Photoionization cross sections of Ethylene Oxide

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In this work a theoretical study for photoionization of Ethylene Oxide is presented. Ethylene oxide, EtO, (C_2H_4O), also called oxyrane, is an important molecule in many areas, such as health, environmental, chemical industry and molecular bio/astrophysics. The photoionization cross sections for each of nine valence orbitals and also the summed cross sections are presented. The calculations are shown in for different approaches: dipole-length/velocity form, static-exchange and static-exchange-polarization levels. A correlation between the ion fragment appearance energies and the different electronic states of parent ion ($C_2H_4O^+$), is proposed. The partial PICS for each orbital shows which symmetry of continuum states are responsible for resonance features and it is also shown how the polarization effects affect the cross sections magnitudes near threshold. The summed PICS presents a maximum peak at 17.4eV in all approaches. The photoionization of C_2H_4O is more efficient at the photon energy of 17.4 eV, in the SEP-L level the contributions of six outermost orbitals to the peak are: $(2b_2)^{-1}$ (12.56%), $(6a_1)^{-1}$ (13.55%), $(3b_1)^{-1}$ (29.50%), $(1a_2)^{-1}$ (15.30%), $(5a_1)^{-1}$ (18.94%); $(1b_2)^{-1}$ (10.15%). The six outermost valence orbital are the ones who contribute the most to the summed PICS and is expected that the correspondent $C_2H_4O^+$ ion states should be the ones leading to major ion fragments. The summed cross section of all valence orbitals of Ethylene Oxide is compared with the results for acetaldehyde and an analysis suggest that the photoionization cross sections, in a given energy range, can be used to identify isomers.