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Encapsulation of cobaltocenium ions in a zeolite-like metal-organic framework

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Experimental Methods

Powder X-ray diffraction (PXRD)

The PXRD patterns were collected on an Ultima IV X-ray diffractometer (Rigaku) equipped with Cu K_α source, with a scan rate of 2°/min and a step size of 0.04°. The simulated XRD pattern of the ZMOF was generated using the crystal structure visualization tool Mercury (CCDC), from the CIF file obtained via SC-XRD results.

Scanning electron microscope (SEM)

The morphology of all crystals was characterized using an SEM (Leo 1530 VP field emission scanning electron microscope). Samples were coated with Au using a Denton Vacuum Desk II sputter-coater for SEM analysis.

Thermogravimetric analysis (TGA)

The TGA was conducted using a SDT Q600 (TA Instruments). The samples were heated from room temperature to 600 °C at a rate of 5 °C/min under nitrogen.

Fourier transform infrared spectroscopy (FT-IR)

The FT-IR spectra was collected using the Nicolet 380 FT-IR ATR spectrometer.

Elemental analysis

The elemental analysis of Cp_2Co^+-*sod*-ZMOF was completed by Galbraith Laboratories, Inc. Found C: 39.11 wt. %, N: 9.18 wt. %, In: 18.80 wt. %, Co: 9.44 wt. %, theoretical C: 39.24, N: 9.15, In:18.75, and Co:9.62 wt. %. The Total Reflection X-ray Fluorescence (TXRF) was measured on the S2 PICOFOX (Bruker) equipped with Mo K_α radiation with a high-efficiency module. The radiation source was operated at 50 kV and 600 µA and data was collected for 300 s. About 20 mg of sample was used for analysis to find metal ratios in Cp_2Co^+-*sod*-ZMOF. The indium to cobalt ratio was found to be Co: 31.8 % and In: 68.1 % which was in agreement with the elemental analysis.

Gas adsorption analysis

The adsorption and desorption isotherms using ultra-high purity CO_2 and N_2 (>99.9999%) were obtained on an ASAP 2020 Plus (Micromeritics instrument corporation). For the surface area and porosity analysis, the MOF crystals were washed three times with fresh DMF and activated at 120°C under vacuum for 24 hours. Activated and dried (~50 mg) samples were transferred to analysis tubes equipped with filler rods and capped with a seal frit. The samples were further dried and evacuated in the instrument for 10 hours at 120°C. Samples were weighed again after the activation step to get the dry sample weight. The isotherms were measured from a relative pressure P/P_o of 0.01 to 1 in a liquid nitrogen (77 K) bath and from 0.0001 to 0.035 for CO_2 (273 K) in an ice bath. The surface area was calculated by the Brunauer–Emmett–Teller (BET) model.

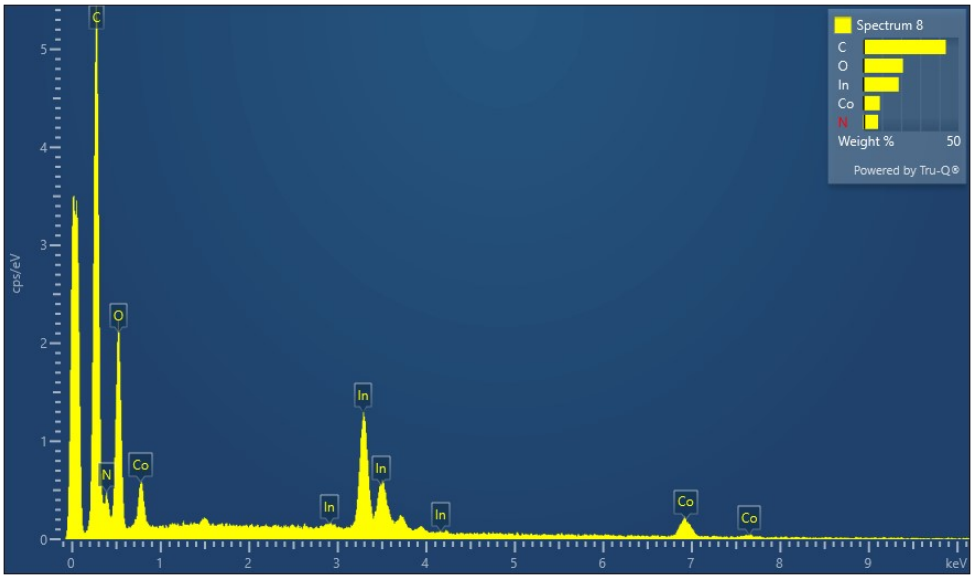

Figure S1. The EDS spectra for **Cp_2Co^+-*sod*-ZMOF**

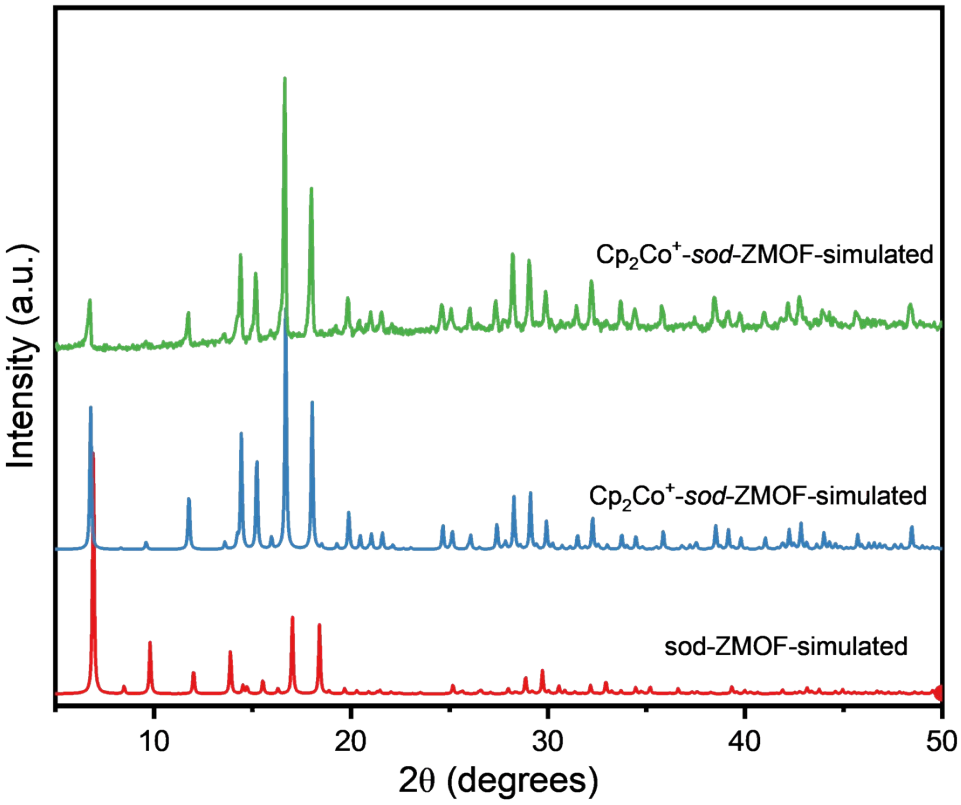

Figure S2. The PXRD comparison of sod-ZMOF, with **Cp_2Co^+-*sod*-ZMOF**, showing the peak shifts in the **Cp_2Co^+-*sod*-ZMOF** as a result of framework expansion.

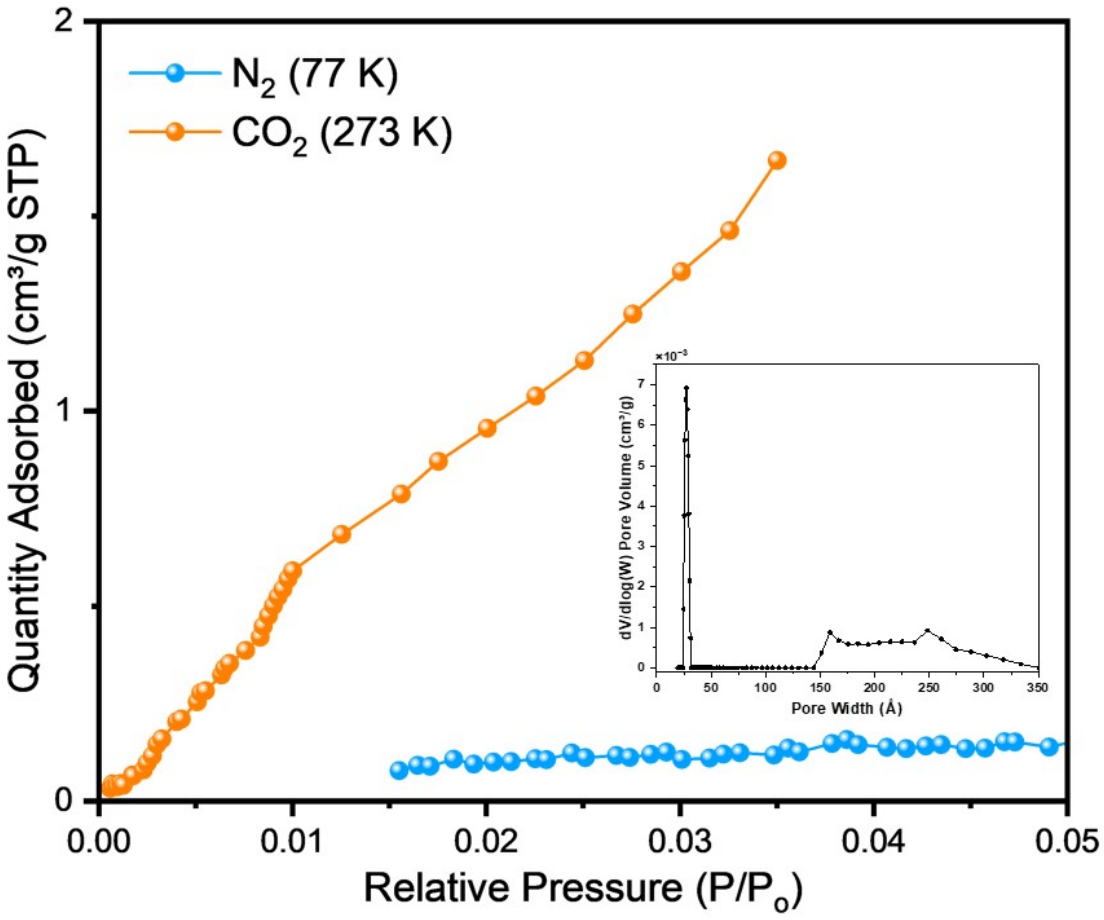

Figure S3. Gas adsorption isotherms of **Cp_2Co^+-sod-ZMOF**

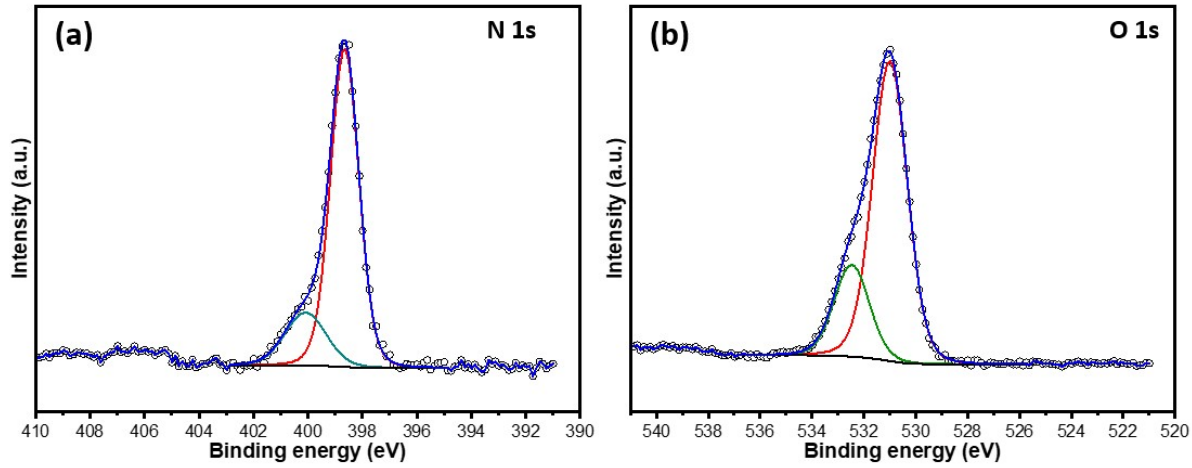

Figure S4. High resolution XPS spectra for **Cp_2Co^+-*sod*-ZMOF** (a) N 1s, and (b) O 1s

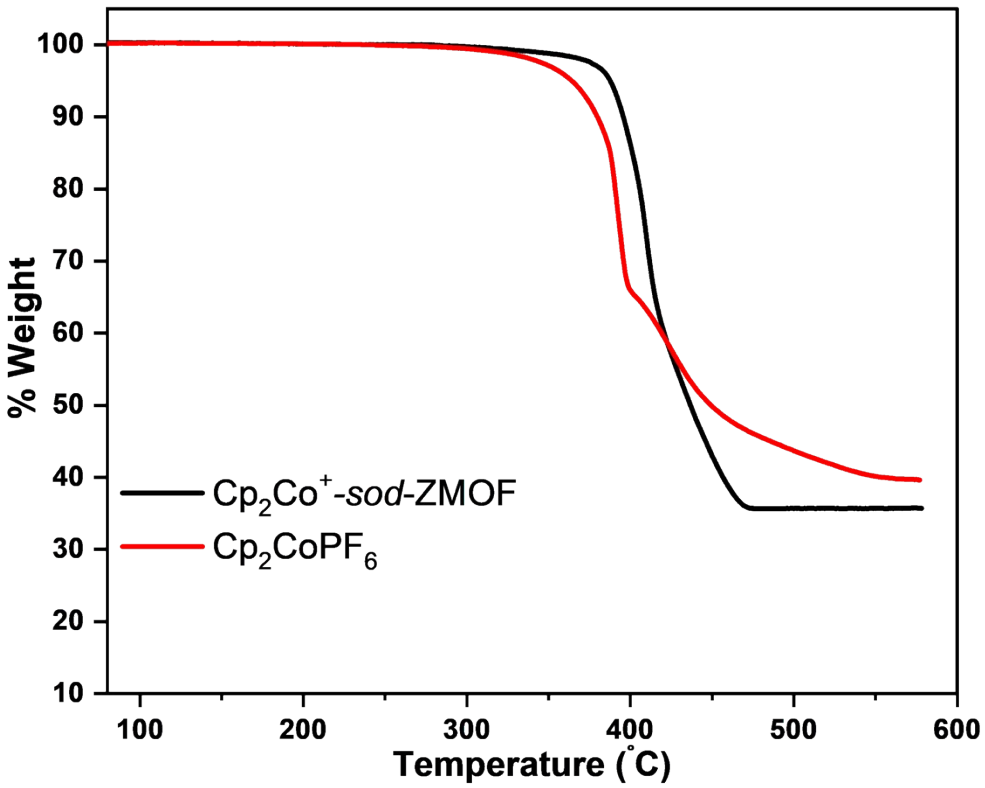

Figure S5. TGA curves of **Cp_2Co^+-*sod*-ZMOF** and the Cp_2CoPF_6 compound.

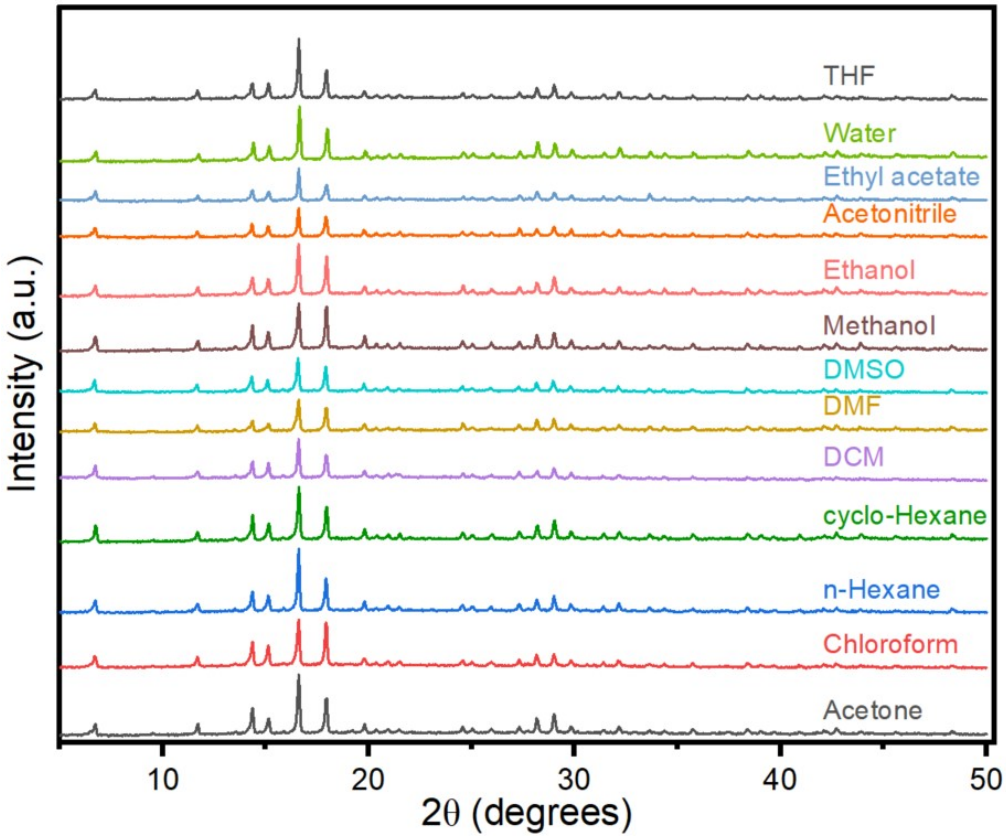

Figure S6. PXRD patterns **Cp_2Co^+-*sod*-ZMOF** in different lab solvents.

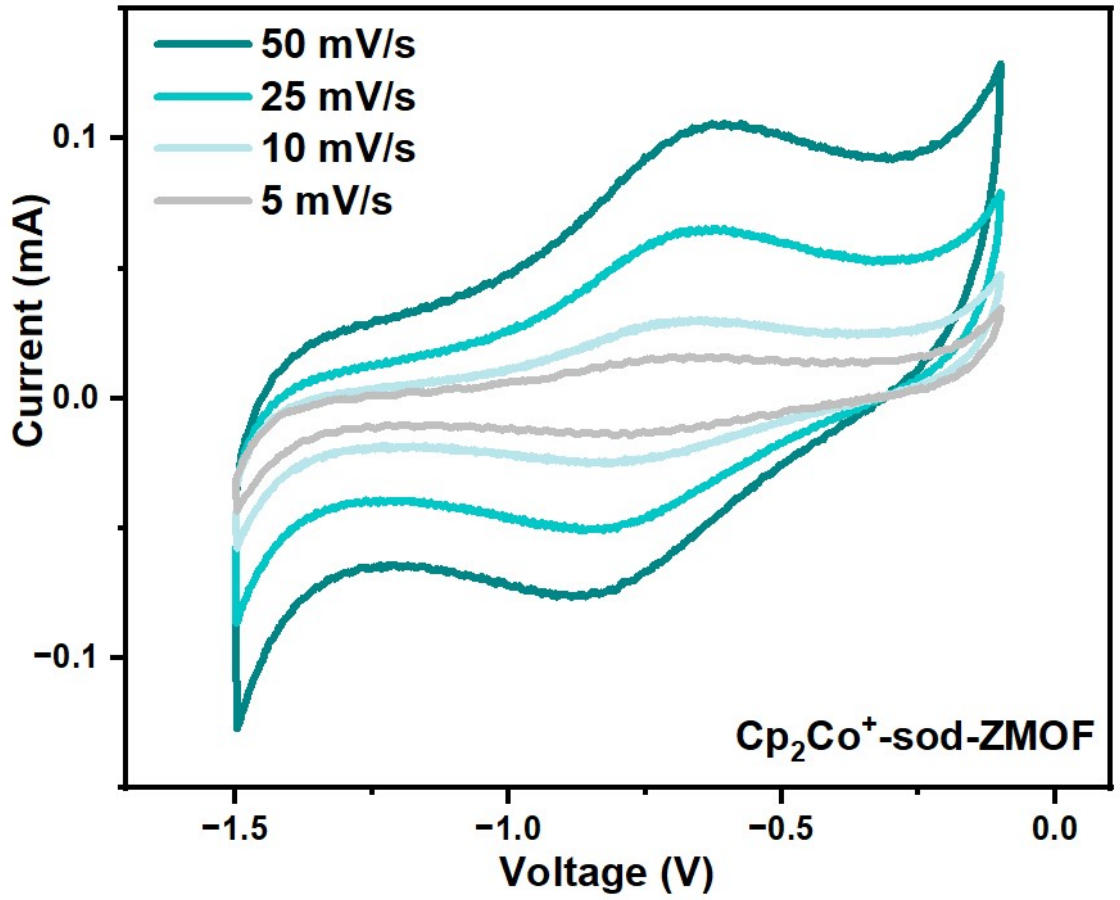

Figure S7. CV curves of **Cp_2Co^+-*sod*-ZMOF** at different scan rates.

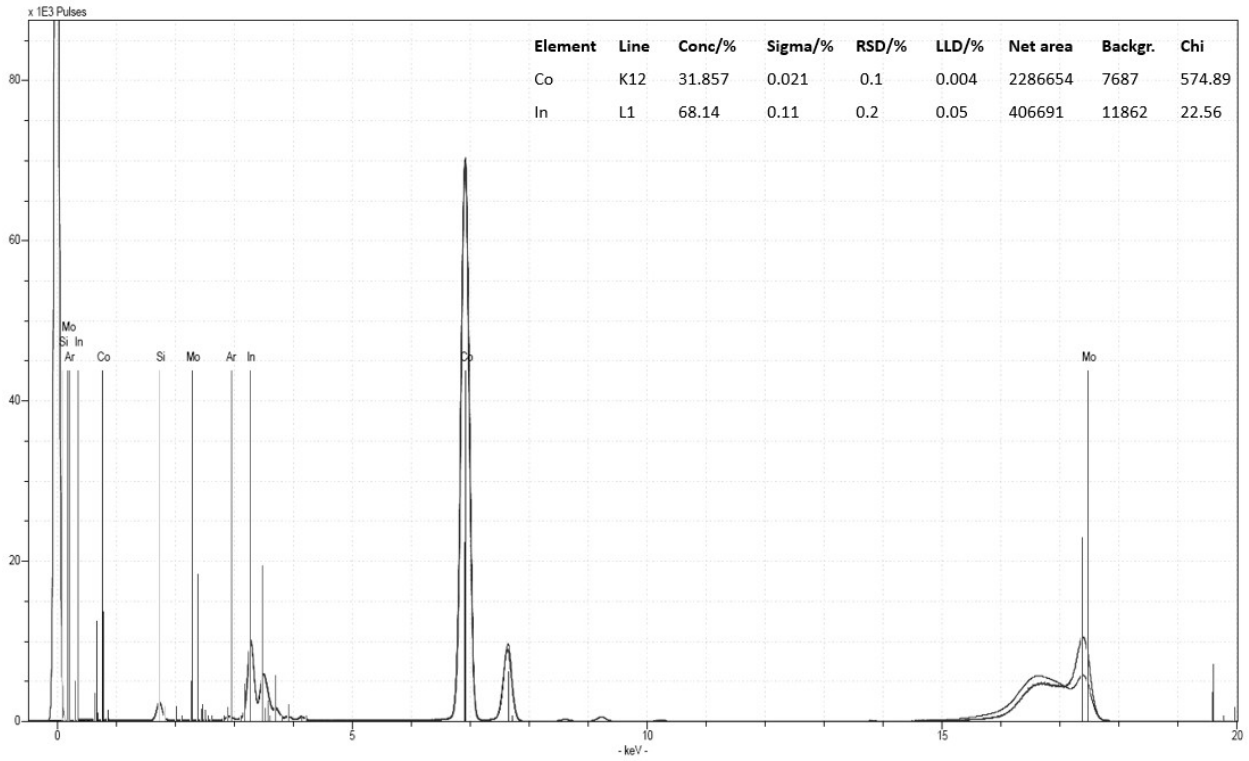

Figure S8. The TXRF spectrum of the **Cp_2Co^+-sod-ZMOF**.

Table S1. Crystal data and structure refinement for **Cp_2Co^+-*sod*-ZMOF**

Identification code	**2261904**	
Empirical formula	$C_{20}H_{14}CoInN_4O_8$	
Formula weight	612.10	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Cubic	
Space group	F d -3 c	
Unit cell dimensions	a = 36.778(4) Å	a= 90°
	b = 36.778(4) Å	b= 90°
	c = 36.778(4) Å	g = 90°
Volume	49745(17) $Å^3$	
Z	96	
Density (calculated)	1.962 Mg/m^3	
Absorption coefficient	1.972 mm^{-1}	
F(000)	28992	
Crystal size	0.100 x 0.070 x 0.070 mm^3	
Theta range for data collection	2.713 to 28.687°.	
Index ranges	-49<=h<=29, -46<=k<=48, -46<=l<=38	
Reflections collected	48380	
Independent reflections	2681 [R(int) = 0.0371]	
Completeness to theta = 25.242°	99.4 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2681 / 511 / 312	
Goodness-of-fit on F^2	1.228	
Final R indices [I>2sigma(I)]	R1 = 0.0273, wR2 = 0.0586	
R indices (all data)	R1 = 0.0335, wR2 = 0.0632	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.371 and -0.480 $e.Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **Cp_2Co^+-*sod*-ZMOF**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
In(1)	5000	6193(1)	3693(1)	29(1)
O(1)	6364(1)	7202(1)	3107(1)	44(1)
O(3)	5258(1)	6084(1)	3133(1)	37(1)
N(1)	5827(1)	7057(1)	3620(1)	30(1)
N(2)	5403(1)	6623(1)	3616(1)	29(1)
C(1)	5547(1)	6904(1)	3796(1)	30(1)
C(2)	5863(1)	6861(1)	3303(1)	33(1)
C(3)	5602(1)	6594(1)	3302(1)	33(1)
C(4)	5500(1)	6306(1)	3037(1)	41(1)
C(5)	6146(1)	6962(1)	3038(1)	43(1)
O(2B)	6115(9)	6813(8)	2711(5)	56(3)
O(4B)	5632(8)	6335(9)	2722(4)	52(3)
O(2A)	6194(15)	6744(14)	2760(13)	53(6)
O(4A)	5713(15)	6258(13)	2761(12)	49(6)
Co(1)	5526(1)	5526(1)	1974(1)	29(1)
C(16)	5104(8)	5539(9)	2323(13)	35(4)
C(17)	5422(9)	5430(8)	2510(5)	28(3)
C(18)	5549(8)	5105(8)	2344(12)	31(4)
C(19)	5314(16)	5023(9)	2052(8)	36(4)
C(20)	5042(9)	5292(17)	2036(8)	39(4)
C(21)	5948(6)	5912(7)	1996(6)	30(4)
C(22)	5617(5)	6069(4)	1874(7)	25(2)
C(23)	5502(6)	5872(9)	1566(6)	31(3)
C(24)	5760(10)	5597(6)	1496(6)	35(3)
C(25)	6025(7)	5611(6)	1766(10)	37(4)
Co(2)	5000	7500	2500	38(1)
C(6)	4793(11)	7573(8)	3014(9)	46(7)
C(7)	4918(9)	7212(8)	2956(8)	45(5)
C(8)	4716(8)	7061(6)	2661(8)	47(5)
C(9)	4464(7)	7327(8)	2541(7)	48(6)
C(10)	4529(9)	7653(7)	2741(10)	48(7)

C(11)	5454(8)	7789(9)	2409(8)	50(6)
C(12)	5509(8)	7437(8)	2275(11)	53(7)
C(13)	5228(11)	7361(8)	2028(11)	55(8)
C(14)	5036(8)	7685(9)	1969(8)	56(7)
C(15)	5163(9)	7943(7)	2217(8)	53(6)

Table S3. Bond lengths [Å] and angles [°] for **Cp_2Co^+-*sod*-ZMOF**.

In(1)-N(2)#1	2.185(2)
In(1)-N(2)	2.185(2)
In(1)-N(1)#2	2.223(2)
In(1)-N(1)#3	2.223(2)
In(1)-O(3)#1	2.302(2)
In(1)-O(3)	2.3025(19)
O(1)-C(5)	1.219(4)
O(3)-C(4)	1.257(4)
N(1)-C(1)	1.339(3)
N(1)-C(2)	1.377(3)
N(2)-C(1)	1.339(3)
N(2)-C(3)	1.370(3)
C(1)-H(1)	0.9500
C(2)-C(3)	1.374(4)
C(2)-C(5)	1.475(4)
C(3)-C(4)	1.486(4)
C(4)-O(4B)	1.263(14)
C(4)-O(4A)	1.30(3)
C(5)-O(2A)	1.31(3)
C(5)-O(2B)	1.326(16)
O(2B)-H(2B)	0.8400
O(2A)-H(2A)	0.8400
Co(1)-C(23)	1.97(2)
Co(1)-C(24)	1.973(13)
Co(1)-C(20)	1.992(16)
Co(1)-C(25)	2.012(18)
Co(1)-C(16)	2.02(3)
Co(1)-C(19)	2.030(19)
Co(1)-C(17)	2.040(19)
Co(1)-C(22)	2.055(16)
Co(1)-C(18)	2.06(3)
Co(1)-C(21)	2.102(19)
C(16)-C(20)	1.409(11)
C(16)-C(17)	1.418(12)

C(16)-H(16)	0.9500
C(17)-C(18)	1.422(11)
C(17)-H(17)	0.9500
C(18)-C(19)	1.410(11)
C(18)-H(18)	0.9500
C(19)-C(20)	1.412(11)
C(19)-H(19)	0.9500
C(20)-H(20)	1.0000
C(21)-C(25)	1.418(11)
C(21)-C(22)	1.420(11)
C(21)-H(21)	0.9500
C(22)-C(23)	1.409(11)
C(22)-H(22)	0.9500
C(23)-C(24)	1.413(11)
C(23)-H(23)	0.9500
C(24)-C(25)	1.393(11)
C(24)-H(24)	1.0000
C(25)-H(25)	0.9500
Co(2)-C(13)	2.00(4)
Co(2)-C(7)	2.01(3)
Co(2)-C(11)	2.01(3)
Co(2)-C(8)	2.01(2)
Co(2)-C(10)	2.02(4)
Co(2)-C(15)	2.03(2)
Co(2)-C(6)	2.05(4)
Co(2)-C(12)	2.06(3)
Co(2)-C(14)	2.07(3)
Co(2)-C(9)	2.08(3)
C(6)-C(7)	1.42(2)
C(6)-C(10)	1.43(2)
C(6)-H(6)	0.9500
C(7)-C(8)	1.425(19)
C(7)-H(7)	0.9500
C(8)-C(9)	1.42(2)
C(8)-H(8)	0.9500
C(9)-C(10)	1.43(2)

C(9)-H(9)	0.9500
C(10)-H(10)	0.9500
C(11)-C(15)	1.40(2)
C(11)-C(12)	1.40(2)
C(11)-H(11)	0.9500
C(12)-C(13)	1.40(2)
C(12)-H(12)	0.9500
C(13)-C(14)	1.40(2)
C(13)-H(13)	0.9500
C(14)-C(15)	1.40(2)
C(14)-H(14)	0.9500
C(15)-H(15)	0.9500

N(2)#1-In(1)-N(2)	130.41(11)
N(2)#1-In(1)-N(1)#2	88.91(8)
N(2)-In(1)-N(1)#2	101.24(8)
N(2)#1-In(1)-N(1)#3	101.24(8)
N(2)-In(1)-N(1)#3	88.91(8)
N(1)#2-In(1)-N(1)#3	155.80(11)
N(2)#1-In(1)-O(3)#1	74.32(7)
N(2)-In(1)-O(3)#1	154.67(8)
N(1)#2-In(1)-O(3)#1	82.51(8)
N(1)#3-In(1)-O(3)#1	79.27(8)
N(2)#1-In(1)-O(3)	154.66(8)
N(2)-In(1)-O(3)	74.32(7)
N(1)#2-In(1)-O(3)	79.27(8)
N(1)#3-In(1)-O(3)	82.51(8)
O(3)#1-In(1)-O(3)	81.92(10)
C(4)-O(3)-In(1)	115.45(17)
C(1)-N(1)-C(2)	105.3(2)
C(1)-N(1)-In(1)#4	128.53(17)
C(2)-N(1)-In(1)#4	125.99(18)
C(1)-N(2)-C(3)	105.4(2)
C(1)-N(2)-In(1)	139.79(18)
C(3)-N(2)-In(1)	114.50(17)
N(2)-C(1)-N(1)	112.9(2)

N(2)-C(1)-H(1)	123.6
N(1)-C(1)-H(1)	123.6
C(3)-C(2)-N(1)	108.0(2)
C(3)-C(2)-C(5)	132.3(3)
N(1)-C(2)-C(5)	119.7(3)
N(2)-C(3)-C(2)	108.4(2)
N(2)-C(3)-C(4)	118.3(3)
C(2)-C(3)-C(4)	133.4(3)
O(3)-C(4)-O(4B)	125.7(9)
O(3)-C(4)-O(4A)	123.9(15)
O(3)-C(4)-C(3)	117.2(3)
O(4B)-C(4)-C(3)	116.5(10)
O(4A)-C(4)-C(3)	117.4(16)
O(1)-C(5)-O(2A)	121.1(16)
O(1)-C(5)-O(2B)	123.0(10)
O(1)-C(5)-C(2)	120.6(3)
O(2A)-C(5)-C(2)	117.1(15)
O(2B)-C(5)-C(2)	115.8(10)
C(5)-O(2B)-H(2B)	109.5
C(5)-O(2A)-H(2A)	109.5
C(23)-Co(1)-C(24)	42.0(4)
C(23)-Co(1)-C(20)	109.1(10)
C(24)-Co(1)-C(20)	123.3(14)
C(23)-Co(1)-C(25)	69.6(5)
C(24)-Co(1)-C(25)	40.9(3)
C(20)-Co(1)-C(25)	158(2)
C(23)-Co(1)-C(16)	115.8(12)
C(24)-Co(1)-C(16)	154.1(17)
C(20)-Co(1)-C(16)	41.1(5)
C(25)-Co(1)-C(16)	160(2)
C(23)-Co(1)-C(19)	132.9(15)
C(24)-Co(1)-C(19)	114.4(6)
C(20)-Co(1)-C(19)	41.1(4)
C(25)-Co(1)-C(19)	123.1(16)
C(16)-Co(1)-C(19)	68.6(6)
C(23)-Co(1)-C(17)	147.2(14)

C(24)-Co(1)-C(17)	164.8(17)
C(20)-Co(1)-C(17)	69.2(4)
C(25)-Co(1)-C(17)	124.4(15)
C(16)-Co(1)-C(17)	40.9(4)
C(19)-Co(1)-C(17)	68.4(4)
C(23)-Co(1)-C(22)	40.9(4)
C(24)-Co(1)-C(22)	69.1(4)
C(20)-Co(1)-C(22)	125.7(19)
C(25)-Co(1)-C(22)	68.5(4)
C(16)-Co(1)-C(22)	102.4(10)
C(19)-Co(1)-C(22)	167(2)
C(17)-Co(1)-C(22)	111.8(9)
C(23)-Co(1)-C(18)	171.6(16)
C(24)-Co(1)-C(18)	131.8(13)
C(20)-Co(1)-C(18)	68.7(6)
C(25)-Co(1)-C(18)	109.2(10)
C(16)-Co(1)-C(18)	68.3(4)
C(19)-Co(1)-C(18)	40.3(5)
C(17)-Co(1)-C(18)	40.5(4)
C(22)-Co(1)-C(18)	147.1(15)
C(23)-Co(1)-C(21)	68.1(4)
C(24)-Co(1)-C(21)	67.9(5)
C(20)-Co(1)-C(21)	161(2)
C(25)-Co(1)-C(21)	40.2(4)
C(16)-Co(1)-C(21)	121.9(18)
C(19)-Co(1)-C(21)	153(2)
C(17)-Co(1)-C(21)	102.6(8)
C(22)-Co(1)-C(21)	39.9(4)
C(18)-Co(1)-C(21)	116.8(13)
C(20)-C(16)-C(17)	108.3(7)
C(20)-C(16)-Co(1)	68.5(11)
C(17)-C(16)-Co(1)	70.4(12)
C(20)-C(16)-H(16)	125.8
C(17)-C(16)-H(16)	125.9
Co(1)-C(16)-H(16)	126.8
C(16)-C(17)-C(18)	107.5(7)

C(16)-C(17)-Co(1)	68.7(13)
C(18)-C(17)-Co(1)	70.6(14)
C(16)-C(17)-H(17)	126.2
C(18)-C(17)-H(17)	126.3
Co(1)-C(17)-H(17)	126.0
C(19)-C(18)-C(17)	107.8(7)
C(19)-C(18)-Co(1)	68.6(11)
C(17)-C(18)-Co(1)	68.8(13)
C(19)-C(18)-H(18)	126.1
C(17)-C(18)-H(18)	126.1
Co(1)-C(18)-H(18)	128.0
C(18)-C(19)-C(20)	108.4(7)
C(18)-C(19)-Co(1)	71.1(13)
C(20)-C(19)-Co(1)	68.0(10)
C(18)-C(19)-H(19)	125.8
C(20)-C(19)-H(19)	125.8
Co(1)-C(19)-H(19)	126.6
C(16)-C(20)-C(19)	107.9(7)
C(16)-C(20)-Co(1)	70.4(13)
C(19)-C(20)-Co(1)	70.9(11)
C(16)-C(20)-H(20)	126.1
C(19)-C(20)-H(20)	126.0
Co(1)-C(20)-H(20)	126.0
C(25)-C(21)-C(22)	107.6(7)
C(25)-C(21)-Co(1)	66.5(9)
C(22)-C(21)-Co(1)	68.3(10)
C(25)-C(21)-H(21)	126.2
C(22)-C(21)-H(21)	126.2
Co(1)-C(21)-H(21)	130.6
C(23)-C(22)-C(21)	107.6(7)
C(23)-C(22)-Co(1)	66.3(11)
C(21)-C(22)-Co(1)	71.8(10)
C(23)-C(22)-H(22)	126.2
C(21)-C(22)-H(22)	126.2
Co(1)-C(22)-H(22)	127.1
C(22)-C(23)-C(24)	108.2(7)

C(22)-C(23)-Co(1)	72.8(11)
C(24)-C(23)-Co(1)	69.1(9)
C(22)-C(23)-H(23)	125.9
C(24)-C(23)-H(23)	125.9
Co(1)-C(23)-H(23)	123.8
C(25)-C(24)-C(23)	108.3(7)
C(25)-C(24)-Co(1)	71.1(10)
C(23)-C(24)-Co(1)	68.9(10)
C(25)-C(24)-H(24)	125.9
C(23)-C(24)-H(24)	125.9
Co(1)-C(24)-H(24)	125.9
C(24)-C(25)-C(21)	108.3(7)
C(24)-C(25)-Co(1)	68.0(9)
C(21)-C(25)-Co(1)	73.3(10)
C(24)-C(25)-H(25)	125.9
C(21)-C(25)-H(25)	125.9
Co(1)-C(25)-H(25)	124.4
C(13)-Co(2)-C(7)	130.9(13)
C(13)-Co(2)-C(11)	69.0(12)
C(7)-Co(2)-C(11)	123.0(9)
C(13)-Co(2)-C(8)	105.6(13)
C(7)-Co(2)-C(8)	41.5(6)
C(11)-Co(2)-C(8)	154.9(9)
C(13)-Co(2)-C(10)	144.3(15)
C(7)-Co(2)-C(10)	69.7(11)
C(11)-Co(2)-C(10)	129.5(12)
C(8)-Co(2)-C(10)	69.5(10)
C(13)-Co(2)-C(15)	68.5(11)
C(7)-Co(2)-C(15)	154.1(8)
C(11)-Co(2)-C(15)	40.6(6)
C(8)-Co(2)-C(15)	162.0(6)
C(10)-Co(2)-C(15)	104.8(12)
C(13)-Co(2)-C(6)	171.8(14)
C(7)-Co(2)-C(6)	41.0(7)
C(11)-Co(2)-C(6)	113.0(14)
C(8)-Co(2)-C(6)	69.0(11)

C(10)-Co(2)-C(6)	40.9(8)
C(15)-Co(2)-C(6)	118.5(11)
C(13)-Co(2)-C(12)	40.5(8)
C(7)-Co(2)-C(12)	114.4(13)
C(11)-Co(2)-C(12)	40.3(7)
C(8)-Co(2)-C(12)	120.0(11)
C(10)-Co(2)-C(12)	169.8(13)
C(15)-Co(2)-C(12)	67.3(10)
C(6)-Co(2)-C(12)	136.1(16)
C(13)-Co(2)-C(14)	40.3(7)
C(7)-Co(2)-C(14)	166.0(9)
C(11)-Co(2)-C(14)	67.4(10)
C(8)-Co(2)-C(14)	125.0(8)
C(10)-Co(2)-C(14)	112.1(13)
C(15)-Co(2)-C(14)	39.9(6)
C(6)-Co(2)-C(14)	147.9(13)
C(12)-Co(2)-C(14)	66.4(11)
C(13)-Co(2)-C(9)	112.6(13)
C(7)-Co(2)-C(9)	68.6(10)
C(11)-Co(2)-C(9)	164.4(9)
C(8)-Co(2)-C(9)	40.6(6)
C(10)-Co(2)-C(9)	40.7(7)
C(15)-Co(2)-C(9)	124.4(8)
C(6)-Co(2)-C(9)	67.8(11)
C(12)-Co(2)-C(9)	149.0(12)
C(14)-Co(2)-C(9)	103.2(9)
C(7)-C(6)-C(10)	107.8(8)
C(7)-C(6)-Co(2)	67.7(17)
C(10)-C(6)-Co(2)	68.5(18)
C(7)-C(6)-H(6)	126.1
C(10)-C(6)-H(6)	126.1
Co(2)-C(6)-H(6)	129.4
C(6)-C(7)-C(8)	108.1(8)
C(6)-C(7)-Co(2)	71.3(19)
C(8)-C(7)-Co(2)	69.5(13)
C(6)-C(7)-H(7)	125.9

C(8)-C(7)-H(7)	125.9
Co(2)-C(7)-H(7)	124.8
C(9)-C(8)-C(7)	107.9(8)
C(9)-C(8)-Co(2)	72.0(13)
C(7)-C(8)-Co(2)	68.9(13)
C(9)-C(8)-H(8)	126.1
C(7)-C(8)-H(8)	126.1
Co(2)-C(8)-H(8)	124.6
C(8)-C(9)-C(10)	108.0(8)
C(8)-C(9)-Co(2)	67.3(12)
C(10)-C(9)-Co(2)	67.7(17)
C(8)-C(9)-H(9)	126.0
C(10)-C(9)-H(9)	126.0
Co(2)-C(9)-H(9)	130.5
C(9)-C(10)-C(6)	107.8(8)
C(9)-C(10)-Co(2)	71.6(16)
C(6)-C(10)-Co(2)	70.6(18)
C(9)-C(10)-H(10)	126.1
C(6)-C(10)-H(10)	126.1
Co(2)-C(10)-H(10)	123.3
C(15)-C(11)-C(12)	107.8(8)
C(15)-C(11)-Co(2)	70.4(13)
C(12)-C(11)-Co(2)	71.9(17)
C(15)-C(11)-H(11)	126.1
C(12)-C(11)-H(11)	126.1
Co(2)-C(11)-H(11)	123.3
C(11)-C(12)-C(13)	107.8(8)
C(11)-C(12)-Co(2)	67.8(16)
C(13)-C(12)-Co(2)	67(2)
C(11)-C(12)-H(12)	126.1
C(13)-C(12)-H(12)	126.1
Co(2)-C(12)-H(12)	130.4
C(14)-C(13)-C(12)	107.5(9)
C(14)-C(13)-Co(2)	72.8(19)
C(12)-C(13)-Co(2)	72.3(18)
C(14)-C(13)-H(13)	126.2

C(12)-C(13)-H(13)	126.2
Co(2)-C(13)-H(13)	120.5
C(15)-C(14)-C(13)	108.0(8)
C(15)-C(14)-Co(2)	68.3(13)
C(13)-C(14)-Co(2)	67(2)
C(15)-C(14)-H(14)	126.0
C(13)-C(14)-H(14)	126.0
Co(2)-C(14)-H(14)	130.3
C(14)-C(15)-C(11)	108.1(8)
C(14)-C(15)-Co(2)	71.9(14)
C(11)-C(15)-Co(2)	69.0(13)
C(14)-C(15)-H(15)	126.0
C(11)-C(15)-H(15)	126.0
Co(2)-C(15)-H(15)	124.8

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,z+1/4,y-1/4 #2 y-1/4,-z+1,x-1/4 #3 -y+5/4,x,-z+3/4

#4 z+1/4,x+1/4,-y+1

Table S4. Anisotropic displacement parameters ($Å^2$x 10^3)for **Cp_2Co^+-*sod*-ZMOF**. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
In(1)	27(1)	30(1)	30(1)	-8(1)	-1(1)	1(1)
O(1)	46(1)	43(1)	45(1)	5(1)	18(1)	1(1)
O(3)	39(1)	41(1)	31(1)	-16(1)	-2(1)	3(1)
N(1)	34(1)	30(1)	26(1)	-6(1)	7(1)	-1(1)
N(2)	31(1)	31(1)	26(1)	-9(1)	5(1)	-2(1)
C(1)	32(1)	32(1)	25(1)	-7(1)	7(1)	-2(1)
C(2)	39(1)	37(1)	24(1)	-5(1)	9(1)	3(1)
C(3)	37(1)	38(1)	24(1)	-8(1)	6(1)	1(1)
C(4)	47(2)	48(2)	28(1)	-14(1)	3(1)	5(1)
C(5)	49(2)	43(2)	35(2)	-1(1)	16(1)	3(1)
O(2B)	69(8)	69(6)	30(4)	-8(4)	22(4)	2(6)
O(4B)	65(6)	62(7)	28(3)	-18(3)	12(3)	3(5)
O(2A)	59(12)	60(10)	39(8)	-11(7)	25(7)	-8(8)
O(4A)	64(12)	50(11)	34(7)	-22(6)	19(8)	-5(7)
Co(1)	29(1)	29(1)	29(1)	2(1)	2(1)	-2(1)
C(16)	28(8)	41(9)	36(11)	7(6)	6(7)	6(7)
C(17)	32(8)	21(7)	31(5)	0(4)	0(5)	1(5)
C(18)	43(8)	19(6)	30(10)	3(5)	1(5)	3(6)
C(19)	44(12)	34(7)	30(8)	-6(6)	6(7)	-16(5)
C(20)	33(7)	46(12)	38(9)	6(7)	-5(6)	-14(5)
C(21)	17(6)	25(8)	48(8)	-4(5)	-4(6)	-10(5)
C(22)	28(6)	22(4)	26(7)	-3(4)	-4(5)	-2(4)
C(23)	31(7)	27(9)	33(7)	-3(5)	-4(5)	-10(4)
C(24)	34(9)	34(7)	38(7)	-14(5)	13(5)	-8(6)
C(25)	27(6)	36(8)	48(11)	1(7)	13(5)	4(6)
Co(2)	38(1)	38(1)	38(1)	2(1)	-2(1)	-2(1)
C(6)	51(13)	58(11)	29(9)	1(8)	0(8)	-5(11)
C(7)	53(13)	49(11)	32(10)	8(8)	-8(7)	-12(9)
C(8)	44(12)	54(10)	45(12)	6(8)	-5(10)	-23(8)
C(9)	43(10)	69(15)	33(10)	13(10)	-4(7)	-18(8)
C(10)	41(11)	59(13)	43(13)	13(9)	3(9)	-8(9)

C(11)	34(10)	67(14)	48(13)	9(10)	-7(8)	-16(9)
C(12)	32(9)	73(14)	55(14)	4(12)	3(8)	-10(9)
C(13)	47(14)	76(15)	41(12)	1(10)	7(10)	-26(10)
C(14)	43(11)	89(19)	36(10)	19(9)	-3(7)	-24(11)
C(15)	47(13)	66(11)	46(13)	22(9)	-5(10)	-15(8)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **Cp_2Co^+-*sod*-ZMOF**.

	x	y	z	U(eq)
H(1)	5460	6987	4025	36
H(2B)	5941	6665	2711	84
H(2A)	6016	6602	2743	79
H(16)	4957	5743	2381	42
H(17)	5531	5551	2710	34
H(18)	5756	4968	2416	37
H(19)	5336	4820	1893	43
H(20)	4835	5301	1859	47
H(21)	6091	5993	2194	36
H(22)	5494	6269	1982	31
H(23)	5288	5918	1428	37
H(24)	5754	5421	1288	42
H(25)	6224	5448	1792	44
H(6)	4872	7733	3200	55
H(7)	5103	7092	3090	54
H(8)	4745	6823	2564	57
H(9)	4284	7295	2358	58
H(10)	4417	7882	2700	57
H(11)	5589	7904	2597	60
H(12)	5702	7278	2339	64
H(13)	5178	7132	1920	66
H(14)	4852	7722	1792	67
H(15)	5069	8182	2249	63

Table S6. Torsion angles [°] for **Cp_2Co^+-*sod*-ZMOF**.

C(3)-N(2)-C(1)-N(1)	-0.5(3)
In(1)-N(2)-C(1)-N(1)	172.9(2)
C(2)-N(1)-C(1)-N(2)	0.4(3)
In(1)#4-N(1)-C(1)-N(2)	-174.67(19)
C(1)-N(1)-C(2)-C(3)	-0.2(3)
In(1)#4-N(1)-C(2)-C(3)	175.05(19)
C(1)-N(1)-C(2)-C(5)	178.9(3)
In(1)#4-N(1)-C(2)-C(5)	-5.9(4)
C(1)-N(2)-C(3)-C(2)	0.3(3)
In(1)-N(2)-C(3)-C(2)	-175.0(2)
C(1)-N(2)-C(3)-C(4)	-178.7(3)
In(1)-N(2)-C(3)-C(4)	6.0(3)
N(1)-C(2)-C(3)-N(2)	-0.1(4)
C(5)-C(2)-C(3)-N(2)	-179.0(3)
N(1)-C(2)-C(3)-C(4)	178.7(3)
C(5)-C(2)-C(3)-C(4)	-0.3(6)
In(1)-O(3)-C(4)-O(4B)	-167(2)
In(1)-O(3)-C(4)-O(4A)	169(4)
In(1)-O(3)-C(4)-C(3)	3.2(4)
N(2)-C(3)-C(4)-O(3)	-6.3(4)
C(2)-C(3)-C(4)-O(3)	175.0(3)
N(2)-C(3)-C(4)-O(4B)	165.2(19)
C(2)-C(3)-C(4)-O(4B)	-14(2)
N(2)-C(3)-C(4)-O(4A)	-173(4)
C(2)-C(3)-C(4)-O(4A)	8(4)
C(3)-C(2)-C(5)-O(1)	-176.3(3)
N(1)-C(2)-C(5)-O(1)	4.9(5)
C(3)-C(2)-C(5)-O(2A)	-8(4)
N(1)-C(2)-C(5)-O(2A)	173(4)
C(3)-C(2)-C(5)-O(2B)	13(2)
N(1)-C(2)-C(5)-O(2B)	-166(2)
C(20)-C(16)-C(17)-C(18)	-2.1(18)
Co(1)-C(16)-C(17)-C(18)	-60.2(14)
C(20)-C(16)-C(17)-Co(1)	58.1(17)

C(16)-C(17)-C(18)-C(19)	1.4(17)
Co(1)-C(17)-C(18)-C(19)	-57.6(17)
C(16)-C(17)-C(18)-Co(1)	59.0(13)
C(17)-C(18)-C(19)-C(20)	0(2)
Co(1)-C(18)-C(19)-C(20)	-58.0(14)
C(17)-C(18)-C(19)-Co(1)	57.8(18)
C(17)-C(16)-C(20)-C(19)	2(3)
Co(1)-C(16)-C(20)-C(19)	61.3(13)
C(17)-C(16)-C(20)-Co(1)	-59.3(18)
C(18)-C(19)-C(20)-C(16)	-1(3)
Co(1)-C(19)-C(20)-C(16)	-61.0(15)
C(18)-C(19)-C(20)-Co(1)	59.9(16)
C(25)-C(21)-C(22)-C(23)	-2.1(14)
Co(1)-C(21)-C(22)-C(23)	-56.8(11)
C(25)-C(21)-C(22)-Co(1)	54.7(13)
C(21)-C(22)-C(23)-C(24)	-0.1(16)
Co(1)-C(22)-C(23)-C(24)	-60.3(13)
C(21)-C(22)-C(23)-Co(1)	60.3(11)
C(22)-C(23)-C(24)-C(25)	2(2)
Co(1)-C(23)-C(24)-C(25)	-60.4(13)
C(22)-C(23)-C(24)-Co(1)	62.7(15)
C(23)-C(24)-C(25)-C(21)	-4(2)
Co(1)-C(24)-C(25)-C(21)	-62.6(14)
C(23)-C(24)-C(25)-Co(1)	59.1(13)
C(22)-C(21)-C(25)-C(24)	3(2)
Co(1)-C(21)-C(25)-C(24)	59.3(13)
C(22)-C(21)-C(25)-Co(1)	-55.8(13)
C(10)-C(6)-C(7)-C(8)	-3(4)
Co(2)-C(6)-C(7)-C(8)	-60(2)
C(10)-C(6)-C(7)-Co(2)	57(3)
C(6)-C(7)-C(8)-C(9)	-1(3)
Co(2)-C(7)-C(8)-C(9)	-61.8(18)
C(6)-C(7)-C(8)-Co(2)	61(3)
C(7)-C(8)-C(9)-C(10)	4(3)
Co(2)-C(8)-C(9)-C(10)	-55(2)
C(7)-C(8)-C(9)-Co(2)	59.9(18)

C(8)-C(9)-C(10)-C(6)	-6(4)
Co(2)-C(9)-C(10)-C(6)	-62(3)
C(8)-C(9)-C(10)-Co(2)	55.2(19)
C(7)-C(6)-C(10)-C(9)	6(4)
Co(2)-C(6)-C(10)-C(9)	62(2)
C(7)-C(6)-C(10)-Co(2)	-56(3)
C(15)-C(11)-C(12)-C(13)	-6(4)
Co(2)-C(11)-C(12)-C(13)	55(3)
C(15)-C(11)-C(12)-Co(2)	-62(2)
C(11)-C(12)-C(13)-C(14)	9(4)
Co(2)-C(12)-C(13)-C(14)	65(3)
C(11)-C(12)-C(13)-Co(2)	-56(2)
C(12)-C(13)-C(14)-C(15)	-8(4)
Co(2)-C(13)-C(14)-C(15)	56(2)
C(12)-C(13)-C(14)-Co(2)	-64(3)
C(13)-C(14)-C(15)-C(11)	5(4)
Co(2)-C(14)-C(15)-C(11)	59.8(18)
C(13)-C(14)-C(15)-Co(2)	-55(3)
C(12)-C(11)-C(15)-C(14)	1(3)
Co(2)-C(11)-C(15)-C(14)	-61.6(19)
C(12)-C(11)-C(15)-Co(2)	63(2)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,z+1/4,y-1/4 #2 y-1/4,-z+1,x-1/4 #3 -y+5/4,x,-z+3/4

#4 z+1/4,x+1/4,-y+1

Table S7. Hydrogen bonds for **Cp_2Co^+-*sod*-ZMOF** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(2B^a)-H(2B^a)...O(4B^a)	0.84	1.66	2.50(3)	173.5
O(2A^b)-H(2A^b)...O(4A^b)	0.84	1.69	2.52(5)	168.0

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,z+1/4,y-1/4 #2 y-1/4,-z+1,x-1/4 #3 -y+5/4,x,-z+3/4

#4 z+1/4,x+1/4,-y+1