Magn. Reson. Discuss.,
https://doi.org/10.5194/mr-2020-14-RC1, 2020

Open Access MAGNETIC RESONANCE Discussions

Interactive comment on "Surprising absence of strong homonuclear coupling at low magnetic field explored by two-field NMR spectroscopy" *by* Ivan V. Zhukov et al.

Anonymous Referee #1

Received and published: 22 July 2020

The authors of this manuscript describe phenomena of generating coherences and oscillations between the associated populations in homo-nuclear J-coupled spin systems under fast transition conditions through the level anti-crossings (LAC). Such transitions are introduced by shuttling the sample between high (14.1 T) and low (0.33 T) magnetic fields. While these phenomena have been studied before, this manuscript focusses on effects of hetero-nuclear scalar couplings that are switched on and off using composite pulse decoupling (WALTZ-64). As pointed out in the on-line discussion of this article, effects of heteronuclear couplings on homonuclear spin systems are indeed a common knowledge, the proton spectrum of dioxane being a classical example. However, the technique of switching between high and low magnetic fields offers new ways of obtain-

ing a better insight into the dynamics of such phenomena. In general, the manuscript is well written, the theoretical treatment is sound, the literature is well cited and the figures are of good quality. As usual, there are a few points to be addressed before the final version of the manuscript can be published. 1. Obviously, the authors have made an effort to maximize the efficiency of the hetero-nuclear decoupling by expanding the original 16 step supercycle to 64 steps and by applying a very high RF field strength of 24 kHz, covering the bandwidth in excess of 60 kHz (4000 ppm at 0.33 T, 14 MHz 1H). Since the CH proton chemical shift range at this field strength is less than 42 Hz (3 ppm) perhaps a simple CW decoupling would have been more efficient. It would also offer means of altering the size of the effective hetero-nuclear coupling. 2. Introduction: when describing slow and fast passage through the LAC the authors should indicate the time scale that is used to define what is fast and what is slow. I would guess it is the J-coupling (H-C, C-C, multiplet structure, etc.) that defines the desired time scale. Please clarify. 3. Page 3, section B, lines 2 and 3: the proton resonance frequency is provided for the 14.1 T field, but not for the more unusual 0.33 T field. Please correct. 4. Page 3, section B, paragraph 2: the authors use RE-BURP refocusing pulse for inversion - nothing wrong with that, except the reader might be curious about the selection of the pulse shape, e.g. why not use an inversion pulse, such as I-BURP or G3 ? 5. Page 3, line 112: "WALTZ-64 supercycle" should be "WALTZ decoupling with MLEV-64 supercycle". A reference to MLEV-64 should be given along with that for the WALTZ decoupling. 6. Caption to Figure 2: the RF field strength for the 0.56 W decoupling at B(HF) should be given. 7. Page 11, lines 346-348, the last statement before the section V (Conclusions): please indicate that this statement is for abundant (or labelled) spins only. Technical Corrections: 1. Page 3, line 102: "multiplet overlay" should read "multiplet overlap". 2. Caption to Figure 1: "non-decoupled" is simpler defined as "coupled". 3. Caption to Figure 2: "The delay ... was varied..." should read "The delay ... was incremented..." 4. Page 4, line 132: the authors should use the capital Delta to avoid confusion with the chemical shifts. See also line 161 on page 6. 5. Page 7, line 202: "semi-selective" should read "band-selective". 6. Page 11, paragraph 2 in Concluions: "We can clearly demonstrate the polarization transfer ... " should read "We can clearly demonstrate that the polarization transfer...".

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