MICROWAVE SPECTRA AND STRUCTURE OF H_2–CuF: OVERVIEW OF THE COMPLEXES OF HYDROGEN WITH METAL-CONTAINING DIATOMICS

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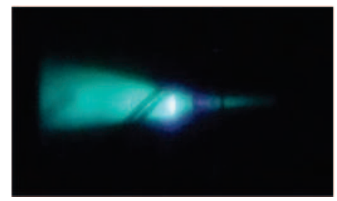

We present here the FTMW spectra of the various isotopologues of the intermediate strength bound complex of dihydrogen with copper fluoride.[a] The bond between the two moieties is surprisingly strong, the H–H forming the cross of the T with the Cu closest to H_2 in the C_{2v} structure. Laser ablation was used to produce both copper isotopologues of *p*-H_2–CuF, *o*-D_2–CuF, and HD–CuF whose $J = 1 - 0$ transitions were observed. Significant changes in the nuclear quadrupole coupling constants for the copper nucleus in H_2–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 H_2 metal containing diatomics.

[a] D. J. Frohman, G. S. Grubbs II, Z. Yu, S. E. Novick, *Inorg. Chem.*, **52**, 816-822 (2013).