

Supporting Information

Two Tetranuclear Butterfly Shaped Co(II) Complexes: Structure, Mass Spectrometric, and Magnetism

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Table S1. Correlative bond distances (Å) and angles (°) of **1** and **2**.

1					
Co3—O1	2.106 (6)	Co1—O3	1.954 (6)	Co4—O5	1.923 (6)
Co3—O6	2.087 (6)	Co1—O2	1.934 (6)	Co2—O1	2.099 (6)
Co3—O4	2.098 (6)	Co1—N2	2.058 (7)	Co2—O6	2.098 (6)
Co3—O3	2.068 (7)	Co4—Cl2	2.465 (6)	Co2—O2	2.072 (6)
Co3—N8	2.136 (7)	Co4—O6	2.288 (6)	Co2—N10	2.129 (7)
Co3—N6	2.110 (6)	Co4—O4	1.942 (6)	Co2—O5	2.085 (6)
Co1—Cl1	2.372 (4)	Co4—N12	2.043 (7)	Co2—N4	2.123 (8)
Co1—O1	2.271 (6)				
O1—Co3—N8	96.3 (2)	O2—Co1—O1	77.8 (2)	O2—Co2—O1	79.0 (2)
O1—Co3—N6	156.6 (3)	O2—Co1—O3	121.7 (3)	O2—Co2—O6	104.2 (3)
O6—Co3—O1	79.3 (2)	O2—Co1—N2	119.5 (3)	O2—Co2—N10	98.5 (3)
O6—Co3—O4	80.4 (2)	N2—Co1—Cl1	104.5 (2)	O2—Co2—O5	175.6 (3)
O6—Co3—N8	154.8 (2)	N2—Co1—O1	77.1 (3)	O2—Co2—N4	77.6 (3)
O6—Co3—N6	97.5 (3)	O6—Co4—Cl2	177.3 (2)	O5—Co2—O1	101.6 (3)
O4—Co3—O1	106.6 (2)	O4—Co4—Cl2	99.0 (2)	O5—Co2—O6	80.3 (2)
O4—Co3—N8	77.1 (3)	O4—Co4—O6	78.9 (2)	O5—Co2—N10	77.1 (3)
O4—Co3—N6	95.7 (3)	O4—Co4—N12	120.4 (3)	O5—Co2—N4	102.5 (3)
O3—Co3—O1	80.4 (2)	N12—Co4—Cl2	105.6 (3)	N4—Co2—N10	94.4 (3)
O3—Co3—O6	99.6 (3)	N12—Co4—O6	77.1 (3)	Co3—O1—Co1	93.7 (2)
O3—Co3—O4	172.8 (3)	O5—Co4—Cl2	100.6 (2)	Co2—O1—Co3	100.4 (2)
O3—Co3—N8	104.1 (3)	O5—Co4—O6	79.1 (2)	Co2—O1—Co1	93.5 (2)
O3—Co3—N6	77.2 (3)	O5—Co4—O4	120.3 (3)	Co3—O6—Co4	93.2 (2)
N6—Co3—N8	95.9 (3)	O5—Co4—N12	107.3 (3)	Co3—O6—Co2	101.1 (2)
O1—Co1—Cl1	177.78 (19)	O1—Co2—N10	99.3 (3)	Co2—O6—Co4	93.5 (2)
O3—Co1—Cl1	99.1 (2)	O1—Co2—N4	154.4 (3)	Co4—O4—Co3	103.9 (3)
O3—Co1—O1	78.9 (2)	O6—Co2—O1	79.2 (2)	Co1—O3—Co3	105.1 (3)
O3—Co1—N2	105.9 (3)	O6—Co2—N10	156.5 (3)	Co1—O2—Co2	105.3 (3)
O2—Co1—Cl1	102.5 (2)	O6—Co2—N4	96.5 (3)	Co4—O5—Co2	105.8 (3)
2					

Br1—Co2	2.515 (2)	Co1—O3 ⁱ	2.054 (9)	Co2—N2	2.025 (9)
Co1—O1	2.080 (7)	Co1—O2	2.123 (9)	Co2—O3	1.935 (8)
Co1—O1 ⁱ	2.119 (7)	Co1—N4	2.097 (9)	Co2—O2	1.954 (9)
Co1—N6 ⁱ	2.100 (9)	Co2—O1	2.278 (8)	O1—Co1 ⁱ	2.119 (7)
N6—Co1 ⁱ	2.100 (9)	O3—Co1 ⁱ	2.054 (9)		
O1—Co1—O1 ⁱ	79.1 (3)	O3 ⁱ —Co1—O2	175.7 (3)	O3—Co2—N2	117.7 (4)
O1—Co1—N6 ⁱ	94.5 (3)	O3 ⁱ —Co1—N4	98.9 (4)	O3—Co2—O2	119.4 (4)
O1—Co1—O2	80.1 (3)	N4—Co1—O1 ⁱ	96.1 (3)	O2—Co2—Br1	98.9 (3)
O1 ⁱ —Co1—O2	100.5 (3)	N4—Co1—N6 ⁱ	99.1 (4)	O2—Co2—O1	79.0 (3)
O1—Co1—N4	155.2 (4)	N4—Co1—O2	76.9 (4)	O2—Co2—N2	111.9 (4)
N6 ⁱ —Co1—O1 ⁱ	155.3 (4)	O1—Co2—Br1	177.39 (19)	Co1—O1—Co1 ⁱ	100.9 (3)
N6 ⁱ —Co1—O2	101.9 (4)	N2—Co2—Br1	103.9 (3)	Co1—O1—Co2	95.0 (3)
O3 ⁱ —Co1—O1 ⁱ	80.4 (3)	N2—Co2—O1	78.4 (3)	Co1 ⁱ —O1—Co2	92.5 (3)
O3 ⁱ —Co1—O1	104.2 (3)	O3—Co2—Br1	100.8 (3)	Co2—O3—Co1 ⁱ	105.6 (4)
O3 ⁱ —Co1—N6 ⁱ	78.1 (4)	O3—Co2—O1	79.0 (3)	Co2—O2—Co1	104.1 (3)

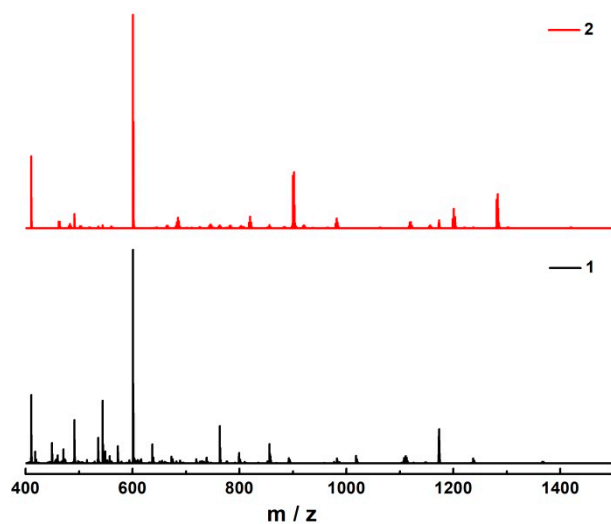
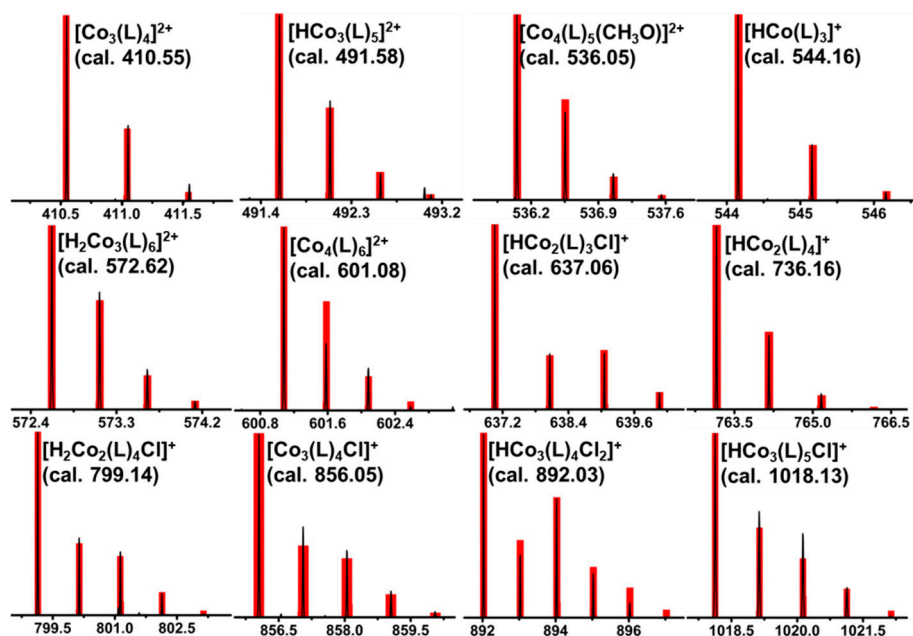


Figure S1. ESI-MS peaks of dissolved crystals of **1** and **2** in methanol.

Table S2. Major peaks distributed in the ESI-MS of **1** and **2** in positive mode.

1			
Peaks	Relative Intensity	Obs. <i>m/z</i>	Calc. <i>m/z</i>
[Co ₃ (L) ₄] ²⁺	0.499	410.55	410.54
[HCo ₃ (L) ₅] ²⁺	0.316	491.58	491.58

$[\text{Co}_4(\text{L})_5(\text{CH}_3\text{O})]^{2+}$	0.187	536.05	536.06
$[\text{H}_2\text{Co}(\text{L})_3]^+$	0.457	544.16	544.16
$[\text{H}_2\text{Co}_3(\text{L})_6]^{2+}$	0.125	572.62	572.62
$[\text{Co}_4(\text{L})_6]^{2+}$	1	601.08	601.08
$[\text{HCo}_2(\text{L})_3\text{Cl}]^+$	0.090	637.06	637.06
$[\text{HCo}_2(\text{L})_4]^+$	0.175	763.16	763.16
$[\text{H}_2\text{Co}_2(\text{L})_4\text{Cl}]^+$	0.049	799.14	799.14
$[\text{Co}_3(\text{L})_4\text{Cl}]^+$	0.091	856.05	856.05
$[\text{HCo}_3(\text{L})_4\text{Cl}_2]^+$	0.025	892.03	892.03
$[\text{HCo}_3(\text{L})_5\text{Cl}]^+$	0.036	1018.13	1018.13
$[\text{Co}_7(\text{L})_{11}(\text{CH}_3\text{O})]^{2+}$	0.035	1108.17	1108.17
$[\text{Co}_4(\text{L})_5\text{Cl}_2]^+$	0.026	1111.03	1111.03
$[\text{Co}_7(\text{L})_{12}]^{2+}$	0.161	1173.19	1173.20
$[\text{Co}_4(\text{L})_6\text{Cl}]^+$	0.024	1237.13	1237.13
2			
Peaks	Relative Intensity	Obs. <i>m/z</i>	Calc. <i>m/z</i>
$[\text{Co}_3(\text{L})_4]^{2+}$	0.338	410.54	410.55
$[\text{HCo}_3(\text{L})_5]^{2+}$	0.068	491.58	491.58
$[\text{Co}_4(\text{L})_6]^{2+}$	1	601.08	601.08
$[\text{Co}_3(\text{L})_4\text{Br}]^+$	0.248	900.01	900.00
$[\text{Co}_7(\text{L})_{12}]^{2+}$	0.118	1173.19	1173.20
$[\text{Co}_4(\text{L})_6\text{Br}]^+$	0.160	1283.06	1283.08



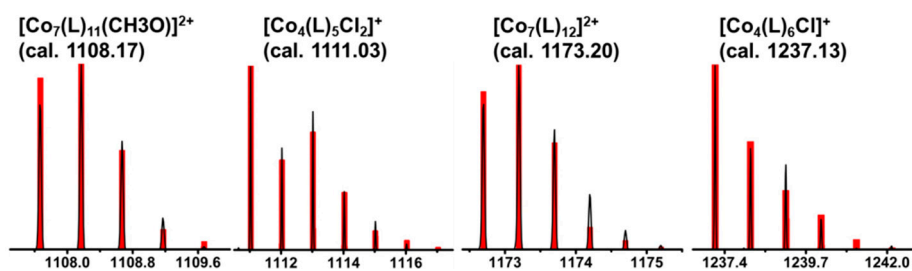


Figure S2. The overlapped calculative and experimental spectra of some peaks for 1.

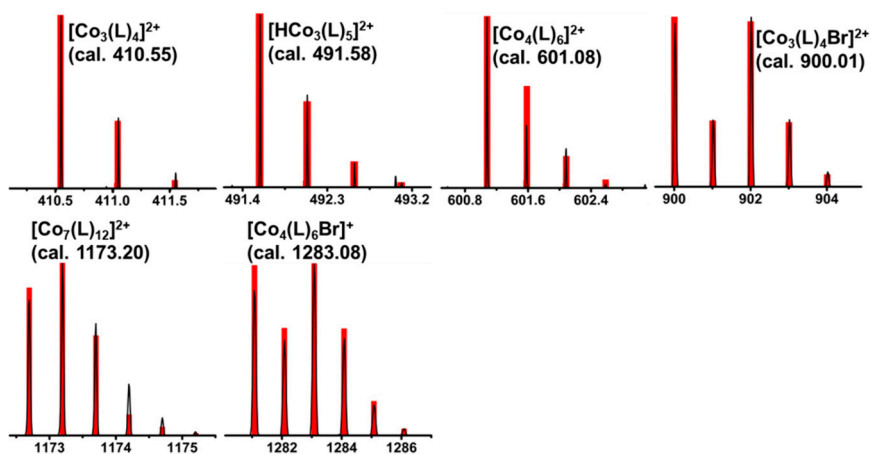


Figure S3. The overlapped calculative and experimental spectra of some peaks for 2.

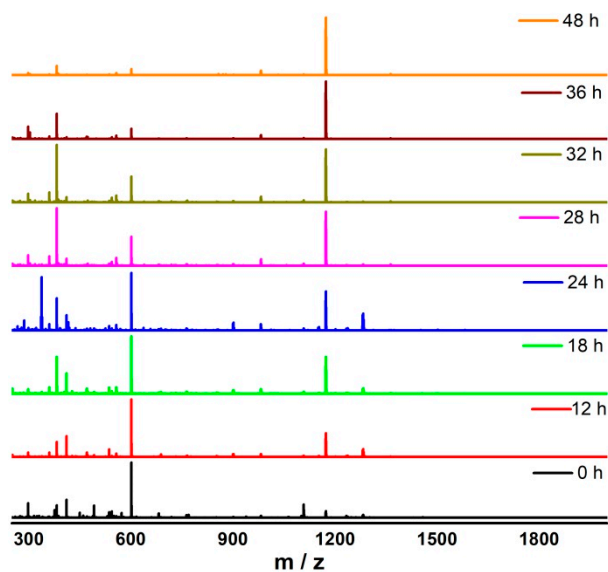


Figure S4. The process of transformation from complex 1 to high nuclear peaks.

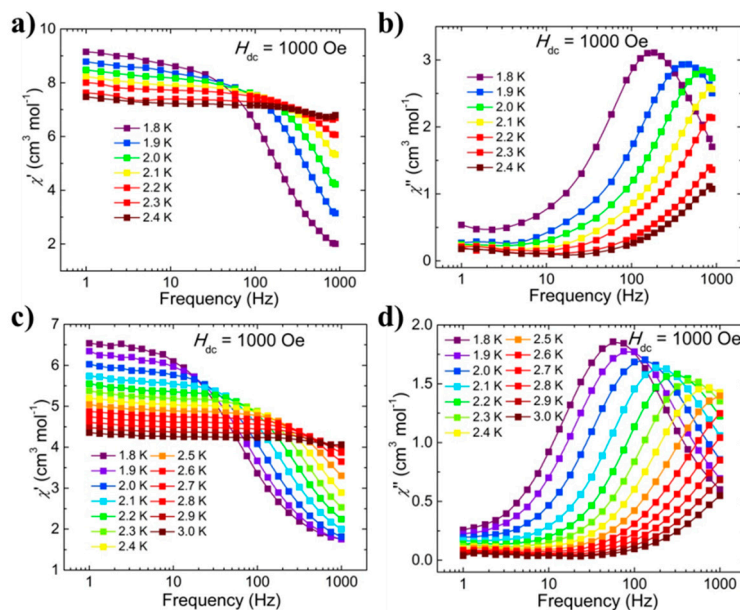


Figure S5. Alterable frequencies ac-susceptibilities ($H_{dc} = 1000$ Oe) at the limit of temperatures for (a and b) **1** and (c and d) **2**.

Table S3. Selected parameters from the fitting results of the Cole-Cole plots for **1** and **2** under 1000 Oe field.

<i>Temp.</i> (K)	1			2		
	τ	α	residual	τ	α	residual
1.8	8.70E-04	0.166	1.27E-01	2.49E-03	0.206	3.87E-02
1.9	5.85E-04	0.168	1.31E-01	1.80E-03	0.205	3.90E-02
2.0	3.53E-04	0.179	1.26E-01	1.17E-03	0.195	5.78E-02
2.1	1.88E-04	0.208	9.88E-02	7.19E-04	0.172	6.94E-02
2.2	1.02E-04	0.222	4.85E-02	4.78E-04	0.153	6.59E-02
2.3	6.44E-05	0.233	7.73E-02	3.31E-04	0.143	5.65E-02
2.4	4.51E-05	0.232	9.17E-02	2.22E-04	0.147	4.92E-02
2.5	3.13E-05	0.228	1.12E-01	1.40E-04	0.164	4.07E-02
2.6	2.30E-05	0.217	9.88E-02	8.34E-05	0.194	3.36E-02