

FOURIER TRANSFORM MICROWAVE SPECTROSCOPY OF Sc^{13}C_2 AND $\text{Sc}^{12}\text{C}^{13}\text{C}$: ESTABLISHING AN ACCURATE STRUCTURE OF ScC_2 ($\tilde{X}^2\text{A}_1$)

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Pure rotational spectra of Sc^{13}C_2 and $\text{Sc}^{12}\text{C}^{13}\text{C}$ ($\tilde{X}^2\text{A}_1$) have been obtained using Fourier Transform Microwave methods. These molecules were created from scandium vapor in combination with $^{13}\text{CH}_4$ and/or $^{12}\text{CH}_4$, diluted in argon, using a Discharge Assisted Laser Ablation Source (DALAS). Transitions in the frequency range of 14-30 GHz were observed for both species including hyperfine splitting due to the nuclear spin of Sc ($I = 7/2$) and ^{13}C ($I = 1/2$). Rotational, spin-rotational, and hyperfine constants have been determined for Sc^{13}C_2 and $\text{Sc}^{12}\text{C}^{13}\text{C}$, as well as a refined structure for ScC_2 . In agreement with theoretical calculations and previous Sc^{12}C_2 results, these data confirm a cyclic (or T-shaped) structure for this molecule.

Scandium carbides have been shown to form endohedral-doped fullerenes, which have unique electrical and magnetic properties due to electron transfer between the metal and the carbon-cage. Spectroscopy of ScC_2 provides data on model systems for comparison with theory.