BROADBAND ROTATIONAL SPECTRUM AND MOLECULAR GEOMETRY OF OC···AgI

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Pure rotational spectra of the ground vibrational states of six isotopologues of OC···AgI have been measured by chirped-pulse Fourier transform microwave spectroscopy. The spectra are assigned to determine the rotational constant, B_0, and the centrifugal distortion constant, D_J, of the complex. The nuclear quadrupole coupling constant of the iodine atom, χ_{aa}(I), has also been measured. The complex is linear. The length of the C—O bond, r(CO), in the r_0 geometry for OC···AgI is 0.008 Å shorter than that found in the free CO molecule. The length of the Ag—I bond, *r*(AgI), is 0.013 Å shorter than in free AgI. The nuclear quadrupole coupling constant of the iodine atom is determined to be -769.84(22) MHz for OC···^{107}AgI implying an ionic character of 0.66 for the metal halide bond. The molecular structure and spectroscopic parameters determined from the experimental data are presented alongside the results of calculations at the explicitly-correlated CCSD(T) level. The design features of a laser ablation source constructed for the present work will be described.