Abstract

"The NMR parameters characterizing the spectra of trans- and cis- decalins are determined from theoretical calculations and experimental spectra. The calculated values of the shielding constants are in good agreement with the measured chemical shifts, with a small but noticeable difference in accuracy for the bridgehead atoms. Out of all the spin-spin coupling constants, only most of $^{1}J_{CC}$ and $^{1}J_{CH}$ values could be extracted from the spectra, and the corresponding computed values are in good agreement with the experiment. It appears that the applied Density Functional (DFT) approach overestimates slightly the $J_{CC}$ coupling and underestimates the differences between one-bond $^{1}J_{CH}$ coupling constants. For all these constants ($J_{CC}$, $J_{CH}$ and $J_{HH}$) through one to three bonds, which could not be obtained experimentally, the predicted values are in good agreement with the general rules relating spin-spin coupling to the number and spatial arrangement of the intervening bonds."