

MICROWAVE SPECTRUM AND STRUCTURE OF THIOBENZOIC ACID (C₆H₅COSH)

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We report the characterization of thiobenzoic acid (C₆H₅COSH) by broadband and cavity microwave spectroscopy. Assignment of the chirped-pulse spectrum was carried out with the DAPPERS software. Using cavity spectroscopy, isotopologue spectra were observed for all carbons (¹³C), the oxygen (¹⁸O), and the sulfur (³⁴S and ³³S). Hyperfine structure for ³³S was observed and quadrupole coupling constants were determined. Spectra of the deuterated species were obtained via H/D exchange in a mixture of thiobenzoic acid and D₂O. A Kraitchman analysis was performed using all heavy-atom isotopic data, and yielded excellent agreement with M06-2X 6-311++G(d,p) calculations. No conformers or tautomers were observed.