Supporting information for

Suppression of ghost distances in multiple-spin double electron-electron resonance

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1 Triradical T111_{inv} in toluene matrix

DEER measurement on triradical T111_{inv} at X-band frequency were additionally conducted in a toluene matrix, whereas all other systems were solely measured in an o-terphenyl matrix. Time and distance domain data are shown in Figure S 1.

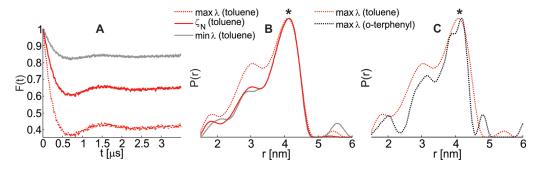


Figure S 1 Time (A) and distance (B,C) domain data of model triradical T111_{inv} measured in a toluene matrix measured at maximum (dashed red) and minimum inversion efficiency (grey) and power scaling of the data with ζ_N (red) compared with the distance distribution in an o-terphenyl matrix (C). A) Form factors in toluene with maximum $\lambda \approx 0.4$ (dashed red), minimum $\lambda \approx 0.1$ (red) and power scaled with $\zeta_N = 1/2$ (grey). B) Distance distributions in toluene obtained from the form factors. Scaling with ζ_N (red) and measuring at lowered inversion efficiency (grey) reduce the ghost peak to the same extent. C) Distance distributions at maximum λ in toluene (dashed red) and o-terphenyl (dashed black).

The emergence and the power scaling behaviour of ghost contributions at maximum inversion is not strongly biased by matrix changes. We tentatively assign the slight change of the magnitude of the ghost peak to matrix effects which may come about by differences in the pair distance distribution at the different glass transition temperatures of the solvents 1 . Slight differences in the numerical value of the inversion efficiency might also come from experimental uncertainties. In toluene as well as in o-terphenyl, the result of power scaling with ζ_N is equally good as the measurement at minimum λ .

References

1 G. Jeschke, M. Sajid, M. Schulte, N. Ramezanian, A. Volkov, H. Zimmermann and A. Godt, J. Am. Chem. Soc., 2010, 132, 10107–10117.