ROTATIONAL SPECTRA AND STRUCTURAL PARAMETERS OF BIS(η_5-CYCLOPENTADIENYL)TUNGSTEN DIHYDRIDE[a]

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Microwave spectroscopy measurements and density functional theory calculations are reported for the bis(η_5-cyclopentadienyl)tungsten dihyride complex and its deuterium substituted isotopomers. Rotational transition frequencies were measured in the 4-18 GHz range using a Flygare-Balle-type pulsed beam spectrometer. $(C_5H_5)_2WH_2$ is a near-prolate asymmetric top with preliminary rotational constants of A= 2062, B= 855, and C= 844 MHz for the main ^{184}W isotopomer. Measurements were made to obtain the M-H bond and H-H distances to determine if this a dihydrogen complex.

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