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

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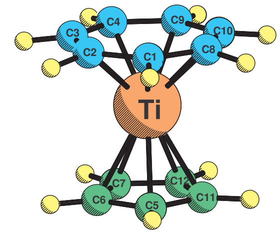

Microwave spectroscopy measurements and density functional theory calculations are reported for the cyclopentadienylcycloheptatrienyltitanium complex, $C_5H_5TiC_7H_7$. This appears to be the first microwave work on a complex containing the cycloheptatrienyl ligand. Rotational transition frequencies 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 0.02Å 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)=2.21Å) than for the C_5H_5 ligand (r(Ti-C)=2.34Å), and the C_7H_7 H atoms are displaced 0.15Å out of the C7 plane, toward the Ti atom.

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