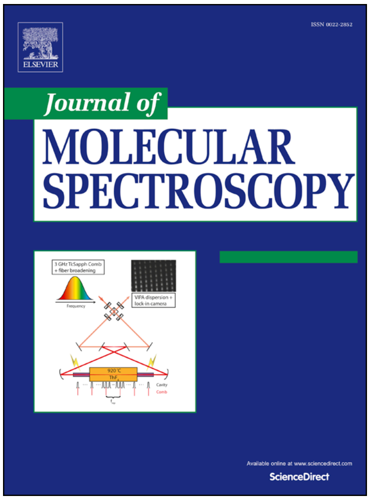

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Vibrationally-Resolved Photoelectron Spectroscopy and Photoelectron Circular Dichroism of Bicyclic Monoterpene Enantiomers

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Abstract

The photoionization of four chiral bicyclic monoterpene isomers, α-pinene, β-pinene, 3-carene and sabinene — all commonly found constituents in essential natural oils — has been studied using synchrotron radiation and compared to recent findings for the cyclic isomer limonene. Slow photoelectron spectra (SPES) are recorded between threshold and an energy of 10.5 eV. In the case of limonene, α-pinene, and 3-carene, vibrational structure is observed in the ground ionic state and attributed to a C=C double bond stretching in the cation, using Franck-Condon vibrational band simulations. The photoelectron circular dichroism (PECD) is examined for specific enantiomers of these terpenes, and vibrational modification of the forward-backward photoelectron asymmetry detected by PECD can be tentatively identified, even when the corresponding SPES is unstructured. Large chiral asymmetry factors are found at low binding energies for the pinenes and 3-carene, with α-pinene in particular displaying a 37% forward-backward photoelectron asymmetry, believed to be a record chiroptical asymmetry for randomly-oriented, non-interacting molecules.