

Supplementary Materials: Hybrid Molecular Compound Exhibiting Slow Magnetic Relaxation and Electrical Conductivity

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Table S1. Crystallographic data of 1.

Formula	$C_{30}H_{19}DyF_{12}NO_8S_{16}$	$a/\text{\AA}$	8.702(9)
Space group	$P\bar{1}$	$b/\text{\AA}$	11.541(12)
Z	2	$c/\text{\AA}$	24.05(2)
T/K	100	$\alpha/^\circ$	76.99(2)
R_{int} , $R1$, $wR2/\%$	3.88, 6.20, 14.02	$\beta/^\circ$	85.55(3)
		$\gamma/^\circ$	80.34(3)

Table S2. Coordination geometry deviation obtained by SHAPE2.1.

Symmetry	Shape	Label	Value
$D4d$	Square antiprism	SAPR-8	0.029
$C2v$	Biaugmented trigonal prism	BTPR-8	2.091
$D2d$	Triangular dodecahedron	TDD-8	2.663
$C2v$	Biaugmented trigonal prism J50	JBTPR-8	2.680
$D2d$	Snub diphenoid J84	JSD-8	5.091
Oh	Cube	CU-8	10.797
Td	Triakis tetrahedron	TT-8	11.591
$D2d$	Johnson gyrobifastigium J26	JGBF-8	16.652
$D6h$	Hexagonal bipyramid	HBPY-8	18.051
$D3h$	Elongated trigonal bipyramid	ETBPY-8	23.291
$C7v$	Heptagonal pyramid	HPY-8	23.945
$D8h$	Octagon	OP-8	26.257
$D3h$	Johnson elongated triangular bipyramid J14	JETBPY-8	27.677

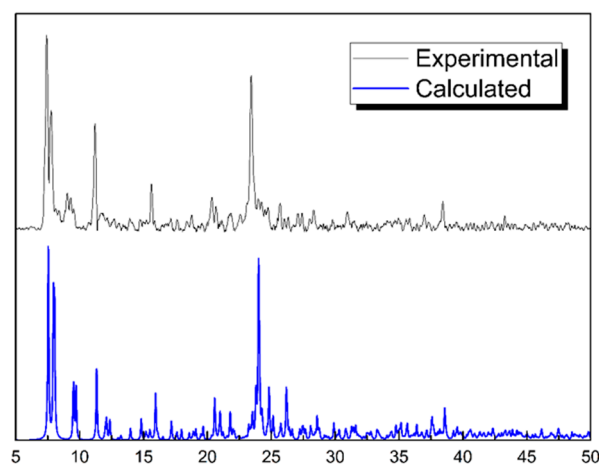


Figure S1. Comparison of the experimental and simulated powder X-ray diffraction spectra for 1.

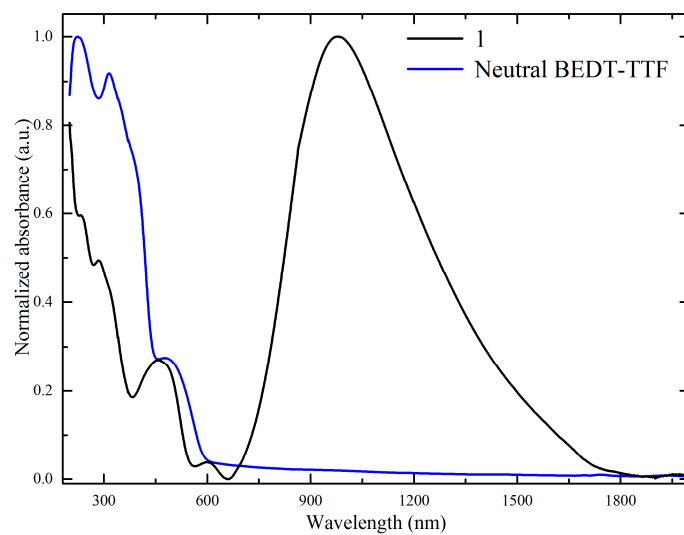


Figure S2. Solid state absorption spectroscopy of **1** and neutral BEDT-TTF for comparison.

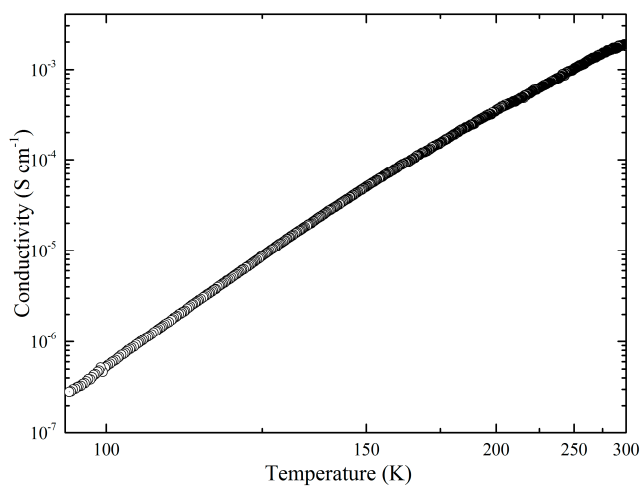


Figure S3. Temperature dependence of resistivity with single crystal using a two-probe method.

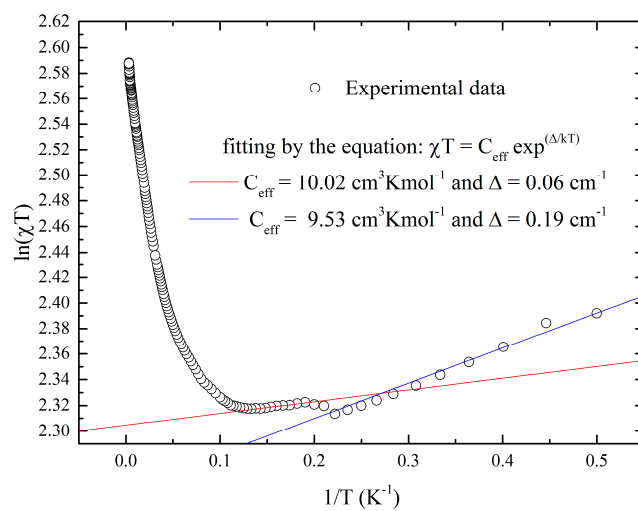


Figure S4. Plots of $\ln(\chi T)$ versus $1/T$.

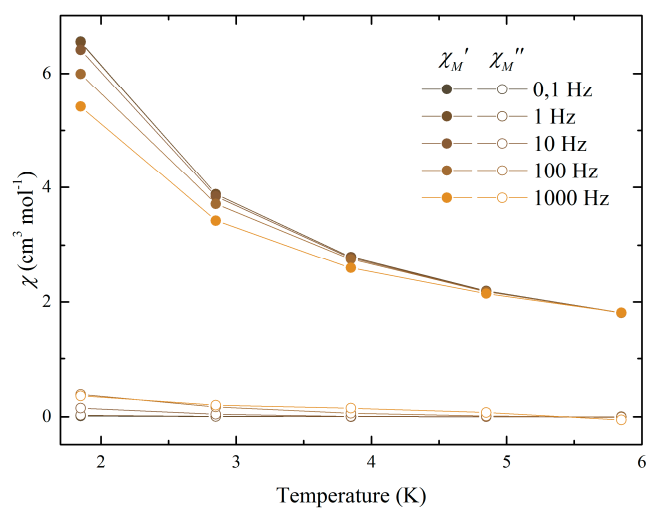


Figure S5. Temperature dependence of ac susceptibility measured in 0 Oe dc fields.

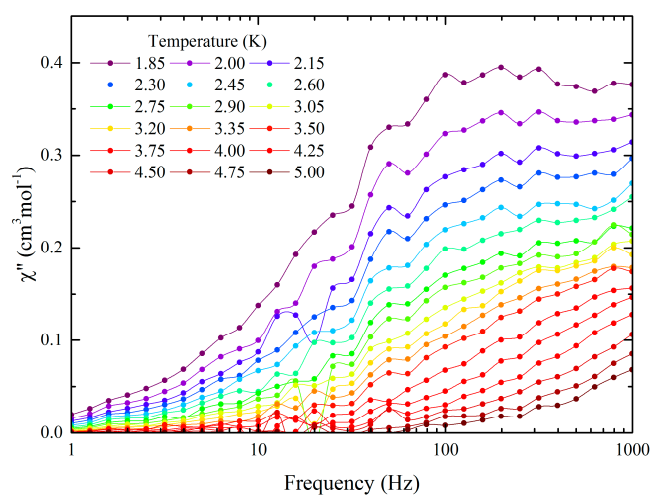


Figure S6. Out-of-phase signal of the susceptibility of complex **1** without external field.

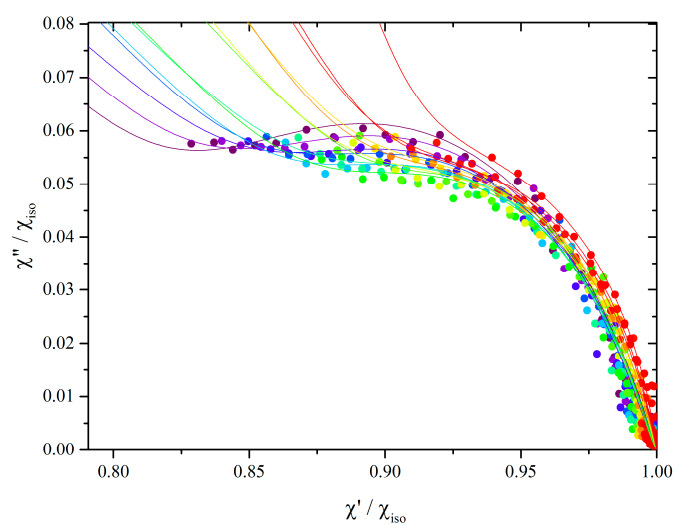


Figure S7. Normalized Argand plot of complex **1** without external field. Lines represent the best fit.

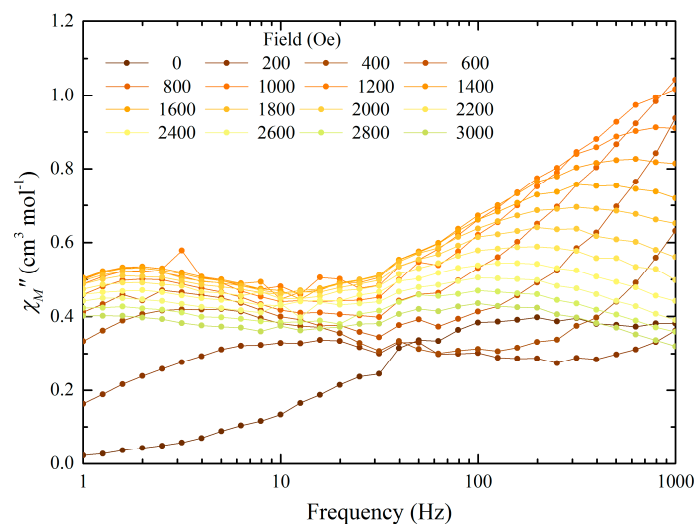


Figure S8. Frequency dependence of χ'' at 1.85 K as a function of dc field.

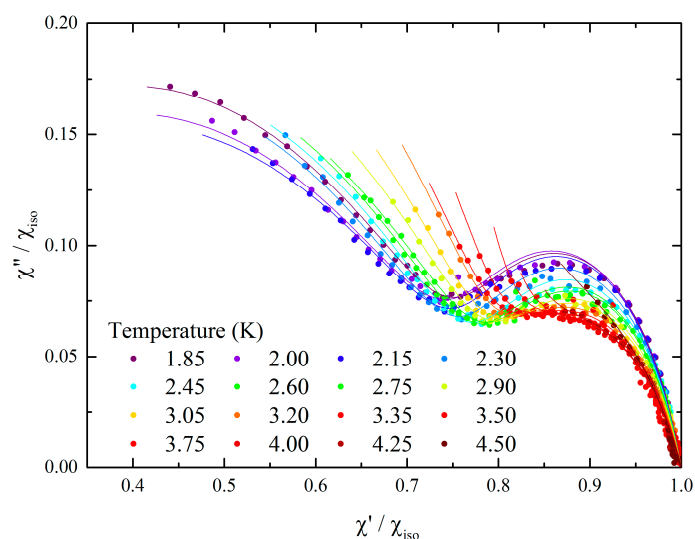


Figure S9. Normalized Argand plot for complex **1** in a 1000 Oe external field.

Table S3. Fitting parameter of frequency dependence of susceptibility for **1** in 0 Oe field.

Temperature	χ_{dia}	χ_{iso1}	χ_{iso2}	τ_1	τ_2	α_1	α_2	Reduced Chi-Sqr	Adj. R-Square
K	$\text{cm}^3\cdot\text{mol}^{-1}$	$\text{cm}^3\cdot\text{mol}^{-1}$	$\text{cm}^3\cdot\text{mol}^{-1}$	s	s				
1.85	0	0.99	5.55	1.26×10^{-3}	4.29×10^{-7}	0.28	0.52	1.84×10^{-4}	0.99998
2	0	0.79	5.13	1.18×10^{-3}	4.32×10^{-7}	0.27	0.54	1.61×10^{-4}	0.99998
2.15	0	0.59	4.82	1.16×10^{-3}	4.34×10^{-7}	0.24	0.56	2.00×10^{-4}	0.99997
2.3	0	0.58	4.46	1.04×10^{-3}	5.57×10^{-7}	0.26	0.52	9.08×10^{-5}	0.99998
2.45	0	0.49	4.17	1.02×10^{-3}	4.72×10^{-7}	0.24	0.53	8.23×10^{-5}	0.99998
2.6	0	0.39	3.94	9.69×10^{-4}	5.10×10^{-7}	0.22	0.55	8.26×10^{-5}	0.99998
2.75	0	0.38	3.66	8.20×10^{-4}	4.11×10^{-7}	0.23	0.53	7.50×10^{-5}	0.99998
2.9	0	0.25	3.56	9.03×10^{-4}	7.23×10^{-7}	0.11	0.53	1.59×10^{-4}	0.99995
3.05	0	0.31	3.28	6.98×10^{-4}	7.33×10^{-7}	0.2	0.47	3.75×10^{-5}	0.99999
3.2	0	0.29	3.11	5.95×10^{-4}	9.31×10^{-7}	0.19	0.44	4.83×10^{-5}	0.99998
3.35	0	0.31	2.92	4.83×10^{-4}	8.34×10^{-7}	0.21	0.4	2.52×10^{-5}	0.99999
3.5	0	0.28	2.8	4.17×10^{-4}	1.16×10^{-6}	0.19	0.35	2.06×10^{-5}	0.99999
3.75	0	0.24	2.61	3.06×10^{-4}	8.20×10^{-7}	0.16	0.35	1.94×10^{-5}	0.99999
4	0	0.24	2.42	2.14×10^{-4}	1.75×10^{-6}	0.15	0.16	2.53×10^{-5}	0.99999

Table S4. Fitting parameter of frequency dependence of susceptibility for **1** in 1000 Oe field.

Temperature	χ_{adia}	χ_{iso1}	χ_{iso2}	τ_1	τ_2	α_1	α_2	Reduced	Adj. R-Square
K	$\text{cm}^3\cdot\text{mol}^{-1}$	$\text{cm}^3\cdot\text{mol}^{-1}$	$\text{cm}^3\cdot\text{mol}^{-1}$	s	s			Chi-Sqr	
1.85	0	1.23	4.53	9.51×10^{-2}	1.07×10^{-4}	0.18	0.48	1.27×10^{-4}	0.99997
2	0	1.15	4.22	7.52×10^{-2}	6.75×10^{-5}	0.19	0.51	1.80×10^{-4}	0.99996
2.15	0	1.04	3.98	6.22×10^{-2}	4.32×10^{-5}	0.18	0.58	1.42×10^{-4}	0.99996
2.3	0	1.01	3.71	5.00×10^{-2}	3.41×10^{-5}	0.21	0.48	2.01×10^{-4}	0.99994
2.45	0	0.89	3.5	3.88×10^{-2}	2.51×10^{-5}	0.22	0.48	1.18×10^{-4}	0.99996
2.6	0	0.82	3.31	2.89×10^{-2}	1.93×10^{-5}	0.23	0.47	9.34×10^{-5}	0.99997
2.75	0	0.75	3.14	2.06×10^{-2}	1.44×10^{-5}	0.23	0.47	7.92×10^{-5}	0.99997
2.9	0	0.71	2.96	1.48×10^{-2}	1.35×10^{-5}	0.26	0.43	5.07×10^{-5}	0.99998
3.05	0	0.69	2.79	9.87×10^{-3}	1.25×10^{-5}	0.28	0.37	3.08×10^{-5}	0.99999
3.2	0	0.67	2.64	6.27×10^{-3}	1.23×10^{-5}	0.9	0.3	2.44×10^{-5}	0.99999
3.35	0	0.64	2.52	4.06×10^{-3}	9.17×10^{-6}	0.32	0.29	5.37×10^{-5}	0.99997
3.5	0	0.62	2.39	2.59×10^{-3}	9.11×10^{-6}	0.34	0.2	2.30×10^{-5}	0.99999
3.75	0	0.6	2.22	1.18×10^{-3}	8.21×10^{-6}	0.36	0.07	1.99×10^{-5}	0.99999
4	0	0.5	2.13	6.89×10^{-4}	4.72×10^{-6}	0.34	0.11	2.43×10^{-5}	0.99998
4.25	0	0.49	1.97	3.27×10^{-4}	3.99×10^{-6}	0.35	0	3.51×10^{-5}	0.99997
4.5	0	0.55	1.78	1.18×10^{-4}	3.36×10^{-6}	0.37	0	2.32×10^{-5}	0.99998
4.75	0	0.34	1.86	1.51×10^{-4}	2.07×10^{-6}	0.25	0	4.42×10^{-5}	0.99996