High-resolution MRS via intermolecular double-quantum coherences in fields inhomogeneous in both B_0 and B_1

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Introduction

Magnetic resonance spectroscopy (MRS) experiments are ideally performed in homogeneous static magnetic field B_0 and RF field B_1, resulting in spectra with narrow resonance lines. However, there are many circumstances where B_0 and/or B_1 fields are inhomogeneous. The spatial homogeneity of magnetic fields is always degraded in a large volume of human or animal tissues or in volumes with mixed tissues. RF fields B_1 across the samples are highly inhomogeneous when surface coils are used. Intermolecular zero- and double-quantum coherences, which originate from dipolar interactions among spins in different molecules, can almost remove the effects of static field inhomogeneity [1-3]. In this work, we show the feasibility to obtain high-resolution MRS via detecting intermolecular double-quantum coherences (iDQCs) in fields inhomogeneous in both B_0 and B_1.

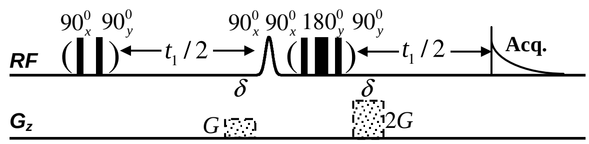

Fig. 1. Modified IDEAL-II pulse sequence.

Methods

The IDEAL-II pulse sequence we proposed previously [3] is utilized. This sequence holds the advantages of high efficiency in acquisition time and small data size. As shown in Fig 1, for this application the first and third pulses are replaced by composite pulses, i.e. the first 90°(x) is replaced by [90^0(x) 90^0(y)], and 180^0(x) by [90^0(x) 180^0(y) 90^0(x)]. The gauss-shaped pulse is selective for solvent and dash rectangles represent correlation selection gradients. Experiments were performed on a Varian INOVA 600 MHz NMR spectrometer at 298 K, equipped with self-shielded x, y, and z gradient coils and a 5 mm HCN triple-resonance RF coil of 1.5 cm effective length. A sample of mixture of methyl ethyl ketone and cyclohexane was used. It has been shown that high-resolution MRS can be obtained with higher signal intensity when a proper phase cycling instead of coherence selection gradients is employed [4]. Therefore, IDEAL-II was performed both with and without coherence selection gradients. To remove the unwanted coherence transfer pathways caused by imperfect pulses, an eight-step phase cycling scheme on the first RF pulse (x, y, -x, -y, x, y, -x, -y), the third RF pulse (x, x, x, x, -x, -x, -x, -x), and the receiver (x, -x, x, -x, x, -x, x, -x) was used. This phase cycling scheme was also employed to select iDQCs when coherence selection gradients were not used.

To simulate a case with both inhomogeneous B_0 and B_1 fields, the sample tube was lifted up to position the bottom of sample tube to the center of the effective range. 1D spectra obtained by a conventional single pulse sequence with different pulse widths were acquired (Fig. 2). Compare spectra (c) to (a), it can be seen that the blue part of spectrum in Fig. 2(c) experiences a RF pulse more than 180^0, while the green part smaller than 180^0. It is clear that B_1 field is inhomogeneous across the sample. The broaden line widths are caused by the inhomogeneous static B_0 field. It is almost impossible to extract correct information for chemical shifts, and even less so for J coupling constants, multiplet patterns and relative peak areas, from the 1D spectra in Fig. 2.

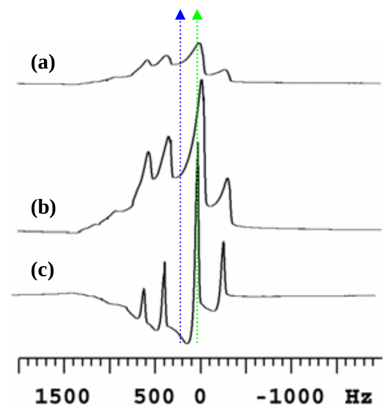

Fig. 2. 1D ^{1}H NMR spectra (phase mode) obtained by a conventional single pulse sequence with increasing pulse durations: (a) 4 µs, (b) 24 µs and (c) 44 µs.

Results and Discussion

The IDEAL-II experimental results for the same sample setting as in Fig 2 are shown in Fig. 3. It can be seen from Figs. 3(c) and (f) that 1D projection spectra hold the high-resolution information of chemical shifts, patterns of multiplicity, and relative areas. The apparent J coupling constants are 21.9 Hz in Figs. 3(c) and (f), while the original ones are 7.3 Hz. Therefore, the scaling factor for J coupling constants is 3, which is consistent with the theoretical value [3]. This allows more accurate measurements of small J coupling constants in weakly coupled spin systems. Noting that Figs. 3(c) and (f) are with the same scale, it can be seen that higher signal intensity can be obtained when coherence selection gradients which can cause additional attenuation are unemployed. When combined with J-scaling technique [5], the method will be more flexible for J coupling constant measurements. This study suggests that iDQCs provide a promising way to obtain high-resolution MRS in fields inhomogeneous both in B_0 and B_1.

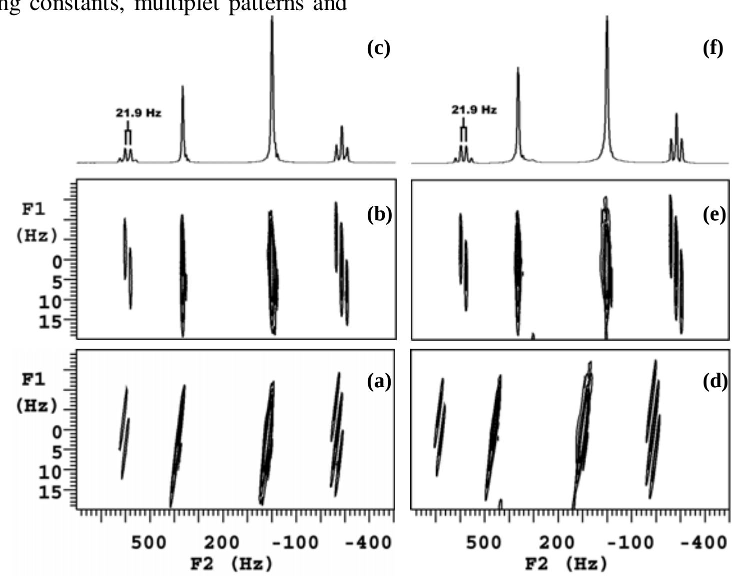

Fig. 3. (a) 2D ^{1}H NMR spectrum (magnitude mode) obtained by IDEAL-II shown in Fig. 1, (b) sheared spectrum of (a) after counterclockwise rotation by 63.4^0, (c) cumulated projection spectrum on the F2 dimension from (b), (d) ~ (f), corresponding to (a) ~ (c) except that IDEAL-II performed with phase cycling but no coherence selection gradients.

Acknowledgments

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References

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