EVIDENCE FOR NOBLE GAS-METAL CHEMICAL BONDING: FT-MICROWAVE SPECTRA, GEOMETRIES AND HYPERFINE CONSTANTS OF THE COMPLEXES Ar-CuX (X=F, Cl, Br).

COREY J. EVANS and MICHAEL C. L. GERRY, *Department of Chemistry, University of British Columbia, 2036 Main Mall, Vancouver, B. C., Canada, V6T 1Z1*.

The rotational spectra of the complexes Ar-CuF, Ar-CuCl and Ar-CuBr have been measured between 5-22 GHz using a cavity pulsed jet Fourier transform microwave spectrometer. They were prepared by ablating Cu metal with a Nd:YAG laser (532 nm) and allowing the vapour to react with a suitable precursor contained as <1% in the Ar backing gas of the jet. The complexes are linear and rather rigid, with the Ar-Cu stretching frequency estimated as ∼200 cm^{-1}. Ground state effective (r_0) and, where possible, substitution (r_s) and double substitution (r_d) geometries have been obtained. The Ar-Cu bonds are short (2.22-2.30Å). Large changes in the Cu nuclear quadrupole coupling constants indicate extensive charge rearrangement on complex formation. *Ab initio* calculations at the MP2 level of theory predict an Ar-Cu bond energy in Ar-CuF of ∼47 kJ mol^{-1}, along with a transfer of ∼0.1 electron from Ar to Cu. The whole picture is consistent with weak Ar-Cu covalent bonding.