

Theoretical studies on the molecular structure, conformational preferences, topological and vibrational analysis of allicin.

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The molecular structure, conformational preferences, topological and vibrational analysis of allicin has been investigated at two different approaches. Calculations have been carried out on static (DFT and MP2) levels with an assortment of Dunning's basis sets and dynamic CPMD simulations. In this both case within the isolated molecule approximation. The results point out that at least twenty different conformers coexist on the PES as confirmed by the flexible character of this molecule. The topological analysis of ELF showed very similar nature of the S—S and S—O bonds. The infrared spectrum has been calculated, and a comparative vibrational analysis has been performed.

Słowa kluczowe

Allicin, Garlic, 2-Propene-1-sulphinothioic acid S-2-propenyl ester, Disulphides, Disulphide bond (bridge), Car–Parrinello molecular dynamics (CPMD), Electron localization function (ELF), Potential energy surface (PES)

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