# Dissociative Electron Attachment to Carbon Tetrachloride Molecules

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The carbon tetrachloride molecule ($CCl_4$) is considered to be a key molecule in electron attachment studies where it is used as a calibrating compound. In the paper, the fragmentation of the $CCl_4$ molecule upon the electron capture is investigated. The low energy electron attachment to $CCl_4$ was studied in the electron energy range from about 0 up to 10 eV with an electron energy beam resolution of about 50 meV. The electron attachment is shown to be a purely dissociative process for this molecule. In the experiment, four anionic fragments were detected: $Cl^-$, $Cl_2^-$, $CCl_3^-$, and $CCl_2^-$. The most abundant anion fragments formed through the dissociative electron attachment to $CCl_4$ is $Cl^-$. Based on the energetic properties of the fragments involved in anion formation, the respective energy thresholds for the reactions leading to the observed anion formation are provided and discussed. Additionally, rough values of cross-section for the detected anion are estimated.

topics: mass spectrometry, electron capture, dissociative electron attachment, carbon tetrachloride

## 1. Introduction

Since the explanation of the formation of the ozone hole by the reaction of ozone with free halogen radicals [1], an increase of scientific interest in the generation of negative ion has been observed [2–6].

Electron–molecule interactions play an important role in many areas of science and life. Detailed knowledge of the processes occurring during the impact of an electron on an atom and a molecule, is a basic requirement for various research problems in physics, biophysics, chemistry, atmospheric physics, technology, etc. [7–10].

The interactions of a low-energy electron with a molecule in the gas phase under the low-pressure condition (when multiple collisions between molecules do not proceed) can be divided into:

- direct scattering,
- resonant scattering.

In direct elastic scattering, the total kinetic energy of the electron–molecule system is retained. In direct inelastic scattering process, the conversion of the kinetic energy of the electron into the internal energy of the molecule takes place. Energy transfer changes the rotational and vibrational states of the molecule. For this reason, direct inelastic scattering causes predominantly electronic excitation of the target molecule.

Resonant scattering occurs when an incoming electron is trapped in the vicinity of AB molecule for a time considerably longer than the time it takes for an electron to fly a distance comparable with the diameter of the molecule. In this case, the electron–molecule system can be treated as an excited negatively charged system — temporary negative ion (TNI) denoted as $(AB^-)^*$. Hence, resonant scattering could be considered as the attachment (capture) of an electron to the molecule AB

$$e^- + AB \rightarrow (AB^-)^*. \qquad (1)$$

Such a process can proceed in the case of low-energy interactions (usually below 10 eV) of electrons with molecules. Obviously, the energy of TNI is higher than the ground state energy of the molecule and electron in the continuum state, so the temporary negative ion is unstable. Energy excess in TNI can most probably be released in two processes:

- autodetachment

$$(AB^-)^* \longrightarrow \begin{cases} A + B^-, \\ A^- + B, \end{cases} \qquad (2)$$
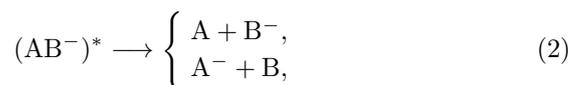
- dissociative electron attachment (DEA)

$$(AB^-)^* \rightarrow e^- + AB^*. \qquad (3)$$

In the DEA process, TNI dissociates into fragments, one of which is an anion and the remaining fragments are neutral. In such a situation,

a characteristic peak is observed in the energy spectrum of the formed ions. The autodetachment process causes the rejection of an additional electron. Such a process is possible until the distance between the atoms in the molecule is smaller than the cross point of the potential energy curves of AB and $(AB^-)^*$ (for more details see [11, 12]). Due to the longer time for the electron to stay in the vicinity of the molecule, after the electron detachment, the molecule can be left in the excited vibrational state. This is the case when TNI is characterized by a substantial change in geometry compared to the geometry of as neutral molecule. Thereby the electron capture changes the electron and nuclei motion in the molecule.

According to the uncertainty principle, the TNI lifetime is related to the energy width of the discrete state of TNI. The lifetime of TNI depends on the energy of the resonance and the size of the molecule. It ranges from about $10^{-14}$ s for $N_2^-$ to several or hundreds of $\mu$s for large polyatomic molecules (e.g. $SF_6^-$) [13].

In the case of electron attachment, two quantities are important: the dissociation energy of the molecule ($D(AB)$) and its electron affinity (EA). A positive EA value indicates the existence of a stable anion in which an extra electron exists in the bound state. In the case of a negative EA, the negative ion in the ground state in unstable in respect to the extra electron ejection. Many molecules are not able to form thermodynamically stable anions (e.g. $N_2$ or $CO_2$), however, they can form short living TNIs [13].

Taking into account the dissociative attachment of an electron to the molecule, one can derive the energy balance

$$AE(B^-) = D(AB) - EA(B) + E_{kin} + E_{exc},$$
(4)

where $AE(B^-)$ is the appearance energy of the $B^-$ ion, $D(AB)$ is the bond dissociation energy of the AB molecule, $E_{kin}$ is the kinetic energy of the formed fragments (A and $B^-$), $E_{exc}$ is the excitation energy of the generated fragments (A and $B^-$).

In the present studies, the formation of negative ion as a result of electron attachment to carbon tetrachloride ($CCl_4$) molecules in the gaseous phase was investigated. This compound is of special importance in the studies of the process of electron capture by molecules, because the formation of the $Cl^-$ anion from $CCl_4$ serves as a calibrant fragmentation pattern. Many investigations proved that the $Cl^-$ ion is formed by DEA (dissociative electron attachment) to $CCl_4$ at two resonant electron energies of about 0 eV and 0.8 eV [14–16]. Nevertheless, in most papers, only the formation of $Cl^-$ in DEA to $CCl_4$ is mentioned or described. After an extensive search in the literature, only three papers [11, 17, 18] were found with data regarding another DEA channels to $CCl_4$. This paper presents the results of anion generation from $CCl_4$
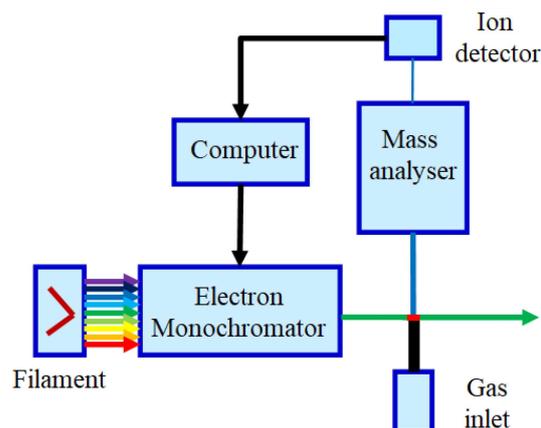


Fig. 1. Schematic view of the electron attachment spectrometer.

with a discussion of possible reaction channels leading to the ion formation and their energy thresholds. The first values of cross-section for the formation of the observed ions are estimated.

## 2. Experimental setups

In the free electron attachment by a molecule, electron attachment spectroscopy (EAS) was applied. A schematic view of the apparatus is shown in Fig. 1. In the EAS method, two crossed beams of electron and molecules interact. The formed anions are then analyzed using a mass spectrometer — in most cases by a quadrupole mass filter. The major advantage of the EAS apparatus is the possibility to measure the efficiency of the respective ion formation as a function of the incoming electrons energy, which allows to distinguish the types of formed anions as well as their resonant energies.

Using the EAS method, partial cross-sections of the electron attachment process leading to the specified ion formation can be measured. By summing up all partial cross-sections, total cross-section can be obtained. The great lack of the EAS technique is the difficulty in direct measurements of the absolute cross-section of the electron attachment. This difficulty is associated with the problems of determining the gas density in the interaction chamber, the gas volume in which the electron–molecule interactions proceed, the ion extraction efficiency from the interaction chamber and the efficiency of anion transmission and detection of the mass spectrometer.

For these reasons, the measured relative cross-sections of DEA processes in experiments with molecular beam are calibrated with the absolute cross-sections obtained by the ETS technique. Comparative methods are also used for this purpose, employing direct measurements of two cross-sections for two compounds, one with the known DEA cross-section and the other with the unknown cross-section in the same experiment.

Such useful and well-recognized compounds in the electron attachment experiments are $CCl_4$ and $SF_6$. The attachment of $s$-wave electron to these molecules leads to the formation of long-lived parent ions $SF_6^-/SF_6$ [13, 19] or stable fragmentary ions formed in the dissociative electron attachment — $Cl^-/CCl_4$ [14–16].

$CCl_4$ is the most frequently used calibrating gas. Many investigations have proved that the $Cl^-$ ion is formed by DEA (dissociative electron attachment) to $CCl_4$ at two resonant electron energies around 0 eV and 0.8 eV [14–16]. The first resonance (at 0 eV) could be used as the electron energy scale correction. The formation of $Cl^-$ at 0.8 eV with a well-known cross-section of $5 \times 10^{-20}$ $m^2$ [20] is used to estimate cross-sections of electron attachment to other molecules and atoms. In this method of cross-section estimation, the ion signals of $Cl^-$ at 0.8 eV and other ions formed in the DEA process to the molecule under study are compared. In the presented results, the method of cross-section estimation was used.

The fundamental of all experimental techniques in which the cross-section of DEA processes is determined is the control of the energy of the captured electron and its spread energy. For accurate results, an electron beam with a low energy spread must be used. It is especially important to obtain a beam of electrons with very low energies close to 0 eV. For the above reasons, electron energy monochromators of different types are applied in experimental setups for the electron attachment studies. In the present studies, the so-called trochoidal electron monochromator (TEM) was used. The main feature of such type of monochromator is the application of a magnetic field parallel to the direction of the electron velocity. In such an arrangement, electrons are guided by the magnetic field, hence slow electrons with the energy close to 0 eV can be admitted to the interaction chamber [21]. A pair of Helmholz coils mounted outside the apparatus generates the magnetic field, which is necessary for the operation of TEM. Energy dispersion proceeds in the region of crossed (at the right angle) electric and magnetic fields. In this region, electrons with lower energy are deflected more strongly than those with higher energy. Using displaced apertures to and out of the dispersion region, electrons with a narrow energy distribution are selected [22]. After proper adjustment of TEM, an electron beam with the energy of about 0 to 20 eV and the minimal spread of about 30 meV (at full width at half maximum — FWHM) can be obtained. In the present experiments, FWHM and the electron current were $\sim$ 50 meV and $\sim$ 10 nA, respectively. The electron energy resolution used represents a reasonable compromise between product ion intensity and energy spread to resolve resonances in the measured ion yields. TEM was continuously heated to the temperature of 360 K in order to prevent surface charging.
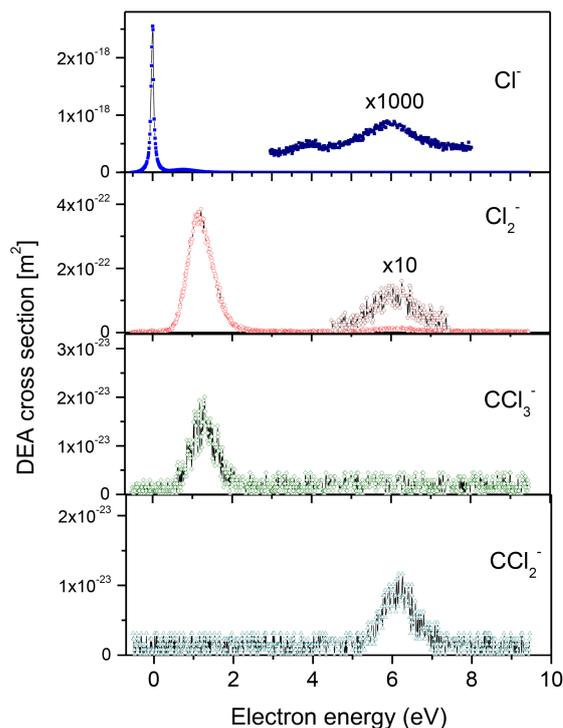


Fig. 2. Partial cross-sections for the all observed anions in the case of DEA to $CCl_4$.

The gas was introduced to the ion chamber through a capillary with a small orifice (20 $\mu$m in diameter) at its end. Ions formed due to electron–molecule interactions were then extracted by ion optics towards a quadruple mass spectrometer, where they were analyzed with respect to the mass to charge ratio (m/z). A channeltron was used for the detection of selected anions. The carbon tetrachloride sample of 99% purity was purchased from Sigma Aldrich.

## 3. Results and discussion

The present studies show that electron attachment to carbon tetrachloride is a purely dissociative process with the formation of four anionic fragments, namely $Cl^-$, $Cl_2^-$, $CCl_3^-$, and $CCl_2^-$. The measured intensity ratios $Cl^-:Cl_2^-:CCl_3^-:CCl_2^-$ (for the most efficient resonances) are 100000:12:0, 65:0, 45. The parent anion $CCl_4^-$ is not observable in the present experiment. The lifetime of this TNI anion is determined to be 30 ps [23], while anions in the mass spectrometer are detected in a few tens of $\mu$s after being formed in the ion source. Moreover, by studying the positive ionisation, Sierra et al. [24] detected 7 types of ions: $C^+$, $Cl^+$, $Cl_2^+$, $CCl^+$, $CCl_2^+$, $CCl_3^+$, and $CCl_3^{2+}$ and did not observe the parent positive anion due to its low stability and fast dissociative ionisation. The cross-section curves for all negatively charged fragments observed from $CCl_4$ in the electron energy range of about 0 to 10 eV are presented in Fig. 2.

The energetic properties of possible fragments from $CCl_4$ (standard enthalpy of formation ($\Delta H^\circ_{f\,gas}$) and electron affinity (EA)) [17, 25] as well as resonance and appearance energies (AE) (in the parenthesis) of the observed anionic counterparts.

| Molecule | $\Delta H^\circ_{f\,gas}$ [eV] | EA [eV] | Resonance and AE [eV] |
|---|---|---|---|
| C | $7.43 \pm 0.005$ | 1.26 | |
| Cl | 1.26 | 3.61 | 0; 0.8(0.3); 3.9(3.2); 6(4.5) $\pm 0.1$ |
| $Cl_2$ | | $2.5 \pm 0.2$ | 1.2(0.6); 6(5.2) $\pm 0.1$ |
| CCl | 5.2 | 0.04 or $-0.14$ [17] | |
| $CCl_2$ | 2.47 | $1.593 \pm 0.006$ | 6.2(5.2) $\pm 0.1$ |
| $CCl_3$ | 0.78 | $2.16 \pm 0.096$ | 1.2(0.7) $\pm 0.1$ |
| $CCl_4$ | $-0.99 \pm 0.03$ | $2.00 \pm 0.2$ | |

Additionally, the appearance and resonant energies as well as the energetic properties (standard enthalpy of formation and electron affinity [17, 25]) of the corresponding neutrals are collected in Table I. A detailed discussion on the formation of all measured fragment anions will be provided in the next paragraphs.

### 3.1. $Cl^-$

The chlorine atom possesses the extremely large electron affinity of 3.61 eV (see Table I), hence the formation of the $Cl^-$ anion is the most efficient in DEA to $CCl_4$. The same situation was also observed in the case of other chlorinated molecules, for which $Cl^-$ was also the most abundantly formed anion [18, 26–28]. The possible DEA channels leading to the $Cl^-$ formation, together with the calculated (based on the data from Table I) reaction energy thresholds ($\Delta E_r$), are

$$CCl_4 + e \rightarrow Cl^- + CCl_3, \quad \Delta E_r = -0.58 \text{ eV}, \tag{5}$$

$$CCl_4 + e \rightarrow Cl^- + CCl_2 + Cl, \quad \Delta E_r = 2.37 \text{ eV}, \tag{6}$$

$$CCl_4 + e \rightarrow Cl^- + CCl + Cl_2, \quad \Delta E_r = 3.84 \text{ eV}, \tag{7}$$

$$CCl_4 + e \rightarrow Cl^- + CCl + 2Cl, \quad \Delta E_r = 6.36 \text{ eV}, \tag{8}$$

$$CCl_4 + e \rightarrow Cl^- + C + Cl_2 + Cl, \quad \Delta E_r = 7.33 \text{ eV}, \tag{9}$$

$$CCl_4 + e \rightarrow Cl^- + C + 3Cl, \quad \Delta E_r = 8.59 \text{ eV}. \tag{10}$$
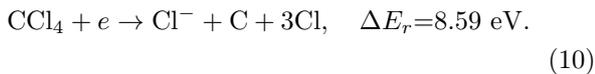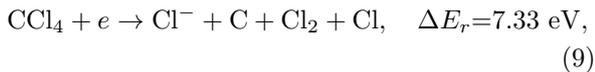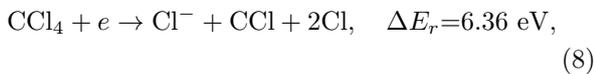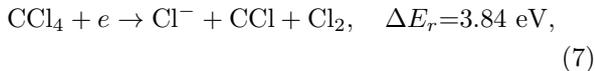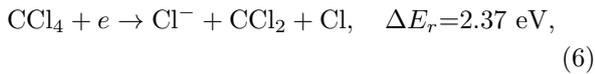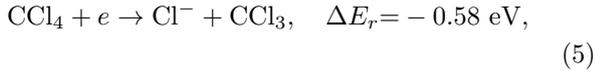
The reaction (5) is exothermic by 0.58 eV, whilst the occurrence of other reactions is possible when additional energy (from 2.37 to 8.59 eV) is supplied to the system by an electron. The measured $Cl^-$ signal shows that this anion is formed mostly in the low energy region between 0 and 1.5 eV, with the resonances at about 0 eV and at 0.8 eV with the appearance energies of 0 eV and 0.3 eV, respectively. A closer inspection of the ion yield indicates another weakly abundant features with the maxima at 3.9 eV and 6.0 eV. The appearance energies AEs derived from experimental data for resonances at higher energies are 3.2 eV and 5.5 eV, respectively. In comparison to the previous studies [11, 17, 18], an additional resonance was observed at 3.9 eV.

Taking into account both, the experimental AE and the obtained $\Delta E_r$, the first resonance peaking at 0 eV corresponds to the reaction (5). The second resonance with a maximum at 0.8 eV corresponds to the dissociative electron attachment to an excited molecule. Its AE is significantly lower than the thermodynamic energy threshold for the reaction (6), hence this DEA channel is not accessible to the formation of $Cl^-$ at 0.8 eV. In such a process, the extra electron is bound to an electronically excited state of the neutral molecule and corresponds to the reaction (5). This statement was also confirmed in earlier studies of the swarm experiment by Modelli et al. [24] and in [17].

The resonance at the energy of 3.9 eV has a higher experimental AE (of 3.2 eV) than $\Delta E_r$ of the reaction (6), whilst AE (4.5 eV) of the resonance at 6.0 eV is higher than $\Delta E_r$ of the reaction (7). Considering the above, it can be assumed that the resonance at 3.9 eV is related to the formation of $CCl_2$ (reaction (6)), while DEA at 6.0 eV causes fragmentation of the molecule leading to the formation of CCl fragment (reaction (7)). However, the exact assignment of a given reaction channel to the observed resonances requires additional research.

### 3.2. $Cl_2^-$

The formation of $Cl_2^-$ anion can be described by the following reactions:

$$CCl_4 + e \rightarrow Cl_2^- + CCl_2, \quad \Delta E_r = 0.96 \pm 0.2 \text{ eV}, \tag{11}$$

$$CCl_4 + e \rightarrow Cl_2^- + CCl + Cl, \quad \Delta E_r = 4.95 \pm 0.2 \text{ eV}, \tag{12}$$

$$CCl_4 + e \rightarrow Cl_2^- + C + Cl_2, \quad \Delta E_r = 5.92 \pm 0.2 \text{ eV}, \tag{13}$$

$$CCl_4 + e \rightarrow Cl_2^- + C + 2Cl, \quad \Delta E_r = 8.44 \pm 0.2 \text{ eV}. \tag{14}$$
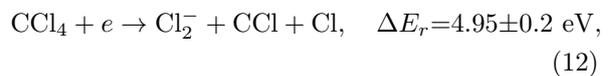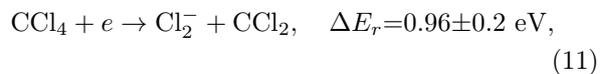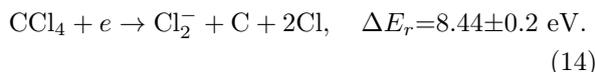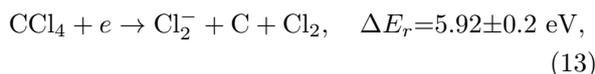
It is worth emphasizing that there is no direct bond between the chlorine atoms in the $CCl_4$ molecule. Thereby, the formation of $Cl_2^-$ requires not only fragmentation of the molecule, but also its reorganization. Such a process of molecule reorganization has been observed before, e.g. the formation of $F_2^-$ from $SF_6$ [30] or $CH_2F_2$ [31].

Two resonances leading to the generation of the $Cl_2^-$ ion were observed in the experiments. The energetic maxima of these resonances are 1.2 eV and 6.0 eV and the corresponding appearance energies are 0.6 eV and 5.2 eV, respectively. The energetic positions of these resonances are in good agreement with those observed previously [11, 17, 18]. Taking into consideration the thermodynamic thresholds of the specific DEA channels, it can be assumed that the low-energy resonance can be described by the reaction (11) if we consider the uncertainties of AE and the $\Delta E_r$ estimations. The formation of $Cl_2^-$ at 6.0 eV is most likely associated with the DEA reaction (12).

### 3.3. $CCl_3^-$ and $CCl_2^-$

The generation of $CCl_3^-$ and $CCl_2$ anions is associated with the formation of their neutral counterparts Cl and $Cl_2$, respectively. Therefore, the formation of these ions competes with the generation of their respective counterpart anions. As can be seen in Table I, the electron affinity values of $CCl_3$ and $CCl_2$ are significantly lower than the corresponding values for Cl and $Cl_2$. This fact causes that the abundances of $CCl_3^-$ and $CCl_2$ anions are definitely lower than in the case of anions generated in competing DEA channels (see (5) and (11)).

The complementary anion to $Cl^-$ with respect to breaking of the C–Cl bond is the anion $CCl_3^-$. The following reaction channel can be considered for its formation with a respective calculated reaction threshold

$$CCl_4 + e \rightarrow CCl_3^- + Cl, \quad \Delta E_r = 0.87 \text{ eV}. \tag{15}$$
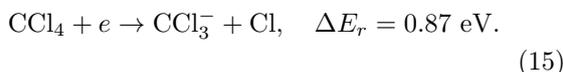
In the present experiment, cross-section of the $CCl_3^-$ formation is characterized by only one resonance peaking at 1.2 eV. For this resonance, AE is $0.7 \pm 0.1$ eV. The $\Delta E_r$ value of the reaction (15) exceeds the observed AE of this channel by about 0.07 eV (if uncertainty is taken into consideration). Kumar et al. [17] calculated $\Delta E_r$ of the reaction (15) to be 0.79 eV. This shows that there are some additional uncertainties in the $\Delta E_r$ estimation, at least for this channel. Additionally, it should be added here that in the present study, the resonance at 6.1 eV (described by Kumar et al. [17]) was not detected. This resonance was not observed in other previous studies of DEA to $CCl_4$ [11, 18]. This may be due to the lower efficiency of the electron capture process in the currently used electron beam apparatus with an energy spread of 50 meV, as opposed to the previously used ones, where this spread was greater than 100 meV. Another possible reason for this may be the extraction discrimination of the ion optics of the quadrupole filter of the ions with higher kinetic energies. For the resonance at 6.1 eV, the fragments will have about 6 eV of excess energy, which can be divided into the excitation energy as well as the kinetic energy of the molecules involved in the DEA process.

The $CCl_2^-$ anion may be formed via the following reaction channels:

$$CCl_4 + e \rightarrow CCl_2^- + Cl_2, \quad \Delta E_r = 1.87 \text{ eV}, \tag{16}$$

$$CCl_4 + e \rightarrow CCl_2^- + 2Cl, \quad \Delta E_r = 4.39 \text{ eV}. \tag{17}$$
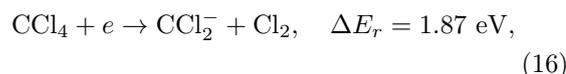
In the present study, the anion $CCl_2^-$ was observed in one resonance energy region peaking at 6.2 eV. The estimated AE value for this resonance is 5.2 eV. This shows that both DEA channels are accessible to formation of $CCl_2^-$ at this resonance. The same resonance was also observed previously. Nevertheless, in earlier studies, another resonance was also observed with a maximum between 1.65 to 1.8 eV and the value of AE between 0.9 to 1.2 eV [11, 17, 18]. Kumar et al. [17] give the value of $\Delta E_r$ for this resonance to be in the range from 1.6 to 1.71 eV, which is also far too high (even taking into account the possible uncertainties of $\Delta E_r$) to be responsible for this anion generation at the low energy resonance.

### 4. Conclusions

Using electron attachment spectroscopy, DEA to carbon tetrachloride in the gas phase was studied. In the electron energy range of about 0 to 10 eV, four complementary anionic species: $Cl^-$, $CCl_3^-$, $Cl_2^-$, and $CCl_2^-$, were detected. The most abundant anion was $Cl^-$ with an estimated cross-section of the order of $10^{-18}$ m$^2$. The other anions are formed at much lower cross-section in the range of $10^{-22}$ to $10^{-23}$ m$^2$. The resonance energies at the formation of individual anions also have similar values, i.e., anions are formed at the electron energies of around 0, 0.8, 1.2, 3.9, and 6 eV. Additionally, for the obtained anions, a detailed discussion of the fragmentation channels leading to their formation was conducted.

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