

Vibrational spectra of racemic and enantiomeric malic acids.

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The IR and Raman spectra of racemic (DL-) and both enantiomeric (L-andD-) forms of malic acids and also their silver salts and deuterated analogues were measured in the polycrystalline state in the range $4000 - 100 \text{ cm}^{-1}$. Significant differences in the spectra of the racemic and enantiomeric forms of malic acid were described for the first time and are discussed in relation to the structural features, including crystal symmetry, geometric parameter distinctions and hydrogen bonding. The most significant spectral differences were noted in the ranges $3000 - 2800$ and $1740 - 1630 \text{ cm}^{-1}$. In the (CH) stretching region distinctions were strongly pronounced in the Raman spectra and the observed pattern was ascribed to crystal symmetry differences. In the second region differences were visible in both the IR and Raman spectra and they were explained as a result of distinctions in the geometric properties of carboxyl-dimer rings of the L-and DL-forms, namely two non-equivalent types of H-bonded carboxyl-dimer rings are present in the crystal of DL-form, which results in a doublet in the (CO) stretching region. In the case of the enantiomeric form, all H-bonded carboxyl-dimer rings are equivalent, so a single (CO) band is observed in their spectra. Other differences in the spectra of these species were observed in the region below 1500 cm^{-1} but their explanation is less straightforward.

Słowa kluczowe

malic acid enantiomers, deuterated malic acid, silver malate, Raman spectra, infrared spectra

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