SPECTROSCOPY OF NbO: CHARACTERIZATION OF THE DOUBLET MANIFOLD

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Doublet bands of NbO in the near infrared have been recorded in emission with FTS techniques using an electrodeless 2450 MHz discharge through He(Ar) + O_2 + $NbCl_5$. Color *Loomis-Wood* diagrams have been used extensively throughout the analysis of the bands. The observed transitions involve the vibrational levels v = 0-4 of a new low-lying $a^2\Delta$ state of configuration $\sigma^2\delta$, with T_e = 4025.5597, ω_e = 1015.2016, A_e = 471.3000 and B_e = 0.4418661 cm^{-1}, as well as four additional doublet states [$c^2\Pi$, $d^2\Delta_i$, $e^2\Phi$ and $f^2\Pi_i$]. Furthermore, a $^2\Sigma$ state, assigned as $b^2\Sigma^-$, has been observed through the $c^2\Pi(v = 0) \rightarrow b^2\Sigma^-(v = 0,1)$ transitions in the 1.6 μm region. The energy levels of the doublet states of this work have been linked to calculated $X^4\Sigma^-$ ground state energy levels using the narrow lines around J'' = 35.5 of the $c^2\Pi \rightarrow X^4\Sigma^-$ intercombination system near 700 nm as a bridge between quartet and doublet manifolds. The linkage is believed to be accurate to within 0.005 cm^{-1}, and will hopefully permit a future systematic search for other intercombination transitions through LIF methods. The $c^2\Pi_{1/2}$ (v = 0-2) levels are locally perturbed. Evidence is presented suggesting that the perturbing levels are the vibrational levels v = 14-16 of the $X^4\Sigma^-$ ground state. Most of the excited doublet states lie only slightly above or below the well-known $B^4\Pi$ state near 15000 cm^{-1}. This gives rise to a surprisingly high density of states in this energy region. Case (*a*) parameters have been derived for all the states involved in the present work. Nuclear hyperfine effects are very weak in the orbitally degenerate states of the doublet manifold, manifested only through slight line broadenings at low *J*. On the other hand, the $b^2\Sigma^-$ state shows considerable magnetic hyperfine structure (b = -0.08196 cm^{-1}), and is for this reason probably a pure $\sigma\delta^2$ state, where the σ molecular orbital is closely related to the Nb_{5s} atomic orbital. High-level calculations, including spin-orbit effects, have been performed on NbO, and the results are in fair agreement with the observations. However, the predicted low-lying $^2\Sigma^+$ state has not been located experimentally. The same calculations suggest that the doublet manifold also contains a low-lying $^2\Gamma$ state. An unanalyzed band in the 11900 cm^{-1} region with impressive hyperfine structure has been preliminarily assigned as the $A^4\Pi \rightarrow X^4\Sigma^-$ transition. The analysis of the doublet manifold of NbS has also been carried out, and preliminary results of this analysis will be presented.