Electron-impact total ionization cross sections for neutral Erythrulose $C_4H_8O_4$

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Electron-impact total ionization cross sections for neutral Erythrulose ($C_4H_8O_4$) were calculated over 11–5000 eV using the orbital-resolved Binary-Encounter-Bethe (BEB) model. The BEB orbital parameters were obtained from a pure single-point calculation at the ωB97X-D4/aug-cc-pVTZ optimized geometry. The calculated first ionization potential 10.175 eV was used for the HOMO ionization threshold. The total ionization cross section increases rapidly above threshold, reaches a broad maximum of 17.14×10^{-16} cm^2 at 87 eV and decreases smoothly at higher incident electron energies, consistent with the expected BEB energy dependence. Orbital-resolved analysis of 32 occupied molecular orbitals shows that ionization is dominated by the frontier valence region, the HOMO through HOMO-7 together contribute 51.8% of the total cross section at the peak energy. The HOMO and HOMO-1 channels individually provide 8.16% and 7.72%, respectively, of the peak cross section, demonstrating the importance of the least-bound valence electrons in electron-impact ionization of this oxygen rich molecule. In the absence of direct experimental ionization data for erythrulose, the present results provide a consistent theoretical reference dataset for future measurements and comparison with structurally related oxygenated molecules. Molecular-orbital population or visualization analysis should be used separately before assigning the frontier orbitals specifically to oxygen lone-pair or antibonding character.

References

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