Evaluation of Cross Section for Electron Impact with hydrogen/helium and Their Combination Molecules in Fusion Plasma

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1. Based on previous research for H₂, D₂, HD (experimental data)
   - Cross sections for electron collisions with hydrogen molecules
   - Electron impact cross sections for deuterated hydrogen and deuterium molecules
     Report on Progress in Physics, 73, 116401 (2010)
   + Electron impact cross sections of vibrationally and electronically excited diatomic molecules
   + Theoretical and experimental data survey
   + Evaluation (only experimental data)

2. Making general data evaluation procedures
   - organized several evaluation meeting → how to evaluate data
   - Still working
Total and elastic scattering and momentum transfer CS

- Cross section data are available for electron-impact elastic scattering collisions in the case of D$_2$ and HD at low electron energies only.
- The elastic momentum transfer cross sections for the two molecules where no measurements have been reported.
- However, cross sections for some inelastic processes for these molecules are available in the literature.

- Absolute elastic scattering cross sections have been measured by Ferch for H$_2$, D$_2$, and HD molecules in the energy range 0.02 – 2 eV.
- The measurements were made with an electron TOF spectrometer and the isotopes H$_2$, D$_2$ and HD were found to have identical cross sections within the uncertainty of $\pm$2% for H$_2$ and D$_2$ and $\pm$2.5% for HD.

The elastic electron scattering cross sections for H\textsubscript{2} and D\textsubscript{2} have also been measured by Golden et al, as a function of electron-impact energy from 0.25 to 15 eV with an estimated uncertainty of ±3%.

Within the experimental uncertainty, the H\textsubscript{2} and D\textsubscript{2} cross sections were found to be identical.

Golden D E, Bandel H W and Salerno J A 1966 *Phys. Rev.* **146** 40

- Momentum transfer cross section for H$_2$ and D$_2$ from near 0 to 2 eV electron energy (by Engelhardt and Phelps (Frost and Phelps))
- The cross sections for the two molecules were found to be identical within the stipulated experimental uncertainty.
- The well-validated momentum transfer cross sections for H$_2$ by Elford at electron energy from 0.01 to 100 eV have been adopted for HD and D$_2$ molecules.

Engelhardt A G and Phelps A V 1963 Phys. Rev. 131 2115,
Rotational, vibrational and electronic excitation

- The rotational excitation cross sections for J=0 to J=2 and J=1 to J=3 and vibrational excitation cross sections for the v=0 to v=1 and v=0 to v=2 transitions for H_2 and D_2 have been compiled by Buckman and Phelps.

  Buckman S J and Phelps A V 1
  985 J. Chem. Phys. 82 4999 (1985)

- The electronic excitation cross sections are the same for H_2 and its isotopomers.

- The electronic excitation cross sections for b^3Σ_u^+ and a^3Σ_g^+ states of H_2 have been compiled by Yoon.


At higher electron energies, the dissociation cross sections computed by Celiberto, for H$_2$ and D$_2$ *(Chem. Phys. 133 355, 1988, At. Data Nucl. Data Tables 77 161, 2001) are the only ones available in the literature.

In the absence of any other data, it is difficult to recommended the cross section values at these electron energies.
The total electron-impact ionization cross sections for HD have not been reported in the literature so far, only D₂

Experiment
- Buckman S J and Phelps A V Joint Institute for Laboratory Astrophysics Information Center Report 27 p 1 (1985)

Theory

The electron-impact ionization cross sections for D₂ as reported by Rapp and Englander-Golden.
Dissociative electron attachment

\[
e^- + H_2, D_2(v, J) = (H_2^-, D_2^-) \\
e^- + HD(v, J) = (HD)^- = H + D^- \\
= D + H^-.
\]

- Schematically, the dissociative electron attachment process for \(H_2, D_2,\) and HD target molecule written as a two-step process
- There are three main dissociative electron attachment processes occurring at low electron-impact energies

1. Known as 4 eV process has a threshold at 3.73±0.07 and proceeds through the attractive potential of lowest \(X^2\Sigma_u^+\) resonant \(H_2^-, D_2^-, HD^-\) state.
2. Proceeds between 5 and 13 eV electron-impact energy through the repulsive state \((^2\Sigma_g^+)\) of the respective negative ions.
3. Known as 14 eV process with the threshold around 13.9 eV proceeds through another attractive resonant state of \(^2\Sigma_g^+\) symmetry.

- The electron-impact dissociative attachment cross sections for negative ion formation in \(H_2, D_2,\) and HD in the 8-18 eV energy range region after subtracting background.
- More detail information is given Rep. Prog. Phys. 73, 116401 (2010)
Summary (H₂, D₂, HD)

- All efforts have been made to compile almost all(?) data whatever available in the literature and subsequently evaluate and validate the same.
- Therefore, the present work should serve as a complete update for e + D₂ and e + HD collisions at different electron-impact energies.
- But unfortunately there is a paucity of data for both HD and D₂ molecules, more particularly for HD.
- As a result, the electron-impact cross sections for some of the different processes for these molecules could not be reviewed in this paper. This has left us with a partially incomplete picture of the subject.

①  Total and elastic scattering and momentum transfer cross sections
②  Rotational, vibrational and electronical excitation
③  Emission cross section
④  Dissociation
⑤  Ionization
⑥  Dissociative electron attachment
Summary (H₂, D₂, HD)

- To obtain a real comprehensive picture, the following few problems have to be addressed in the near future:

1. Total electron-impact scattering cross sections (elastic + inelastic) have not been measured so far for both HD and D₂ molecules. Such measurements using the latest technology are required at all electron energies from 0 to 1000 eV.
2. The rotational and vibrational excitation cross sections for D₂ reported in the literature are the old sets of measured values. Also, such cross sections are not available for HD molecules at all. These cross sections need to be measured again using a new technique.
3. No measurements for the appearance energies of HD⁺, H⁺ /HD and D⁺ /HD are available. Also, total electron-impact ionization cross sections for HD molecules have not been reported in the literature.
4. The absolute dissociative electron attachment cross sections for HD and D₂ molecules at 300 K and at higher temperatures in the case of the 4 eV process have been measured earlier but have been found in uncertainty estimation. So, these need to be measured again. Also, no effort has been made to measure these cross sections at higher temperatures for the 8 and 14 eV processes.
In the Second RCM, Vienna, 03-05 July 2013,

Proposal

Electron-Impact Cross sections of vibrationally and electronically excited diatomic molecules (H\textsubscript{2}, D\textsubscript{2}, N\textsubscript{2}, O\textsubscript{2}, Cl\textsubscript{2}, F\textsubscript{2}, I\textsubscript{2})

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Proposal

The electron impact studies of ground state molecules have been extensively carried out, both experimentally and theoretically, since the last few decades. However, work on excited states has been initiated in the relatively recent past. Also, there is paucity of experimental data in this field in spite of the recent technological developments achieved at various stages of electron-collision experiments. Interest in the subject has also grown tremendously because of its applications in many scientific disciplines and semiconductor and other related industry. The main reason for experimental data being scarce in this field is the difficulty of producing sufficiently large number of molecules in excited states under controlled conditions. Also, in many situations, it is required to produce excited molecules in large numbers in well-characterized and precisely defined states. This was not possible previously as the vibrational/rotational levels in the same electronic state are closely spaced. Over and above, dissociation and pre-dissociation, especially in the case of polyatomic molecules, create additional problems like depletion of excited state populations. But fortunately, with the advent and availability of high-powered tuneable pulsed lasers, the situation has considerably improved.
Electron impact cross sections of vibrationally and electronically excited molecules

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ABSTRACT

It is well known that the electron impact cross sections for elastic and inelastic processes for the vibrationally and electronically excited molecules are predominantly different than those for molecules in the ground state. Collisions of low energy electrons with excited molecules play an important role in explaining the behavior of gas discharges in laser and plasma physics, in planetary atmospheres, stars, and interstellar medium and in plasmas widely used in the fabrication of microelectronics. This explains as to why there is a need for having validated sets of electron impact cross sections for different processes. This work reviews the subject of electron collisions with vibrationally and electronically excited molecules in a comprehensive way. The survey has been carried out for a few excited molecules such as H2, D2, T2, HD, HT, DT, N2, O2, and CO2.

This review includes the discussion on the methods to produce and detect vibrationally and electronically excited molecules. We will take up the cross section data available in the literature for such molecules on electron scattering, dissociation, ionization and attachment processes and will discuss, evaluate and well-validate the same wherever and whenever possible.

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Cross section for $O$ excited targets than for the ground state molecules. Again, the threshold energy of these cross sections is much lower for molecular oxygen in the ground and low-lying singlet states

been related with the size of the target at each vibrational level. Also, the ionization cross sections of vibrationally excited

measurements.

methods, both thermal and super-thermal excited molecules in the rovibrational and electronic states can be produced

and electron beam excitation. Electric discharges (DC, RF or microwave), both transverse or coaxial, and laser beams,

considerably improved.

state populations. But fortunately, with the advent and availability of high powered tunable pulsed lasers, the situation has

not possible previously as the vibrational/rotational levels in the same electronic state are closely spaced. The dissociation

it is required to produce excited molecules in large number in well-characterized and precisely defined states. This was

stages of electron-collision experiments. The main reason for experimental data being scarce in this field is the difficulty

Acknowledgment
After the publication of JPCRD90, a few comprehensive experimental measurements of the excitation cross section of $\text{H}_2$ have been reported. Considering the results of those measurements, the evaluation of the cross section data was made to revise the cross sections reported in JPCRD90 for $b^3\Sigma_u^+$, $a^3\Sigma_u^+$, $c^3\Pi_u$, $B^1\Sigma_u^+$, $C^1\Pi_u$, $E$, $F^1\Sigma_g^+$, and $e^3\Sigma_u^+$. For other states, no substantially new information is available.

(JPCRD90) H. Tawara, Y. Itikawa, H. Nishimura, and M. Yoshino,

(JPCRD08) J. S. Yoon and et. al.,
Three different EELS measurements have been reported for the excitation of the $B^1\Sigma_u^+$ state. The experiment by Srivastava and Jensen\textsuperscript{43} is too old and the result of Khakoo and Trajmar\textsuperscript{23} is superseded by a new measurement of the same group.\textsuperscript{40} Liu \textit{et al.}\textsuperscript{44} derived $Q_{\text{exc}}$ from their measurement of the $B$-$X$ emission. They took much care about possible cascade effects and normalized their cross sections with the optical oscillator strength at the high-energy limit. The resultant $Q_{\text{exc}}$ of Liu \textit{et al.} agrees very well with the corresponding cross section obtained from the EELS measurement by Wrkich \textit{et al.} (Fig. 11). We take the result of Liu \textit{et al.} as the recommended values for the excitation (shown in Table 8). They estimated the errors of their cross sections to be $\pm (15-25)\%$ for 20–500 eV of electron energy, $\pm (7-15)\%$ for the energies above that, and $\pm 30\%$ for the energies below 20 eV.

We have the same situation for the excitation of the $C^1\Pi_u$ state as for the $B^1\Sigma_u^+$ state (Fig. 12). That is, we take the result of Liu \textit{et al.}\textsuperscript{44} for the recommended cross sections for the $C^1\Pi_u$ state (shown in Table 8).
Summary (H₂)

1. total scattering cross section
2. elastic scattering cross section
3. momentum transfer cross section
4. rotational cross section for the transition \( J=0 \rightarrow 2 \)
5. Vibrational cross section for the transition \( v=0 \rightarrow 1 \)
6. A few representative cross sections for the excitation of electronic states (i.e., the excitations of \( b^3 \Sigma_u^+, B^1 \Sigma_u^+, E, F^1 \Sigma_g^+ \) states)
7. Dissociation cross sections
8. Total ionization cross sections
9. Ionization cross section for the production of \( H^+ \)
Appendix ($H_2$)

- Electronically excited states (except for metastable one) of hydrogen molecules rapidly decay to the lower states by emission of radiation.
- For an application of detailed collisional-radiative model, however, information on the rate of collisional transition between those excited states is needed.
- All the experimental cross sections are summarized. On the other hand, extensive effort has been spent on obtaining theoretical cross sections for the vibrationally or electronically excited targets.
- Since no corresponding experimental results are available, it is very difficult to evaluate the accuracy of those theoretical cross sections.
- For this reason, we do not make any recommendation on the cross section for the hydrogen molecules in their excited states.
- Instead we simply give here a list of those theoretical papers reporting cross sections for excited targets.
- Electron-impact dissociative attachment of $H_2$ has a peculiarity. Cross sections for the process strongly depend on the vibrational state of the target.
- Very extensive theoretical studies have been made for the process. The following list does not include the papers concerning the dissociative attachment process.

12.1. Collisions with vibrationally excited $H_2$ (in its ground electronic state)

Papers on the dissociative attachment are not included; see Sec. 10.

(i) $H_2(X,v) \rightarrow H_2^*(n) \rightarrow H+H$

$n=I^1\Sigma_u^+, C^3\Pi_u, B^1\Sigma_u^+, D^1\Pi_u, B'^1\Sigma_u^+, D'^1\Pi_u,$

$n=b^3\Sigma_u^+ (\text{Ref. 63})$

(ii) $H_2(X,v) \rightarrow H_2^*(n)$

$n=B^1\Sigma_u^+, C^3\Pi_u, B^1\Sigma_u^+, D^1\Pi_u, B'^1\Sigma_u^+, D'^1\Pi_u$ (Ref. 63)

(iii) $H_2(X,v) \rightarrow H_2^*(n) \rightarrow H+H^+$

$n=X^3\Sigma_g^+ (\text{Ref. 63})$

(iv) $H_2(X,v) \rightarrow H_2^*(n) \rightarrow H_2(X,v') + h\nu$

$n=B^1\Sigma_u^+, C^3\Pi_u (\text{Ref. 63})$

(v) $H_2(X,v) \rightarrow H_2^*(n) \rightarrow H+H+h\nu$

$n=B^1\Sigma_u^+, C^3\Pi_u (\text{Ref. 63})$

(vi) $H_2(X,v) \rightarrow H_2(X^2\Sigma_u^+) \rightarrow H_2(X,v')$ (Ref. 68)

12.2. Collisions with electronically excited $H_2$

(i) $H_2^*(B^1\Sigma_u^+,v) \rightarrow H_2^*(n) \rightarrow H+H$

$n=I^1\Pi_u (\text{Ref. 63})$

(ii) $H_2^*(B^1\Sigma_u^+,v) \rightarrow H_2^*(n)$

$n=I^1\Pi_u (\text{Ref. 63})$

(iii) $H_2^*(a^3\Sigma_u^+,v) \rightarrow H_2^*(n) \rightarrow H+H$

$n=d^3\Pi_u (\text{Ref. 69})$

(iv) $H_2^*(a^3\Sigma_u^+,v) \rightarrow H_2^*(n)$

$n=d^3\Pi_u (\text{Ref. 69})$

(v) $H_2^*(c^3\Pi_u,v) \rightarrow H_2^*(n) \rightarrow H+H$

$n=g^3\Sigma_u^+, h^3\Sigma_u^+ (\text{Ref. 69})$

(vi) $H_2^*(c^3\Pi_u,v) \rightarrow H_2^*(n)$

$n=g^3\Sigma_u^+, h^3\Sigma_u^+ (\text{Ref. 69})$

(vii) $H_2^*(c^3\Pi_u,v) \rightarrow H_2^*(n)$

$n=a^3\Sigma_u^+, b^3\Sigma_u^+, c^3\Pi_u, X^1\Sigma_g^+ (\text{Ref. 70})$

(viii) $H_2^*(a^3\Sigma_u^+,v) \rightarrow H_2^*(n)$

$n=a^3\Sigma_u^+, b^3\Sigma_u^+, c^3\Pi_u, X^1\Sigma_g^+ (\text{Ref. 71})$