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REDUCED MOBILITY OF H^+ IONS IN n-BUTANOL GAS

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Abstract. In this paper we show predictions for the low energy cross sections and transport properties for the H^+ ions in n-Butanol gas. These data are needed for modelling in numerous applications of technologically importance. Appropriate gas phase enthalpies of formation for the products were used to calculate scattering cross section as a function of kinetic energy. Calculated cross sections can be used to obtain reduced mobility as a function of *E/N* (*E* -electric field strength; *N*-gas density) for H^+ in n-Butanol gas.

1. INTRODUCTION

n-Butanol occurs naturally as a minor product of the fermentation of sugars and other carbohydrates and is present in many foods and beverages as well as in a wide range of consumer products. Although most volatile organic compounds can be detected by fast methods such as ion mobility spectroscopy, precise determination is possible only if reaction of specific ions with targeted compound is well known.

The goal of this work is to calculate transport parameters of fragment ions of n-Butanol. We employ Denpoh-Nanbu's theory (DNT) see Denpoh et al. 1998 to calculate transport cross section sets for H^+ ions scattering on n-Butanol appropriate for low energies of H^+ ions. By using Monte Carlo technique that properly takes into account thermal collisions see Ristivojević et al. 2012 we calculated transport parameters as a function of *E/N*.

2. CROSS SECTION SETS

The scattering cross sections of H^+ on n-Butanol are calculated by using the DNT see Denpoh et al. 1998. separating elastic from reactive collisions. The induced dipole polarizability of 8.9×10^{-24} cm^3 see Ababneh et al. 2003 is used for the n-Butanol target. In resemblance with our recent work see Stojanović et al. 2013 DNT method is used to separate elastic from reactive endothermic collisions by accounting for the thermodynamic threshold energy and branching ratio according to the Rice-Rampsperger- Kassel (RRK) theory see Rice et al. 1928. Within the RRK theory the internal energy is being distributed among an empirical number of ***s*** equivalent effective modes of the complex selected from the total number of atoms involved in the complex.

Appropriate gas phase enthalpies of formation for the products see Lias et al. 1988 were used to calculate thermodynamic thresholds.

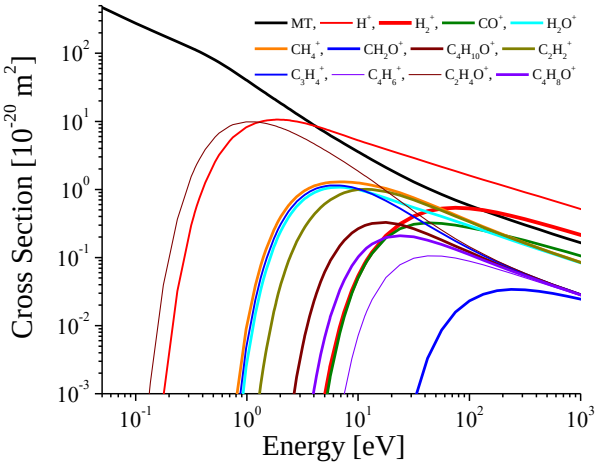

Figure 1: Cross section sets for H^+in n-Butanol gas.

The cross section sets for endothermic and exothermic reactions of H^+ with n-Butanol is presented in Figure 1.

2. RESULTS AND DISCUSSION

The transport properties of species in gas plasma are of great importance for understanding the nature of molecular and ionic interactions in gas mixtures see Todd et al. 2002, Mason et al. 1957. These properties include mean energy, drift velocity, diffusion coefficients, ionization and chemical reaction coefficients, ion chemical reaction coefficients and rarely excitation coefficients, and are very useful in the chemical industry for the design of many types of transport and process equipment. Swarm parameters, which are functions of the reduced electric field *E/N* (E-electric field strength, N-gas density) in direct electric fields are usually used for plasma modeling and simulation.

The flux and bulk drift velocities for H^+ in n-Butanol gas as a function of *E/N* are given in Figure 2. The drift velocities obtained by the Monte Carlo simulation are calculated in real space (bulk) and in velocity space (flux) values which are obtained as $\langle v \rangle$ and $d\langle x \rangle/dt$, respectively. As *E/N* increases, the high-energy ions from the distribution function increasingly have non-conservative collisions in which the H^+ ions disappear, shifting the center of mass of the swarm backward, resulting in a bulk velocity less than the flux.

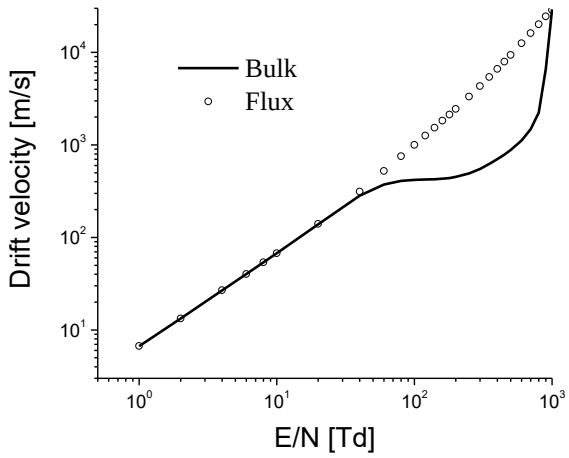

Figure 2: Drift velocity of H^+ ions in n-Butanol gas as a function of *E/N* at $T = 300$ K.

In Figure 3. we show the results of Monte Carlo simulation for reduced mobility as a function of *E/N*. Due to reactive collisions bulk and flux values of reduced mobility are separated.

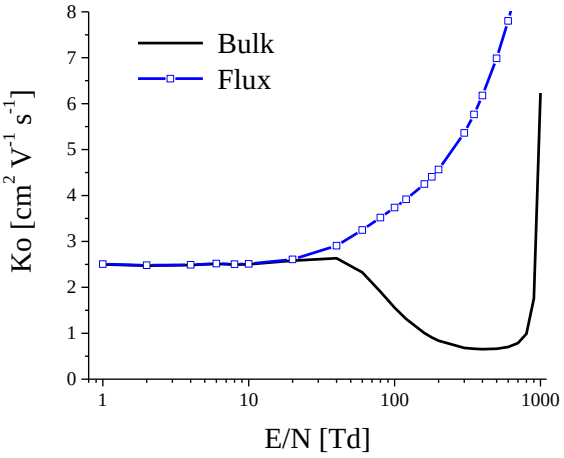

Figure 3: Reduced mobility of H^+ ions in n-Butanol gas as a function of *E/N* at *T*=300 K.

The mobility *K* of an ion is the quantity defined as the velocity attained by an ion moving through a gas under the unit electric field. One often exploits the reduced or standard mobility defined as:

$$K_0 = \frac{v_d}{N_0 E} N \,, \qquad (1)$$

where v_d is the drift velocity of the ion, *N* is the gas density at elevated temperature *T* and *E* is the electric field.

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