ACTIVATION OF C-H BONDS: PURE ROTATIONAL SPECTROSCOPY OF $HZnCH_3$ ($\tilde{X}\ ^1A_1$)

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The pure rotational spectrum of $HZnCH_3$ has been observed in its ground electronic state ($\tilde{X}\ ^1A_1$) 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 $Zn(CH_3)_2$ in an AC discharge and also from Zn (vapor) + CH_4 with a DC discharge. From measurements of the spectra of various isotopic species (^{66}Zn, ^{67}Zn, ^{68}Zn, ^{13}C, and ^{2}H), an accurate structure has been determined. The H-C-H bond angle was found to be $108.7°$, slightly smaller than that in $ZnCH_3$ or CH_4. In addition, nuclear spin-rotation (I · J) interactions with the methyl hydrogen nuclei and electric quadrupole coupling from the ^{67}Zn 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 + CH_4 pathway, is a good indication of the ability of metal atoms to insert into C-H bonds.