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Experimental and theoretical UV characterizations of acetylacetone and its isomers.

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Kolekcja

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Streszczenie

Cryogenic matrix isolation experiments have allowed the measurement of the UV absorption spectra of the high-energy non-chelated isomers of acetylacetone, these isomers being produced by UV irradiation of the stable chelated form. Their identification has been done by coupling selective UV-induced isomerization, infrared spectroscopy, and harmonic vibrational frequency calculations using density functional theory. The relative energies of the chelated and non-chelated forms of acetylacetone in the S_0 state have been obtained using density functional theory and coupled-cluster methods. For each isomer of acetylacetone, we have calculated the UV transition energies and dipole oscillator strengths using the excited-state coupled-cluster methods, including EOMCCSD (equation-of-motion coupled-cluster method with singles and doubles) and CR-EOMCCSD(T) (the completely renormalized EOMCC approach with singles, doubles, and non-iterative triples). For dipole-allowed transition energies, there is a very good agreement between experiment and theory. In particular, the CR-EOMCCSD(T) approach explains the blue shift in the electronic spectrum due to the formation of the non-chelated species after the UV irradiation of the chelated form of acetylacetone. Both experiment and CR-EOMCCSD(T) theory identify two among the seven non-chelated forms to be characterized by red-shifted UV transitions relative to the remaining five non-chelated isomers.

Słowa kluczowe

Chemical calculations, Energy, Irradiation, Molecular structure, Quantum mechanics

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