A novel series of giant cobalt-calixarene macrocycles: Ring-expansion and modulation of pore apertures through recrystallization

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Materials and Characterization

H_4TC4A was synthesized according to the literature method.[1] Other chemicals were purchased and without further purification before use. FT-IR spectra were recorded on a PerkinElmer Spectrum One spectrometer using KBr as pellets. Elemental analyses (C, H, and N) were carried out with a vario EL cube elemental analyzer. UV-Vis absorption spectra were detected by a Perkin-Elmer Lambda950 UV/Vis/NIR spectrophotometer. TG analysis was performed on a NETZSCH STA 449C instrument. X-ray photoelectron spectroscopic (XPS) measurements were carried out with an ESCALAB 250Xi using a monochromatic Al Kα X-ray source. Gas sorption measurements were carried out on Micromeritics ASAP 2020 gas adsorption analyzer.

Absorption of dyes

Before absorption tests, the samples were activated by soaking with MeOH for one day and drying in vacuum. In a typical adsorption experiment, 10 mg activated sample was dispersed in a 10 mL solution of dye (10 ppm). After 30 min of stirring, the solution was sampled by filtration and was analyzed by the UV-Vis spectrophotometer.

Synthesis of the metallomacrocycles

Synthesis of {Co_{30}-A}

A mixture of H_4TC4A (0.1 mmol, 72 mg), H_3pdc (0.15 mmol, 26 mg), $Co(ClO_4)_2 \cdot 6H_2O$

(0.42 mmol, 154 mg), MeOH (9 mL), DMF (1 mL) and several drops of TEA was sealed in a 23 mL Teflon-lined autoclave without stirring (Fig. S9, left) and then kept at 130℃ for 3 days. After cooling it to room temperature for one day, crimson block crystals of {**Co_{30}-A**} were collected by filtration and washed with MeOH/DMF (v:v = 9:1). The average yield for 6 attempts was about 68.7 mg, 66.8% based on H_3pdc. Elemental analysis (%) for $C_{325}H_{374}Co_{30}N_{30}O_{92}S_{24}$ (including 6 $(CH_3)_2NH_2^+$ cations): calculated C 44.77, H 4.30, N 4.82; found (after soaking with MeOH and drying in vacuum) C 44.85, H 4.41, N 4.86.

Synthesis of {Co_{30}-B}

The synthetic procedure was similar to that for the synthesis of {**Co_{30}-A**}, except that the mixture was stirred for 10 min before heating (Fig. S9, right). The average yield for 6 attempts was about 40.3 mg, 39.3% based on H_3pdc. Elemental analysis (%) for $C_{318}H_{366}Co_{30}N_{30}O_{90}S_{24}$ (including 6 $(CH_3)_2NH_2^+$ cations): calculated C 44.58, H 4.28, N 4.91; found (after soaking with MeOH and drying in vacuum) C 44.62, H 4.38, N 5.04.

Synthesis of {Co_{32}-A}

The synthetic procedure was similar to that for the synthesis of {**Co_{30}-A**}, except that $CoCl_2 \cdot 6H_2O$ (100 mg) was used instead of $Co(ClO_4)_2 \cdot 6H_2O$ and DMF was replaced by NMP. Purple rod-like crystals of {**Co_{32}-A**} were collected by filtration and washed with MeOH/NMP (v:v = 9:2). The average yield for 6 attempts was about 75.8 mg, 64.4% based on H_4TC4A. Elemental analysis (%) for $C_{360}H_{392}Cl_8Co_{32}N_{16}O_{80}S_{32}$: calculated C 45.87, H 4.06, N 2.38; found (after soaking with MeOH and drying in vacuum) C 45.92, H 4.24, N 2.51.

Synthesis of {Co_{32}-B}

Route 1: 30 mg {**Co_{32}-A**} was dissolved in 1 mL DMF. After evaporating in air for several days. Crystals of {**Co_{32}-B**} were collected by filtration and washed with CH_3CN. The average yield for 3 attempts: ~20.4 mg, 68.0% based on {**Co_{32}-A**}.

Route 2: NaCl (10 mg) was added into 1 mL DMF solution of {**Co_{30}-A**} (30 mg) and the mixture was heated at 130℃. Crystals of {**Co_{32}-B**} were produced after one day. The average yield for 3 attempts: ~10.1 mg, 37.9% based on {**Co_{30}-A**}. Elemental

analysis (%) for $C_{360}H_{392}Cl_8Co_{32}N_{16}O_{80}S_{32}$: calculated C 45.87, H 4.06, N 2.38; found (after soaking with MeOH and drying in vacuum) C 45.96, H 4.22, N 2.44.

Synthesis of {Co_{32}-C}.

1 mL DMF solution containing 30 mg {**Co_{32}-A**} was sealed in a 5 mL screw glass bottle and heated at 130℃. After several days, enumerable crystals of {**Co_{32}-C**} were collected and washed with CH_3CN. The average yield for 3 attempts: ~2.0 mg, 6.7% based on {**Co_{30}-A**}.

Synthesis of {Co_{40}}.

{**Co_{32}-A**} (30 mg) in 5 mL DMF was sealed in a 5 mL screw glass bottle and stored at RT for about 2 months, a small amount of{**Co_{40}**} crystals were produced. Yield: 5.2 mg, 3.4% based on {**Co_{32}-A**}. Heat the DMF solution of {**Co_{32}-A**} at 60 ℃ for two weeks increased the yield of {**Co_{40}**} (the average yield for 3 attempts: ~8.0 mg, 5.1% based on {**Co_{30}-A**}).

Caution! There is a risk of explosion when perchlorates are heated directly. Ensure the leakproofness of the hydrothermal reactor to avoid the evaporation of the solvents. Stainless steel linings are also needed in the solvothermal reactions.

Single Crystal X-ray Diffraction

Single crystal X-ray diffraction data of {**Co_{32}-A**} was collected on a XtaLAB Synergy R diffractometer with Cu K_α radiation (λ = 1.54184 Å) at 100 K while those of {**Co_{30}-A/B**}, {**Co_{32}-B/C**} and {**Co_{40}**} were collected on a Rigaku ROD, Synergy Custom system, HyPix diffractometer equipped with mirror-monochromatic Ga Kα radiation (λ = 1.3405 Å) at 120 K. The data collection and reduction were performed on the *CrysAlis^{Pro}* program.[2] The structures were solved by SHELXT methods with the Olex2 program[3,4], and non-hydrogen atoms were refined anisotropically by least-squares on F^2 using SHELXL.[3] Although the diffractions were carried out at low temperature, solvents within the lattice interstices were difficult to fix based on the current data. Hence, the data were treated by the "SQUEEZE" method as implemented in PLATON.[5] Appropriate restraints or constraints were applied to the geometry and the atomic displacement parameters of the atoms in the compounds. The hydrogen atoms attached to C and N atoms were placed in idealized positions and refined using a riding model

to the atom to which they were attached. The *R* factors in the final structural refinement are relatively large but are typical for such systems.[6,7] Pertinent crystallographic data collection and refinement parameters are collected in Table S7. Selected bond lengths are collected in Table S8-S13.

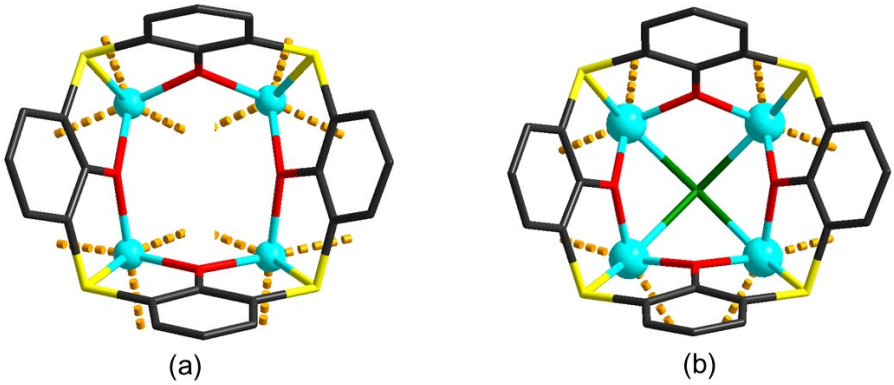

Fig. S1 Illustration of two common SBUs for the metal-TC4A coordination cages and metallomacrocycles. M_4-TC4A (a) and M_4Cl-TC4A (b). H toms and t-butyl groups are omitted for clarity.

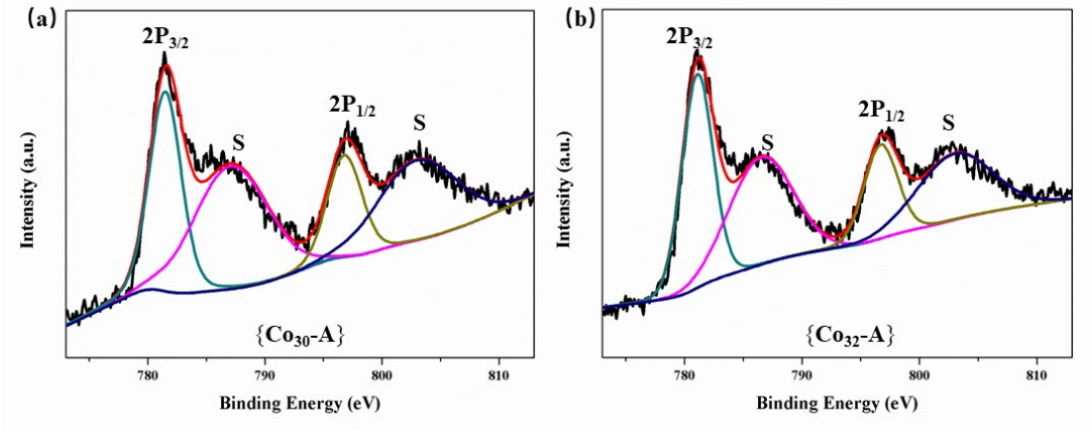

Fig. S2 Co 2p XPS spectra of {**Co_{30}-A**} and {**Co_{32}-A**}.

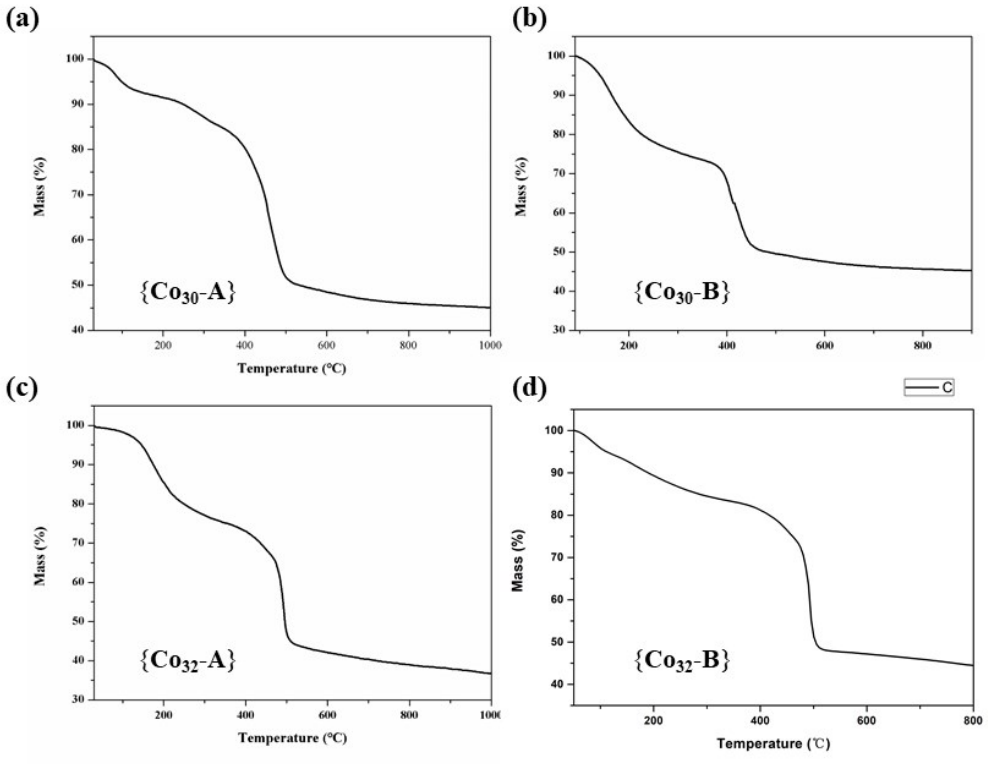

Fig. S3 TGA curves of the metallomacrocycles.

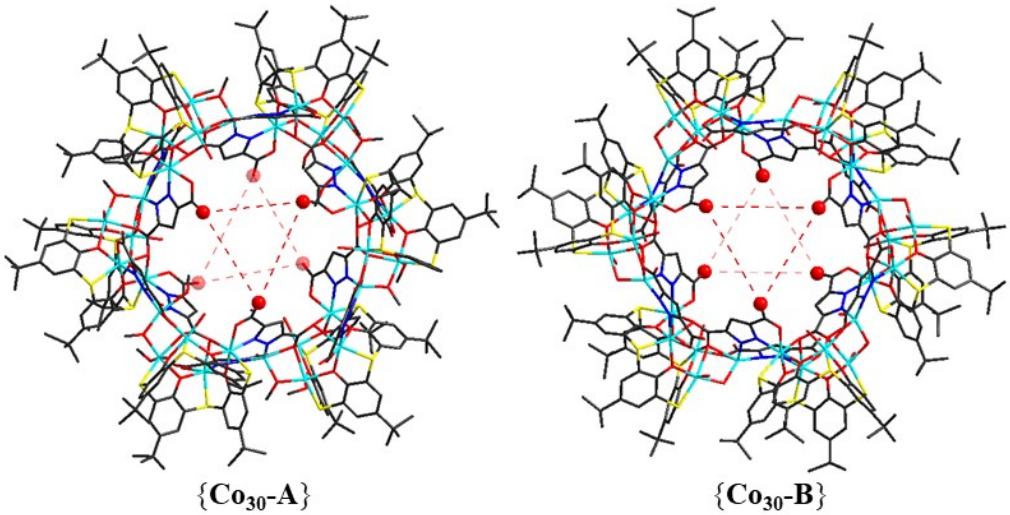

Fig. S4 Structures of {**Co$_{30}$-A/B**} showing the uncoordinated carboxylate O atoms of pdc^{3-} inside the ring cavities. H atoms are omitted for clarity. Color code: C, black; O, red; N, blue; S, yellow; Co, turquoise.

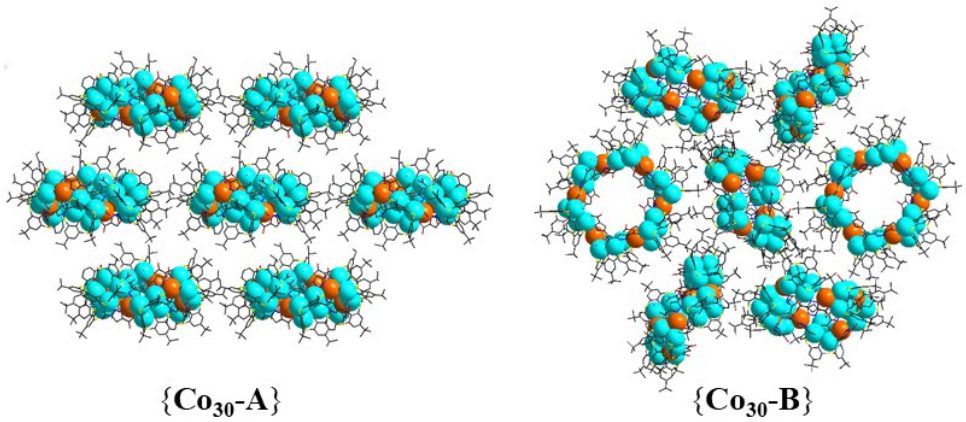

Fig. S5 packing modes of {**Co$_{30}$-A/B**}.

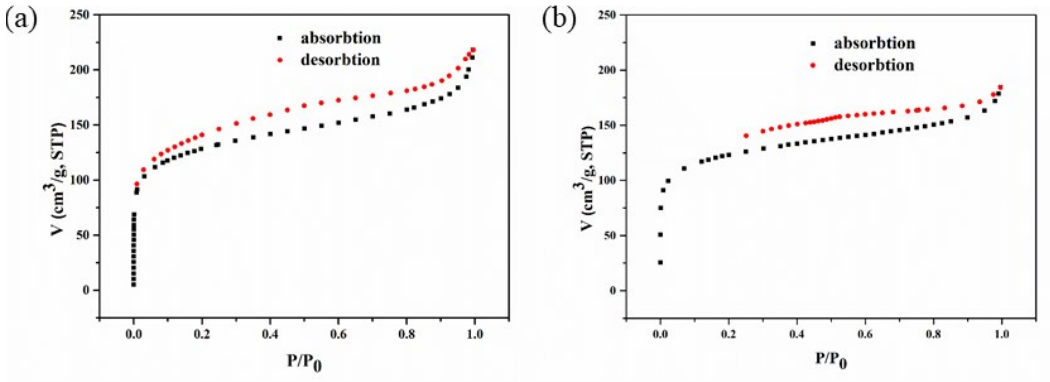

Fig. 6 N_2 adsorption isotherms (77 K) of {**Co$_{32}$-A**} (a) and {**Co$_{32}$-B**} (b).

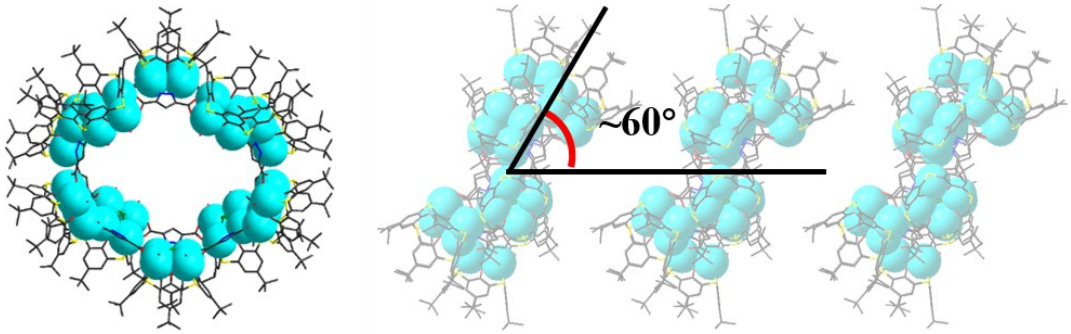

Fig. 7 Top and side view of the tubular structures in {**Co$_{40}$**}.

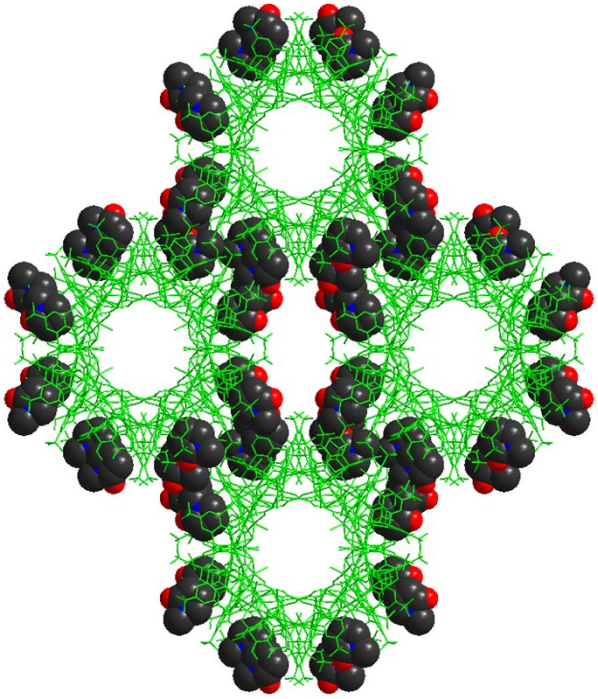

Fig. S8 Stacking of {**Co_{32}-A**} rings showing trapped NMP molecules in the cavities.

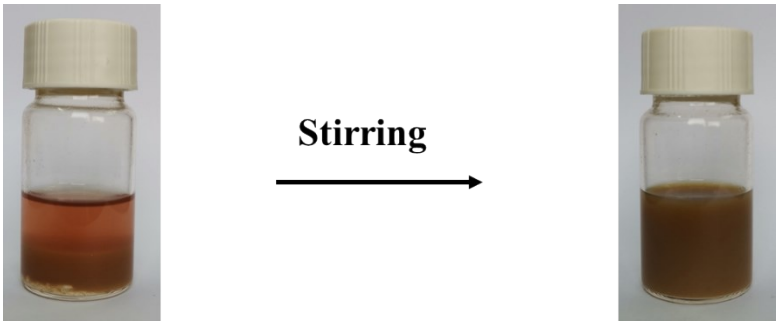

Fig. S9 Photos of the mixture before and after stirring in synthesizing {**Co_{30}-B**}.

Table S1 Bond valence sum values for Co atoms in {**Co_{30}-A**}.

Co1	2.01	Co11	1.80	Co21	2.00
Co2	1.87	Co12	1.86	Co22	1.81
Co3	1.78	Co13	1.90	Co23	2.09
Co4	1.99	Co14	1.95	Co24	2.12
Co5	2.03	Co15	1.94	Co25	2.02
Co6	2.13	Co16	1.90	Co26	2.06
Co7	1.95	Co17	1.95	Co27	2.04
Co8	2.07	Co18	1.80	Co28	1.81
Co9	2.00	Co19	1.99	Co29	1.89
Co10	1.98	Co20	1.87	Co30	1.89

Table S2 Bond valence sum values for Co atoms in {**Co_{30}-B**}.

Co1	1.89	Co3	2.07	Co5	2.17

Co2	1.95	Co4	1.97		

Table S3 Bond valence sum values for Co atoms in {**Co_{32}-A**}.

Co1	1.92	Co7	1.86	Co13	2.04
Co2	1.88	Co8	1.90	Co14	2.00
Co3	1.88	Co9	2.05	Co15	2.01
Co4	1.88	Co10	1.89	Co16	2.01
Co5	1.89	Co11	2.00		
Co6	2.04	Co12	2.05		

Table S4 Bond valence sum values for Co atoms in {**Co_{32}-B**}.

Co1	1.95	Co23	1.93	Co45	1.93
Co2	1.94	Co24	1.87	Co46	2.12
Co3	1.95	Co25	2.07	Co47	2.01
Co4	2.01	Co26	1.83	Co48	2.07
Co5	1.85	Co27	1.90	Co49	1.94
Co6	1.93	Co28	1.97	Co50	2.05
Co7	2.17	Co29	1.94	Co51	1.98
Co8	1.93	Co30	2.01	Co52	2.04
Co9	1.90	Co31	1.97	Co53	1.97
Co10	1.86	Co32	2.04	Co54	1.87
Co11	1.90	Co33	1.89	Co55	1.96
Co12	1.92	Co34	1.96	Co56	1.89
Co13	1.90	Co35	2.09	Co57	1.85
Co14	1.98	Co36	2.06	Co58	1.83
Co15	1.95	Co37	2.06	Co59	2.07
Co16	1.99	Co38	2.01	Co60	1.95
Co17	1.87	Co39	2.89	Co61	2.01
Co18	2.00	Co40	1.93	Co62	1.98
Co19	1.95	Co41	2.13	Co63	2.01
Co20	1.95	Co42	1.90	Co64	2.04
Co21	2.13	Co43	1.92		
Co22	1.86	Co44	2.09		

Table S5 Bond valence sum values for Co atoms in {**Co_{32}-C**}.

Co1	1.88	Co7	1.90	Co13	1.98
Co2	1.85	Co8	2.01	Co14	2.05
Co3	1.88	Co9	1.85	Co15	1.87
Co4	1.87	Co10	1.88	Co16	1.96
Co5	1.85	Co11	1.89		
Co6	1.99	Co12	1.94		

Table S6 Bond valence sum values for Co atoms in {**Co_{40}**}.

Co1	1.85	Co8	1.88	Co15	2.03
Co2	1.87	Co9	1.88	Co16	1.93
Co3	1.83	Co10	2.00	Co17	1.99
Co4	2.02	Co11	2.04	Co18	1.94
Co5	1.86	Co12	2.00	Co19	1.98
Co6	1.91	Co13	1.92	Co20	2.05
Co7	1.89	Co14	1.88		

PLATON SQUEEZE Results

The SQUEEZE results from the platon program as follows:

loop_
  _platon_squeeze_void_nr
  _platon_squeeze_void_average_x
  _platon_squeeze_void_average_y
  _platon_squeeze_void_average_z
  _platon_squeeze_void_volume
  _platon_squeeze_void_count_electrons
  _platon_squeeze_void_content

{**Co_{30}-A**}

1 -0.016 0.766 0.010 30861 11865 ' '

{**Co_{30}-B**}

1 -0.003 -0.007 -0.002 19870 5225 ' '
2 0.500 0.000 0.000 900 157 ' '
3 1.000 0.000 0.500 900 157 ' '
4 0.500 0.500 0.500 900 157 ' '
5 1.000 0.500 1.000 900 157 ' '

{**Co_{32}-A**}

1 -0.001 -0.006 -0.002 39420 8584 ' '
2 0.214 0.203 0.653 19 0 ' '
3 0.786 0.203 0.847 19 0 ' '
4 0.333 0.232 0.797 10 -1 ' '
5 0.667 0.232 0.703 10 -1 ' '
6 0.271 0.238 0.843 13 -1 ' '
7 0.729 0.238 0.657 13 -1 ' '
8 0.229 0.262 0.157 13 -1 ' '
9 0.771 0.262 0.343 13 -1 ' '
10 0.167 0.268 0.203 10 -1 ' '
11 0.833 0.268 0.297 10 -1 ' '
12 0.286 0.297 0.347 19 0 ' '
13 0.714 0.297 0.153 19 0 ' '
14 0.286 0.703 0.847 19 0 ' '
15 0.714 0.703 0.653 19 0 ' '

16	0.167	0.732	0.703	10	-1 ''
17	0.833	0.732	0.797	10	-1 ''
18	0.229	0.738	0.657	13	-1 ''
19	0.771	0.738	0.843	13	-1 ''
20	0.271	0.762	0.343	13	-1 ''
21	0.729	0.762	0.157	13	-1 ''
22	0.333	0.768	0.297	10	-1 ''
23	0.667	0.768	0.203	10	-1 ''
24	0.214	0.797	0.153	19	0 ''
25	0.786	0.797	0.347	19	0 ''

{**Co_{32}-B**}

1	0.023	0.376	0.020	64221	5948 ''
2	0.269	0.639	0.303	8	0 ''
3	0.769	0.361	0.303	7	0 ''
4	0.190	0.135	0.345	10	1 ''
5	0.690	0.865	0.345	10	1 ''
6	0.231	0.639	0.803	8	-1 ''
7	0.731	0.361	0.803	7	-1 ''
8	0.310	0.135	0.845	10	1 ''
9	0.810	0.865	0.845	10	1 ''

{**Co_{32}-C**}

1	-0.111	0.637	0.075	27486	8098 ''
2	0.107	0.088	0.470	15	-1 ''
3	0.107	0.912	0.970	15	-1 ''
4	0.131	0.851	0.002	9	0 ''
5	0.131	0.149	0.502	10	0 ''
6	0.224	0.410	0.141	12	0 ''
7	0.224	0.590	0.641	11	0 ''
8	0.276	0.910	0.359	11	0 ''
9	0.276	0.090	0.859	11	0 ''
10	0.369	0.648	-0.002	10	0 ''
11	0.369	0.352	0.498	10	0 ''
12	0.393	0.587	0.030	14	0 ''
13	0.393	0.413	0.530	15	-1 ''
14	0.607	0.588	0.470	15	-1 ''
15	0.607	0.412	0.970	15	-1 ''
16	0.631	0.351	0.002	9	0 ''
17	0.631	0.649	0.502	10	0 ''
18	0.724	0.910	0.141	12	0 ''
19	0.724	0.090	0.641	11	0 ''
20	0.776	0.410	0.359	11	0 ''
21	0.776	0.590	0.859	11	0 ''
22	0.869	0.148	-0.002	10	0 ''
23	0.869	0.852	0.498	10	0 ''

24	0.893	0.087	0.030	14	0	' '
25	0.893	0.913	0.530	15	-1	' '

{**Co_{40}**}

1	-0.304	-0.775	0.728	10964.0	2561.2	' '
2	0.082	0.964	0.535	14.8	0.0	' '
3	0.395	0.329	0.151	12.5	3.4	' '
4	0.605	0.671	0.849	12.5	3.6	' '
5	0.918	0.036	0.465	14.8	0.0	' '

According to the SQUEEZE analysis and TGA measurements, the formula for the compounds are estimated as follows:

Based on molecular electrons:

Notes: The counter ions in Co30-A/B are highly disordered, and the cation is assumed to be $[(CH_3)_2NH_2]^+$ which is a common counter ion in solvothermal reactions with DMF as a solvent.

Electron numbers for the molecules: $(CH_3)_2NH_2$ = 27 e^-, DMF = 48 e^-, MeOH = 26 e^-, NMP = 62 e^-

Co30-A: $[Co_{30}(TC4A)_6(pdc)_{12}(\mu_2\text{-}OMe)_6(MeOH)_8(H_2O)_6]\cdot[(CH_3)_2NH_2]_6(DMF)_x(MeOH)_y$

x=58, y=0 or x=0, y=108. **(1)**

Co30-B: $[Co_{30}(TC4A)_6(pdc)_{12}(\mu_2\text{-}OMe)_6(H_2O)_{12}]\cdot[(CH_3)_2NH_2]_6(DMF)_x(MeOH)_y$

x=27, y=0 or x=0, y=50. **(2)**

Co32-A: $[Co_{32}Cl_8(TC4A)_8(pdc)_8(H_2O)_{16}](NMP)_{8+x}(MeOH)_y$

x=34, y=0 or x=0, y=82. **(3)**

Co32-B: $[Co_{32}Cl_8(TC4A)_8(pdc)_8(H_2O)_{16}]\ (DMF)_{4.5+x}$

x=31. **(4)**

Co32-C: $[Co_{32}Cl_8(TC4A)_8(pdc)_8(H_2O)_{13.4}(DMF)_{0.8}(dma)_{0.5}(HCOOH)_{1.3}]\ (DMF)_{14+x}$

x=42. **(5)**

Co40: $[Co_{40}Cl_{10}(TC4A)_{10}(pdc)_{10}(H_2O)_{20}]\ (DMF)_{24+x}$

x=53. **(6)**

Based on TGA results:

Co30-A: $[Co_{30}(TC4A)_6(pdc)_{12}(\mu_2\text{-}OMe)_6(MeOH)_8(H_2O)_6]\cdot[(CH_3)_2NH_2]_6(DMF)_x(MeOH)_y$

x=32, y=0 or x=0, y=73 (21.1% weight loss assigned to solvents). **(7)**

Co30-B: $[Co_{30}(TC4A)_6(pdc)_{12}(\mu_2\text{-}OMe)_6(H_2O)_{12}]\cdot[(CH_3)_2NH_2]_6(DMF)_x(MeOH)_y$

x=8, y=0 or x=0, y=17 (6% weight loss assigned to solvents). **(8)**

Co32-A: $[Co_{32}Cl_8(TC4A)_8(pdc)_8(H_2O)_{16}](NMP)_{8+x}(MeOH)_y$

x=16, y=0 or x=0, y=36 (21.7% weight loss assigned to solvents) **(9)**

Co32-B: $[Co_{32}Cl_8(TC4A)_8(pdc)_8(H_2O)_{16}]\ (DMF)_{4.5+x}$

x=35 (23.1% weight loss assigned to solvents). **(10)**

Take both SQUEEZE results and TGA tests in to consideration, the possible formula for the compounds are (7) for {**Co_{30}-A**}, (8) for {**Co_{30}-B**}, (9) for **{Co_{32}-A**}, (10) for {**Co_{32}-B**}, (5) for {**Co_{32}-C**}, (6) for {**Co_{40}**}.

Table 7 Crystallographic data of the compounds

	{**Co$_{30}$-A**}	{**Co$_{30}$-B**}	{**Co$_{32}$-A**}	{**Co$_{32}$-B**}	{**Co$_{32}$-C**}	{**Co$_{40}$**}
CCDC number	2062188	2062189	2062190	2062191	2062192	2062193
Crystal Formula*	$C_{325}H_{374}Co_{30}N_{30}O_{92}S_{24}$	$C_{318}H_{366}Co_{30}N_{30}O_{90}S_{24}$	$C_{400}H_{464}Cl_8Co_{32}N_2O_{88}S_{32}$	$C_{935}H_{1283}Cl_{16}Co_{64}N_{87}O_{167}S_{64}$	$C_{430.73}H_{548.5}Cl_8Co_3{}_2N_{39.3}O_{108.83}S_{32}$	$C_{521}H_{652}Cl_{10}Co_{40}N_{44}O_{124}S_{40}$
Formula weight	8710.13	8586.00	10211.2	22804.76	11213.15	13508.89
crystal system	triclinic	cubic	monoclinic	orthorhombic	monoclinic	triclinic
space group	Cc	Pa-3	C2/c	Pca21	C2/c	P-1
a [Å]	54.4788(9)	37.3887(2)	66.638(2)	65.4426(5)	49.3116(10)	23.7232(3)
b [Å]	30.7508(3)	37.3887(2)	51.3655(4)	35.1245(3)	26.6728(4)	31.4851(4)
c [Å]	38.3160(8)	37.3887(2)	36.3667(12)	59.0133(5)	56.2706(10)	36.7204(5)
α [°]	90	90	90	90	90	69.6330(10)
β [°]	110.400(2)	90	143.163(7)	90	97.979(2)	71.5790(10)
γ [°]	90	90	90	90	90	84.6960(10)
V [Å^3]	60163.7(19)	52266.2(8)	74630(8)	135650.2(19)	73295(2)	24390.5(6)
Z	4	4	4	4	4	1
T[K]	120	110	100	100	120	120
D_c[g/cm^3]*	0.961	1.091	0.909	1.117	1.233	1.184
μ[mm^{-1}]	5.183	5.970	6.865	0.934	4.865	4.579
reflns coll.	103131	82632	73304	665146	81978	109466
unique reflns	60114	19762	39366	259511	81463	87328
GOF	0.999	1.505	1.006	0.955	1.150	1.046
R1[I>2σ(I)][a]	7.40%	15.71%	7.79%	10.37%	10.00%	8.28%
wR2[I>2σ(I)][b]	22.42%	44.10%	26.34%	27.68%	32.56%	28.78%

[a] $R1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. [b] $wR2 = \{\Sigma[w(F_o^2 - Fc^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$; *The formula and D_c do not include the unidentified disordered solvents in {**Co$_{30}$-A/B**} and {**Co$_{32}$-A**}.

Table S8 Selected bond lengths for {**Co_{30}-A**}.

Atom	Atom	Length (Å)	Atom	Atom	Length (Å)
Co1	S5	2.4338	Co15	N14	2.1013
Co1	O1	2.0649	Co16	S15	2.4636
Co1	O3	2.0524	Co16	O14	2.086
Co1	O4	2.0812	Co16	O19	2.3759
Co1	O8	2.0067	Co16	O35	1.9842
Co1	O17	2.2469	Co16	N10	2.0494
Co2	S1	2.4755	Co16	O66	2.0728
Co2	O2	2.0981	Co17	S11	2.4487
Co2	O3	2.1008	Co17	O30	2.1047
Co2	O12	2.0061	Co17	O43	2.3277
Co2	N1	2.0896	Co17	O53	2.1403
Co2	O34	2.2267	Co17	O56	1.9776
Co3	O1	2.0693	Co17	O60	2.0025
Co3	O15	1.9749	Co18	S12	2.4372
Co3	O17	2.2073	Co18	O25	2.0082
Co3	N3	2.0131	Co18	O44	2.1163
Co3	N5	2.0558	Co18	N16	2.116
Co4	S8	2.4357	Co18	O75	2.0542
Co4	O10	2.2971	Co19	S14	2.4573
Co4	O20	1.9643	Co19	O29	1.9928
Co4	O28	2.0986	Co19	O44	2.1099
Co4	O32	2.0252	Co19	O48	1.9348
Co4	O41	2.1222	Co19	O57	2.3982
Co5	S3	2.4466	Co19	O61	2.1205
Co5	O7	2.0781	Co20	S17	2.4918
Co5	O8	1.9905	Co20	O13	2.1394
Co5	O15	1.9547	Co20	O38	1.9601
Co5	O17	2.3378	Co20	O49	2.2969
Co5	O31	2.1271	Co20	O51	2.0304
Co6	S2	2.4318	Co20	N23	2.1334
Co6	O5	2.0249	Co21	O43	2.2003
Co6	O6	2.0179	Co21	O56	1.9684
Co6	O9	1.9542	Co21	N9	2.0009
Co6	O39	2.1065	Co21	O59	2.0588
Co6	O46	2.2489	Co21	O85	2.3944
Co7	O10	2.2001	Co21	N24	2.0234
Co7	O20	1.9486	Co22	O18	2.0456
Co7	N2	2.0469	Co22	O48	1.9385
Co7	O27	2.0681	Co22	N6	2.0835
Co7	O45	2.3706	Co22	O57	2.2122
Co7	N12	2.0549	Co22	N11	2.0298

Co8	S9	2.4279	Co23	S19	2.448
Co8	O10	2.2125	Co23	O18	2.0674
Co8	O23	2.0692	Co23	O29	1.9909
Co8	O27	2.077	Co23	O40	2.0147
Co8	O32	1.9715	Co23	O57	2.1742
Co8	O37	2.052	Co23	O63	2.0977
Co9	S4	2.4384	Co24	S24	2.436
Co9	O9	2.0256	Co24	O54	2.0773
Co9	O11	1.9534	Co24	O55	1.9345
Co9	O14	2.1311	Co24	O64	1.9833
Co9	O21	2.0742	Co24	O67	2.1122
Co9	O46	2.3366	Co24	O71	2.2663
Co10	S7	2.4582	Co25	S13	2.4645
Co10	O7	2.134	Co25	O13	2.0393
Co10	O12	1.9591	Co25	O43	2.2944
Co10	O24	2.0249	Co25	O59	2.0729
Co10	O34	2.4074	Co25	O60	1.9903
Co10	N8	1.9933	Co25	O72	2.0461
Co11	O6	2.0545	Co26	S21	2.4358
Co11	O11	1.9668	Co26	O36	1.9963
Co11	O46	2.1866	Co26	O52	2.0769
Co11	N7	2.051	Co26	O58	2.0961
Co11	N15	2.0367	Co26	O64	1.991
Co12	S10	2.4282	Co26	O71	2.2493
Co12	O22	2.0086	Co27	S18	2.4307
Co12	O28	2.1113	Co27	O16	1.9645
Co12	O33	2.3977	Co27	O54	2.0535
Co12	N4	2.0658	Co27	O88	1.9684
Co12	O68	2.0566	Co27	N25	2.058
Co13	S6	2.4472	Co28	S23	2.4758
Co13	O38	1.9806	Co28	O25	1.9916
Co13	O42	2.0868	Co28	O40	2.1307
Co13	O49	2.3306	Co28	O74	2.2038
Co13	O53	2.0756	Co28	N20	2.1841
Co13	N17	2.0816	Co28	O82	2.0978
Co14	S20	2.4597	Co29	O52	2.0342
Co14	O5	2.0681	Co29	O55	1.9177
Co14	O19	2.2097	Co29	O71	2.2277
Co14	O35	1.9797	Co29	N18	2.0802
Co14	O62	2.1247	Co29	N22	1.985
Co14	N13	2.0673	Co30	S22	2.4784
Co15	S16	2.4677	Co30	O16	2.0123
Co15	O22	1.9845	Co30	O36	2.0457

Co15	O23	2.0795	Co30	N19	2.14
Co15	O33	2.2064	Co30	O79	2.0292
Co15	O50	2.0801	Co30	O81	2.3274

Table S9 Selected bond lengths for {**Co_{30}-B**}.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Co1	O1	1.953(9)	Co3	O2	2.350(9)
Co1	N3	1.987(6)	Co3	S2	2.414(4)
Co1	N2	2.007(9)	Co4	O11	2.034(9)
Co1	O3	2.056(8)	Co4	O7	2.041(11)
Co1	O2	2.219(7)	Co4	O3	2.043(8)
Co2	O5	1.980(10)	Co4	O2	2.150(8)
Co2	N1[1]	2.007(9)	Co4	O13	2.203(11)
Co2	O4	2.045(8)	Co4	S3	2.437(5)
Co2	O9[1]	2.105(8)	Co5	O5	1.954(11)
Co2	O6	2.407(9)	Co5	O11	2.027(10)
Co2	S1	2.442(3)	Co5	N4[1]	2.042(8)
Co3	O7	1.954(10)	Co5	O6	2.093(9)
Co3	O1	2.000(7)	Co5	O15[1]	2.112(10)
Co3	O8	2.076(9)	Co5	S4	2.431(6)
Co3	O4	2.084(8)			

Symmetry code for 1: $3/2 - x, 1/2 + y, z$

Table S10 Selected bond lengths for {**Co_{32}-A**}.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Co1	O6	2.007(4)	Co9	S11	2.5293(18)
Co1	O10	2.065(4)	Co9	O9	1.993(4)
Co1	O20	1.989(4)	Co9	O13	2.009(4)
Co1	N2[1]	2.084(4)	Co9	O15	2.023(4)
Co2	Cl1	2.7140(15)	Co9	O33	2.101(4)
Co2	S6	2.5424(16)	Co10	Cl4	2.7174(18)
Co2	O1	2.017(3)	Co10	S8	2.5184(18)
Co2	O13	2.067(4)	Co10	O4	2.009(4)
Co2	O30	1.989(4)	Co10	O26	1.994(4)
Co2	N3[1]	2.090(5)	Co10	O29	2.063(4)
Co3	Cl1	2.7270(15)	Co10	N7[1]	2.087(5)
Co3	S2	2.5326(16)	Co11	Cl2	2.5914(16)
Co3	O1	2.018(3)	Co11	S14	2.5316(18)
Co3	O8	1.982(3)	Co11	O10	2.020(4)
Co3	O11	2.065(4)	Co11	O27	2.036(4)
Co3	N6[1]	2.098(5)	Co11	O32	2.017(4)
Co4	Cl3	2.7337(16)	Co11	O36	2.091(5)
Co4	S7	2.5356(16)	Co12	Cl3	2.6002(17)

Co4	O3	2.011(3)	Co12	S10	2.5127(19)
Co4	O12	2.081(4)	Co12	O12	2.026(4)
Co4	O18	1.976(4)	Co12	O17	2.013(4)
Co4	N5[1]	2.103(5)	Co12	O22	2.002(4)
Co5	Cl3	2.7134(17)	Co12	O35	2.090(5)
Co5	S5	2.5207(16)	Co13	Cl4	2.5881(17)
Co5	O3	2.020(4)	Co13	S13	2.5360(18)
Co5	O14	2.071(4)	Co13	O5	2.017(4)
Co5	O19	1.998(4)	Co13	O21	2.028(4)
Co5	N4[1]	2.098(5)	Co13	O31	2.012(4)
Co6	Cl1	2.6148(17)	Co13	O38	2.039(5)
Co6	S9	2.5171(18)	Co14	Cl2	2.6077(16)
Co6	O2	1.999(4)	Co14	S15	2.5344(19)
Co6	O9	2.004(4)	Co14	O7	2.016(4)
Co6	O11	2.011(4)	Co14	O24	2.024(4)
Co6	O34	2.099(4)	Co14	O32	2.002(4)
Co7	Cl2	2.7071(17)	Co14	O39	2.085(5)
Co7	S1	2.5235(17)	Co15	Cl3	2.5991(16)
Co7	O6	2.024(3)	Co15	S12	2.5337(18)
Co7	O7	2.076(4)	Co15	O14	2.016(4)
Co7	O23	1.998(4)	Co15	O16	2.023(4)
Co7	N1[1]	2.097(4)	Co15	O22	2.009(4)
Co8	S4	2.5227(17)	Co15	O37	2.094(5)
Co8	Cl4	2.7189(18)	Co16	Cl4	2.6179(19)
Co8	O4	2.009(4)	Co16	S16	2.541(2)
Co8	O21	2.076(4)	Co16	O25	2.041(4)
Co8	O28	1.979(4)	Co16	O29	1.999(5)
Co8	N8[1]	2.085(5)	Co16	O31	2.020(4)
Co9	Cl1	2.5991(16)	Co16	O40	2.080(6)

Symmetry code for 1: $1 - x, y, 1/2 - z$

Table S11 Selected bond lengths for {**Co_{32}-B**}.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Co1	S5	2.499(4)	Co33	O7	2.011(10)
Co1	O6	2.001(10)	Co33	O9	2.047(10)
Co1	O17	2.066(9)	Co33	O54	2.039(10)
Co1	O67	2.012(9)	Co33	N10	2.084(12)
Co1	N11	2.048(12)	Co34	Cl11	2.740(5)
Co2	S2	2.546(4)	Co34	S34	2.528(5)
Co2	O29	2.003(10)	Co34	O44	1.983(9)
Co2	O71	1.985(9)	Co34	O53	2.025(9)
Co2	N18	2.094(13)	Co34	N12	2.106(12)
Co2	O126	1.989(9)	Co34	O122	2.066(10)
Co3	Cl4	2.713(4)	Co35	Cl5	2.737(4)

Co3	S7	2.507(4)	Co35	S42	2.542(4)
Co3	O4	2.002(10)	Co35	O51	2.006(10)
Co3	O86	2.045(10)	Co35	O55	2.036(10)
Co3	O126	1.997(10)	Co35	N19	2.099(12)
Co3	N26	2.059(12)	Co35	O128	2.006(10)
Co4	Cl1	2.584(4)	Co36	S14	2.499(4)
Co4	S52	2.541(5)	Co36	Cl8	2.730(4)
Co4	O16	1.998(10)	Co36	O30	2.018(10)
Co4	O61	2.013(10)	Co36	O60	2.009(10)
Co4	O69	2.044(10)	Co36	O68	1.991(9)
Co4	O146	2.090(12)	Co36	N20	2.105(12)
Co5	S6	2.514(4)	Co37	S26	2.518(4)
Co5	Cl9	2.729(4)	Co37	Cl15	2.627(4)
Co5	O13	2.057(10)	Co37	O9	1.994(10)
Co5	O49	2.027(9)	Co37	O20	2.014(10)
Co5	O114	2.041(10)	Co37	O21	2.003(10)
Co5	N29	2.106(12)	Co37	O149	2.067(10)
Co6	S55	2.499(4)	Co38	S30	2.523(4)
Co6	O34	1.955(9)	Co38	O56	1.953(11)
Co6	N3	2.078(12)	Co38	O98	1.998(10)
Co6	O64	2.082(10)	Co38	N24	2.133(12)
Co6	O75	2.031(9)	Co38	O134	2.008(10)
Co7	Cl2	2.625(4)	Co39	Cl5	2.713(5)
Co7	S10	2.553(4)	Co39	S48	2.526(4)
Co7	O6	1.996(10)	Co39	N7	2.081(12)
Co7	O23	1.951(10)	Co39	O85	2.062(10)
Co7	O125	2.028(9)	Co39	O128	2.067(10)
Co7	O156	2.025(11)	Co39	O129	2.045(10)
Co8	Cl3	2.720(4)	Co40	Cl13	2.705(4)
Co8	S1	2.536(4)	Co40	S62	2.520(4)
Co8	O15	1.986(9)	Co40	O32	1.967(9)
Co8	O33	2.047(9)	Co40	O42	2.040(10)
Co8	N1	2.110(12)	Co40	O57	2.081(11)
Co8	O66	1.983(9)	Co40	N17	2.099(12)
Co9	Cl12	2.699(4)	Co41	Cl11	2.619(4)
Co9	S49	2.520(4)	Co41	S41	2.516(5)
Co9	O25	1.974(9)	Co41	O78	2.034(9)
Co9	N5	2.087(12)	Co41	O97	1.993(10)
Co9	O102	2.053(10)	Co41	O122	2.014(10)
Co9	O145	1.999(9)	Co41	O132	2.086(11)
Co10	Cl1	2.711(4)	Co42	Cl7	2.591(4)
Co10	S54	2.510(4)	Co42	S50	2.528(4)
Co10	O16	2.032(10)	Co42	O12	2.024(11)
Co10	O62	2.021(9)	Co42	O72	2.019(11)
Co10	O75	1.997(8)	Co42	O96	2.149(11)
Co10	N35	2.062(12)	Co42	O134	2.027(10)
Co11	Cl6	2.703(4)	Co43	Cl10	2.631(4)

Co11	S12	2.537(4)	Co43	S27	2.552(4)
Co11	O31	2.015(9)	Co43	O38	2.018(12)
Co11	O46	2.007(10)	Co43	O43	2.027(10)
Co11	O131	2.018(9)	Co43	O58	2.083(10)
Co11	N33	2.063(12)	Co43	O150	2.052(12)
Co12	Cl12	2.582(4)	Co44	S9	2.518(4)
Co12	S51	2.532(4)	Co44	Cl15	2.722(4)
Co12	O22	2.038(9)	Co44	O11	2.074(10)
Co12	O102	2.024(10)	Co44	O54	2.021(10)
Co12	O143	1.989(9)	Co44	O65	1.967(9)
Co12	O157	2.080(12)	Co44	N23	2.051(12)
Co13	Cl3	2.610(4)	Co45	S44	2.525(4)
Co13	S38	2.543(4)	Co45	O81	1.978(10)
Co13	O33	2.029(9)	Co45	O82	2.035(11)
Co13	O63	2.033(9)	Co45	O87	2.055(10)
Co13	O83	2.121(10)	Co45	Cl16	2.629(4)
Co13	O93	1.988(10)	Co45	O141	2.084(11)
Co14	Cl3	2.583(4)	Co46	Cl10	2.570(4)
Co14	S46	2.498(5)	Co46	S45	2.526(5)
Co14	O2	2.014(10)	Co46	O58	1.940(10)
Co14	O36	2.023(9)	Co46	O70	2.001(10)
Co14	O89	2.130(11)	Co46	O109	2.095(11)
Co14	O93	2.025(9)	Co46	O138	2.051(10)
Co15	S4	2.527(4)	Co47	Cl5	2.607(4)
Co15	Cl9	2.598(4)	Co47	S53	2.530(5)
Co15	O40	2.073(10)	Co47	O55	2.030(10)
Co15	O94	2.055(10)	Co47	O77	2.055(10)
Co15	O114	1.978(10)	Co47	O101	2.080(9)
Co15	O133	2.001(11)	Co47	C252	1.995(14)
Co16	Cl4	2.607(4)	Co48	S43	2.520(4)
Co16	S13	2.540(4)	Co48	O52	1.998(10)
Co16	O10	2.017(10)	Co48	O53	2.015(10)
Co16	O24	2.019(11)	Co48	O84	2.061(10)
Co16	O86	2.010(10)	Co48	N34	2.086(12)
Co16	O92	2.098(10)	Co49	Cl13	2.593(4)
Co17	S47	2.513(4)	Co49	S58	2.557(5)
Co17	O18	2.106(10)	Co49	O57	2.027(11)
Co17	O48	1.992(9)	Co49	O106	1.914(11)
Co17	N27	2.058(12)	Co49	O115	2.021(12)
Co17	O145	2.027(9)	Co49	O140	2.027(10)
Co18	S59	2.511(4)	Co50	S21	2.519(4)
Co18	O2	2.023(10)	Co50	Cl8	2.731(4)
Co18	O15	2.001(8)	Co50	O60	2.006(10)
Co18	N2	2.082(12)	Co50	O95	2.040(10)
Co18	O74	1.997(9)	Co50	N31	2.120(12)
Co19	Cl4	2.588(4)	Co50	O139	2.016(10)
Co19	S15	2.514(5)	Co51	S29	2.510(4)

Co19	O10	1.986(9)	Co51	N8	2.075(12)
Co19	O29	2.037(10)	Co51	O79	1.992(11)
Co19	O80	2.053(10)	Co51	O81	2.007(10)
Co19	O105	2.036(9)	Co51	Cl16	2.725(4)
Co20	S18	2.521(4)	Co51	O123	2.022(10)
Co20	O31	1.940(9)	Co52	S22	2.542(5)
Co20	N9	2.090(12)	Co52	Cl8	2.595(4)
Co20	O124	1.982(10)	Co52	O41	1.928(11)
Co20	O142	2.030(11)	Co52	O95	2.094(10)
Co21	Cl2	2.617(4)	Co52	O100	1.971(11)
Co21	S25	2.496(4)	Co52	O155	2.132(12)
Co21	O5	2.041(10)	Co53	S39	2.531(5)
Co21	O23	1.999(10)	Co53	O82	2.007(10)
Co21	O112	2.031(10)	Co53	O90	2.026(10)
Co21	O130	2.055(11)	Co53	Cl16	2.607(4)
Co22	Cl6	2.603(4)	Co53	O144	2.144(12)
Co22	S17	2.517(5)	Co53	O147	1.960(10)
Co22	O26	1.985(10)	Co54	Cl8	2.642(4)
Co22	O142	2.044(11)	Co54	S24	2.503(5)
Co22	O151	2.131(13)	Co54	O30	2.010(11)
Co22	O152	2.061(11)	Co54	O35	1.977(10)
Co23	S3	2.538(4)	Co54	O41	1.988(10)
Co23	O8	2.004(9)	Co54	O148	2.079(12)
Co23	O47	2.022(9)	Co55	Cl11	2.613(4)
Co23	N14	2.199(13)	Co55	S35	2.554(5)
Co23	C121	2.032(15)	Co55	O84	1.964(10)
Co24	Cl2	2.731(4)	Co55	O88	2.074(10)
Co24	S31	2.518(4)	Co55	O97	1.993(10)
Co24	O5	2.021(10)	Co55	O113	2.147(13)
Co24	O17	2.008(10)	Co56	Cl5	2.633(4)
Co24	O39	1.980(9)	Co56	S37	2.536(5)
Co24	N6	2.096(12)	Co56	O85	2.037(10)
Co25	Cl9	2.734(4)	Co56	O91	2.073(11)
Co25	S40	2.520(4)	Co56	C239	2.016(14)
Co25	O1	2.100(10)	Co56	C252	1.975(14)
Co25	O13	1.996(10)	Co57	Cl10	2.715(4)
Co25	O14	1.973(10)	Co57	S33	2.524(4)
Co25	N30	2.092(13)	Co57	O43	2.035(10)
Co26	Cl1	2.631(4)	Co57	O50	2.012(10)
Co26	S60	2.535(6)	Co57	O73	1.976(10)
Co26	O59	2.044(10)	Co57	N28	2.098(11)
Co26	O61	2.026(10)	Co58	S63	2.513(5)
Co26	O64	1.993(11)	Co58	N4	2.134(13)
Co26	O108	1.936(12)	Co58	O104	1.994(10)
Co27	S16	2.527(6)	Co58	Cl16	2.725(5)
Co27	Cl14	2.614(4)	Co58	O123	2.041(10)
Co27	O27	2.044(10)	Co58	O147	2.038(10)

Co27	O76	1.967(10)	Co59	S32	2.529(4)
Co27	O127	2.006(10)	Co59	O45	1.997(9)
Co27	O158	2.149(9)	Co59	O50	2.038(9)
Co28	S19	2.518(5)	Co59	O70	2.053(10)
Co28	Cl14	2.581(5)	Co59	N32	2.061(12)
Co28	O3	2.055(9)	Co60	Cl7	2.724(4)
Co28	O76	2.009(10)	Co60	O28	2.112(10)
Co28	C121	2.044(15)	Co60	O98	1.997(10)
Co28	O159	2.098(9)	Co60	N25	2.078(12)
Co29	Cl6	2.618(4)	Co60	S64	2.521(4)
Co29	S23	2.550(5)	Co60	O137	1.933(10)
Co29	O26	1.995(11)	Co61	S8	2.570(5)
Co29	O46	2.038(10)	Co61	Cl7	2.590(4)
Co29	O107	2.067(11)	Co61	O12	2.027(10)
Co29	O136	2.015(9)	Co61	O28	1.983(10)
Co30	Cl9	2.622(4)	Co61	O116	2.002(10)
Co30	S57	2.516(5)	Co61	O118	2.017(12)
Co30	O1	1.954(10)	Co62	S20	2.523(4)
Co30	O19	2.008(11)	Co62	Cl15	2.609(4)
Co30	O99	2.131(13)	Co62	O11	2.020(10)
Co30	O133	2.012(11)	Co62	O20	1.996(10)
Co31	Cl12	2.624(4)	Co62	O110	2.116(11)
Co31	S56	2.525(5)	Co62	O117	2.075(10)
Co31	O18	1.970(10)	Co63	S36	2.516(5)
Co31	O37	2.024(9)	Co63	Cl13	2.620(4)
Co31	O121	2.138(11)	Co63	O106	2.043(11)
Co31	O143	2.041(9)	Co63	O111	2.002(11)
Co32	S28	2.509(4)	Co63	O120	1.962(11)
Co32	Cl14	2.715(4)	Co63	O153	2.083(13)
Co32	O27	1.988(10)	Co64	S61	2.530(4)
Co32	O47	2.012(10)	Co64	O42	2.024(11)
Co32	O119	2.011(11)	Co64	N16	2.110(12)
Co32	N36	2.085(13)	Co64	O120	2.134(11)
Co33	S11	2.515(4)	Co64	O135	2.003(11)

Table S12 Selected bond lengths for {**Co_{32}-C**}.

Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
Co1	Cl1	2.7041(14)	Co9	O2	2.029(3)
Co1	S9	2.5158(15)	Co9	O12	2.058(4)
Co1	O1	2.016(3)	Co9	N5	2.083(4)
Co1	O5	1.996(3)	Co9	O39[1]	1.990(4)
Co1	O16	2.069(3)	Co10	Cl3	2.7178(15)
Co1	N1	2.103(4)	Co10	S6	2.5147(16)
Co2	S7	2.5078(15)	Co10	O7	1.972(4)
Co2	Cl4	2.7332(15)	Co10	O11	2.068(4)
Co2	O12	2.069(3)	Co10	O19	2.025(3)

Co2	O18	2.031(3)	Co10	N7	2.113(5)
Co2	O21	2.019(4)	Co11	S3	2.5123(15)
Co2	N3	2.080(4)	Co11	Cl3	2.7378(15)
Co3	Cl2	2.7081(14)	Co11	O13	2.076(3)
Co3	S8	2.5105(15)	Co11	O19	2.014(4)
Co3	O3	2.032(3)	Co11	O29[1]	1.986(4)
Co3	O6	2.006(3)	Co11	N8	2.104(4)
Co3	O26	2.058(3)	Co12	Cl2	2.5889(14)
Co3	N2	2.103(4)	Co12	S14	2.5245(15)
Co4	S5	2.5335(15)	Co12	O14	2.029(3)
Co4	O3	2.019(4)	Co12	O25	2.070(4)
Co4	O27	2.047(3)	Co12	O27	2.023(4)
Co4	O28	1.983(4)	Co12	O36	2.095(4)
Co4	N4	2.087(4)	Co13	Cl4	2.5883(15)
Co5	S1	2.5416(15)	Co13	S12	2.5503(16)
Co5	O1	2.017(4)	Co13	O15	2.064(4)
Co5	O23	2.059(3)	Co13	O18	2.001(4)
Co5	O24	1.989(4)	Co13	O30	2.028(4)
Co5	N6	2.103(4)	Co13	O38	2.071(4)
Co6	Cl1	2.6189(14)	Co14	Cl4	2.5994(15)
Co6	S13	2.5247(15)	Co14	S10	2.5577(15)
Co6	O8	1.997(3)	Co14	O2	2.001(4)
Co6	O9	2.006(4)	Co14	O30	2.038(4)
Co6	O16	2.016(3)	Co14	O32[1]	2.071(4)
Co6	O33	2.109(4)	Co14	O40	2.091(4)
Co7	Cl2	2.6477(14)	Co15	Cl3	2.5885(14)
Co7	S16	2.5678(15)	Co15	S11	2.5321(15)
Co7	O4	2.072(3)	Co15	O10[1]	2.015(4)
Co7	O14	2.032(3)	Co15	O13	2.025(4)
Co7	O26	2.007(4)	Co15	O22	2.009(4)
Co7	O35	2.070(5)	Co15	O34	2.119(5)
Co8	Cl1	2.6115(14)	Co15	N15	2.119(5)
Co8	S2	2.5182(15)	Co16	Cl3	2.6569(15)
Co8	O8	1.991(4)	Co16	S15	2.5443(17)
Co8	O17	2.021(4)	Co16	O11	1.996(4)
Co8	O23	2.013(4)	Co16	O20	2.033(4)
Co8	O37	2.114(4)	Co16	O22	2.017(4)
Co9	S4	2.5231(15)	Co16	O31	2.087(4)

Symmetry code for 1: $1 - x, y, 1/2 - z$

Table S13 Selected bond lengths for {**Co$_{40}$**}.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Co1	S3	2.54	Co11	O11	1.9961
Co1	O2	2.0107	Co11	O22	1.9985
Co1	O4	2.058	Co11	O40	2.0921
Co1	O12	1.9984	Co12	Cl2	2.5761
Co1	N7[1]	2.1096	Co12	S12	2.5118
Co2	S1	2.5182	Co12	O5	2.0207
Co2	Cl2	2.7236	Co12	O11	2.0288
Co2	O1	2.0049	Co12	O23	2.0447
Co2	O8	2.0942	Co12	O42	2.0718
Co2	O10	1.9866	Co13	S16	2.525
Co2	N3[1]	2.1072	Co13	O25	2.0027
Co3	S4	2.554	Co13	O32	2.0545
Co3	O1	1.9997	Co13	O39	1.9812
Co3	O5	2.0797	Co13	N10[1]	2.0853
Co3	O14	1.994	Co14	S15	2.5476
Co3	N4[1]	2.1185	Co14	O20	2.003
Co4	Cl1	2.5912	Co14	O25	1.9919
Co4	S5	2.5145	Co14	N8[1]	2.1029
Co4	O4	2.0125	Co14	O58	2.0523
Co4	O6	2.0551	Co15	Cl3	2.6035
Co4	O19	1.9965	Co15	S13	2.5388
Co4	O31	2.0766	Co15	O9	1.9973
Co5	S6	2.5276	Co15	O21	1.9963
Co5	O2	2.0084	Co15	O30	2.0497
Co5	O7	2.0728	Co15	O45	2.0653
Co5	O15	1.9913	Co16	Cl3	2.6158
Co5	N9[1]	2.1038	Co16	S14	2.533
Co6	S7	2.5269	Co16	O13	2.0198
Co6	O16	2.0319	Co16	O21	2.0515
Co6	O26	2.0404	Co16	O37	2.0474
Co6	O33	1.9653	Co16	O48	2.0872
Co6	N1[1]	2.0792	Co17	Cl4	2.5989
Co7	S2	2.5163	Co17	S18	2.5177
Co7	O3	2.0231	Co17	O17	2.0234
Co7	O9	2.0716	Co17	O24	2.0494
Co7	O29	1.9765	Co17	O34	2.0042
Co7	N5[1]	2.0904	Co17	O44	2.091
Co8	S8	2.5278	Co18	Cl4	2.6027

Co8	O16	2.0087	Co18	S17	2.5039
Co8	O17	2.0738	Co18	O26	2.0081
Co8	O27	1.9861	Co18	O28	2.071
Co8	N2[1]	2.0923	Co18	O34	2.0261
Co9	S11	2.5493	Co18	O47	2.1186
Co9	O3	2.0093	Co19	Cl5	2.594
Co9	O13	2.0673	Co19	S19	2.5063
Co9	O35	1.9747	Co19	O36	2.0239
Co9	N6[1]	2.0989	Co19	O41	2.0158
Co10	Cl1	2.6004	Co19	O46	2.1177
Co10	S10	2.5187	Co19	O58	2.0254
Co10	O7	2.0025	Co20	Cl5	2.6188
Co10	O18	2.0382	Co20	S20	2.5237
Co10	O19	2.0273	Co20	O32	2.0292
Co10	O43	2.0866	Co20	O38	2.0314
Co11	Cl2	2.626	Co20	O41	2.001
Co11	S9	2.5392	Co20	O49	2.1166
Co11	O8	2.0063			

Symmetry code for 1: $1 - x$, $1 - y$, $1 - z$

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