MICROWAVE SPECTRA, STRUCTURES AND HYPERFINE CONSTANTS OF OCAgX AND OCCuX (X=F,Cl,Br).

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The rotational spectra of OCAgX and OCCuX (where X is F, Cl, Br) have been obtained through Fourier Transform microwave spectroscopy. The molecules were generated via the ablation of a metal rod in the presence of a halogen precursor, and were stabilised within a supersonic jet. Through accurate measurements of the observed line positions, the rotational constants (B_0, D_0) of the species have been evaluated to a high degree of precision. The acquisition of isotopic data has permitted an accurate determination of O-C, M-C, and M-X distances in all species. In each case, the O-C bond is found to be close to that of monomeric CO, and significantly shorter than that predicted by calculation at the MP2 level. An examination of the observed hyperfine structure has permitted the precise determination of nuclear quadrupole coupling constants for species containing chlorine, bromine and copper atoms. Apart from OCCuCl, these are the first experimental observations of these complexes.