

MICROWAVE SPECTRA AND STRUCTURE OF H₂-CuF: OVERVIEW OF THE COMPLEXES OF HYDROGEN WITH METAL-CONTAINING DIATOMICS

G. S. GRUBBS II, DANIEL J. FROHMAN, *Department of Chemistry, Wesleyan University, 52 Lawn Avenue, Middletown, CT, 06459-0180, USA*; ZHENHONG YU, *Aerodyne Research, Inc. 45 Manning Road, Billerica, MA 01821*; STEWART E. NOVICK, *Department of Chemistry, Wesleyan University, 52 Lawn Avenue, Middletown, CT, 06459-0180, USA (email to SEN: snovick@wesleyan.edu)*.

We present here the FTMW spectra of the various isotopologues of the intermediate strength bound complex of dihydrogen with copper fluoride.^a The bond between the two moieties is surprisingly strong, the H-H forming the cross of the T with the Cu closest to H₂ in the C_{2v} structure. Laser ablation was used to produce both copper isotopologues of *p*-H₂-CuF, *o*-D₂-CuF, and HD-CuF whose $J = 1 - 0$ transitions were observed. Significant changes in the nuclear quadrupole coupling constants for the copper nucleus in H₂-CuF compared to that in uncomplexed CuF suggests bonding greater than that typical of van der Waals interactions. This talk will serve as the introduction to presentations at this meeting of other H₂ metal containing diatomics.



^aD. J. Frohman, G. S. Grubbs II, Z. Yu, S. E. Novick, *Inorg. Chem.*, **52**, 816-822 (2013).