COMPREHENSIVE ANALYSIS OF THE A $^4\Pi$ - X $^4\Sigma^-$ TRANSITION OF MOLYBDENUM NITRIDE, MoN: LIMITATIONS OF A HUND'S CASE(a) ANALYSIS

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Transition metal nitrides are of growing interest due to their catalytic, energy storage, sensing, superconducting, and mechanical properties. The (0,0) band of the A $^4\Pi$ - X $^4\Sigma^-$ transition of MoN was recorded at Doppler-limited resolution using intracavity laser spectroscopy (ILS) integrated with a Fourier-transform spectrometer used for detection (ILS-FTS). The target MoN molecules were produced in the plasma discharge of a molybdenum-lined copper hollow cathode, using a gas mixture of Ar with about 1% N_2 in a reaction chamber with about 1 Torr total pressure. Isotopologue structure in the spectrum is clearly visible and analysis is underway for the five abundant isotopologues with no nuclear spin (I_{Mo}=0): ^{92}MoN (14.6%), ^{94}MoN (9.2%), ^{96}MoN (16.7%), ^{98}MoN (24.3%), and ^{100}MoN (9.7%). Hyperfine structure in the spectrum is not resolved, but clearly adds to the profile of each feature. To perform a comprehensive fit, the line positions ^{95}MoN (15.9%) and ^{97}MoN (9.6%) from Cheung et al. [JMS 202, (2000)] were included in the fit. PGOPHER was used with mass-constrained parameters based on ^{98}MoN, using a Hund's case(a) approach for both states. Although the constrained approach worked well for spectral analysis, several parameters needed to be fit individually for each isotopologue.