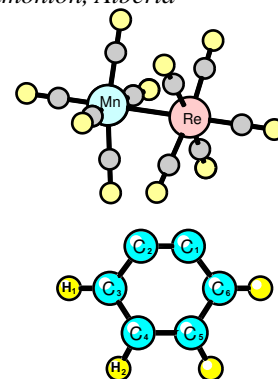


EXPERIMENTAL ROTATIONAL SPECTRA FOR $\text{MnRe}(\text{CO})_{10}$ AND $o\text{-C}_6\text{H}_4$ REQUIRED ACCURATE THEORETICAL CALCULATIONS FOR SUCCESSFUL ANALYSIS^a

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The keys to successfully analysing the high-resolution rotational spectra for manganese-rhenium decacarbonyl and for *o*-benzynes were the results of extensive and accurate theoretical calculations. Obtaining the microwave spectrum of the dinuclear complex $\text{MnRe}(\text{CO})_{10}$ was made difficult by the low rotational constant (200 MHz) resulting in fairly high *J* values for transitions in the normal Flygare-Balle spectrometer region. The assignments were further complicated by the presence of ^{185}Re , ^{187}Re isotopes with $eQq = 391$ and 370 MHz and ^{55}Mn with $eQq = -16.5$ MHz. Large Gaussian orbital basis calculations by Palmer and Guest provided sufficiently accurate predicted molecular constants to assign and fit the spectrum. Although the spectrum for the normal isotopomer of *o*-benzynes could be obtained with reasonable *S/N*, assigning the single-substitution ^{13}C isotopomer spectra, even with an enriched sample, proved to be difficult. The accurate and precise rotational constants for the 7 measured isotopomers for $o\text{-C}_6\text{H}_4$ could not be accurately fit using a planar structure due to the vibrational averaging effects. Using *ab initio* vibrational averaging corrections calculated by Groner, an accurate, near-equilibrium structure was obtained for *o*-benzynes.



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