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Averaged electron collision cross sections for thermal mixtures of β-Alanine conformers in the gas phase

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Abstract: Beta-alanine (3-aminopropanoic acid, NH2-CH2-CH2-COOH) is the simplest β-amino acid; it is an isomer of α-alanine in which the amino group is bonded at the β carbon with the respect of carboxylic group (-COOH). Beta-Alanine is a solid at room temperature and found in zwitterionic form in condensed phase. Beta-alanine vaporizes at temperatures near 360 K and it is well-known that in the gas phase it exists as a mixture of charge-neutral conformers. As is often observed for amino acids, β-alanine is a very flexible molecule and it exists as a great variety of spatial stable conformations. In the gas phase, intramolecular interactions are important for stabilizing different spatial arrangements of atoms.In this work, we report a theoretical study comparing elastic cross sections for the 10 lowest-energy conformers of β-alanine in the gas phase for impact energies ranging from 1 to 10 eV. We also present averaged-cross sections which take into account relative populations of different conformers.The R-matrix method used in this work is the UKRMol implementation of the UK molecular R-matrix codes which is describe in details elsewhere Tennyson [1]. The cross sections are calculated in static-exchange-polarization (SEP level) using the same same approach in our previous work in Fujimoto et al [2] which calculations on two alanine conformers were performed. The eigenphase sums, resonance features, differential and integral cross sections are computed for each individual conformer. Resonance positions for the low-energy p* shape resonance are found to vary from 2.5 eV to 3.3 eV and the resonance widths from 0.2 eV to 0.5 eV. Averaged cross sections for thermal mixtures of the 10 conformers are presented and a comparison with various temperature-dependent sets of relative populations based on relative Gibbs free energies are shown. A comparison with previous results for the α-alanine [3] isomer is also done.We believe that these results should be more reliable for comparison with measured data at temperature where the gas phase molecule is experimentally accessible.

Key-words: cross sections, amino acids, β-alanine
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