

THE PURE ROTATIONAL SPECTRA AND HYPERFINE STRUCTURES OF SCANDIUM MONOHALIDES

WEI LIN, SARA A. BEATON, COREY J. EVANS, and MICHAEL C. L. GERRY, *Department of Chemistry, University of British Columbia, 2036 Main Mall, Vancouver, B. C., Canada, V6T 1Z1.*

The pure rotational spectra of ScF, ScCl and ScBr have been recorded using Fourier transform microwave spectroscopy in the frequency range 6-26 GHz. The molecules were generated by laser ablation of a solid Sc rod in the presence of a low percentage of SF₆, Cl₂ or Br₂, respectively, in argon. They are the first measurements of the pure rotational spectra of the X¹Σ⁺ states for all three molecules. For ScF, only the $J=1-0$ rotational transition could be observed in the frequency range of our spectrometer. The electric quadrupole coupling constant and the spin-rotation constant for Sc have been determined. For ScCl, the two lowest rotational transitions were measured. The electric quadrupole constants and the spin-rotation constants of Sc and both isotopes of Cl have been determined. For ScBr, for which there had previously been no rotational spectrum of any kind, transitions of both Br isotopes have been measured. The rotational constants have been used to evaluate its geometry. The hyperfine parameters for the three molecules are interpreted in terms of the electronic structure and chemical bonding. Comparisons will be made to similar molecules.