Supporting Information

An Cobalt Complex with 2,4,6-Tris(di-2-pyridy;amine)-1,3,5-triazine: Antiferromagnetic Couple Governed Single-molecule-magnet Behaviour

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Content

Table S1. Crystallographic data and structural refinement parameters for complexes **1**.

	Co_2
Formula	$C_{66}H_{68}Co_2N_{24}O_{26}Cl_4$
f w	1873.10
T / K	193(2)
λ / Å	1.34139
Crystal system	Monoclinic
Space group	$P2_1/n$
a / Å	13.483(3)
b / Å	14.312(3)
c / Å	20.482(4)
α / º	90
β / º	101.02
γ / º	90
V / Å^3	3879.5(15)
Z	2
D_c / g cm^{-3}	1.604
μ / mm^{-1}	3.680
F(000)	1924
θ / °	3.158 to 53.982
Reflns collected	65724
Reflns unique	7070
R_{int}	0.0917
GOF on F^2	1.049
R_1 [I> 2σ(I)][a]	0.0467
wR_2 [I>2σ(I))][b]	0.1106
R_1 (all data)[a]	0.0654
wR_2 (all data)[b]	0.1249
Largest diff. Peak, hole / (e Å^{-3})	0.722 and -0.777

[a]$R_1 = \Sigma$ ||Fo| – |Fc||/Σ|Fo|; [b]$wR_2 = [\Sigma w(Fo^2 - Fc^2)^2/\Sigma w(Fo^2)^2]^{½}$.

Table S2. Bond lengths [A] and angles [deg] for **1**.

Co(1)-N(11)	2.120(3)	N(7)-C(14)	1.435(4)
Co(1)-O(2)	2.122(2)	N(4)-C(1)	1.381(4)
Co(1)-N(8)A	2.132(3)	N(4)-C(9)	1.421(4)
Co(1)-N(12)	2.133(2)	N(4)-C(4)	1.440(4)
Co(1)-N(9)A	2.148(3)	N(6)-C(9)	1.331(4)
Co(1)-O(1)	2.155(2)	N(6)-C(13)	1.347(4)
Cl(2)-O(8)	1.393(4)	N(5)-C(4)	1.326(4)
Cl(2)-O(9)	1.401(4)	N(5)-C(8)	1.346(4)
Cl(2)-O(7)	1.418(3)	C(24)-C(25)	1.383(4)
Cl(2)-O(10)	1.425(3)	C(29)-C(30)	1.381(4)
Cl(1)-O(3)	1.393(4)	C(19)-C(20)	1.380(4)
Cl(1)-O(6)	1.408(3)	C(4)-C(5)	1.377(4)
Cl(1)-O(4)	1.408(3)	C(20)-C(21)	1.380(4)
Cl(1)-O(5)	1.413(4)	C(14)-C(15)	1.382(4)
N(8)-C(14)	1.338(4)	C(9)-C(10)	1.391(4)
N(8)-C(18)	1.347(4)	C(33)-C(32)	1.375(5)
N(10)-C(3)	1.393(4)	C(23)-C(22)	1.374(5)
N(10)-C(29)	1.432(4)	C(25)-C(26)	1.383(5)
N(10)-C(24)	1.441(4)	C(18)-C(17)	1.372(5)
N(11)-C(24)	1.336(4)	C(30)-C(31)	1.379(5)
N(11)-C(28)	1.356(4)	C(5)-C(6)	1.382(5)
N(2)-C(3)	1.331(4)	C(16)-C(15)	1.390(5)
N(2)-C(2)	1.344(4)	C(16)-C(17)	1.390(5)
N(9)-C(19)	1.340(4)	C(22)-C(21)	1.381(5)
N(9)-C(23)	1.354(4)	C(32)-C(31)	1.381(5)
N(12)-C(29)	1.343(4)	C(28)-C(27)	1.371(5)
N(12)-C(33)	1.351(4)	C(6)-C(7)	1.378(5)
N(1)-C(2)	1.324(4)	C(13)-C(12)	1.367(5)
N(1)-C(1)	1.329(4)	C(10)-C(11)	1.382(5)
N(3)-C(3)	1.332(4)	C(11)-C(12)	1.383(5)
N(3)-C(1)	1.341(4)	C(27)-C(26)	1.385(5)
N(7)-C(2)	1.383(4)	C(7)-C(8)	1.371(5)
N(7)-C(19)	1.432(4)		
N(11)-Co(1)-O(2)	90.00(9)	C(4)-N(5)-C(8)	116.5(3)
N(11)-Co(1)-N(8)A	178.29(10)	N(11)-C(24)-C(25)	123.1(3)
O(2)-Co(1)-N(8)A	91.68(9)	N(11)-C(24)-N(10)	117.1(3)
N(11)-Co(1)-N(12)	87.24(10)	C(25)-C(24)-N(10)	119.8(3)
O(2)-Co(1)-N(12)	87.31(9)	N(12)-C(29)-C(30)	122.5(3)
N(8)A-Co(1)-N(12)	92.51(10)	N(12)-C(29)-N(10)	115.7(3)
N(11)-Co(1)-N(9)A	91.75(10)	C(30)-C(29)-N(10)	121.7(3)
O(2)-Co(1)-N(9)A	171.72(9)	N(9)-C(19)-C(20)	123.8(3)
N(8)A-Co(1)-N(9)A	86.63(10)	N(9)-C(19)-N(7)	115.2(3)

N(12)-Co(1)-N(9)A	100.86(9)	C(20)-C(19)-N(7)	121.0(3)
N(11)-Co(1)-O(1)	92.07(9)	N(1)-C(1)-N(3)	126.1(3)
O(2)-Co(1)-O(1)	85.33(9)	N(1)-C(1)-N(4)	118.5(3)
N(8)A-Co(1)-O(1)	88.39(9)	N(3)-C(1)-N(4)	115.5(3)
N(12)-Co(1)-O(1)	172.61(9)	N(5)-C(4)-C(5)	124.3(3)
N(9)A-Co(1)-O(1)	86.52(9)	N(5)-C(4)-N(4)	115.0(3)
O(8)-Cl(2)-O(9)	108.6(3)	C(5)-C(4)-N(4)	120.7(3)
O(8)-Cl(2)-O(7)	111.6(3)	C(19)-C(20)-C(21)	118.6(3)
O(9)-Cl(2)-O(7)	107.7(3)	N(8)-C(14)-C(15)	123.3(3)
O(8)-Cl(2)-O(10)	110.1(2)	N(8)-C(14)-N(7)	115.6(3)
O(9)-Cl(2)-O(10)	108.7(2)	C(15)-C(14)-N(7)	121.0(3)
O(7)-Cl(2)-O(10)	109.9(2)	N(2)-C(3)-N(3)	126.9(3)
O(3)-Cl(1)-O(6)	112.1(3)	N(2)-C(3)-N(10)	118.3(3)
O(3)-Cl(1)-O(4)	110.6(3)	N(3)-C(3)-N(10)	114.8(3)
O(6)-Cl(1)-O(4)	108.3(2)	N(6)-C(9)-C(10)	122.9(3)
O(3)-Cl(1)-O(5)	105.3(3)	N(6)-C(9)-N(4)	115.4(3)
O(6)-Cl(1)-O(5)	111.2(3)	C(10)-C(9)-N(4)	121.7(3)
O(4)-Cl(1)-O(5)	109.3(3)	N(1)-C(2)-N(2)	127.3(3)
C(14)-N(8)-C(18)	117.7(3)	N(1)-C(2)-N(7)	115.5(3)
C(14)-N(8)-Co(1)A	119.65(19)	N(2)-C(2)-N(7)	117.1(3)
C(18)-N(8)-Co(1)A	122.6(2)	N(12)-C(33)-C(32)	123.4(3)
C(3)-N(10)-C(29)	121.9(2)	N(9)-C(23)-C(22)	122.8(3)
C(3)-N(10)-C(24)	117.6(2)	C(24)-C(25)-C(26)	118.4(3)
C(29)-N(10)-C(24)	118.8(2)	N(8)-C(18)-C(17)	123.1(3)
C(24)-N(11)-C(28)	117.5(3)	C(31)-C(30)-C(29)	118.9(3)
C(24)-N(11)-Co(1)	122.3(2)	C(4)-C(5)-C(6)	117.9(3)
C(28)-N(11)-Co(1)	119.9(2)	C(15)-C(16)-C(17)	119.1(3)
C(3)-N(2)-C(2)	112.3(3)	C(14)-C(15)-C(16)	118.2(3)
C(19)-N(9)-C(23)	116.8(3)	C(23)-C(22)-C(21)	119.5(3)
C(19)-N(9)-Co(1)A	119.24(19)	C(33)-C(32)-C(31)	118.2(3)
C(23)-N(9)-Co(1)A	122.9(2)	N(11)-C(28)-C(27)	123.1(3)
C(29)-N(12)-C(33)	117.4(3)	C(7)-C(6)-C(5)	119.2(3)
C(29)-N(12)-Co(1)	122.64(19)	C(20)-C(21)-C(22)	118.6(3)
C(33)-N(12)-Co(1)	119.1(2)	N(6)-C(13)-C(12)	123.4(3)
C(2)-N(1)-C(1)	113.5(3)	C(11)-C(10)-C(9)	118.0(3)
C(3)-N(3)-C(1)	113.6(2)	C(10)-C(11)-C(12)	119.4(3)
C(2)-N(7)-C(19)	121.3(2)	C(28)-C(27)-C(26)	118.4(3)
C(2)-N(7)-C(14)	120.4(2)	C(18)-C(17)-C(16)	118.6(3)
C(19)-N(7)-C(14)	117.3(2)	C(8)-C(7)-C(6)	118.3(3)
C(1)-N(4)-C(9)	123.0(2)	C(30)-C(31)-C(32)	119.4(3)
C(1)-N(4)-C(4)	117.0(2)	C(25)-C(26)-C(27)	119.5(3)
C(9)-N(4)-C(4)	119.6(2)	C(13)-C(12)-C(11)	118.4(3)
C(9)-N(6)-C(13)	117.4(3)	N(5)-C(8)-C(7)	123.7(3)

Table S3. The fit parameters obtained from analyses of the ac susceptibilities of **1** under 0.8 kOe bias dc field.

T / K	χ_T/cm^3 mol^{-1}	χ_S /cm^3 mol^{-1}	ln(τ / s)	a	R^2
1.8	1.84E+00	2.01E-01	-9.28893	9.45E-02	4.60E-03
1.9	1.76E+00	1.81E-01	-9.4279	1.06E-01	5.20E-04
2	1.67E+00	1.76E-01	-9.56709	1.01E-01	6.01E-04
2.1	1.59E+00	1.71E-01	-9.69883	9.49E-02	1.03E-03
2.2	1.53E+00	1.64E-01	-9.80241	1.01E-01	6.43E-04
2.4	1.41E+00	1.57E-01	-10.0145	9.50E-02	5.88E-04
2.6	1.31E+00	1.59E-01	-10.1894	8.74E-02	4.67E-04
2.8	1.22E+00	1.64E-01	-10.3429	7.80E-02	5.02E-04
3	1.14E+00	1.51E-01	-10.5037	7.79E-02	5.00E-04
3.2	1.07E+00	1.55E-01	-10.6254	7.25E-02	3.44E-04
3.4	1.01E+00	1.55E-01	-10.7591	6.52E-02	2.86E-04
3.6	9.57E-01	1.55E-01	-10.8688	6.25E-02	1.57E-04
3.8	9.10E-01	1.37E-01	-10.9587	7.05E-02	1.23E-04
4	8.64E-01	1.55E-01	-11.0457	5.04E-02	1.34E-04
4.2	8.24E-01	1.46E-01	-11.1355	5.29E-02	1.40E-04

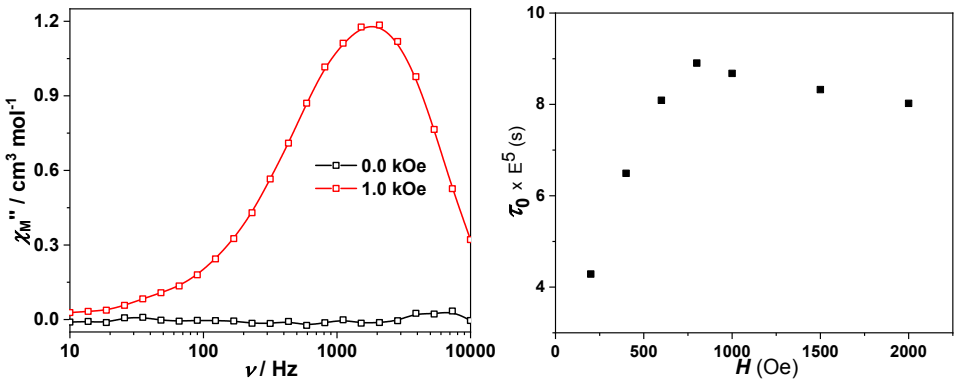

Figure S1. Left: Isothermal field sweep measurement performed on polycrystalline sample of complex **1**. Right: The plots τ_0 *vs.* H for complex **1**.

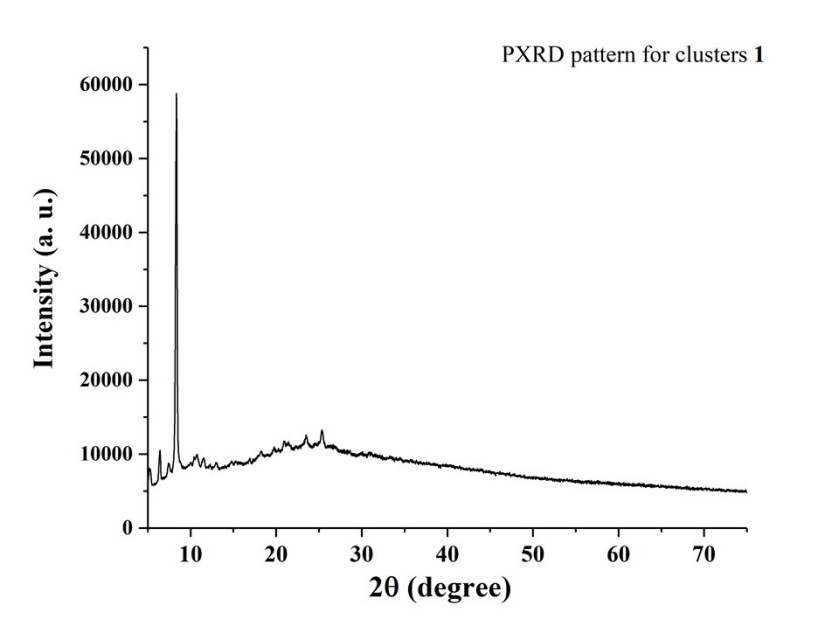

Figure S2. PXRD pattern for cluster **1**.

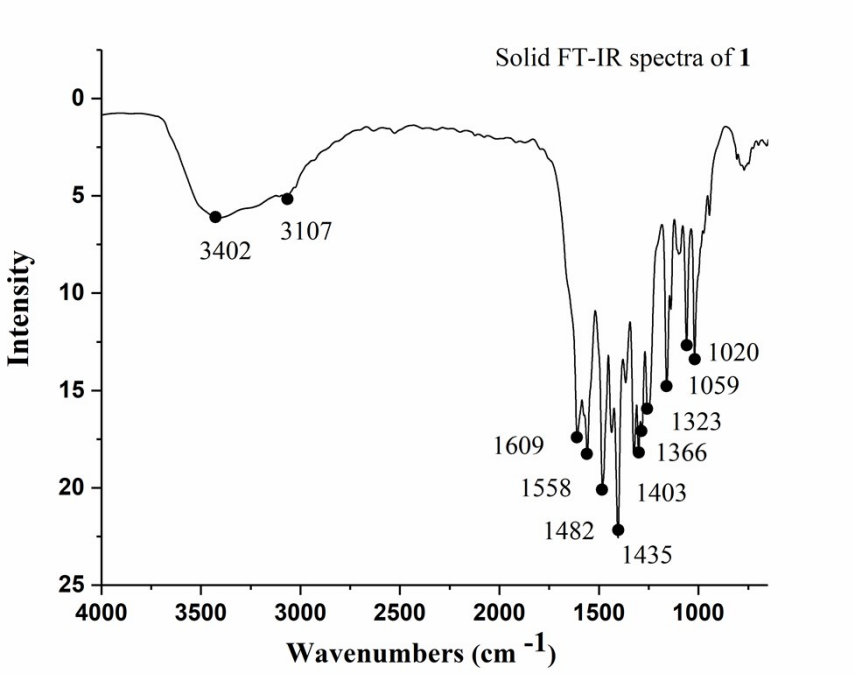

Figure S3. ATR-FTIR spectra of cluster **1**.