The IST-LISBON database on LXCat

L L Alves
Instituto de Plasmas e Fusão Nuclear, Instituto Superior Técnico, Universidade de Lisboa, Av Rovisco Pais, 1049-001 Lisboa, Portugal

llalves@tecnico.ulisboa.pt

Abstract. LXCat is a web-based, community-wide project on the curation of data needed in the modelling of low-temperature plasmas. LXCat is organized in databases, contributed by members of the community around the world and indicated by the contributor's chosen title. This paper presents the status of the data available on the IST-LISBON database with LXCat. IST-LISBON contains up-to-date electron-neutral collisional data (together with the measured swarm parameters used to validate these data) resulting from the research effort of the Group of Gas Discharges and Gaseous Electronics with Instituto de Plasmas e Fusão Nuclear, Instituto Superior Técnico, Lisbon, Portugal. Presently, the IST-LISBON database includes complete and consistent sets of electron scattering cross sections for argon, helium, nitrogen, oxygen, hydrogen and methane.

1. Introduction. The LXCat project
Electrons are the prime species to convey energy into a gas, producing plasma, and thus knowledge of reliable electron–neutral scattering cross sections is of paramount importance to accurately describe the electron kinetics in low-temperature plasmas, bringing extra credibility to modelling results. The LXCat project (www.lxcat.net) [1] is an open-access website for collecting, displaying, and downloading electron and ion scattering cross sections for binary encounters (swarm-derived, measured or calculated using quantum mechanical theory), electron and ion swarm parameters (measured transport parameters and rate coefficients), interaction potentials, optical oscillator strengths and other data essential for modeling low-temperature plasmas. LXCat is organized in databases, contributed by members of the community around the world and indicated by the contributor's chosen title.

At present LXCat offers 21 databases (managed by approximately 30 contributors from 11 countries), 17 of which contain sets of cross sections for electron scattering from ground-state neutral atoms and molecules, covering a range of energies from thermal up to 100’s of eV and higher. Some of the databases present complete and consistent sets of cross sections [2-4], with interest for modelling and/or diagnostic studies (e.g. based on optical measurements), corresponding to much more than a simple compilation of data. Complete cross section sets stand for arrangements able to describe the main electron momentum-loss, energy-loss and number-changing processes (ionization, attachment, recombination), either individually or grouped together. In this sense, cross sections for only one particular excitation process and/or for a limited energy range, as often encountered in the literature, are not relevant by themselves. Consistent sets are those able to reproduce measured values of swarm parameters when used as input data to evaluate the electron energy distribution function (eedf) from a Boltzmann solver or Monte Carlo/Particle-in-Cell codes.
The most popular strategy to determine a complete, consistent cross section set in gaseous electronics uses an iterative process to perform educated adjustments onto an initial compilation of data, as follows: (i) a set of cross sections is collected from the literature; (ii) the cross sections are used as input data to calculate eedfs and to evaluate electron transport parameters and rate coefficients; (iii) the magnitudes of the cross sections are adjusted (within experimental error or theoretical uncertainty, if possible), to improve the agreement between calculated and measured swarm data. Such an iterative procedure embeds a global consistency check, since it relies on reproducing measured electron parameters, but cannot be used to ensure either the uniqueness of the cross section set or the validation of the cross section for any individual process. Despite the poor resolution of the swarm method and the fact that it only allows adjusting integral cross sections, the procedure is highly meaningful for plasma modelling, since it provides a consistent estimation of transport parameters and macroscopic (excitation and ionization) rate coefficients. In fact, cross section compilations that lack this consistency check with swarm experiments are of limited interest in low-temperature simulations.

LXCat offers also a series of on-line tools enabling: (i) uploading / downloading data in ASCII format; (ii) selecting and displaying multiple data sets graphically; (iii) rescaling and downloading graphs; (iv) calculating electron swarm parameters from selected cross section data, in pure gases or in gas mixtures, using the Boltzmann equation solver BOLSIG+ [5]; and (v) displaying of calculated swarm parameters along with selected experimental values of these quantities obtained from the databases.

The LXCat team has been making systematic inter-comparisons of cross section data and comparisons of calculated and measured swarm parameters. These were published for noble gases [2-4] and reported in about 10 communications to conferences, also for common molecular gases (H₂, N₂ and O₂).

2. The IST-LISBON database

One of LXCat’s databases is IST-LISBON, which contains up-to-date electron-neutral collisional data (together with the measured swarm parameters used to validate these data) resulting from the research effort of the Group of Gas Discharges and Gaseous Electronics with Instituto de Plasmas e Fusão Nuclear, Instituto Superior Técnico, Lisbon, Portugal.

Presently, IST-LISBON includes complete and consistent sets of electron scattering cross sections, and measured swarm parameters, for argon, helium, nitrogen (atomic and molecular, including also electron-impact rotational and vibrational excitation cross-sections), molecular oxygen (including also electron-impact rotational and vibrational excitation cross-sections), hydrogen (atomic and molecular, including also electron-impact rotational and vibrational excitation cross-sections) and methane. In general, our cross sections yield predictions for the electron transport parameters and rate coefficients, calculated with a two-term Boltzmann solver, which agree within less than 20% with measurements, for reduced electric fields $E/N \sim 10^{-4} – 500$ Td (where $E$ is the electric field intensity and $N$ is the neutral gas density; 1 Td = $10^{-17}$ V cm²). This kind of agreement is acceptable in many plasma applications, although for highly accurate swarm experiments a minimum accuracy of 1% is required [6-8].

2.1. Argon

The compilation and adjustment of the complete set of electron–neutral scattering cross sections from ground-state argon is reported in [9]. The set includes 39 cross sections (elastic momentum-transfer, 37 excitations and ionization) up to 1 keV. Figure 1 summarizes the argon cross section set with IST-LISBON.

The elastic momentum-transfer cross section was obtained from [10]. Direct excitation cross sections up to 100 eV were obtained: from [11], for the 4s metastable and resonance levels (multiplied by a factor 0.5); from [12], for the 4p levels; from [13], for the 3d, 3d’, 5s and 5s’ levels; from [14], for the 5p levels; for the 4d, 6s and 4d’ levels, only optically allowed transitions were considered using the expressions and data of [15-17]. The previous direct excitation cross sections were extended to 1
keV, by using analytical asymptotic expressions similar to those proposed in [17-18]. Direct ionization
adopted the cross section measured in [19].

When these cross sections are used as input data in a two-term Boltzmann solver, they yield swarm
parameters (reduced mobility $\mu_N$, characteristic energy $u_k$ and Townsend ionization coefficient $\alpha/N$) in
general agreement with measurements, within the 2-25% experimental uncertainties reported. Note
that calculations agree also with measurements (25-30% errors) of the total excitation coefficients
(including cascade contributions coherent with the proposed cross section set) for the 4s-metastable,
the 4s-resonance and the 4p levels. More details can be found in [2].

![Figure 1. Summary of the argon cross section set with IST-LISBON, as a
function of the electron kinetic energy. Elastic momentum-transfer (solid
magenta line and A; multiplied by factor 0.1), excitation to 4s-metastable
levels (solid blue and B; x10), excitation to 4s-resonance levels (dashed
blue and C; x10), excitation to 2p levels (dotted blue and D), total
excitation (solid black and E), and ionization (solid red and F).](image)

2.2. Helium
The compilation and adjustment of the complete set of electron–neutral scattering cross sections from
ground-state helium is reported in [20-21]. The set includes 44 cross sections (elastic momentum-
transfer, 42 excitations and ionization) up to 100 eV. Figure 2 summarizes the helium cross section set
with IST-LISBON.

The elastic momentum-transfer cross section was obtained from [22-23] at low energies, [24] at
intermediate energies, and [25] at high energies. Total (direct plus cascade) excitation cross sections
were obtained: for the $2^3S + 2^1S$ metastable levels (cross section multiplied by a factor 0.65), from
[26] near threshold, from [27] at low energies and from [28] at high energies; for the $2^1P$ and $3^1P$
levels (x1.12), from [29]; for the $4^1P$ level (x1.2), from [30]; for the $2^3P$ level (x0.89) from [31]; for
the $3^3P$ level (x0.89), from [32]. Direct cross sections for the $n^{1/2}S,D$ ($n = 3-7$), $n^{1}P$ ($n = 5-7$), $n^{3}P$ ($n = 4-7$) and $n^{1/2}FGHI$ ($n < 7$) levels were obtained from [33-34]. The direct cross sections for the low-
lying levels $2^{1,3}S$, $n^{1}P$ ($n = 2-4$) and $n^{3}P$ ($n = 2-3$) were calculated from the corresponding total cross
sections by correcting for the cascade transitions. The individual excitation cross sections for the $2^1S$
and $2^3S$ metastable levels were obtained from the corresponding lumped cross section by using the
deconvolution parameter proposed in [33-34]. Direct ionization adopted the cross section measured in [19]. A review of this cross section set was recently published [35] (including also the extension of its maximum energy to 1 keV), and it will soon be used in updating the IST-LISBON database.

When these cross sections are used as input data in a two-term Boltzmann solver, they yield swarm parameters in general agreement with measurements, within the 5-10% experimental uncertainties reported and considering the dispersion observed in the measurements, reaching differences as high as factors of 4-5. More details can be found in [3].

![Figure 2. Summary of the helium cross section set with IST-LISBON, as a function of the electron kinetic energy. Elastic momentum-transfer (solid magenta line and A; multiplied by factor 0.1), excitation to metastable 2^3S+2^1S levels (solid blue and B; x10), excitation to 2^3P+2^1P levels (dashed blue and C), total excitation (solid black and D), and ionization (solid red and E).](image)

**2.3. Nitrogen**

The complete set of electron–neutral scattering cross sections from ground-state molecular nitrogen was initially reported in [36]. The set includes 23 cross sections (effective; excitations to 10 vibrational levels and 11 electronic levels; and ionization), and it was compiled mostly from [37-38]. Originally, the set was limited to 40 eV kinetic energy, but prior to its publication on LXCat it was reviewed and extended to 1 keV, using information from the databases BIAGI-v8.9 and PHELPS. Figure 3 summarizes the N\(_2\) cross section set with IST-LISBON.

The *effective* momentum-transfer cross section [37-38] corresponds to the sum of the elastic momentum-transfer, the total excitation and the ionization cross sections. This quantity appears in the collision term of the electron Boltzmann equation, after expansion in Legendre polynomials and if higher order anisotropies in the differential cross sections for inelastic scattering are neglected [9], as it is commonly assumed in two-term Boltzmann solvers.

Direct excitation cross sections (up to 40 eV) to electronic levels were obtained: from [37-38], for A^3\(\Sigma_u^+\) (v=0-4; v=5-9; v>9), C^3\(\Pi_u^+\), E^3\(\Sigma_u^+\), and a^3\(\Sigma_g^+\) levels; from [39], for B^3\(\Pi_g\), W^3\(\Delta_u\), B^3\(\Sigma_u^+\), a^1\(\Pi_g\), a^1\(\Sigma_g^+\) and w^1\(\Delta_u\) levels; from [40], for N\(_2\) higher lying levels. The cross section for the N\(_2\)(v=0)-N\(_2\)(v=1) vibrational excitation was adjusted using also the results of [41-45]. The cross sections for the
N$_2$(v=0)-N$_2$(v=2-8) excitations were adjusted using also the results of [36-37], and those for the
N$_2$(v=0)-N$_2$(9-10) excitations, not included in PHELPS database, were adjusted using also the results
of [36-37,46]. Direct ionization adopted the cross section measured in [19].

![Figure 3](image.png)

**Figure 3.** Summary of the N$_2$ cross section set with IST-LISBON, as a function of the electron kinetic energy. Effective momentum-transfer (solid magenta line and A), first vibrational excitation v=0→v=1 as an example (solid blue and B), first rotational excitation J=0→J=2 as an example (dashed blue and C), total excitation (solid black and D), and ionization (solid red and E).

When this complete set of cross sections (extended to 1 keV) is used as input data in a two-term Boltzmann solver, it yields calculated swarm parameters in agreement with measurements for $E/N$ values between 10 and 1000 Td. Maximum deviations are of 27% for $u_k$ and 22% for $\mu N$, between 300-400 Td, and of 45% for $\alpha/N$ around 150 Td. Below 10 Td the set must be further completed to include rotational excitation / de-excitation mechanisms, in order to reproduce measured swarm data. Here, we have adopted the rotational excitation cross sections of [47] for the $J \rightarrow J + 2$ transitions ($J=0,\ldots,30$), taking $Q = 1.09$ and $B = 2.5 \times 10^{-4}$ eV [48] for the N$_2$ quadruple moment and rotational constant, respectively, assuming a Boltzmann distribution at gas temperature $T_g$ for the rotational populations with the electronic ground-state. With the inclusion of the supplementary rotational mechanisms, the deviations between calculated and measured values of $u_k$ and $\mu N$ are well below 10%, in the low $E/N$ region at $T_g = 77, 300$ K.

The IST-LISBON dataset for nitrogen includes also electron–neutral cross sections for the atomic system [49]. This set was compiled from [50] and [51], for the elastic momentum-transfer and the excitation of N(4D) and N(3P) levels from ground-state N(4S), respectively.

## 2.4. Oxygen

The complete set of electron–neutral scattering cross sections from ground-state molecular oxygen was initially reported in [52]. The set was compiled mostly from [53], and it includes the following 14 cross sections: elastic momentum-transfer; excitations to 4 vibrational levels; excitations to 7 electronic levels (a'Î'; b'Î', a'Î'g, A'Î'g, C'Î'g and c'Î'g bound states; A'Î'u, C'Î'u and c'Î'u; yielding dissociation into 2O(3P) and continuum Herzberg bands; B'Î'u; yielding dissociation into O(3P)+O(3P);
radiative levels with thresholds at 9.97 eV and 14.7 eV); dissociative attachment; and ionization. Originally, the set was limited to 40 eV kinetic energy, but prior to its publication on LXCat it was reviewed and extended to 1 keV, using information mainly from the databases PHELPS and BIAGI-v8.9. The exception is the cross section for the excitation of O$_2$(a$^1\Delta_g$), which was extended up to 200 eV using the results of [54] and then extrapolated up to 1 keV. Figure 4 summarizes the O$_2$ cross section set with IST-LISBON.

![Figure 4. Summary of the O$_2$ cross section set with IST-LISBON, as a function of the electron kinetic energy. Effective momentum-transfer (solid magenta line and A), first vibrational excitation v=0→v=1 as an example (solid blue and B), first rotational excitation J=1→J=3 as an example (dashed blue and C), dissociative attachment (solid green and D), total excitation (solid black and E), and ionization (solid red and F).](image)

When this complete set of cross sections (extended to 1 keV) is used as input data in a two-term Boltzmann solver, it yields calculated swarm parameters in agreement with measurements for $E/N$ values between 10 and 1000 Td. The maximum deviations observed are the following: for $u_k$, 5% between 10-100 Td; for $\mu N$, 21% between 10-100 Td (where a 44% dispersion is found in the experimental values); for the reduced attachment Townsend coefficient, a factor of 2 difference in the region 10-100 Td, equivalent to the experimental dispersion; for the reduced ionization Townsend coefficient, a factor of 1.5 difference in the region 100-400 Td, also equivalent to the experimental dispersion. Below 10 Td the set must be further completed to include rotational excitation / de-excitation mechanisms, in order to reproduce measured swarm data. Here, we have adopted the rotational excitation cross sections of [47] for the $J \rightarrow J + 2$ transitions ($J=1,3,5,...,29$), taking $Q = 1.4$ and $B = 1.8 \times 10^4$ eV [55], and assuming a Boltzmann distribution at $T_g$ for the rotational populations with the electronic ground-state. With the inclusion of the supplementary rotational mechanisms, the deviations between calculated and measured values of $u_k$ and $\mu N$ in the low $E/N$ region are found below the 20% experimental dispersion observed.

2.5. Hydrogen

The compilation of the complete set of electron–neutral scattering cross sections from ground-state hydrogen is reported in [56]. The set was compiled mostly from [57-58], and it includes the following
25 cross sections up to 1 keV: elastic momentum-transfer [59]; 4 rotational excitations (for \( J=0 \rightarrow J=2 \), obtained from the swarm measurements of [60], at low energies, and from the theoretical expressions of [61], at intermediate energies; for \( J \rightarrow J+2 \) with \( J=1-3 \), obtained from the swarm measurements of [62], at low energies, and from the data proposed in [63], at intermediate energies); excitations to 3 vibrational levels [64]; excitation to 4 triplet dissociative levels (\( b^3\Sigma_u^+; c^3\Pi_u; a^3\Sigma_g^+ \) and \( e^3\Sigma_u^+ \)) and to 7 singlet partially dissociative Rydberg levels (\( B^1\Sigma_u^+; C^1\Pi_u; E^1\Sigma_g^+; F^1\Sigma_g^+; B''^1\Sigma_u^+; D^1\Pi_u; B''''^1\Sigma_u^+ \) and \( D''^1\Pi_u \)); dissociation into \( \text{H}(1s)+\text{H}(2s,2p,3,4,5) \) [65-67]; and ionization [68-70]. Figure 5 summarizes the \( \text{H}_2 \) cross section set with IST-LISBON.

**Figure 5.** Summary of the \( \text{H}_2 \) cross section set with IST-LISBON, as a function of the electron kinetic energy. Elastic momentum-transfer (solid magenta line and A); total vibrational excitation (solid blue and B); first (\( J=0 \rightarrow J=2 \), dashed blue and C) and second (\( J=1 \rightarrow J=3 \), dotted blue and D) rotational excitations, as examples; total excitation to singlet levels (solid black and E) and to triplet levels (dashed black and F); and ionization (solid red and G).

When these cross sections are used as input data in a two-term Boltzmann solver, they yield swarm parameters in general agreement with measurements, for reduced electric fields in the range \( 10^{-3} \) to \( 1000 \) Td and gas temperatures of 300, 77 K. At low \( E/N \), the agreement can only be obtained by including inelastic stepwise and superelastic transitions between the rotational levels considered, assuming a Boltzmann distribution at \( T_g \) for their populations. The maximum deviations observed are the following: for \( u_a \), 8\% in the region \( 10^{-2}-1 \) Td and 19\% at 150 Td (for a 30\% dispersion in the experimental values), this deviation increasing with \( E/N \); for \( \mu_\ell N \), 6\% in the region \( 10^{-3}-1 \) Td and 16\% at 180 Td; for \( \alpha/N \), ~50\% in the region 150-850 Td. A similar agreement is also observed between calculated and measured values of the total dissociation coefficient and the excitation coefficient for all singlet levels.

The IST-LISBON dataset for hydrogen includes also electron–neutral cross sections for the atomic system [56]. This set was compiled from [71-72] for the elastic momentum-transfer, and adjusted from [15] for the excitation of \( \text{H}(2s,2p,3,4,5) \) levels and for the ionization from ground-state \( \text{H}(1s) \).
2.6. Methane

The complete set of swarm-derived electron–neutral cross sections for methane was initially reported in [73], for kinetic energies up to 40 eV. Prior to its publication on LXCat, this set was substantially reviewed and extended up to energies of at least 400 eV. The present set, mainly based on the works [74-77], includes the following 9 cross sections: elastic momentum-transfer [74]; excitation of 2 vibrational modes (1,3) and (2,4) [74-75], obtained from [78-79] at low energies and from [80] at high energies; dissociation into CH$_3$ and CH$_2$ [75], obtained by subtracting the dissociative ionization cross section proposed in [77] to the total dissociation cross section reported in [81], and estimating the CH$_3$/CH$_2$ branching ratio from [76]; dissociative attachment into CH$_2^-$ and H$^-$ [74] (not shown in figure 6, due to the small value of the corresponding cross section); and ionization into CH$_4^+$ and CH$_3^+$ [77], yielding a total ionization cross section that agrees with the results of [19,75].

When this complete set of cross sections is used as input data in a two-term Boltzmann solver, it yields calculated swarm parameters in agreement with measurements, for $E/N$ values in the range $10^1$ to 400 Td. The maximum deviations observed are the following: for $u_k$, 12% around 30 Td and 30-40% below 1 Td (similar to the dispersion in the experimental values); for $\mu_N$, 10-15% in the region 10-300 Td and 28-40% below 1 Td (again, similar to the dispersion in the experimental values); for $\alpha/N$, 25% at 150 Td.

![Figure 6](image)

**Figure 6.** Summary of the methane cross section set with IST-LISBON, as a function of the electron kinetic energy. Elastic momentum-transfer (solid magenta line and A); vibrational excitations (1,3) (solid blue and B) and (2,4) (dashed blue and C); dissociation into CH$_3$ (solid black and D) and CH$_2$ (dashed black and E); and ionization into CH$_4^+$ (solid red and F) and CH$_3^+$ (dashed red and G).

3. Final remarks

This paper has presented the current status of the IST-LISBON database with LXCat, summarizing its complete and consistent sets of electron-neutral scattering cross sections for argon, helium, nitrogen, oxygen, hydrogen and methane. We have also reported on the quality of the calculated swarm parameters (characteristic energy, reduced mobility and excitation / ionization coefficients) obtained with these cross sections, when used as input data in a two-term Boltzmann solver, giving indication
of the maximum deviations observed with respect to experimental values of these parameters, also available on LXCat. The IST-LISBON database will continue to be updated with the most recent data on cross sections and swarm parameters compiled, adjusted and checked by the Lisbon’s group. Future work involves the update of helium cross sections and the upload of data for CO$_2$.

This paper has also briefly presented the web-based, open-access LXCat project. Our future plans include continuing the enlargement of LXCat databases (attracting new contributors and/or introducing new data types) and pursuing the evaluation / checking of the data published on-line. We are also committed to give each contributor a proper recognition for his/her work, by setting a consistent format for referencing among editors of journals (eventually, including citations of the original papers where the data was obtained from) and/or by introducing DOI numbers for the individual databases.

Acknowledgments

This work was partially supported by Fundação para a Ciência e a Tecnologia, under Project Pest-OE/SADG/LA0 010/2013.

References

[1] Pancheshnyi S, Biagi S F, Bordage M C, Hagelaar G J L, Morgan W L, Phelps A V and Pitchford L C 2012 Chem. Phys. 398 148
[2] Pitchford L C et al 2013 J. Phys. D: Appl. Phys. 46 334001
[3] Alves L L et al 2013 J. Phys. D: Appl. Phys. 46 334002
[4] Bordage M C et al 2013 J. Phys. D: Appl. Phys. 46 334003
[5] Bolsig 2005 www.bolsig.laplace.univ-tlse.fr/
[6] Petrović et al 2009 J. Phys. D: Appl. Phys. 42 194002
[7] Petrović et al 2007 Plasma Sources Sci. Technol. 16 S1
[8] White et al 2003 J. Phys. D: Appl. Phys. 36 3125
[9] Yanguas-Gil A, Cotrino J and Alves L L 2005 J. Phys. D: Appl. Phys. 38 1588
[10] Yamabe C, Buckman S J and Phelps A V 1983 Phys. Rev. A 27 1345
[11] Khakoo M A et al 2004 J. Phys. B: At. Mol. Opt. Phys. 37 247
[12] Chilton J E, Boffard J B, Schappe R S and Lin C C 1998 Phys. Rev. A 57 267
[13] Hayashi M 2003 Report NIFS-DAT-72, National Institute for Fusion Science of Japan
[14] Weber T, Boffard J B and Lin C C 2003 Phys. Rev. A 68 032719
[15] Drawin H W 1967 Report No EUR-CEA-FC-383, Fontenay-aux-Roses
[16] Lee C M and Lu K T 1973 Phys. Rev. A 8 1241
[17] Bretagne J, Callède G, Legentil M and Puech V 1986 J. Phys. D: Appl. Phys. 19 761
[18] Bretagne J, Godart J and Puech V 1982 J. Phys. D: Appl. Phys. 15 2205
[19] Rapp D and Englander-Golden P 1965 J. Chem. Phys. 43 1464
[20] Alves L L and Ferreira C M 1991 J. Phys. D: Appl. Phys. 24 581
[21] Alves L L, Gousset G and Ferreira C M 1992 J. Phys. D: Appl. Phys. 25 1713
[22] Crompton R W, Elford M T and Jory R L 1967 Aust. J. Phys. 20 369
[23] Crompton R W, Elford M T and Robertson A G 1970 Aust. J. Phys. 23 667
[24] Milloy H B and Crompton R W 1977 Phys. Rev. A 15 1847
[25] Register D F, Trajmar S and Srivastava S K 1980 Phys. Rev. A 21 1134
[26] Schulz G J and Fox R E 1957 Phys. Rev. 106 1179
[27] Schulz G J and Philbrick J W 1964 Phys. Rev. Lett. 13 477
[28] Mason N J and Newell W R 1987 J. Phys. B: At. Mol. Phys. 20 1357
[29] Westerveld W B, Heideman H G M and Van Eck J 1979 J. Phys. B: At. Mol. Phys. 12 115
[30] Donaldson F G, Hender M A and McConkey J W 1972 J. Phys. B: At. Mol. Phys. 5 1192
[31] Jobe J D and St John R M 1967 Phys. Rev. 164 117
[32] de Heer F J and Jansen R H J 1977 J. Phys. B: At. Mol. Phys. 10 3741
[33] Gousset G and Boulmer-Leborgne C 1984 J. Physique 45 689
[34] Daviaud S 1989 *PhD Thesis* University Paris-Sud, Orsay, France
[35] Santos M, Noël C, Belmonte T and Alves L L 2014 *J. Phys. D: Appl. Phys.* 47 265201
[36] Loureiro J and Ferreira C M 1986 *J. Phys. D: Appl. Phys.* 19 17
[37] Pitchford L C and Phelps A V 1982 *Bull. Am. Phys. Soc.* 27 109
[38] Tachibana K and Phelps A V 1979 *J. Chem. Phys.* 71 3544
[39] Cartwright D C, Trajmar S, Chutjian A and Williams W 1977 *Phys. Rev. A* 16 1041
[40] Zipf E C and McLaughlin R W 1978 *Planet. Space Sci.* 26 449
[41] Schulz G J 1962 *Phys. Rev.* 135 229
[42] Schulz G J 1964 *Phys. Rev.* A 8 2883
[43] Gerjouy E and Stein S 1955 *Phys. Rev.* 97 1671
[44] Huber K P and Herzberg G 1979 *Molecular Spectra and Molecular Structure. IV. Constants of Diatomic Molecules* (D. van Nostrand Reinhold Co., Princeton:New Jersey)
[45] Marques L, Jolly J and Alves L L 2007 *J. Appl. Phys.* 102 063305
[46] Phelps A V, private communication
[47] Winters H F 1975 *J. Chem. Phys.* 63 3462
[48] Simko T, Martisovits M, Bretagne J and Gousset G 1997 *Phys. Rev. E* 56 5908