Supporting Information For:

Lanthanide Single Molecule Magnets: Relation Between Crystal Packing and Tunnelling Relaxation Time

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*** Calculated tunnelling rates for the complete dataset are available as separate plain text files.**

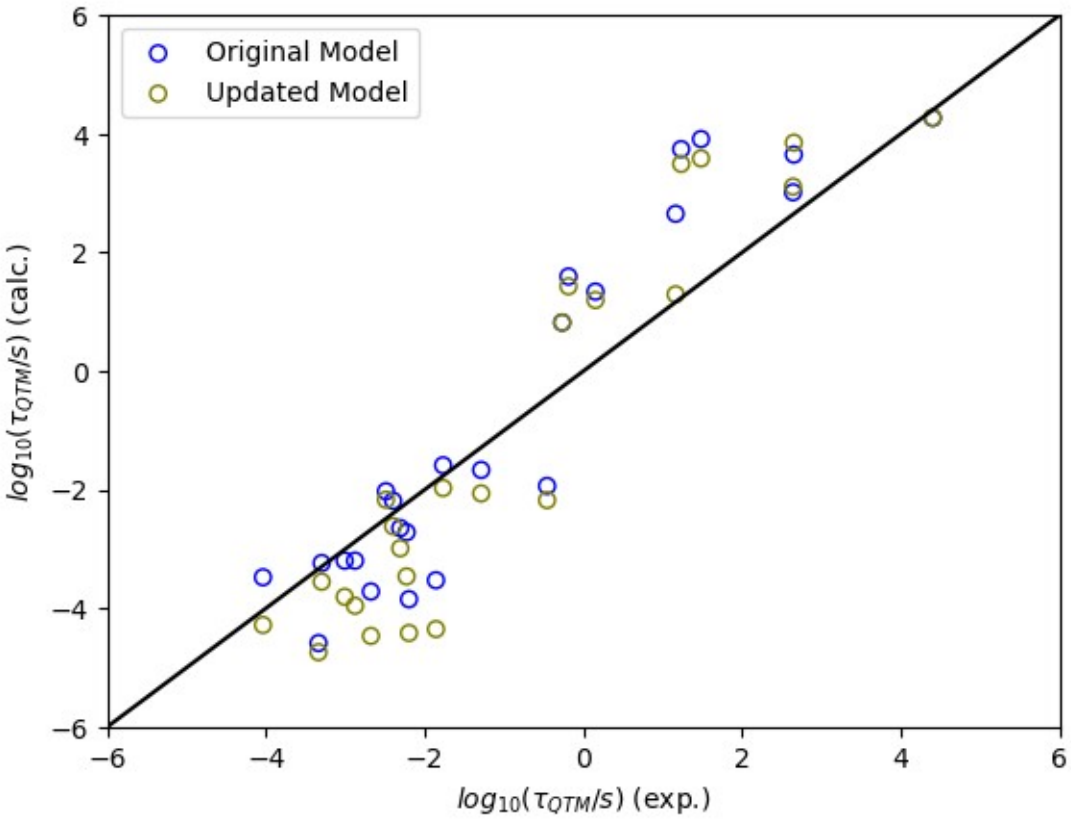

Figure S1. Experimental and calculated tunnelling relaxation times for a set of 24 molecular complexes. Blue and green circles correspond to values calculated with the original and updated model of the spin-dipolar model.

Table S1. Experimental and calculated tunnelling relaxation time for the 24 molecular systems of the model benchmark set.

REFCODE	$log_{10}(\tau/s)$			Reference
	Experimental	Calculated		
		Old Model	New Model	
BAJSIQ	-3.34	-4.59	-4.74	[1]
DARTOH	-2.20	-3.85	-4.42	[2]
DARTUN	-1.86	-3.53	-4.35	[2]
EJASIT	-3.01	-3.20	-3.81	[3]
FUMCUN01	1.16	2.65	1.29	[4]
GAQGOX	-2.31	-2.65	-2.99	[5]
GUYRAU	-2.68	-3.72	-4.47	[6]
IMOVAJ	-0.46	-1.94	-2.18	[7]
LIRQUB	4.40	4.27	4.27	[8]
NAFMIT	1.48	3.91	3.58	[4]
OLUJEM	-4.04	-3.48	-4.28	[9]
PAXRIS	-3.30	-3.24	-3.56	[10]
PUKFAF	-1.77	-1.59	-1.98	[11]
QUQKUK	-1.29	-1.67	-2.07	[12]
QUQLEV	-2.40	-2.19	-2.62	[12]
TEKXUF	-2.49	-2.03	-2.17	[13]
TEKYAM	-0.27	0.82	0.82	[13]
UCEZUZ	-2.88	-3.20	-3.96	[14]
UCIBAL	-2.23	-2.72	-3.47	[14]
VORCUD	-0.19	1.59	1.43	[15]
WIRHAJ	2.64	3.01	3.11	[16]
WIRHEN	2.65	3.65	3.85	[16]
ZAVSOH	1.23	3.74	3.49	[17]
ZIFPIQ	0.15	1.34	1.19	[18]

Table S2. Selected crystallographic information and calculated tunnelling relaxation times for the ten coordination polymers with the highest positive departure from the expected tunnelling relaxation time. Several repetitions of the system with Refcode DOGFEO13 were cleared from the list as they presented essentially identical parameters.

CCDC Refcode	Lattice Parameters						$\log_{10}(\tau)$/s (average)
	a	b	c	α	β	γ	
GAPFIM	11.670	5.440	21.841	90	90	90	-4.48
NUCPOS	7.671	6.820	25.658	90	94.011	90	-3.40
DOGFEO13	5.829	5.829	19.214	90	90	120	-4.14
PEBZAA01	6.551	6.551	18.517	90	90	120	-4.10
OLIDUK	6.691	6.691	18.601	90	90	120	-4.07
WUYTIV	6.669	6.669	18.371	90	90	120	-4.09
POSYIJ	6.648	6.648	19.091	90	90	120	-4.04
PICQIF	6.568	6.568	18.640	90	90	120	-4.09
NIGROM	11.569	6.756	12.088	90	103.44	90	-3.80
NIGRAY	11.636	6.824	12.168	90	103.76	90	-3.79

References

1 M. Jeletic, P.-H. Lin, J. J. Le Roy, I. Korobkov, S. I. Gorelsky and M. Murugesu, *J. Am. Chem. Soc.*, 2011, **133**, 19286–19289.

2 G. Chen, Y. Guo, J. Tian, J. Tang, W. Gu, X. Liu, S. Yan, P. Cheng and D. Liao, *Chemistry – A European Journal*, 2012, **18**, 2484–2487.

3 Y.-S. Meng, C.-H. Wang, Y.-Q. Zhang, X.-B. Leng, B.-W. Wang, Y.-F. Chen and S. Gao, *Inorg. Chem. Front.*, 2016, **3**, 828–835.

4 Y.-C. Chen, J.-L. Liu, L. Ungur, J. Liu, Q.-W. Li, L.-F. Wang, Z.-P. Ni, L. F. Chibotaru, X.-M. Chen and M.-L. Tong, *J. Am. Chem. Soc.*, 2016, **138**, 2829–2837.

5 Y. Kishi, F. Pointillart, B. Lefeuvre, F. Riobé, B. Le Guennic, S. Golhen, O. Cador, O. Maury, H. Fujiwara and L. Ouahab, *Chemical Communications*, 2017, **53**, 3575–3578.

6 S. Jiang, B. Wang, G. Su, Z. Wang and S. Gao, *Angew. Chem. Int. Ed.*, 2010, **49**, 7448–7451.

7 J. Liu, Y.-C. Chen, J.-L. Liu, V. Vieru, L. Ungur, J.-H. Jia, L. F. Chibotaru, Y. Lan, W. Wernsdorfer, S. Gao, X.-M. Chen and M.-L. Tong, *J. Am. Chem. Soc.*, 2016, **138**, 5441–5450.

8 F.-S. Guo, B. M. Day, Y.-C. Chen, M.-L. Tong, A. Mansikkamäki and R. A. Layfield, *Science*, 2018, **362**, 1400–1403.

9 E. Lucaccini, M. Briganti, M. Perfetti, L. Vendier, J. Costes, F. Totti, R. Sessoli and L. Sorace, *Chemistry – A European Journal*, 2016, **22**, 5552–5562.

10 S.-S. Liu, Y.-S. Meng, Y.-Q. Zhang, Z.-S. Meng, K. Lang, Z.-L. Zhu, C.-F. Shang, B.-W. Wang and S. Gao, *Inorg. Chem.*, 2017, **56**, 7320–7323.

11 A. B. Canaj, S. Dey, O. Céspedes, C. Wilson, G. Rajaraman and M. Murrie, *Chemical Communications*, 2020, **56**, 1533–1536.

12 W.-B. Sun, P.-F. Yan, S.-D. Jiang, B.-W. Wang, Y.-Q. Zhang, H.-F. Li, P. Chen, Z.-M. Wang and S. Gao, *Chem. Sci.*, 2016, **7**, 684–691.

13 H. Zhang, R. Nakanishi, K. Katoh, B. K. Breedlove, Y. Kitagawa and M. Yamashita, *Dalton Transactions*, 2018, **47**, 302–305.

14 Y. Bi, Y. Guo, L. Zhao, Y. Guo, S. Lin, S. Jiang, J. Tang, B. Wang and S. Gao, *Chemistry – A European Journal*, 2011, **17**, 12476–12481.

15 S. Bala, G.-Z. Huang, Z.-Y. Ruan, S.-G. Wu, Y. Liu, L.-F. Wang, J.-L. Liu and M.-L. Tong, *Chemical Communications*, 2019, **55**, 9939–9942.

16 K. Randall McClain, C. A. Gould, K. Chakarawet, S. J. Teat, T. J. Groshens, J. R. Long and B. G. Harvey, *Chem. Sci.*, 2018, **9**, 8492–8503.

17 Y. Chen, J. Liu, Y. Lan, Z. Zhong, A. Mansikkamäki, L. Ungur, Q. Li, J. Jia, L. F. Chibotaru, J. Han, W. Wernsdorfer, X. Chen and M. Tong, *Chemistry – A European Journal*, 2017, **23**, 5708–5715.

18 Y.-S. Ding, K.-X. Yu, D. Reta, F. Ortu, R. E. P. Winpenny, Y.-Z. Zheng and N. F. Chilton, *Nat. Commun.*, 2018, **9**, 3134.