilitate calculation of the production of N_2 1st negative band emission. This cross section set was originally derived using the Continuous Approximation for Rotation (CAR) which is not yet implemented in LXCat. The "single level approximation for rotation" (SLAR) as been used in its place. See Hake and Phelps, Phys. Rev. 158, 60 (1967).
Biagi -v8.9	**15 vibrational levels in the ground state, 9 triplet states, 8 singlet states, ionization. Some of the excited states are separated into individual vibrational levels.**	Transcribed from SF Biagi's Fortran code MagBoltz v8.9 neglecting rotational (de)excitation from the 39 levels included in the original code. Therefore these data should not be used below 0.5 Td. We are presently transcribing the more detailed cross sections into LXCat. Developed using a Monte Carlo simulation. Cross sections for certain transitions have been grouped according to vibrational levels and the energy loss is weighted accordingly. Therefore the energy loss does not always correspond to the threshold energy.
IST-Lisbon	**10 vibrational levels, 6 triplet states, 4 singlet states, ionization, rotational (de)excitation J – J+2 for J=0-24.**	Cross sections compiled mostly from LC Pitchford and AV Phelps (1982), and K Tachibana and AV Phelps (1979) [see J Loureiro and CM Ferreira, 1986 J. Phys. D **19** 17]. Recommended for 1 Td < E/N < 100 Td. See comments on LXCat for how to use these data.
Itikawa	**1 rotational level, 1 vibrational level, 6 triplet levels, 6 singlet levels, dissociation, and 3 separate ionization levels. Total scattering and total elastic cross sections are also given.**	Cross section set recommended on the basis of available beam experiments and theory as described "Cross Sections for Electron Collisions with Nitrogen Molecules" Y. Itikawa, J Phys Chem Ref Data, **35** 31 (2006) This cross section set is flagged as "partial" on LXCat and thus is not available for use with the on-line Boltzmann solver. These cross sections are downloadable.



Comparisons of momentum transfer, summed vibrational excitation and ionization cross sections

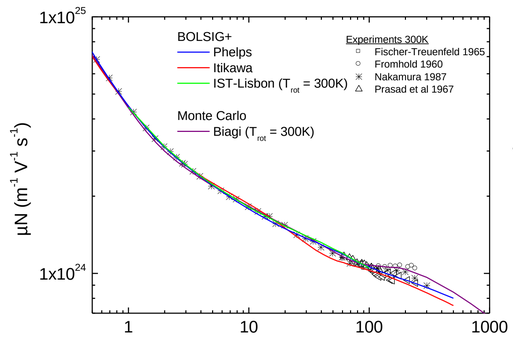


Comparisons of summed triplet and singlet excitation cross sections

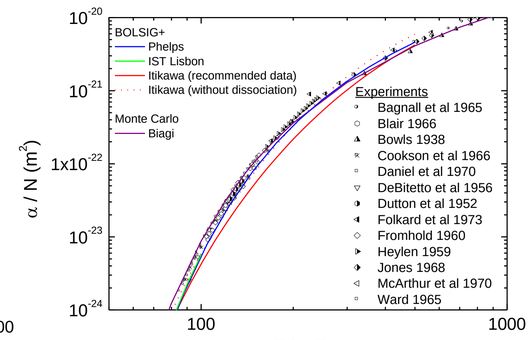
Note the distinction between elastic and effective momentum transfer (see H_2 poster).
The ionization cross sections are essentially the same in all data sets.

Transport and rate coefficients for N_2 calculated using cross sections LXCat and comparisons with selected experimental results

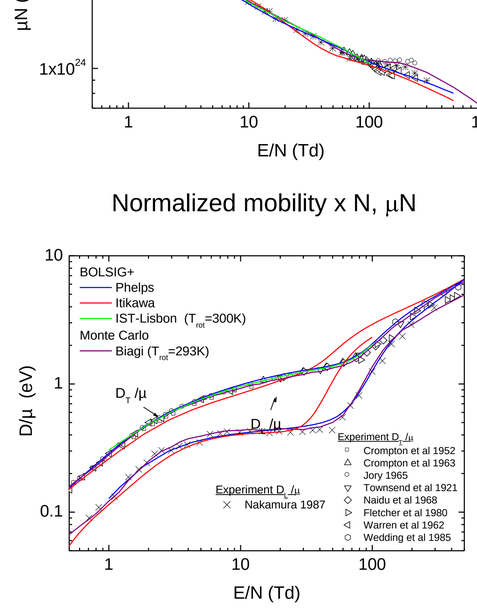
BOLSIG+ is a 2-term Boltzmann solver available on-line on the LXCat site.



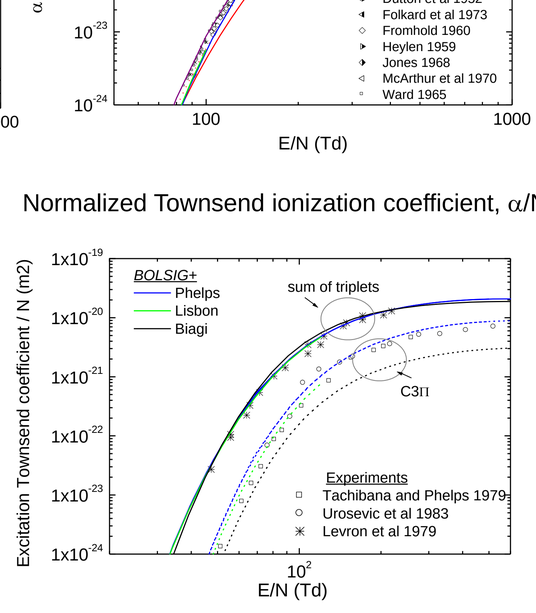
Normalized mobility x N, μN



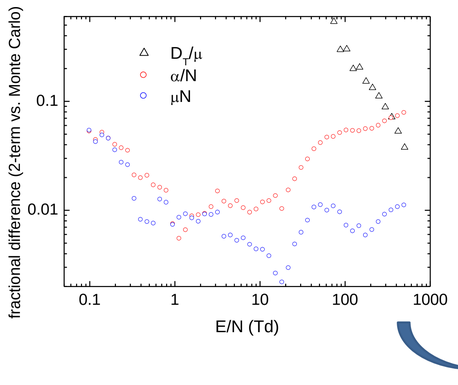
Normalized Townsend ionization coefficient, α/N



Characteristic energy, D_T/μ, and D_L/μ



Excitation coefficients for $A^3\Sigma$ and $C^3\Pi$ states



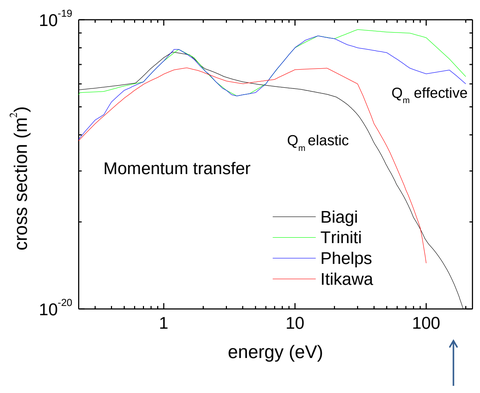
Treatment of rotational excitation : Comparisons of results of calculations using the Single Level Approximation to Rotation (SLAR) of Hake and Phelps with a full treatment (39 levels) at Trot = 300K confirms validity of the SLAR for E/N > 1 Td. Inclusion of superelastic scattering from this level may extend the range of usefulness. Tests are in progress.

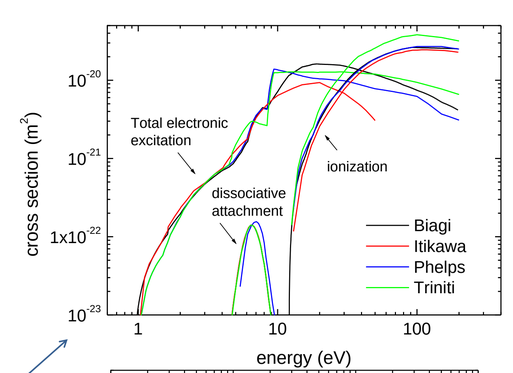
- The 2-term approximation (and use of BOLSIG+) is adequate for our purposes.

Sets of cross sections available on LXCat for O_2

Database	Level of detail for excitation	Comments
Phelps	**1 rotational level, 4 vibrational levels, 6 electronic levels (some are dissociative), dissociative attachment, 3-body attachment and ionization**	From Lawton and Phelps, J Chem Phys 69, 1055 (1978) and tabulated in the JILA Information Center Report No 28. Developed using a two-term Boltzmann solver. The 3-body cross section is converted to a 2-body cross section by assuming a gas number density of 1/cm3. Developed for use with a two-term Boltzmann solver. Not to be used with BOLSIG+ below 0.5 Td unless continuous approximation or single level approximation to rotation is included.
Biagi -v8.9	**Same grouping as Phelps**	Transcribed from SF Biagi's Fortran code MagBoltz v8.9 using the subroutine "Oxygen 2003". Developed using a Monte Carlo simulation. The 3-body cross section is converted to a 2-body cross section by assuming a gas number density of 1/cm3.
Triniti	**1 effective vibrational level, 3 electronic levels, 2 dissociative processes, dissociative ionization, and 2 ionization processes** **+1 effective rotational level (not included in the BOLSIG+ calculations shown below)**	From "Physics and engineering of singlet delta oxygen production in low-temperature plasmas", by A A Ionin et al, J Phys D 40 525 (2007) and based in part on Eliasson & Kogelschatz 1986 Brown Boveri report on "Basic data for modelling electric discharges in gases" Developed using a two-term Boltzmann solver. The implementation of "effective" rotational excitation in the Triniti Boltzmann code gives the correct zero field limit.
Itikawa	**3 vibrational levels, 6 electronic levels (some are dissociative), dissociative attachment and ionization. Total scattering and total elastic cross sections are also given.**	Cross section set recommended on the basis of available beam experiments and theory as described in "Cross sections for electron collisions with oxygen molecules", by Y Itikawa, J Phys Chem Ref Data, 38 1 (2009) This cross section set is flagged as "partial" on LXCat and thus is unavailable for use with the on-line Boltzmann solver. These cross sections are downloadable.

Additional databases on LXCat containing data for N_2 and/or O_2 :
MORGAN : Same as Phelps for N_2 but with one ionization level and no rescaling of the $C^3\Pi$ state. Rotational excitation is included explicitly but via a CAR (continuous approximation for rotation) parameter not yet implemented in BOLSIG+ Same as Phelps for O_2
SIGLO : Same as Phelps for N_2 but some slight differences appear in the rotational excitation at resonance; and the two ionization levels have been combined into one. The O_2 cross sections have been removed from the SIGLO database because they were the same as Phelps.

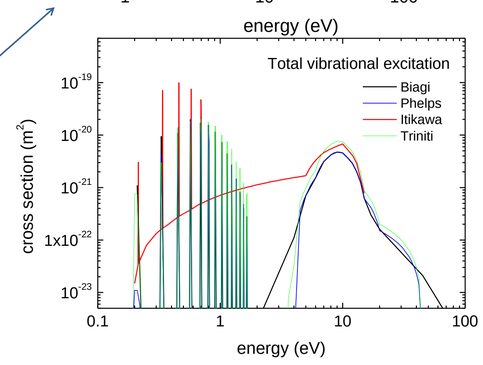




Comparisons of momentum transfer cross sections.

Comparisons of total electronic excitation, dissociative attachment and ionization (top) and vibrational excitation cross sections (bottom)

The cross section for 3-body attachment (not shown) peaks at low energies and is spiked, similar to the low energy vibrational excitation.



Transport and rate coefficients for O_2 calculated using cross sections LXCat and comparisons with selected experimental results

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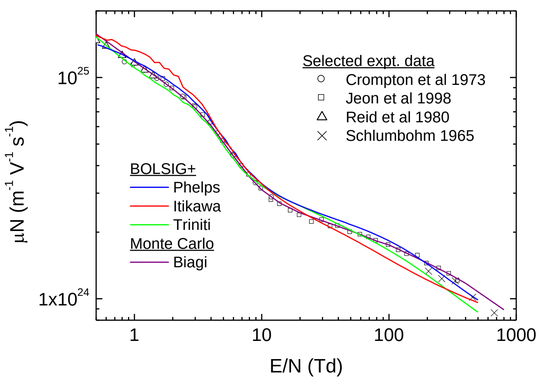
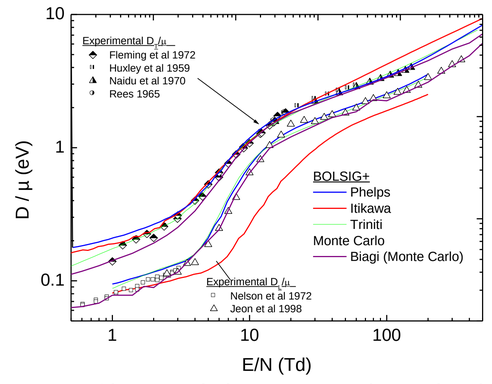


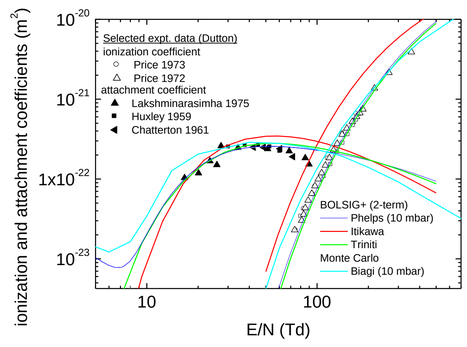
Normalized mobility x N, μN



Characteristic energy, D_T/μ, and D_L/μ

Conclusions

- All experimental data and all cross section sets described here are available on the open-access website, LXCat (www.lxcat.net).
- The cross section sets developed specifically for calculations of swarm parameters and available on LXCat each yield generally good agreement with measurements when used appropriately (see comments on the LXCat site for correct usage for each).
- More work is needed to incorporate and validate simplified treatments of rotational excitation into the on-line software.
- This work brings together compilations of data for N2 and O2 based purely on "best" cross sections in the literature with those assembled with the requirement that the cross sections be consistent with swarm parameters. Efforts are being made to add to Itikawa's partial set of cross sections in order to obtain a complete set yielding more accurate swarm parameters when used with Boltzmann equation solvers



Normalized Townsend ionization and attachment coefficients

The 3-body attachment coefficient , important at low E/N, is shown here for 10 mbar . The differences between the 3-body attachment rate for Biagi (Monte Carlo) and Phelps (2-term) are due to differences in the 3-body attachment cross sections. The 2-term approximation introduces very little error in this region.