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REFERENCE: Short visit grant, EIPAM

Beneficiary: Prof. Oddur Ingolfsson, Science Institute, University of Iceland, Reykjavik, Iceland.

Host: Prof. Stefan Matejcek, Comenius University, Bratislava, Slovakia.

Period: from 09/10/05 to 17/10/05; Duration 9 days; Place: Bratislava, Slovakia.

Reference code: EIPAM 766

SCIENTIFIC REPORT***Purpose of visit***

The purpose of the visit is to study dissociative electron attachment DEA to the amino acid L-Valine. The study is to be conducted in the gas phase using the crossed electron/molecule beams apparatus in Bratislava. This study is a part of the effort to better understand the intrinsic mechanism of anion and radical formation and fragmentation on the molecular level. We hope this study may contribute to our understanding of radiation damage to biomolecules as well as the processes of radical formation in the crystalline and polycrystalline valine under ionizing radiation.

Work carried out

During the visit we studied the dissociative electron attachment (DEA) to the amino acid L-Valine. The study was conducted in the gas phase using the crossed electron/molecule beams apparatus in Bratislava. The dissociative electron attachment to valine was studied in the gas phase in the energy range from 0-14 eV incident electron energy. In this energy range we recorded the electron energy dependency of fragments with the mass to charge ratio (m/Z): 116, 100, 74, 56, 45 26 and 17.

Results

We studied the energy dependency of the fragment formation in dissociative electron attachment to valine in the energy range from 0-14 eV incident electron energy. In this energy range dissociative electron attachment to valine was found to lead to the formation of fragments with the mass to charge ratio (m/Z) of 116, 100, 74, 56, 45 26 and 17. We attribute these mass to charge ratios to the fragments $(M-H)^-$, $(M-OH)^-$, $C_2H_4O_2N^-$, $C_4H_8^-$, $COOH^-$, CN^- and OH^- . The most pronounced of these fragments is the molecular ion that has lost one hydrogen $(M-H)^-$. This fragment is predominantly formed via a low energy resonance, reflected in the ion yield curve by an intensity maximum at about 1.2 eV. In addition to $M-H^-$ the fragment $M-OH^-$, $COOH^-$ and OH^- also show maxima at low energies, i.e. resonances at sub excitation energies located close to 2 eV. Core excited resonances are also observed in electron attachment to valine around 5-6 eV and about 8.5 eV. The later contribution is visible to some extent in all ion yield curves

except for $M-H^-$ the former on the other hand appears only through $(M-H)^-$, $(M-OH)^-$, $COOH^-$ and with low intensities through CN^- and OH^- formation. In addition a contribution close to 0 eV is observed in the COO^- and OH^- ion yield curves.

Interpretation of the data is in progress.

Colaborations.

Collaboration in the field of charged induced fragmentation of biologically relevant molecules was established between Prof. Stefan Matejcik, Comenius University, Bratislava, Slovakia and Prof. Oddur Ingolfsson, Science Institute, University of Iceland, Reykjavik, Iceland. Furthermore, the bases for collaboration is being explored between Prof. Pavel Mach, Comenius University, Bratislava, Slovakia and Prof. Oddur Ingolfsson, Science Institute, University of Iceland, Reykjavik, Iceland.

Publications

A publication of the results obtained during the visit is in preparation. Oral presentation will be given at the University of Iceland and conference contribution in oral or poster form might result from this work.