PCCP

ROYAL SOCIETY OF CHEMISTRY

CORRECTION

View Article Online
View Journal | View Issue

Cite this: *Phys. Chem. Chem. Phys.*, 2021, **23**, 13768

Correction: *De novo* prediction of cross-effect efficiency for magic angle spinning dynamic nuclear polarization

Frédéric Mentink-Vigier,[ab] Anne-Laure Barra,[c] Johan van Tol,[b] Sabine Hediger,[a] Daniel Lee[a] and Gaël De Paëpe*[a]

DOI: 10.1039/d1cp90117f

rsc.li/pccp

Correction for '*De novo* prediction of cross-effect efficiency for magic angle spinning dynamic nuclear polarization' by Frédéric Mentink-Vigier *et al.*, *Phys. Chem. Chem. Phys.*, 2019, **21**, 2166–2176, DOI: 10.1039/C8CP06819D.

The authors wish to correct the sign of the *J*-exchange interaction in Table 1 in order to match the convention defined in the Supporting Information. The *J*-exchange interaction values are all negative under the convention $\left(\hat{H}_{\text{exchange}} = -2J_{a,b}\,\overrightarrow{\hat{S}_a}\cdot\overrightarrow{\hat{S}_b}\right)$. The corrected version of Table 1 is shown below.

Table 1 List of the calculated (DFT) and experimental geometric parameters (after fitting) for the TEKPol and AMUPol biradicals. Euler angles are given in degrees with respect to the first *g*-tensor, using Easyspin's v 5.1 rotation convention (active rotation).[67] The *g*-strains for the simulations are proportional to ([1.3 × (g_x − 2), g_y − 2, g_z − 2] × 6%) and are [0.8, 0.35, 0.13] × 10^{-3} for TEKPol and [0.8, 0.3, 0.12] × 10^{-3} for AMUPol

Biradical	*g*-Tensor [g_x, g_y, g_z]	*g*-Tensor relative orientation (α, β, γ)	^{14}N hyperfine coupling (MHz)	Dipolar coupling/ *J*-exchange interaction (MHz)	Dipolar orientation (ϕ, θ)
TEKPol DFT	[2.0094, 2.0070, 2.0024]	[−70.4, 79.7, −63.7]	n.c.[a]	30.5/n.c.	[10, 66.3]
TEKPol Exp.	[2.0095, 2.0060, 2.0021] ± 2 × 10^{-4}	[−75.4, 79.6, −58.6] ± 2.5	[18, 16, 98] ± 2	30.5 ± 1/−1 ± 1	[10, 66.3] ± 3
AMUPol DFT	[2.0091, 2.0067, 2.0024]	[125.1, 129.7, −46.6]	n.c.[a]	34.75/n.c.	[−174.6, 74]
AMUPol Exp.	[2.0092, 2.0061, 2.0020] ± 2 × 10^{-4}	[123.1, 129.8, −46] ± [2.5, 5, 2.5]	[18, 17, 100] ± 2	35 ± 2/−16 ± 2	[−174, 76] ± 5

[a] n.c. = not calculated.

A sentence in the conclusion should also be modified to: "it clearly confirms the presence of an exchange interaction of ∼−15 MHz and a dipolar coupling of ∼35 MHz for AMUPol, as initially reported,[23,30] although it was a matter of debate[78] until recently.[68]"

In addition, Fig. 4 was incorrect: the grey overlay representing the error was shifted. The corrected figure is shown below.

[a] *Univ. Grenoble Alpes, CEA, CNRS, INAC-MEM, F-38000 Grenoble, France. E-mail: gael.depaepe@cea.fr*
[b] *National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL, 32310, USA*
[c] *Laboratoire National des Champs Magnétiques Intenses – CNRS, Univ. Grenoble Alpes, F-38042 Grenoble, France*

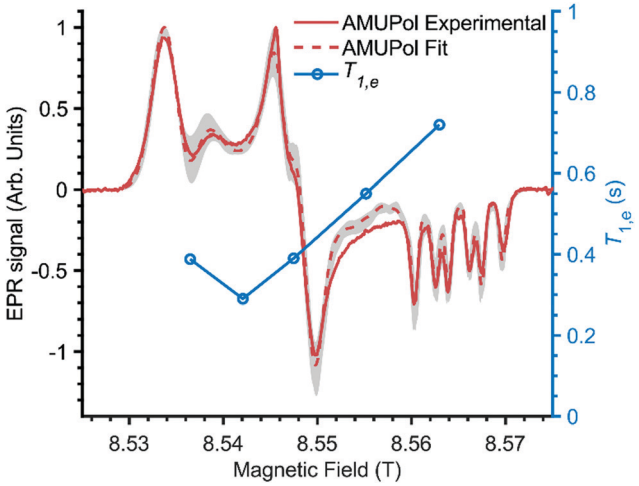

Fig. 4 High-field EPR spectrum of 10 mM of AMUPol in D_8-glycerol/D_2O/H_2O (60/30/10 v%) + 2M ^{13}C-urea, recorded at 100 K, for a microwave frequency of 240 GHz. The red curve represents the experimental spectrum and the red dashed line represents the theoretical EPR spectrum obtained with fitted parameters reported in Table 1. The blue dots correspond to the measured electron spin–lattice relaxation times, T_{1e} (right axis).

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.