

Electronic Supplementary Material (ESI) for New Journal of Chemistry. This journal is © The Royal Society of Chemistry and the Centre National de la Recherche Scientifique 2021

Supporting Information

Magnetic relaxation in two chain-like Zn₂Dy₂ Schiff base coordination polymers bridged by tetraoxolene and its one-electron reduced radical

Cai-Ming Liu^{a,b} and Xiang Hao^a*

^a *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, Beijing 100190, China. E-mail: cmliu@iccas.ac.cn*

^b *School of Chemical Sciences, University of Chinese Academy of Sciences, Beijing 100049, China.*

Table S1. Continuous shape measures calculation for Dy1 atom in **1**.

Dy1 structure

EP-9	1 D9h	Enneagon
OPY-9	2 C8v	Octagonal pyramid
HBPY-9	3 D7h	Heptagonal bipyramid
JTC-9	4 C3v	Johnson triangular cupola J3
JCCU-9	5 C4v	Capped cube J8
CCU-9	6 C4v	Spherical-relaxed capped cube
JCSAPR-9	7 C4v	Capped square antiprism J10
CSAPR-9	8 C4v	Spherical capped square antiprism
JTCTPR-9	9 D3h	Tricapped trigonal prism J51
TCTPR-9	10 D3h	Spherical tricapped trigonal prism
JTDIC-9	11 C3v	Tridiminished icosahedron J63
HH-9	12 C2v	Hula-hoop
MFF-9	13 Cs	Muffin

Structure [ML9]	EP-9	OPY-9	HBPY-9	JTC-9	JCCU-9	CCU-9	JCSAPR-9	CSAPR-9	JTCTPR-9	TCTPR-9	JTDIC-9	HH-9	MFF-9
ABOXIY,	36.639,	22.989,	18.848,	15.565,	10.777,	9.076,	1.640,	1.147,	3.407,	1.777,	12.575,	9.054,	0.983

Table S2. Continuous shape measures calculation for Dy2 atom in **1**.

Dy2 structure

EP-9	1 D9h	Enneagon
OPY-9	2 C8v	Octagonal pyramid
HBPY-9	3 D7h	Heptagonal bipyramid
JTC-9	4 C3v	Johnson triangular cupola J3
JCCU-9	5 C4v	Capped cube J8
CCU-9	6 C4v	Spherical-relaxed capped cube
JCSAPR-9	7 C4v	Capped square antiprism J10
CSAPR-9	8 C4v	Spherical capped square antiprism
JTCTPR-9	9 D3h	Tricapped trigonal prism J51
TCTPR-9	10 D3h	Spherical tricapped trigonal prism
JTDIC-9	11 C3v	Tridiminished icosahedron J63
HH-9	12 C2v	Hula-hoop
MFF-9	13 Cs	Muffin

Structure [ML9]	EP-9	OPY-9	HBPY-9	JTC-9	JCCU-9	CCU-9	JCSAPR-9	CSAPR-9	JTCTPR-9	TCTPR-9	JTDIC-9	HH-9	MFF-9
ABOXIY,	35.080,	23.099,	17.937,	15.686,	11.046,	9.393,	2.433,	1.795,	3.713,	2.698,	13.592,	7.728,	1.261

Table S3. Continuous shape measures calculation for Dy1 atom in **2**.

Dy1 structure

EP-9	1 D9h	Enneagon
OPY-9	2 C8v	Octagonal pyramid
HBPY-9	3 D7h	Heptagonal bipyramid
JTC-9	4 C3v	Johnson triangular cupola J3
JCCU-9	5 C4v	Capped cube J8
CCU-9	6 C4v	Spherical-relaxed capped cube
JCSAPR-9	7 C4v	Capped square antiprism J10
CSAPR-9	8 C4v	Spherical capped square antiprism
JTCTPR-9	9 D3h	Tricapped trigonal prism J51
TCTPR-9	10 D3h	Spherical tricapped trigonal prism
JTDIC-9	11 C3v	Tridiminished icosahedron J63
HH-9	12 C2v	Hula-hoop
MFF-9	13 Cs	Muffin

Structure [ML9]	EP-9	OPY-9	HBPY-9	JTC-9	JCCU-9	CCU-9	JCSAPR-9	CSAPR-9	JTCTPR-9	TCTPR-9	JTDIC-9	HH-9	MFF-9
ABOXIY,	36.361,	23.009,	18.393,	15.770,	10.589,	9.526,	1.567,	1.092,	3.288,	1.750,	12.605,	9.342,	1.019

Table S4. Continuous shape measures calculation for Dy2 atom in **2**.

Dy2 structure

EP-9	1 D9h	Enneagon
OPY-9	2 C8v	Octagonal pyramid
HBPY-9	3 D7h	Heptagonal bipyramid
JTC-9	4 C3v	Johnson triangular cupola J3
JCCU-9	5 C4v	Capped cube J8
CCU-9	6 C4v	Spherical-relaxed capped cube
JCSAPR-9	7 C4v	Capped square antiprism J10
CSAPR-9	8 C4v	Spherical capped square antiprism
JTCTPR-9	9 D3h	Tricapped trigonal prism J51
TCTPR-9	10 D3h	Spherical tricapped trigonal prism
JTDIC-9	11 C3v	Tridiminished icosahedron J63
HH-9	12 C2v	Hula-hoop
MFF-9	13 Cs	Muffin

Structure [ML9]	EP-9	OPY-9	HBPY-9	JTC-9	JCCU-9	CCU-9	JCSAPR-9	CSAPR-9	JTCTPR-9	TCTPR-9	JTDIC-9	HH-9	MFF-9
ABOXIY,	36.361,	23.009,	18.393,	15.770,	10.589,	9.526,	1.567,	1.092,	3.288,	1.750,	12.605,	9.342,	1.305

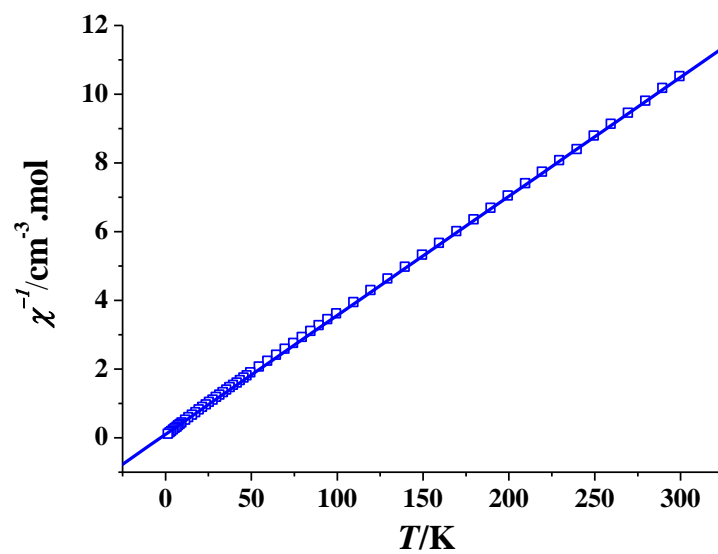


Fig. S1. $1/\chi$ versus T plot of **1**.

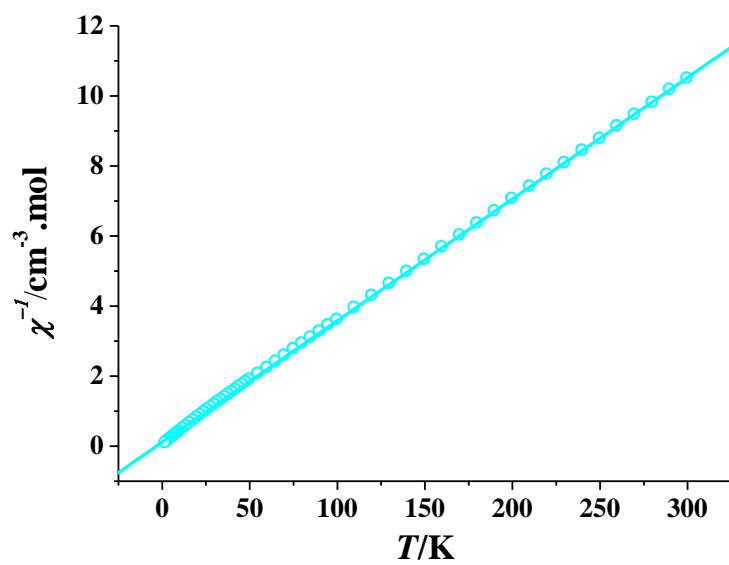


Fig. S2. $1/\chi$ versus T plot of **2**.

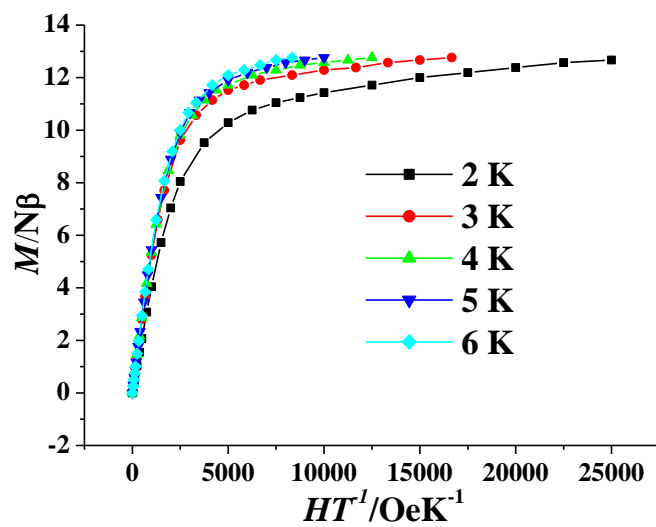


Fig. S3. M versus H/T plots at 2-6 K of 1.

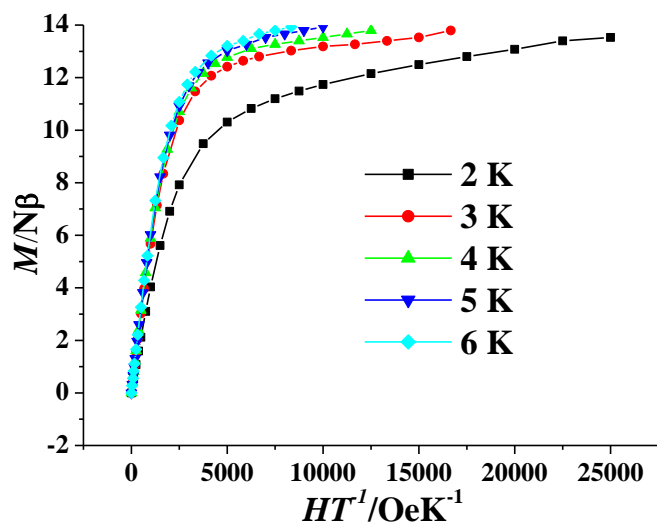


Fig. S4. M versus H/T plots at 2-6 K of 2.

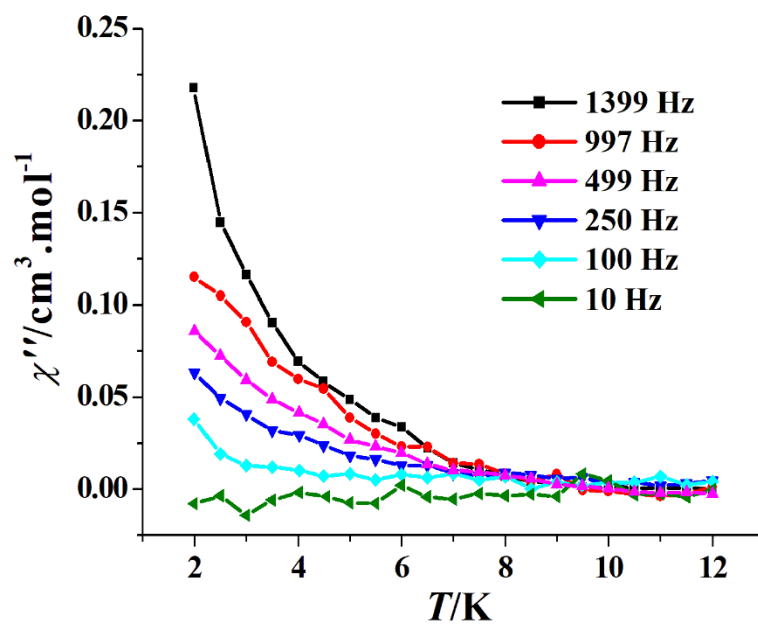


Fig. S5. Temperature dependence of χ'' for **1** under zero dc field.

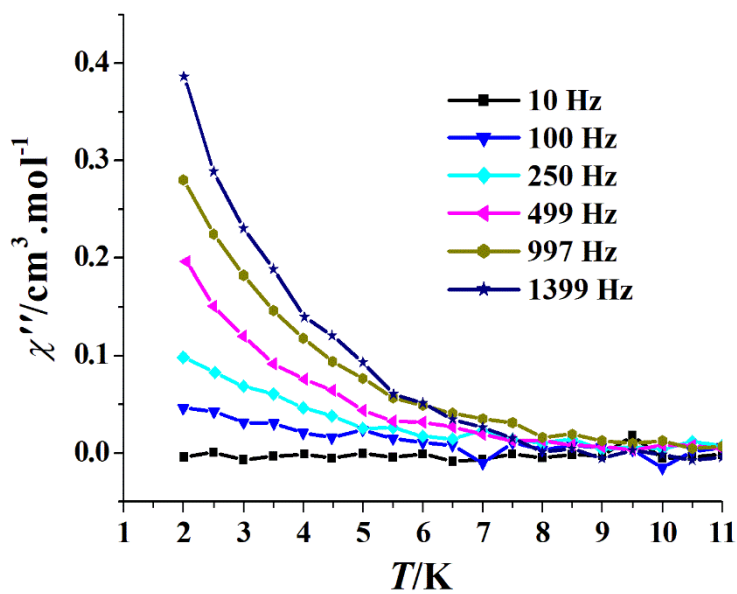


Fig. S6. Temperature dependence of χ'' for **2** under zero dc field.

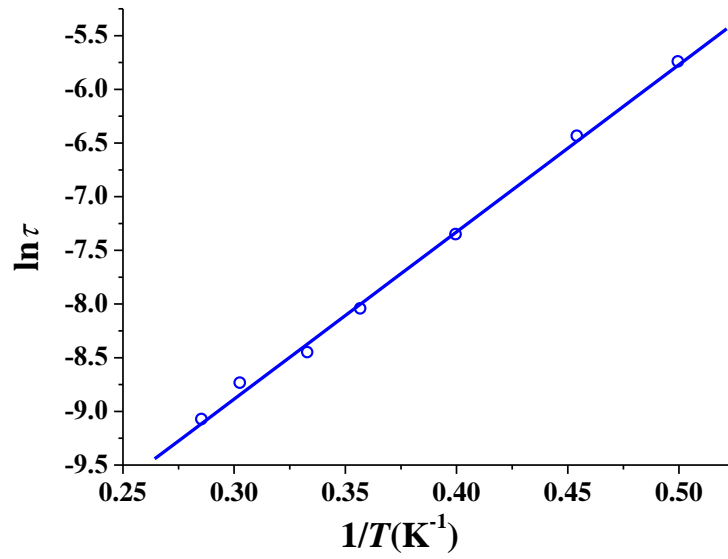


Fig. S7. Plot of $\ln(\tau)$ versus $1/T$ for **1** ($H_{\text{dc}} = 1500$ Oe), the solid line represents the best fitting with the Arrhenius law.

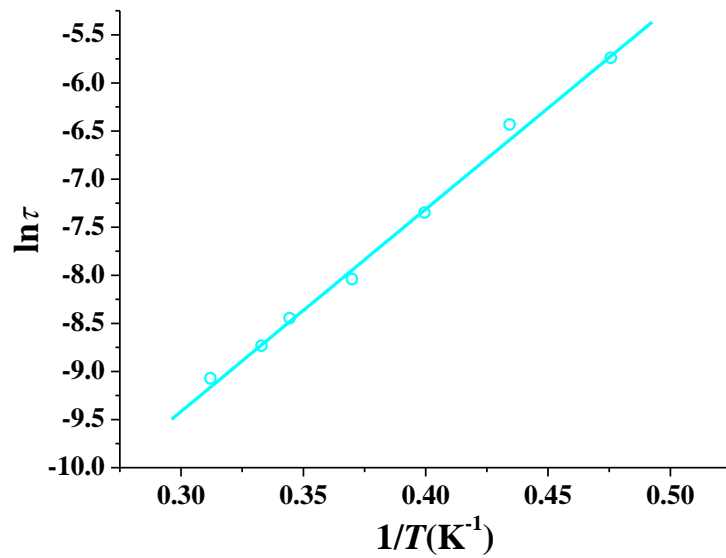


Fig. S8. Plot of $\ln(\tau)$ versus $1/T$ for **2** ($H_{\text{dc}} = 1500$ Oe), the solid line represents the best fitting with the Arrhenius law.

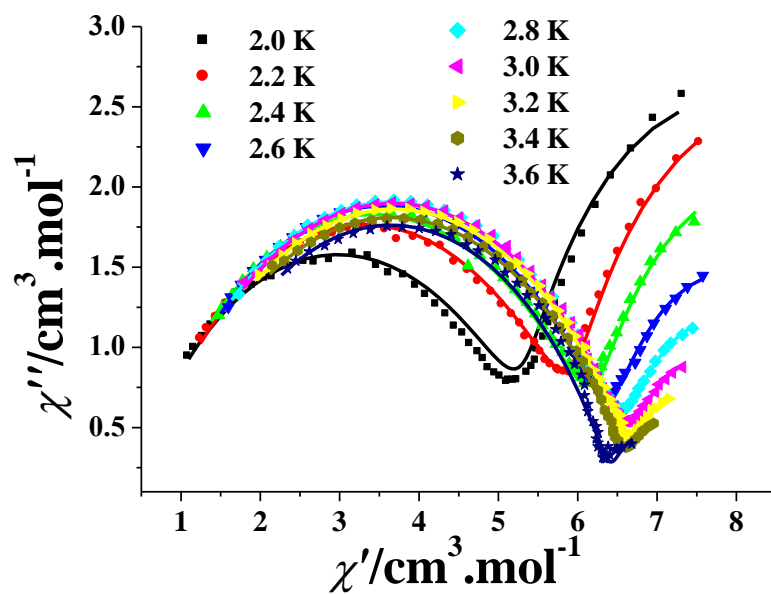


Fig. S9. Cole-Cole plots at 2.0-3.6 K for **1** ($H_{\text{dc}} = 1500$ Oe and $H_{\text{ac}} = 2.5$ Oe), the solid lines represent the best fitting with the sum of two modified Debye functions.

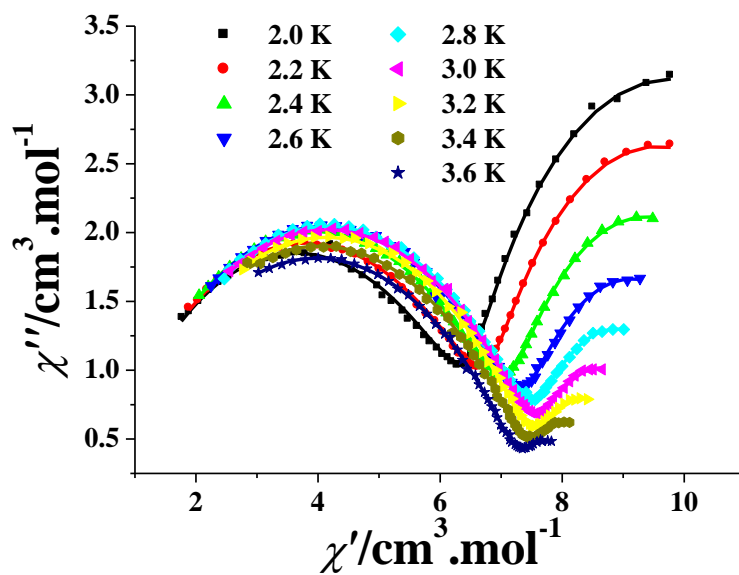


Fig. S10. Cole-Cole plots at 2.0-3.6 K for **2** ($H_{\text{dc}} = 1500$ Oe and $H_{\text{ac}} = 2.5$ Oe), the solid lines represent the best fitting with the sum of two modified Debye functions.

Table S5. Linear combination of two modified Debye model fitting parameters from 2.0 K to 3.6 K of **1** at 1500 Oe.

$T(K)$	$\chi_2(\text{cm}^3.\text{mol}^{-1})$	$\chi_1(\text{cm}^3.\text{mol}^{-1})$	$\chi_0(\text{cm}^3.\text{mol}^{-1})$	$\tau_1(\text{s})$	α_1	$\tau_2(\text{s})$	α_2
2.0	11.10054	5.28038	0.32256	0.21202	0.00737	0.00074	0.31356
2.2	10.49602	5.40027	0.42377	0.25053	0.02296	0.00071	0.29922
2.4	10.44035	4.4324	0.38549	0.26156	0.02995	0.00062	0.30714
2.6	9.38677	3.24554	0.46696	0.20775	0.0098	0.00059	0.30184
2.8	8.96897	2.70296	0.48632	0.22236	0.01498	0.00053	0.30564
3.0	8.49696	2.19058	0.50371	0.22516	0.00687	0.00047	0.31094
3.2	8.17045	1.89678	0.54327	0.25232	0.00014	0.00042	0.31828
3.4	7.68757	1.52191	0.57166	0.23717	0.00009	0.00036	0.3244
3.6	7.30255	1.49754	0.58971	0.26036	0.00003	0.00032	0.29545

Table S6. Linear combination of two modified Debye model fitting parameters from 2.0 K to 3.6 K of **2** at 1500 Oe.

$T(K)$	$\chi_2(\text{cm}^3.\text{mol}^{-1})$	$\chi_1(\text{cm}^3.\text{mol}^{-1})$	$\chi_0(\text{cm}^3.\text{mol}^{-1})$	$\tau_1(\text{s})$	α_1	$\tau_2(\text{s})$	α_2
2.0	13.13252	6.76395	0.39132	0.16448	0.03753	0.00048	0.33663
2.2	12.39254	5.70179	0.39942	0.15192	0.03681	0.00046	0.34127
2.4	11.72278	4.80594	0.45508	0.15776	0.05377	0.00043	0.33503
2.6	11.00678	3.8953	0.50343	0.15506	0.05967	0.00041	0.33864
2.8	10.37649	3.13763	0.51235	0.15715	0.06738	0.00037	0.34752
3.0	9.90424	2.65131	0.4995	0.17512	0.10641	0.00033	0.35474
3.2	9.27892	2.1066	0.53543	0.16297	0.08714	0.00029	0.36275
3.4	8.82681	1.67405	0.44631	0.1713	0.10873	0.00025	0.37857
3.6	8.35111	1.38775	0.48582	0.16695	0.10285	0.00022	0.38923