

Partial Ionization Cross Sections for 1-Propanol and 1-Butanol

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Electron interactions with 1-propanol and 1-butanol are important for understanding the physical-chemical aspects in many technological applications, such as in pesticide formulations, among others. Accurate experimental measurements are also required to compare with, and assess theoretical predictions, as well as, for use as the input data for modelling applications. Electron collisions resulting in molecule ionization create a plethora of ionic fragments, radicals and neutral molecules. Therefore, understanding electron interactions with these alcohols is essential.

Experimental measurements of the cation created in electron impact ionization have been undertaken for the primary isomers of propanol and butanol using a Hidden Quadrupole Mass Spectrometer (EPIC 300). The mass spectra obtained reveals the relative probability of forming the various cations by either direct ionization, as well as dissociative ionization, using incident electrons of 70 eV. For many of the m/z values, more than one cation is possible, thus making the assignment of each peak observed difficult. In these cases, the appearance energy helps us to determine the identity of the fragments recorded. Partial ionization cross sections (PICS) were measured for a number of ionic fragments for 1-propanol and 1-butanol (shown in Figure 2), over the energy range 10-100 eV. PICS for 1-propanol were compared to the only data available in the literature, published by R. Rejoub *et al.* (shown in Figure 1), obtaining excellent agreement. As far as we know, we are reporting for the first time the PICS for 1-butanol in this work. Total ionization cross sections were also obtained by adding up the PICS for all cations measured for both molecular targets.

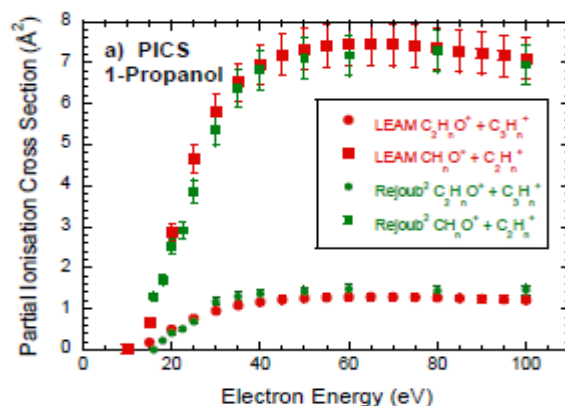


Figure 1. Partial Ionization Cross Section (PICS) for cations grouped within similar m/z to enable comparison with the data from Rejoub.

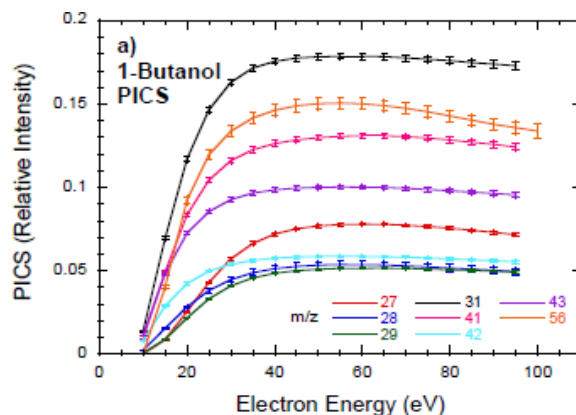


Figure 2. Partial Ionization Cross Section (PICS) for 8 most cations.

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Reference:

- [1] R. Rejoub, C. D. Morton, B. G. Lindsay and R. F. Stebbings, *J. Chem. Phys.*, vol. 118, p. 1756, 2003.