

Electronic supporting Information

A new family of high nuclearity Co^{II}/Dy^{III} coordination clusters possessing robust and unseen topologies

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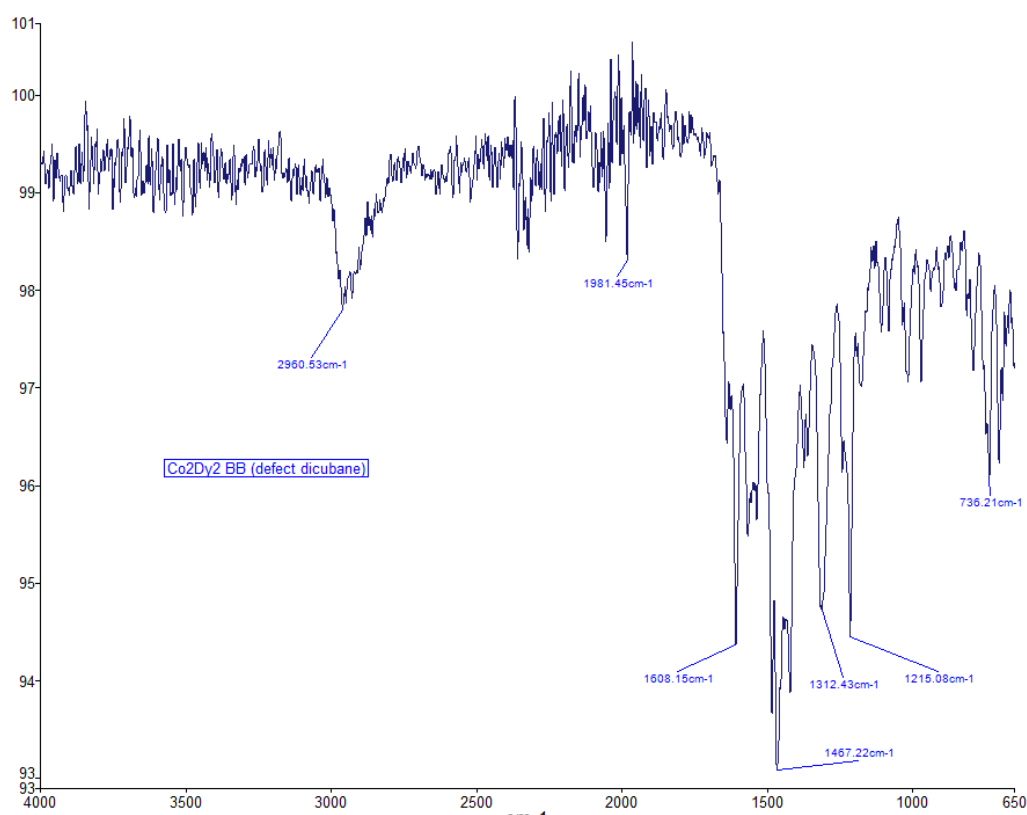


Fig S1. IR of **3**

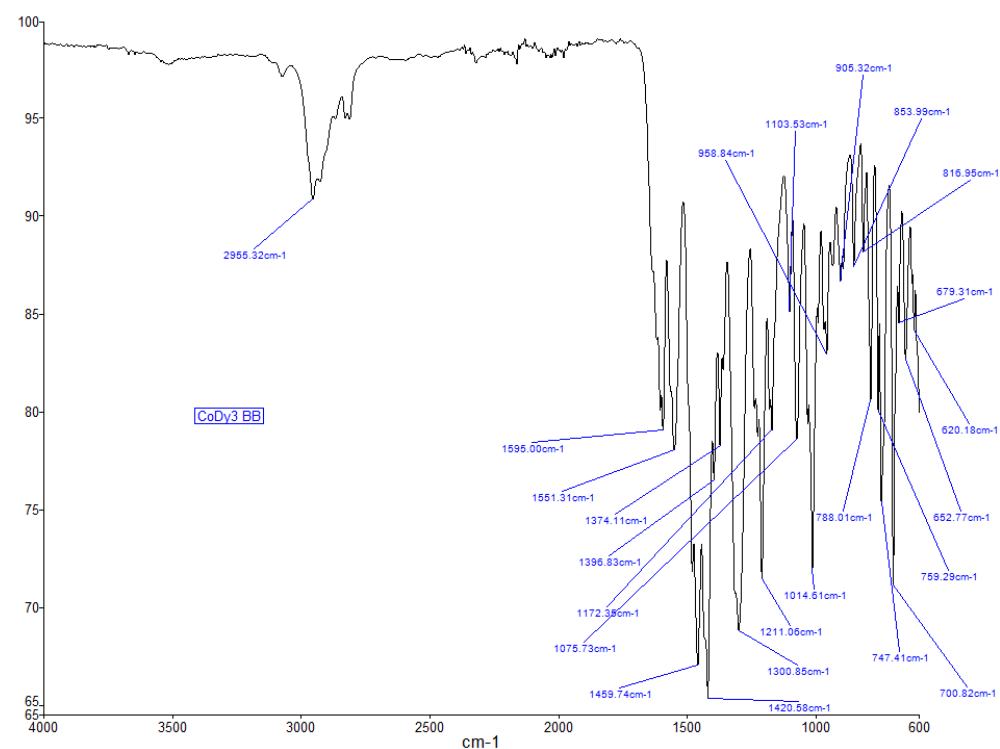


Fig S2. IR of 4

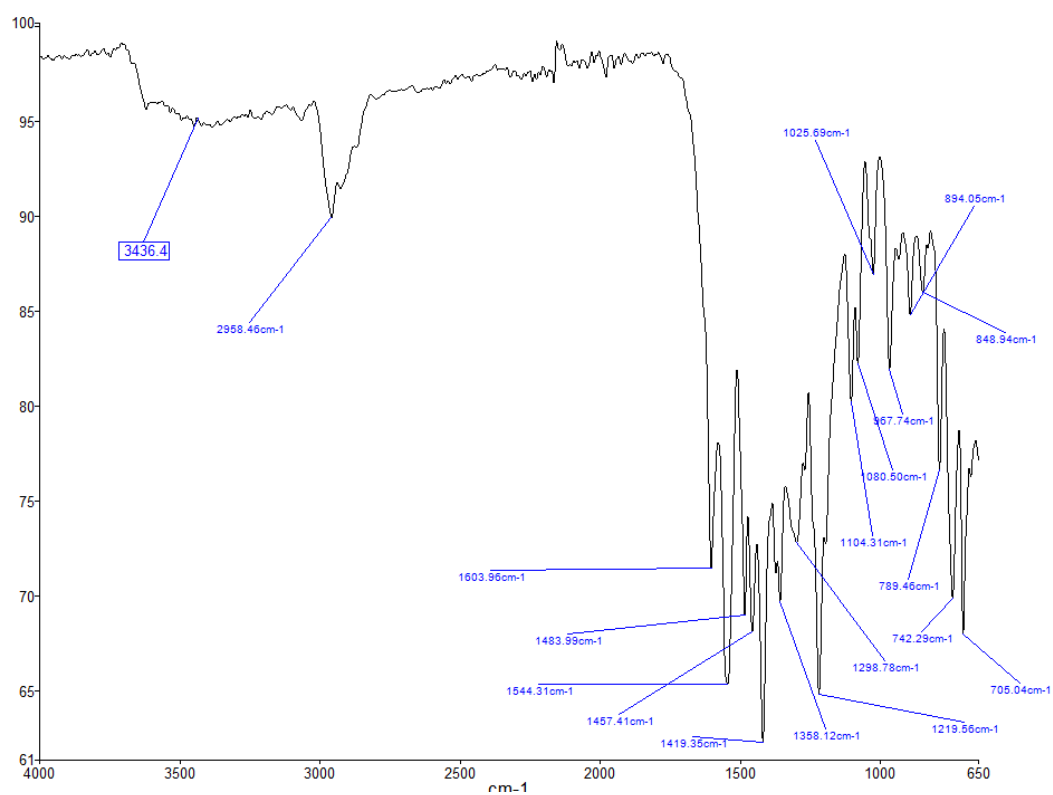


Fig S3. IR of 6

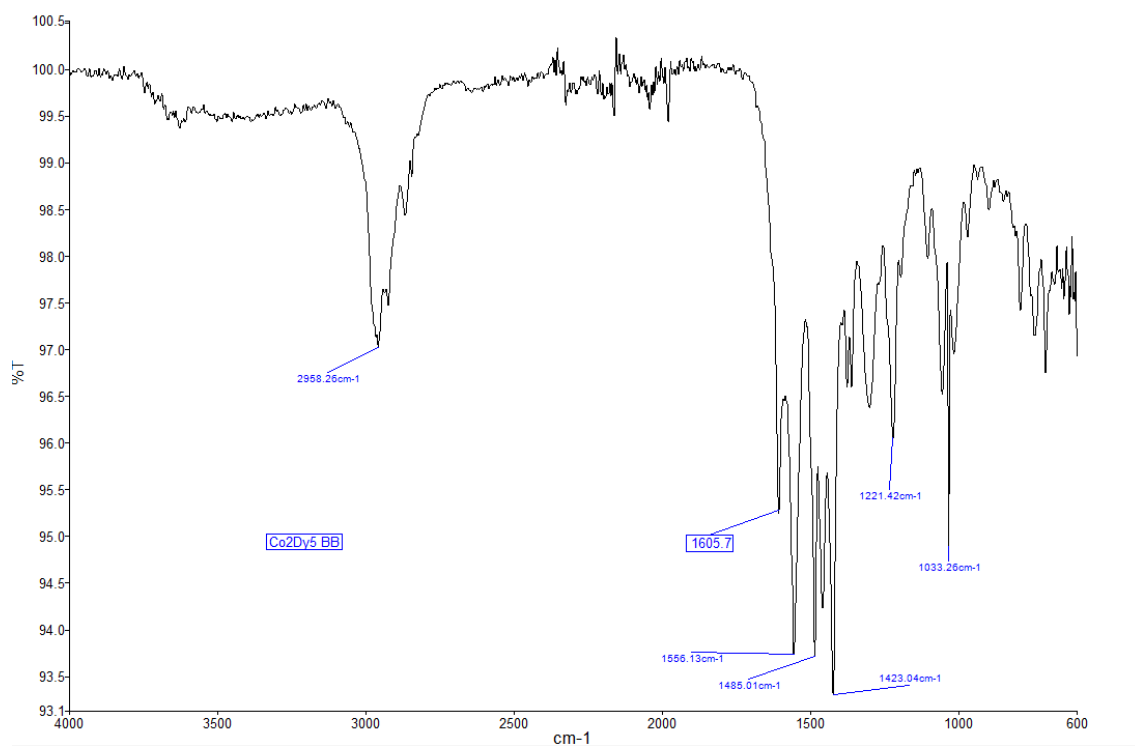


Fig S4. IR of **7**

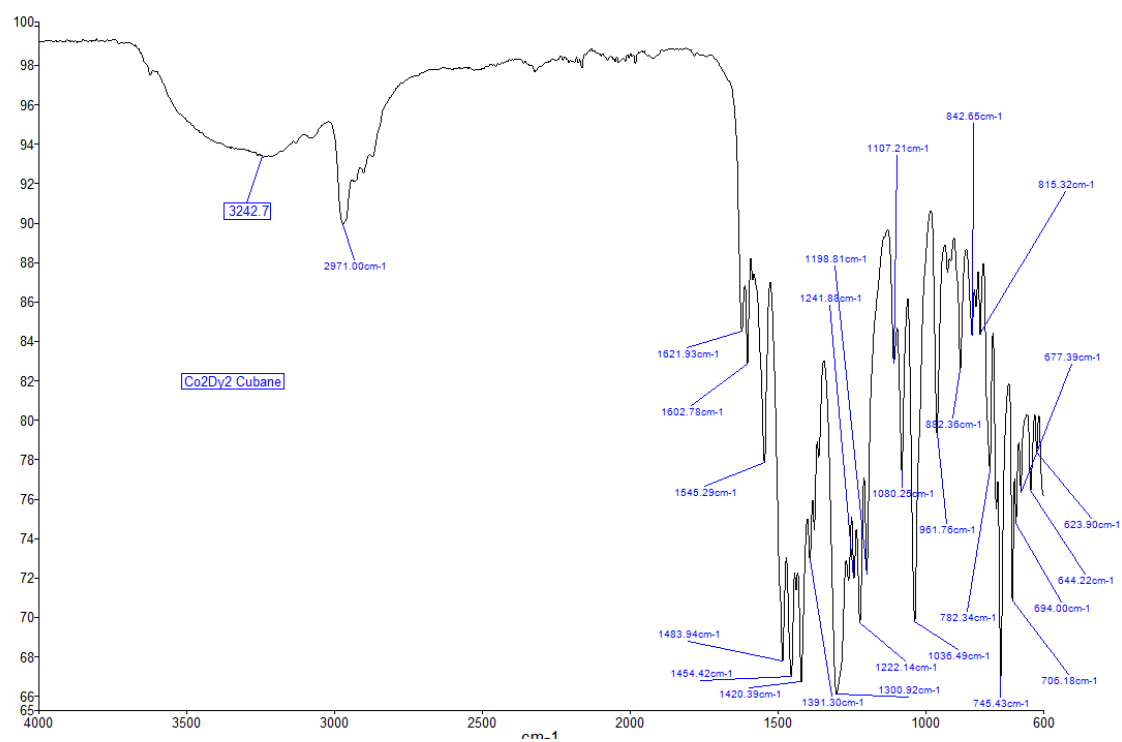


Fig S5. IR of **8**

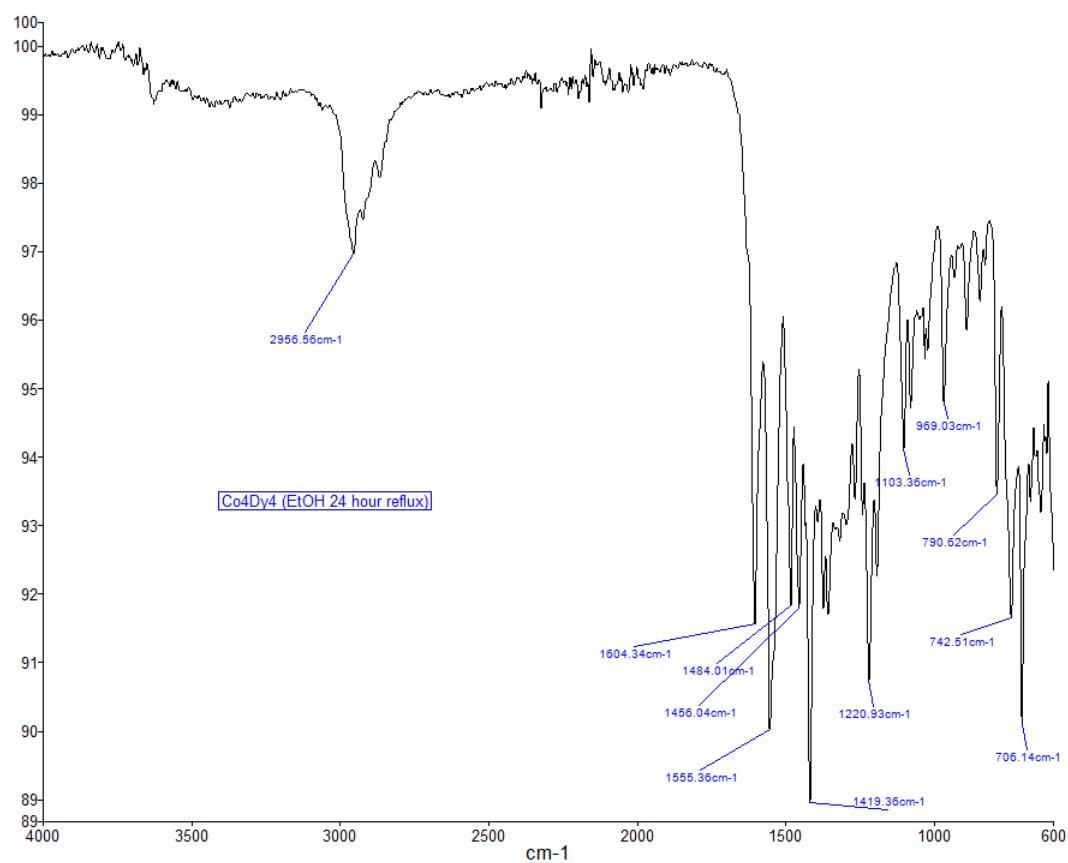


Fig S6. IR of **9**

W7D5 3BB

BEN4538 35 (0.667) Cm (30:37)

1: TOF MS ES+
1.10e4

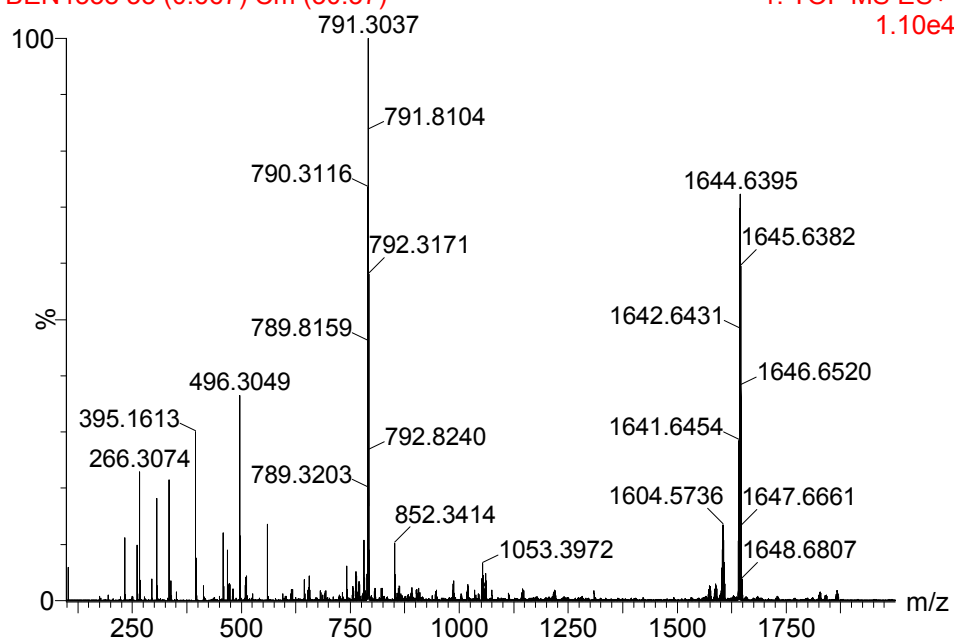


Fig S7. ESI-MS of **3**

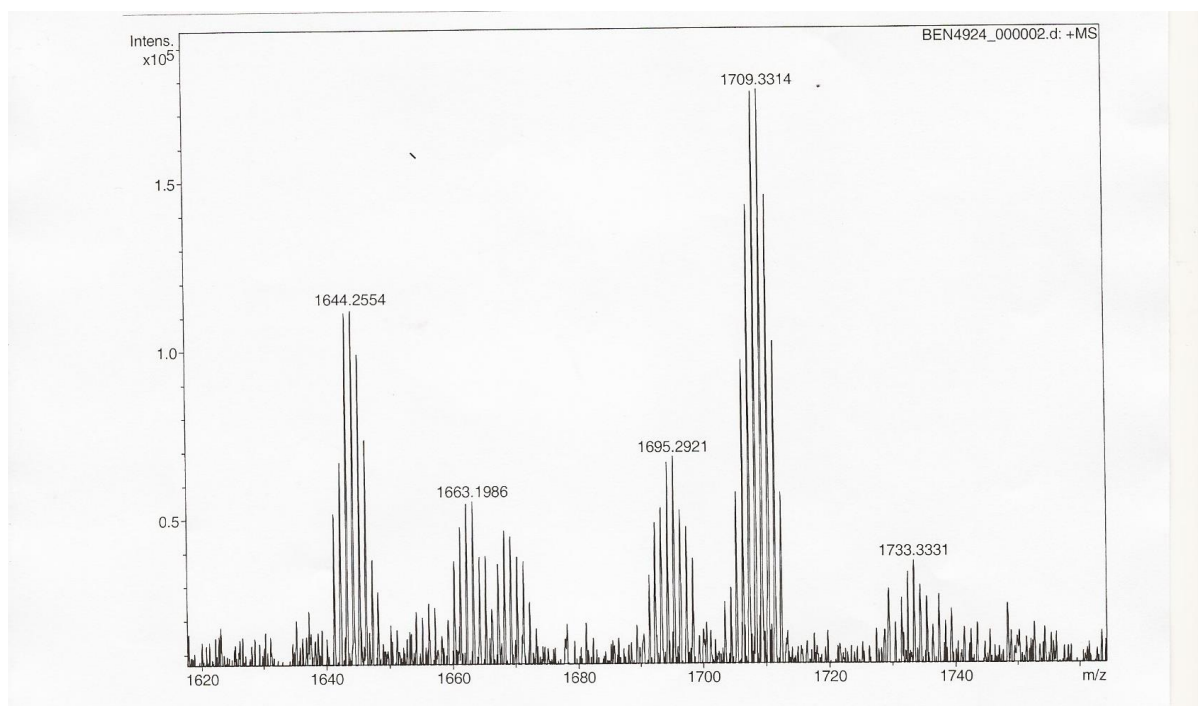
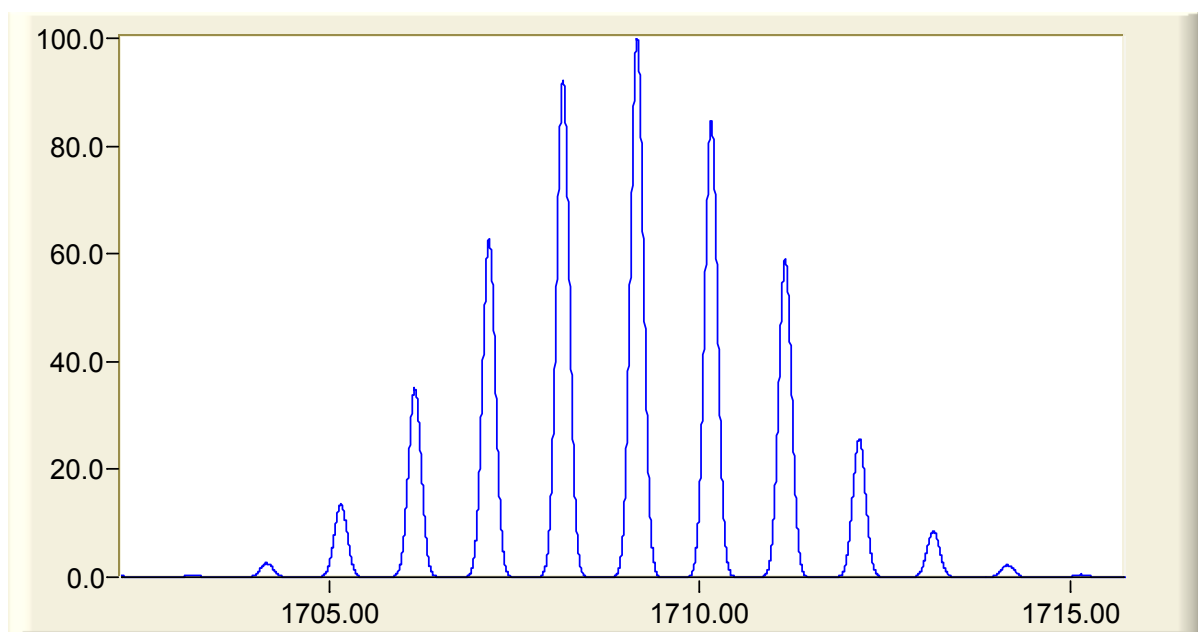


Fig S8. ESI-MS of **8**



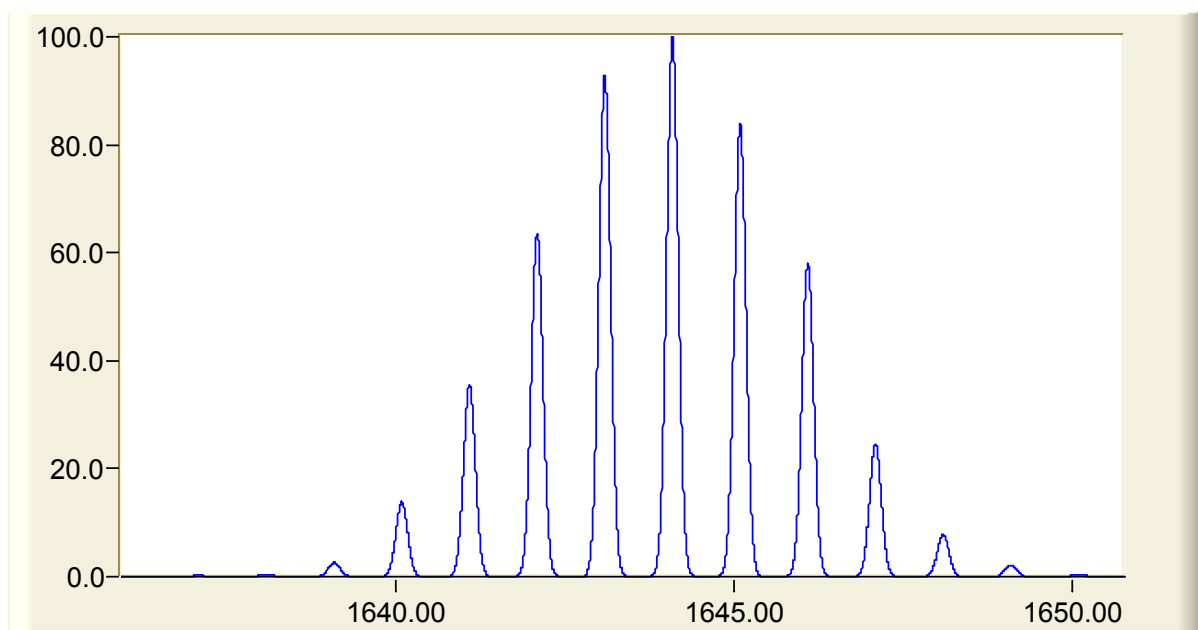


Fig S8. ESI-MS of **8** (upper), Isotopic distribution for the two fragments $[\text{Co}^{\text{II}}_2\text{Dy}^{\text{III}}_2(\text{OH})_2(\text{L})_2(\text{piv})_2(\text{NO}_3)_4(\text{EtOH})_2(\text{H}_2\text{O})] + \text{H}^+$ (center) and $[\text{Co}^{\text{II}}_2\text{Dy}^{\text{III}}_2(\text{OH})_2(\text{L})_2(\text{piv})_2(\text{NO}_3)_4(\text{EtOH})]^+$ (lower)

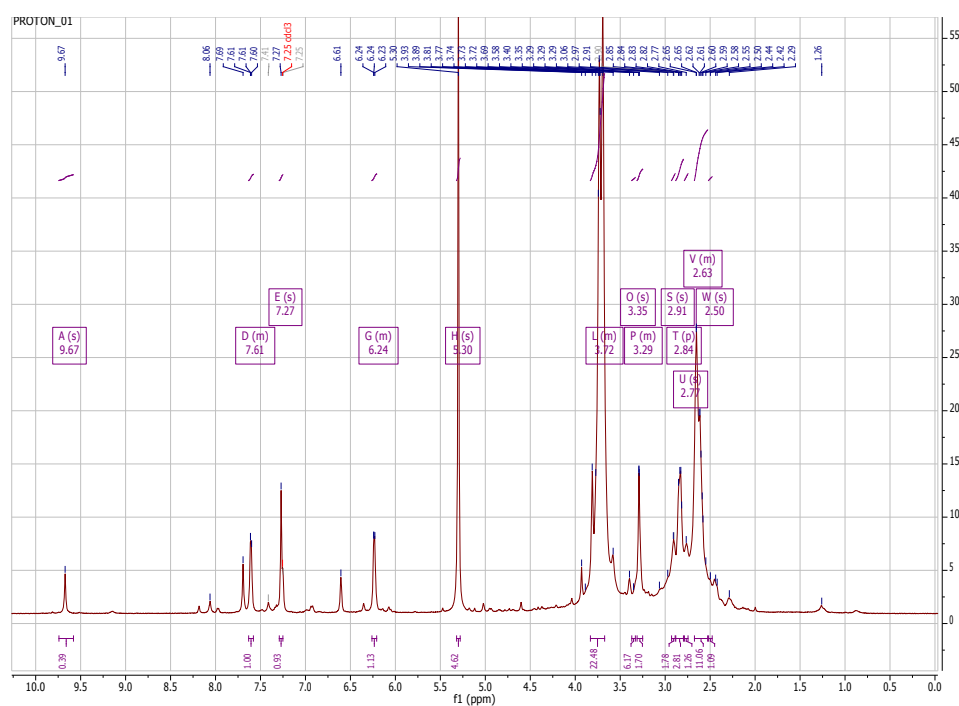


Fig S9. ^1H -NMR of reaction studied. Loading 2.5% of **3** for 2h. Similar patterns were observed for the other reactions.

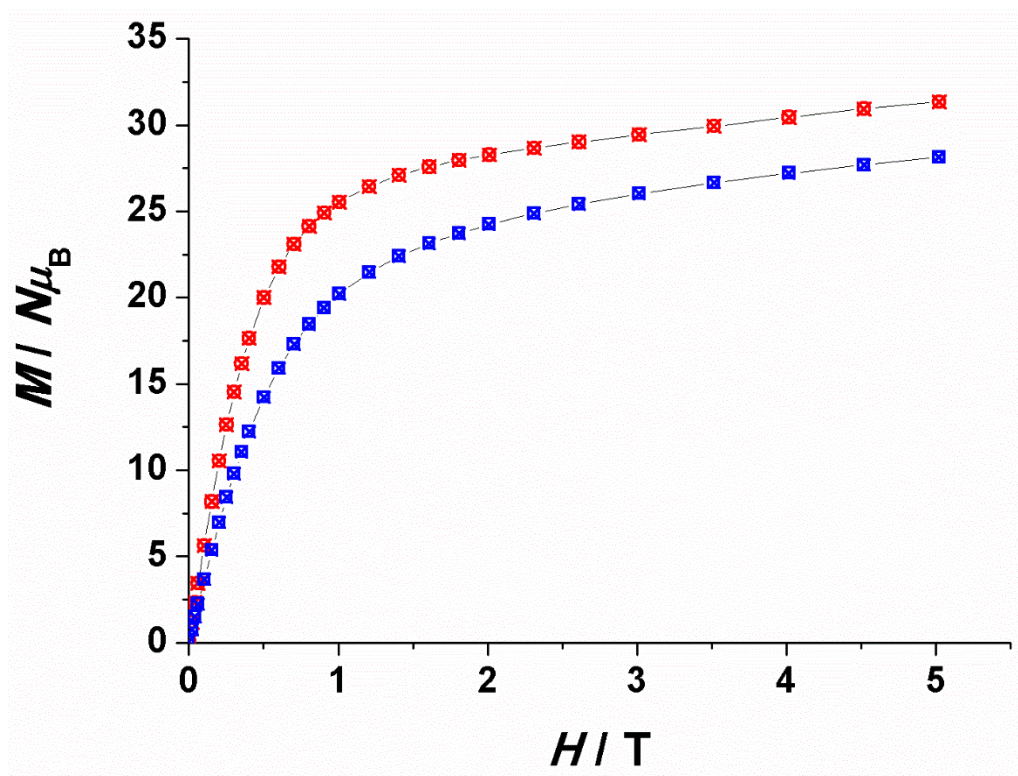


Fig. S10. Magnetization plot for **6** (blue) and **7** (red)

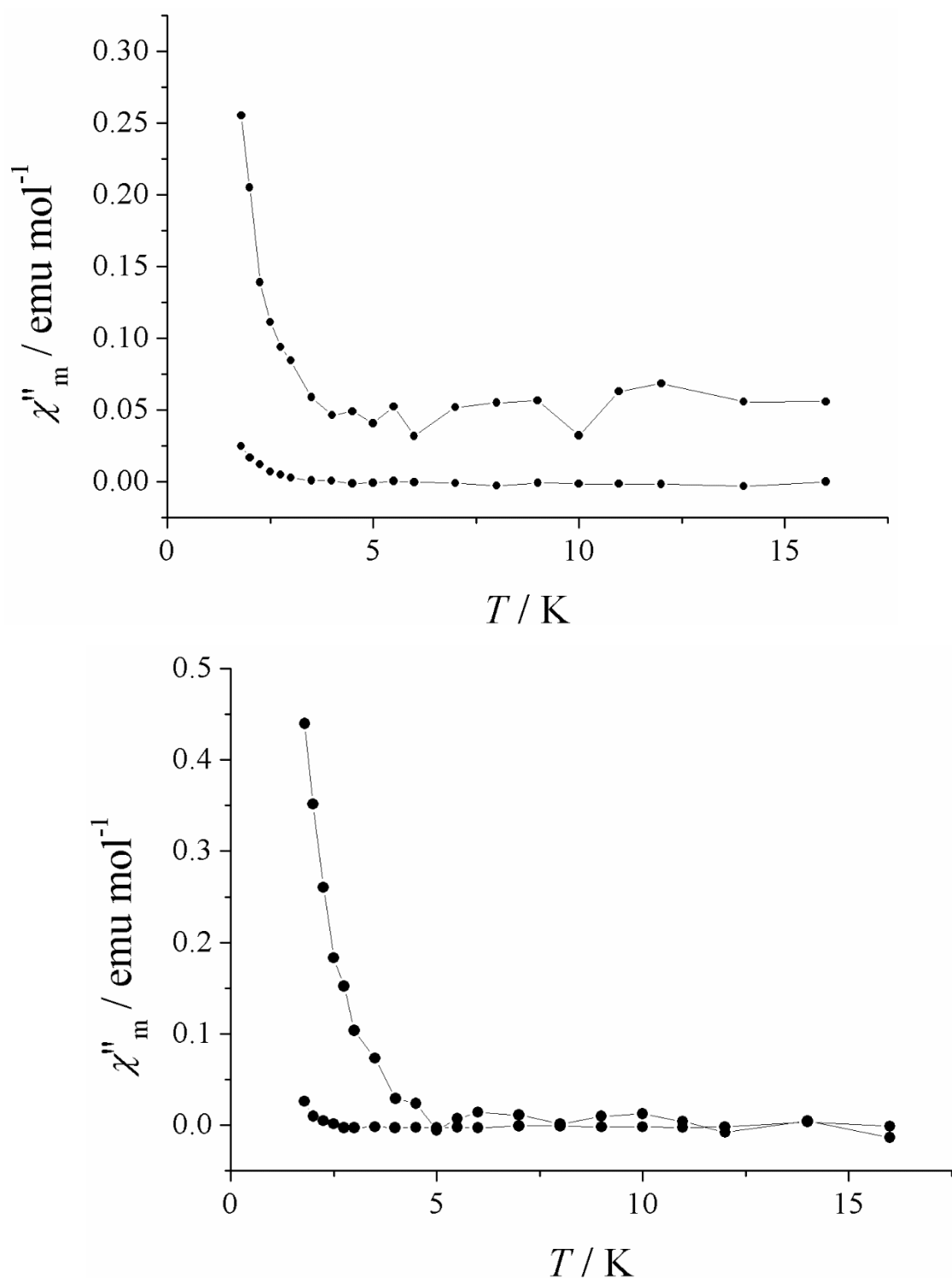


Fig. S11. χ''_m / T under dc field and a 4 G ac field oscillating at 1000 and 10 Hz for **6** (above) and **7** (below)

Table S1. Crystallographic parameters for compounds **3 – 9**.

Crystal	3	4	5	6
Empirical Formula	C ₁₂₃ H ₁₇₂ Co ₄ Dy ₄ N ₁₆ O ₄₈	C ₅₄ H ₇₄ CoDy ₃ N ₉ O ₂₅	C ₃₁₀ H ₄₀₄ Co ₁₀ Dy ₁₃ N ₃₃ O ₁₀₅	C ₁₂₀ H ₁₅₄ Co ₄ Dy ₄ N ₁₄ O ₃₄
Formula wt/ g mol ⁻¹	3528.48	1795.65	8974.44	3222.28
Crystal System,	triclinic	monoclinic	triclinic	hexagonal
space group	P -1	C2/c	P -1	P6/m
a/Å	14.0680(2)	17.0866(7)	13.7063(10)	27.7587(6)
b/Å	21.3940(3)	19.9394(7)	25.9590(18)	27.7587(6)
c/Å	26.2804(4)	20.2635(9)	32.551(2)	22.5433(9)
α/°	67.4228(15)	90	73.030(2)	90
β/°	86.9557(13)	109.693(5)	88.444(3)	90
γ/°	89.2403(12)	90	89.026(3)	120
Vol/Å ³	7292.9(2)	6499.9(5)	11072.7(14)	15043.4(9)
Z, Calc density (Mgm ⁻³)	2, 1.607	4, 1.835	1, 1.346	3, 1.067
Abs coeff (mm ⁻¹)	2.551	3.746	2.594	1.845
F(000)	3556	3544	4463	4848
Crystal	Orange plate	Orange plate	Orange needle	Orange plate
Crystal Dimensions/ mm ³	0.11x0.11x0.01	0.26x0.14x0.08	0.16x0.02x0.01	0.05x0.03x0.01
θ range (°)	27.5	26.0	25.242	26.0
No. of reflections collected	117090	16618	156032	108985
R _{int}	0.0498	0.0300	0.1105	0.1782
No. of data/restraints/parameters	36189/32/1666	7502/0/427	44922/58/2116	10477/0/375
Final R indices [<i>F</i> ² > 2σ(<i>F</i> ²)] : R ₁ , wR ₂	0.0838, 0.1858	0.0327, 0.0705	0.0760, 0.1931	0.0580, 0.1401
R indices (all data) : R ₁ , wR ₂	0.1027, 0.1945	0.0438, 0.0759	0.1111, 0.2120	0.1002, 0.1533
Largest diff. peak and hole/e Å ⁻³	6.752, -4.744	1.465, -0.946	2.661, -2.277	1.045, -0.684

Table S1. Crystallographic parameters for compounds **3 – 9** (continued).

Crystal	7	8	8'	9
Empirical Formula	C ₉ H ₁₂₉ Co ₂ DyN ₁₀ O ₃₇	C ₅₂ H ₇₂ Co ₂ Dy ₂ N ₁₀ O ₂₈	C ₅₄ H ₇₈ Co ₂ Dy ₂ N ₁₀ O ₂₉	C ₁₁₆ H ₁₆₀ Co ₄ Dy ₄ N ₁₂ O ₃₄
Formula wt/ g mol ⁻¹	2897.40	1728.05	1774.12	3152.27
Crystal System,	orthorhombic	monoclinic	monoclinic	hexagonal
space group	Pbca	C2/c	P2/n	P6/m
a/Å	28.3983(4)	24.6279(17)	24.026(3)	27.6952(19)
b/Å	17.1091(3)	12.2953(5)	12.2884(14)	27.6952(19)
c/Å	23.8614(6)	26.851(2)	26.741(3)	22.6753(16)
α/°	90	90	90	90
β/°	90	115.817(9)	116.1429(18)	90
γ/°	90	90	90	120
Vol/Å ³	11593.6(4)	7319.1(9)	7087.5(15)	15062(2)
Z, Calc density (Mgm ⁻³)	4, 1.660	4, 1.568	4, 1.663	3, 1.043
Abs coeff (mm ⁻¹)	3.538	2.545	2.632	1.841
F(000)	5724	3456	3560	4752
Crystal	Orange block	Orange block	Orange block	Orange plate
Crystal Dimensions/ mm ³	0.10x0.07x0.02	0.21x0.14x0.10	0.07x0.06x0.04	0.13x0.13x0.03
θ range (°)	25.242	26.0	25.242	25.242
No. of reflections collected	150674	21059	85427	103612
R _{int}	0.1091	0.0453	0.0849	0.0537
No. of data/restraints/parameters	13272/711/1593	8459/21/435	16099/8/869	10422/878/392
Final R indices [<i>F</i> ² > 2σ(<i>F</i> ²)] : R ₁ , wR ₂	0.0911, 0.2129	0.0505, 0.1226	0.0578, 0.1556	0.0378, 0.1073
R indices (all data) : R ₁ , wR ₂	0.1005, 0.2165	0.0739, 0.1348	0.0625, 0.1608	0.0469, 0.1118
Largest diff. peak and hole/e Å ⁻³	3.679, -1.425	1.565, -0.988	3.378, -2.919	0.897, -0.359