MILLIMETER-WAVE STUDIES OF THE ISOTOPOLOGUES OF $IZnCH_3(X^1A_1)$: GEOMETRIC PARAMETERS AND EVIDENCE FOR ZINC INSERTION

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The laboratory detection of gas-phase $IZnCH_3$ (X^1A_1), using millimeter-wave direct absorption methods, was reported previously. This work has been extended by the measurement of the pure rotational spectrum of several isotopolgues: $I^{64}ZnCH_3$, $I^{66}ZnCH_3$, $I^{64}ZnCD_3$, and $I^{64}Zn^{13}CH_3$. These species were all created by the reaction of zinc vapor with CH_3I, CD_3I, or $^{13}CH_3I$ in the presence of a DC discharge. The zinc isotopolgues were observed in natural abundance. Rotational transitions in the range $256-293$ GHz (J = 109 $\leftarrow$ 108 to J = 132 $\leftarrow$ 131, for K = 0 to 6) have been recorded for each species. From these measurements, an r_0 structure has been determined. This structure was found to be in good agreement with previous DFT calculations. Interestingly, the 110.2° Zn – C – H bond angle of $IZnCH_3$ is identical to that of the hydrogen substituted zinc insertion complex $HZnCH_3$ (X^1A_1). These data are further evidence that $IZnCH_3$ is not created by the generation of free radical fragments, but by the direct insertion of atomic zinc into the C – I bond of iodomethane.