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FTIR matrix isolation and theoretical studies of glycolic acid dimers.

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Streszczenie

Glycolic acid (GA) dimers were studied in low temperature argon matrices by means of FTIR spectroscopy. Experimentally, the dimers were produced when monomeric glycolic acid molecules were thermally mobilized upon annealing of argon matrices at 25–35K. The experimental spectra observed upon annealing indicate the presence of three different dimer structures. Computationally, MP2 and DFT calculations were used to study the potential dimer species in order to scrutinize the possible dimer structures, their energetics and their spectral features. Altogether 27 local minima were found for dimer structures for the three lowest conformers of glycolic acid considered based on previous studies on glycolic monomer in argon matrices. Comparing the computational and the experimental spectra especially in the OH and CO stretching regions it was possible to assign the experimental observations to the three most stable dimer species.

Słowa kluczowe

infrared spectra, Hydrogen bond, MP2, DFT

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