Electron transfer to phenyl boronic acid upon potassium collisions

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The degrading effect of low-energy electrons on biological tissue is acknowledged in the scientific community. These free or weakly bounded electrons may appear as a secondary product of irradiation and promote physiological molecules' dissociation through electronic attachment or electron transfer [1, 2]. It is extremely relevant to know how this dissociation pattern behaves with energy, not only from a toxicological perspective, but also as potential application for molecular manipulation and drug design. Boronic acids have been recently explored as promising pharmaceutical agents and as compounds with widespread biomedical applications, including enzyme inhibition, fluorescent dyes and cancer irradiation agents [3, 4]. Being so, it is of great interest to study the behaviour of these compounds after interaction with weakly bounded electrons that might exist in physiological medium.

In this study we characterize the fragmentation pattern of phenylboronic acid upon electron transfer, leading to the understanding of the existent dissociation channels and fundamentally contributing to medicinal chemistry applied to drug design. The experimental work was carried out in a crossed-beam atom-molecule apparatus, using the potassium atom as electron donor. The negative ions resultant of the target molecule's dissociation due to electron transfer were analysed with reflectron time-of-flight mass spectrometry. The fragmentation pattern of phenylboronic acid was traced as function of collision energy (10-1000 eV), described in figure 1. The two most yielded fragments were identified as BO^- and BO_2^-. Moreover, the reaction was shown to be selective, *i.e.* at energies below 100 eV it is mostly formed BO^-, while at energies above 100 eV it is mostly formed BO_2^-. To analyse the influence of the hybridization state of the boron atom, cyclohexylboronic acid's dissociation was also studied, which resulted in predominant formation of BO_2^-.

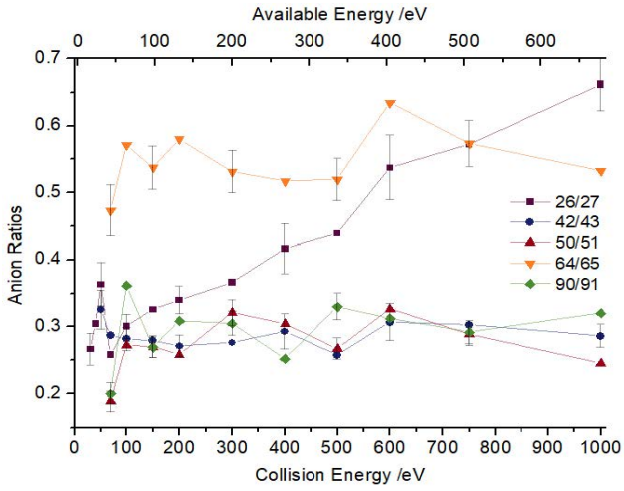

Figure 1: Branching ratio of boron containing anions formed upon electron transfer in potassium collisions as a function of energy.

[1] Boudaiffa B *et al* 2000 *Science* **287** 1658
[2] Alizadeh E *et al* 2015 *Annu. Rev. Phys. Chem.* **66** 379
[3] Brooks W L A and Sumerlin B S 2016 *Chem. Rev.* **116** 1375
[4] Trippier P C and McGuigan C 2010 *MedChemComm* **1** 183