

## THE LOW-LYING ELECTRONIC STATES OF SCANDIUM MONOCARBIDE, ScC

CHIAO-WEI CHEN, ANTHONY MERER, YEN-CHU HSU, *Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, Taiwan.*

Extensive wavelength-resolved fluorescence studies have been carried out for the electronic bands of ScC and Sc<sup>13</sup>C lying in the range 14000 - 16000 cm<sup>-1</sup>. 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<sup>-1</sup>, and the first excited electronic state is an  $\Omega = 5/2$  state, with a frequency of 712 cm<sup>-1</sup>, lying 155.54 cm<sup>-1</sup> higher. These states are assigned as the lowest spin-orbit components of X<sup>2</sup>Π<sub>i</sub> and a<sup>4</sup>Π<sub>i</sub>, respectively. The quartet nature of the a state is confirmed by the observation of the <sup>4</sup>Π<sub>3/2</sub> component, 18.71 cm<sup>-1</sup> above the <sup>4</sup>Π<sub>5/2</sub> component. The strongest bands in the region studied are two <sup>4</sup>Δ<sub>7/2</sub> - <sup>4</sup>Π<sub>5/2</sub> transitions, where the upper states lie 14355 and 15445 cm<sup>-1</sup> above X<sup>2</sup>Π<sub>3/2</sub>. Extensive doublet-quartet mixing occurs, which results in some complicated emission patterns. The energy order, a<sup>4</sup>Π above X<sup>2</sup>Π, is consistent with the ab initio calculations of Kalemios et al.,<sup>a</sup> but differs from that found by Simard et al in the isoelectronic YC molecule.<sup>b</sup>

---

<sup>a</sup>A. Kalemios, A. Mavridis and J.F. Harrison, *J. Phys. Chem.* **A155**, 755 (2001).

<sup>b</sup>B. Simard, P.A. Hackett and W.J. Balfour, *Chem. Phys. Lett.*, **230**, 103 (1994).