THE STRUCTURE OF ScC_2 ($\tilde{X}^2A_1$): A COMBINED FOURIER TRANSFORM MICROWAVE/MILLIMETER-WAVE SPECTROSCOPY AND COMPUTATIONAL STUDY

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Pure rotational spectra of $Sc^{13}C_2$ ($\tilde{X}^2A_1$) and $Sc^{12}C^{13}C$ ($\tilde{X}^2A'$) have been obtained using Fourier Transform microwave/millimeter-wave methods. These molecules were synthesized from the combination of scandium vapor, produce via laser ablation, with mixtures of $^{13}CH_4$ or $^{13}CH_4/^{12}CH_4$, diluted in argon. The four lowest a-type rotational transitions were observed for both species in the frequency range of 14 – 61 GHz. Each exhibit hyperfine splittings due to the nuclear spins of ^{13}C (I = 1/2) and/or Sc (I = 7/2). Rotational, spin-rotation, and hyperfine parameters have been determined for these isotopologues, and a refined structure for ScC_2 established. In addition, a quartic force field was calculated for ScC_2 and its isotopologues using a highly accurate coupled cluster-based composite method, incorporating complete basis set extrapolation, scalar relativistic corrections, outer core and inner core electron correlation, and higher-order valence correlation effects. The ratio of experimental to theoretical (B+C) values is 1.005 for all calculated isotopologues, yielding a promising route towards predictive gas phase rotational spectroscopy for new metal-carbon bearing radicals.