Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Highly efficient ^{19}F heteronuclear decoupling in solid-state NMR spectroscopy using supercycled refocused-CW irradiation

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Details on experiments

All the experiments mentioned here were recorded on a Bruker Avance II widebore 400 MHz instrument.		
Figure2	Decoupling condition: *r*CW$^{[0p]}$: $\tau_A = \tau_r$, $\nu_1{}^{cw} = \nu_1{}^{\pi} = \nu_1$ *r*CW$^{[0p90p]}$: $\tau_A = 1.01\tau_r$, $\nu_1{}^{cw} = \nu_1{}^{\pi} = \nu_1$ *r*CW$^{[0p180p0m180m]}$: $\tau_A = 1.02\tau_r$, $\nu_1{}^{cw} = \nu_1{}^{\pi} = \nu_1$ *r*CW$^{[0p180m0m180p]}$: $\tau_A = 0.98\tau_r$, $\nu_1{}^{cw} = \nu_1{}^{\pi} = \nu_1$ SPINAL64: $\tau = 4.00$ μs (flip angle 180^o), Phase: $\Theta = 10^o$, $\alpha = 5^o$, $\beta = 10^o$ TPPM: $\tau = 3.75$ μs(flip angle 169^o), Phase: $\Theta = 20^o$	$\nu_1 = 125$ kHz $\nu_r = 25$ kHz
Figure3	Decoupling condition: *r*CW$^{[0p90p]}$: $\tau_A = 1.03\tau_r$, $\nu_1{}^{cw} = \nu_1{}^{\pi} = \nu_1$ SPINAL64: $\tau = 4.30$ μs(flip angle 171^o), Phase: $\Theta = 10^o$, $\alpha = 5^o$, $\beta = 10^o$ TPPM: $\tau = 3.75$ μs(flip angle 149^o), Phase: $\Theta = 25^o$	$\nu_1 = 110$ kHz $\nu_r = 15$ kHz

Fig.SI-1: Numerical simulations for a larger ^{19}F-CSA in a $^{13}CF_2$ spin system.
Here, we show the numerically simulated decoupling profile of (a) *r*CW$^{[0p180p0m180m]}$ and (b) *r*CW$^{[0p90p]}$ for a CF_2 system (same parameters as in Fig.4a-b except an increased ^{19}F-CSA of 100 ppm (~40 kHz)) as a function of τ_A/τ_r and ν_1 with ν_r = 15 kHz.

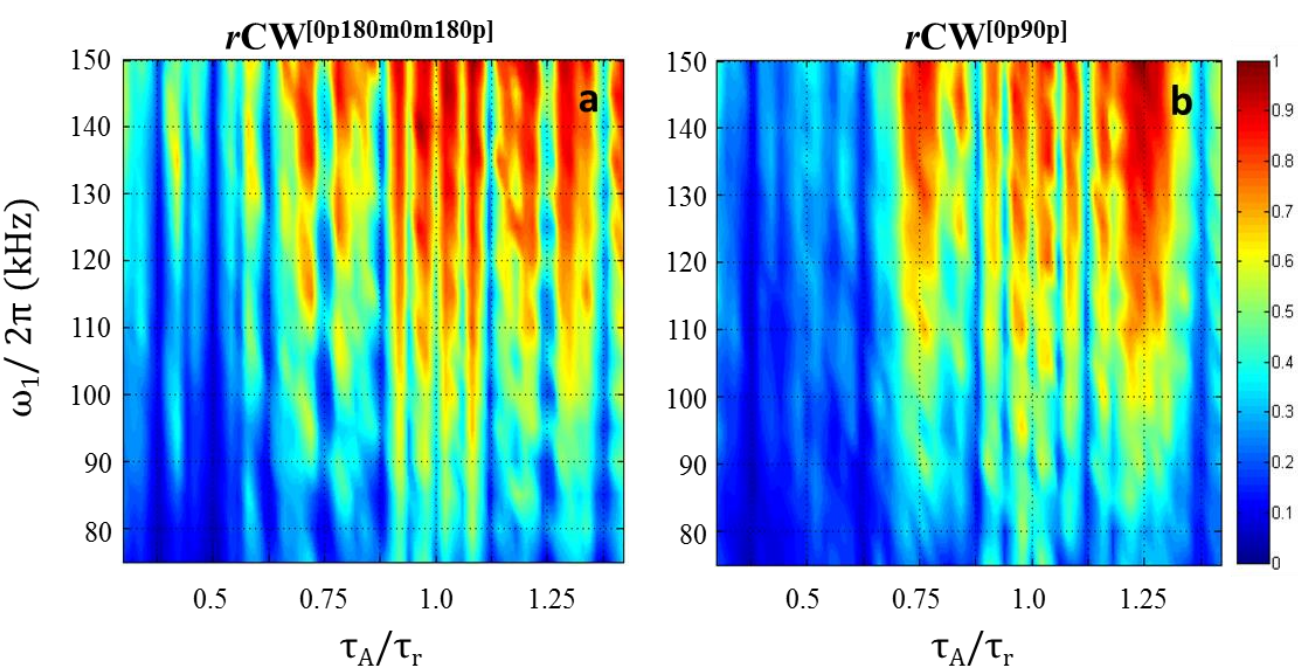
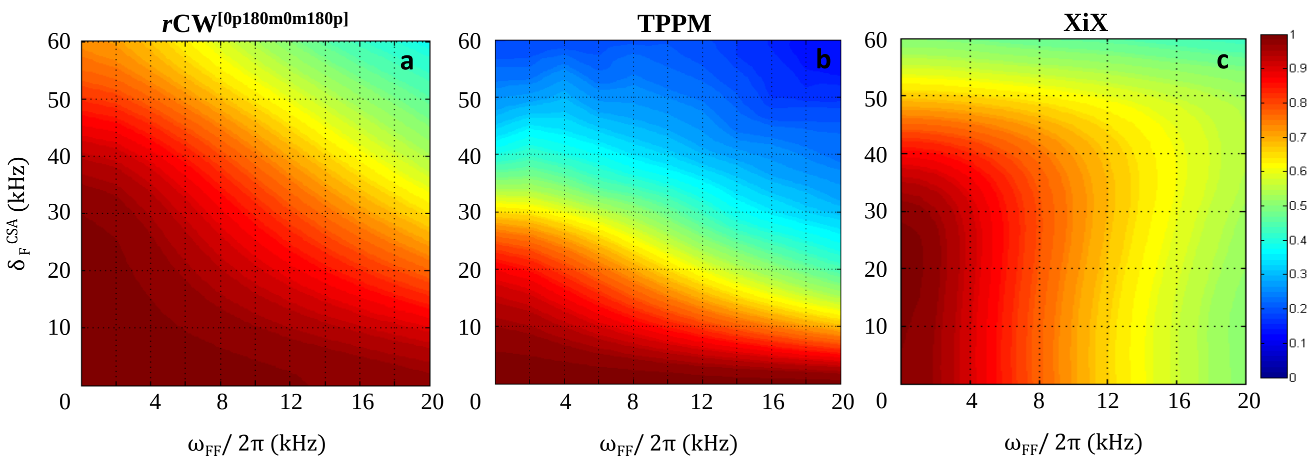


Fig.SI-2: Numerical simulations for varying ^{19}F-CSA and ^{19}F-^{19}F dipole coupling strength in a CF_2 spin system.

Numerically simulated normalized peak height observed for the ^{13}C resonance of a CF_2 spin system as a function of ^{19}F-CSA and ^{19}F-^{19}F dipole coupling strength under (a) *r*CW$^{[0p180m0m180p]}$, (b) TPPM, and (c) XiX irradiation with ν_1 = 125 kHz kHz, ν_r = 15 kHz, and a magnetic field strength of 400 MHz. While TPPM is not tolerant towards high CSA, XiX performance is hindered by homonuclear interaction.



Floquet analysis

The form of the effective dipolar Hamiltonian induced by the cross term between the *II* homonuclear dipolar coupling and the *IS* heteronuclear dipolar coupling is given by

$$H_{(II-IS)}^{(0,0)} = -\sum_{\mu,\nu,\sigma,\gamma\equiv x,y,z}\sum_{i,j}\sum_{n,k}\frac{a_k^{\mu\nu}a_{-k}^{\sigma}\omega_{I_iI_j}^{(n)}\omega_{I_iS}^{(-n)}}{n\omega_r+k\omega_c}I_{i\gamma}I_{j\nu}S_z$$

Here, the indices *i* and *j* represent different spins of *I* and the indices μ, σ, and γ follow the Levi-Civita permutation relations.