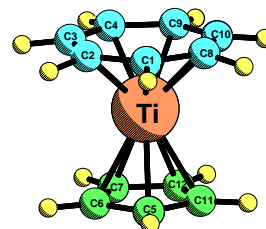


ROTATIONAL SPECTRA AND HYPERFINE STRUCTURE FOR A TITANIUM SANDWICH COMPLEX,
 $C_5H_5TiC_7H_7^a$

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Microwave spectroscopy measurements and density functional theory calculations are reported for the cyclopentadienylcycloheptatrienyltitanium complex, $C_5H_5TiC_7H_7$. 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 $B = 771.78907(38)$, $D_J = 0.0000295(41)$, and $D_{JK} = 0.001584(73)$ MHz. The quadrupole hyperfine splittings for $C_5H_5^{48}TiC_7H_7$ were clearly observed, and $eQq_{aa} = 18.432(90)$ MHz. Analysis of the rotational constants indicates that bond lengths in the gas phase are about 0.02\AA longer than those reported for the solid-state X-ray structure. The calculated Ti-C bond lengths are shorter for the C_7H_7 ligand ($r(Ti-C) = 2.21\text{\AA}$) than for the C_5H_5 ligand ($r(Ti-C) = 2.34\text{\AA}$), and the C_7H_7 H atoms are displaced 0.15\AA out of the C_7 plane, toward the Ti atom.



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