THE ARGON-CYCLOPENTADIENYL THALLIUM WEAKLY-BOUND COMPLEX, ROTATIONAL SPECTRUM AND STRUCTURE

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The symmetric-top rotational spectrum of the neutral argon-cyclopentadienyl thallium complex was measured using a Flygare-Balle-type Fourier transform microwave spectrometer. This appears to be the first rotational spectrum for a noble gas-organometallic complex. The rotational constants are B = 372.45 MHz for Ar-$C_5H_5^{205}$Tl and 373.35 MHz for Ar-$C_5H_5^{203}$Tl isotopomers. D_J = 0.1 kHz and D_{JK} = 0.4 kHz, indicating a fairly rigid structure. The argon atom is located on top of the cyclopentadienyl ring, on the a-axis of the C_5H_5Tl monomer, opposite the thallium atom. The separation distance between argon and the cyclopentadienyl ring is 3.56 Å. The binding energy of Ar-C_5H_5Tl was estimated to be about 1-3 kJ mol^{-1} using low-level MP2 theory.