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Supporting Information

Construction of Lanthanide Single-Molecule Magnets with the Magnetic Motif $[Dy(MQ)_4]^-$

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CONTENT:

Table S1. Continuous Shape Measures calculation for **1** and **2** by SHAPE v2.1*.

1							
Dy1	OP-8	HPY-8	HBPY-8	CU-8	SAPR-8	TDD-8	JGBF-8
	30.581	22.810	13.706	8.342	2.327	3.687	14.590
	JETBPY-8	JBTPR-8	BTPR-8	JSD-8	TT-8	ETBPY-8	
	25.762	4.557	3.801	6.505	8.797	20.903	
Dy2	EP-9	OPY-9	HBPY-9	JTC-9	JCCU-9	CCU-9	JCSAPR-9
	36.298	22.317	19.178	12.912	10.340	9.169	3.519
	CSAPR-9	JTCTPR-9	TCTPR-9	JTDIC-9	HH-9	MFF-9	
	2.578	3.749	2.102	9.565	12.273	2.706	
2							
Dy1	OP-8	HPY-8	HBPY-8	CU-8	SAPR-8	TDD-8	JGBF-8
	33.703	22.030	14.734	10.571	3.582	3.627	15.439
	JETBPY-8	JBTPR-8	BTPR-8	JSD-8	TT-8	ETBPY-8	
	25.648	4.738	3.403	6.326	11.144	21.655	
Dy2	OP-8	HPY-8	HBPY-8	CU-8	SAPR-8	TDD-8	JGBF-8
	22.830	22.000	15.446	11.959	1.394	3.341	14.366
	JETBPY-8	JBTPR-8	BTPR-8	JSD-8	TT-8	ETBPY-8	
	24.682	3.264	2.520	5.146	12.721	20.481	
Dy3	OP-8	HPY-8	HBPY-8	CU-8	SAPR-8	TDD-8	JGBF-8
	32.442	22.083	14.770	9.683	2.766	3.265	16.088
	JETBPY-8	JBTPR-8	BTPR-8	JSD-8	TT-8	ETBPY-8	
	26.083	4.700	3.309	6.634	10.156	21.678	

* OP-8 = Octagon (D8h), HPY-8 = Heptagonal pyramid (C7v), HBPY-8 = Hexagonal bipyramid (D6h), CU-8 = Cube (Oh), SAPR-8 = Square antiprism (D4d), TDD-8 = Triangular dodecahedron (D2d), JGBF-8 = Johnson gyrobifastigium (D2d), JETBPY-8 = Johnson elongated triangular bipyramid (D3h), JBTPR-8 = Biaugmented trigonal prism (C2v), BTPR-8 = Biaugmented trigonal prism (C2v), JSD-8 = Snub diphenoid (D2d), TT-8 = Triakis tetrahedron (Td), ETBPY-8 = Elongated trigonal bipyramid (D3h). EP-9 = Enneagon (D9h), OPY-9 = Octagonal pyramid (C8v), HBPY-9 = Heptagonal bipyramid (D7h), JTC-9 = Johnson triangular cupola (C3v), JCCU-9 = Capped cube (C4v), CCU-9 = Spherical-relaxed capped cube (C4v), JCSAPR-9 = Capped square antiprism (C4v), CSAPR-9 = Spherical capped square antiprism (C4v), JTCTPR-9 = Tricapped trigonal prism (D3h), TCTPR-9 = Spherical tricapped trigonal prism (D3h), JTDIC-9 = Tridiminished icosahedron (C3v), HH-9 = Hula-hoop (C2v), MFF-9 = Muffin (Cs).

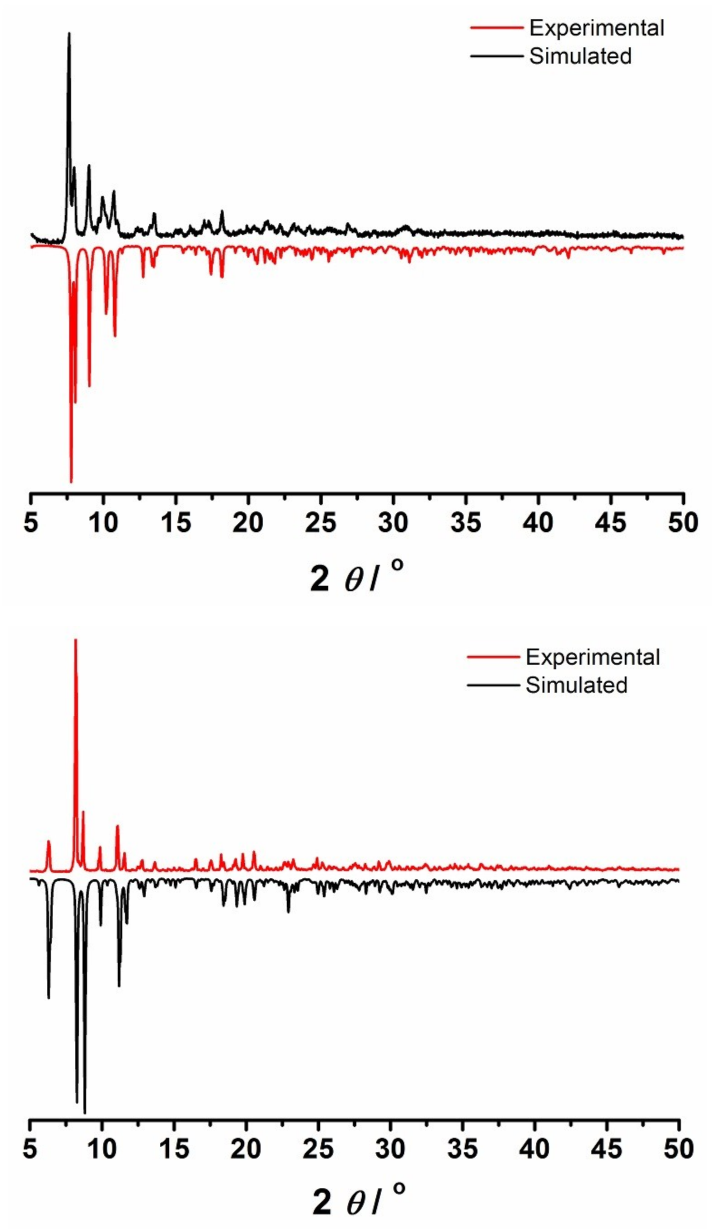


Figure S1. Experimental (*red lines*) and simulated (*black lines*) PXRD patterns of **1** (*top*) and **2** (*bottom*).

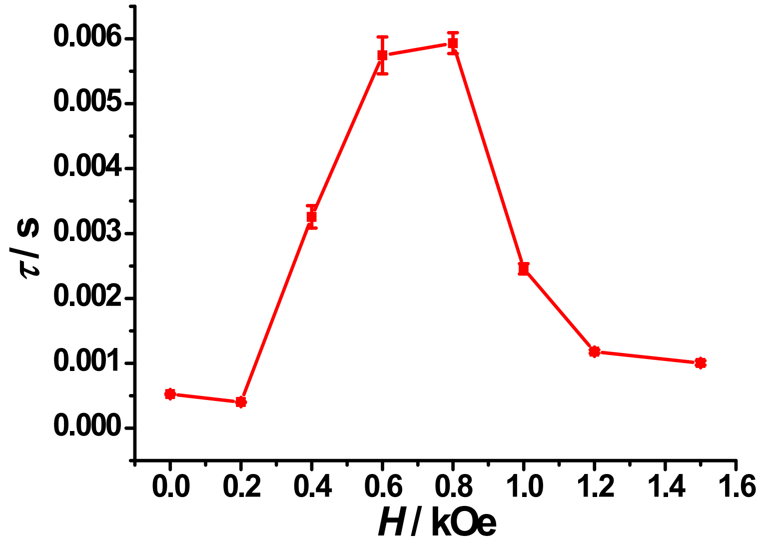
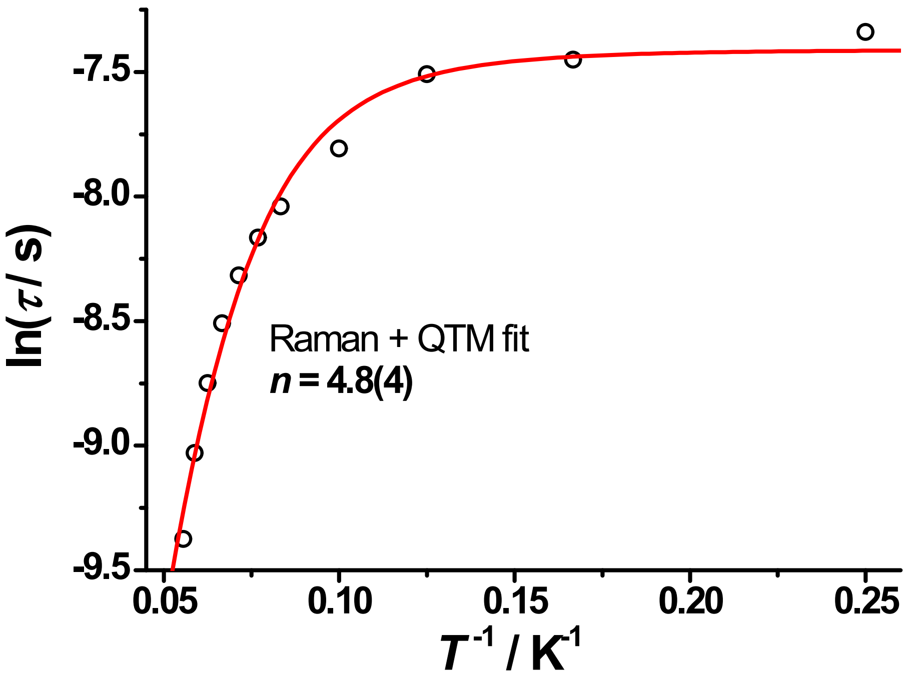
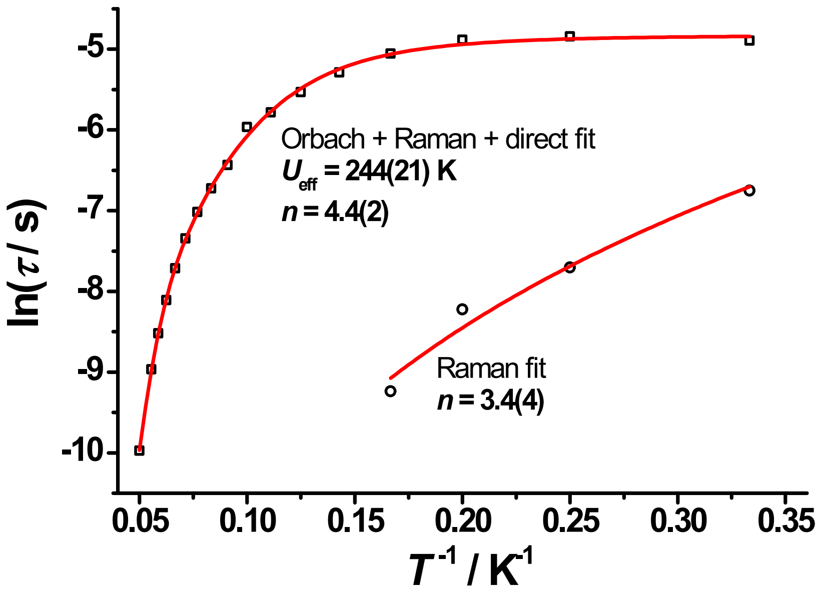


Figure S2. Dc field dependence of the relaxation time for 2 at 2 K. The optimum field is 800 Oe. The solid line is a guide for eye.



Model	nTao_Tfenzhiyi_CTn_QTM (User)		
Equation	-ln(C*Tfenzhiyi^(-n)+1/taoQTM)		
Reduced Chi-Sqr	0.00609		
Adj. R-Squar	0.98629		
		Value	Standard Err
lntao	C	0.00907	0.01022
lntao	n	4.7724	0.40066
lntao	taoQTM	6.04761E-	3.20207E-5

Figure S3. Relaxation time τ versus T^{-1} plots for complex **2** under zero dc magnetic field.



Model	lnTao_Tfenzhiyi_Ueff_CTn_AT1 (User)		
Equation	-ln(C*Tfenzhiyi^(-n)+1/tao0*exp(-U_k*Tfenzhiyi)+A*T)		
Reduced Chi-Sqr	0.00225		
Adj. R-Square	0.9991		
		Value	Standard Error
lntao	tao0	3.30801E-10	3.54488E-10
lntao	U_k	244.72373	21.57221
lntao	C	0.01249	0.00532
lntao	n	4.39512	0.17308
lntao	A	29.16971	0.94031

Model	lnTao_Tfenzhiyi_CTn_AT1 (User)		
Equation	-ln(C*Tfenzhiyi^(-n)+A*T)		
Reduced Chi-Sqr	0.04055		
Adj. R-Square	0.96224		
		Value	Standard Error
lntao	C	18.92485	11.02819
lntao	n	3.42402	0.38905
lntao	A	0	0

Figure S4. Relaxation time τ versus T^{-1} plots for complex **2** under an 800 Oe dc magnetic field.