Electronic Supplementary Material (ESI) for Dalton Transactions.

Supplementary Information

High relaxation barrier in Neodymium furoate-based field-induced SMMs

E. Bartolomé[a,*], A. Arauzo[b,c], S J. Luzón[b,d], S. Melnic[e], S. Shova[f], D. Prodius[g], I. C. Nlebedim[g], F. Bartolomé[b], J. Bartolomé[b]

S1. *Ab initio* results

Weight composition of the 5 Kramer's doublets (KD) as a function of the free ion states for Nd(III) in the two complexes.

Table S1. *Ab initio* calculated eigenstates of Nd(III) in terms of the free ion wave functions. The numbers in the table indicate the weight of the combined $\pm M_J$ states.

Complex (**1**)

Levels	Energy (K)	±9/2	±7/2	±5/2	±3/2	±1/2
KD1	0	0.554	0.149	0.012	0.162	0.123
KD2	125.496	0.135	0.086	0.192	0.272	0.315
KD3	270.225	0.031	0.094	0.687	0.123	0.065
KD4	341.208	0.199	0.110	0.012	0.309	0.371
KD5	498.804	0.081	0.560	0.098	0.135	0.127

Complex (**2**)

Levels	Energy (K)	±9/2	±7/2	±5/2	±3/2	±1/2
KD1	0	0.561	0.032	0.023	0.281	0.102
KD2	58.800	0.103	0.160	0.611	0.097	0.029
KD3	197.715	0.147	0.283	0.252	0.228	0.089
KD4	334.262	0.130	0.459	0.059	0.254	0.098
KD5	362.732	0.058	0.065	0.055	0.140	0.682

S2. Susceptibility *vs.* temperature for complex (2)

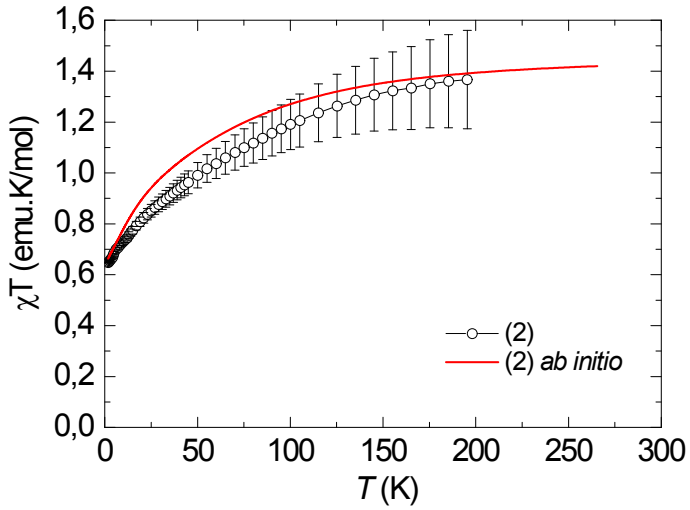

Fig. S1. Temperature dependence of the susceptibility product for complex (**2**) and *ab initio* fit.

S3. Bottleneck effect relaxation experiments

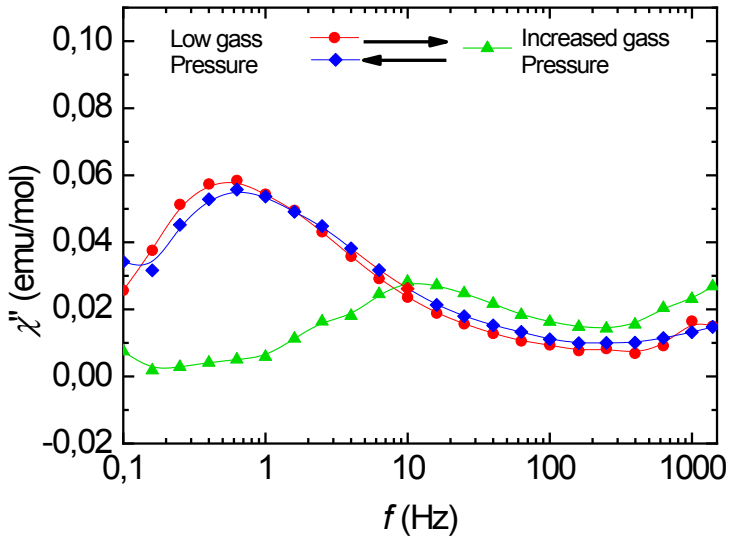

Fig. S2. $\chi''(f)$ at T=3 K, H=10 kOe measured for complex (**1**) in the SQUID susceptometer under different pressure conditions: experiments were performed with the chamber purged (low pressure) or vented (high pressure); the $\chi''(f)$ curve is recovered one the chamber is purged again.