EXPERIMENTAL ROTATIONAL SPECTRA FOR $MnRe(CO)_{10}$ AND o-C_6H_4 REQUIRED ACCURATE THEORETICAL CALCULATIONS FOR SUCCESSFUL ANALYSIS[a]

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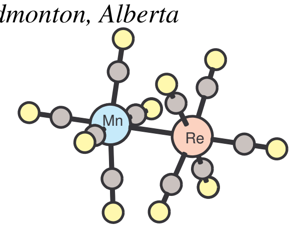

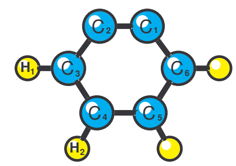

The keys to successfully analysing the high-resolution rotational spectra for manganese-rhenium decacarbonyl and for o-benzyne were the results of extensive and accurate theoretical calculations. Obtaining the microwave spectrum of the dinuclear complex $MnRe(CO)_{10}$ was made difficult by the low rotational 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-benzyne 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-C_6H_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-benzyne.

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