

Measurement of Carbon-Carbon Coupling between Chemically Equivalent Nuclei.

Blechta, Vratislav 2016

Dostupný z http://www.nusl.cz/ntk/nusl-263129

Dílo je chráněno podle autorského zákona č. 121/2000 Sb.

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Datum stažení: 13.09.2024

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MEASUREMENT OF CARBON-CARBON COUPLINGS BETWEEN CHEMICALLY EQUIVALENT NUCLEI

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Carbon-carbon couplings are useful quantities for testing quality of quantum chemical calculations. In some cases homonuclear couplings between chemically equivalent nuclei can be desired for this task. On the other hand, such couplings 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 heteronucler 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.

Acknowledgement

For the financial support, the Czech Science Foundation (Project No. 15-12719S) is gratefully acknowledged.

References

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