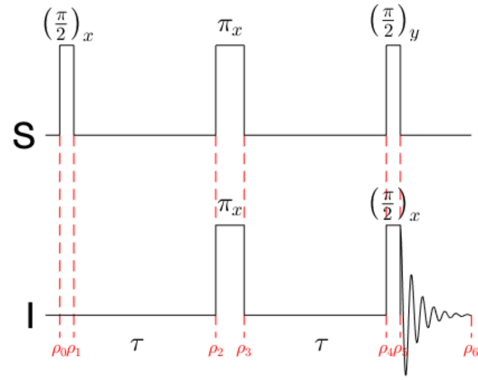
December 2021 NMR Topic of the Month: The INEPT Pulse Sequence



If this sequence is inept, why use it?

No, no! This sequence is not inept, it is The INEPT pulse sequence. INEPT is short for Insensitive Nuclei Enhanced by Polarization Transfer, and it is a very clever way to improve the signal acquired from low-sensitivity nuclei. As such, the INEPT sequence is often a building block within other sequences.

What is a low-sensitivity nucleus?

In general, nuclei with larger gyromagnetic ratios (γ) are easier to observe. Larger γ means larger magnitude of the magnetic moment, Boltzmann polarization, Larmor frequency, and couplings. The magnetic moment and Boltzmann population relate directly to the magnitude of the signal. The Larmor frequency is a rate of change of the magnetic moment in the coil, and a higher frequency facilitates detection. The couplings tend to allow the nuclei to relax more quickly, so more transients can be acquired in a given period of time. In other words, the couplings do not enhance the signal shot-to-shot, but allow for more shots over time, which means more overall signal in the same amount of time.

How does the INEPT work?

The INEPT sequence moves magnetization from the sensitive (S) spins to the insensitive (I) spins through the scalar (J) coupling. It does this by starting with bilinear terms detectable on channel S and converting them to bilinear terms detectable on channel I. Specifically, where $c_X = \frac{1}{4}\left(\gamma_X B_0 / k_B T\right)$:

$$\rho_0 = c_I I_z + c_S S_z \rightarrow \rho_1 = c_I I_z - c_S S_y \rightarrow$$

$$\rho_2 = c_I I_z - c_S S_y cos\left(\omega_S \tau\right) cos(\pi J \tau) + c_S 2 I_z S_x cos\left(\omega_S \tau\right) sin(\pi J \tau) + c_S S_x sin\left(\omega_S \tau\right) cos(\pi J \tau) + c_S 2 I_z S_y sin\left(\omega_S \tau\right) sin(\pi J \tau) \rightarrow$$

$$\rho_3 = - c_I I_z + c_S S_y cos\left(\omega_S \tau\right) cos(\pi J \tau) - c_S 2 I_z S_x cos\left(\omega_S \tau\right) sin(\pi J \tau) + c_S S_x sin\left(\omega_S \tau\right) cos(\pi J \tau) + c_S 2 I_z S_y sin\left(\omega_S \tau\right) sin(\pi J \tau) \rightarrow$$

$$\rho_4 = - c_I I_z + c_S S_y cos(2\pi J \tau) - c_S 2 I_z S_x sin(2\pi J \tau) \rightarrow \rho_5 = c_I I_y + c_S S_y cos(2\pi J \tau) - c_S 2 I_y S_z sin(2\pi J \tau)$$

Notice that the last term in ρ_5 is observable on the insensitive channel, but has the constant from the sensitive nuclei. Also notice that the maximum of the final term occurs when $\tau = 1/|4J|$, then $\rho_5(\tau = 1/|4J|) = c_I I_y - sgn[J] c_S 2 I_y S_z$, which is why sequences that utilize The INEPT require an input for the scalar coupling. Finally, if the coupling (J) is small and/or the system relaxes too quickly, The INEPT sequence will perform no better than the simple one pulse experiment.

References

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3. G.A. Morris and R. Feeman, *J. Am. Chem. Soc.* **101**, 760-762 (1979).