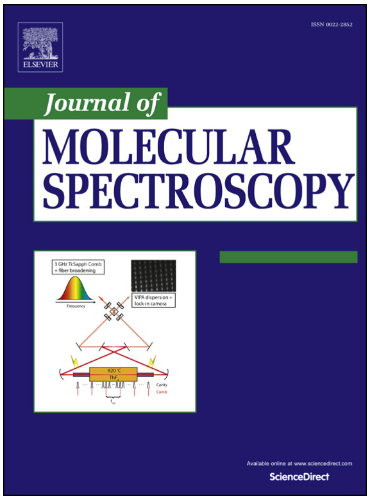

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The complete molecular geometry and electric dipole moment of salicyl aldehyde from rotational spectroscopy

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Abstract

The pure rotational spectrum of salicyl aldehyde, $C_7H_6O_2$, a classic molecule with an OH$\cdots$O intramolecular hydrogen bond, was investigated in detail with several different spectrometers. Supersonic expansion measurements at 8-18 GHz were used to determine rotational constants for 26 different isotopologues, either in natural abundance or prepared synthetically, and including single substitution of each of the 15 atoms in the molecule. Further measurements of the room temperature rotational spectrum at 8-230 GHz allowed assignment of the five lowest excited vibrational states. Their rotational constants were used to calibrate anharmonic force field calculations, which were then used to determine the semi-experimental equilibrium r_e^{SE} geometry. This is compared with several other structural determinations and with quantum chemistry calculations. In addition, Stark measurements in supersonic expansion were used to determine the electric dipole moment of salicyl aldehyde.

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