Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Formation of Nanocluster {Dy_{12}} Containing Dy-Exclusive Vertex-Sharing [$Dy_4(\mu_3\text{-}OH)_4$] Cubanes via Simultaneous Multitemplate Guided and Step-by-Step Assembly

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Table S1a. 27 examples of high-nuclear lanthanide clusters are known with nuclearity ≥10 was queried using CCDC2018 (2.00) until 15 Jan. 2019.

No	Complex	Ref.
1	$[Ln_{14}(CO_3)_{13}(ccnm)_9(OH)(H_2O)_6(phen)_{13}(NO_3)]\cdot(CO_3)_{2.5}\cdot(phen)_{0.5}$ ($\mathbf{Ln_{14}}$)	1
2	$[Ln_{24}(DMC)_{36}(\mu_4\text{-}CO_3)_{18}(\mu_3\text{-}H_2O)_2]$ ($\mathbf{Ln_{24}}$)	2, 3
3	$[(CO_3)_2@Ln_{37}(LH_3)_8(CH_3COO)_{21}(CO_3)_{12}(\mu_3\text{-}OH)_{41}(\mu_2\text{-}H_2O)_5(H_2O)_{40}]\cdot(ClO_4)_{21}\cdot100(H_2O)$ ($\mathbf{Ln_{37}}$)	4
4	$[Er_{60}(L\text{-}thre)_{34}(\mu_6\text{-}CO_3)_8(\mu_3\text{-}OH)_{96}(\mu_2\text{-}O)_2(H_2O)_{18}]\cdot Br_{12}\cdot(ClO_4)_{18}\cdot40(H_2O)$ ($\mathbf{Ln_{60}}$)	5
5	$[Dy_{72}(mda)_{24}(mdaH)_8(OH)_{120}(O)_8(NO_3)_{16}]\cdot(NO_3)_8$ ($\mathbf{Ln_{72}}$)	6
6	$[Gd_{38}(\mu\text{-}O)(\mu_8\text{-}ClO_4)_6(\mu_3\text{-}OH)_{42}(CAA)_{37}(H_2O)_{36}(EtOH)_6]\cdot(ClO_4)_{10}\cdot(OH)_{17}\cdot14DMSO\cdot13H_2O$ ($\mathbf{Ln_{38}}$)	7
7	$[Gd_{48}(\mu_4\text{-}O)_6(\mu_3\text{-}OH)_{84}(CAA)_{36}(NO_3)_6(H_2O)_{24}(EtOH)_{12}(NO_3)Cl_2]\cdot Cl_3$ ($\mathbf{Ln_{48}}$)	
8	$[Ln_{104}(ClO_4)_6(CH_3COO)_{56}(\mu_3\text{-}OH)_{168}(\mu_4\text{-}O)_{30}(H_2O)_{112}]\cdot(ClO_4)_{22}$ ($\mathbf{Ln_{104}}$)	8
9	$\{[Ln_{36}(NA)_{36}(OH)_{49}(O)_6(NO_3)_6(N_3)_3(H_2O)_{20}]Cl_2\cdot28H_2O\}_n$ ($\mathbf{Ln_{36}}$)	9
10	$\{[Cl_2\&(NO_3)]@[Er_{48}(NA)_{44}(OH)_{90}(N_3)(H_2O)_{24}]\}_n$ ($\mathbf{Ln_{48}}$)	10
11	$K_2[Ho_{48}(IN)_{46}(\mu_3\text{-}OH)_{84}(\mu_4\text{-}OH)_4(\mu_5\text{-}O)_2(OAc)_4(H_2O)_{14}(CO_3)Br_2]$ ($\mathbf{Ln_{48}}$)	11
12	$[(ClO_4)@Ln_{27}(\mu_3\text{-}OH)_{32}(CO_3)_8(CH_3CH_2COO)_{20}(H_2O)_{40}]\cdot(ClO_4)_{12}\cdot(H_2O)_{50}$ ($\mathbf{Ln_{27}}$)	12
13	$[Ln_{15}(\mu_3\text{-}OH)_{20}(\mu_5\text{-}X)]^{24+}$ ($\mathbf{Ln_{15}}$)	13, 14
14	$[Dy_{19}(\mathbf{1}\text{-}3H)(\mathbf{1}\text{-}2H)_{11}(CH_3CO_2)_6(OH)_{26}(H_2O)_{30}]$ ($\mathbf{Ln_{19}}$)	15
15	$Ln_{14}(\mu_4\text{-}OH)_2(\mu_3\text{-}OH)_{16}(\mu\text{-}\eta^2\text{-}acac)_8(\eta^2\text{-}acac)_{16}$ ($\mathbf{Ln_{14}}$)	16
16	$H_{18}[Ln_{14}(\mu\text{-}\eta2\text{-}O_2N\text{-}C_6H_4\text{-}O)_8(\eta2\text{-}O_2N\text{-}C_6H_4\text{-}O)_{16}(\mu_4\text{-}O)_2(\mu_3\text{-}O)_{16}]$ ($\mathbf{Ln_{14}}$)	17
17	$Ln_{14}(\mu_4\text{-}OH)_2(\mu_3\text{-}OH)_{16}(\mu\text{-}\eta^2\text{-}acac)_8(\eta^2\text{-}acac)_{16}\cdot6H_2O$ ($\mathbf{Ln_{14}}$)	18
18	$[Ho_{26}(IN)_{28}(CH_3COO)_4(CO_3)_{10}(OH)_{26}(H_2O)_{18}]\cdot20H_2O$ ($\mathbf{Ln_{26}}$)	19
19	$[Dy_{26}(\mu_3\text{-}OH)_{20}(\mu_3\text{-}O)_6(NO_3)_9I]^{36+}$ ($\mathbf{Ln_{26}}$)	20
20	$[Gd_{10}(\mu_3\text{-}OH)_8]^{22+}$ ($\mathbf{Ln_{10}}$)	21
21	$[Dy_{10}O_2(OH)_6(o\text{-}van)_6(ISO)_{13}(H_2O)_2](NO_3)$ ($\mathbf{Ln_{10}}$)	22
22	$[Ln_{10}(TBC8A)_2(PhPO_3)_4(OH)_2(HCO_3)(HCOO)(DMF)_{14}]\cdot(H_6TBC8A)\cdot8CH_3OH$ ($\mathbf{Ln_{10}}$)	23
23	$[Ln_{16}As_{16}W_{164}O_{576}(OH)_8(H_2O)_{42}]^{80-}$ ($\mathbf{Ln_{16}}$)	24
24	$[Ln_{27}Ge_{10}W_{106}O_{406}(OH)_4(H_2O)_{24}]^{59-}$ ($\mathbf{Ln_{26}}$)	25
25	$[Ln_{12}(L)_6(OH)_4O_2(CO_3)_6][Ln_{12}(L)_6(OH)_4O_4(CO_3)_6]\cdot(ClO_4)_4\cdot xH_2O$ ($\mathbf{Ln_{12}}$)	26
26	$[Dy_{11}(OH)_{11}(phendox)_6(phenda)_3(OAc)_3]\cdot(OH)\cdot40H_2O\cdot7MeOH$ ($\mathbf{Ln_{11}}$)	27
27	$[Gd_{60}(CO_3)_8(CH_3COO)_{12}(\mu_2\text{-}OH)_{24}(\mu_3\text{-}OH)_{96}(H_2O)_{56}](NO_3)_{15}\cdot Br_{12}\cdot(dmp)_5\cdot30CH_3OH\cdot20Hdmp$ ($\mathbf{Ln_{60}}$)	28

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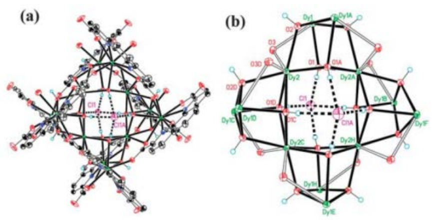
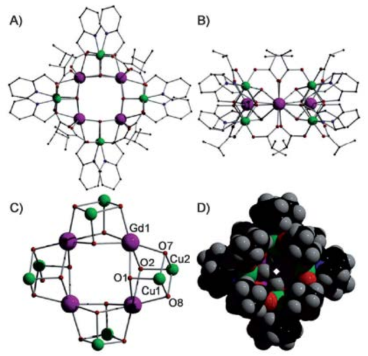
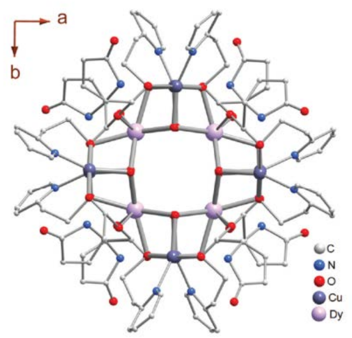
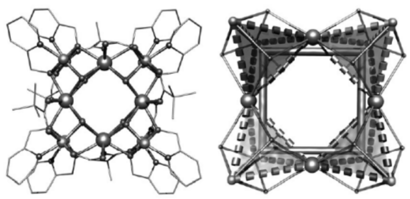
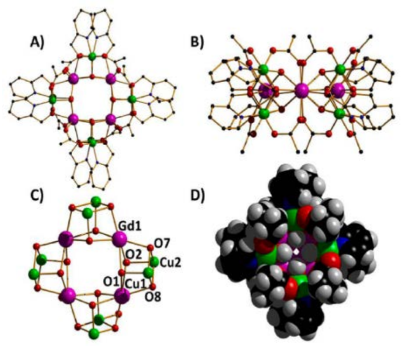
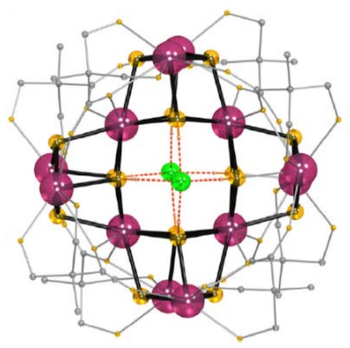
Table S1b. The M_{12} structure containing Vertex-Sharing $\{M_4O_4\}$ Cubanes was queried using CCDC2018 (2.00) until 15 Jan. 2019.

No	Title	Structure	Ref.
1	Chloride templated formation of$\{Dy_{12}(OH)_{16}\}^{20+}$ cluster core incorporating1,10-phenanthroline -2,9-dicarboxylate		*CrystEngComm*, **2011**, **13**, 3345–3348.

2	The Importance of Being Exchanged: $[Gd^{III}_4M^{II}_8(OH)_8(L)_8(O_2CR)_8]^{4+}$Clusters for MagneticRefrigeration		*Angew. Chem. Int. Ed.* **2012**, *51*, 4633 –4636.
3	Chiral biomolecule based dodecanucleardysprosium(III)–copper(II)clusters: structuralanalyses and magnetic properties		*Inorg. Chem. Front.* **2015**, *2*, 854–859.
4	$Cu^{II}Gd^{III}$ Cryogenic Magnetic Refrigerants and Cu_8Dy_9 Single-MoleculeMagnet Generated by In Situ Reactions of Picolinaldehyde and Acetylpyridine: Experimental and Theoretical Study		*Chem. Eur. J.* **2013**, *19*, 17567–17577.
5	Structurally Flexible and Solution Stable$[Ln_4TM_8(OH)_8(L)_8(O_2CR)_8(MeOH)_y](ClO_4)_4$: A Play ground for Magnetic Refrigeration		*Inorg. Chem.* **2016**, *55*, 10535−10546.
6	Filling the Missing Links of M_{3n} Prototype 3d-4f and 4f Cyclic Coordination Cages: Syntheses, Structures, and Magnetic Properties of the $Ni_{10}Ln_5$ and the Er_{3n}Wheels		*Inorg. Chem.* **2017**, *56*, 12821−12829.

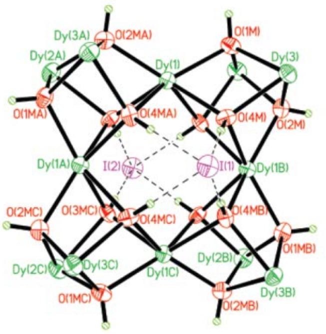
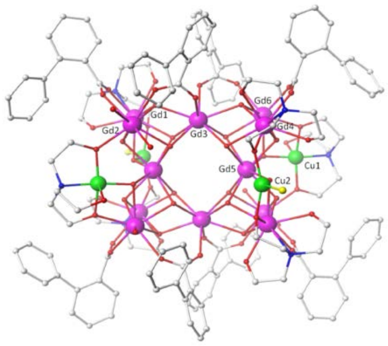
7	Halide-Templated Assembly of Polynuclear Lanthanide-Hydroxo Complexes		*Inorg. Chem.* **2002**, *41*, 278-286.
8	Synthesis, Structure, and Magnetism of a Family of Heterometallic{Cu_2Ln_7} and {Cu_4Ln_{12}} (Ln = Gd, Tb, and Dy) Complexes: The Gd Analogues Exhibiting a Large Magnetocaloric Effect		*Inorg. Chem.* **2014**, *53*,13154−13161.

Table S2a. Crystallographic data of the complex **Dy**$_{12}$.

Complex	**Dy**$_{12}$
Formula	$C_{92}H_{116}Dy_{12}N_8O_{52}$
Formula weight	4115.92
T (K)	153.15
Crystal system	Monoclinic
Space group	$C2/c$
a (Å)	23.2979(3)
b (Å)	20.7928(2)
c (Å)	27.2160(5)
α (°)	90
β (°)	97.7266(14)
γ (°)	90
V (Å^3)	13064.5(3)
Z	4
D_c(g cm^{-3})	2.093
μ (mm^{-1})	36.678

Reflns coll.	47464
Unique reflns	13210
R_{int}	0.0617
$^{a}R_1[I \geq 2\sigma(I)]$	0.0254
$^{b}wR_2$(all data)	0.0820
GOF	1.076

$^{a}R_1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$, $^{b}wR_2 = [\Sigma w(F_o^2-F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$

Table S2b. Selected bond lengths (Å) and angles (°) of complex **Dy12**.

Bond lengths (Å)					
Dy1—O10^{i}	2.310 (3)	Dy2—O15^{i}	2.305 (3)	Dy3—O18	2.219 (2)
Dy1—O16^{i}	2.345 (3)	Dy2—O20	2.333 (2)	Dy3—O12^{i}	2.365 (3)
Dy1—O15	2.349 (2)	Dy2—O15	2.362 (2)	Dy3—O19	2.368 (2)
Dy1—O16	2.389 (2)	Dy2—O16	2.363 (2)	Dy3—O17	2.394 (2)
Dy1—O7	2.472 (2)	Dy2—O7	2.390 (2)	Dy3—O9	2.466 (3)
Dy1—O1	2.482 (3)	Dy2—O19	2.401 (2)	Dy3—O2	2.482 (3)
Dy1—O1W	2.575 (2)	Dy2—O17	2.401 (2)	Dy3—O2W	2.560 (3)
Dy1—N1	2.655 (3)	Dy2—O9	2.449 (2)	Dy3—N2	2.613 (3)
Dy4—O21	2.302 (2)	Dy5—O14	2.361 (2)	Dy6—O17	2.331 (2)
Dy4—O19	2.330 (2)	Dy5—O21	2.371 (2)	Dy6—O8	2.348 (2)
Dy4—O22	2.336 (2)	Dy5—O22	2.371 (2)	Dy6—O20	2.377 (2)
Dy4—O11^{i}	2.337 (3)	Dy5—O22^{i}	2.376 (2)	Dy6—O13	2.488 (2)
Dy4—O21^{i}	2.369 (2)	Dy5—O11	2.434 (3)	Dy6—O4	2.510 (3)
Dy4—O13	2.393 (2)	Dy5—O3	2.449 (3)	Dy6—O4W	2.604 (2)
Dy4—O20	2.412 (2)	Dy5—O3W	2.600 (2)	Dy6—O18	2.614 (2)
Dy4—O18	2.553 (2)	Dy5—N3	2.618 (3)	Dy6—N4	2.627 (3)
Bond angles (°)					
O10^{i}—Dy1—O16^{i}	85.87 (9)	O15^{i}—Dy2—O20	115.93 (8)	O18—Dy3—O12^{i}	82.59 (10)
O10^{i}—Dy1—O15	75.27 (9)	O15^{i}—Dy2—O15	67.61 (11)	O18—Dy3—O19	76.70 (8)
O16^{i}—Dy1—O15	70.46 (9)	O20—Dy2—O15	77.08 (9)	O12^{i}—Dy3—O19	76.07 (9)
O10^{i}—Dy1—O16	146.06 (9)	O15^{i}—Dy2—O16	70.90 (9)	O18—Dy3—O17	73.90 (9)
O16^{i}—Dy1—O16	68.68 (11)	O20—Dy2—O16	145.92 (8)	O12^{i}—Dy3—O17	148.69 (8)

O15—Dy1—O16	75.23 (9)	O15—Dy2—O16	75.50 (8)	O19—Dy3—O17	78.57 (8)
O10^{i}—Dy1—O7	113.48 (8)	O15^{i}—Dy2—O7	125.13 (9)	O18—Dy3—O9	133.18 (8)
O16^{i}—Dy1—O7	123.93 (8)	O20—Dy2—O7	81.13 (9)	O12^{i}—Dy3—O9	114.45 (9)
O15—Dy1—O7	65.55 (8)	O15—Dy2—O7	66.69 (9)	O19—Dy3—O9	66.98 (7)
O16—Dy1—O7	67.88 (8)	O16—Dy2—O7	69.67 (8)	O17—Dy3—O9	70.85 (8)
O10^{i}—Dy1—O1	151.64 (10)	O15^{i}—Dy2—O19	78.30 (8)	O18—Dy3—O2	109.78 (10)
O16^{i}—Dy1—O1	108.85 (11)	O20—Dy2—O19	70.67 (8)	O12^{i}—Dy3—O2	148.78 (10)
O15—Dy1—O1	132.02 (9)	O15—Dy2—O19	115.04 (8)	O19—Dy3—O2	133.87 (10)
O16—Dy1—O1	61.61 (10)	O16—Dy2—O19	140.39 (8)	O17—Dy3—O2	61.20 (10)
O7—Dy1—O1	78.95 (10)	O7—Dy2—O19	149.89 (8)	O9—Dy3—O2	78.59 (10)
O10^{i}—Dy1—O1W	86.81 (8)	O15^{i}—Dy2—O17	149.91 (8)	O18—Dy3—O2W	63.43 (9)
O16^{i}—Dy1—O1W	75.72 (8)	O20—Dy2—O17	72.33 (8)	O12^{i}—Dy3—O2W	88.35 (10)
O15—Dy1—O1W	142.52 (8)	O15—Dy2—O17	140.29 (9)	O19—Dy3—O2W	138.78 (8)
O16—Dy1—O1W	107.11 (8)	O16—Dy2—O17	119.73 (9)	O17—Dy3—O2W	98.98 (10)
O7—Dy1—O1W	151.12 (8)	O7—Dy2—O17	83.91 (8)	O9—Dy3—O2W	151.47 (9)
O1—Dy1—O1W	74.19 (10)	O19—Dy2—O17	77.80 (9)	O2—Dy3—O2W	73.28 (11)
O10^{i}—Dy1—N1	74.34 (9)	O15^{i}—Dy2—O9	82.88 (9)	O18—Dy3—N2	154.02 (10)
O16^{i}—Dy1—N1	159.30 (10)	O20—Dy2—O9	128.17 (9)	O12^{i}—Dy3—N2	71.50 (10)
O15—Dy1—N1	98.08 (10)	O15—Dy2—O9	148.52 (9)	O19—Dy3—N2	94.85 (9)
O16—Dy1—N1	126.35 (9)	O16—Dy2—O9	84.93 (9)	O17—Dy3—N2	129.12 (10)
O7—Dy1—N1	61.46 (8)	O7—Dy2—O9	128.82 (8)	O9—Dy3—N2	60.54 (9)
O1—Dy1—N1	91.66 (12)	O19—Dy2—O9	66.75 (8)	O2—Dy3—N2	93.89 (11)
O1W—Dy1—N1	108.53 (9)	O17—Dy2—O9	71.02 (8)	O2W—Dy3—N2	116.26 (10)
O21—Dy4—O19	116.39 (8)	O14—Dy5—O21	73.90 (8)	O17—Dy6—O8	84.89 (8)
O21—Dy4—O22	71.60 (8)	O14—Dy5—O22	84.99 (8)	O17—Dy6—O20	72.81 (8)
O19—Dy4—O22	146.31 (9)	O21—Dy5—O22	69.80 (8)	O8—Dy6—O20	74.33 (8)
O21—Dy4—O11^{i}	126.10 (9)	O14—Dy5—O22^{i}	144.28 (8)	O17—Dy6—O13	125.44 (8)
O19—Dy4—O11^{i}	83.30 (8)	O21—Dy5—O22^{i}	75.23 (9)	O8—Dy6—O13	113.39 (8)
O22—Dy4—O11^{i}	67.94 (8)	O22—Dy5—O22^{i}	67.71 (10)	O20—Dy6—O13	64.88 (7)
O21—Dy4—O21^{i}	69.11 (10)	O14—Dy5—O11	115.82 (9)	O17—Dy6—O4	107.58 (10)
O19—Dy4—O21^{i}	77.10 (9)	O21—Dy5—O11	66.15 (8)	O8—Dy6—O4	144.66 (9)
O22—Dy4—O21^{i}	76.00 (9)	O22—Dy5—O11	121.78 (9)	O20—Dy6—O4	140.63 (9)
O11^{i}—Dy4—O21^{i}	67.73 (8)	O22^{i}—Dy5—O11	65.74 (8)	O13—Dy6—O4	86.64 (10)

O21—Dy4—O13	80.39 (8)	O14—Dy5—O3	89.57 (10)	O17—Dy6—O4W	70.46 (8)
O19—Dy4—O13	127.74 (9)	O21—Dy5—O3	137.11 (9)	O8—Dy6—O4W	85.97 (8)
O22—Dy4—O13	85.11 (8)	O22—Dy5—O3	69.53 (9)	O20—Dy6—O4W	139.52 (7)
O11^{i}—Dy4—O13	128.31 (8)	O22^{i}—Dy5—O3	101.17 (9)	O13—Dy6—O4W	154.45 (7)
O21^{i}—Dy4—O13	147.85 (8)	O11—Dy5—O3	151.89 (9)	O4—Dy6—O4W	68.52 (9)
O21—Dy4—O20	77.10 (8)	O14—Dy5—O3W	139.36 (8)	O17—Dy6—O18	68.04 (8)
O19—Dy4—O20	70.53 (9)	O21—Dy5—O3W	144.94 (8)	O8—Dy6—O18	147.99 (8)
O22—Dy4—O20	140.29 (8)	O22—Dy5—O3W	114.96 (8)	O20—Dy6—O18	81.33 (8)
O11^{i}—Dy4—O20	151.65 (8)	O22^{i}—Dy5—O3W	75.32 (8)	O13—Dy6—O18	72.85 (7)
O21^{i}—Dy4—O20	114.74 (8)	O11—Dy5—O3W	84.58 (8)	O4—Dy6—O18	63.88 (9)
O13—Dy4—O20	65.83 (8)	O3—Dy5—O3W	67.71 (10)	O4W—Dy6—O18	99.94 (7)
O21—Dy4—O18	152.95 (8)	O14—Dy5—N3	74.74 (9)	O17—Dy6—N4	159.20 (9)
O19—Dy4—O18	71.19 (8)	O21—Dy5—N3	99.51 (9)	O8—Dy6—N4	74.53 (9)
O22—Dy4—O18	117.68 (8)	O22—Dy5—N3	159.20 (9)	O20—Dy6—N4	98.18 (8)
O11^{i}—Dy4—O18	79.40 (8)	O22^{i}—Dy5—N3	128.25 (9)	O13—Dy6—N4	62.72 (8)
O21^{i}—Dy4—O18	136.42 (8)	O11—Dy5—N3	65.38 (9)	O4—Dy6—N4	91.34 (11)
O13—Dy4—O18	75.50 (8)	O3—Dy5—N3	114.15(10)	O4W—Dy6—N4	110.31 (9)
O20—Dy4—O18	81.93 (8)	O3W—Dy5—N3	84.23 (9)	O18—Dy6—N4	130.25 (8)
Symmetry code: (i) -*x*, *y*, -*z*+1/2.					

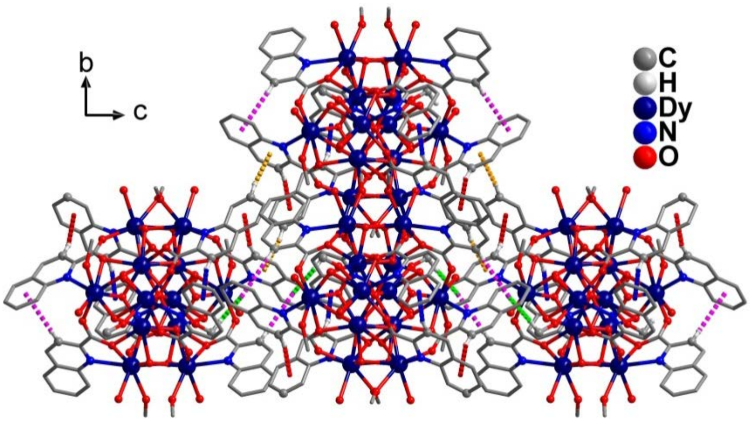


Figure S1. The weak interaction bonds for complex **Dy_{12}**.

Table S3. Hydrogen-bonds for **Dy_{12}** complex.

Dy_{12}		
Hydrogen bond	**Distance[a], Å**	**Angle[b], °**

$C_2–H_2···\pi$	2.84	161
$C_7–H_7···\pi$	2.52	172
$C_{11}–H_{11}···\pi$	2.94	163
$C_{20}–H_{20}···\pi$	2.95	152
$C_{44}–H_{44A}···\pi$	2.96	154

[a] Distance between acceptor and donor; [b] Angle of acceptor–hydrogen–donor.

Table S4. *SHAPE* analysis of the Dy1 ion in **Dy_{12}**.

Label	**Shape**	**Symmetry**	**Distortion(°)**
OP-8	D_{8h}	Octagon	35.358
HPY-8	C_{7v}	Heptagonalpyramid	22.662
HBPY-8	D_{6h}	Hexagonal bipyramid	14.952
CU-8	O_h	Cube	8.177
SAPR-8	D_{4d}	Square antiprism	3.085
TDD-8	D_{2d}	Triangular dodecahedron	2.859
JGBF-8	D_{2d}	Johnson gyrobifastigium J26	16.164
JETBPY-8	D_{3h}	Johnsonelongatedtriangular bipyramid J14	26.369
JBTPR-8	C_{2v}	Biaugmented trigonal prism J50	4.820
BTPR-8	C_{2v}	Biaugmented trigonal prism	3.989
JSD-8	D_{2d}	Snub diphenoid J84	6.861
TT-8	T_d	Triakis tetrahedron	8.663
ETBPY-8	D_{3h}	Elongated trigonal bipyramid	22.258

Table S5. *SHAPE* analysis of the Dy2 ion in **Dy_{12}**.

Label	**Shape**	**Symmetry**	**Distortion(°)**
OP-8	D_{8h}	Octagon	25.970
HPY-8	C_{7v}	Heptagonalpyramid	23.138
HBPY-8	D_{6h}	Hexagonal bipyramid	15.134
CU-8	O_h	Cube	8.041
SAPR-8	D_{4d}	Square antiprism	0.998

TDD-8	D_{2d}	Triangular dodecahedron	2.223
JGBF-8	D_{2d}	Johnson gyrobifastigium J26	15.377
JETBPY-8	D_{3h}	Johnsonelongatedtriangular bipyramid J14	26.661
JBTPR-8	C_{2v}	Biaugmented trigonal prism J50	3.389
BTPR-8	C_{2v}	Biaugmented trigonal prism	2.712
JSD-8	D_{2d}	Snub diphenoid J84	5.458
TT-8	T_d	Triakis tetrahedron	8.763
ETBPY-8	D_{3h}	Elongated trigonal bipyramid	21.197

Table S6. *SHAPE* analysis of the Dy3 ion in $\mathbf{Dy_{12}}$.

Label	**Shape**	**Symmetry**	**Distortion(°)**
OP-8	D_{8h}	Octagon	31.564
HPY-8	C_{7v}	Heptagonalpyramid	21.989
HBPY-8	D_{6h}	Hexagonal bipyramid	14.927
CU-8	O_h	Cube	8.917
SAPR-8	D_{4d}	Square antiprism	3.867
TDD-8	D_{2d}	Triangular dodecahedron	2.854
JGBF-8	D_{2d}	Johnson gyrobifastigium J26	15.684
JETBPY-8	D_{3h}	Johnsonelongatedtriangular bipyramid J14	25.674
JBTPR-8	C_{2v}	Biaugmented trigonal prism J50	5.224
BTPR-8	C_{2v}	Biaugmented trigonal prism	4.275
JSD-8	D_{2d}	Snub diphenoid J84	6.657
TT-8	T_d	Triakis tetrahedron	9.336
ETBPY-8	D_{3h}	Elongated trigonal bipyramid	20.904

Table S7. *SHAPE* analysis of the Dy4 ion in $\mathbf{Dy_{12}}$.

Label	**Shape**	**Symmetry**	**Distortion(°)**
OP-8	D_{8h}	Octagon	26.542

HPY-8	C_{7v}	Heptagonalpyramid	22.705
HBPY-8	D_{6h}	Hexagonal bipyramid	14.395
CU-8	O_h	Cube	7.530
SAPR-8	D_{4d}	Square antiprism	1.132
TDD-8	D_{2d}	Triangular dodecahedron	2.079
JGBF-8	D_{2d}	Johnson gyrobifastigium J26	15.272
JETBPY-8	D_{3h}	Johnsonelongatedtriangular bipyramid J14	26.269
JBTPR-8	C_{2v}	Biaugmented trigonal prism J50	3.580
BTPR-8	C_{2v}	Biaugmented trigonal prism	2.853
JSD-8	D_{2d}	Snub diphenoid J84	5.807
TT-8	T_d	Triakis tetrahedron	8.254
ETBPY-8	D_{3h}	Elongated trigonal bipyramid	20.479

Table S8. *SHAPE* analysis of the Dy5 ion in $\mathbf{Dy_{12}}$.

Label	**Shape**	**Symmetry**	**Distortion(^{o})**
OP-8	D_{8h}	Octagon	35.428
HPY-8	C_{7v}	Heptagonalpyramid	22.343
HBPY-8	D_{6h}	Hexagonal bipyramid	13.038
CU-8	O_h	Cube	6.630
SAPR-8	D_{4d}	Square antiprism	3.577
TDD-8	D_{2d}	Triangular dodecahedron	2.213
JGBF-8	D_{2d}	Johnson gyrobifastigium J26	14.798
JETBPY-8	D_{3h}	Johnsonelongatedtriangular bipyramid J14	26.532
JBTPR-8	C_{2v}	Biaugmented trigonal prism J50	5.044
BTPR-8	C_{2v}	Biaugmented trigonal prism	3.697
JSD-8	D_{2d}	Snub diphenoid J84	5.851
TT-8	T_d	Triakis tetrahedron	7.452
ETBPY-8	D_{3h}	Elongated trigonal bipyramid	21.271

Table S9. *SHAPE* analysis of the Dy6 ion in **Dy_{12}**.

Label	Shape	Symmetry	Distortion(°)
OP-8	D_{8h}	Octagon	34.393
HPY-8	C_{7v}	Heptagonalpyramid	22.959
HBPY-8	D_{6h}	Hexagonal bipyramid	13.977
CU-8	O_h	Cube	6.797
SAPR-8	D_{4d}	Square antiprism	3.291
TDD-8	D_{2d}	Triangular dodecahedron	2.324
JGBF-8	D_{2d}	Johnson gyrobifastigium J26	16.377
JETBPY-8	D_{3h}	Johnsonelongatedtriangular bipyramid J14	26.054
JBTPR-8	C_{2v}	Biaugmented trigonal prism J50	5.096
BTPR-8	C_{2v}	Biaugmented trigonal prism	4.328
JSD-8	D_{2d}	Snub diphenoid J84	6.897
TT-8	T_d	Triakis tetrahedron	7.195
ETBPY-8	D_{3h}	Elongated trigonal bipyramid	23.568

Thermal analysis

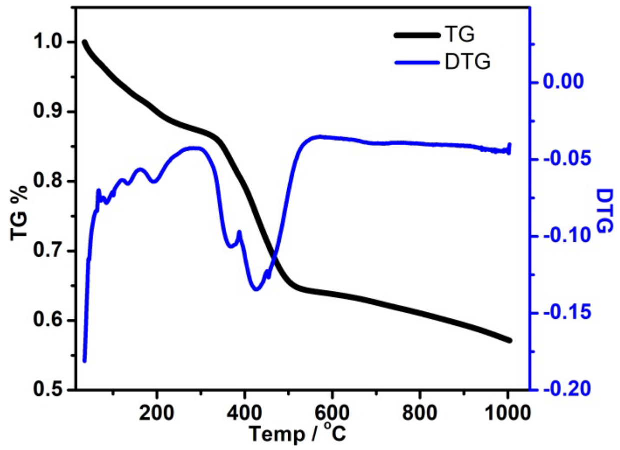


Figure S2a. The TG curve of **Dy_{12}** under heating in flowing N_2 at 5 °C·min^{-1} over the temperature range of 35-1000 °C.

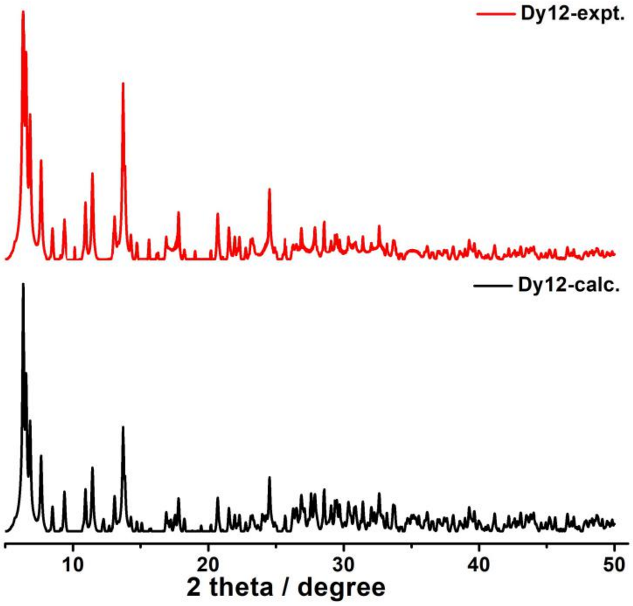


Figure S2b. Powdered X-ray diffraction (XRD) patterns for complex **Dy_{12}**.

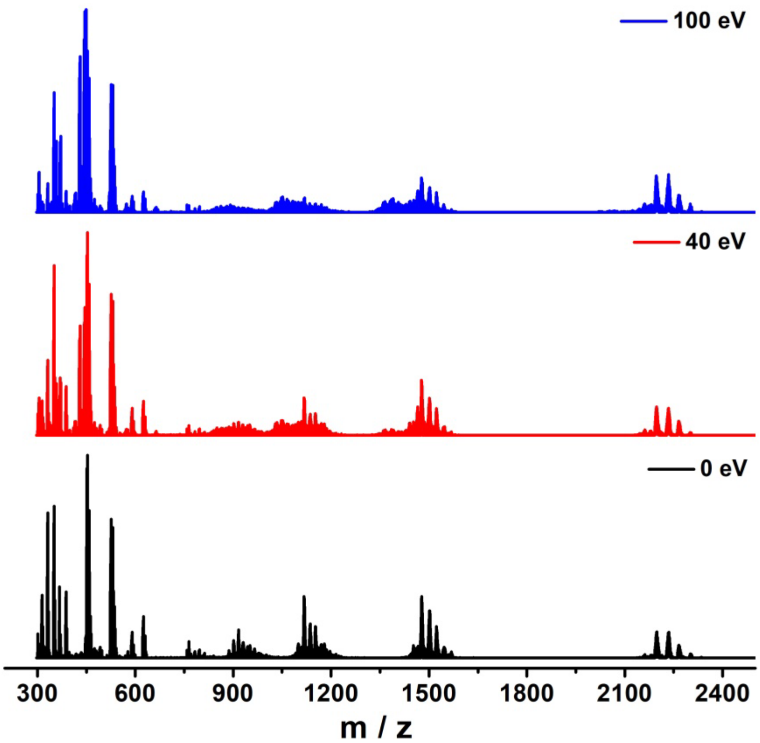
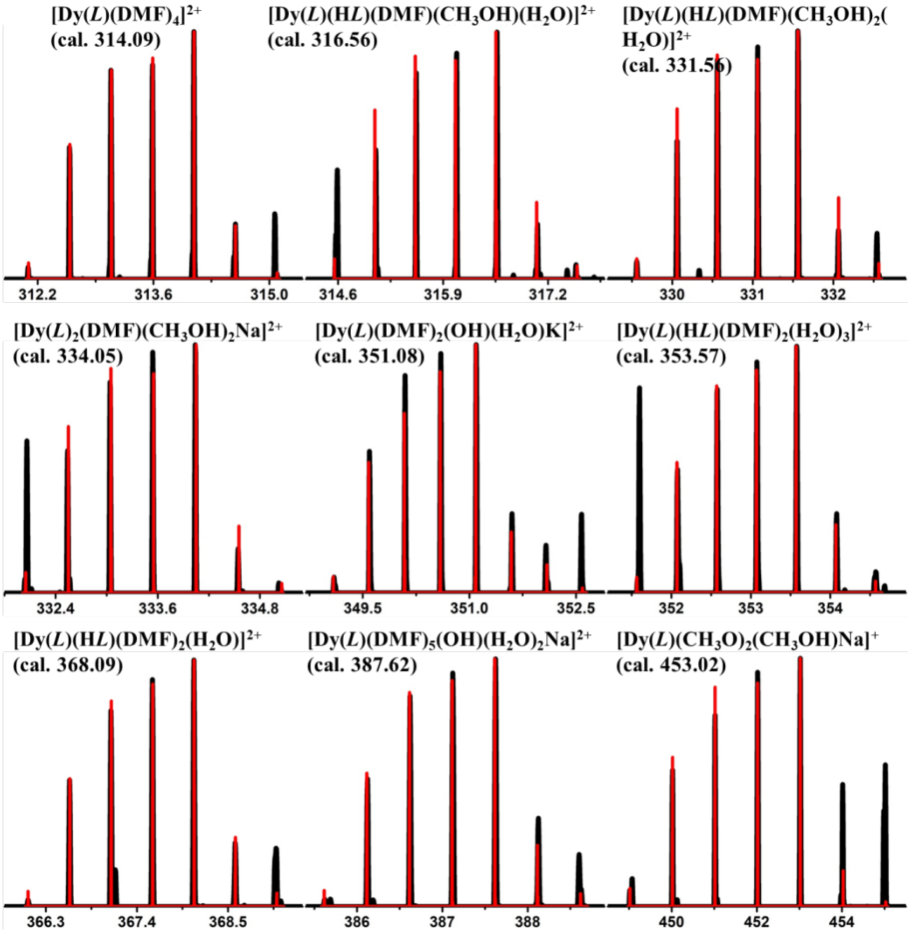


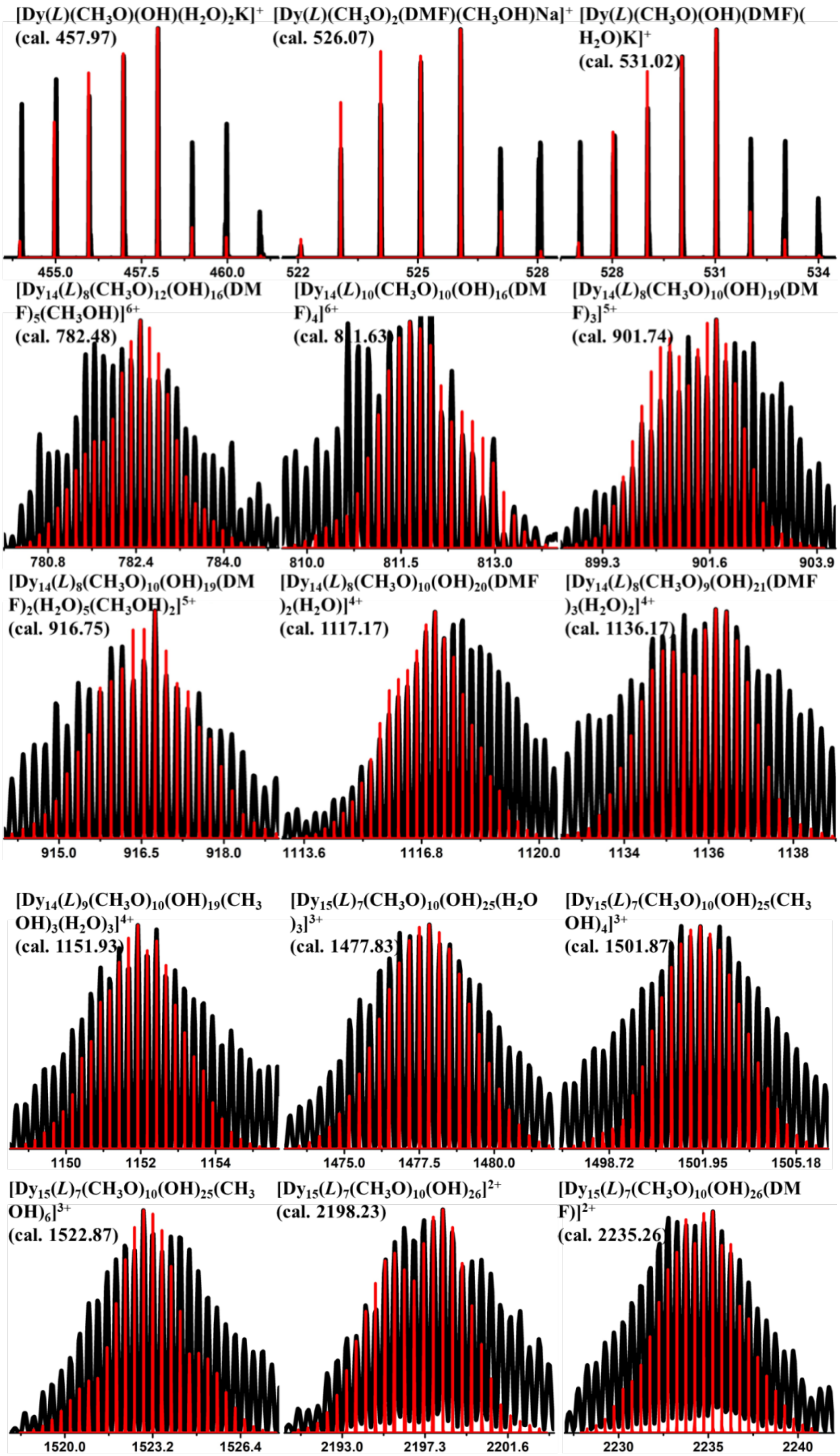
Figure S3. Positive ESI-MS spectra of **Dy_{12}** in DMF (In-Source CID 0, 40 and 100 eV).

Table S10. Major species assigned in the ESI-MS of **Dy_{12}** in positive mode (Since the **Dy_{12}** crystal is easily weathered, a small amount of the reaction solution is retained during sampling to cause introduction of Dy^{3+} ions).

Dy_{12} (In-Source CID 0 eV)			
Peaks	Relative Intensity	*Obs.m/z*	*Calc.m/z*
$[Dy(L)(DMF)_4]^{2+}$	0.311	314.09	314.09
$[Dy(L)(HL)(DMF)(CH_3OH)(H_2O)]^{2+}$	0.157	316.57	316.56
$[Dy(L)(HL)(DMF)(CH_3OH)_2(H_2O)]^{2+}$	0.720	331.56	331.56
$[Dy(L)_2(DMF)(CH_3OH)_2Na]^{2+}$	0.231	334.04	334.05
$[Dy(L)(OH)(DMF)_4(H_2O)K]^{2+}$	0.751	351.09	351.08
$[Dy(L)(HL)(DMF)_2(H_2O)_3]^{2+}$	0.288	353.58	353.57
$[Dy(L)(HL)(DMF)_2(CH_3OH)_2(H_2O)]^{2+}$	0.354	368.09	368.09
$[Dy(L)(OH)(DMF)_5(H2O)_2Na]^{2+}$	0.326	387.62	387.62
$[Dy(L)(CH_3O)_2(CH_3OH)Na]^{+}$	1	453.02	453.02
$[Dy(L)(CH_3O)(OH)(H_2O)_2K]^{+}$	0.735	457.98	457.97
$[Dy(L)(CH_3O)_2(DMF)(CH_3OH)Na]^{+}$	0.690	526.07	526.07
$[Dy(L)(CH_3O)(OH)_2(DMF)(H_2O)K]^{+}$	0.650	531.03	531.02
$[Dy_{12}(L)_8(CH_3O)_{12}(OH)_{16}(DMF)_5(CH_3OH)+2Dy^{3+}]^{6+}$	0.032	782.48	782.48
$[Dy_{12}(L)_{10}(CH_3O)_{10}(OH)_{16}(DMF)_4+2Dy^{3+}]^{6+}$	0.020	811.64	811.63
$[Dy_{12}(L)_8(CH_3O)_{10}(OH)_{19}(DMF)_3+2Dy^{3+}]^{5+}$	0.082	901.74	901.74
$[Dy_{12}(L)_8(CH_3O)_{10}(OH)_{19}(DMF)_2(H_2O)_5(CH_3OH)_2+2Dy^{3+}]^{5+}$	0.142	916.75	916.75
$[Dy_{12}(L)_8(CH_3O)_{10}(OH)_{20}(DMF)_2(H_2O)+2Dy^{3+}]^{4+}$	0.311	1117.16	1117.17
$[Dy_{12}(L)_8(CH_3O)_9(OH)_{21}(DMF)_3(H_2O)_2+2Dy^{3+}]^{4+}$	0.170	1136.16	1136.17
$[Dy_{12}(L)_9(CH_3O)_{10}(OH)_{19}(CH_3OH)_3(H_2O)_3+2Dy^{3+}]^{4+}$	0.159	1151.92	1151.93
$[Dy_{12}(L)_7(CH_3O)_{10}(OH)_{25}(H_2O)_3+3Dy^{3+}]^{3+}$	0.306	1477.84	1477.83
$[Dy_{12}(L)_7(CH_3O)_{10}(OH)_{25}(CH_3OH)_4+3Dy^{3+}]^{3+}$	0.235	1501.87	1501.87
$[Dy_{12}(L)_7(CH_3O)_{10}(OH)_{25}(CH3OH)_6+3Dy^{3+}]^{3+}$	0.157	1522.86	1522.87
$[Dy_{12}(L)_7(CH_3O)_{10}(OH)_{26}+3Dy^{3+}]^{2+}$	0.131	2198.22	2198.23
$[Dy_{12}(L)_7(CH_3O)_{10}(OH)_{26}(DMF)+3Dy^{3+}]^{2+}$	0.129	2235.26	2235.26
$[Dy_{12}(L)_7(CH_3O)_{10}(OH)_{26}(DMF)(CH_3OH)_2+3Dy^{3+}]^{2+}$	0.063	2266.28	2266.28



[Dy(L)(DMF)4]2+ (cal. 314.09)
[Dy(L)(HL)(DMF)(CH3OH)(H2O)]2+ (cal. 316.56)
[Dy(L)(HL)(DMF)(CH3OH)2(H2O)]2+ (cal. 331.56)
312.2 313.6 315.0 314.6 315.9 317.2 330 331 332
[Dy(L)2(DMF)(CH3OH)2Na]2+ (cal. 334.05)
[Dy(L)(DMF)2(OH)(H2O)K]2+ (cal. 351.08)
[Dy(L)(HL)(DMF)2(H2O)3]2+ (cal. 353.57)
332.4 333.6 334.8 349.5 351.0 352.5 352 353 354
[Dy(L)(HL)(DMF)2(H2O)]2+ (cal. 368.09)
[Dy(L)(DMF)5(OH)(H2O)2Na]2+ (cal. 387.62)
[Dy(L)(CH3O)2(CH3OH)Na]+ (cal. 453.02)
366.3 367.4 368.5 386 387 388 450 452 454


$[Dy(L)(CH_3O)(OH)(H_2O)_2K]^+$
(cal. 457.97)
455.0 457.5 460.0
$[Dy(L)(CH_3O)_2(DMF)(CH_3OH)Na]^+$
(cal. 526.07)
522 525 528
$[Dy(L)(CH_3O)(OH)(DMF)(H_2O)K]^+$
(cal. 531.02)
528 531 534
$[Dy_{14}(L)_8(CH_3O)_{12}(OH)_{16}(DMF)_5(CH_3OH)]^{6+}$
(cal. 782.48)
780.8 782.4 784.0
$[Dy_{14}(L)_{10}(CH_3O)_{10}(OH)_{16}(DMF)_4]^{6+}$
(cal. 811.63)
810.0 811.5 813.0
$[Dy_{14}(L)_8(CH_3O)_{10}(OH)_{19}(DMF)_3]^{5+}$
(cal. 901.74)
899.3 901.6 903.9
$[Dy_{14}(L)_8(CH_3O)_{10}(OH)_{19}(DMF)_2(H_2O)_5(CH_3OH)_2]^{5+}$
(cal. 916.75)
915.0 916.5 918.0
$[Dy_{14}(L)_8(CH_3O)_{10}(OH)_{20}(DMF)_2(H_2O)]^{4+}$
(cal. 1117.17)
1113.6 1116.8 1120.0
$[Dy_{14}(L)_8(CH_3O)_9(OH)_{21}(DMF)_3(H_2O)_2]^{4+}$
(cal. 1136.17)
1134 1136 1138
$[Dy_{14}(L)_9(CH_3O)_{10}(OH)_{19}(CH_3OH)_3(H_2O)_3]^{4+}$
(cal. 1151.93)
1150 1152 1154
$[Dy_{15}(L)_7(CH_3O)_{10}(OH)_{25}(H_2O)_3]^{3+}$
(cal. 1477.83)
1475.0 1477.5 1480.0
$[Dy_{15}(L)_7(CH_3O)_{10}(OH)_{25}(CH_3OH)_4]^{3+}$
(cal. 1501.87)
1498.72 1501.95 1505.18
$[Dy_{15}(L)_7(CH_3O)_{10}(OH)_{25}(CH_3OH)_6]^{3+}$
(cal. 1522.87)
1520.0 1523.2 1526.4
$[Dy_{15}(L)_7(CH_3O)_{10}(OH)_{26}]^{2+}$
(cal. 2198.23)
2193.0 2197.3 2201.6
$[Dy_{15}(L)_7(CH_3O)_{10}(OH)_{26}(DMF)]^{2+}$
(cal. 2235.26)
2230 2235 2240

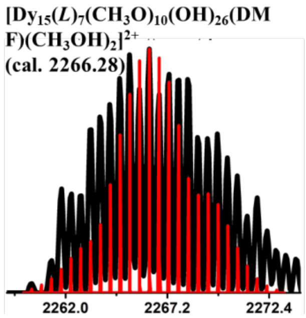
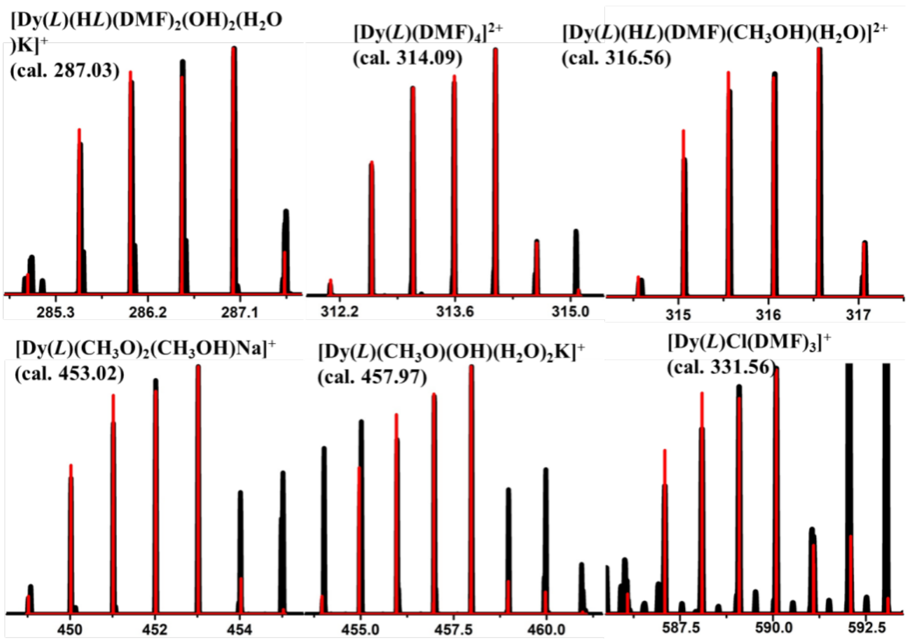


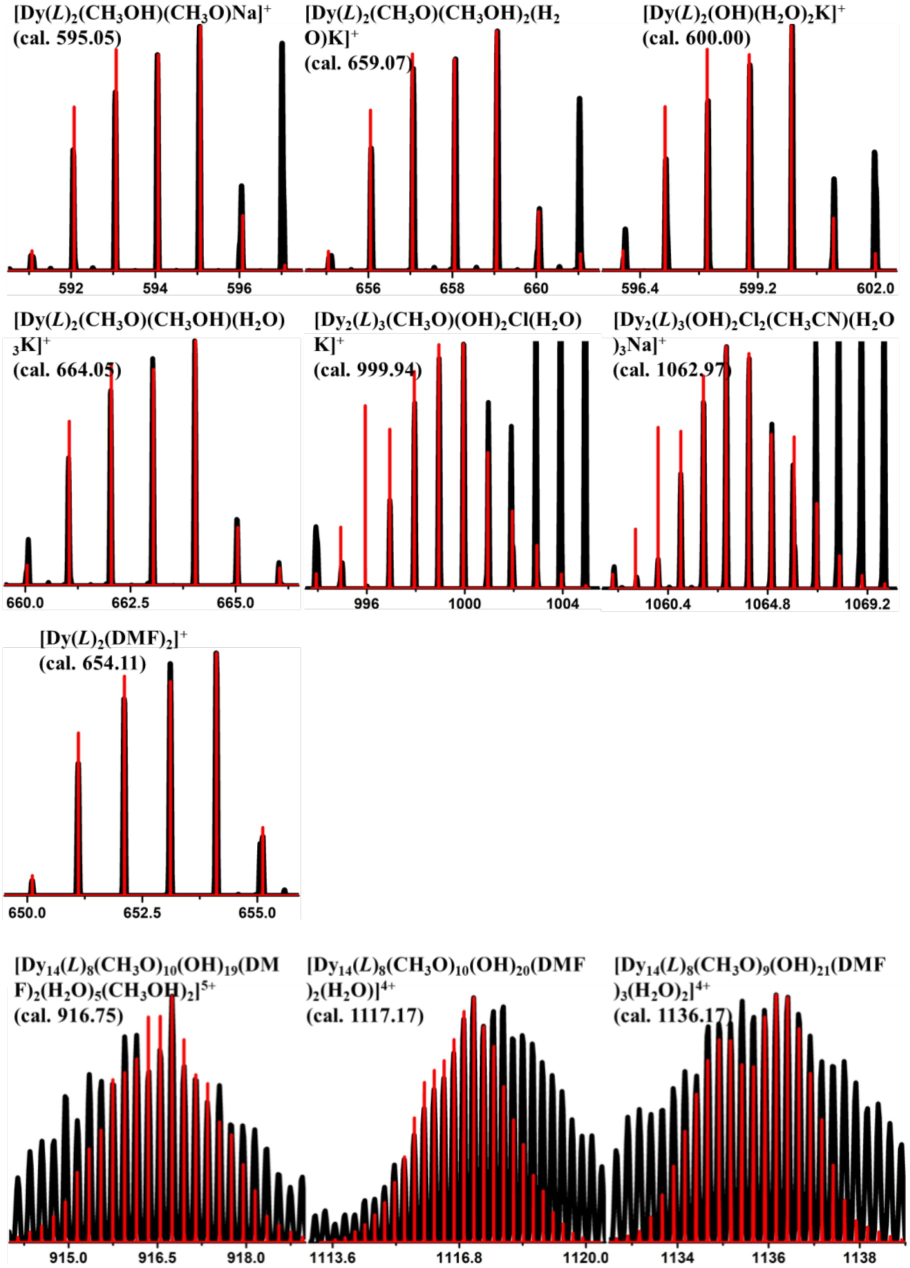
Figure S4. The superposed simulated and observed spectra of several species for **Dy12** (In-Source CID 0 eV).

Table S11. Major species assigned in the Time-dependent ESI-MS of **Dy12** in positivemode.

m/z	**Fragment**	**Relative Intensity**						
		1min	15min	40min	60min	2.5h	8 h	12h
210.05	$[(L+H)(H_2O)_2]^+$ (cal.210.07)	1	1	0.569	0.437	0.249	0	0
287.04	$[KDy(L)(OH)(DMF)_2(H_2O)_2]^{2+}$ (cal.287.03)	0.087	0.021	0	0	0	0	0
314.09	$[Dy(L)(DMF)_4]^{2+}$ (cal.314.09)	0.107	0	0	0	0	0	0
316.57	$[KDy(L)(OH)(DMF)_2(CH_3CN)(H_2O)_3]^{2+}$(cal.316.55)	0.156	0.029	0	0	0	0	0
453.02	$[Dy(L)(CH_3O)_2(CH_3OH)Na]^+$ (cal.453.02)	0.032	0.349	1	1	1	1	1
457.98	$[Dy(L)(CH_3O)(OH)(H_2O)_2K]^+$ (cal.457.97)	0.090	0.256	0.735	0.752	0.587	0.271	0.116
462.94	$[Dy(L)(OH)_2(H_2O)_3K]^+$ (cal.462.97)	0.092	0.073	0.209	0.320	0.167	0.077	0.033
590.09	$[Dy(L)Cl(DMF)_3]^+$ (cal.590.10)	0.083	0	0	0	0	0	0
595.05	$[Dy(L)_2(CH_3OH)(H_2O)_3+H]^+$ (cal.595.07)	0.148	0.052	0	0	0	0	0
600.01	$[KDy(L)_2(OH)(H_2O)_2]^+$ (cal.600.00)	0.109	0.228	0.091	0.107	0.036	0.004	
654.11	$[Dy(L)_2(DMF)_2]^+$ (cal.654.11)	0.033	0	0	0	0	0	0
659.07	$[Dy(L)_2K(H_2O)(CH_3O)(CH_3OH)_2]^+$ (cal.659.06)	0.040	0.078	0.021	0.026	0.008	0	0
664.03	$[Dy(L)_2K(H_2O)_3(CH_3O)(CH_3OH)]^+$ (cal.664.05)	0.019	0.252	0.172	0.245	0.106	0.010	0
998.95	$[KDy_2(L)_3(OH)_2Cl(CH_3OH)(H_2O)]^+$ (cal.998.94)	0.011	0.002	0	0	0	0	0
1062.97	$[NaDy_2(L)_3(OH)Cl_2(H_2O)_4(CH_3CN)]^+$ (cal.1062.98)	0.007	0.006	0	0	0	0	0
901.74	$[Dy_{12}(L)_8(CH_3O)_{10}(OH)_{19}(DMF)_3+2Dy^{3+}]^{5+}$ (cal.901.74)	0	0	0	0.019	0.046	0.088	0.066
916.75	$[Dy_{12}(L)_8(CH_3O)_{10}(OH)_{19}(DMF)_2(H_2O)_5(CH_3OH)_2+2Dy^{3+}]^{5+}$	0	0	0	0.013	0.046	0.107	0.066

	(cal.916.75)							
1117.16	$[Dy_{12}(L)_8(CH_3O)_{10}(OH)_{20}(DMF)_2(H_2O)+2Dy^{3+}]^{4+}$ (cal.1117.17)	0	0	0	0.031	0.115	0.352	0.167
1136.16	$[Dy_{12}(L)_8(CH_3O)_9(OH)_{21}(DMF)_3(H_2O)_2+2Dy^{3+}]^{4+}$ (cal.1136.17)	0	0	0	0.013	0.079	0.201	0.116
1151.92	$[Dy_{12}(L)_9(CH_3O)_{10}(OH)_{19}(CH_3OH)_3(H_2O)_3+2Dy^{3+}]^{4+}$ (cal.1151.93)	0	0	0	0	0.064	0.195	0.094
1477.84	$[Dy_{12}(L)_7(CH_3O)_{10}(OH)_{25}(H_2O)_3+3Dy^{3+}]^{3+}$ (cal.1477.83)	0	0	0	0.035	0.118	0.527	0.173
1501.87	$[Dy_{12}(L)_7(CH_3O)_{10}(OH)_{25}(CH_3OH)_4+3Dy^{3+}]^{3+}$ (cal.1501.87)	0	0	0	0.020	0.127	0.388	0.185
1522.86	$[Dy_{12}(L)_7(CH_3O)_{10}(OH)_{25}(CH3OH)_6+3Dy^{3+}]^{3+}$ (cal.1522.87)	0	0	0	0	0.075	0.272	0.109
2198.22	$[Dy_{12}(L)_7(CH_3O)_{10}(OH)_{26}+3Dy^{3+}]^{2+}$ (cal.2198.23)	0	0	0	0.014	0.027	0.276	0.505
2235.26	$[Dy_{12}(L)_7(CH_3O)_{10}(OH)_{26}(DMF)+3Dy^{3+}]^{2+}$ (cal.2235.26)	0	0	0	0	0.038	0.276	0.511
2266.28	$[Dy_{12}(L)_7(CH_3O)_{10}(OH)_{26}(DMF)(CH_3OH)_2+3Dy^{3+}]^{2+}$ (cal.2266.28)	0	0	0	0	0.016	0.141	0.262




$[Dy(L)_2(CH_3OH)(CH_3O)Na]^+$ (cal. 595.05)
592
594
596
$[Dy(L)_2(CH_3O)(CH_3OH)_2(H_2O)K]^+$ (cal. 659.07)
656
658
660
$[Dy(L)_2(OH)(H_2O)_2K]^+$ (cal. 600.00)
596.4
599.2
602.0
$[Dy(L)_2(CH_3O)(CH_3OH)(H_2O)_3K]^+$ (cal. 664.05)
660.0
662.5
665.0
$[Dy_2(L)_3(CH_3O)(OH)_2Cl(H_2O)K]^+$ (cal. 999.94)
996
1000
1004
$[Dy_2(L)_3(OH)_2Cl_2(CH_3CN)(H_2O)_3Na]^+$ (cal. 1062.97)
1060.4
1064.8
1069.2
$[Dy(L)_2(DMF)_2]^+$ (cal. 654.11)
650.0
652.5
655.0
$[Dy_{14}(L)_8(CH_3O)_{10}(OH)_{19}(DMF)_2(H_2O)_5(CH_3OH)_2]^{5+}$ (cal. 916.75)
915.0
916.5
918.0
$[Dy_{14}(L)_8(CH_3O)_{10}(OH)_{20}(DMF)_2(H_2O)]^{4+}$ (cal. 1117.17)
1113.6
1116.8
1120.0
$[Dy_{14}(L)_8(CH_3O)_9(OH)_{21}(DMF)_3(H_2O)_2]^{4+}$ (cal. 1136.17)
1134
1136
1138

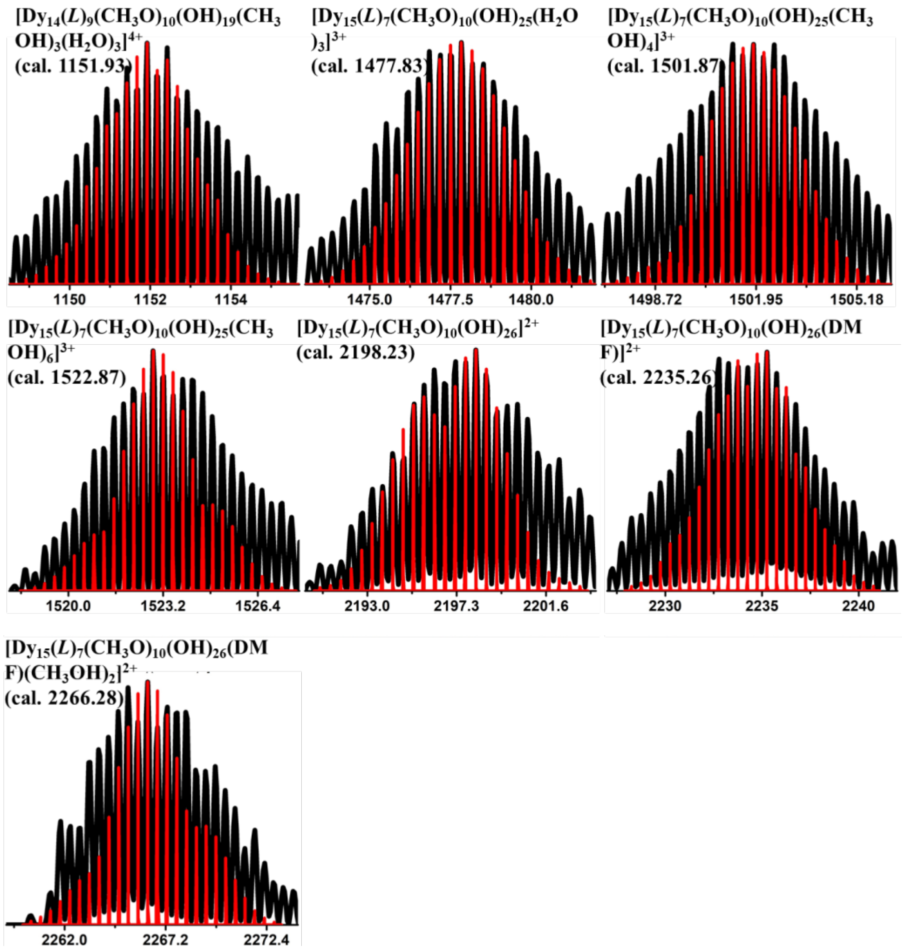


Figure S5. The superposed simulated and observed spectra of several species in the Time-dependent ESI-MS of **Dy12**.

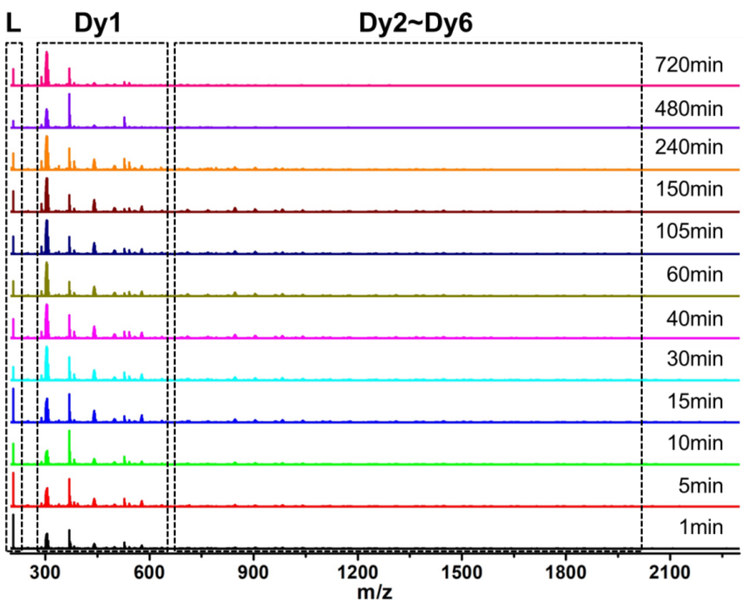
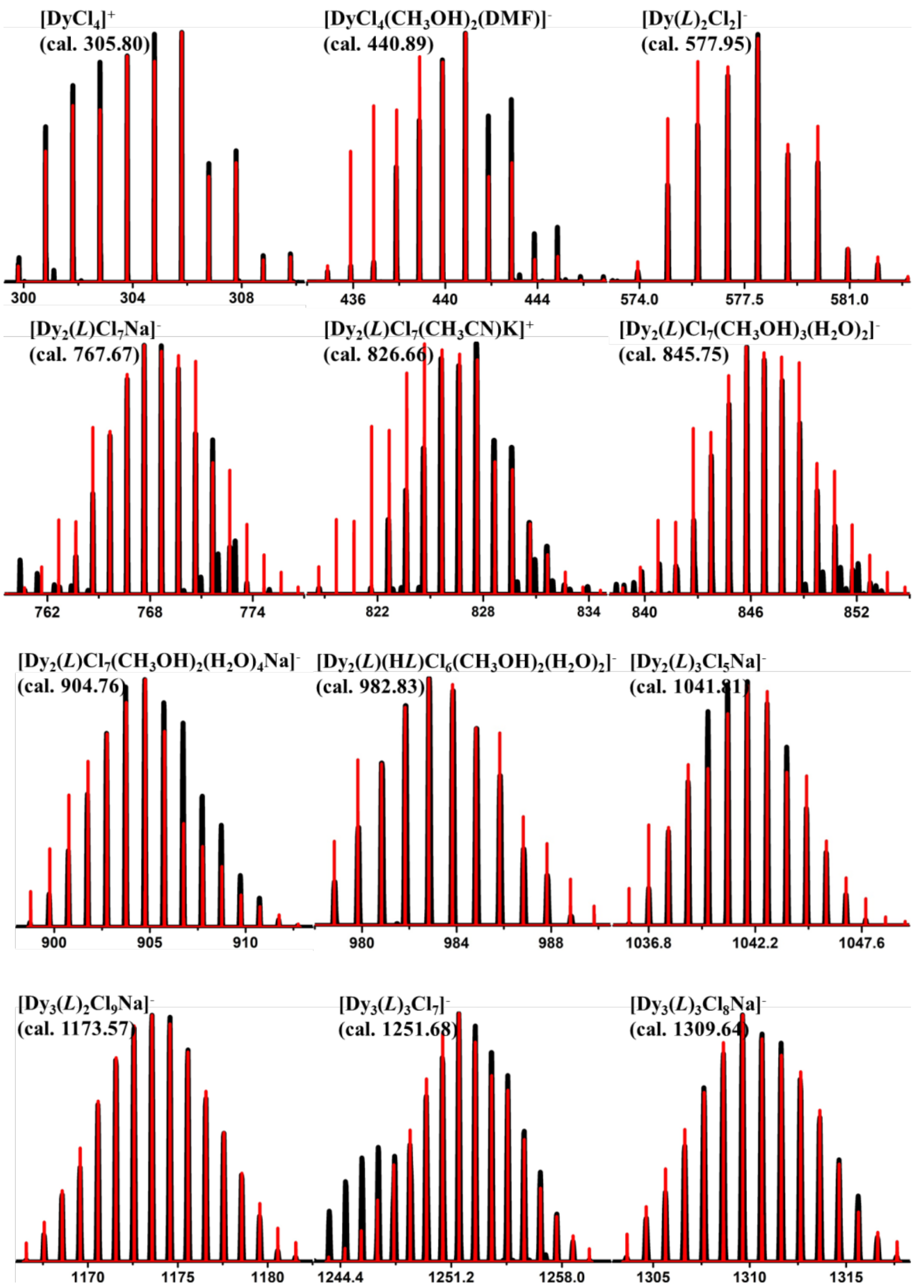


Figure S6. Time-dependent HRESI-MS spectra for the stepwise assembly of **Dy12** in negative mode.

Table S12. Major species assigned in the Time-dependent ESI-MS of **Dy$_{12}$** in negative mode.

m/z	Fragment	Relative Intensity						
		1min	15min	40min	60min	2.5h	8 h	12h
305.80	$[DyCl_4]^-$ (cal.305.80)	0.442	0.703	1	1	1	1	1
440.87	$[DyCl_4(DMF)(CH_3O)_2]^-$ (cal.440.89)	0.103	0.344	0.342	0.279	0.354	0.068	0.080
577.95	$[Dy(L)_2Cl_2]^-$ (cal.577.95)	0.087	0.209	0.165	0.134	0.166	0.015	0.009
767.66	$[Dy_2Cl_7(L)Na]^-$ (cal.767.66)	0.010	0.026	0.038	0.040	0.044	0.012	0.022
826.66	$[Dy_2Cl_7(L)K(CH_3CN)]^-$ (cal.826.66)	0.006	0.013	0.022	0.019	0.024	0.009	0.018
845.75	$[Dy_2Cl_7(HL)(CH_3OH)_2(H_2O)_2]^-$ (cal.845.75)	0.025	0.085	0.093	0.102	0.114	0.011	0.007
962.69	$[Dy_2Cl_8(HL)(H_2O)_8K]^-$ (cal.962.69)	0.012	0.026	0.033	0.025	0.033	0.005	0.006
983.83	$[Dy_2Cl_6(L)(HL)(CH_3OH)_2(H_2O)_2]^-$ (cal.983.83)	0.020	0.067	0.062	0.058	0.068	0.003	0
1041.81	$[Dy_2Cl_5(L)_3Na]^-$ (cal.1041.81)	0.016	0.046	0.042	0.035	0.043	0.002	0.005
1173.57	$[Dy_3Cl_9(L)_2Na]^-$ (cal.1173.57)	0.004	0.013	0.018	0.020	0.021	0.004	0.005
1251.68	$[Dy_3Cl_7(L)_3]^-$ (cal.1251.68)	0.006	0.018	0.020	0.023	0.026	0.002	0
1309.64	$[Dy_3Cl_8(L)_3Na]^-$ (cal.1309.64)	0.008	0.024	0.022	0.024	0.028	0.002	0
1369.63	$[Dy_3Cl_8(L)_3K(N_3)H]^-$ (cal.1369.63)	0.007	0.019	0.024	0.021	0.026	0.003	0.002
1446.71	$[Dy_3Cl_7(L)_4Na]^-$ (cal.1446.71)	0.009	0.030	0.030	0.028	0.035	0.001	0
1715.54	$[Dy_4Cl_{10}(L)_4Na]^-$ (cal.1715.54)	0.001	0.007	0.008	0.008	0.010	0	0
1775.50	$[Dy_5Cl_{10}(L)_3(CH_3O)_3]^-$ (cal.1775.50)	0.002	0.007	0.009	0.009	0.010	0.001	0
1852.58	$[Dy_5Cl_9(L)_3(CH_3O)_2(OH)_2(H_2O)_6]^-$ (cal.1852.58)	0.003	0.013	0.011	0.013	0.015	0	0
1980.41	$[Dy_6Cl_{10}(L)_3(OH)_5(CH_3O)(H_2O)]^-$ (cal.1980.41)	0	0.005	0.006	0.006	0.010	0.005	0
2025.45	$[Dy_6Cl_{10}(L)_3(OH)_5(CH_3O)(CH_3OH)_2]^-$ (cal.12025.45)	0	0.003	0.004	0.005	0.003	0.001	0
2058.48	$[Dy_6Cl_{10}(L)_3(OH)_5(CH_3O)(CH_3OH)_3]^-$ (cal.2058.48)	0	0.002	0.003	0.002	0.002	0	0



$[DyCl_4]^+$
(cal. 305.80)
$[DyCl_4(CH_3OH)_2(DMF)]^-$
(cal. 440.89)
$[Dy(L)_2Cl_2]^-$
(cal. 577.95)
300 304 308
436 440 444
574.0 577.5 581.0
$[Dy_2(L)Cl_7Na]^-$
(cal. 767.67)
$[Dy_2(L)Cl_7(CH_3CN)K]^+$
(cal. 826.66)
$[Dy_2(L)Cl_7(CH_3OH)_3(H_2O)_2]^-$
(cal. 845.75)
762 768 774
822 828 834
840 846 852
$[Dy_2(L)Cl_7(CH_3OH)_2(H_2O)_4Na]^-$
(cal. 904.76)
$[Dy_2(L)(HL)Cl_6(CH_3OH)_2(H_2O)_2]^-$
(cal. 982.83)
$[Dy_2(L)_3Cl_5Na]^-$
(cal. 1041.81)
900 905 910
980 984 988
1036.8 1042.2 1047.6
$[Dy_3(L)_2Cl_9Na]^-$
(cal. 1173.57)
$[Dy_3(L)_3Cl_7]^-$
(cal. 1251.68)
$[Dy_3(L)_3Cl_8Na]^-$
(cal. 1309.64)
1170 1175 1180
1244.4 1251.2 1258.0
1305 1310 1315

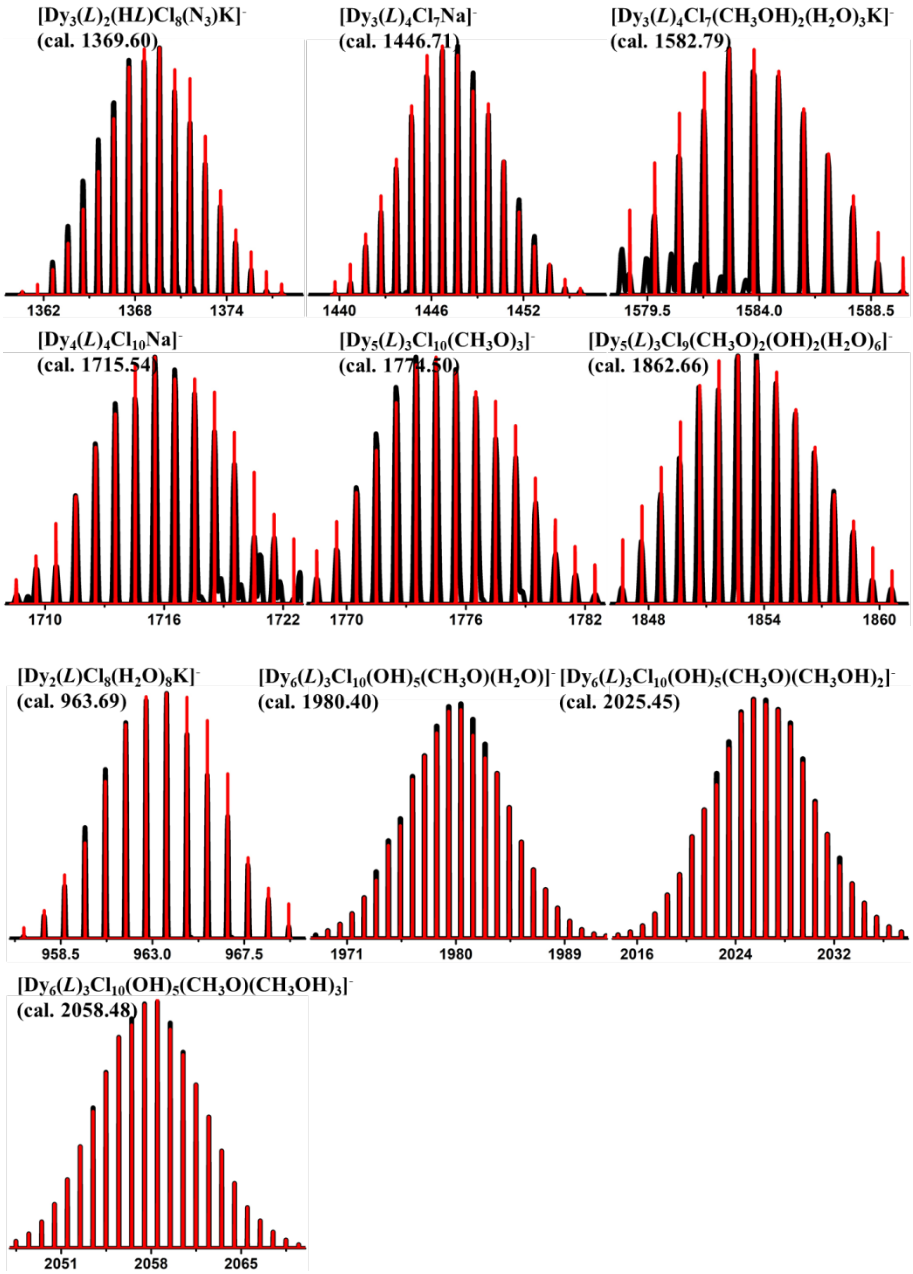


Figure S7. The superposed simulated and observed spectra of several species in the Time-dependent ESI-MS of **Dy12**.

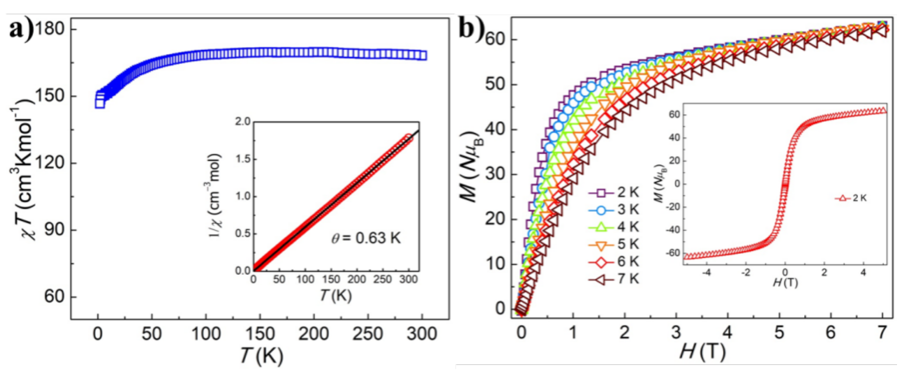


Figure S8. Temperature dependence of $\chi_m T$ (a) and field dependence of the magnetization (b) for **Dy12**.

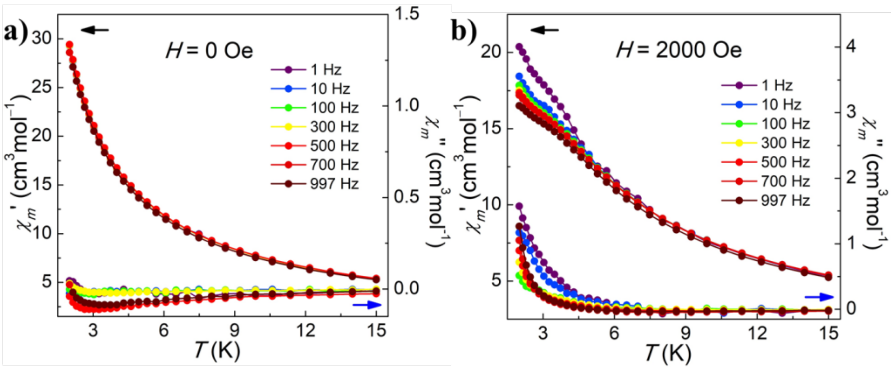


Figure S9. The temperature dependence of the in-phase (χ') and out-of-phase (χ'') ac-susceptibilities for different frequencies in 0 (a) and 2000 Oe (b) dc-field for **Dy12**.

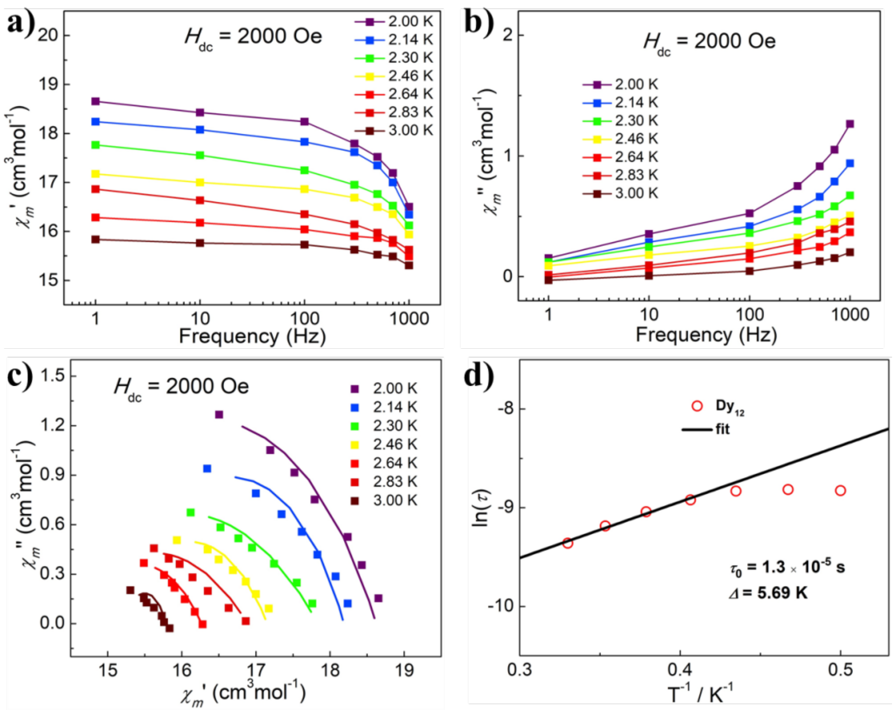


Figure S10. Variable-frequency dependent ac susceptibilities for **Dy12** under 2000 Oe (a and b) dc-field; c) Cole–Cole plots from ac susceptibilities; d) Arrhenius plots generated from the temperature-dependent relaxation times extracted from the ac-susceptibilities Cole-Cole fits in H_{dc} = 2000 Oe, The symbols and lines represent the extracted times and least-square fits.

Table S13. Selected parameters from the fitting results of the Cole-Cole plots for **Dy12** under 2000 Oe dc-field.

	H_{dc}=2000 Oe

T (K)	τ	α	residual
2.00	1.47E-04	3.60E-01	2.43E-01
2.14	1.48E-04	4.23E-01	3.02E-01
2.30	1.46E-04	5.49E-01	3.08E-01
2.46	1.33E-04	5.60E-01	4.15E-01
2.64	1.18E-04	4.82E-01	5.02E-02
2.83	1.03E-04	5.82E-01	5.81E-02
3.03	8.62E-05	2.69E-01	5.41E-02