Electronic Supplementary Material (ESI) for CrystEngComm.

Crystal Structure of the Meta-Stable Intermediate in the Photomechanical, Crystal-to-Crystal Reaction of 9-Tertbutyl Anthracene Ester

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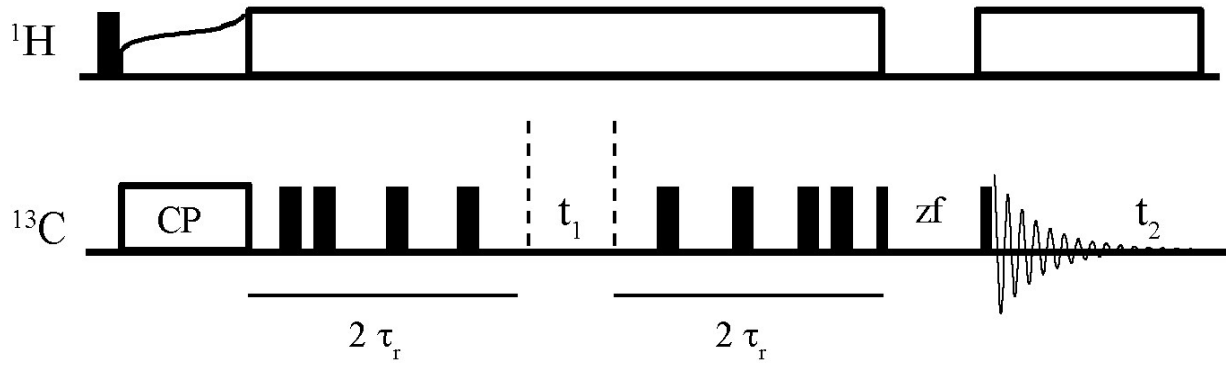


Figure S1. The modified TOSS-deTOSS pulse sequence[1] includes cog-wheel phase cycling[2] (COG16(0,1,0,1,0,1,0,1,0;0)) of the 8 π pulses on carbon comprising the TOSS and deTOSS periods and the addition of the final z-filter (zf).

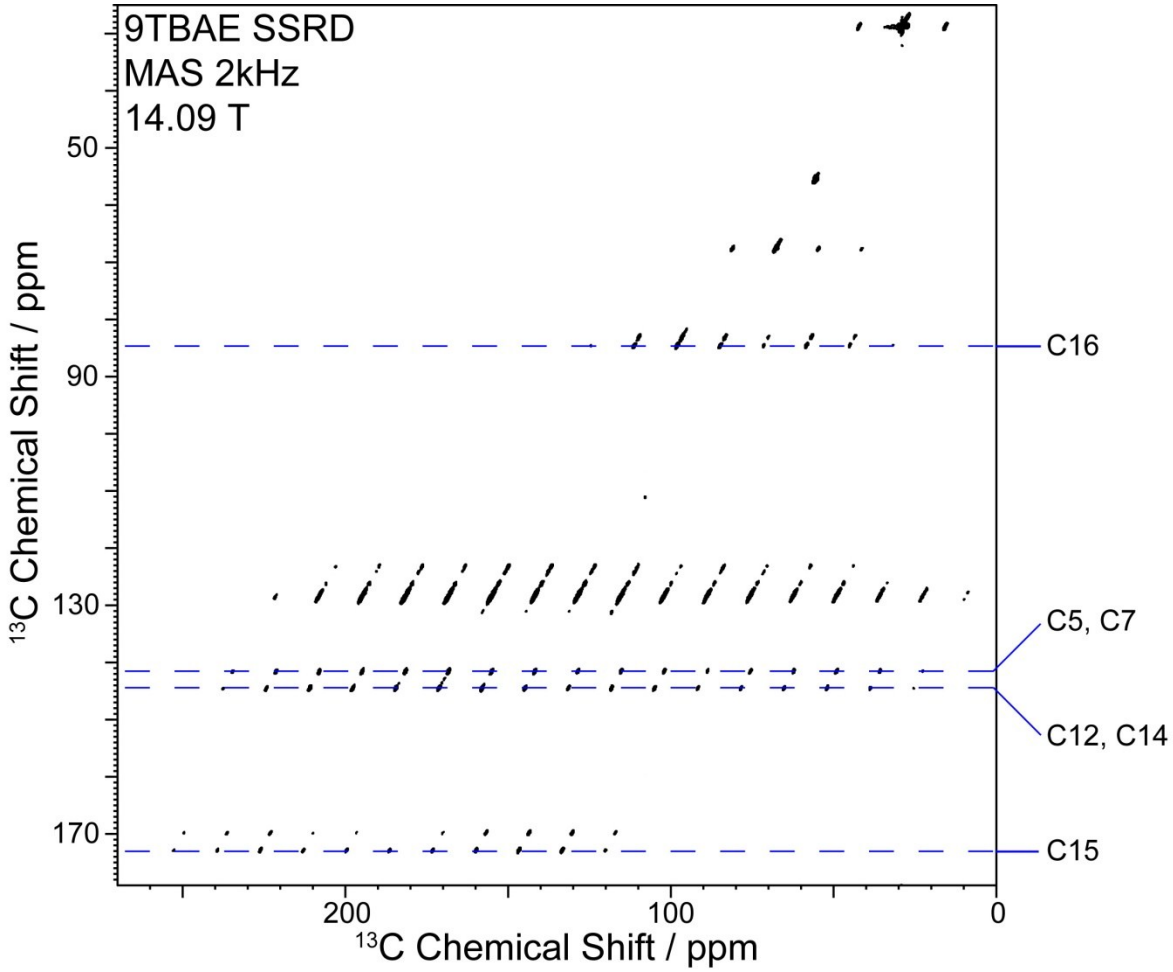
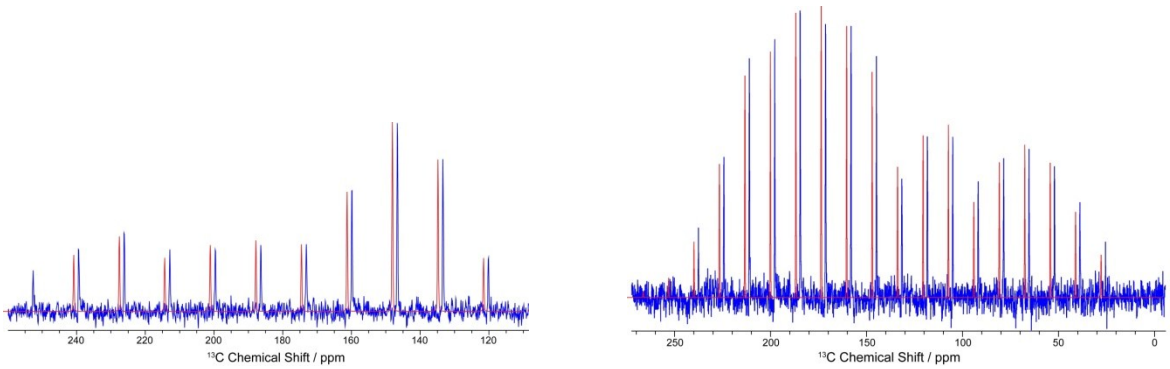


Figure S2. The TOSS-deTOSS spectrum of the SSRD at 14.09 T and 2 kHz MAS. The sideband-free isotropic chemical shift appears on vertical (f1) axis, while chemical shift anisotropies are encoded along the horizontal (f2) axis. Four traces were selected for fitting and are shown in Figure S3. 2D data were acquired as 2048 complex-valued points in t2 (spectral width 50 kHz, total acquisition time 41.02 ms) and 512 complex points in t1 (spectral width 25 kHz, total acquisition time 20.48 ms); 16 transients were co-added at each t1 point with a recycle delay of 3 s, for a total experiment time of 7 hours.

a) C15

b) C5, C7



c) C12, C14

d) C15

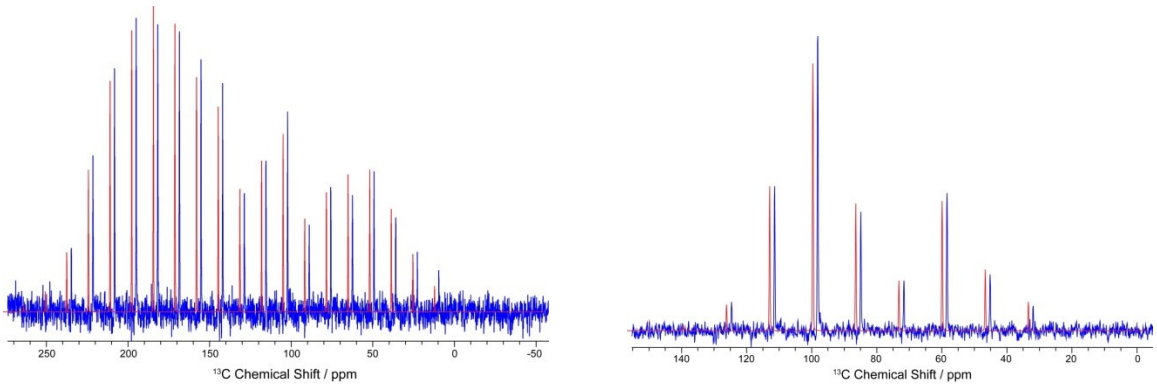


Figure S3. 1D traces (blue) from the SSRD TOSS-deTOSS spectrum used for extracting the CSA tensors via Herzfeld-Berger analysis (red) for the indicated carbon sites.

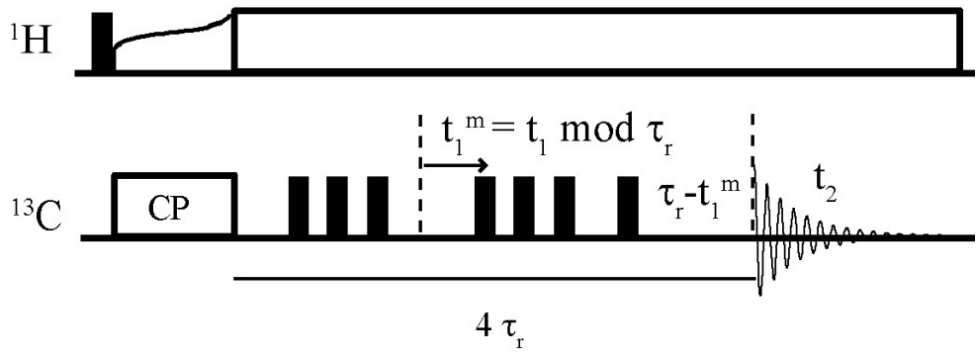


Figure S4. The xCSA[3] pulse sequence modified for extended t_1 acquisition. This sequence makes use of modula acquisition to experimentally extend the t_1 signal (which is periodic over one rotor period) and allow for full resolution of the sidebands and better definition of the baseline in the spectra shown in Figures S5/S6.

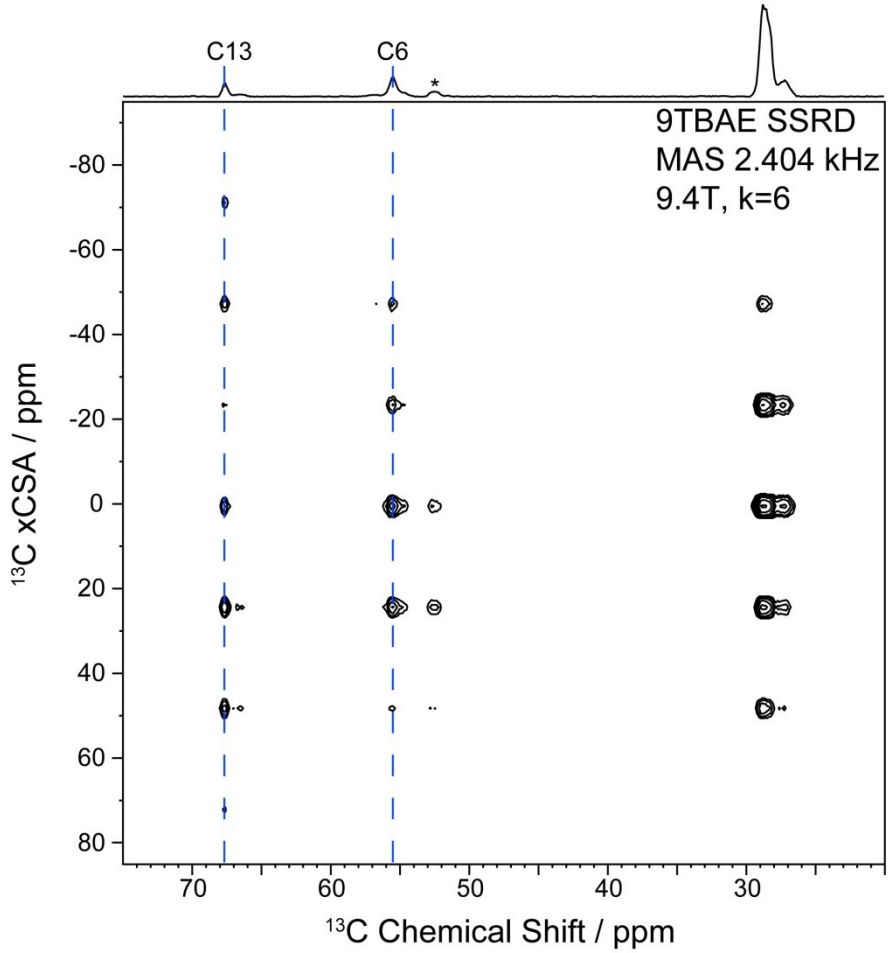


Figure S5. The xCSA spectrum of the SSRD at 9.4 T and 2.404 kHz MAS. The sideband-free isotropic chemical shift is on horizontal (f2) axis, while chemical shift anisotropies are encoded along the vertical (f1). Two traces were selected for fitting and are shown in Figure S6. 2D data were acquired as 2048 complex-valued points in t2 (spectral width 50 kHz, total acquisition time 40.96 ms) and 128 real-valued points in t1 (26 μs dwell, total acquisition time 3.328 ms); 64 transients were co-added at each t1 point with a recycle delay of 4 s, for a total experiment time of 15.5 hours.

C6 C13

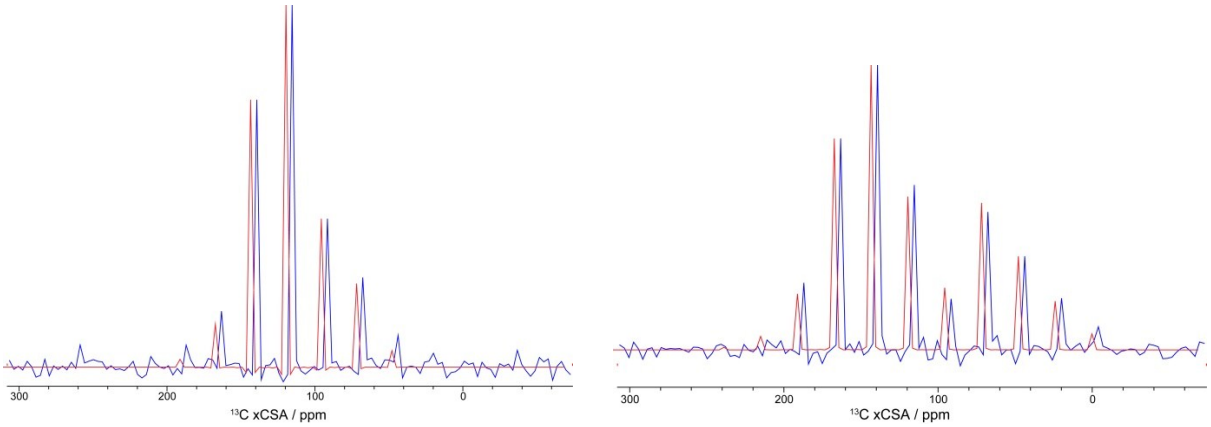


Figure S6. 1D traces (blue) from the SSRD xCSA spectrum used for extracting the CSA tensors via Herzfeld-Berger analysis (red) for the indicated carbon sites.

References

1. A. C. Kolbert and R. G. Griffin, *Chemical Physics Letters*, 1990, **166**, 87-91.
2. N. Ivchenko, C. E. Hughes and M. H. Levitt, *Journal of Magnetic Resonance*, 2003, **164**, 286-293.
3. I. Hung and Z. H. Gan, *J. Magn. Reson.*, 2011, **213**, 196-199.