Microwave spectroscopy measurements and density functional theory calculations are reported for the cyclopentadienylcycloheptatrienyltitanium complex, \( \text{C}_5\text{H}_5\text{TiC}_7\text{H}_7 \). This appears to be the first microwave work on a complex containing the cycloheptatrienyl ligand. Rotational transition frequencies for this symmetric-top complex were measured in the 4-13 GHz range using a Flygare-Balle-type pulsed beam spectrometer. The spectroscopic constants obtained for the normal isotopomer are \( B = 771.78907(38) \) GHz, \( D_J = 0.0000295(41) \) MHz, and \( D_{JK'K} = 0.001584(73) \) MHz. The quadrupole hyperfine splittings for \( \text{C}_5\text{H}_5\text{TiC}_7\text{H}_7 \) were clearly observed, and \( e^{Qq}_a = 18.432(90) \) MHz. Analysis of the rotational constants indicates that bond lengths in the gas phase are about 0.02 Å longer than those reported for the solid-state X-ray structure. The calculated Ti-C bond lengths are shorter for the \( \text{C}_7\text{H}_7 \) ligand (\( r(\text{Ti-C}) = 2.21 \) Å) than for the \( \text{C}_5\text{H}_5 \) ligand (\( r(\text{Ti-C}) = 2.34 \) Å), and the \( \text{C}_7\text{H}_7 \) H atoms are displaced 0.15 Å out of the \( \text{C}_7 \) plane, toward the Ti atom.

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