Canadian Association of Physicists

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Contribution ID: **68** Type: **Oral Competition (Graduate Student) / Compétition orale (Étudiant(e) du 2e ou 3e cycle)**

(G*) Magic-angle orientation selectivity in two-pulse EPR COSY (correlation spectroscopy) sequence: Distance measurements in biological systems

Thursday 10 June 2021 12:00 (3 minutes)

Two-pulse COSY (correlation spectroscopy) EPR (Electron Paramagnetic resonance) sequence, utilized for distance measurements in biological systems using nitroxide biradicals, is investigated both analytically and numerically. The analytical expressions derived here for any orientations of the two nitroxide dipoles with respect to the dipolar axis, oriented at an angle \theta with respect to the magnetic field with respect to the dipolar axis joining the two nitroxide dipoles at the angle, \theta, show that, in general, the coherence transfer from p=0 to the single quantum p=1 state is peaked at the orientation \theta being the magic-angle, {54.7}^\circle, and its supplementary angle, {125.3}^\circle, with a narrow width, implying that there is produced orientational selectivity, by the first \pi/2 pulse. This results in the signal being predominantly determined by those biradicals, whose dipolar axes are at, or near, the magic and its supplementary angle. This is entirely a novel finding, not published in the literature. Furthermore, the analytical treatment shows that the Fourier transforms of the two-pulse COSY signal exhibit peaks at \pm d\times \left(3cos^2\theta-1\right); here d=\frac{2}{3}D, with D being the dipolar-coupling constant.). In addition, there occurs also structural sensitivity of the signal, i.e., its dependence on the orientations of the two nitroxide dipoles during to free evolution over the two coherence states p=+1 and -1. The powder (polycrystalline) averages over the unit sphere, accumulated over 20 sets of Monte-Carlo orientations of the two nitroxide dipole moments reveal that the Pake doublets occur at \pm d. It is concluded that the two-pulse COSY experiment is a preferred technique for distance measurements as compared to other multi-pulse (four, five, six) sequences, as well as two-pulse DQ (double quantum) and five-pulse DQM (double quantum modulation) sequences, because its Pake doublet is the most intense of all the other multi-pulse sequences.

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