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# RATE COEFFICIENTS FOR $Ar^+$ IN $Ar/BF_3$ MIXTURES

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**Abstract.**In this paper we present most probable reactions of $Ar^+$ ion with $Ar/BF_3$mixtures. Appropriate gas phase enthalpies of formation for the products were used to calculate scattering cross section as a function of kinetic energy. These data are needed for modeling in numerous applications of technologically important $BF_3$discharges. Results for transport coefficients as a function of *E/N* (*E* -electric field; *N*-gas density), specially rate coefficients were obtained by using the Monte Carlo technique.

## 1. INTRODUCTION

Cold plasmas are frequently used in new technologies where they open up the possibilities of non-intrusive production or modification of various substances (Makabe et al. 2006.). These plasmas have a high electron temperature and low gas temperature so non-equilibrium behavior of a large number of species becomes important (Robson et al. 2005.). Current computer resources allow studies of complex global models (Murakami et al. 2013.) which describe the behavior of such plasmas by taking into account a very large number of particles. The knowledge of ion-neutral reactions is generally available (see https://nl.lxcat.net/data/set_type.php) although the effects of reactions on transport parameters of particular ions are much less studied due to non-detectability of rapidly vanishing ionic fluxes. This especially holds for ions whose transport is affected by fast reactions (Stojanović et al. 2014. andNikitović et al. 2016.).

In this paper we firstly selected the most probable reactions of $Ar^+$ with $BF_3$ gases for thermodynamic threshold energies below about 15 eV.

## 2. CROSS SECTION SETS

Complete cross section sets for ion transport are scarce in spite of a broad range of specific methods relevant for quantification of particular cross sections. The main problem in heavy particle scattering, easily and precisely selecting the state of the projectile and target before the collision, is still very complicated for a range of conditions, so databases for ion scattering (Murakami et al. 2013. and https://nl.lxcat.net/data/set_type.php) are still devoid of such data. Phelps established the first worldwide accessible database with cross section sets (see https://nl.lxcat.net/cache/5b33772b61cf9/) tested for each particular case either for swarm conditions of spatially resolved measurements of emission or ion mobility values. In order to focus on effects of reactive processes introduced by $BF_3$ we neglected all but these two components of the $Ar^+$ + Ar cross section set. Complete cross section sets used in this work are shown in Figure 1.

Appropriate gas phase enthalpies of formation for the products (Table 1) were used to calculate thermodynamic thresholds.

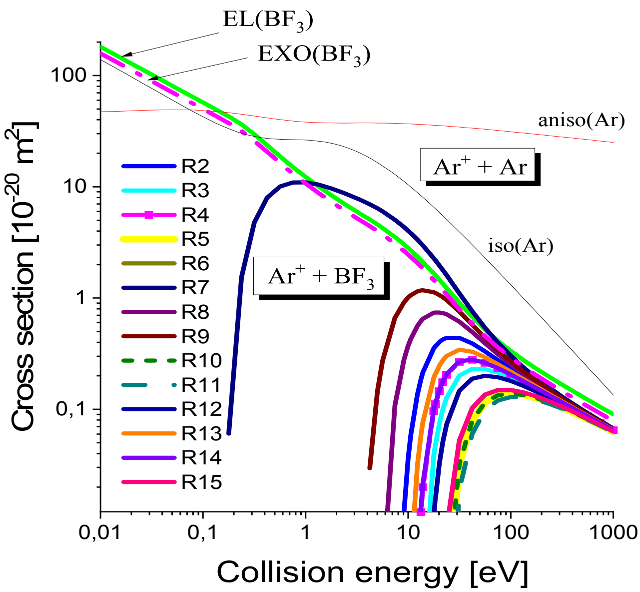



Figure 1: Cross section sets for $Ar^+$in $BF_3$.

| Ion/neutral | $\Delta H_f$(ion) kJ/mol (room temperature) | $\Delta H_f$(neutral) kJ/mol (room temperature) |
|---|---|---|
| $Ar^+/Ar$ | 1520.57 | 0 |
| $Ar_2^+/ Ar_2$ | 1398.1 | -1.01 |
| $B^+/B$ | 1363.3 | 562.7 |
| $BF^+/BF$ | 957 | -115.8 |
| $BF_2^+/BF_2$ | 314 | -589.9 |
| $BF_3^+/BF_3$ | 364.3 | -1137.0 |
| $F^+/F$ | 1760.2 | 79.4 |
| $F_2^+/F_2$ | 1514.5 | 0 |

Table 1: Heats of formation $\Delta_f \mathbf{H}^0$ at 298 K (kJ/mol).

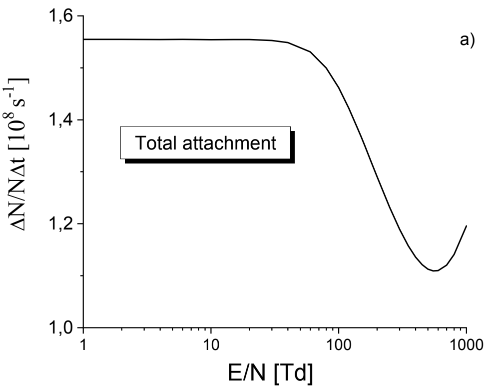
## 3. DISCUSSION AND RESULTS

Monte Carlo Simulations (MCS) have many applications for analysis of the transport of charged particles in plasmas. MCS provide swarm data with the only the uncertainty due to statistical fluctuations and uncertainties in the cross sections. In addition, MCS is the basis of hybrid models of plasmas allowing easy and accurate representation of the end effects and of the non-local high energy groups of particles which are essential in production of plasmas and treatment of surfaces.The MC code used in our analysis is based on the null collisions method.

In Figure 2 we show rate coefficients for reactions of $Ar^+$ ions with $Ar/BF_3$ mixtures at $T$=300K, calculated by Monte Carlo simulations. Rate coefficients are important for applications of the global model to $Ar/BF_3$ mixtures. We are presenting reaction products and thermodynamic thresholds for $Ar^+$ + $BF_3$(Nikitović et al. 2019.)formation a) total attachment and b) attachment for endothermic and exothermic reaction products.

## 4. CONCLUSION

In addition to presenting the data we show here the effects of non-conservative collisions to ion transport. Data for swarm parameters for ions are needed for hybrid and fluid codes and the current focus on liquids or liquids in the mixtures with rare gases dictates the need to produce data compatible with those models.



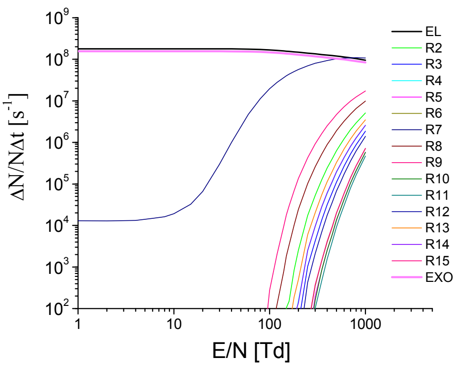




Figure 2: Rate coefficients of $Ar^+$ in $Ar/BF_3$ mixtures.

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