Electron scattering from pyrimidine

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Synopsis

Electron scattering from pyrimidine (C₄H₄N₂) was investigated over a wide range of energies. Following different experimental and theoretical approaches, total, elastic and ionization cross sections as well as electron energy loss distributions were obtained.

Being the molecular base of biomolecules like cytosine, thymine, uracil, thiamin, and alloxan, pyrimidine is an interesting candidate for studying its electron interaction properties.

Here, we present experimental and theoretical results on electron scattering from gaseous pyrimidine in different energy ranges. First, total cross sections (CS) were determined by measuring the beam attenuation in the energy range 10-500 eV. This was done using a newly-constructed apparatus confining the electron beam magnetically along the central axis before, during and after scattering.

Electron-impact ionization experiments were carried out combining simultaneous electron and ion measurements with a time of flight analysis of the ionic fragments produced.

With an optical potential method based on the independent atom model and including the screening-corrected additivity rule [1], total and integral elastic and inelastic CS (1 eV - 10 keV) were also calculated in order to complement the experimental data. Generally, good agreement with our experimental results is observed in the common energy range. Furthermore, IAM-SCAR elastic differential CS are presented.

Electron Energy Loss (EEL) spectra were measured in the range 30-2000 eV using a transmission beam technique that measures a mixture of small angles [2]. In fig. 1, some examples of the energy loss distributions obtained are displayed. The average energy loss calculated from these spectra, together with our calculated inelastic cross section, has been used for computing the electron stopping power of pyrimidine for energies of 20-3000 eV.

Finally, the present theoretical and experimental results, complemented by data available in the literature where appropriate, will be used as the input data for the Low-Energy Particle Track Simulation (LEPTS), a Monte Carlo programme code capable of simulating electron and positron interactions in different media at the molecular level.

Figure 1. Electron energy loss distributions measured for pyrimidine at various incident energies.

References