Proton Detection of Carbon-Carbon Couplings between Chemically Equivalent Nuclei.

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PROTON DETECTION OF CARBON-CARBON COUPLINGS BETWEEN CHEMICALLY EQUIVALENT NUCLEI

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Coupling constants between equivalent carbons in symmetrical compounds are uneasy to measure due to a collapse of their signals to single lines in standard decoupled spectra. In spite of this fact 2QHMBC experiment was proposed for indirect detection of carbon-carbon couplings in symmetrical molecules but the explanation of the 2QHMBC operation on symmetrical molecules appears to be unclear and incorrect.

Analytical formulas for time development of density matrix of strongly coupled symmetrical HC-C'H' spin systems were derived. Optimal polarization delay length for maximal signal in 2QHMBC is discussed and it is found as substantially different from the originally proposed value $1/(2*{}^{1}J(C,H))$. New values of polarization transfer delay can help to increase signal-to-noise ratio by about hundreds of percent in 2QHMBC experiment. Based on the analytical formulas a new version of indirect detection experiment, called SYMONA is proposed for carbon-carbon coupling constants and connectivities detection. The new sequence has more flat position of a signal maximum ($t=1/[{}^{1}J(C,C)+{}^{3}J(H,H)]$) and it is less prone to bad setting of polarization transfer delay length and consequently to lowered signal-to-noise ratio.