

THE LOW-LYING ELECTRONIC STATES OF SCANDIUM MONOCARBIDE, ScC

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Extensive wavelength-resolved fluorescence studies have been carried out for the electronic bands of ScC and Sc¹³C lying in the range 14000 - 16000 cm⁻¹. Taken together with detailed rotational analyses of these bands, these studies have clarified the natures of the low-lying electronic states. The ground state is an $\Omega = 3/2$ state, with a vibrational frequency of 648 cm⁻¹, and the first excited electronic state is an $\Omega = 5/2$ state, with a frequency of 712 cm⁻¹, lying 155.54 cm⁻¹ higher. These states are assigned as the lowest spin-orbit components of X²Π_i and a⁴Π_i, respectively. The quartet nature of the a state is confirmed by the observation of the ⁴Π_{3/2} component, 18.71 cm⁻¹ above the ⁴Π_{5/2} component. The strongest bands in the region studied are two ⁴Δ_{7/2} - ⁴Π_{5/2} transitions, where the upper states lie 14355 and 15445 cm⁻¹ above X²Π_{3/2}. Extensive doublet-quartet mixing occurs, which results in some complicated emission patterns. The energy order, a⁴Π above X²Π, is consistent with the ab initio calculations of Kalemios et al.,^a but differs from that found by Simard et al in the isoelectronic YC molecule.^b

^aA. Kalemios, A. Mavridis and J.F. Harrison, *J. Phys. Chem.* **A155**, 755 (2001).

^bB. Simard, P.A. Hackett and W.J. Balfour, *Chem. Phys. Lett.*, **230**, 103 (1994).