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

Supplementary Information for Uncertainty estimates for magnetic relaxation times and magnetic relaxation parameters

Daniel Reta[a,*] and Nicholas F. Chilton[a,*]

[a] The School of Chemistry, The University of Manchester, Oxford Road, M13 9PL, UK

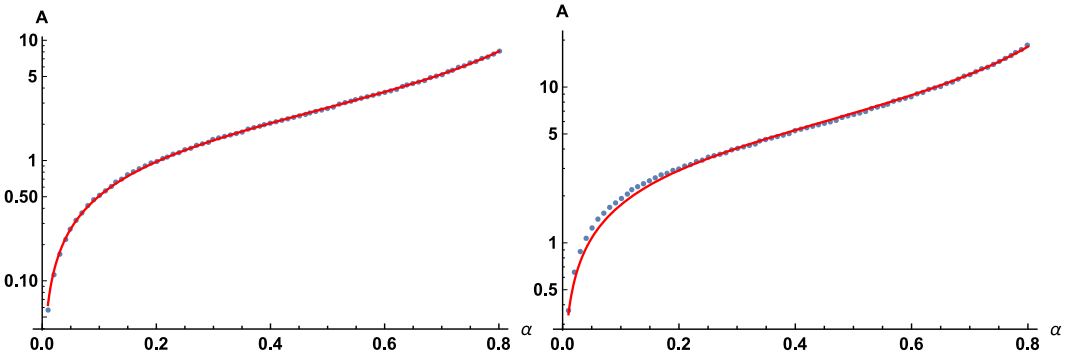

Figure S1 – Range of $\pm A$ required to encapsulate 1σ (left) and 2σ (right) populations as a function of α from the Fuoss-Kirkwood distribution. Note the logarithmic scale.

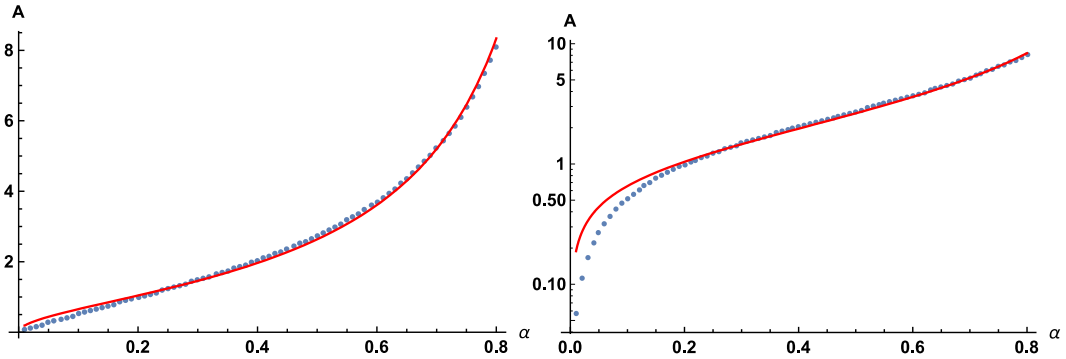

Figure S2 – Range of $\pm A$ required to encapsulate 1σ populations as a function of α from the Fuoss-Kirkwood distribution on a linear y-scale (left) and a logarithmic y-scale (right). Red line is a fit with the square-root model ($A \approx \frac{1.86\sqrt{\alpha}}{1-\alpha}$).

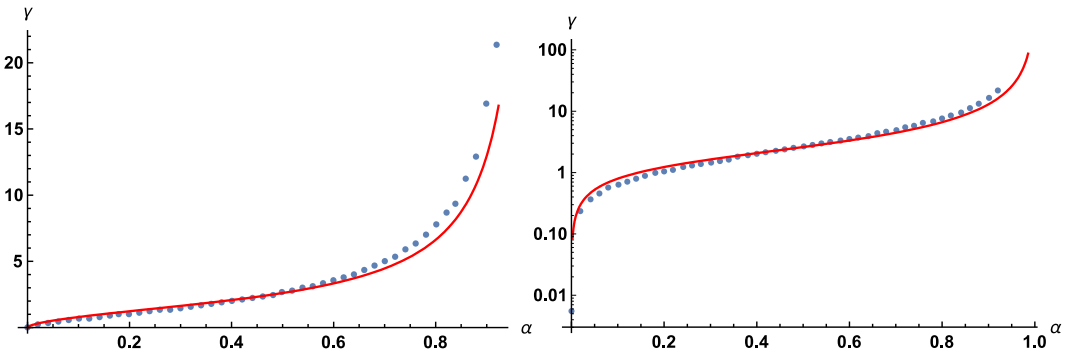

Figure S3 – Equivalence of γ as a function of α on a linear y-scale (left) and a logarithmic y-scale (right). Red line is a fit with the tangential model ($\gamma \approx \frac{1.97\ tan[\frac{\alpha\pi}{2}]}{\alpha^{0.41}}$).

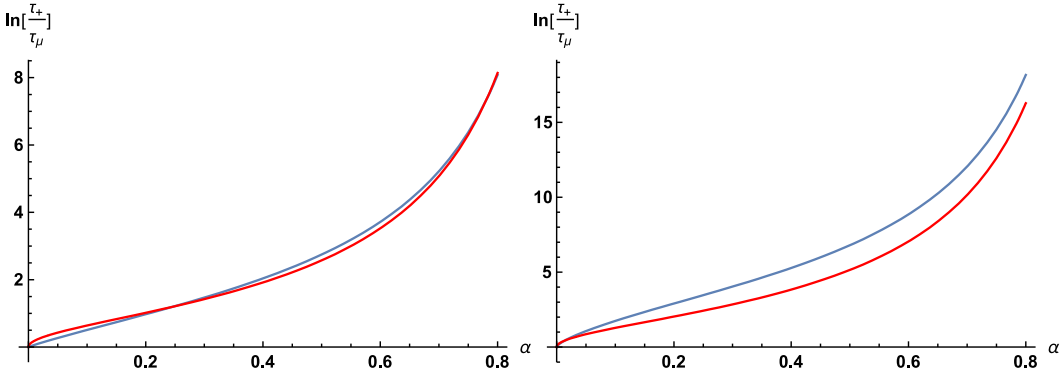

Figure S4 – Comparison between the Fuoss-Kirkwood (blue) and log-normal (red) models at 1σ (left) and 2σ (right) levels.

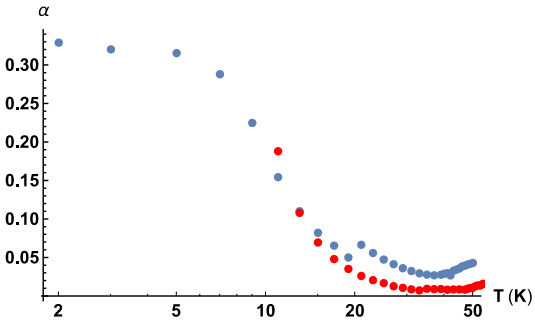

Figure S5 – Temperature dependence of α for [Dy(bbpen)Cl] (blue) and [Dy(bbpen)Br] (red).

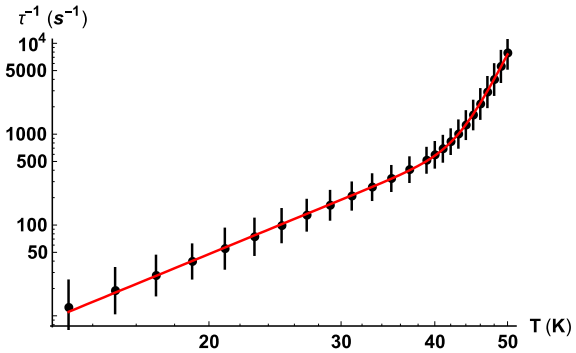

Figure S6 – Relaxation dynamics for [Dy(bbpen)Cl], note the log-log scale. Error bars are calculated using the log-normal distribution model at the 1σ level. Red line is a fit to Equation 10 with the 1σ level parameters given in Table S1.

Table S1 – Magnetic relaxation parameters accounting for distributions in the relaxation time. First row for each compound is without considering any uncertainty in the τ values (*i.e.* 0σ). Numbers in parentheses are standard errors (*i.e.* 1σ parameter ranges).

Compound	Range	U_{eff} (K)	A (log[s])	R (log[s^{-1} K^{-n}])	n	Q (log[s])
[Dy(bbpen)Cl][6] [a] (all temperatures)	0σ	920(10)	-11.8(1)	-2.97(2)	3.55(2)	-0.358(6)
	1σ	900(200)	-12(2)	-3.0(6)	3.5(4)	-0.4(4)
[Dy(bbpen)Cl][6] [a] (> 13 K only)	0σ	880(20)	-11.4(2)	-2.67(4)	3.35(3)	-
	1σ	900(200)	-12(2)	-2.7(5)	3.4(4)	-

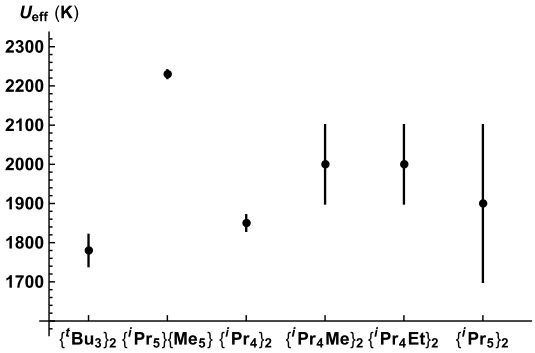

Figure S7 – U_{eff} values for the [DyCpCp']$^{+}$ cations with uncertainties determined at the 1σ level.