# Determination of Inelastic Collision Cross Sections for $C_3F_8$ Molecule by Multi-term Boltzmann Equation Analysis

Byung-Hoon Jeon and Sung-Chul Ha†

**Abstract**

We measured the electron transport coefficients, the electron drift velocity W and the longitudinal diffusion coefficient $D_L$ in the 0.526% and 5.05% $C_3F_8$-Ar mixtures over the E/N range from 0.01 Td to 100 Td by the double shutter drift tube, and compared the measured results by Hunter *et al.* with those. We determined the inelastic collision cross sections for the $C_3F_8$ molecule by the comparison of the present measurements and the calculation of electron transport coefficients in the $C_3F_8$-Ar mixtures by using a multi-term Boltzmann equation analysis.

**Key Words** : Inelastic collision cross sections for $C_3F_8$ molecule, Electron drift velocity, Electron longitudinal diffusion coefficient, Multi-term Boltzmann equation analysis

## 1. Introduction

Perfluropropane($C_3F_8$) in the perfluoroalkanes, $C_nF_{2n+2}$(n=1,2,3,4), is frequently used as one of effective etchants in semiconductor etching processes and it is also used as gaseous media in diffuse discharge switches for pulsed-power inductive energy storage application $C_3F_8$.[1]

Because of physical and industrial importance of perfluoropropane($C_3F_8$), there have been a small number of investigations on electron transport coefficients in $C_3F_8$ gas[2] and on electron collision cross sections of the $C_3F_8$ molecule[3]. Recently, Christophrou and Olthoff[4] compiled a set from available cross sections data, but their compilation was rather scanty for use in any quantitative computer modeling of related plasma phenomena.

In this paper, first, we measured electron drift velocity and the longitudinal diffusion coefficient in the 0.526% and 5.05% $C_3F_8$-Ar mixtures and, secondly, determined the inelastic collision cross sections for the $C_3F_8$ molecule by the comparison of the present measurements and the calculation of electron transport coefficients in the both mixtures by using a multi-term Boltzmann equation analysis.

Joongbu Univ., Computer Aided Design
Kumsan-Gun, Chungnam, 312-940
E-mail : bhjeon@joongbu.ac.kr

†Dongguk Univ., Electrical engineering
Chung-Ku, Seoul

## 2. Experiments

The apparatus and the data processing procedure used in the present measurement of the drift velocity and the longitudinal diffusion coefficient were the same as those used in the works of Jeon[5, 6].

Measurements were repeated at least at three different gas densities at each E/N value. All measurements were carried out at room temperature, 300±2K.

The mixtures were composed of pure $C_3F_8$ (purity 99.99%) and Ar (99.9999%) and the actual mix ratio was determined by using a gas chromatography test.

## 3. Experimental Results

The mean values of the measured electron transport coefficients, the drift velocity **W**, product of the gas number density and the longitudinal diffusion coefficient **ND**$_L$, and the ratio of the longitudinal diffusion coefficient to the electron mobility $D_L/\mu$, as a function of E/N in the 0.526% and 5.05% $C_3F_8$-Ar mixtures over the E/N range 0.01 to 100 Td and over the gas pressure from 0.133 to 122 kPa (1 to 900 torr, 1torr = 133.322 Pa) are shown by solid symbols in Figures 1 to 3 (● and ■ are measured results in the 0.526% and 5.05% $C_3F_8$-Ar mixtures, respectively.). And these figures also shown are the respective transport coefficients in pure Ar by open triangles for comparison.

The present measured drift velocity in $C_3F_8$-Ar mixtures is only compared with experimental result in 0.5% $C_3F_8$-Ar mixture by Hunter *et al.*[7] The present result is higher than that over the E/N range from 0.2 to 0.8 Td by about 18% at most.

The measured longitudinal diffusion coefficient in each mixture was also enhanced in the same E/N range as the drift velocity, and showed a small hump over the E/N range from 2 to 9 Td in the 0.526% mixture and from 6 to 35 Td in the 5.05% mixture. And this E/N dependence also indicates the effect caused by the inelastic collision cross sections of the $C_3F_8$ molecule.

## 4. Boltzmann equation analysis

The electron transport coefficients in both mixtures were calculated by a multi-term Boltzmann equation analysis code developed by Robson and Ness in James-Cook university[8].

The cross sections set for the Ar atom determined by Nakamura and Kurachi[9] was used throughout the present study. At the beginning, we assumed an initial cross sections set for the $C_3F_8$ molecule which consisted of the elastic momentum transfer (Qm) by Pirgov and Stefanov[3], the total attachment (Qatt) by Hunter and Christophorou[10], the total ionization (Qi) by Chantry and Chen[11] and the total vibrational excitation (Qv) by Pirgov and Stefanov[3].

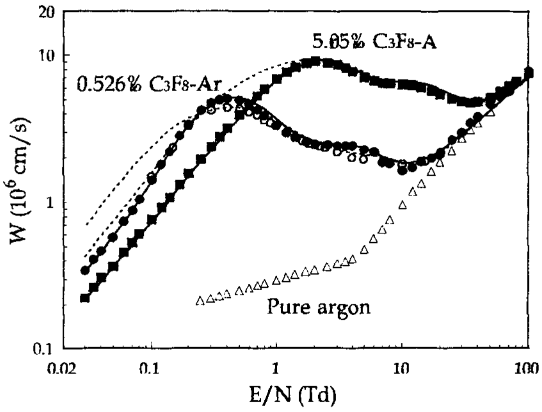


Figure 1 **W** as a function of E/N in 0.526% and 5.05% $C_3F_8$-Ar mixtures. The broken and the solid curves show calculated values using an initial and the present cross sections set, respectively, for $C_3F_8$ molecule. And ○ is measured result in 0.5% $C_3F_8$-Ar mixture by Hunter *et al.*,.

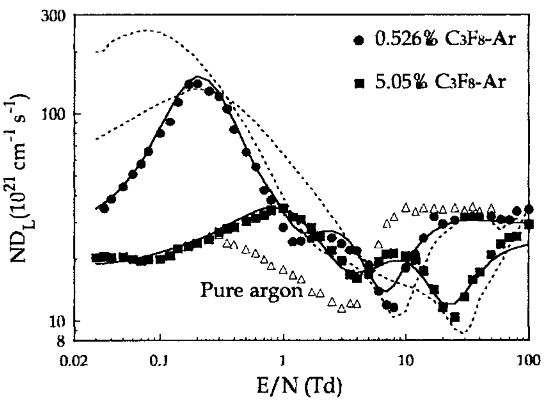


Figure 2 **ND**$_L$ as a function of E/N in 0.526% and 5.05% $C_3F_8$-Ar mixtures. The broken and the solid curves show calculated values using an initial and the present cross sections set, respectively, for $C_3F_8$ molecule.

The calculated **W**, **ND**$_L$ and $D_L/\mu$ using thses cross sections are shown by the broken curves in Figures 1 to 3. The results showed fair agreement in higher E/N but there was substantial disagreement in lower E/N. These disagreement indicated that the present values of the threshold energies for the additional vibrational excitations are wrong, and a need for inclusion of additional inelastic cross sections over the lower electron energy.

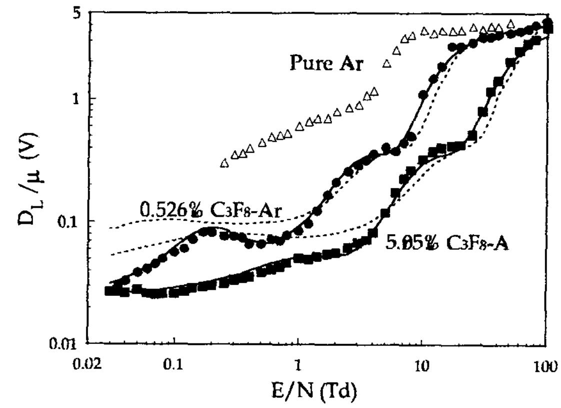


Figure 3 $D_L/\mu$ as a function of E/N in 0.526% and 5.05% $C_3F_8$-Ar mixtures. The broken and the solid curves show calculated values using an initial and the present cross sections set, respectively, for $C_3F_8$ molecule.

Therefore, we started our trial-and-error amendment procedure for agreement of the electron transport coefficients in the $C_3F_8$-Ar mixtures between the measurement and the calculation.

The determined cross sections set for $C_3F_8$ molecule by these procedure is shown by the solid and the thick solid curves in Figure 4.

And, the calculated electron transport coefficients by using this set are shown by solid curves in Figures 1 to 3, and the maximum difference between these and the measurements of the electron transport coefficients reduced to about 10%.

The present set as shown in Figure 4 include the cross section of the momentum transfer compiled by Christophorou and Olthoff[4] over the electron energy range 1.5-100 eV and of the neutral dissociation by Motlagh and Moore[12], both of which did not have appreciable effect on the electron transport coefficients in the 0.526% and 5.05% $C_3F_8$-Ar mixtures in the measured range. And this figure also shows initial cross sections set by broken and solid curves.

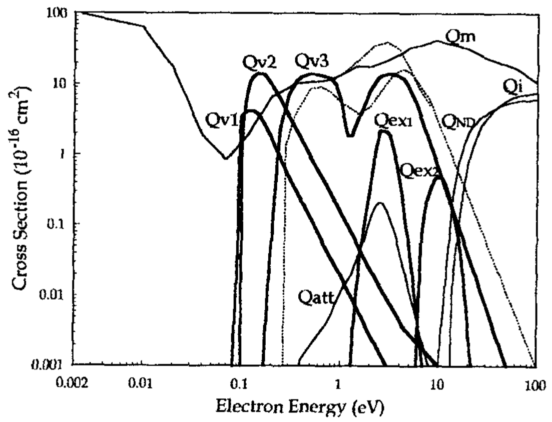


Figure 4 The present set of electron collision cross sections for $C_3F_8$ molecule (by the solid and the thick solid curves). the broken and the solid curves show initial cross sections for $C_3F_8$ molecule.

## 5. Conclusions

We measured the drift velocity and the longitudinal diffusion coefficient in the 0.526% and 5.05% $C_3F_8$-Ar mixtures over the wide E/N range from 0.03 to 100 Td. There has been no measurement of the longitudinal diffusion coefficient in the $C_3F_8$-Ar mixtures so far.

The electron transport coefficients in these mixtures sensitively reflect the inelastic (vibrational excitations and excitations) cross sections, and nearly insensitive to the elastic momentum transfer cross section for the molecule. By utilizing this advantage, the measured transport coefficients were used to determine the inelastic collision cross sections for the $C_3F_8$ molecule over the energy range where the electron beam experiment may be difficult to carry out.

For complete set of cross sections of the $C_3F_8$ molecule, it is further necessary to measure the electron transport coefficients in pure $C_3F_8$, and to determine the elastic momentum transfer cross section by analyzing them, when the present inelastic cross sections should be utilized.

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