CHEMICAL BONDING BETWEEN Ar/Kr AND Au: FTMW SPECTRA, GEOMETRIES AND HYPERFINE CONSTANTS OF THE COMPLEXES Ar-AuX (X=F,Cl,Br) AND Kr-AuCl.

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The microwave rotational spectra of Ar-AuX(X=F,Cl,Br) and of Kr-AuCl were measured in the 5-22 GHz range using a cavity pulsed-jet Fourier transform microwave spectrometer. All complexes were found to be linear and rather rigid. Ground state effective (r_0) geometries were found for all complexes, while for Kr-AuCl a substitution (r_s) structure was obtained. The Ar-Au distance ranges from 2.39 to 2.50 Å in going from Ar-AuF to Ar-AuBr while for Kr-AuCl, the Kr-Au distance is 2.52Å. The Au nuclear quadrupole coupling constant was found to change radically on complex formation. For Ar-AuCl, eQq(Au)=-259.8 MHz while for Kr-AuCl, eQq(Au)=-349.7 MHz, is in contrast with that of monomeric AuCl where eQq(Au)=+9.6 MHz. *Ab initio* calculations at the MP2 level of theory predict a Ar-Au bond energy of 46 kJ mol^{-1} for Ar-AuCl with a transfer of 0.1 electrons from Ar to Au, while for Kr-AuCl the bond energy is 71 kJ mol^{-1} with a transfer of 0.2 electrons from Kr to Au. The whole picture is consistent with weak Ng-Au covalent bonding.