Ladder-type 1D coordination polymer of Dy(III): Synthesis and investigation of magnetic behaviours

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Table S1. Crystallographic data and refinement parameters for **1-Dy$_{poly}$**.

Complex	**1-Dy$_{poly}$**
Empirical formula	$C_{25}H_{25}ClDyN_5O_5$
Formula weight	673.45
Temperature/K	100(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	7.54622(4)
b/Å	25.77176(17)
c/Å	13.72571(7)
α/°	90
β/°	94.0002(5)
γ/°	90
Volume/Å^3	2662.86(3)
Z	4
ρ_{calc}g/cm^3	1.680
μ/mm^{-1}	16.312
F(000)	1332.0
Crystal size/mm^3	0.35 × 0.24 × 0.18
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	6.86 to 160.148
Index ranges	$-6 \le h \le 9$, $-32 \le k \le 32$, $-17 \le l \le 17$
Reflections collected	53033
Independent reflections	5746 [R_{int} = 0.0337, R_{sigma} = 0.0175]
Data/restraints/parameters	5746/3/341
Goodness-of-fit on F^2	1.108
Final R indexes [I>=2σ (I)]	R_1 = 0.0256, wR_2 = 0.0672
Final R indexes [all data]	R_1 = 0.0264, wR_2 = 0.0677
Largest diff. peak/hole / e Å^{-3}	0.77/-0.97
CCDC	2433773

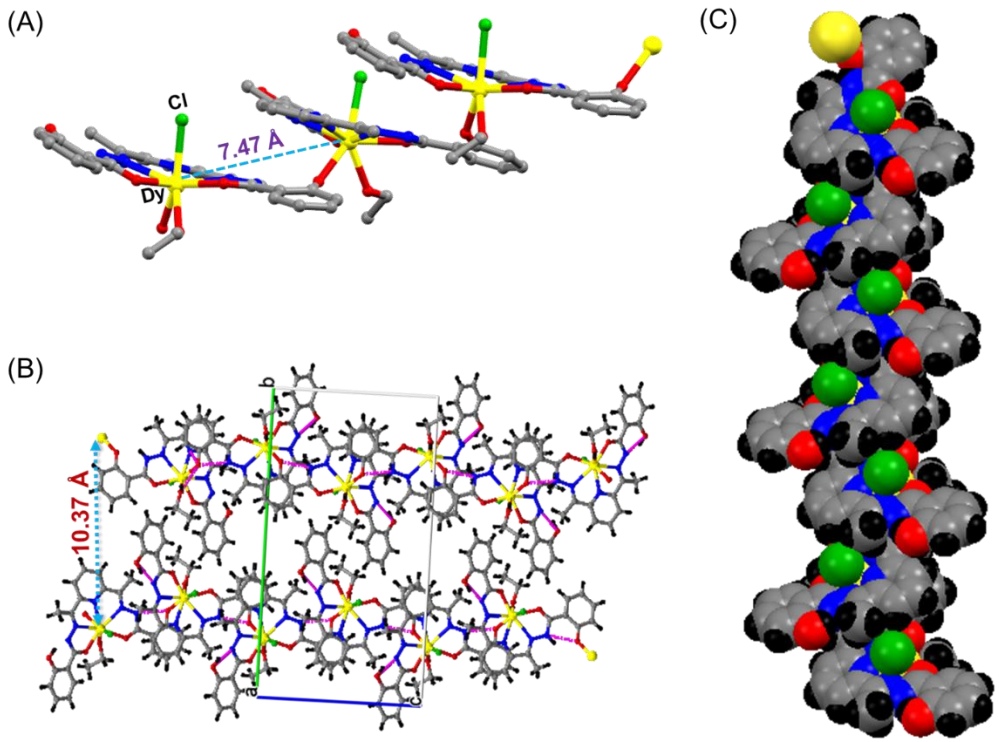

Figure S1. Ladder type propagation (A), packing structure (B) and the spacefill diagram (C) for **1-Dy$_{poly}$**.

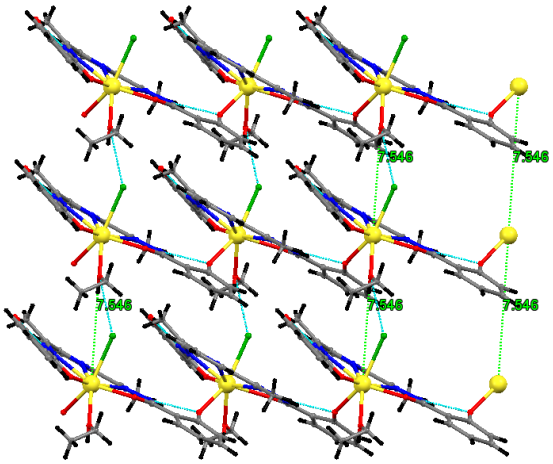

Figure S2. Interchain hydrogen bonding through axially coordinated ethanol and Cl ¯ ligands. Dy···Dy shown in Å.

Table S2: Selected bond lengths and bond angle parameters for **1-Dy$_{poly}$**.

Atom	Atom	Length/Å	Atom	Atom	Atom	Bond Angle/˚
Dy1	Cl1	2.6955(6)	O4	Dy1	Cl1	84.55(5)
Dy1	O4	2.2736(17)	O4	Dy1	O1^1	104.93(6)
Dy1	O1^1	2.3054(17)	O4	Dy1	O2	102.54(6)
Dy1	O2	2.3810(17)	O4	Dy1	O5	72.91(7)
Dy1	O5	2.3934(18)	O4	Dy1	N1	128.69(6)
Dy1	N1	2.524(2)	O4	Dy1	N4	64.95(6)
Dy1	N4	2.456(2)	O4	Dy1	N2	163.74(6)
Dy1	N2	2.543(2)	O1^1	Dy1	Cl1	151.15(4)

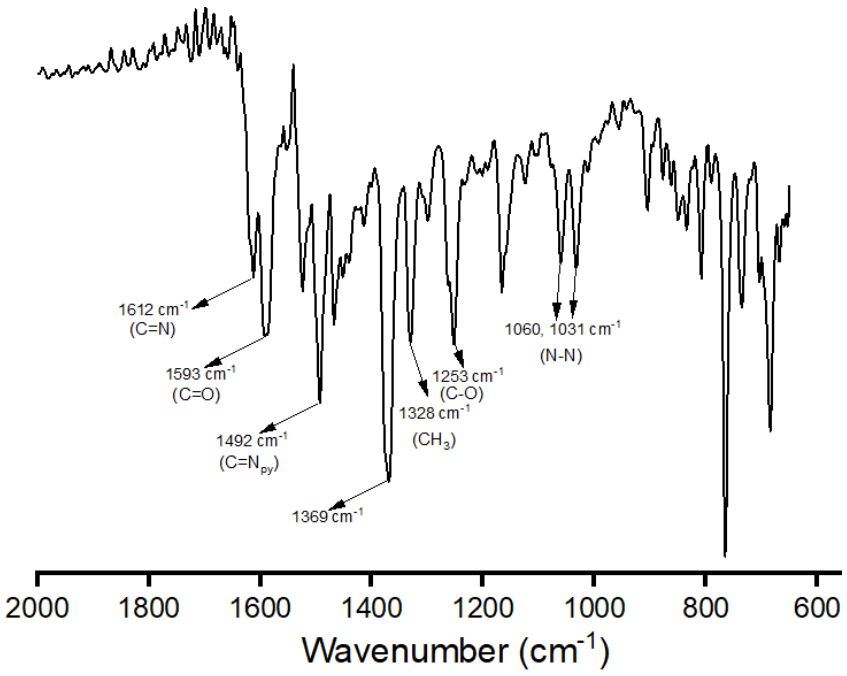

Figure S3. Solid state FT-IR data recorded for **1-Dy$_{poly}$**.

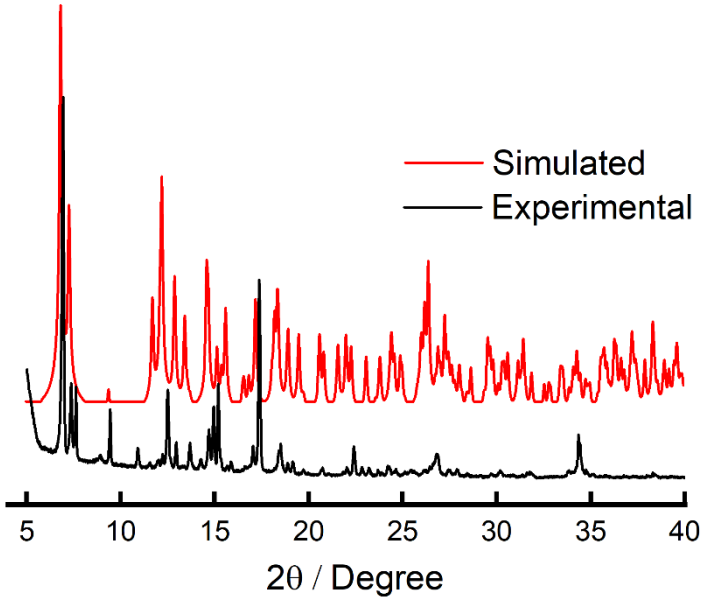

Figure S4. Powder X-ray diffraction data for **1-Dy$_{poly}$**.

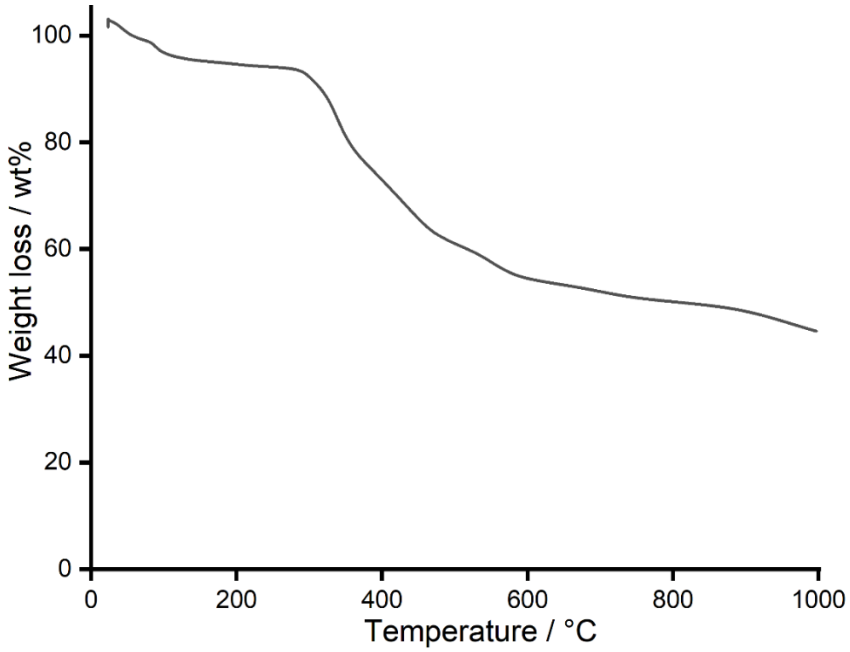

Figure S5. Thermogravimetric analysis (TGA) data for **1-Dy$_{poly}$**.

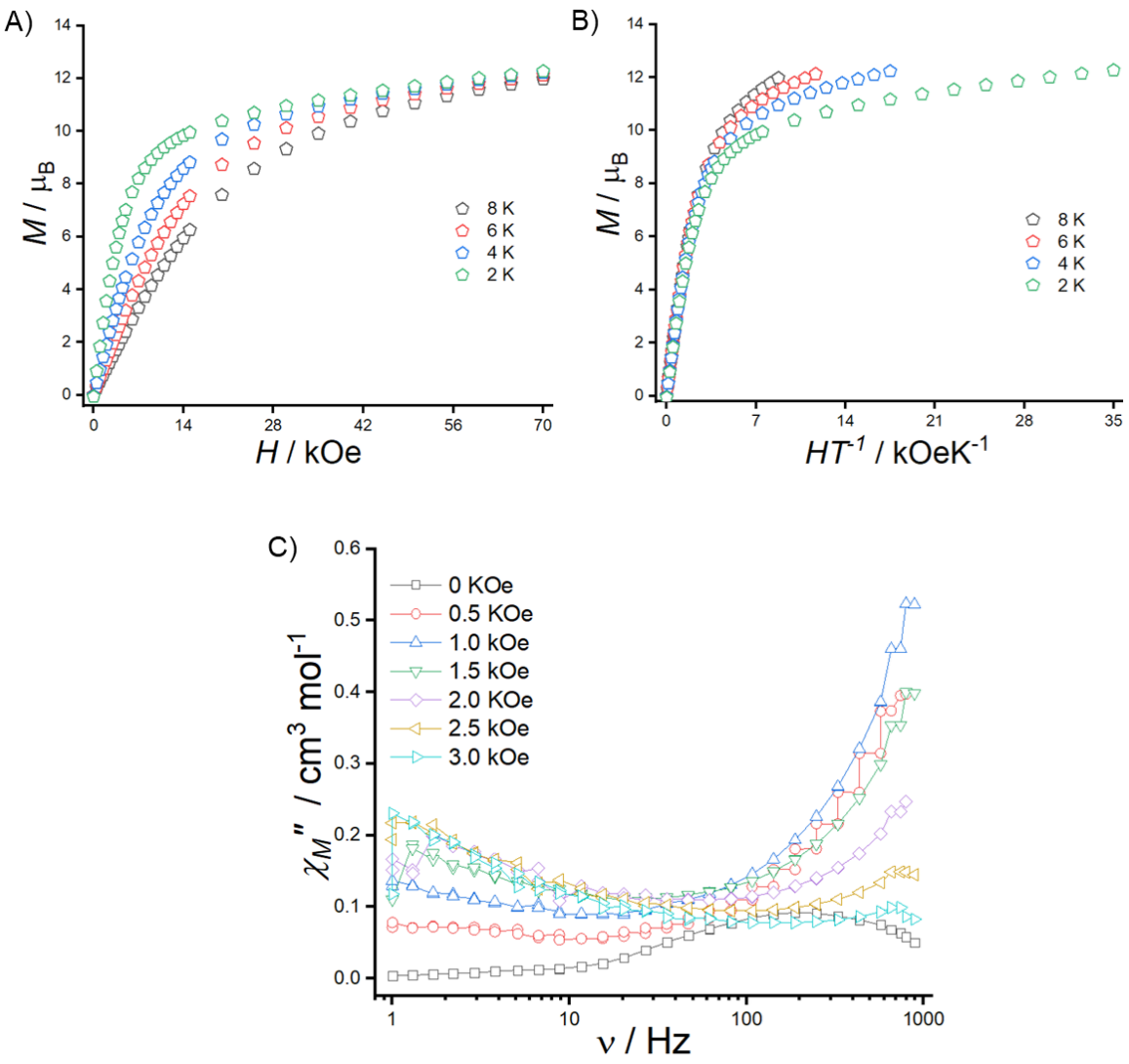

Figure S6. Magnetization (A), reduced magnetization (B), and field-dependent ac magnetic susceptibility data at the indicated magnetic fields for **1-Dy$_{poly}$**.

Table S3. Computed energies of spin-free states for Dy(III) ion in **1-Dy$_{poly}$.**

Spin-free states	Relative EMIN(au)	Rel lowest level(eV)	Energy (cm^{-1})
1	0	0	0
2	0.000101973	0.002774821	22.3804
3	0.000540207	0.014699789	118.5618
4	0.000846079	0.023022981	185.6929
5	0.001014161	0.027596733	222.5827
6	0.00126214	0.034344576	277.0077
7	0.001278472	0.034788981	280.5921
8	0.001988536	0.054110811	436.4331
9	0.002349968	0.063945874	515.7583
10	0.002520673	0.068591012	553.2238

11	0.002746913	0.074747309	602.8777
12	0.034399913	0.936069314	7549.9082
13	0.035061519	0.954072539	7695.114
14	0.035217497	0.958316924	7729.3473
15	0.035340065	0.961652169	7756.2478
16	0.035615485	0.969146721	7816.6955
17	0.035700372	0.971456607	7835.3259
18	0.035833842	0.975088513	7864.6192
19	0.158909434	4.324145976	34876.5894
20	0.159884286	4.350673058	35090.5447
21	0.160117698	4.357024532	35141.7728

Table S4: Computed energies of spin-orbit states for Dy(III) ion **1-Dy$_{poly}$**.

Spin-orbit states	Relative EMIN(au)	Rel lowest level(eV)	Energy (cm^{-1})
1	-0.022233149	0	0
2	-0.022233149	0	0
3	-0.021708722	0.014270375	115.0983
4	-0.021708722	0.014270375	115.0983
5	-0.021532677	0.019060817	153.7359
6	-0.021532677	0.019060817	153.7359
7	-0.021414786	0.022268778	179.6098
8	-0.021414786	0.022268778	179.6098
9	-0.021246242	0.026855105	216.601
10	-0.021246242	0.026855105	216.601
11	-0.020859188	0.03738738	301.5496
12	-0.020859188	0.03738738	301.5496
13	-0.020443402	0.048701495	392.8041
14	-0.020443402	0.048701495	392.8041
15	-0.020338232	0.051563297	415.886
16	-0.020338232	0.051563297	415.886
17	-0.008248979	0.380528638	3069.1705
18	-0.008248979	0.380528638	3069.1705
19	-0.007952111	0.38860683	3134.3255
20	-0.007952111	0.38860683	3134.3255
21	-0.007822019	0.392146813	3162.8773
22	-0.007822019	0.392146813	3162.8773
23	-0.007726011	0.394759331	3183.9487
24	-0.007726011	0.394759331	3183.9487
25	-0.007485634	0.401300309	3236.7053
26	-0.007485634	0.401300309	3236.7053
27	-0.007336889	0.405347868	3269.351

28	-0.007336889	0.405347868	3269.351
29	-0.007186745	0.409433509	3302.304
30	-0.007186745	0.409433509	3302.304
31	0.003532022	0.701106005	5654.8013
32	0.003532022	0.701106005	5654.8013
33	0.003703913	0.705783407	5692.5271
34	0.003703913	0.705783407	5692.5271
35	0.00381991	0.708939839	5717.9854
36	0.00381991	0.708939839	5717.9854
37	0.004248702	0.720607858	5812.0943
38	0.004248702	0.720607858	5812.0943
39	0.004381999	0.724235066	5841.3497
40	0.004381999	0.724235066	5841.3497
41	0.004494194	0.727288053	5865.9737
42	0.004494194	0.727288053	5865.9737
43	0.013371546	0.96885309	7814.3272
44	0.013371546	0.96885309	7814.3272
45	0.013601549	0.97511181	7864.8071
46	0.013601549	0.97511181	7864.8071
47	0.014129792	0.989486029	7980.743
48	0.014129792	0.989486029	7980.743
49	0.01421069	0.991687366	7998.498
50	0.01421069	0.991687366	7998.498
51	0.01431668	0.994571491	8021.7601
52	0.01431668	0.994571491	8021.7601
53	0.021256544	1.183414818	9544.8842
54	0.021256544	1.183414818	9544.8842
55	0.021479015	1.189468569	9593.711
56	0.021479015	1.189468569	9593.711
57	0.021539506	1.191114608	9606.9872
58	0.021539506	1.191114608	9606.9872
59	0.021623682	1.193405165	9625.4618
60	0.021623682	1.193405165	9625.4618
61	0.02170296	1.195562432	9642.8613
62	0.02170296	1.195562432	9642.8613
63	0.021863828	1.199939857	9678.1676
64	0.021863828	1.199939857	9678.1676
65	0.022070776	1.205571198	9723.5875
66	0.022070776	1.205571198	9723.5875
67	0.02234288	1.21297553	9783.3074
68	0.02234288	1.21297553	9783.3074
69	0.02247562	1.216587574	9812.4405
70	0.02247562	1.216587574	9812.4405
71	0.022604583	1.220096845	9840.7447
72	0.022604583	1.220096845	9840.7447

73	0.02796199	1.365879314	11016.5596
74	0.02796199	1.365879314	11016.5596
75	0.028419959	1.37834128	11117.0722
76	0.028419959	1.37834128	11117.0722
77	0.028705988	1.386124533	11179.8483
78	0.028705988	1.386124533	11179.8483
79	0.031497477	1.462084792	11792.5091
80	0.031497477	1.462084792	11792.5091
81	0.031614368	1.465265584	11818.1639
82	0.031614368	1.465265584	11818.1639
83	0.031761649	1.469273301	11850.4884
84	0.031761649	1.469273301	11850.4884
85	0.031854809	1.471808318	11870.9347
86	0.031854809	1.471808318	11870.9347
87	0.032036661	1.476756756	11910.8465
88	0.032036661	1.476756756	11910.8465
89	0.039485273	1.67944381	13545.6278
90	0.039485273	1.67944381	13545.6278
91	0.039813454	1.688374063	13617.6552
92	0.039813454	1.688374063	13617.6552
93	0.039948734	1.692055215	13647.3457
94	0.039948734	1.692055215	13647.3457
95	0.040087347	1.695827086	13677.7679
96	0.040087347	1.695827086	13677.7679
97	0.045978297	1.856127981	14970.6818
98	0.045978297	1.856127981	14970.6818
99	0.046111015	1.859739424	14999.81
100	0.046111015	1.859739424	14999.81
101	0.046300858	1.864905314	15041.4758
102	0.046300858	1.864905314	15041.4758
103	0.050629227	1.982686252	15991.4431
104	0.050629227	1.982686252	15991.4431
105	0.050664274	1.983639933	15999.135
106	0.050664274	1.983639933	15999.135
107	0.053345136	2.056589886	16587.5161
108	0.053345136	2.056589886	16587.5161
109	0.154825889	4.818021866	38859.9671
110	0.154825889	4.818021866	38859.9671
111	0.154947789	4.821338932	38886.721
112	0.154947789	4.821338932	38886.721
113	0.155144169	4.826682712	38929.8215
114	0.155144169	4.826682712	38929.8215
115	0.15549492	4.836227128	39006.8024
116	0.15549492	4.836227128	39006.8024
117	0.161062493	4.987728509	40228.7434

118	0.161062493	4.987728509	40228.7434
119	0.161515285	5.000049591	40328.1197
120	0.161515285	5.000049591	40328.1197
121	0.16179148	5.007565244	40388.7375
122	0.16179148	5.007565244	40388.7375
123	0.165902034	5.119419122	41290.8999
124	0.165902034	5.119419122	41290.8999
125	0.166051514	5.12348669	41323.707
126	0.166051514	5.12348669	41323.707

Table S5: Computed LoProp charges on the atoms in **1-Dy$_{poly}$**.

Dy1	Cl1	O1	O2	O3	O4	H1	N1	N2	H2
2.462	**-0.874**	**-0.801**	-0.481	-0.637	-0.611	0.348	-0.324	-0.218	0.255
O5	H3	N3	N4	N5	C1	C2	C3	C4	H4
-0.510	0.341	-0.230	-0.240	-0.415	-0.104	0.129	-0.105	-0.060	0.154
C5	C6	H5	C7	C8	C9	H6	C10	H7	C11
0.160	-0.152	0.134	0.202	0.457	-0.133	0.137	-0.076	0.137	0.509
C12	C13	H8	C14	H9	C15	C16	C17	H10	C18
0.224	-0.148	0.139	-0.174	0.134	0.264	0.146	-0.069	0.139	-0.364
H11	H12	H13	C19	H14	C20	H15	H16	H17	C21
0.152	0.116	0.145	-0.172	0.122	-0.370	0.155	0.146	0.122	-0.087
H18	C22	H19	C23	H20	H21	C24	H22	C25	H23
0.127	-0.053	0.139	0.034	0.101	0.141	-0.172	0.134	-0.352	0.141
H24	H25	O6	C26	C27	C28	H26	C29	H27	C30
0.115	0.118	-0.882	0.300	-0.200	-0.106	0.122	-0.206	0.115	-0.122
C31	H28	H29	H30	H31					
-0.238	0.114	0.106	0.344	0.106					

Table S6. SINGLE_ANISO computed wave function decomposition analysis for Dy(III) in **1-Dy$_{poly}$**. The bold ones correspond to major contributions.

$\pm m_J$	Wave function decomposition analysis
KD1	**94.40**% |±15/2› + 3.3% |±11/2›
KD2	**35.10**% |±13/2› + 6.30% |±11/2› + 6.80% |±9/2› + 10.90% |±5/2› + 22.1% |±1/2›
KD3	**31.70**% |±3/2› + 22.10% |±13/2› + 18.50% |±9/2› + 11.40% |±5/2›
KD4	**32.50**% |±5/2› + 6.1% |±11/2› + 30.60% |±7/2› + 18.50% |±9/2› + 20.1% |±1/2›
KD5	**24.4**% |±13/2› + 19.0% |±11/2› + 20.1% |±3/2› + 17.20% |±1/2› + 10.4% |±9/2›
KD6	**38.0**% |±11/2› + 23.6% |±9/2› + 11.7% |±13/2› + 12.20% |±1/2›
KD7	**19.0**% |±3/2› + 18.3% |±1/2› + 12.7% |±11/2› + 15.60% |±5/2›
KD8	**27.9**% |±7/2› + 24.3% |±5/2› + 21.9% |±9/2› + 12.10% |±3/2›

Table S7. Computed crystal-field parameters for Dy^{III} in **1-Dy$_{poly}$**.

k	q	(K)^2	B(k,q)
2	-2	1.5	-2.54E-01
	-1	6	**1.34E+00**
	0	1	**-1.12E+00**
	1	6	6.72E-01
	2	1.5	-3.05E-01
4	-4	17.5	-1.91E-02
	-3	140	-5.33E-02
	-2	10	1.67E-02
	-1	20	-1.06E-02
	0	1	-5.38E-03
	1	20	-1.54E-02
	2	10	-4.07E-03
	3	140	-9.59E-04
	4	17.5	3.61E-03
6	-6	57.75	-4.64E-04
	-5	693	-1.53E-04
	-4	31.5	-6.83E-05
	-3	105	-3.80E-05
	-2	26.25	6.41E-05
	-1	42	-2.01E-05
	0	1	-2.11E-06
	1	42	1.38E-04
	2	26.25	7.81E-05
	3	105	2.20E-06
	4	31.5	-3.71E-05
	5	693	6.26E-04
	6	57.75	-5.50E-04

Table S8: Computed spin densities for high-spin and broken symmetry for **Gd_2^{mod-1}** and **Gd_2^{mod-2}**.

Spin State	Atom	Mulliken Charge	Spin density
Gd_2^{mod-1}			
HS	Gd1	1.514	7.038
	Gd2	1.498	7.039
BS1	Gd1	1.514	-7.038
	Gd2	1.498	7.039
BS2	Gd1	1.514	7.038
	Gd2	1.498	-7.039
Gd_2^{mod-2}			
HS	Gd1	1.521	7.042
	Gd2	1.470	7.043
BS1	Gd1	1.521	-7.042
	Gd2	1.470	7.042
BS2	Gd1	1.521	7.042
	Gd2	1.470	-7.042