

Abstract Submitted
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Formation of H_3^+ in methanol : an intramolecular bond rearrangement study SANKAR DE, JYOTI RAJPUT, A. ROY, C.P. SAFVAN, Inter-University Accelerator Centre, New Delhi - 110067, India, P.N. GHOSH, Dept. of Physics, University of Calcutta, Kolkata - 700009, India — We report here results of TOF multi-hit coincidence experiment [1] that provide evidence for intramolecular reactions involving proton coagulation in methanol [2] after interaction with 1.2 MeV Ar^{8+} projectiles produced from the ECR ion source in the LEIBF laboratory of Inter-University Accelerator Centre, India. Quite remarkably, we have observed the formation of H_3^+ due to movement of protons within the multiply charged parent molecular ion through two-body process ($CH_3OH^{2+} \rightarrow H_3^+ + COH^+$) and such bond formation occurs before the Coulomb repulsion makes the fragment ions to fly apart. Analysis of the fragmentation pattern of CH_3OH^{2+} has been carried out using *ab initio* quantum chemical techniques. Structural calculations indicate that the formation of H_3^+ is the preferred pathway in the overall fragmentation dynamics of the ground state of this alcohol. The field generated from highly charged ions induces the system to rearrange its structure following a minimum energy pathway and form hydrogen molecular ions. Repeating the experiment with CH_3OD confirm our bond rearrangement phenomenon and establish that H_3^+ formation occurs only within the methyl group of the alcohol. Ref: [1] S. De et. al. NIMB, 243, 435 (2006) [2] Sankar De et. al. PRL, 97, 213201 (2006)

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