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RESEARCH PAPER

Properties of Electron Swarm Parameters in Tetrahydrofuran

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A B S T R A C T:
Reported electron collision cross sections data in the energy range ~ 0 to 300 eV from gaseous biomolecule Tetrahydrofuran (THF) have been used to calculate the electron energy distribution function (EEDF) and swarm parameters for electrically excited of THF, using a two-term solution of the Boltzmann equation. The electron swarm parameters namely (mean energy, drift velocity, diffusion coefficient, electron mobility, characteristic energy, attachment and ionization coefficient), at room temperature and atmospheric pressure are presented over a wide range of applied electric field strength E/N (E is the electric field and N is the gas number density) varying from 0.1 Td to 1000 Td (1Td = 10^{-17} Vcm^2). The EEDF found to be non-Maxwellian. The electron swarm parameters are compared with those calculated using multi term kinetic theory and experimentally using the pulsed Townsend technique. The influence of inelastic cross section on the calculated transport parameters is also explained.

KEY WORDS: THF, swarm parameters, cross sections, kinetics, electron Boltzmann equation.
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1.INTRODUCTION :

High-energy ionizing radiation e.g., α-particles, protons, heavy ions, γ-rays, and X-rays, use in radiotherapy and radiodiagonistic exams, when incident the biomolecule model systems or living cells leads to loss genetic information, cell death and genetic mutation (Hall and Giaccia, 2018) by secondary electrons when the energy of low-energy electrons (LEEs) below 20 eV, it can induce damage to DNA. (Martin et al., 2004) show that the low-energy electrons (LEEs) induce damage in DNA, as well as to basic DNA components such as bases (Abdul-Carime et al., 2004), deoxyribose sugar (Ptasinska et al., 2004) and the phosphate group (Elahe-Alizadeh et al., 2015; Pan and Sanche, 2005) via the formation of negative ions or resonances, these processes occurs via dissociative electron attachment (DNA).

The interaction of positron with biological matter and human tissue is important key for the medical field, in fact as the electron and positrons are thermalize in biological matter and human tissue, the annihilation γ-rays emitted by annihilation of two particles such technique used in imaging application called positron emission tomography (PET) (Cherry et al., 2003). Furthermore, the interaction of electrons with water is important to study the behavior of biomolecules, water vapour used as a replacement for the bimolecular in process of radiolysis tracks (Muñoz et al., 2008). Tetrahydrofuran molecule (THF, C_4H_8O), or oxolane, is the most best matter in gas phase used to study the biomolecules matter after water (Stokes et al., 2020), can be viewed as a sugar-like component of the backbone of DNA. The backbone of DNA consists as a series of Tetrahydrofuran (THF) molecules held together by phosphate bonds, also Tetrahydrofuran (THF) is an important component of RNA (Thiemer et al., 2003).

More recently, Tetrahydrofuran has been investigated experimentally and theoretically to understanding the low energy electron collisions

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and the dynamic of energy deposition in DNA (White et al., 2018; White et al., 2014; White et al., 2014a), For plasma interaction with biological matter, the electron collision cross sections play the important role to study the electron transport parameters in gaseous systems. Several electron collision cross sections have been measured experimentally and derived theoretically for Tetrahydrofuran. These includes, six full sets of Tetrahydrofuran (THF) cross sections (momentum transfer, vibrational excitation, electronic excitation ionization and attachment cross sections) have been proposed experimentally and theoretically over various electron energy ranges: by (Garland et al., 2013) for electron incident energies between 0.1 eV to 300 eV, (Fuss et al., 2014) for electron incident energies from 1 eV to 10KeV, (Bug et al., 2017) for energies ranging from 30 eV to 1000 eV, (Swadia et al., 2017, 2017a) for electron energies between the ionization threshold to 5000 eV, and (Casey et al., 2017) modified the (Garland et al., 2013) cross-section sets by the first measurement of electron swarm parameters in pure gaseous Tetrahydrofuran (THF), using inverse swarm method. Thereafter, (de Urquijo et al., 2019) who refined the (Casey et al., 2017) cross-section sets by performing and analyzing the swarm parameters of THF-Ar and THF-N_2 mixtures.

The swarm parameters have a long history from the early studies (Frost and Phelps, 1962; Engelhardt and Phelps, 1964; Engelhardt, et al., 1964; Huxley and Crompton, 1974) to more recent investigation (Šaši´c, et al., 2013; Deng and Xiao, 2014). Theoretically swarm parameters may be calculated using Monte Carlo Simulation or Boltzmann equation analysis using electron energy distribution function (EEDF) with the available sets of cross sections. The EEDF calculated by the electron energy gain and loss due to acceleration with electric field and electrons collision (Itikawa, 2007).

The electron swarm parameters of THF, namely, drift velocity, electron mean energy, ionization and attachment coefficients, are widely studied in the literature (Garland et al., 2013; Duque et al., 2015; Casey et al., 2017). These swarm parameters are also calculated in THF-H_2O (White et al., 2014) and THF-Ar and THF-N_2 (Wolff et al., 2019) gas mixtures. More recently, the binary mixtures of THF-Ar are studied by (Stokes et al., 2020).

In the present work we have calculated the electron swarm parameters of Tetrahydrofuran (THF) at room temperature based on the two term solution of Boltzmann transport equation that is solved for values of E/N ranging from 0.1 Td to 1000 Td using the NOMAD code (Rockwood and Greene, 1980).

2. The Boltzmann equation

The basic of Boltzmann transport equation used in this study is given as (Frost and Phelps, 1962,

$$\frac{E^2}{3}\frac{d}{du}\left(\frac{u}{NQ_m^e(u)}\frac{df_0(u)}{du}\right)+\frac{2m}{M}\frac{d}{du}\left(u^2NQ_m^e(u)f_0(u)\right)$$
$$+\frac{2mK_BT_g}{Me}\left(u^2NQ_m^e(u)\frac{df_0(u)}{du}\right) \qquad (1)$$
$$+\sum_J\left[(u+u_J)f_o(u+u_J)N_oQ_J(u+u_J)-uf_o(u)N_oQ_J(u)\right]$$
$$+\sum_J\left[(u-u_J)f_o(u-u_j)N_JQ_{-J}(u-u_J)-uf_o(u)NQ_{-J}(u)\right]=0$$

Here,

$$Q_m^e(u)=Q_m(u)+\sum_J Q_J(u)+Q_i(u)+Q_a(u) \qquad (2)$$

Where $Q_m^e(u)$ denotes an effective collision frequency for momentum transfer, M, K_B, E, u, N are the molecular mass, Boltzmann constant, applied dc electric field, electron energy and the gas density respectively, T_g is gas temperature, $Q_m(u)$ is the momentum transfer cross-sections related to the total cross section $Q_m(u)= Q_T(u)(1-\cos\theta)$, θ is scattering angle (Lucas, et al., 1973). $Q_J(u)$, $Q_i(u)$, $Q_a(u)$ are the electron cross sections for excitation (rotational, vibrational, electronic), ionization, and attachment respectively, and u_j is

the energy loss due to collisional excitation. The last two term is the influence of superelastic collision it occurs at low electric field, $Q_{-J}(u)$ is superelastic cross-section, u_J energy gain due to superelastic collision. The superelastic cross-section Q_{-J} can be written as (Mitchel and Zemansky,1971),

$$Q_{-J} = \frac{u+u_J}{u} Q_J(u+u_J) \quad (3)$$

The initial electron energy distribution function EEDF with a mean electron energy $\bar{u} = 1.5K_BT_e$ was chosen as Maxwellian with temperature T_e (Nighan, 1970),

$$f(u) = \left(\frac{2}{\sqrt{\pi}}\right)(K_BT_e)^{\frac{-3}{2}} \exp\left(\frac{-u}{K_BT_e}\right) \quad (4)$$

Using the electron energy distribution function one can calculate the electron swarm parameters as follows (Othman, et al., 2019; Hagelaar and Pitchford, 2005; Nakamura and Lucas, 1978) where the electron energy distribution function $f(u)$ obeys to the normalization condition,

$$\int_0^\infty f(u)\sqrt{u}du = 1 \quad (5)$$

The mean electron energy,

$$\bar{u} = \int_0^\infty u^{\frac{3}{2}} f_o(u)du \quad (6)$$

The density-normalized electron mobility μ_e

$$\mu_e N = -\frac{1}{3}\left(\frac{2e}{m}\right)^{1/2}\int_0^\infty \frac{u}{Q_m^e(u)}\frac{df_o(u)}{du}du \quad (7)$$

The electrons drift velocity,

$$v_d = \mu E \quad (8)$$

The density-normalized transverse diffusion coefficient,

$$D_T N = \frac{1}{3}\left(\frac{2e}{m}\right)^{1/2}\int_0^\infty \frac{uf_o(u)}{Q_m^e(u)}du \quad (9)$$

The characteristic energy u_k,

$$u_k = \frac{D_T e}{\mu_e} \quad (10)$$

The reduced-density ionization coefficient α/N is given by (Othman, et al., 2020; Morgan and Penetrante, 1990; Láska, et al., 1984)

$$\frac{\alpha}{N} = \frac{1}{v_d}\left(\frac{2e}{m}\right)^{1/2}\int_i^\infty Q_i(u)uf_o(u)du \quad (11)$$

where $Q_i(u)$ is the ionization cross-section.

The reduced-density attachment coefficient η/N is given by:

$$\frac{\eta}{N} = \frac{1}{v_d}\left(\frac{2e}{m}\right)^{1/2}\int_a^\infty Q_a(u)uf_o(u)du \quad (12)$$

where $Q_a(u)$ is the attachment cross-section.

Electron swarm parameters were calculate using collision cross section for a THF vapour number density N=7.3765x10^{21} cm^{-3}, which is equivalent to 1 atm at 298 K.

3. Cross Section

The electron energy distribution function (EEDF) and electron swarm parameters in gaseous Tetrahydrofuran (THF, C_4H_8O) was calculated from the sets of cross section (elastic and inelastic) this sets includes 21 collision processes: one momentum transfer cross section (Q_m) taken from (Trevisan, et al., 2006; Garland, et al., 2013; Casy, et al., 2017 and Stokes, et al., 2020), 12 vibration excitation (Q_{v1}, Q_{v2}, Q_{v3}, Q_{v4}, Q_{v5}, Q_{v6}, Q_{v7}, Q_{v8}, Q_{v9}, Q_{v10}, Q_{v11}, Q_{v12}) with threshold energy 0.228, 0.72 0.114, 0.134, 0.18, 0.363, 0.45, 0.65, 0.15, 0.083, 0.27 and 0.330 eV respectively are taken from (Duque, et al., 2015) and six electronic excitation cross sections of (Garland, et al., 2013) have been used based on the energy loss spectra of (Do, et al., 2011). The attachment cross sections of (Stokes, et al., 2020) have been used, these lies between the values of (Garland, et al., 2013) and the values of (de Urquijo, et al., 2019) with threshold energy of 0.28 eV, lying between the threshold energy of 1 eV for (Garland et al., 2013) and 0.08 eV for (de Urquijo et al., 2019). The ionization cross sections with threshold energy 0.955 eV of (Garland, et al., 2013) have been used, and these cross-sections are in good agreement with (Mozejko and Sanche, 2005), (Fuss, et al., 2009) and (Dampc et al., 2011).

4. Results and Discussion

To solve the electron energy distribution function (EEDF) which was based on the two-term solution of Boltzmann equation, the data of electron collision cross-sections of THF is explained in previous section, used as main input data to calculated electron swarm parameters.

The electron energy distribution function EEDF as function of electron energy, are obtained by using two-term approximation solution of Boltzmann equation method (Eq. 1) at different values of electric field strength E/N (E: electric field, N: gas number density) electric field strength E/N, expressed in unit of Townsend.

The calculated electron energy distribution function EEDF for a dc field in THF at different values of E/N at temperature 298 K and pressure 1 atm are shown in figure 1. It is found that at lowest electric field strength E/N, the electron energies are thermal and the electron energy distribution function EEDF is Maxwellian as shown in equation 4 with mean electron energy $\bar{u} = 1.5K_B T_e$, the Maxwellian distribution function normalized by equation 5 where T_e is electron temperature in unit of eV. At E/N<20 Td, EEDF drops sharply after several (eV) the Maxwellian function's will appear as straight lines, because the elastic cross-section is constant at low electric field and the vibrational cross section increases around 0.1 eV and decrease when electron energy greater than 1 eV. Therefore, in this region the degree of ionization is very small and the energy created from electric field is mainly used for vibrational excitation. However, as the E/N is increased the EEDF located at higher energy range, the EEDF is clearly non-Maxwellian, and has a shoulder at about 2 eV when E/N≥20 Td, due to the large electronic excitation and vibrational cross-section. The tail of the distribution function shift to higher energy due to inelastic collision which reflects the dominant electron-molecule energy exchange processes in this region more ionization or excitation collision occurs.

Figures 2-8, present results for electron swarm parameters in THF, including mean energy, drift velocity, diffusion coefficient, mobility, ionization and attachment coefficient. The results presented are calculated and analyzed using two-term solution of the Boltzmann equation by a balance between power input from an applied electric field E and energy loss rate via electron collisions. All results are calculated as a function of the reduced electric field E/N over a wide range varying from 0.1Td to 1000 Td, (1 Td = 10^{-17} Vcm^2) at fixed temperature 298 K and pressure 1 atm. Figure 2 demonstrated mean electron energy as a function of E/N, at low electric field strength E/N>10 Td the mean energy is in thermal equilibrium, it is essentially isotropic remain nearly constant, as we move to higher field the mean energy rapidly increases with increasing E/N, this is because at high energy region the inelastic processes are dominated. The behavior of the mean electron energy is also reflected in the electron drift velocity and diffusion coefficient. It is seen the present calculation agree well with the

theoretical values of (Garland, et al., 2013; White, et al., 2014) and (Duque, et al., 2015).

The present values of drift velocity for THF are shown in figure 3, the previous experimental values of (Casey, et al., 2017; de Urquijo, et al., 2019) and theoretical values of (Stokes, et al., 2020) are displayed in the same figure. A good agreement has been shown over the entire range of E/N. It is evident that the experimental data of (Casey, et al., 2017) fall below present results, the difference is up to about 15% over the range of E/N<40 Td. As shown in this figure, the calculated drift velocity in thermal equilibrium with background THF vapor from 0.1 Td to 10 Td linearly increase, where elastic and vibrational collision are dominating. Around 20 Td to 40 Td a plateau in the drift velocity is observed due to the effect of the electronic excitation. At high reduce electric field strength E/N>100 Td the ionization channel is dominate, the drift velocity increase up to the highest calculated value at 1000 Td.

The reduced transverse diffusion coefficient D_TN for pure THF vapor as function of E/N values is shown in figure 4. The present calculation was found in good agreement with theoretical values of (Garland, et al., 2013) and (White, et al., 2014). The normalized reduced electron mobility μ_eN is shown in figure 5, at low E/N values the electron mobility is in thermal equilibrium, when E/N is around 30 Td, a maximum values can be observed, then the electron mobility start to decrease with increasing E/N, because at E/N>30 Td the attachment coefficient decrease the number of electrons. The behavior of characteristic energy eD_T/μ_e displays in figure 6.

Figure 7 is illustrated the reduced-density attachment coefficient η/N in THF as a function of E/N values, in comparison with the experimental values of (Casey, et al., 2017) and (de Urquijo, et al., 2019), as well as the theoretical values of (Stokes, et al., 2020). Throughout the range of $5 \leq E/N \leq 100$ Td, good agreements have been observed. At low reduced electric field, E/N<20 Td the electronegative region observed, in this region the reduced attachment coefficient decreasing with increasing E/N until approximately 30 Td, the resonance region appear at around 40 Td, then start to increase up to 70 Td, again start to decrease, around 100 Td the ionization channel dominated. This is because around 20.5 eV a large increase in the magnitude of the dissociation electron attachment DEA observed approximately equal to 0.0033×10^{-16} cm^2 (Garland, et al., 2013). The reduced-density ionization coefficient α/N in THF as a function of E/N values is shown in figure 8. The present values are compared with the theoretical values of (Stokes, et al., 2020) and with the measured values of (Casey, et al., 2017; de Urquijo, et al., 2019). Throughout the range of $100 \leq E/N \leq 1000$ Td, the theoretical results of (Stokes, et al., 2020) and experimental results of (Casey, et al., 2017) slightly lower compare with the present results. The coherent results obtained confirmed that two-term solution of Boltzmann equation analysis of the present study is valid.

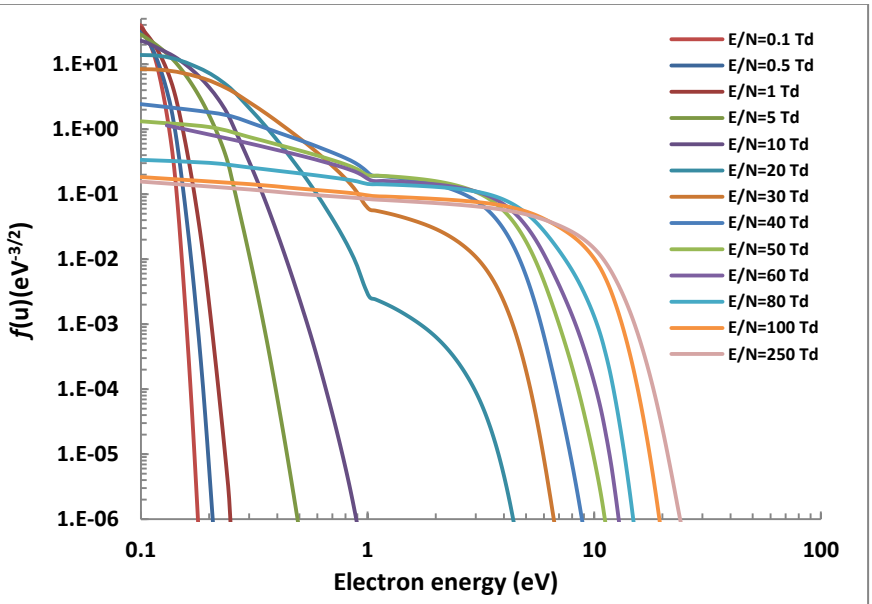

Figure 1. The electron energy distribution function for the THF.

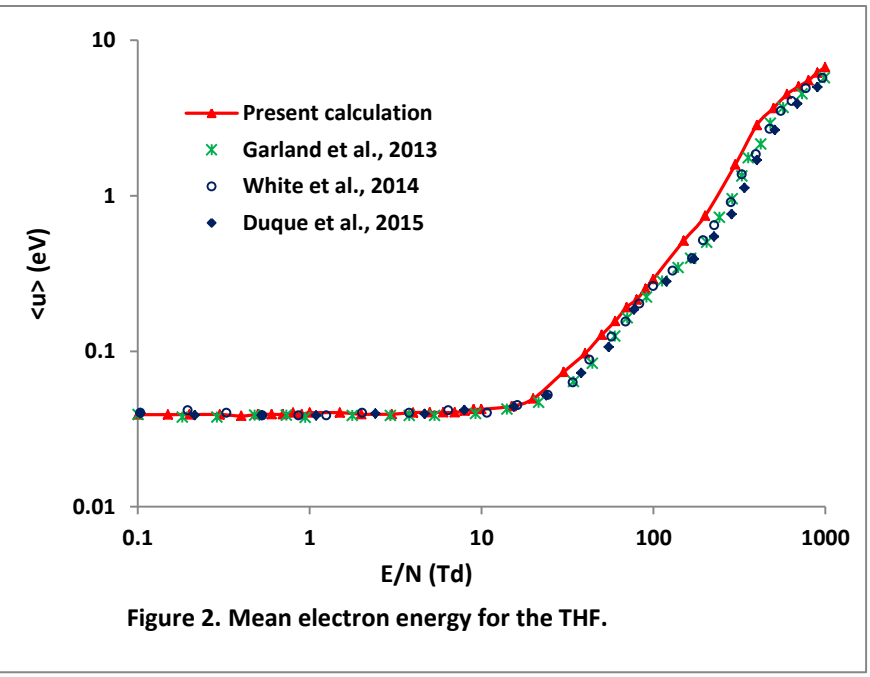

Figure 2. Mean electron energy for the THF.

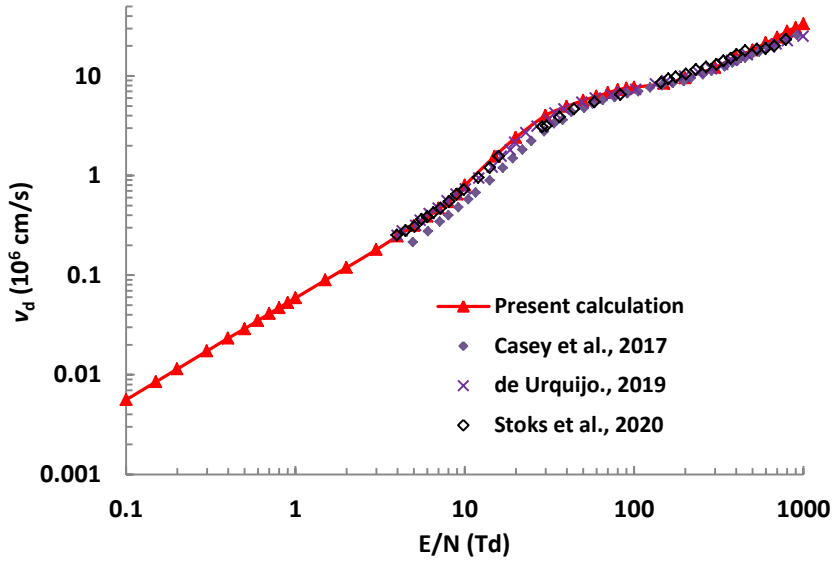

Figure 3. Electrons drift velocity for the THF.

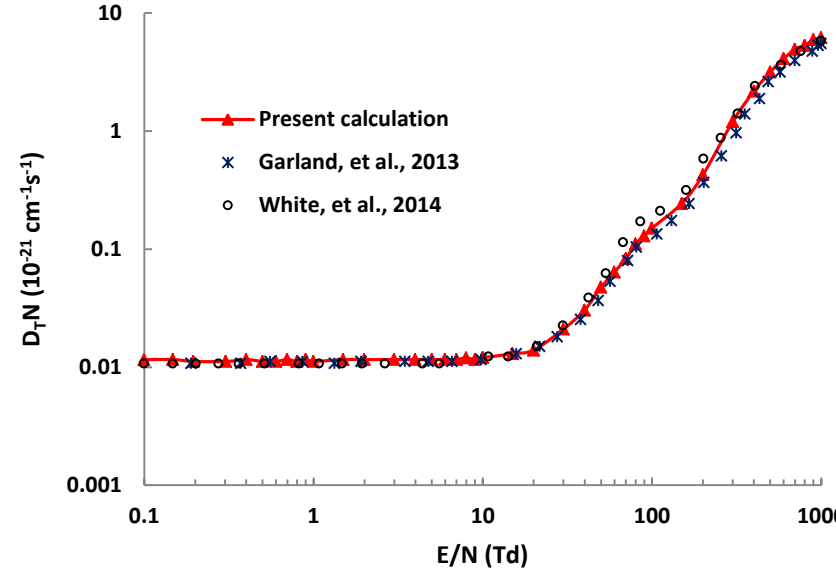

Figure 4. Reduced transverse diffusion coefficient for the THF.

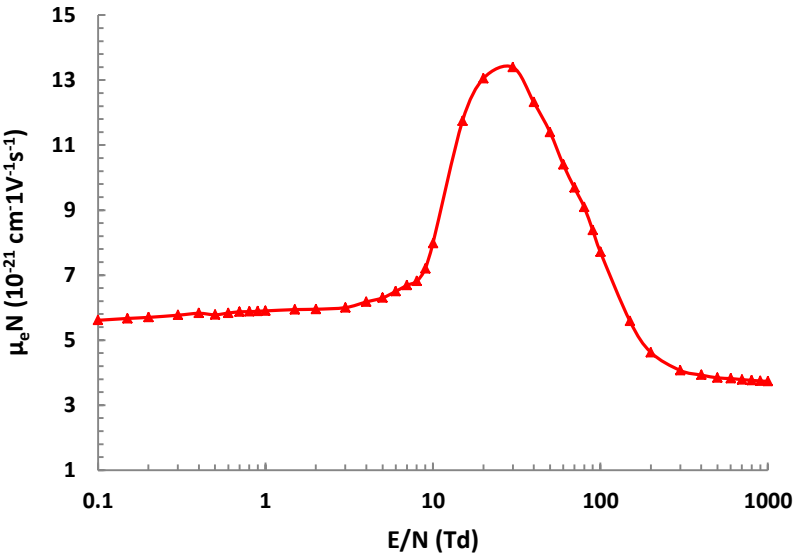

Figure 5. Reduced electron mobility for the THF.

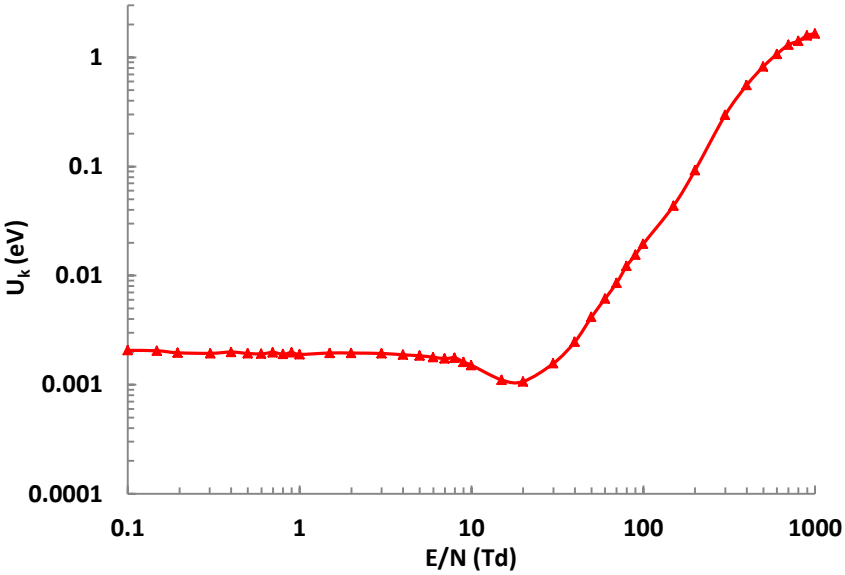

Figure 6. Characteristic energy for the THF.

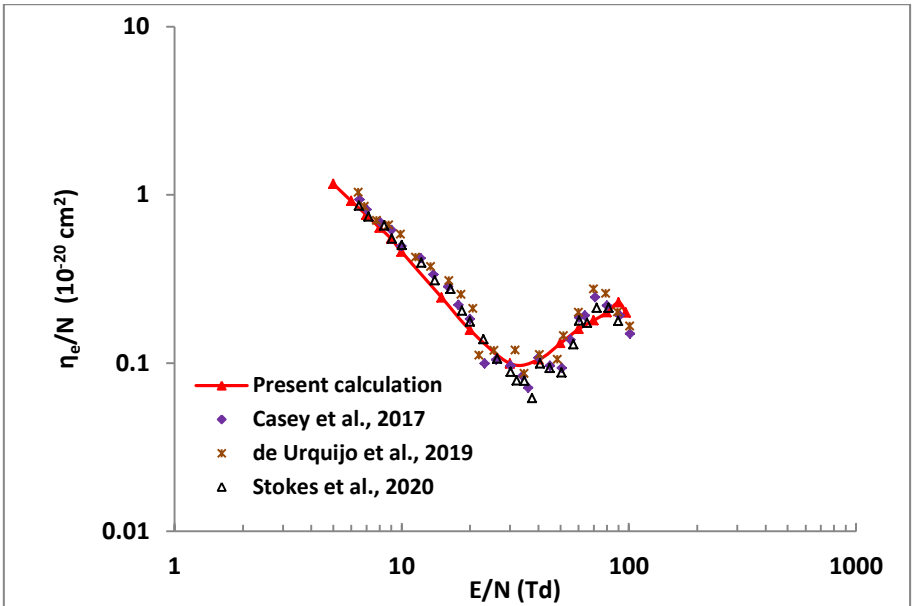

Figure 7. Reduced attachment coefficient for the THF.

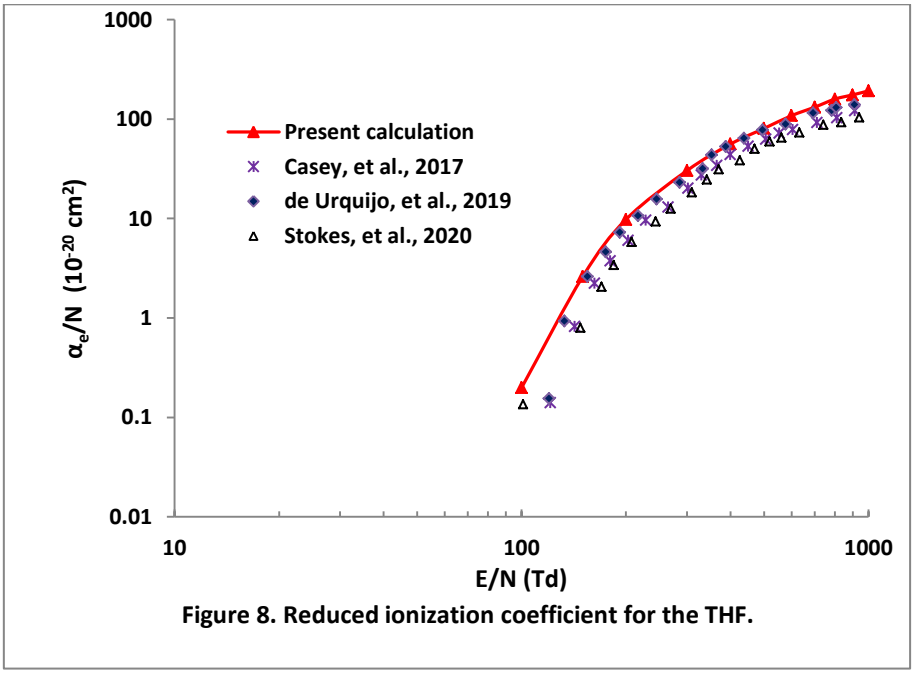

Figure 8. Reduced ionization coefficient for the THF.

5. Conclusion

In the present work, we have examined the behavior of electrons in applied uniform dc electric fields as a function of reduced electric field strength E/N. The two-term solution results give values for EEDF and mean energy, drift velocity, transverse diffusion coefficient, electron mobility, characteristic energy, attachment and ionization coefficient as a function of E/N in the range between 0.1 Td to 1000 Td. These results were obtained based on binary collisions of electrons with THF molecule. A good agreement between the calculated and previous theoretical and experimental values is observed.

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