Supporting Information

Wheel-like Gd42 Polynuclear Complex with Significant Magnetocaloric Effect

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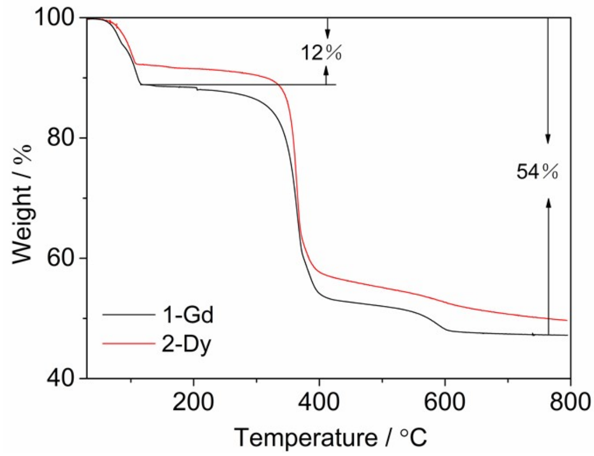


Fig. S1. The thermogravimetric analysis of **1-Gd** and **2-Dy**.

TGA analyses of **1-Gd** and **2-Dy** obtained similar results. For the complex **2-Dy**, at 100 °C, about 10 % weight loss is caused by the escape of uncoordinated solvent molecules (such as H_2O, MeOH) in the pores. As the temperature increases, the cluster compounds begin to decompose around 300 °C and heat to 600 °C, the weight is almost unchanged, and the remaining 48 % is Dy_2O_3, which is basically in line with the theoretical calculation.

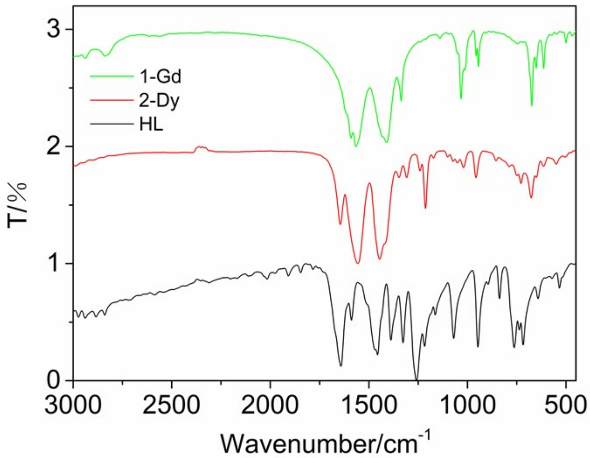
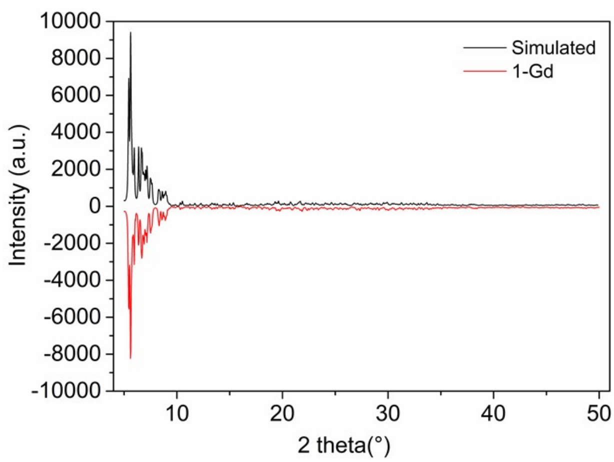


Fig. S2. IR spectra of free ligand H_2L and complexes.



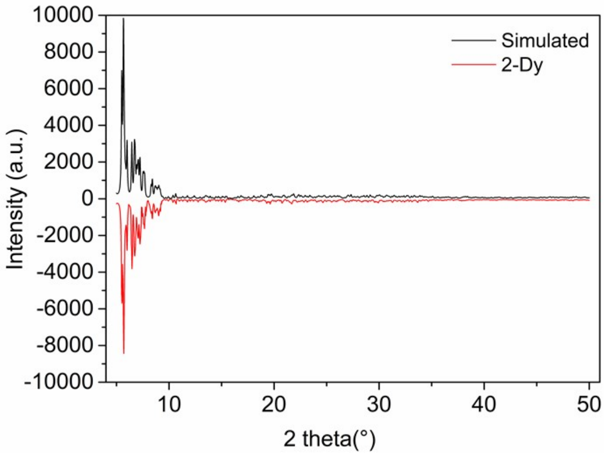


Fig. S3. PXRD curve for complexes **1-Gd**(top) and **2-Dy**(bottom).

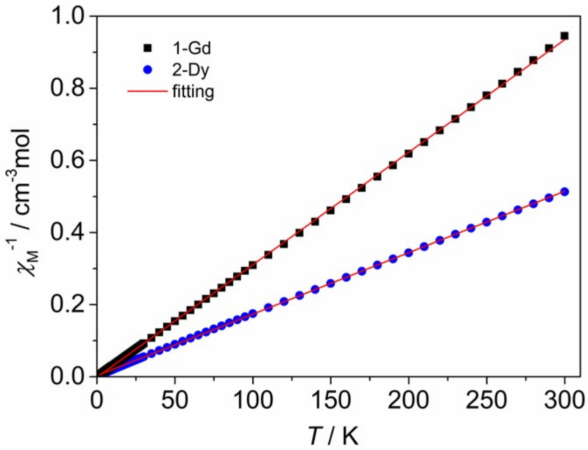


Fig. S4. The χ_M^{-1} *vs* *T* and the Curie-Weiss linear fit for **1-Gd** and **2-Dy**.

The direct current (dc) magnetic properties of the complexes were investigated under 1000 Oe field in the temperature range of 2-300 K and fitted with the Curie-Weiss law. For **1-Gd**, Curie constant C = 320.27 cm^3 K mol^{-1} and Weiss constant θ = + 0.54 K. Positive θ indicates that ferromagnetic interaction between Gd^{3+} ions and vice versa. For **2-Dy**, the Curie constant C = 586.44 cm^3 K mol^{-1} and Weiss constant θ = -1.76 K by fitting the temperature dependence of magnetic susceptibilities.

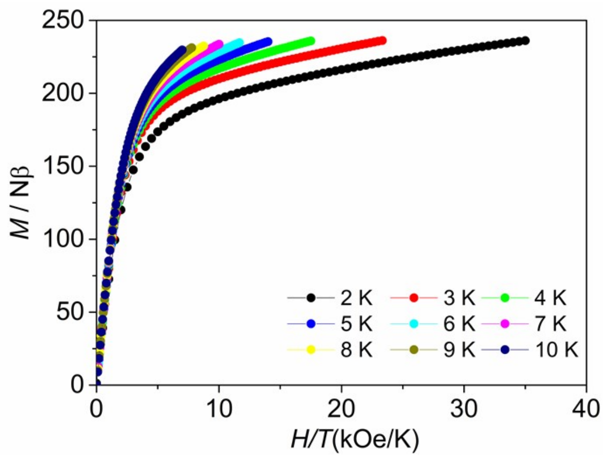


Fig. S5. Magnetization *versus H/T* for **2-Dy** at 2-10 K and 0-7 T dc magnetic field.

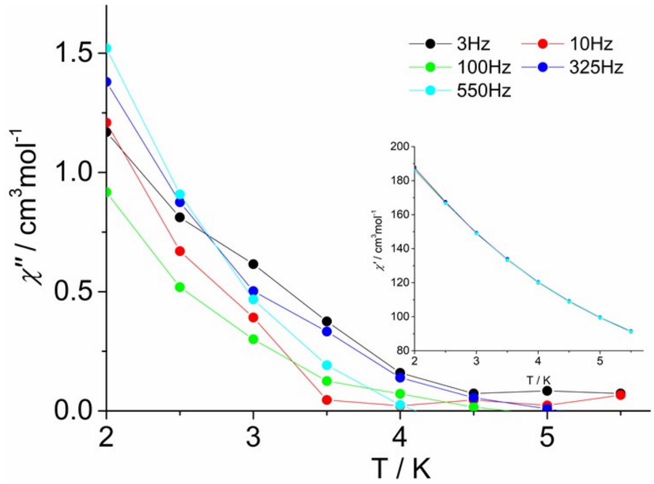


Fig. S6. Temperature dependence of the in-phase (inset) and out-of-phase ac susceptibility at the indicated frequencies with ΔH =1500 Oe for **2-Dy**.

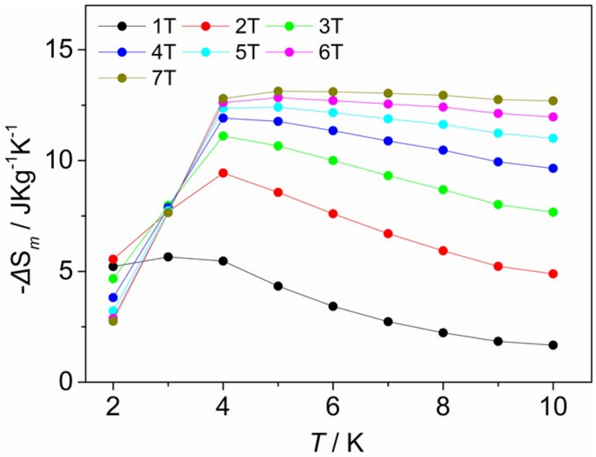


Fig. S7. -ΔS_m calculated by using the magnetization data of **2-Dy** at different fields and temperatures.

Table S1. Selected bond lengths (Å) for **1-Gd**.

Gd1-O2	2.345(2)	Gd11-O44	2.454(2)
Gd1-O10	2.348(2)	Gd11-O49	2.469(2)
Gd1-O9	2.3647(17)	Gd11-O93	2.472(3)
Gd1-O37	2.375(2)	Gd11-O84	2.473(2)
Gd1-O20	2.4218(17)	Gd11-O100	2.480(2)
Gd1-O11	2.4340(19)	Gd11-O62	2.565(2)
Gd1-O15	2.512(2)	Gd12-O22	2.3306(18)
Gd1-Gd2	3.8920(3)	Gd12-O16	2.340(2)
Gd1-Gd9	3.9190(3)	Gd12-O1	2.342(2)
Gd2-O39	2.3484(18)	Gd12-O36	2.349(2)
Gd2-O10	2.373(2)	Gd12-O110	2.3670(18)
Gd2-O97	2.432(2)	Gd12-O50	2.403(2)
Gd2-O32	2.461(2)	Gd12-O96[1]	2.4417(19)
Gd2-O2	2.465(2)	Gd12-O80	2.514(3)
Gd2-O87	2.478(3)	Gd13-O25	2.351(2)
Gd2-O98	2.483(2)	Gd13-O23[1]	2.3725(19)
Gd2-O63	2.485(3)	Gd13-O96	2.422(2)
Gd2-O33	2.5150(17)	Gd13-O40[1]	2.457(2)
Gd3-O12	2.321(2)	Gd13-O95[1]	2.474(2)
Gd3-O5	2.348(2)	Gd13-O65[1]	2.480(2)
Gd3-O7	2.350(2)	Gd13-O36[1]	2.4810(19)
Gd3-O27	2.356(2)	Gd13-O70	2.481(2)
Gd3-O102	2.362(2)	Gd13-O34	2.515(2)
Gd3-O103	2.4156(17)	Gd14-O26	2.303(2)
Gd3-O14	2.4441(16)	Gd14-O67	2.363(2)
Gd3-O111	2.507(2)	Gd14-O24	2.367(2)
Gd4-O113	2.394(2)	Gd14-O3	2.373(2)
Gd4-O7	2.4131(15)	Gd14-O28	2.382(2)
Gd4-O11	2.418(2)	Gd14-O38	2.4329(19)
Gd4-O18	2.425(2)	Gd14-O101	2.4407(18)
Gd4-O103	2.427(2)	Gd14-O115	2.534(3)
Gd4-O99	2.433(2)	Gd15-O45	2.397(2)
Gd4-O107	2.449(2)	Gd15-O23	2.407(2)
Gd4-O21	2.495(2)	Gd15-O60	2.420(2)
Gd4-O37	2.508(2)	Gd15-O96[1]	2.4233(17)
Gd5-O94	2.318(2)	Gd15-O68	2.447(2)
Gd5-O100	2.3565(19)	Gd15-O34[1]	2.449(2)
Gd5-O98	2.359(2)	Gd15-O6	2.456(2)
Gd5-O112	2.365(2)	Gd15-O61	2.487(2)
Gd5-O109	2.3662(19)	Gd15-O110	2.529(2)
Gd5-O19	2.4206(19)	Gd16-O35	2.333(2)
Gd5-O97	2.4498(19)	Gd16-O17	2.362(2)
Gd5-O55	2.515(2)	Gd16-O49	2.367(2)

Gd6-O47	2.351(2)	Gd16-O52	2.3670(18)
Gd6-O16	2.371(2)	Gd16-O8	2.367(2)
Gd6-O101	2.433(2)	Gd16-O57	2.425(2)
Gd6-O43	2.452(2)	Gd16-O13	2.429(2)
Gd6-O72	2.470(2)	Gd16-O118	2.505(3)
Gd6-O1	2.472(2)	Gd17-O46	2.315(2)
Gd6-O28	2.4736(19)	Gd17-O95	2.3518(19)
Gd6-O69	2.478(3)	Gd17-O23	2.360(2)
Gd6-O58	2.532(2)	Gd17-O29	2.380(2)
Gd7-O30	2.3384(18)	Gd17-O106	2.3810(17)
Gd7-O7	2.368(2)	Gd17-O6	2.401(2)
Gd7-O11	2.4273(17)	Gd17-O105[1]	2.451(2)
Gd7-O53	2.458(2)	Gd17-O76	2.519(3)
Gd7-O5	2.462(2)	Gd18-O119	2.385(2)
Gd7-O85	2.477(3)	Gd18-O24	2.3952(18)
Gd7-O116	2.478(3)	Gd18-O14	2.412(2)
Gd7-O9	2.484(2)	Gd18-O51	2.413(2)
Gd7-O99	2.5097(19)	Gd18-O89	2.428(2)
Gd8-O24	2.353(2)	Gd18-O38	2.430(2)
Gd8-O48	2.3561(18)	Gd18-O73	2.449(2)
Gd8-O14	2.4392(19)	Gd18-O83	2.480(3)
Gd8-O31	2.453(3)	Gd18-O27	2.5445(18)
Gd8-O3	2.461(2)	Gd19-O104	2.343(2)
Gd8-O82	2.472(3)	Gd19-O17	2.364(2)
Gd8-O77	2.488(3)	Gd19-O105	2.445(2)
Gd8-O102	2.4941(17)	Gd19-O8	2.472(2)
Gd8-O51	2.514(2)	Gd19-O29[1]	2.472(2)
Gd9-O54	2.385(2)	Gd19-O56	2.4730(19)
Gd9-O97	2.3946(18)	Gd19-O79[1]	2.478(3)
Gd9-O10	2.4090(17)	Gd19-O86	2.488(2)
Gd9-O59	2.409(3)	Gd19-O114	2.537(2)
Gd9-O33	2.428(2)	Gd20-O75	2.387(2)
Gd9-O20	2.433(2)	Gd20-O81	2.405(2)
Gd9-O64	2.4717(19)	Gd20-O101	2.4074(19)
Gd9-O117	2.473(2)	Gd20-O16	2.419(2)
Gd9-O109	2.533(2)	Gd20-O58	2.428(3)
Gd10-O92	2.396(3)	Gd20-O91	2.441(3)
Gd10-O13	2.3979(16)	Gd20-O74	2.459(3)
Gd10-O19	2.400(2)	Gd20-O67	2.537(2)
Gd10-O62	2.420(3)	Gd21-O42	2.394(3)
Gd10-O112	2.4226(19)	Gd21-O105	2.4005(16)
Gd10-O71	2.431(3)	Gd21-O57	2.404(3)
Gd10-O78	2.461(2)	Gd21-O17	2.412(2)
Gd10-O90	2.471(3)	Gd21-O88	2.429(2)

Gd10-O52	2.534(2)	Gd21-O114	2.438(3)
Gd11-O108	2.346(2)	Gd21-O66[1]	2.471(2)
Gd11-O112	2.359(2)	Gd21-O41	2.473(3)
Gd11-O13	2.438(2)	Gd21-O106[1]	2.553(2)

Table S2. Selected bond lengths (Å) for **2-Dy**.

Dy01-O025	2.320(6)	Dy0B-O00M	2.446(6)
Dy01-O00U	2.332(5)	Dy0B-O027	2.457(6)
Dy01-O00Q	2.402(5)	Dy0B-O02R	2.534(6)
Dy01-O01R	2.428(6)	Dy0C-O02C	2.363(6)
Dy01-O02X	2.434(6)	Dy0C-O011	2.380(5)
Dy01-O00S	2.443(5)	Dy0C-O01M	2.384(5)
Dy01-O00W	2.457(5)	Dy0C-O01O	2.396(6)
Dy01-O031	2.463(6)	Dy0C-O01K	2.402(5)
Dy01-O022	2.493(5)	Dy0C-O023	2.405(6)
Dy02-O016	2.292(6)	Dy0C-O02P	2.413(6)
Dy02-O00U	2.324(5)	Dy0C-O02S	2.458(6)
Dy02-O020	2.332(5)	Dy0C-O020	2.490(6)
Dy02-O00S	2.332(5)	Dy0D-O00R	2.300(6)
Dy02-O00N	2.345(5)	Dy0D-O00O	2.320(6)
Dy02-O01B	2.391(6)	Dy0D-O01V	2.325(6)
Dy02-O01M	2.416(5)	Dy0D-O00T	2.334(5)
Dy02-O01F	2.485(6)	Dy0D-O027	2.350(5)
Dy03-O02D	2.369(6)	Dy0D-O02I	2.397(5)
Dy03-O00Z	2.381(5)	Dy0D-O010	2.417(5)
Dy03-O02G	2.389(6)	Dy0D-O02U	2.479(6)
Dy03-O01A	2.390(5)	Dy0E-O01X	2.283(6)
Dy03-O01D	2.403(6)	Dy0E-O03G	2.334(6)
Dy03-O00V	2.405(6)	Dy0E-O029	2.342(6)
Dy03-O038	2.424(6)	Dy0E-O01N	2.338(6)
Dy03-O01U	2.464(6)	Dy0E-O012	2.355(5)
Dy03-O017	2.497(5)	Dy0E-O036	2.409(6)
Dy04-O019	2.304(6)	Dy0E-O018[1]	2.412(5)
Dy04-O01C	2.342(6)	Dy0E-O03K	2.517(6)
Dy04-O015	2.343(5)	Dy0F-O01T[1]	2.330(6)
Dy04-O00Z	2.337(5)	Dy0F-O01N	2.326(5)
Dy04-O024	2.363(6)	Dy0F-O01I	2.419(5)
Dy04-O00V	2.373(5)	Dy0F-O01W	2.427(6)
Dy04-O01L	2.426(5)	Dy0F-O03I	2.438(6)
Dy04-O03A	2.488(5)	Dy0F-O012	2.446(5)
Dy05-O01H	2.303(5)	Dy0F-O03T	2.456(7)
Dy05-O00X	2.334(6)	Dy0F-O021	2.464(5)
Dy05-O011	2.327(5)	Dy0F-O02M	2.488(6)
Dy05-O021	2.340(6)	Dy0G-O010	2.360(5)

Dy05-O02Z	2.352(6)	Dy0G-O035	2.372(6)
Dy05-O01O	2.389(5)	Dy0G-O01J	2.378(6)
Dy05-O01I	2.426(5)	Dy0G-O02R	2.392(6)
Dy05-O02J	2.488(6)	Dy0G-O01E	2.398(5)
Dy06-O00P	2.289(5)	Dy0G-O039	2.410(6)
Dy06-O00M	2.332(6)	Dy0G-O03W	2.433(6)
Dy06-O01E	2.329(5)	Dy0G-O03D	2.440(6)
Dy06-O00W	2.337(6)	Dy0G-O01V	2.515(6)
Dy06-O026	2.346(5)	Dy0H-O01G	2.322(5)
Dy06-O01J	2.401(5)	Dy0H-O014	2.324(5)
Dy06-O00Q	2.435(5)	Dy0H-O018	2.411(5)
Dy06-O02W	2.494(6)	Dy0H-O02A	2.424(5)
Dy07-O01P	2.316(6)	Dy0H-O029[1]	2.438(6)
Dy07-O00Z	2.341(5)	Dy0H-O03L[1]	2.438(7)
Dy07-O01A	2.399(5)	Dy0H-O01Q	2.446(5)
Dy07-O02F	2.422(6)	Dy0H-O03J	2.453(6)
Dy07-O037	2.436(6)	Dy0H-O034	2.509(5)
Dy07-O015	2.438(6)	Dy0I-O028	2.305(6)
Dy07-O02L	2.459(6)	Dy0I-O011	2.349(5)
Dy07-O00Y	2.462(6)	Dy0I-O01M	2.396(5)
Dy07-O01D	2.485(5)	Dy0I-O00X	2.436(5)
Dy08-O02Y	2.365(7)	Dy0I-O02K	2.438(6)
Dy08-O00Q	2.361(5)	Dy0I-O03R	2.448(6)
Dy08-O02H	2.385(6)	Dy0I-O00N	2.448(5)
Dy08-O01B	2.396(6)	Dy0I-O03N	2.449(7)
Dy08-O022	2.396(6)	Dy0I-O023	2.481(6)
Dy08-O00U	2.395(5)	Dy0J-O01S	2.358(6)
Dy08-O02V	2.447(6)	Dy0J-O01L	2.357(5)
Dy08-O02Q	2.448(6)	Dy0J-O00T	2.386(5)
Dy08-O026	2.526(5)	Dy0J-O032	2.394(6)
Dy09-O02B	2.320(5)	Dy0J-O02I	2.398(6)
Dy09-O00T	2.330(5)	Dy0J-O03S	2.404(7)
Dy09-O01L	2.425(5)	Dy0J-O03X	2.435(7)
Dy09-O01Y	2.435(6)	Dy0J-O02N	2.438(5)
Dy09-O02T	2.435(6)	Dy0J-O024	2.537(5)
Dy09-O01C	2.456(5)	Dy0K-O03B	2.369(7)
Dy09-O00O	2.461(5)	Dy0K-O01I	2.372(5)
Dy09-O03C	2.462(6)	Dy0K-O01N	2.382(5)
Dy09-O032	2.499(5)	Dy0K-O036	2.414(7)
Dy0A-O013	2.312(5)	Dy0K-O03P	2.414(6)
Dy0A-O01Q	2.320(5)	Dy0K-O02M	2.413(6)
Dy0A-O014	2.324(5)	Dy0K-O030	2.419(6)
Dy0A-O00Y	2.330(6)	Dy0K-O03Q	2.460(6)
Dy0A-O017	2.343(5)	Dy0K-O02Z	2.512(6)

Dy0A-O02E	2.384(6)	Dy0L-O018	2.372(5)
Dy0A-O01A	2.414(5)	Dy0L-O03F	2.377(7)
Dy0A-O033	2.486(6)	Dy0L-O03M	2.383(7)
Dy0B-O02O	2.307(5)	Dy0L-O02E	2.389(6)
Dy0B-O01E	2.321(5)	Dy0L-O014	2.400(5)
Dy0B-O010	2.410(5)	Dy0L-O034	2.404(7)
Dy0B-O03O	2.431(6)	Dy0L-O03U	2.412(7)
Dy0B-O01Z	2.432(6)	Dy0L-O03H[1]	2.434(6)
Dy0B-O03E	2.445(6)	Dy0L-O03G[1]	2.514(6)