

Fine Tuning the Energy Barrier of Molecular Nanomagnets via Lattice Solvent Molecules

Cai-Ming Liu,* De-Qing Zhang & Dao-Ben Zhu

*Beijing National Laboratory for Molecular Sciences, Center for Molecular Science,
Key Laboratory of Organic Solids, Institute of Chemistry, CAS Research/Education
Center for Excellence in Molecular Science, Chinese Academy of Sciences, No.2 1st
North Street, Zhongguancun, Beijing 100190, China.*

Table S1. Continuous Shape Measures' calculation for the Tb(III) ion in complex 1.

Tb structures

OP-8	1 D8h	Octagon
HPY-8	2 C7v	Heptagonal pyramid
HBPY-8	3 D6h	Hexagonal bipyramid
CU-8	4 Oh	Cube
SAPR-8	5 D4d	Square antiprism
TDD-8	6 D2d	Triangular dodecahedron
JGBF-8	7 D2d	Johnson gyrobifastigium J26
JETBPY-8	8 D3h	Johnson elongated triangular bipyramid J14
JBTPR-8	9 C2v	Biaugmented trigonal prism J50
BTPR-8	10 C2v	Biaugmented trigonal prism
JSD-8	11 D2d	Snub diphenoid J84
TT-8	12 Td	Triakis tetrahedron
ETBPY-8	13 D3h	Elongated trigonal bipyramid

Structure [ML8]	OP-8	HPY-8	HBPY-8	CU-8	SAPR-8	TDD-8	JGBF-8	JETBPY-8	JBTPR-8	BTPR-8	JSD-8	TT-8	ETBPY-8
ABOXIY,	31.698,	23.086,	16.504,	11.444,	3.314,	1.015,	13.017,	27.453,	2.247,	1.756,	2.666,	11.951,	24.368

Table S2. Continuous Shape Measures' calculation for the Tb(III) ion in complex 2.

Tb structures

OP-8	1 D8h	Octagon
HPY-8	2 C7v	Heptagonal pyramid
HBPY-8	3 D6h	Hexagonal bipyramid
CU-8	4 Oh	Cube
SAPR-8	5 D4d	Square antiprism
TDD-8	6 D2d	Triangular dodecahedron
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Structure [ML8]	OP-8	HPY-8	HBPY-8	CU-8	SAPR-8	TDD-8	JGBF-8	JETBPY-8	JBTPR-8	BTPR-8	JSD-8	TT-8	ETBPY-8
ABOXIY,	31.788,	22.983,	16.541,	11.586,	3.073,	1.096,	13.154,	27.344,	2.040,	1.584,	2.756,	12.103,	24.236

Table S3. Continuous Shape Measures' calculation for the Tb(III) ion in complex 3.

Tb structures

OP-8	1 D8h	Octagon
HPY-8	2 C7v	Heptagonal pyramid
HBPY-8	3 D6h	Hexagonal bipyramid
CU-8	4 Oh	Cube
SAPR-8	5 D4d	Square antiprism
TDD-8	6 D2d	Triangular dodecahedron
JGBF-8	7 D2d	Johnson gyrobifastigium J26
JETBPY-8	8 D3h	Johnson elongated triangular bipyramid J14
JBTPR-8	9 C2v	Biaugmented trigonal prism J50
BTPR-8	10 C2v	Biaugmented trigonal prism
JSD-8	11 D2d	Snub diphenoid J84
TT-8	12 Td	Triakis tetrahedron
ETBPY-8	13 D3h	Elongated trigonal bipyramid

Structure [ML8]	OP-8	HPY-8	HBPY-8	CU-8	SAPR-8	TDD-8	JGBF-8	JETBPY-8	JBTPR-8	BTPR-8	JSD-8	TT-8	ETBPY-8
ABOXIY,	31.876,	22.773,	16.416,	11.604,	2.998,	1.163,	13.002,	27.432,	1.920,	1.496,	2.832,	12.121,	24.286

Table S4. Continuous Shape Measures' calculation for the Tb(III) ion in complex 4.

Tb structures

OP-8	1 D8h	Octagon
HPY-8	2 C7v	Heptagonal pyramid
HBPY-8	3 D6h	Hexagonal bipyramid
CU-8	4 Oh	Cube
SAPR-8	5 D4d	Square antiprism
TDD-8	6 D2d	Triangular dodecahedron
JGBF-8	7 D2d	Johnson gyrobifastigium J26
JETBPY-8	8 D3h	Johnson elongated triangular bipyramid J14
JBTPR-8	9 C2v	Biaugmented trigonal prism J50
BTPR-8	10 C2v	Biaugmented trigonal prism
JSD-8	11 D2d	Snub diphenoid J84
TT-8	12 Td	Triakis tetrahedron
ETBPY-8	13 D3h	Elongated trigonal bipyramid

Structure [ML8]	OP-8	HPY-8	HBPY-8	CU-8	SAPR-8	TDD-8	JGBF-8	JETBPY-8	JBTPR-8	BTPR-8	JSD-8	TT-8	ETBPY-8
ABOXIY,	32.125,	23.815,	16.621,	11.722,	3.172,	1.017,	12.868,	27.630,	2.223,	1.735,	2.626,	12.249,	24.210

Table S5. Continuous Shape Measures' calculation for the Dy(III) ion in complex 5.

Dy structures

OP-8	1 D8h	Octagon
HPY-8	2 C7v	Heptagonal pyramid
HBPY-8	3 D6h	Hexagonal bipyramid
CU-8	4 Oh	Cube
SAPR-8	5 D4d	Square antiprism
TDD-8	6 D2d	Triangular dodecahedron
JGBF-8	7 D2d	Johnson gyrobifastigium J26
JETBPY-8	8 D3h	Johnson elongated triangular bipyramid J14
JBTPR-8	9 C2v	Biaugmented trigonal prism J50
BTPR-8	10 C2v	Biaugmented trigonal prism
JSD-8	11 D2d	Snub diphendoid J84
TT-8	12 Td	Triakis tetrahedron
ETBPY-8	13 D3h	Elongated trigonal bipyramid

Structure [ML8]	OP-8	HPY-8	HBPY-8	CU-8	SAPR-8	TDD-8	JGBF-8	JETBPY-8	JBTPR-8	BTPR-8	JSD-8	TT-8	ETBPY-8
ABOXIY,	31.689,	23.108,	16.402,	11.353,	3.273,	0.975,	12.992,	27.566,	2.181,	1.735,	2.599,	11.843,	24.53

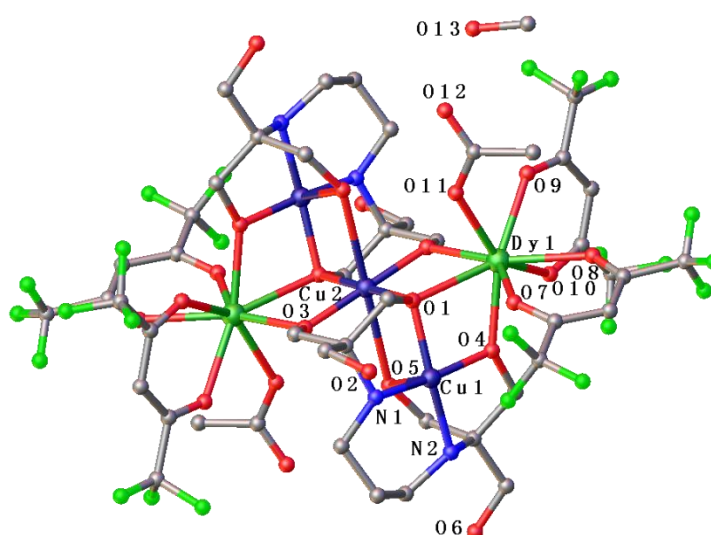


Fig. S1. Crystal structure of 5, all H atoms are omitted for clarity.

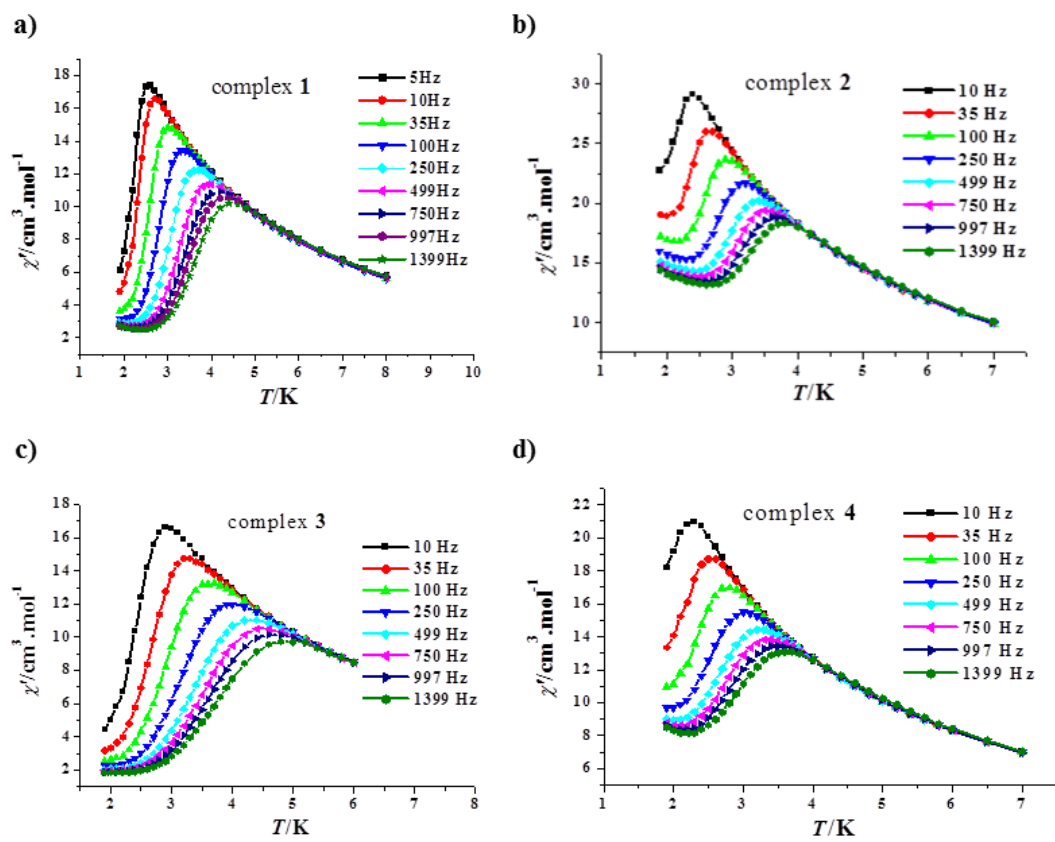


Fig. S2. Plots of χ'' vs T for **1-4** ($H_{\text{dc}} = 0$ Oe, $H_{\text{ac}} = 2.5$ Oe).

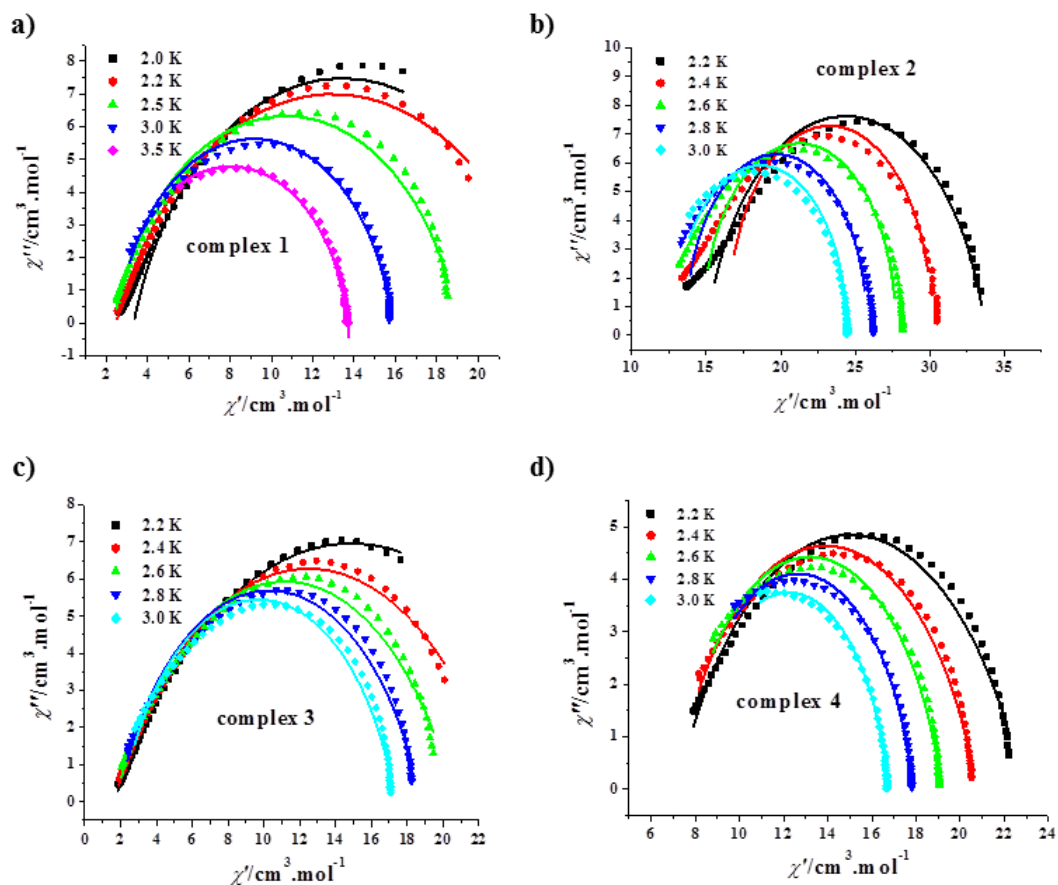


Fig. S3. Cole-Cole plots for **1-4** ($H_{dc} = 0$ Oe and $H_{ac} = 2.5$ Oe). The solid lines represent the best fitting

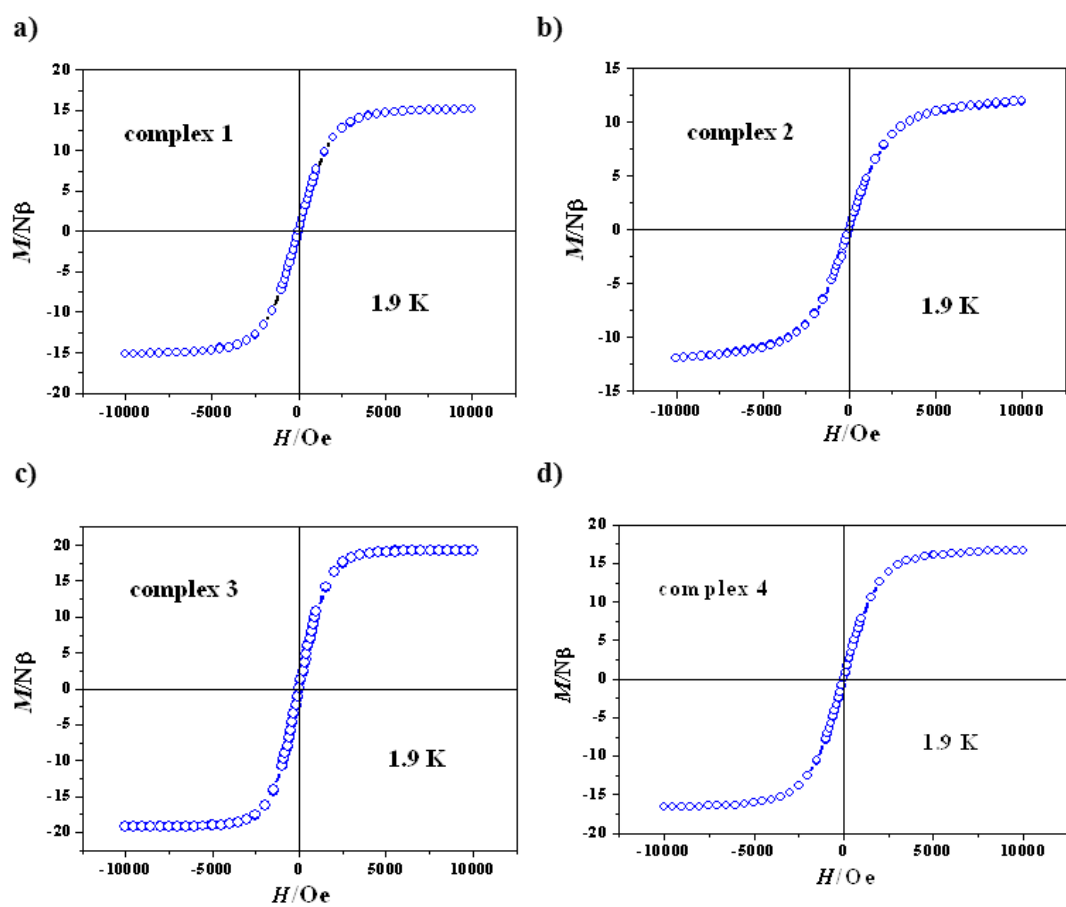


Fig. S4. Plots of M vs H at 1.9 K from -10000 to 10000 Oe for **1-4**.

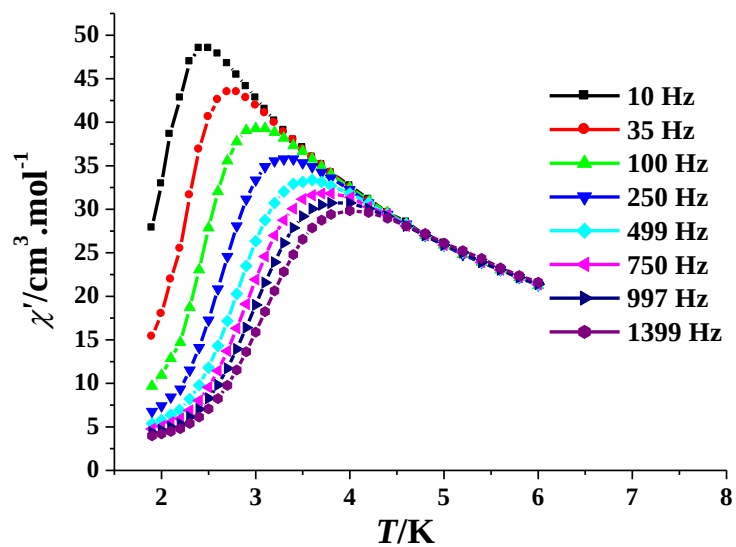


Fig. S5. Plot of χ'' vs T for **5** ($H_{dc} = 0$ Oe, $H_{ac} = 2.5$ Oe).

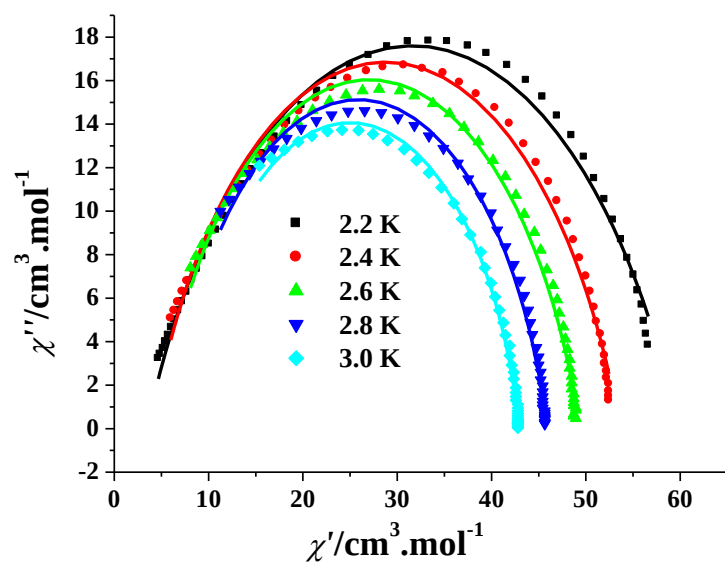


Fig. S6. Cole-Cole plot at 2.2-3.0 K for **5** ($H_{dc} = 0$ Oe and $H_{ac} = 2.5$ Oe). The solid lines represent the best fitting

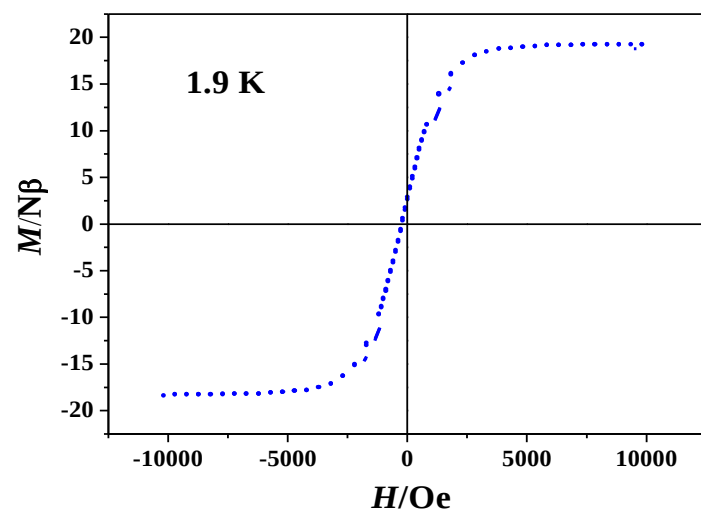


Fig. S7. Plot of M vs H at 1.9 K from -10000 to 10000 Oe for 5.