Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics


**High-resolution through-space correlations between spin-1/2 and half-integer quadrupolar nuclei with the MQ-*D*-R-INEPT NMR experiment.**

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# Electronic Supplementary Information

## Table of content

**Derivation of Eq. 18 for the *D*-R-INEPT transfer efficiency**

In the present section, we calculate the transfer efficiency, $f(\tau)$, of *D*-R-INEPT. For the sake of simplicity, we consider an isolated pair of spin-1/2 nuclei, *I* and *S*. Nevertheless, the dependence of $f(\tau)$ with the Euler angles $\Omega_{PR}^{D,IS} = \{0, \beta_{PR}^{D,IS}, \gamma_{PR}^{D,IS}\}$ is identical for a pair of spin-1/2 and half-integer quadrupolar nuclei since in the *D*-R-INEPT sequence, the RF pulses applied to the quadrupolar nuclei are selective for the central transition (CT) and the terms in the density matrix corresponding to CT can be decomposed onto fictitious spin-1/2 operators $\{\hat{C}_x^I, \hat{C}_y^I, \hat{C}_z^I\}$. Furthermore, the relaxation phenomena and all spin interactions, with the exception of the *I*-*S* dipolar coupling, are disregarded. We assume the initial density operator is $\hat{I}_x$ (or $\hat{C}_x^I$ for a half-integer quadrupolar *I* nucleus). During the R$^3$ ($N$ = 1) recoupling applied on the *S* channel, the density matrix evolves under the effect of the AH given by Eq. S1:

$$\hat{I}_x \xrightarrow{\overline{\hat{H}_{D,IS}}^{(1)}\tau} \cos(\omega_{D,IS}\tau)\hat{I}_x + 2\sin(\omega_{D,IS}\tau)\left[\cos(\phi)\hat{I}_y\hat{S}_z + \sin(\phi)\hat{I}_y\hat{S}_y\right] \qquad \text{Eq. (S1)}$$

After the application of the two 90° pulses of phase x on *I* and *S* channels, the density operator has the following form:

$$\hat{\rho}(t_{90}^+) = \cos(\omega_{D,IS}\tau)\hat{I}_x + 2\sin(\omega_{D,IS}\tau)\left[-\cos(\phi)\hat{I}_z\hat{S}_y + \sin(\phi)\hat{I}_z\hat{S}_z\right] \qquad \text{Eq. (S2)}$$

where $t_{90}^+$ is the time point corresponding to the end of the 90° pulses. The first term in Eq. S2 is not transferred to the *S* nucleus and is discarded in the following. The two other terms in Eq. S2 are transferred and evolve under the Hamiltonian of Eq. 9. In particular, $2\hat{I}_z\hat{S}_y$ and $2\hat{I}_z\hat{S}_z$ operators are transformed into operator $\hat{S}_x$ with respective pre-factors $-\cos(\phi)\sin(\omega_{D,IS}\tau)$ and $\sin(\phi)\sin(\omega_{D,IS}\tau)$. Therefore, the transfer efficiency is:

$$f(\tau) = \left\langle \left(\hat{S}_x \middle| \hat{S}_x\right)^{1} \left(\hat{S}_x \middle| \hat{U}\hat{I}_x\hat{U}^{\dagger}\right) \right\rangle = \left\langle \sin^2\left(\omega_{D,IS}\tau\right)\left\{\cos^2(\phi) + \sin^2(\phi)\right\} \right\rangle \qquad \text{Eq. (S3)}$$

which directly gives Eq. 18.

**Table S1.** P-Al distances ($d_{P-Al}$ < 3.25 Å), $^{31}P$-$^{27}Al$ dipolar ($|b_{P-Al}|/2\pi$) and scalar couplings ($J_{P-Al}$)[1] in $AlPO_4$-VPI-5.

| P | Al | $d_{P-Al}$ (Å) | $b_{P-Al}/2\pi$ (Hz) | $J_{P-Al}$ (Hz) |
|---|---|---|---|---|
| P1 | Al2 | 3.096 | 425 | |
| | Al3 | 3.101 | 423 | |
| | Al1 | 3.276 | 359 | 20 |
| | Al1 | 3.318 | 345 | 25 |
| P2 | Al2 | 3.091 | 427 | |
| | Al1 | 3.113 | 418 | 13 |
| | Al3 | 3.117 | 416 | |
| | Al2 | 3.130 | 411 | |
| P3 | Al3 | 3.087 | 429 | |
| | Al3 | 3.117 | 417 | |
| | Al1 | 3.157 | 401 | 15 |
| | Al2 | 3.242 | 370 | |

## Reference

1 J. Trébosc, J. P. Amoureux, L. Delevoye, J. W. Wiench, M. Pruski, *Solid State Sci.*, 2004, **6**, 1089.