EMISSION SPECTROSCOPY AND *AB INITIO* CALCULATIONS ON TaN

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The emission spectra of TaN have been investigated in the 9000-25000 cm^{-1} region using a Fourier transform spectrometer. The spectra were observed in a tantalum hollow cathode lamp by discharging a mixture of 1.5 Torr of Ne and about 6 mTorr of N_2. In addition to previously known bands, numerous additional bands were observed and assigned to a number of new transitions. The spectroscopic properties of the low-lying electronic states of TaN were also predicted by *ab initio* calculations. A $^1\Sigma^+$ state, with equilibrium constants of B_e=0.457907(11) cm^{-1}, α_e= 0.002350(22) cm^{-1} and r_e=1.682999(20) Å, has been identified as the ground state of TaN based on our experimental observations supported by the *ab initio* results. This state is followed by a $^3\Delta_1$ state at 2827 cm^{-1} above the ground state. The higher energy region consists of several singlet and the triplet states, with the triplet states having Hund's case (c) characteristics. Most of the excited states (Ω states) are affected by strong interactions with nearby states.