Positron Interactions with Nitrogen and Oxygen and Pyridine Molecules: Elastic, Inelastic and Total Cross Sections

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Positrons are difficult to handle experimentally, yet their collisional cross sections are necessary for particle track models of medical techniques such as positron emission tomography and in situ ion therapy dose calculation. The use of relatively simple approximations, many built from the first Born approximation [1], has been shown to provide accurate cross-sectional collision data for electron and positron collisions down to collision energies below 100 eV. The available experimental data [2] are always used to benchmark these calculations, and any changes to an approximation are subject to scrutiny.

Improvements to the IAM-SCAR calculation procedure [3], [4], a theoretical approach based on the optical potential method and the geometry of a molecule, have increased its accuracy well below this limit. When applied to electron-molecule scattering, improvements were seen for the cross-sections of collisions with simple molecules when compared with higher levels of theory. The improvements include the screened interference of the scattering wave due to the multiple scattering from the atoms in the molecule, and are now included for both the electron and positron scattering formulations of the IAM-SCAR+I code.

The changes to positron-molecule scattering are explored here on the N_2, O_2 and pyridine [5] molecules. The effects on the cross section are pronounced in the collisional energy range below 100 eV, and the accuracy of the IAM-SCAR method above 100 eV is maintained. The new calculations are compared to other recent calculations and experimental data.

References

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