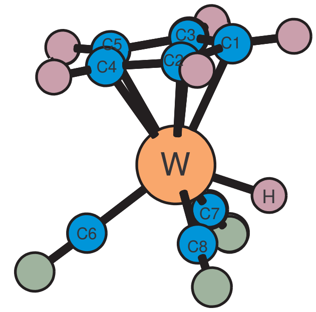
MICROWAVE SPECTROSCOPY MEASUREMENTS OF THE GAS PHASE STRUCTURE OF CYCLOPENTADIENYL TUNGSTENTRICARBONYL HYDRIDE [a]

CHANDANA KARUNATILAKA, CHAKREE TANJAROON, KRISTEN S. KECK, AND STEPHEN G. KUKOLICH, *Department of Chemistry, University of Arizona, Tucson, AZ 85721*.



Microwave spectra for five unique ^{13}C isotopomers of cyclopentadienyltungstentricarbonyl hydride were measured using a Flygare-Balle type microwave spectrometer system. The new rotational constants were combined with the previously obtained rotational constants for normal and deuterium analogues for various tungsten isotopes. A total of fifty-seven rotational constants were acquired and used in the least squares fit to obtain the gas phase structure of this d^4 - metal mono hydride complex. The results from the structural fit yielded the W-H bond length: r_o(W-H)= 1.788(20) Å, which agrees very well with the previously reported Kraitchman value of r_s(W-H)= 1.79(4) Å. The present study also yielded the distance from tungsten to the centroid distance of the C_5H_5 ring: r(W-Cp)= 2.02(1) Å, the ring radius of Cp: r(Cp)= 1.2016(4) Å, the average bond length from tungsten to the carbonyl carbon, r(W-CO)= 1.981(14) Å, and the average cyclopentadienyl C-C bond length of 1.421(4) Å. Results obtained from the structural fit are in much closer agreement with the Kraitchman values than with the DFT results.

[a] Supported by THE NATIONAL SCIENCE FOUNDATION - CHE0304969