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## Fragmentation of tryptophan molecule by low-energy electron-impact

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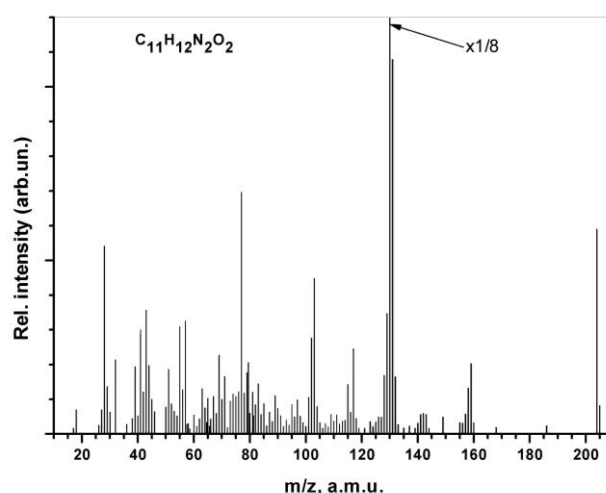
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**Synopsis** The fragmentation of a gas-phase tryptophan molecule by a low-energy (<70 eV) electron impact was studied both experimentally and theoretically. Various positively charged fragments have been observed and analyzed. A special attention is paid to the energy characteristics of the ionic fragment yield.

This paper deals with the studies of the low-energy (<150 eV) electron interaction with the tryptophan ( $C_{11}H_{12}N_2O_2$ ) molecule belonging to the essential amino acids in order to probe the intrinsic properties of the molecule and trace its chemical structure change(s) under the electron impact. Tryptophan is the metabolic precursor of serotonin, which plays an important role in a sleeping process and is necessary for normal growth and nitrogen balance in humans.

The experimental technique used in this work was described in detail in a number of our previous papers (see, e.g. [1]). A crossed-beam technique with the mass separation of the collision products by means of a magnetic mass-spectrometer was applied. The tryptophan molecule mass-spectrum measured by us is (see Fig. 1) generally close to that for the electron-impact ionization quoted in the NIST database [2] and that for the case of photoionization [3]. Structurally, tryptophan, as the aromatic amino acid, could be presented as the indole-3-alanine or the 3-methyleneindole bound at the  $C_\alpha$  position to a residue of a simple amino acid (glycine). The ion fragment  $C_9H_8N^+$  ( $m/z=130$  a.m.u.) corresponding to the dominant mass-spectrum peak (Fig. 1) is produced due to the  $C_\alpha-C_\beta$  ( $C_{10}-C_{11}$ ) bond rupture in the initial molecule. The fraction of the complementary ion with the mass of  $m/z=74$  a.m.u. (i.e.  $C_2H_4NO_2^+$ ) is about 1% of the main peak. Thus, the tryptophan molecule ionization proceeds mainly due to electron elimination by the methyleneindole group of the molecule at which the positive charge is predominantly localized.

In this mass-spectrum, we have found for the first time the production of the  $C_8H_5N_2^+$ ,  $C_9H_7N_2^+$  and  $C_9H_9N_2^+$  doubly charged ions having the  $m/z=57.5$ ,  $64.5$ ,  $65.5$ ,  $79.5$  a.m.u. masses. As our theoretical DFT approach-based analysis shows, some of them could be produced not only due to the direct initial molecule dissociation but also result from the secondary fragmentation of the 3-methyleneindole part of the parent tryptophan molecule.



**Figure 1.** Tryptophan molecule mass-spectrum.

We have also determined the ionization threshold  $E_i$  for the parent tryptophan molecule. Its absolute value of  $8.3\pm 0.1$  eV is slightly lower than the similar one obtained in our previous studies on the other aliphatic amino acids. The appearance potential  $E_{ap}$  for the  $C_9H_8N^+$  ion ( $m/z=130$  a.m.u.) produced from the parent molecule was determined by us to be  $9.1\pm 0.1$  eV and this value by 0.93 eV exceeds that obtained theoretically.

Thus, the analysis of the mass-spectrometric studies of the tryptophan molecule electron-impact fragmentation accompanied by theoretical calculations allowed the main dissociation mechanisms of the above molecule under the low-energy electron impact to be determined. Most of the peaks in the experimental mass spectrum were identified.

### References

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