FOURIER TRANSFORM EMISSION SPECTROSCOPY AND AB INITIO CALCULATIONS ON NbCl AND TaCl

R. S. RAM, *Department of Chemistry, University of Arizona, Tucson, AZ 85721*; A. G. ADAM, *Department of Chemistry, University of New Brunswick, Frederiction, N.B., Canada, E3B 6E2*; N. RINSKOPF and J. LIÉVIN, *Laboratoire de Chimie Physique Moléculaire, CP 160/09, Av. F. D. Roosevelt 50, Bruxelles, Belgium*; and P. F. BERNATH, *Department of Chemistry, University of Waterloo, Waterloo, Ont., Canada N2L 3G1*.

The emission spectra of NbCl and TaCl have been recorded in the 3000-20000 cm^{-1} region using a Fourier transform spectrometer. The bands were observed by microwave excitation of a mixture of $NbCl_5$ or $TaCl_3$ vapor and He. The TaCl bands have also been recorded by laser excitation spectroscopy in a jet expansion source at the University of New Brunswick. Two groups of NbCl bands observed in the 6500-7000 cm^{-1} and 9000-11000 cm^{-1} regions have been assigned as two electronic transitions with $\Delta\Omega = 1$ (R, P and Q branches) and $\Delta\Omega = 0$ (R and P branches), respectively. The 6500-7000 cm^{-1} bands consist of five subbands, while four subbands have been assigned in the 9000-11000 cm^{-1} region. The absence of Ω-doubling in the two transitions or a combination defect in $\Delta\Omega = 1$ transition indicates that high Λ states are involved. Ab initio calculations have been performed on NbCl and the spectroscopic properties of the low-lying electronic states have been predicted. The results of our experimental and theoretical studies will be presented. The observed TaCl bands have been classified into three groups with different lower state molecular constants. Out of the three lower states, the two states with $\Omega = 0^+$ and $\Omega = 2$ have been found to be very close in energy and the ground state of TaCl is one of these two states.