

COMPARISONS OF QUANTEMOL AND MORGAN LXCAT CROSS SECTION SETS FOR ELECTRON-NEUTRAL SCATTERING AND RATE-COEFFICIENTS: HELIUM AND WATER[†]

UDC 539.12...172

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Abstract. *The present work compares cross section sets for electron scattering from ground state helium and ground state water molecule, which are available at LXCat Morgan database and the new Quantemol-DB. These cross section sets are used as an input for numerical solving of Boltzmann equation by using electron Boltzmann solver BOLSIG+, in order to obtain transport coefficients, electron energy distribution function and rate coefficients for electron impact scattering processes. The calculated quantities are compared to examine the quality and completeness of the cross section sets provided by Quantemol database for modeling low-temperature plasmas and interpretation of experimental results.*

Key words: *cross section, electron energy distribution function, rate coefficient*

1. INTRODUCTION

The fast growing realm of applications of low temperature non-equilibrium plasmas in various fields (Adamovich et al., 2017), such as materials processing (Lieberman and Lichtenberg, 2005; Makabe and Petrović, 2006), surface modification (Bhoj and Kushner, 2006; Dorai and Kushner, 2003) and biomedical applications including plasma medicine and plasmas in agriculture (Kong et al., 2009; Weltmann and Woedtke, 2017; Puač et al., 2006; Graves, 2012; Metelmann et al., 2015), requires a detailed analysis and understanding of all important physical and chemical processes in such plasmas.

Received June 10th, 2019; accepted September 25th, 2019

[†] Acknowledgement: This work is supported by MPNTR of Serbia, projects ON171037 and III41011.

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At atmospheric pressure chemistry is much more complex as compared to low pressures, including more than a thousand of processes which develop in a few hundreds of nanoseconds after discharge ignition (Bruggeman et al., 2017). In the case of plasma interaction with liquid water the situation is more complicated due to a large number of chemical processes which develop in the liquid phase and in intermediate interface zone (Bruggeman et al., 2016). Since chemical composition of such plasmas is often difficult to access by measurements, numerical models are used in analysis and understanding of all important processes (Alves et al., 2018), giving the base for developing of new plasma devices and opening further possibilities for application. In order to construct a plasma model, one should, as a start, use appropriate transport and rate coefficients which could be obtained from the cross section set.

Due to a large number of important processes and plasma species which should be included in the model, atmospheric pressure low-temperature plasmas are quite difficult to study by PIC/MC or fluid models. Complex chemical composition can be treated more efficiently with global (spatially averaged) models, based on particle and energy balance in discharges (Hurlbatt et al., 2017). Such models require knowledge of appropriate rate coefficients for all heavy particle collisions and chemical reactions, as for the electron impact processes. Using inadequate values of rate coefficients, possibly due to temperature and pressure dependences or other reasons, may lead to discrepancies of several orders of magnitude in complex plasma models (Turner, 2015; Turner, 2016). Having this fact in mind, in the process of constructing global models all the data taken from the literature or available databases, such as Quantemol-DB (QDB) (Tennyson et al., 2017), should be the subject of a critical evaluation.

The goal of this work is to make a comparison of cross section data for electron scattering from helium ground state atom and water ground state molecule, currently available in the QDB, with W. L. Morgan cross section sets available online under the LXCat project (Pancheshnyi et al., 2012; Morgan database, 2019). The latter set is known to be a reasonable compilation of the best data due to R.W. Crompton and A.V. Phelps and also some new results. On the other hand QDB contains a large number of reaction rates, rates for excited species and cross sections for collisions with excited states. Thus one is motivated to use the data from that database in global models but the initial step of electron-molecule collisions needs to be verified.

A set of cross sections which should be used in calculation of transport/rate coefficients and plasma modeling should be *consistent* and *complete*, which means to be able to describe all important electron momentum, energy and number-losses in collisions and finally to be able to reproduce measured values of electron swarm parameters (Alves et al., 2013; Petrović et al., 2009). The so called swarm-technique to obtain cross sections from the transport coefficients follows the procedure of applying transport theory to model weakly ionized plasmas. Thus application of swarm derived sets guarantees satisfaction of the above mentioned balances provided that the initial experimental data were accurate and well defined. The complete cross section set for molecular gases should include cross sections for elastic/effective momentum transfer, excitation in various rotational, vibrational and electronic states of interest and total ionization.

Electron energy distribution function (EEDF) and rate coefficients for electron scattering processes from helium atom and water molecule are calculated by numerical solving of Boltzmann kinetic equation (BE) with Morgan and QDB cross section sets. BE is solved by electron Boltzmann solver BOLSIG+ (Hagelaar et al., 2005) which calculates

EEDF based on two-term approximation expansion in Legendre polynomials (Lieberman and Lichtenberg, 2005; Makabe and Petrović, 2006). Comparison of results for helium and water is chosen by having in mind the importance of these gases in low-temperature atmospheric pressure plasmas with applications in medicine and agriculture, according to the recent publications (Liu et al., 2010; Bruggeman and Schram, 2010; Murakami et al., 2013; Mladenović et al., 2018; Schroter et al., 2018; Lazović et al., 2010).

2. COMPARISON OF CROSS SECTION SETS PRESENTLY AVAILABLE AT QUANTEMOL-DB WITH CROSS SECTIONS FROM MORGAN (KINEMA RESEARCH) FROM LXCAT

This section presents comparison of cross section sets for electron scattering from ground state helium and water molecule, currently available at Quantemol database (QDB) (Tennyson et al., 2017), with cross section sets from Morgan database at LXCat project (Morgan database, 2019). While there are other sets of cross sections for helium in that database more or less based on the low energy cross section of Crompton and coworkers (Crompton et al., 1967; Milloy and Crompton, 1977) and the higher energy cross sections due to Phelps and coworkers, we have not pursued a more detailed comparisons as the primary goal was to ascertain whether the data presented in QDB are consistent with those obtained by swarm analyses. It is also worth noting that electron helium momentum transfer cross section at low energies (sub excitation) is the most accurately determined cross section as the swarm result has been confirmed by theories with controlled accuracy (Nesbet, 1979; O'Malley et al., 1979).

2.1. Helium

Comparison of cross section sets for electron scattering from ground state helium is presented in Figure 1. Data in Morgan database were developed a few decades ago by W. L. Morgan as swarm derived cross section sets and tested using two-term Boltzmann solver ELENDIF (Morgan and Penetrante, 1990) for calculation of swarm parameters. They are grouped as four scattering processes, referred as elastic momentum transfer, excitation in $2^3S_1+2^1S_0$ states, total excitation (summing all the states with threshold of 20.6eV and higher) and ionization, representing one of the *complete sets* of cross sections for electron scattering in helium (Pancheshnyi et al., 2012). Data currently available at QDB are referred as cross section for electron elastic scattering from ground state helium, excitation in He^* , excitation in He^{**} state and ionization (Tennyson et al., 2017).

QDB cross section for elastic scattering is compared with Morgan momentum transfer cross section in fig. 1a), showing higher differences above 10eV, since anisotropy ($1-\cos\theta$) is assumed, where θ is the scattering angle. Due to anisotropic scattering, momentum transfer cross section is different significantly from the integrated elastic cross section (Alves et al., 2013; Hagelaar et al., 2005). As it is customary to use the cross section sets in a two term Boltzmann code the integrated elastic and the momentum transfer cross sections are often interchanged which may be done only in the case of isotropic scattering. However when the two cross sections differ then one needs to apply anisotropy of scattering together with the total elastic cross section. As momentum transfer cross sections are derived from the drift velocities (mainly) and other transport coefficients, those cross sections include the effect of the anisotropic scattering. Here we shall compare the Morgan set (based on the momentum transfer cross section) with the

QDB elastic scattering set applied incorrectly (with anisotropic scattering), and also corrected for anisotropy in such a way that the momentum transfer cross section from the Morgan set is being used (thus testing the effect of other processes).

Cross sections for electron impact excitation of He^* and He^{**} states, referred to in QDB calculations (HPEM code (Kushner, 2009)), are compared with the Morgan excitation cross sections in $2^3S_1+2^1S_0$ state and total excitation in fig. 1b-c). According to the similarity in shape and magnitude, and to the energy threshold, it can be assumed that these cross sections are related to the same processes. Cross sections for lower threshold processes seem to differ (see fig 1b) by a factor of more than 2. The sums of cross sections for excitation with threshold of 20.6eV and more in the two sets seem to agree well. Finally, fig. 1d) presents electron impact ionization cross sections from Morgan and QDB, which have almost identical values across the entire energy range.

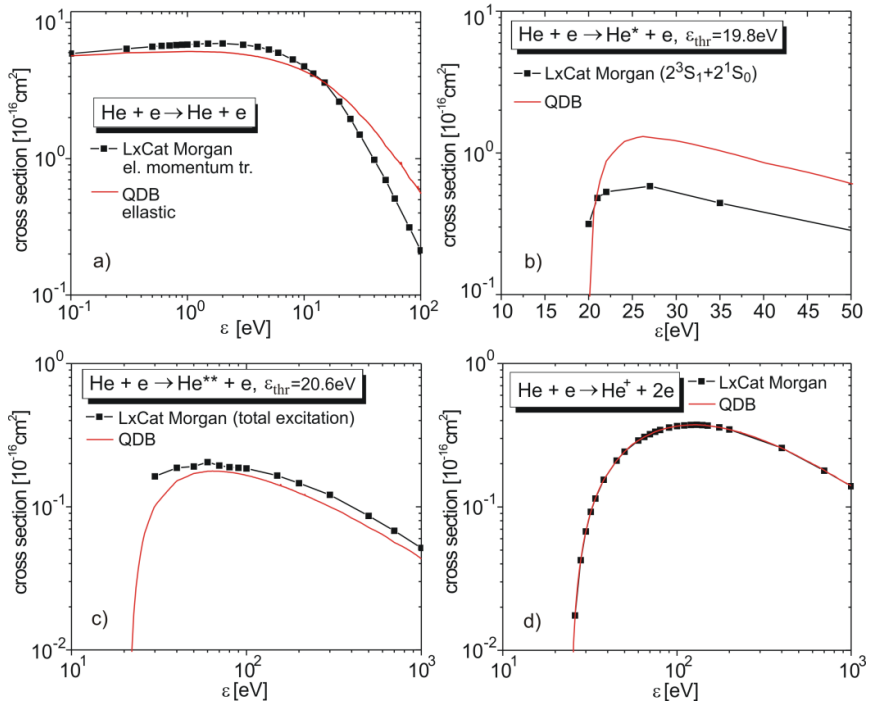


Fig. 1 Cross sections for electron scattering from helium ground state atom, a) momentum transfer and elastic, b) excitation, c) total excitation and d) ionization

2.2. Water

Comparison of cross section sets for electron scattering from water molecule in ground state is presented in Figure 2a-f). Data in QDB are taken from Itikawa and Mason (2005). Figure 2a) shows significant difference between QDB and Morgan momentum transfer cross sections below 1 eV. That difference could be related to rotationally elastic scattering, with cross section presented in Figure 2b). Morgan cross section set for electron scattering from water molecule does not include explicitly cross sections for rotational transitions, as referred in Pancheshnyi et al. (2012) and the Morgan database

(2019). Cross sections for rotational transitions from QDB, presented in Figure 2b) for $j=0-0,1,2,3$ are calculated by Faure et al. (2004) using the R-matrix method. As shown in Itikawa and Mason (2005), rotationally elastic process $j=0-0$ has a sizable contribution to the cross section for elastic scattering, and to momentum transfer (below 1eV after weighting by a factor $(1-\cos\theta)$).

Figure 2c) presents cross sections for electron impact vibrational excitation of water molecule. There is high similarity in shape and magnitude of cross sections from QDB and Morgan for stretching modes (100)-(001) and for (010), although thresholds are slightly different (0.453 eV and 0.3 eV QDB, 0.5 eV and 0.2 eV Morgan).

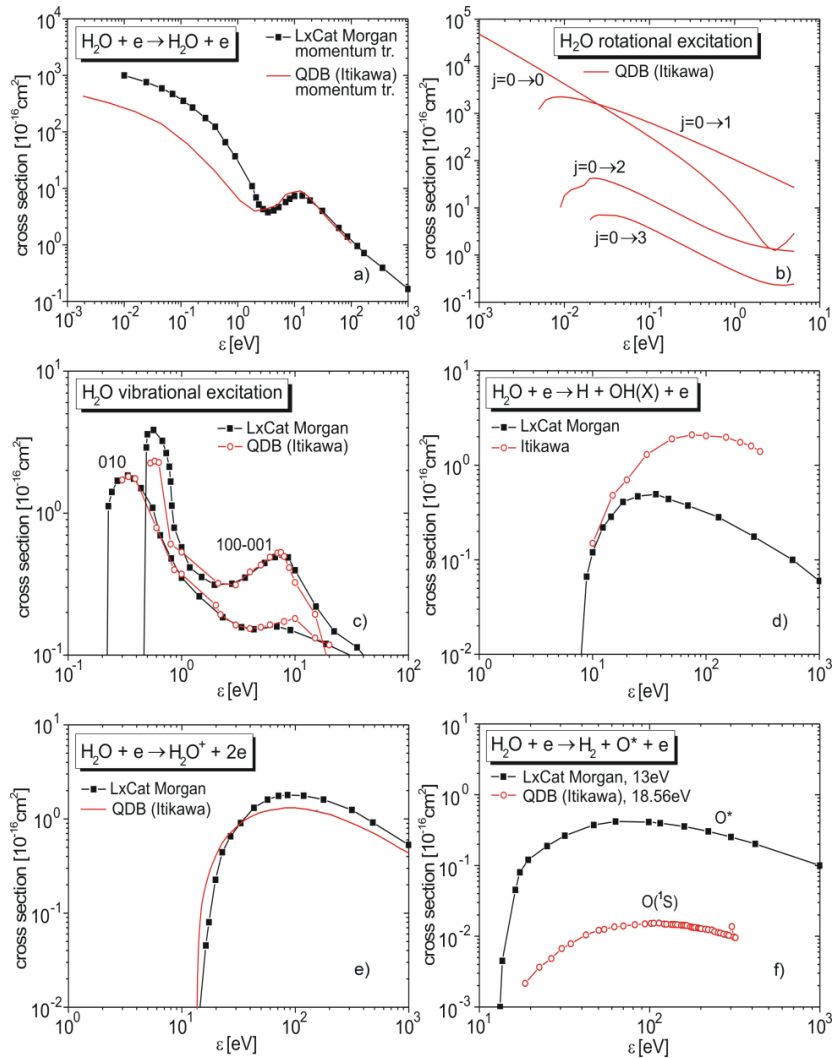


Fig. 2 Cross sections for electron scattering from water ground state molecule, a) momentum transfer, b) rotational excitation, c) vibrational excitation, d) dissociation in OH(X) state, e) ionization and f) dissociation in excited O state.

A greater difference exists between Itikawa and Morgan datasets for electron impact dissociation of water molecule to OH(X) in the ground radical state. This process has its energy threshold of 7.6 eV (as presented in Figure 2d). This process is determined in the literature as the main channel in creation of the OH radical, one of the most important reactive oxygen species for biomedical applications of atmospheric pressure low-temperature plasmas (Bruggeman and Schram, 2010). Having in mind that fact, comparison of two data sets (Itikawa and Morgan) is made in Figure 2d), although neither cross section nor this process is currently available at QDB. The same stands for process of water dissociation in excited OH(A) state as a product, with energy threshold around 9 eV.

QDB and Morgan cross sections for electron impact ionization of water molecule, with energy threshold 12.6 eV, presented in Figure 2e), show similarity in shape and magnitude. Finally, Figure 2f) presents the cross sections for electron impact dissociation of water molecule in excited atomic oxygen state and hydrogen molecule. In Morgan database this process has the threshold of 13 eV, but without exact specification of excited O^* state. For QDB cross section, taken from Itikawa and Mason (2005), it is stated that it is dissociation to the metastable $O(^1S)$ state. It is difficult to understand whether an almost two orders of magnitude difference with the cross section from the Morgan set is due to the latter including other processes as well. This is an important issue as it pertains to the completeness of the set.

Here we make no statements on whether these two sets are the best available or not, which of the two is better. There were several attempts to do swarm based normalization of the cross section data for water molecules (White et al., 2014; de Uguijo et al., 2014; White et al., 2018; Yousfi and Benabdessadok, 1996) but those have been limited to lower energies perhaps not covering the range needed to model plasmas. On the other hand, compilations of the binary collision data (Itikawa and Mason, 2005) may have different cross sections with different quality or uncertainty and some could be missing without effective compensation through other included processes (as common in the swarm analyses). Here we merely wish to point out range of different data that may be used and how those affect plasma chemical modeling.

3. COMPARISON OF ELECTRON ENERGY DISTRIBUTION FUNCTIONS AND RATE COEFFICIENTS USED IN PLASMA MODELLING

Construction of a plasma model requires knowledge of transport and rate coefficients which can be measured directly or calculated from the electron (and ion) energy distribution functions. In many cases for low temperature plasmas it is assumed that all heavy particles, ions and neutrals, have Maxwell-Boltzmann distribution with gas temperature, and distribution function should be determined only for electrons. Electron distribution function $f_e(\vec{r}, \vec{v}, t)$ is defined in such manner that quantity

$$dN|_{\vec{r} \in [\vec{r}+d\vec{r}], \vec{v} \in [\vec{v}+d\vec{v}]} = f_e(\vec{r}, \vec{v}, t) d^3\vec{r} d^3\vec{v} \quad (1)$$

represents the number of electrons in a moment of time t , within a small volume $d^3\vec{r}$ around a position \vec{r} and within $d^3\vec{v}$ around velocity \vec{v} (Lieberman and Lichtenberg, 2005; Makabe and Petrović, 2006). Definition given by eq. (1) is often modified by using the relation $f(\vec{r}, \vec{v}) d^3\vec{r} d^3\vec{v} = f(\vec{r}, \varepsilon) \varepsilon^{1/2} d\varepsilon$, so that electron energy distribution function

(EEDF) is expressed in units [$\text{eV}^{-3/2}$] (Taccogna and Dilecce, 2016). EEDF can be calculated by numerical solving of Boltzmann equation (BE) for a given set of cross sections:

$$\frac{\partial f_e(\vec{r}, \vec{v}, t)}{\partial t} + \vec{v} \cdot \nabla_{\vec{r}} f_e(\vec{r}, \vec{v}, t) + \vec{a} \cdot \nabla_{\vec{v}} f_e(\vec{r}, \vec{v}, t) = J_{coll}(f_e, F_{heavy p.}). \quad (2)$$

Collision term, or collision operator $J_{coll}(f_e, F_{heavy p.})$ is taken in general Boltzmann form, and it is separately defined for every kind of included collision process, based on one appropriately normalized and hopefully complete cross section set (Makabe and Petrović, 2006), which can be provided from swarm experiments (Pancheshnyi et al., 2012; Petrović et al., 2009), beam experiments (Itikawa and Mason, 2005) or numerically calculated (Kushner, 2009). After solving BE, rate coefficients could be calculated from the cross section data using EEDF, and expressed as a function of reduced electric field E/N or mean electron energy (i.e. electron temperature) (Lieberman and Lichtenberg, 2005; Makabe and Petrović, 2006):

$$k_e = \sqrt{2/m_e} \int_{\varepsilon_{thr}}^{+\infty} \sigma(\varepsilon) f_e(\varepsilon) \sqrt{\varepsilon} d\varepsilon. \quad (3)$$

In this section we present the result of solving BE by using the BOLSIG+ program (Hagelaar et al., 2005), where EEDF is represented by the well-known two-term approximation (TTA):

$$f_e(v, \cos\psi, z, t) = f_{e0}(v, z, t) + f_{e1}(v, z, t) \cos\theta, \quad (4)$$

after expansion in series of Legendre polynomials in velocity space. TTA stands for a case of electron swarm drift in weak electric field, oriented along z -axis in eq. (4). f_{e0} denotes isotropic part of the EEDF, f_{e1} denotes anisotropic perturbation as a consequence of a drift (influence of an electric field), while θ represent angle between electron velocity and the field direction. As stated in Lieberman and Lichtenberg (2005), and Makabe and Petrović (2006), the condition for nearly isotropic EEDF in TTA during the drift is that the elastic scattering frequency must be large compared to the frequencies for electron energy gain (from the field) and for inelastic processes. That condition often holds for electrons in low-temperature weakly ionized plasma, because magnitude of the cross section for elastic momentum transfer scattering is appreciably higher than for inelastic scattering processes, although excitations and ionizations, much less frequent, are crucial for plasma sustaining.

3.1. Helium

EEDFs for electrons in pure helium, obtained by solving BE for cross sections from Morgan and QDB are presented in Figure 3 for the same mean energy 2.50eV, which was taken in this work as a representative value for comparison of EEDFs. By using cross sections from QDB we obtain the same mean energy for a lower value of the reduced electric field of 3.76Td.

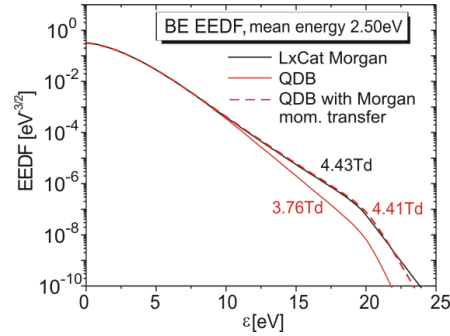


Fig. 3 Electron energy distribution function obtained by solving of Boltzmann equation for He cross section set from Morgan (black line) and Quantemol (red lines).

More importantly, there is a noticeable difference in the high energy tail above 10eV, due to different E/N values for the same mean energy. Different E/N values on the other hand are dictated by difference between elastic scattering cross section and momentum transfer cross section, while assuming isotropic scattering at the same time.

Differences between the two sets of drift velocities are the greatest at the highest energies, as presented in fig. 4a). The actual causes are not clear and differences simply

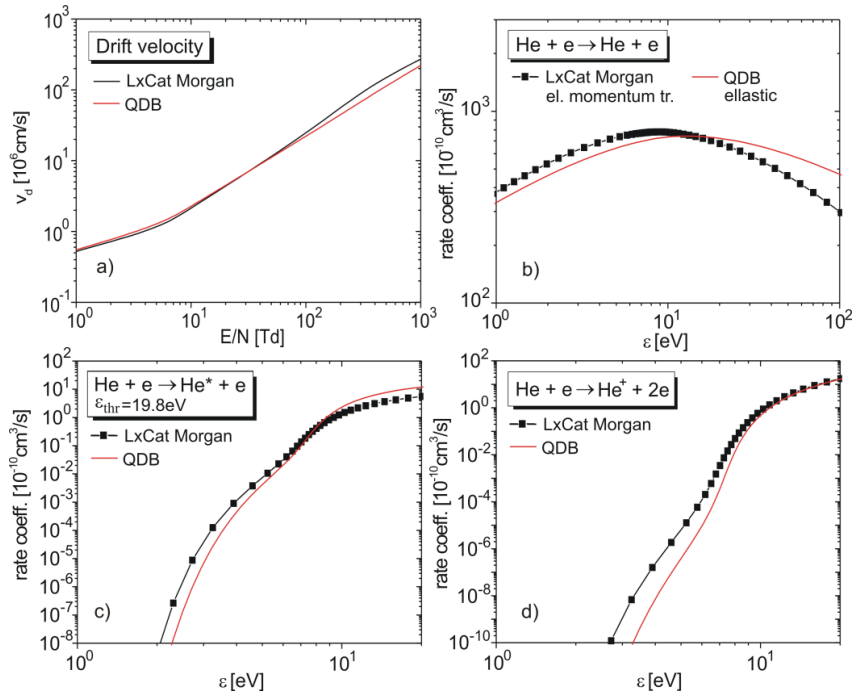


Fig. 4 Drift velocity a) and rate coefficients for: momentum transfer and elastic electron scattering b), excitation c) and ionization of helium d), obtained by solving of BE for He cross section set from Morgan (black lines and scatter) and QDB (red lines).

explained. Rate coefficients for Morgan momentum transfer and QDB elastic electron scattering are compared in fig. 4b), for completeness of comparison, although they are associated to a different kind of scattering process.

The difference in energy tail of EEDFs is higher at energies around 20eV, and has more pronounced influence on the rate coefficients for processes with higher energy threshold. Figures 4c-d) present comparison of rate coefficients for helium excitation (19.8eV) and ionization (24.6eV). The similar conclusions for influence of EEDF on rate coefficients for inelastic processes with high-energy threshold are obtained in Mladenović et al. (2018) and Petrović et al. (2007) as indication of high errors, which can be made by using Maxwell-Boltzmann distribution for electrons in low temperature plasmas. In this work we use only non-equilibrium approach in treatment of electrons based on solving the BE. Since the Morgan dataset for helium is stated to be complete (Pancheshnyi et al., 2012; Morgan database, 2019), the obtained results resolve the influence of QDB cross section set on EEDF and rate coefficients, indicating whether it should be used for plasma modelling.

The values of rate coefficient for ionization differ for more than two orders of magnitude in the energy region 2-3eV, clearly reflecting the differences in EEDFs, since ionization cross sections are the same (Figure 1d) and have a much larger threshold. The difference is less pronounced in the case of excitation (Figure 4c), because of lower threshold and slightly higher cross section for excitation (Figure 1b).

Finally, we perform BE calculations with QDB set, but using the momentum transfer cross section from the Morgan database. Those results are quite close to the Morgan set (dashed line in figure 3, 2.50eV for 4.41Td), reflecting the significant difference between elastic and momentum transfer scattering due to anisotropy related to the weighting factor $(1-\cos\theta)$. The influence of these cross sections on the shape of EEDF is so pronounced because collision frequency of elastic/momentum transfer scattering is appreciably higher than that for the inelastic processes (in low temperature plasmas). As stated in Alves et al. (2013) and Hagelaar et al. (2005), cross section for momentum transfer appears in the collision term of the BE for electrons after expansion in Legendre polynomials, as to be expected in order to describe anisotropy of EEDF in the spatial profile of the drift velocity. This fact clearly indicates that main differences in EEDF and rate coefficients, for the two sets presented in figures 4a-d), are mainly due to the use of the cross section for elastic scattering in the QDB set, due to lack of momentum transfer data.

3.2. Water

EEDFs, obtained by solving BE for cross sections from Morgan (black line) and QDB (red dashed line) are presented in Figure 5 for the same mean energy of 2.50eV. By using QDB data the same mean energy is obtained for a two times lower value of the reduced electric field 36.8Td, with significant difference in the high energy tail of EEDFs above 7.5eV.

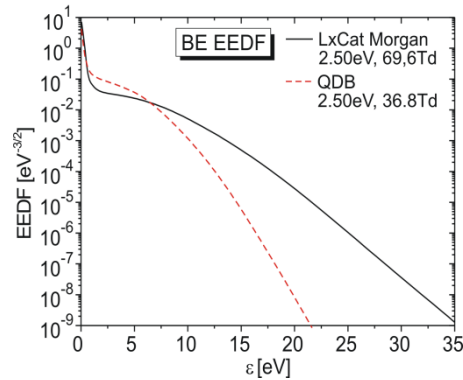


Fig. 5 BE EEDF for H₂O cross section set by Morgan (black line) and QDB (red dashed line).

For the same value of the reduced electric field, in case of using QDB set, BE calculations give almost a two times higher mean electron energy of 4.82eV, with considerably smaller differences in high energy tail but with all the differences in the low energy region present (dashed-dot red line in figure 6a). These differences are partially due to the cross sections for inelastic processes, but mainly caused by differences between Morgan and QDB momentum transfer cross section, as described in figures 2b-f).

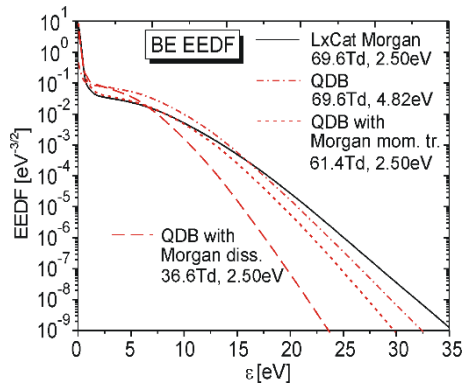


Fig. 6 BE EEDF for H₂O cross section set by Morgan (black line) and QDB (red lines): influence of electric field (dashed-dot), momentum transfer (dot) and dissociation (dashed line).

In both cases, according to Morgan and QDB, calculated EEDF has the characteristic structure in form of a plateau in the lower energy region, starting at energies characteristic for vibrational excitation. In our calculation we have assumed unperturbed gas with only the thermal population of excited states. However, if vibrational states become more populated as in numerous applications (Colonna and Capitelli, 2001; Guerra et al., 2004) the effect of vibrational energy losses would be augmented by the superelastic processes.

In figure 6) we have tried to illustrate how each of the choices to combine the cross sections for inelastic processes affects the EEDF (calculations based on the two databases and

also by replacing elastic cross section from the QDB by that from Morgan's database). Results of BE calculations for QDB cross section set, with only Morgan momentum transfer, show similar values of lower energy plateaus, providing the same mean energy of 2.50eV for a similar value of reduced electric field 61.4Td (dotted red line in figure 6b), as compared with results obtained by using Morgan dataset. A more pronounced plateau in this case provides a considerably higher energy tail, although difference still remains above 7.6eV, indicating the influence of inelastic scattering processes. Although both datasets Morgan and QDB provide cross section for momentum transfer scattering, differences in EEDF induced by differences in the cross sections (see figure 2a) represent the effect similar to that presented in figure 3 for helium.

Figure 6 also shows the influence of Morgan cross section for dissociation in OH(X) state, which is considerably smaller than the Itikawa cross section (figure 2d). It can be concluded that the most important differences are related with momentum transfer and dissociation cross sections.

Figure 7a-d) present comparison of BE rate coefficients, obtained from EEDFs presented in Figure 5 for QDB and Morgan cross section sets. Rate coefficient for elastic momentum transfer is higher in the case of the Morgan database almost by one order of magnitude below 3eV due to the difference in cross section's magnitude (figure 2a) and

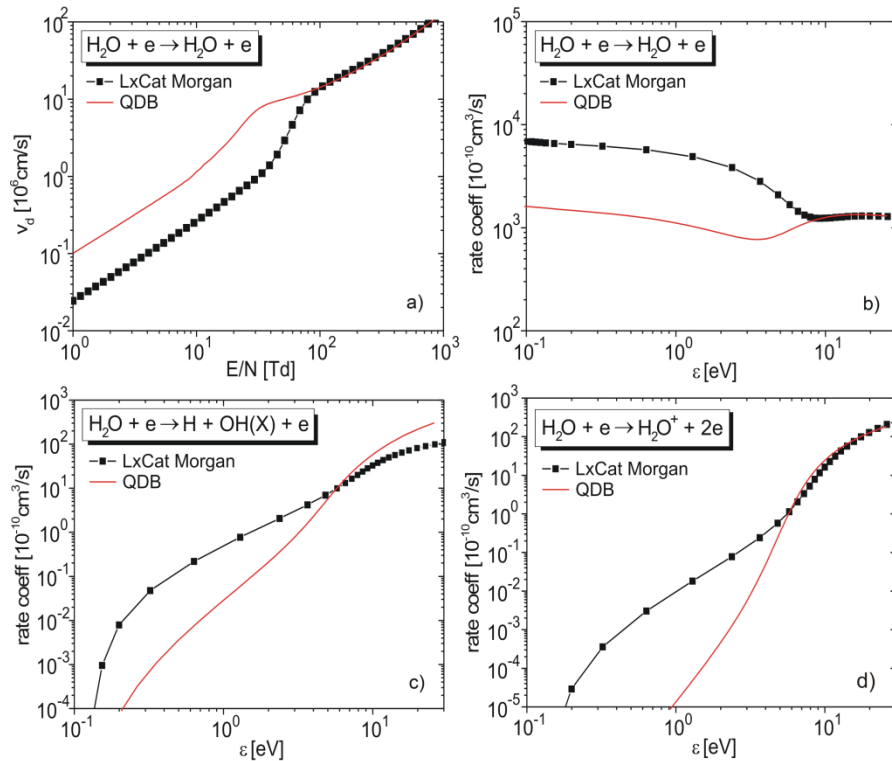


Fig. 7 Drift velocity [10⁶ cm/s] a) and BE rate coefficients for: b) electron impact momentum transfer, c) dissociation and d) ionization of water molecule, for Morgan cross section set (black lines with scatter) and Quantemol/Itikawa database (red lines).

shape of the EEDFs (figure 5). Similarly to results presented in figures 4c-d) for electron scattering from helium, figure 7c-d) shows an influence of EEDF on rate coefficients for processes with higher thresholds. Rate coefficient for electron-impact water dissociation in OH(X) state is higher for the Morgan set, mainly due to the higher EEDF above the threshold of this process 7.6eV, but becomes less than in Itikawa case probably because of the lower cross section (see figure 2d), as presented in figure 7c). The influence of EEDF's tail is more pronounced in the case of electron impact ionization with higher threshold than in dissociation. For explanation one needs to consider overlap of the EEDF with the related cross sections (see figure 2e).

4. CONCLUSION

This work presents a comparison of cross section data for electron scattering from helium and water ground state, currently available at Quantemol database and Morgan database under the LXCat project. The choice of gases is relevant for modeling of atmospheric pressure plasma jets whereby plasma is formed in pure helium and sometimes in mixtures of helium and water vapour to study the effect of humidity on formation of pulsed streamers and other properties.

Boltzmann kinetic equation is numerically solved for electrons, by using generally available Boltzmann solver BOLSIG+. We have chosen two datasets from the LXCat database and from the Quantemol data base without implying that those are the best available sets and comparisons between electron energy distribution functions and rate coefficients are presented. We have selected these two sets as possible foundations for our global modeling of atmospheric pressure plasma jets or other non-equilibrium (cold) plasmas. This is thus the first step towards testing the Quantemol data set as the sole basis for a complex global model.

In the case of helium, Morgan database set is stated to be complete, since it includes cross section for momentum transfer, excitation, total excitation and ionization normalized by the swarm procedure. Differences in results obtained using the Quantemol set are mainly caused by the inappropriate use of the cross section for elastic scattering without added anisotropy to represent properly the momentum transfer in transport. In such a case one may be tempted to assume isotropic scattering for all collisions. We suggest that in absence of explicit verified anisotropy it would be better to use momentum transfer cross section obtained in a swarm analysis. Even for the codes that do not employ momentum transfer but use total elastic cross section one needs to include the differential scattering (and/or to test the set by performing a swarm analysis).

In the case of water, it is stated at LXCat that Morgan database does not include explicitly cross sections for rotational transitions (it uses CARS approximation). Thus it should not be used for calculations by BOLSIG+ without adding the contribution of rotational scattering. Quantemol database includes cross sections from Itikawa's set which contains first four rotational transitions. One should be warned that it may become necessary to include many more rotational transitions to cover the range of thermal energies which may populate several rotational states. In addition, superelastic rotational processes need to be included.

Results presented in this work indicate that the differences between EEDF and rate coefficients obtained from Morgan and Quantemol sets are mainly caused by the differences in momentum transfer cross section, probably induced by the cross section for

rotationally elastic scattering in Itikawa database. Furthermore, Morgan's cross section data for electron impact water dissociation in OH(X) state is appreciably lower than in the Itikawa case. Since this process is stated in the literature as the main production channel for OH radicals, one should be warned to check for the best source of data for this process based on some independent test.

On the other hand water vapour is present in such plasma in small quantities (as a small percentage of the air that is mixed into helium plasma with abundances of few percent). Thus uncertainties in the cross sections should not prevent one from using either of the two sets as the basis for the global model, provided that transport in helium is dealt with accurately.

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**POREĐENJE SETOVA PRESEKA IZ BAZA QUANTEMOL I
MORGAN LXCAT I KOEFICIJENATA BRZINE ZA PROCESSE
RASEJANJA ELEKTRONA NA NEUTRALIMA:
HELIJUM I VODENA PARA**

U radu je prezentovano poređenje setova preseka za rasejanje elektrona na atomu helijuma i molekulu vodene pare u osnovnom stanju, dostupnih u bazi LXCat Morgan i novijoj bazi Quantemol-DB. Ovi setovi preseka su iskorišćeni kao ulazni parametri za numeričko rešavanje Bolcmanove jednačine primenom Bolcman-solvera BOLSIG+, u cilju određivanja transportnih koeficijenata, funkcije raspodele elektrona po energiji i koeficijenata brzine za procese rasejanja elektrona. Izvršeno je poređenje izračunatih koeficijenata u cilju ispitivanja kvaliteta i kompletnosti seta preseka dostupnih u bazi Quantemol za potrebe modelovanja niskotemperaturnih plazmi i interpretacije eksperimentalnih rezultata.

Ključne reči: presek, funkcija raspodele elektrona po energiji, koeficijent brzine