MICROWAVE SPECTRA AND STRUCTURES OF H₂S-CuCl AND H₂O-CuCl.

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A Balle-Flygare FT-MW spectrometer coupled to a laser ablation source has been used to measure the pure rotational spectra of H₂S-CuCl and H₂O-CuCl. Both molecules are generated via laser ablation (532 nm) of a metal rod in the presence of CCl₄, argon, a low partial pressure of H₂S or H₂O and are stabilized by supersonic expansion. Rotational constants and centrifugal distortion constants have been measured for eight isotopologues of H₂S-CuCl with substitutions available at the copper, chlorine and hydrogen atoms. Transitions in the spectra of nine isotopologues of H₂O-CuCl have been measured with isotopic substitutions achieved for every atom. The spectra of both H₂S-CuCl and H₂O-CuCl are consistent with a linear arrangement of sulphur or oxygen, metal and chlorine atoms. The structure of H₂S-CuCl is pyramidal with C_S symmetry. The structure of H₂O-CuCl is either C_{2v} planar at equilibrium or C_S pyramidal but with a low potential-energy barrier to planarity such that the v=0 and 1 states associated with the motion that inverts the configuration at the O atom are well separated. Nuclear quadrupole coupling constants have been measured for the chlorine and copper atoms in each molecule. Nuclear spin-rotation constants have been determined for the copper atom.