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 $\Theta=93.6^{\circ}$, and therefore is different from CuOH, which has a Cu-O-H angle of $\Theta=110.1^{\circ}$. This striking variation in geometry likely results from a lack of hybridization in the CuSH molecule.