Carbon-carbon couplings between chemically equivalent or almost equivalent nuclei

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Coupling constants are useful quantities for testing quality of quantum chemical calculations and for estimation of presence of chemical bonds on unknown samples. In some cases the couplings between chemically equivalent or almost chemically equivalent atoms can be desired for this task. By the term "Almost equivalent atoms" we mean very strongly coupled ones, i.e. in practice directly bonded atoms separated by few Hz difference in the chemical shifts.

Such couplings and connectivity information are impossible to detect under normal conditions. Fortunately there is particular exception if the equivalent nuclei (carbons) are coupled to other heteronuclei (typically to protons). Then, the heteronuclear couplings (i.e. carbon-proton) can be used as artificial chemical shifts separating the two carbons on a frequency axis. The corresponding experiment can be a standard INADEQUATE without proton decoupling during preparation and acquisition periods [1]. This experiment is generally very time consuming since the acquired spectrum is usually split by a number of heteronuclear couplings and therefore it has very low intensity.

We present here a modification of the above experiment with the aim of increasing the sensitivity. This can be achieved by 2D *J*-resolved refocused INADEQUATE without decoupling during preparation period but with decoupling during acquisition and equilibrium periods. The experiment is discussed with respect to the sensitivity and influence of strong couplings.

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References

[1] S. Berger, J. Magn. Reson. 66, 555 (1986).