ACTIVATION OF C-H BONDS: PURE ROTATIONAL SPECTROSCOPY OF HZnCH₃ (\tilde{X}^1A_1)

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The pure rotational spectrum of HZnCH₃ has been observed in its ground electronic state ($\tilde{X}^{1}A_{1}$) using both direct absorption and Fourier transform microwave techniques in the frequency range 18-516 GHz. Twelve rotational transitions of this symmetric top species were recorded in K-ladders up to K = 7. The molecule was synthesized from Zn(CH₃)₂ in an AC discharge and also from Zn (vapor) + CH₄ with a DC discharge. From measurements of the spectra of various isotopic species (⁶⁶Zn, ⁶⁷Zn, ⁶⁸Zn, ¹³C, and ²H), an accurate structure has been determined. The H-C-H bond angle was found to be 108.7°, slightly smaller than that in ZnCH₃ or CH₄. In addition, nuclear spin-rotation (I · J) interactions with the methyl hydrogen nuclei and electric quadrupole coupling from the ⁶⁷Zn nucleus were resolved in the FTMW spectrum. From these data, hyperfine parameters have been established. The value of eqQ = -109.125(11) MHz indicates that the bonds to zinc are primarily covalent. Detection of this species, especially via the Zn + CH₄ pathway, is a good indication of the ability of metal atoms to insert into C-H bonds.