



Supplement of

The decay of the refocused Hahn echo in double electron–electron resonance (DEER) experiments

Thorsten Bahrenberg et al.

Correspondence to: Stefan Stoll (stst@uw.edu) and Daniella Goldfarb (daniella.goldfarb@weizmann.ac.il)

The copyright of individual parts of the supplement might differ from the article licence.

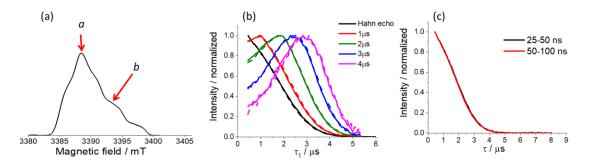


Figure S1. (a) W-band echo-detected EPR spectrum of 100 μ M 3-maleimido-proxyl in H₂O/glycerol (80:20 v/v) measured at 25 K (different batch than that shown in Fig. 3). (b) Normalized echo intensity as a function τ_1 of for several τ_2 values (indicated on the Figure) measured at the two different field positions, *a* (solid lines) and *b* (dashed lines) as indicated in (a), together with a Hahn echo decay. The $\pi/2$ and π pulse durations were 25 and 50 ns. (c) Comparison of the Hahn echo decay recorded at position *a* with different $\pi/2$ and π pulses as noted on the figure.

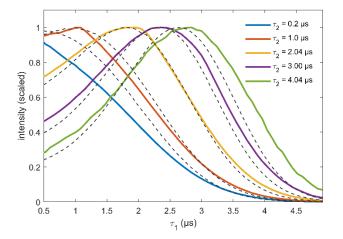


Figure S2. Comparison of the experimental refocused Hahn echo decays for 3-maleimido-proxyl (solid coloured lines; as in Figure 3c) with the CCE simulations (dashed black lines; as in Fig. 9b). The simulations reproduce the experimental trends well. The largest deviations are seen at short and large τ_2 values.

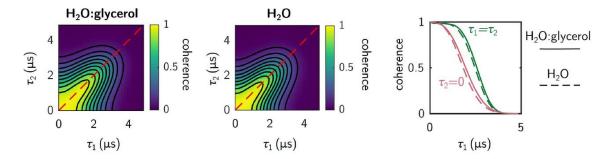


Figure S3. CCE simulations of the refocused echo decay for different solvents: H₂O:glycerol (left) and H₂O (centre), and a comparison of the $\tau_2 = 0$ and $\tau_1 = \tau_2$ traces (right). The H₂O:glycerol simulation is the same 3-CCE simulation as in Figure 10. The H₂O simulation has an identical input, save for the solvent environment, a pure water solvent instead of a mixture of water and glycerol. Consequently, the water-only system has 494 one-clusters, 4,124 two-clusters, and 49,178 three-clusters. Both solvents give very similar decays.

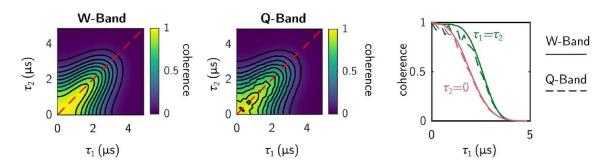


Figure S4. CCE simulations of the refocused Hahn echo for W-band (left) and Q-band (right), and a comparison of the $\tau_2 = 0$ and $\tau_1 = \tau_2$ traces (right). The W-Band simulation is the same 3-CCE simulation as in Figure 10. The Q-Band simulation has an identical input, except for the applied magnetic field; $B_0 = 1.2$ T. While there are more ESEEM modulations in the Q-Band simulation, the decay envelopes are close to identical.