STRUCTURE OF THE MODEL GRIGNARD-TYPE REAGENT $ClZnCH_3$ ($\tilde{X}^1A_1$) BY MILLIMETER-WAVE SPECTROSCOPY

MARK BURTON, *Department of Chemistry and Biochemistry, University of Arizona, Tucson, AZ, USA*; NAZIFA TABASSUM, *Department of Molecular and Cellular Biology, University of Arizona, Tucson, AZ, USA*; LUCY M. ZIURYS, *Department of Chemistry and Biochemistry; Department of Astronomy, Arizona Radio Observatory, University of Arizona, Tuscon, AZ, USA*.

Pure rotational spectra of the $^{37}ClZnCH_3$, $ClZnCD_3$, and $ClZn^{13}CH_3$ isotopologues of monomeric $ClZnCH_3$ ($\tilde{X}^1A_1$) have been recorded using millimeter-wave direct absorption techniques in the frequency range 263 – 303 GHz. These species were synthesized in the gas phase in a DC discharge by the reaction of zinc vapor, produced in a Broida-type oven, with $^{37}ClCH_3$ (in natural chlorine abundance), $ClCD_3$, or $Cl^{13}CH_3$. The data for each isotopologue were analyzed with a symmetric top Hamiltonian and rotational and centrifugal constants determined. In combination with previous measurements of $Cl^{64}ZnCH_3$, $Cl^{66}ZnCH_3$, and $Cl^{68}ZnCH_3$, an $r_m^{(2)}$ structure was determined for this organozinc compound. The bond lengths were calculated to be r_{Cl-Zn} = 2.0831(1) Å, r_{Zn-C} = 1.9085(1) Å, and r_{C-H} = 1.1806(5) Å. The H-C-H bond angle was found to be 110.5° – slightly larger than that in methane. These data serve to benchmark future structure calculations of organozinc compounds, which are widely used in organic synthesis.