Mgr Iwona Kosendiak
Title of PhD thesis „Conformations and photochemistry of glycolic acid and its molecular complexes. Spectroscopic and theoretical research.”
Supervisor: Prof. dr hab. Maria Wierzejewska
Auxiliary supervisor: Dr Justyna Krupa

Abstract

The subject of the research conducted in this study was glycolic acid (GA), its dimers and molecular complexes with dinitrogen. Glycolic acid has been identified as a tropospheric pollution of natural and industrial origin. For this reason, it was decided to investigate the possibility of GA aggregates formation and GA interactions with nitrogen, the main air component. Afterwards it was important to determine the effect of electromagnetic radiation, of different spectral ranges on the acid and its complexes. Although the idea of the dissertation is derived from the atmospheric chemistry, the presented investigations are classified as basic research.

The experimental studies were carried out using the low-temperature matrix isolation technique coupled with FTIR spectroscopy at the Faculty of Chemistry, University of Wrocław or coupled with Raman spectroscopy at the Faculty of Chemistry and Nanoscience Center of the University of Jyväskylä in Finland. Argon, nitrogen and nitrogen doped argon in the ratio N_2:Ar 1:4000 were used as matrix gases. Thermal phenomena occurring in the matrix heating processes were used to study glycolic acid dimers and nitrogen complexes. Monochromatic radiation from the near infrared (NIR), visible light (VIS) and ultraviolet (UV) ranges was used to determine the photochemical processes of GA and its nitrogen complexes.

Interpretation of experimental results was supported by theoretical research carried out at the DFT and MP2 levels with various functional basis sets. These studies provided valuable structural and spectroscopic information for the studied systems. The results of AIM calculations made possible to determine the hydrogen bonds or van der Waals interactions occurring between the studied molecules.The structures of GA dimers were optimized and the interactions between acid molecules were determined. Three dimer structures were identified in the FTIR spectra of GA isolated in argon matrix. Raman spectra of glycolic acid isolated in an argon matrix were obtained and described. The processes of GA isomerization in the argon matrix under the influence of visible light radiation were determined using Raman spectroscopy as a detection system. The structures of glycolic acid dinitrogen complexes were optimized and their interactions were determined. By means of FTIR spectroscopy, the structures of GA···N_2 complexes were identified, the influence of thermal effects, NIR and UV radiation on the complexes were analyzed. Raman spectra of GA···N_2 complexes were obtained and interpreted. Visible light excitation of complexes was determined by Raman spectroscopy. Photoisomerization and photodecomposition under UV

excitation of glycolic acid isolated in argon and nitrogen matrices were observed and described. The products of photolysis were identified in the form of molecular complexes of aldehyde with water, carbon monoxide and carbon dioxide, and a complex of water with carbon monoxide.