Optical Spectroscopy of the Niobium Methylidyne Free Radical, NbCH

David A. Gillett, M. Barnes, G.F. Metha[a], K. Athanassenas and A.J. Merer, *Department of Chemistry, University of British Columbia, 2036 Main Mall, Vancouver, B.C. V6T 1Z1, Canada.*

Pulsed laser excitation spectra of niobium methylidyne (NbCH) have revealed 29 bands for NbCH and 17 for NbCD in the wavelength region 545–625 nm. NbCH was produced in a supersonic free jet expansion in helium by reacting methane with laser ablated niobium (355 nm Nd:YAG).
The band structure can be organised into transitions involving excitation from the $\tilde{X}^3\Delta_1$ ground state to numerous vibronic levels of two close lying excited electronic states with Ω=2 and Ω=1, whose origins are near 16050 cm^{-1} and 16250 cm^{-1} respectively. Upper state assignments are complicated by a large vibronic (Renner-Teller) coupling between the two states and random perturbations due to 'dark' states.
Wavelength resolved fluorescence spectra of NbCH(NbCD) have allowed us to determine two of the three $\tilde{X}$ state vibrational fundamentals:

$$\nu_2 = 603(466)\,\mathrm{cm}^{-1}, \nu_3 = 905(858)\,\mathrm{cm}^{-1}.$$

Work is currently underway to record the $(0,0)$ bands at cw laser resolution, which will allow accurate structural parameters to be determined and will resolve the niobium nuclear hyperfine structure. Modelling of the Renner-Teller interaction between the vibronic levels of the two close lying excited electronic states is also in progress.

[a]Present address: School of Chemistry, University of Sydney, Building F11, Sydney, N.S.W. 2006, Australia