MICROWAVE SPECTRUM AND GEOMETRY OF $H_3P\cdots AgI$

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The pure rotational spectrum of the vibrational ground state of $H_3P\cdots AgI$ has been measured by chirped-pulse FTMW spectroscopy. The complex is generated via laser ablation (532 nm) of a silver rod in the presence of CF_3I, PH_3 and argon. It is subsequently stabilized and interrogated in the cold environment of a supersonic jet. The rotational constant, B_0, and the centrifugal distortion constant, D_J, have been measured for $H_3P\cdots^{107}AgI$ and $H_3P\cdots^{109}AgI$. The spectrum of the complex is consistent with a C_{3v} geometry and a linear arrangement of the P, Ag and C atoms. The measured rotational constants allow a preliminary determination of the geometry of the molecule. The nuclear quadrupole coupling constant of the iodine atom, χ_{aa}(I) , is also established. The experimental results are compared with theory performed at the explicitly-correlated coupled-cluster singles, doubles and perturbative triples level.