MICROWAVE SPECTRA AND GEOMETRIES OF THE CARBONYL GOLD HALIDES, OCAuX (X=F,Cl,Br)

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Microwave spectra of several isotopic species of each of the carbonyl gold halides, OCAuX (X=F,Cl,Br) have been measured with a cavity pulsed jet Fourier transform microwave spectrometer. The frequency range was 5-21 GHz. The samples were prepared by laser ablation of Au metal in the presence of CO (1.5%) and halogen precursor (SF_6,Cl_2,Br_2,0.1%) contained in the Ar backing gas of the jet. These are the first high resolution spectroscopic measurements for all three molecules; for OCAuF this is the first report of any kind. Rotational constants have been evaluated, and used to determine the molecular geometries. The CO bond lengths are very close to that of monomeric CO, and the AuC bonds are relatively long; both results are different from those of the majority of transition metal carbonyls. These geometries agree well in general with ab initio calculations. The Au, Cl and Br nuclear quadrupole coupling constants show major differences from those of the corresponding AuX monomers.