

MASS-INDEPENDENT ROTATIONAL AND DEPERTURBATION ANALYSIS OF THE [15.30]1 AND [14.26]0⁺ ELECTRONIC STATES OF TUNGSTEN SULFIDE (WS)

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The complex electronic structure of transition metal diatomic molecules, such as tungsten monosulfide (WS), makes them intriguing targets for high level spectroscopic analysis. A plethora of electrons and accessible valence orbitals make WS a difficult molecule to model computationally due to the large number of possible electronic interactions. The (0,0) and (1,0) vibrational bands of the [15.30]1 – X ³Σ⁻(0⁺) transition of WS were recorded in absorption at Doppler-limited resolution using intracavity laser spectroscopy integrated with a Fourier-transform spectrometer used for detection (ILS-FTS). The target WS molecules were produced in the plasma discharge of a tungsten-lined copper hollow cathode, using a gas mixture of approximately 70% Ar and 30% H₂, with a trace amount of CS₂, giving a reaction chamber pressure of about 1 torr total. Within each spectrum, evidence of heterogeneous mass- and J-dependent perturbations were observed across all four abundant isotopologues: ¹⁸²W³²S, ¹⁸³W³²S, ¹⁸⁴W³²S, and ¹⁸⁶W³²S. The perturbations observed in the (0,0) and (1,0) bands were attributed to interactions with lines in the v=2 and v=3 vibrational levels of the [14.26]0⁺ state of WS. Rotational and deperturbation analyses incorporated a mass-independent Dunham model built into PGOPHER to fit lines from the two [15.30]1 transition bands, as well as line positions from several bands of the [14.26]0⁺ – X ³Σ⁻(0⁺) transition previously analyzed by our group (J.C. Harms et al., *J. Mol. Spec.* 2020 (374), 111378). The results of this analysis and comparison with previous computational work (J. Zhang et al., *J. Quant. Spectrosc. Radiat. Transfer.* 2020 (256), 107314) will be presented.