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Study of the Different Features of the Conformers of Alkanethiols in Ionization Process Using One-photon Mass Analyzed Threshold Ionization

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In this study we investigated the difference of the conformers of alkanethiols in ionization process by one-photon mass-analyzed threshold ionization spectroscopy. From the experimental results we obtained the adiabatic ionization energies of the molecules and the vibrational frequencies of the cation states. We analyzed the experimental results by using the *ab initio* and density functional calculations. The deuterium substitution effect and calculation of Franck-Condon factors confirm our interpretation of the results.