Simultaneous Acquisition of Signals of Different Orders of Intermolecular Multiple-quantum Coherences

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Introduction

A new pulse sequence was proposed to simultaneously acquire five different intermolecular multiple-quantum coherence (iMQC) signals with coherence order n = 2, 1, 0, -1, -2 in isolated spin-1/2 systems (e.g. water), respectively [1,2,3]. Each signal is uncontaminated by the others, and has the same intensity as acquired from a conventional CRAZED sequence that selects only one order at a time, thus saving much experimental time. Moreover, the simultaneous acquisition of (±2)-quantum (±2Q), (0)-quantum (ZQ), and (±1)-quantum (±1Q) coherence signals permits careful evaluation of the differences in signal intensities. The theoretical predicts are supported by the experimental observations and numerically simulated results.

Methods

The new pulse sequence was depicted in Fig. 1. To obtain a specific coherence order, the phase cycling is necessary. Five cycling schemes were designed as follows: φ is (0, 90, 180, 270) for -1, 0 and +1 orders with receiver phase (0°, 270°, 180°, 90°), $(0°, 180°)_2$ and (0°, 90°, 180°, 270°), respectively; eight-step phase cycling (45° increments) for -2 and +2 orders with receiver phase $(0°, 180°)_4$ and $(0°)_8$, respectively. At first glance, 28 single acquisitions are necessary to obtain all the five signals separately. However, a careful analysis shows that only 10 single acquisitions are actually needed, as listed in Table I. The signals of –1Q, +1Q, ZQ, –2Q, and +2Q coherences can be obtained by combination I (a-i-f+j), II (a+i-e-j), III (a-c+e-g), IV (a+b+c+d+e+f+g+h), and V (a-b+c-d+e-f+g-h), respectively. Here '+' means adding and '-' means subtracting. With the above post-processing schemes, more than half the experimental time can be saved.

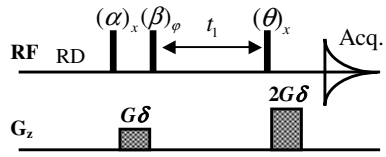

Fig.1 Pulse sequence designed to simultaneously acquire multiple orders of iMQC signals

Table I. Phase settings for acquisition of ±2, 0, ±1 order iMQC signals

Index	a	b	c	d	e	f	g	h	i	j
φ	0°	45°	90°	135°	180°	225°	270°	315°	90°	270°
φ_{rec}	0°	180°	0°	180°	0°	180°	0°	180°	90°	90°

Experiments were carried out at 298 K on a Varian Unity+ 500 NMR spectrometer. The sample was water (80% H_2O, 20% D_2O). Resonance offset was set to 100 Hz. All the RF flip angles were 80°. Ten single acquisitions were performed using the phase settings shown in Table I.

Results and discussion

Experimental observations and simulated results are shown in Fig.2 and Fig.3, respectively. Fig. 2(a) clearly shows different cross-peaks at the indirectly detected dimension corresponding to the ZQ-, ±1Q-, and ±2Q-coherence frequencies. The signals originating from higher order coherences are too small to be observed. With the five phase combination schemes, five iMQC signals with ±2, 0, ±1 orders have been acquired simultaneously, as shown in Figs. 2(b)~(f). Compared to the conventional CRAZED sequence, the signals from 0, ±1 orders are much less susceptible to contamination from signals of other coherence orders, since the conventional SQC signal due to imperfect rf pulse flip angles and the recovered longitudinal magnetization during the evolution period is removed in the new pulse sequence. The corresponding simulated results are given in Fig. 3 [5], in good agreement with the experimental results. In Ref.[2], the simultaneous acquisitions of five signals include conventional SQC, iDQCs and iZQCs, moreover, the obtained iZQCs may contain conventional SQCs which are difficult to be eliminated due to imperfect RF flip angles. The five signals acquired herein are all from intermolecular dipolar interactions, and they are much more pure since they are more insensitive to the precision of the flip angles.

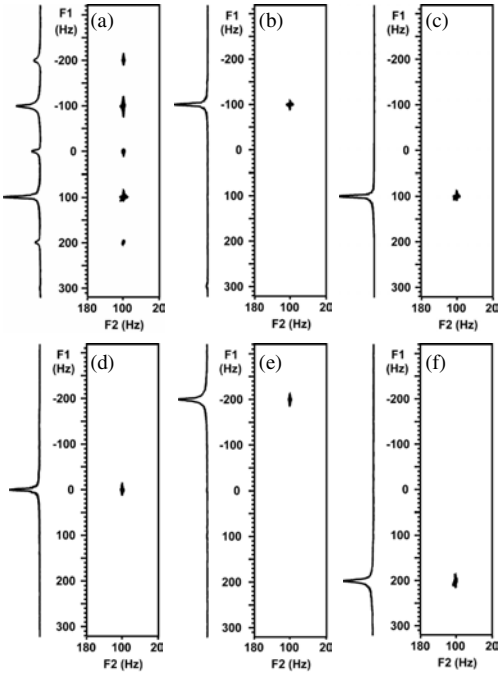

Fig.2 2D experimental spectra of water (a) without the phase cycling; (b) –1Q; (c) +1Q; (d) ZQ; (e) –2Q; (f) +2Q.

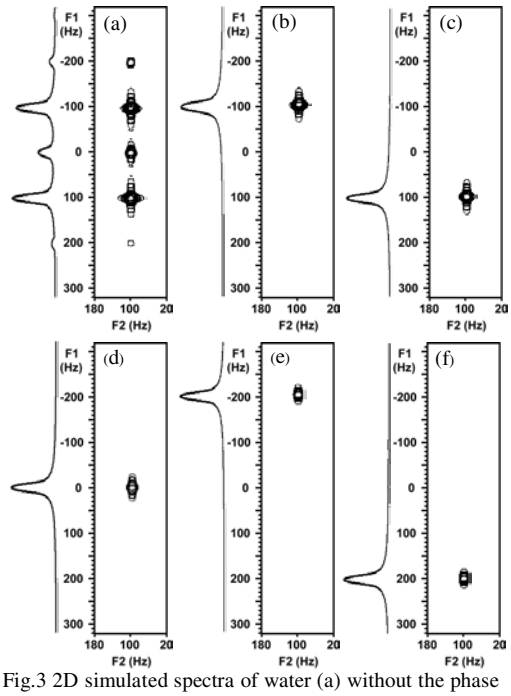

Fig.3 2D simulated spectra of water (a) without the phase cycling; (b) –1Q; (c) +1Q; (d) ZQ; (e) –2Q; (f) +2Q.

Acknowledgment

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