THE MILLIMETER/SUBMILLIMETER SPECTRUM OF CUSH($\tilde{X}^1A'$): INVESTIGATION OF THE TRANSITION METAL SULFUR BOND

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The pure rotational spectra of ^{63}CuSH and ^{65}CuSH and its deuterated isotopomers were recorded using millimeter/submillimeter-wave direct absorption techniques. The molecule was produced by reacting copper vapor with H_2S in the presence of d.c. discharge. Transitions ranging from J = 24 $\rightarrow$ 25 to J = 50 $\rightarrow$ 51 spanning the region of 262 - 538 GHz were measured for ^{63}CuSH and ^{65}CuSH, as well as transitions J = 32 $\rightarrow$ 33 to J = 39 $\rightarrow$ 40 for the deuterated species. The spectra showed extensive K_a ladder structure for all species, which is consistent with the molecule being an asymmetric top. Rotational constants, as well as an r_0 structure, have been determined for the molecule. This study shows that the molecule is bent with a Cu-S-H angle of Θ = 93.6^o, and therefore is different from CuOH, which has a Cu-O-H angle of Θ =110.1^o. This striking variation in geometry likely results from a lack of hybridization in the CuSH molecule.