RATE COEFFICIENTS FOR Ar^+ IN Ar/BF_3 MIXTURES

Ž. Nikitović[1]*, M. Gilić[1], J. Mitrić[1] and M. Raspopović[1]

[1]*Institute of Physics, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia*

***zeljka@ipb.ac.rs**

Abstract

In this paper we present the 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 function of kinetic energy. These data are in need for modeling in numerous applications of technologically important BF3 discharges. Results for transport coefficients as a function of E/N; rate coefficients are obtained by using the Monte Carlo technique.

RESULTS AND DISCUSSION

Phelps established the first worldwide accessible database with cross ection sets (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 Bf3 we neglected all but these two components of the $Ar^+ + Ar$ cross section set. Complete cross section used in this work is shown in Fig. 1. Appropriate gas phase enthalpies of formation for the products (Table 1) were used to calculate thermodynamic thresholds.

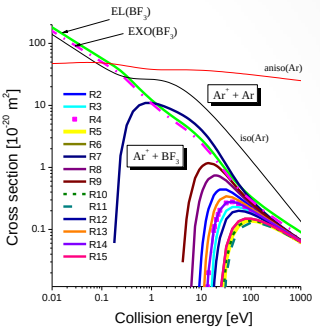

Fig. 1. Cross section sets for Ar^+in BF_3

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

Ion/ neutral	ΔHf (ion) kJ/mol	ΔHf (neutral) kJ/mol
Ar^+/Ar	1520.57	0.00
Ar_2^+/Ar_2	1398.1	- 1.01
B^+/B	1363.3	562.70
BF^+/BF	957.0	- 115.80
BF_2^+/BF_2	34.0	-579.90
BF_3^+/BF_3	364.3	-1137.00
F^+/F	1760.2	79.40
F_2^+/F_2	1514.5	0.00

Monte Carlo method code used in our analysis is based on the null collisions method. In Fig. 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.

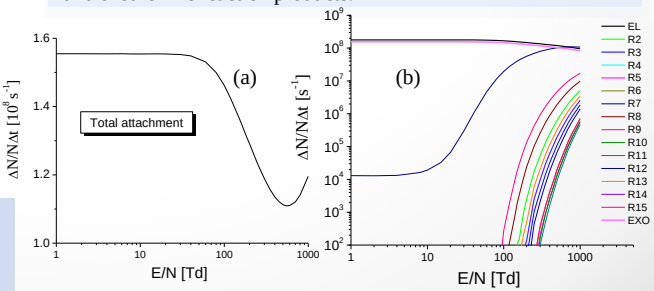

Fig. 2. Rate coefficients of Ar^+ in Ar/BF_3 mixtures.

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.