Supplementary information

COF-Inspired Fabrication of Two-Dimensional Polyoxometalate Based Open Frameworks for Biomimetic Catalysis

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SI-1. Materials and Methods

All reagents were purchased from commercial sources and used without further treatments. The solid phase ^{13}C NMR spectra were obtained on a Varian 300 MHz Solid State Infinityplus 300 NMR spectrometer. ^{1}H NMR and ^{13}C NMR spectra was recorded on Bruker AV42 instruments at 400 MHz. Chemical shifts were reported in parts per million (ppm) down field from internal tetramethylsilane. Powder X-ray diffraction measurements were recorded on a D/Max-2500 X-ray diffractometer using Cu-Kα radiation by depositing powder on glass substrate, 2θ from 3° to 40° with 0.02° increment. Single crystal diffraction data was collected at 120 K via an Oxford Cryo stream system on a SuperNova (Mo) X-ray Source with micro-focus sealed X-ray tube. PLATON/SQUEEZE programme was used to remove disordered solvent molecules. The crystal data files of **MC-Co** and **MC-Mn** were deposited into the Cambrige Crystallographic Data Centre (CCDC) and assigned the number 1997411, 1997412, respectively. The surface areas of tested materials were determined using a Micromeritics ASAP-2460. Fourier transform infrared spectra (FT-IR) spectra were recorded on a Nicolet iS 50 ATR-FTIR instrument. Ultraviolet-visible absorption spectra of solution samples are collected using an Agilent Cary 100 UV/Vis spectrophotometer with background correction. Scanning electron microscopy (SEM) images were taken with Hitachi JSM-7500F scanning electron microscopy. Transmission electron microscopy images were characterized on a Tecnai G2 F20 electron microscope. Samples were dried using a Tousimis Samdri-PVT-3D supercritical carbon dioxide dryer. Element analysis was carried out on Vario EL cube. Atomic Force Microscopy (AFM) was carried out on Bruker Dimension Icon. ICP-OES were conducted on a SpectroBlue of 27.12MHz.

SI-2. Synthetic Procedures

2.1 Synthesis of $MnMo_6$, $CoMo_6$.

$[MnMo_6O_{18}\{(OCH_2)_3CNH_2\}_2]\cdot[N(C_4H_9)_4]_3$ (**$MnMo_6$**) and $[CoMo_6O_{18}\{(OCH_2)_3CNH_2\}_2]\cdot[N(C_4H_9)_4]_3$ (**$CoMo_6$**) were synthesized according to the literature.[1,2]

2.2 Synthesis of NKPOM-OF-1(Mn).

A Pyrex tube was charged with **$MnMo_6$** (76.6 mg, 0.04 mmol), **TFPB** (8.9 mg, 0.02 mmol), 1.5 mL 1,4-dioxane and 0.2 mL 6 M aqueous acetic acid. The tube was flash frozen at 77 K (liquid N_2 bath), evacuated and flame sealed. Upon sealing the length of the tube was reduced to ca. 13 cm. The reaction was heated at 120 °C for 72 h and orange solids were isolated by centrifugation and washed with acetonitrile. The powder was soaked in methanol for five days and dried using supercritical carbon dioxide to yield **NKPOM-OF-1(Mn)** (53.0 mg, 63% based on {$MnMo_6$}). Anal. Calcd for ($C_{130}H_{227}Mn_2Mo_{12}N_9O_{48}$): C, 39.50%; H, 5.79%; N, 3.19%; Mn, 2.78%; Mo, 29.18%. Found: C, 39.38%; H, 6.03%; N, 3.19%; Mn, 2.69%; Mo, 29.28%. The good agreement of calculated and found elemental analysis results confirmed that there were no unreacted monomers remained in NKPOM-OFs, indicative the high purity of the material.

2.3 Synthesis of NKPOM-OF-1(Co).

The preparation of **NKPOM-OF-1(Co)** was similar to that of **NKPOM-OF-1(Mn)**, except that **$MnMo_6$** was replaced by **$CoMo_6$** (75.9 mg, 0.04 mmol). Green solids were obtained (56.6 mg, 67%). Anal. Calcd for ($C_{146}H_{262}Co_2Mo_{12}N_{10}O_{48}$): C, 41.80%; H, 6.30%; N, 3.34%; Co, 2.81%; Mo, 27.45%. Found: C, 41.98%; H, 6.50%; N, 3.39%; Co, 2.61%; Mo, 27.54%.

2.4 Synthesis of NKPOM-OF-2(Mn).

The preparation of **NKPOM-OF-2(Mn)** was similar to that of **NKPOM-OF-1(Mn)**, except that TFPB was replaced by ETTBA (8.9 mg, 0.02 mmol). Yellow solids were obtained (52.8 mg, 62.9%). Anal. Calcd for: ($C_{134}H_{242.5}Mn_2Mo_{12}N_{9.5}O_{48}$): C, 40.07%; H, 6.08%; N, 3.31%; Mn, 2.74%; Mo, 28.67%. Found: C, 39.86%; H, 6.39%; N, 3.30%; Mn, 2.60%; Mo, 28.87%.

2.5 Synthesis of NKPOM-OF-2(Co).

The preparation of **NKPOM-OF-2(Co)** was similar to that of **NKPOM-OF-1(Co)**, except that TFPB was replaced by ETTEA (8.9 mg, 0.02 mmol). Yellow green solids were obtained (55.0 mg, 65%). Anal. Calcd for: ($C_{134}H_{242.5}Co_2Mo_{12}N_{9.5}O_{48}$): C, 39.99%; H, 6.07%; N, 3.31%; Co, 2.91%; Mo, 28.46%. Found: C, 39.65%; H, 6.24%;

N, 3.33%; Co, 2.80%; Mo, 28.60%.

2.6 Synthesis of MC-Mn.

$MnMo_6$ (150.0 mg, 0.08 mmol) and benzaldehyde (85.0 mg, 0.8 mmol) were dissolved in 20 mL acetonitrile. The system was refluxed at 100 ℃ for 48 h. After the reaction, the solution was cooled to room temperature. 105.0 mg block orange crystals were obtained through evaporation of ether, yield 65%.

2.7 Synthesis of MC-Co.

The preparation of **MC-Co** was similar to that of **MC-Mn**, except that **$MnMo_6$** was replaced by **$CoMo_6$** (151.8 mg, 0.08 mmol). 112.0 mg block green crystals were obtained as product, yield 70%.

SI-3. Characterization of MC-Co.

MC-Co: ^{1}H NMR (400 MHz, DMSO-d6) δ 8.36 (s, 2H), 7.79 (dt, J = 6.7, 1.7 Hz, 4H), 7.47-7.39 (m, 6H), 4.06 (s, 12H), 3.18-3.12 (m, 24H), 1.60-1.51 (m, 24H), 1.31 (h, J = 7.3 Hz, 24H), 0.92 (t, J = 7.3 Hz, 32H). ^{13}C NMR (400 MHz, DMSO) δ 160.15, 136.08, 131.16, 128.56, 127.88, 74.79, 69.88, 57.50, 23.06, 19.20, 13.49.

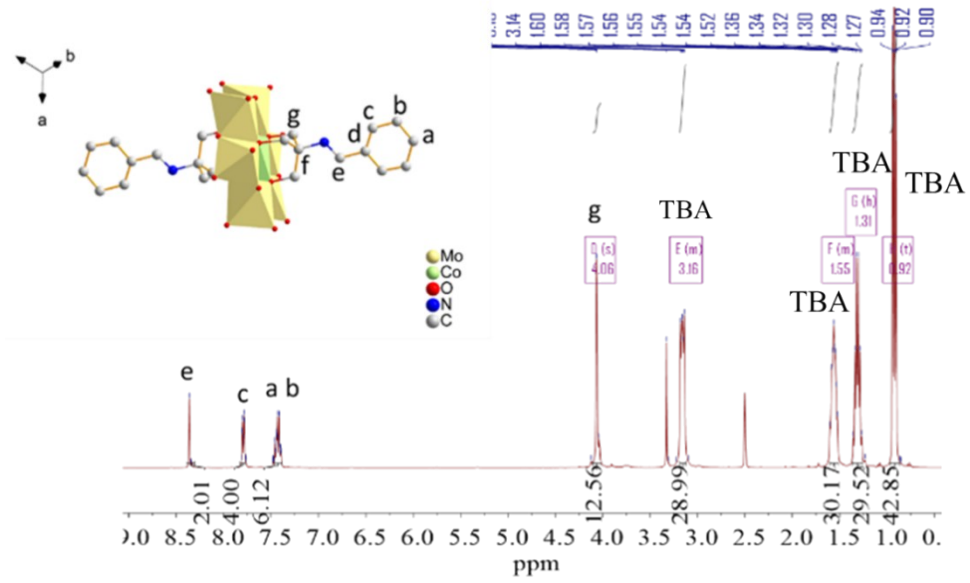

Fig. S1 | ^{1}H NMR spectrum of **MC-Co**.

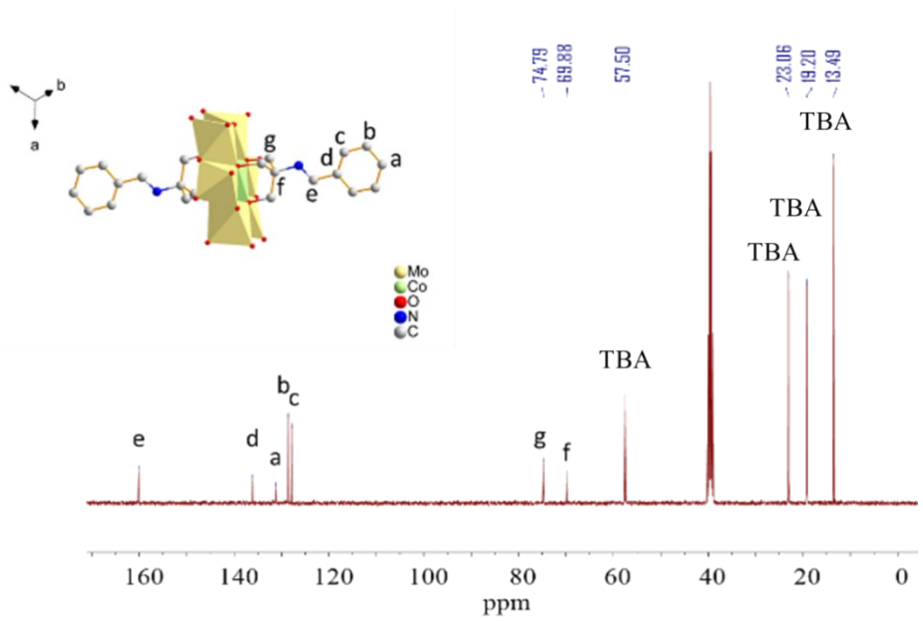

Fig. S2 | ^{13}C NMR spectrum of **MC-Co**.

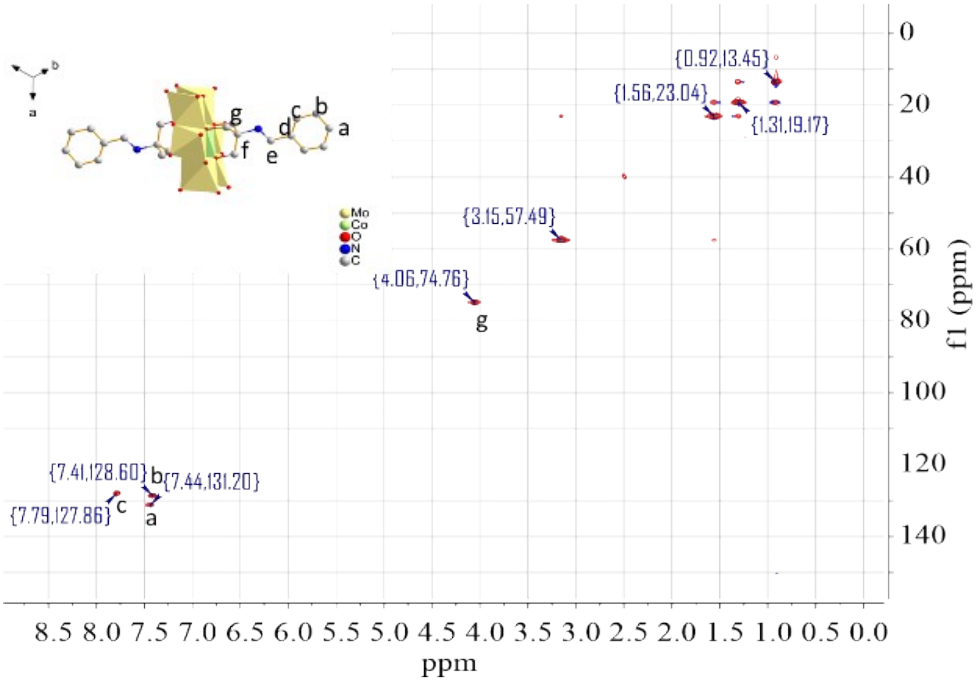

Fig. S3 | ^{1}H-^{13}C HSQC spectrum of **MC-Co**.

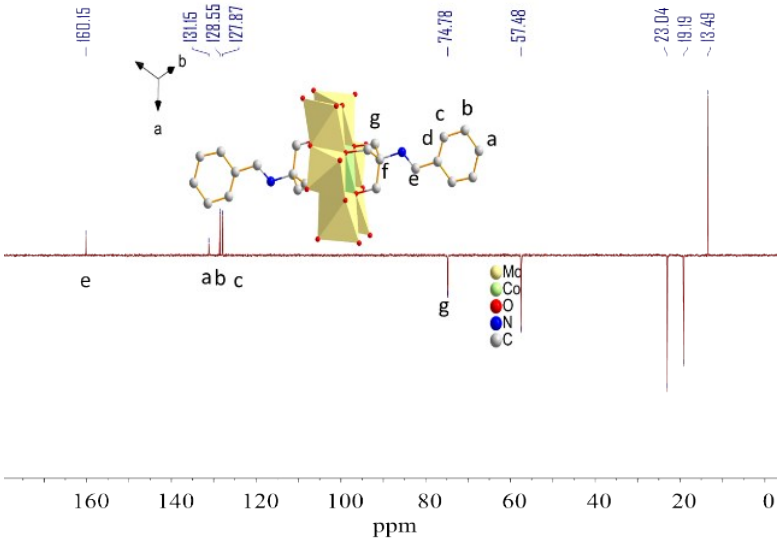

Fig. S4 | DEPT 135 spectrum of **MC-Co**.

SI-4. Characterization of NKPOM-OF-1(Co)

Stability of **NKPOM-OF-1(Co)**: We tested the stability of **NKPOM-OF-1(Co)** with various solvents (water, DMSO, DMF and methanol). 100 mg NKPOM-OFs were soaked in 10 mL solvent. After 48 h, the **NKPOM-OF-1(Co)** was collected by centrifugation, washed by acetonitrile and dried under ambient conditions. There is no significant weight loss or color change. PXRD patterns reveal that **NKPOM-OF-1(Co)** remained high crystallinity in these solvents.

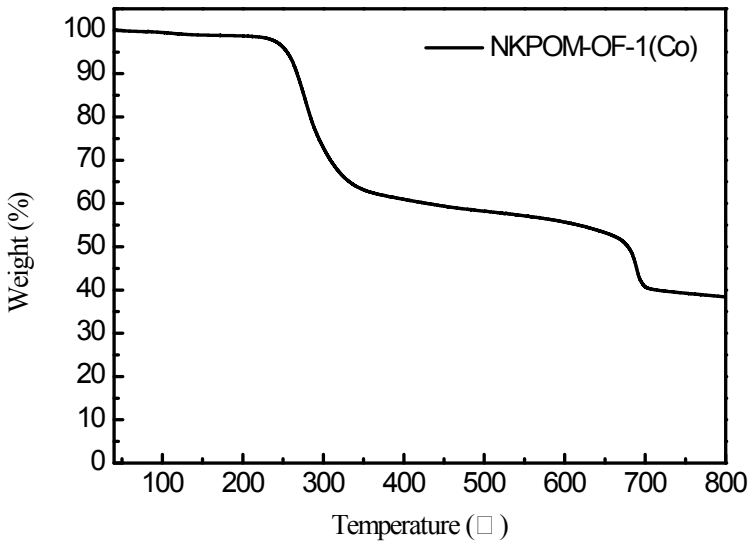

Fig. S5 | TGA curve of **NKPOM-OF-1(Co)**.

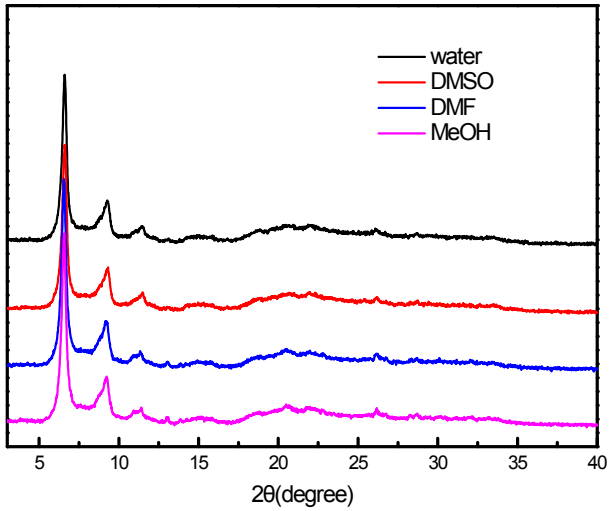

Fig. S6 | Powder X-ray diffraction (PXRD) pattern of **NKPOM-OF-1(Co)** after the treatment in various solvents for 48 h.

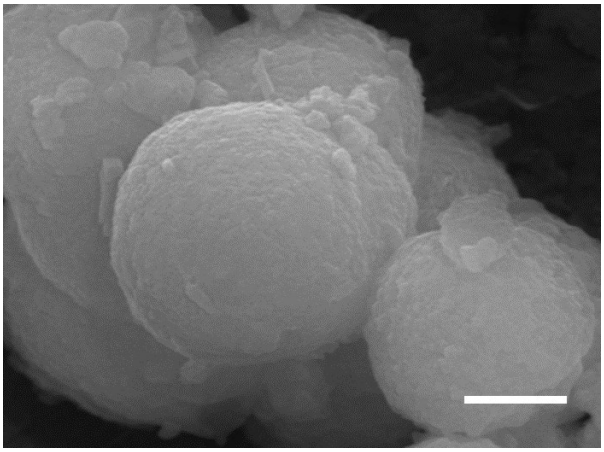

Fig. S7 | SEM image of **NKPOM-OF-1(Co)**, Scale bar 1 μm.

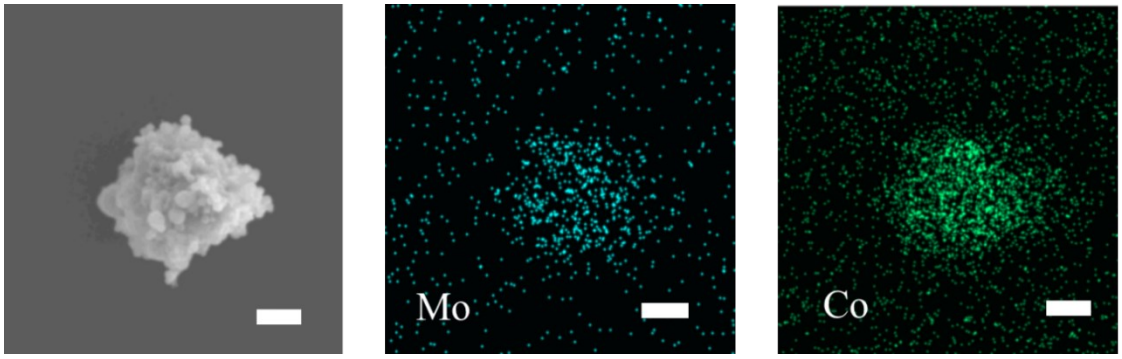

Fig. S8 | SEM mapping images of **NKPOM-OF-1(Co),** Scale bar 20 μm.

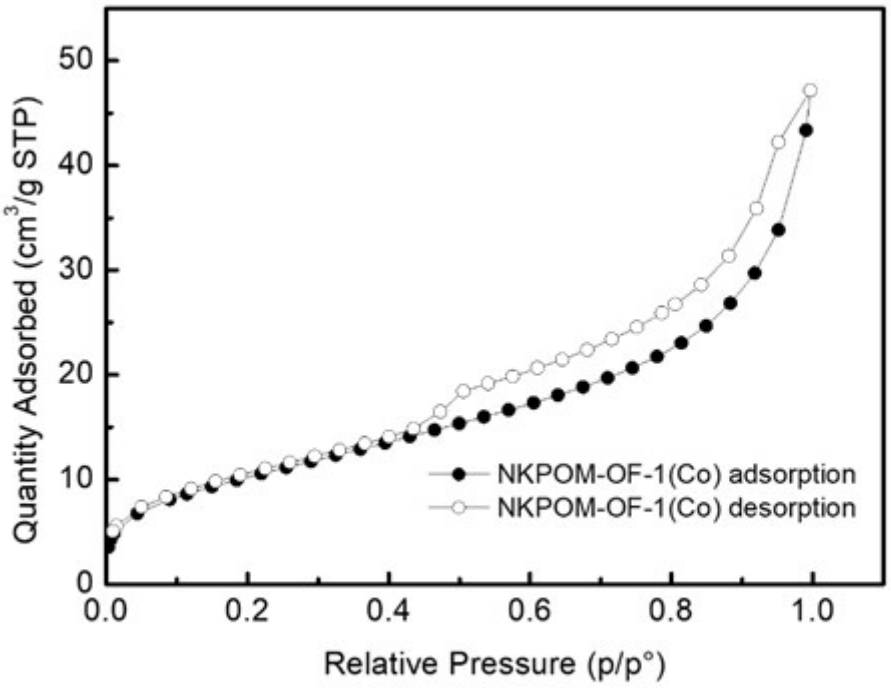

Fig. S9 | N_2 adsorption and desorption isotherms of **NKPOM-OF-1(Co)** at 77 K. The inset is the pore size distributions of **NKPOM-OF-1(Co)**.

Table S1 | Calculated Surface Area of **NKPOM-OFs** using material studio software and experimental results.

	NKPOM-OF-1(Co)	**NKPOM-OF-1(Mn)**
Calculated Surface Area (m^2/g)	**180**	**180**
Experimental Langmuir Surface Area (m^2/g)	**134**	**134**

SI-5. Characterization of MC-Mn

MC-Mn: ^{1}H NMR (400 MHz, DMSO-d6) δ 8.75 (s, 2H), 7.70 (d, J = 7.0 Hz, 4H), 7.55 (d, J = 6.9 Hz, 4H), 7.28 (t, J = 7.2 Hz, 2H), 3.16 (q, J = 4.9 Hz, 24H), 1.56 (dq, J

= 11.5, 6.4, 5.4 Hz, 24H), 1.31 (q, J = 7.1 Hz, 24H), 0.92 (t, J = 7.0 Hz, 36H). ^{13}C NMR (400 MHz, DMSO-d6) δ 204.96 , 134.74 , 132.80 , 130.37 , 128.23 , 58.12 (d, J = 3.3 Hz), 23.66 , 19.93 , 14.18 .

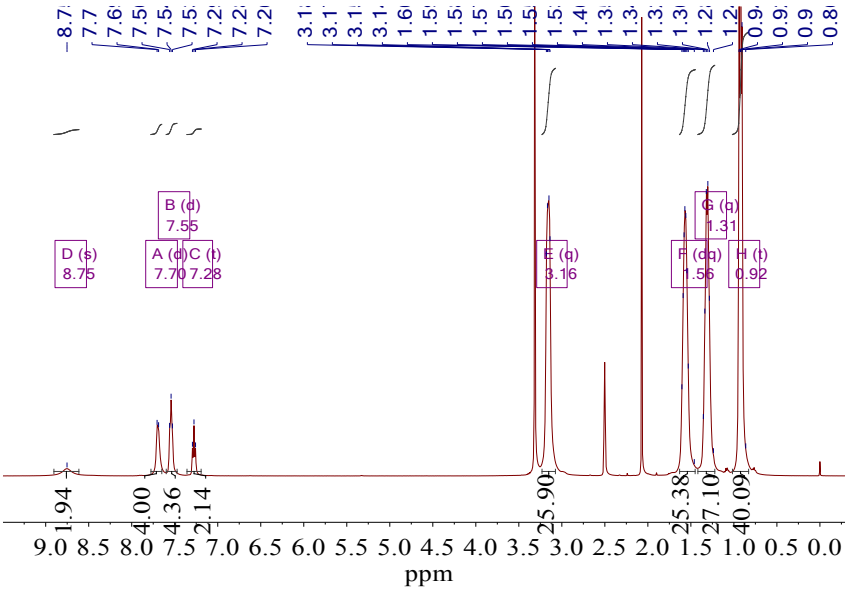

Fig. S10 | ^{1}H NMR spectrum of **MC-Mn**.

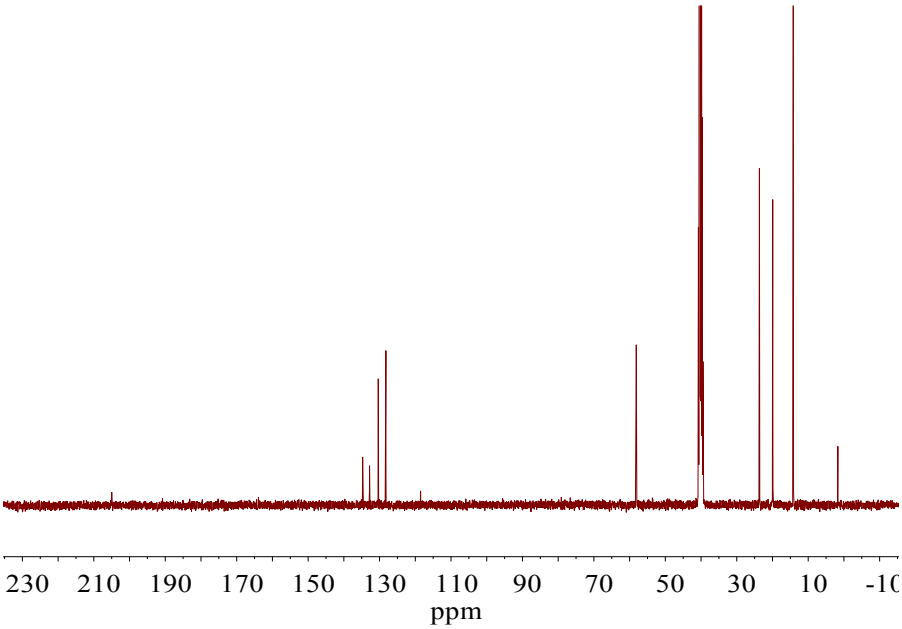

Fig. S11 | ^{13}C NMR spectrum of **MC-Mn**.

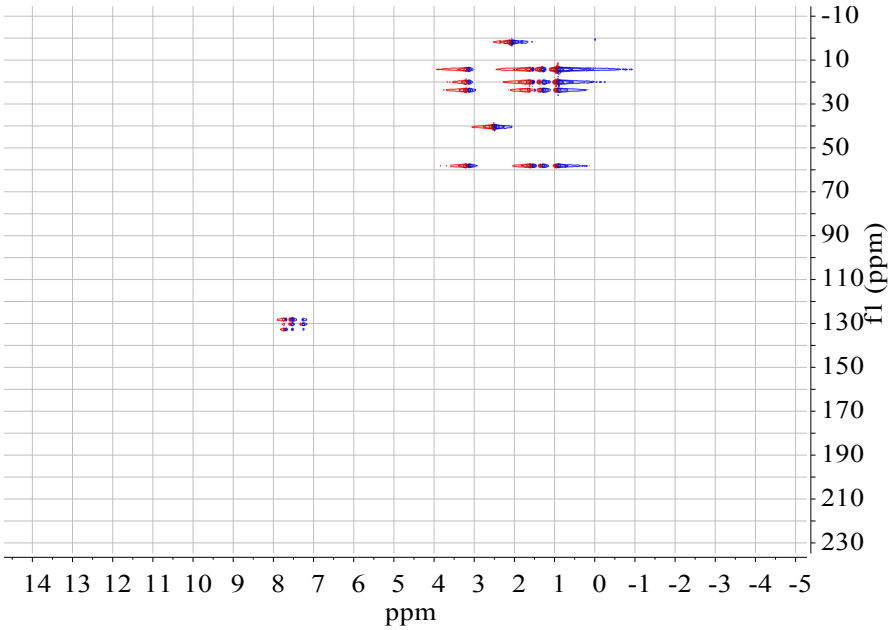

Fig. S12 | ^{1}H-^{13}C HSQC spectrum of **MC-Mn**.

SI-6. Characterization of NKPOM-OF-1(Mn), NKPOM-OF-2(Co) and NKPOM-OF-2(Mn)

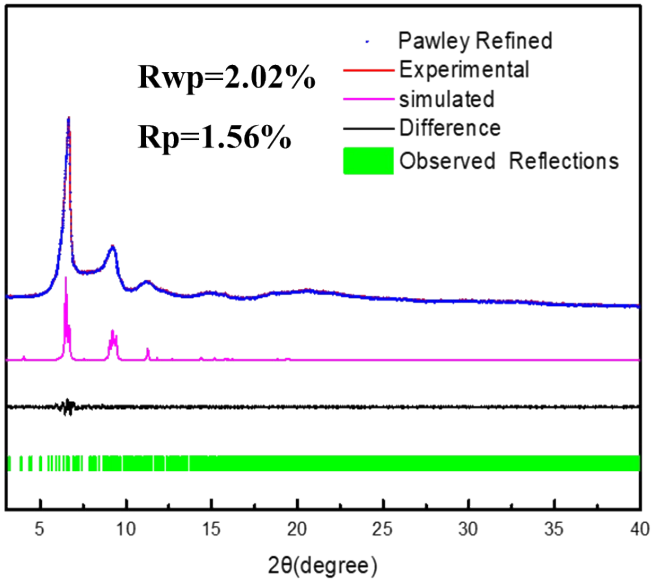

Fig. S13 | Experimental and simulated PXRD patterns of **NKPOM-OF-1(Mn)**.

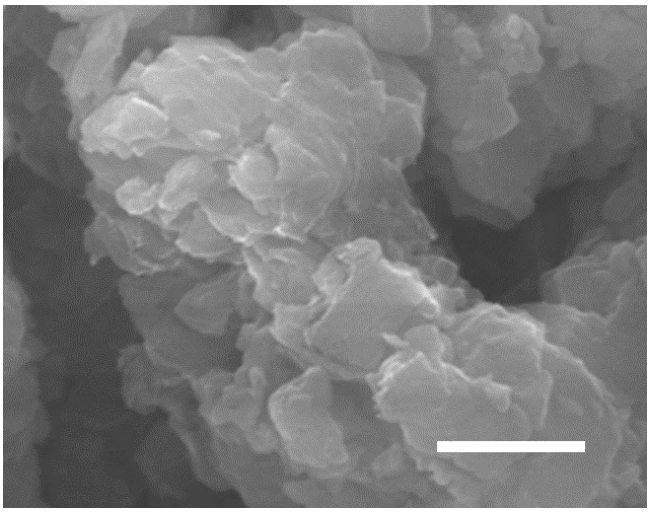

Fig. S14 | SEM image of (a) **NKPOM-OF-1(Mn)**, Scale bar 1 μm.

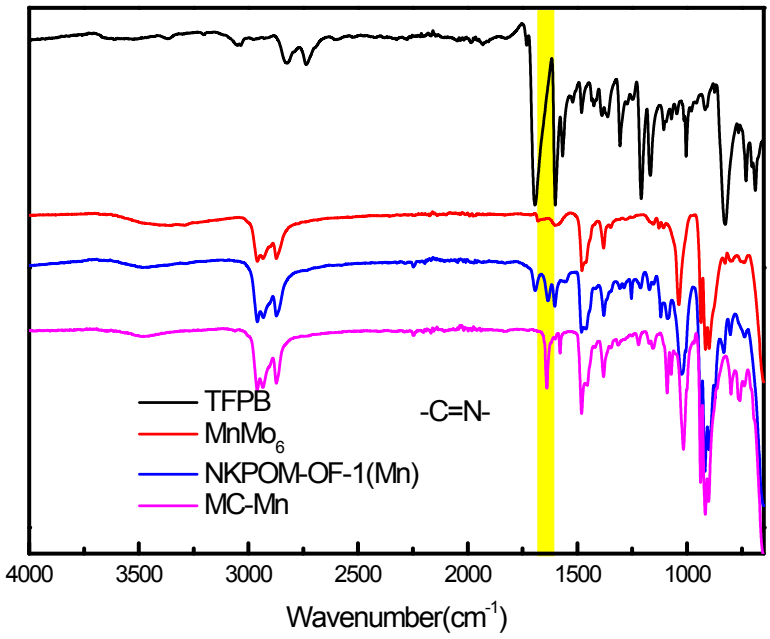

Fig. S15 | FT-IR spectra of TFPB, **$MnMo_6$**, **NKPOM-OF-1(Mn)** and **MC-Mn**.

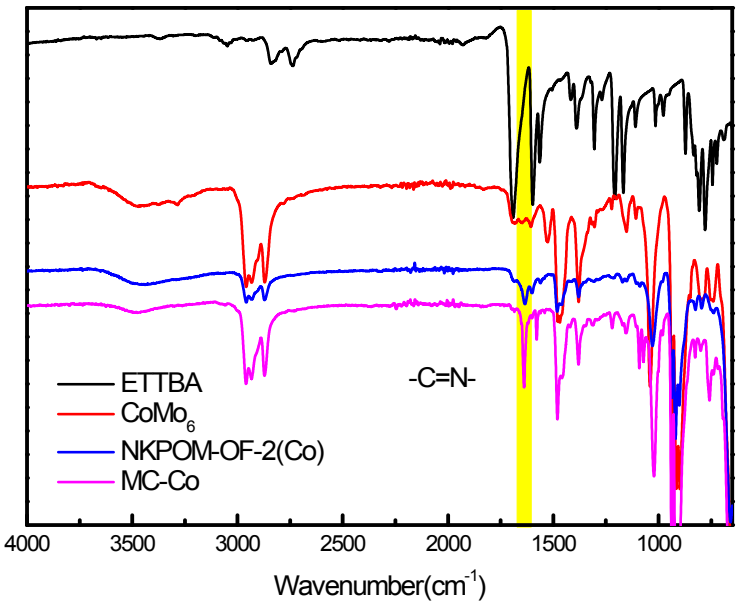

Fig. S16 | FT-IR spectra of ETTBA, **$CoMo_6$**, **NKPOM-OF-2(Co) MC-Co**.

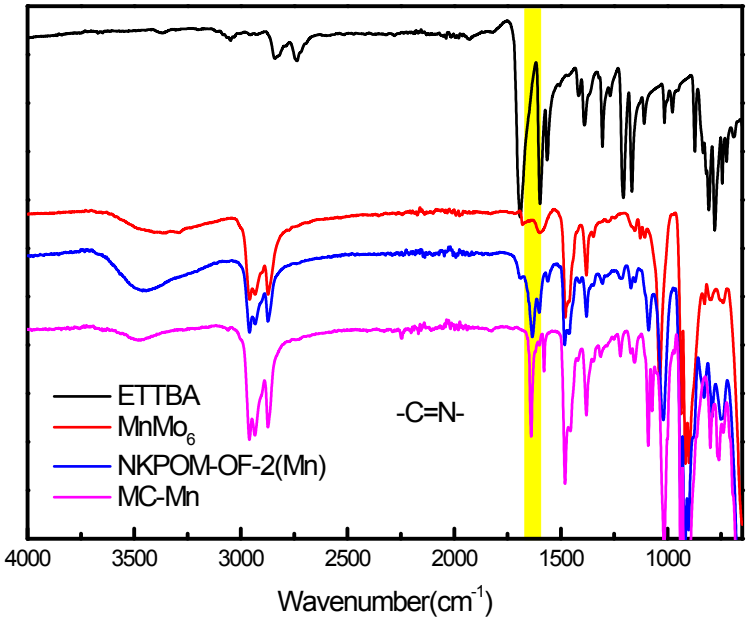

Fig. S17 | FT-IR spectra of ETTBA, **$MnMo_6$**, **NKPOM-OF-2(Mn)**, **MC-Mn**.

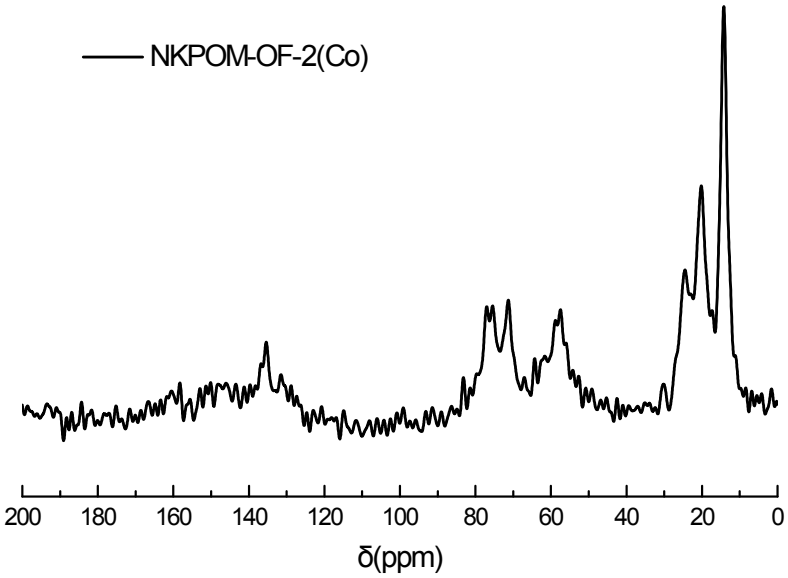

Fig. S18 | ^{13}C CP/MAS NMR spectrum of **NKPOM-OF-2(Co)**.

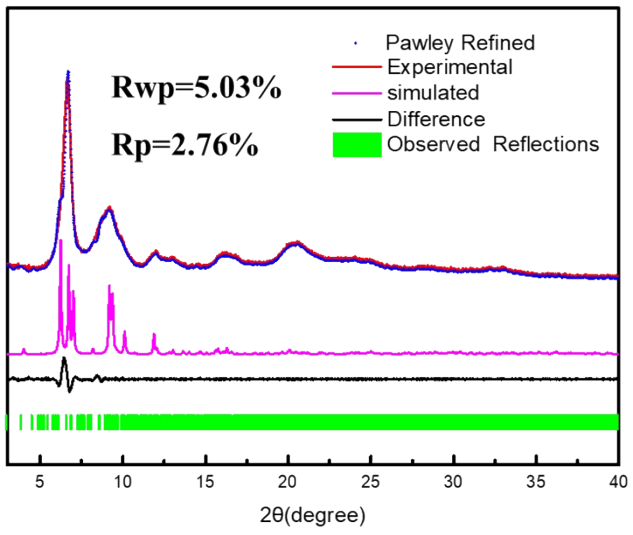

Fig. S19 | Experimental and simulated PXRD patterns of **NKPOM-OF-2(Mn)**.

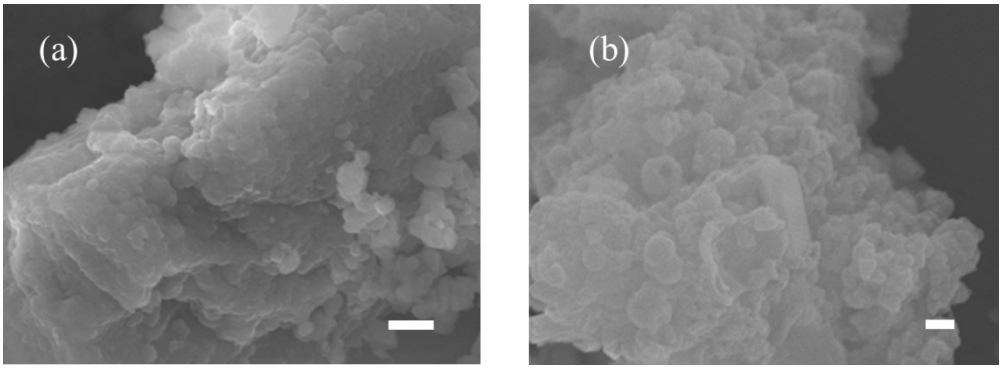

Fig. S20 | SEM images of (a) **NKPOM-OF-2(Co)**, (b) **NKPOM-OF-2(Mn)**. Scale bar 1 μm.

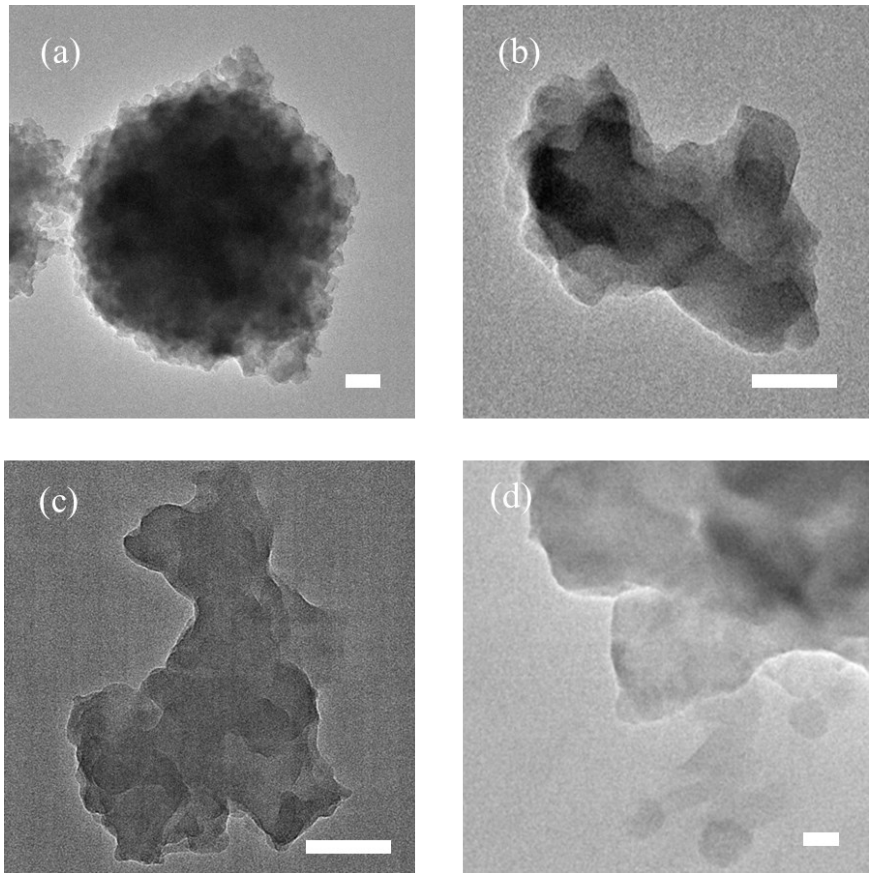

Fig. S21 | TEM images of (a) **NKPOM-OF-1(Co)**, (b) **NKPOM-OF-1(Mn)**, (c) **NKPOM-OF-2(Co)** and (d) **NKPOM-OF-2(Mn)**. Scale bar 100 nm.

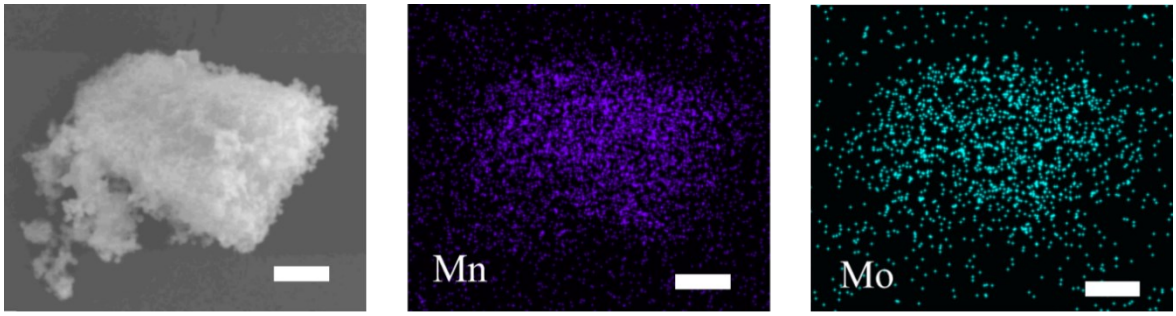

Fig. S22 | SEM mapping images of **NKPOM-OF-1(Mn)**, Scale bar 10 μm.

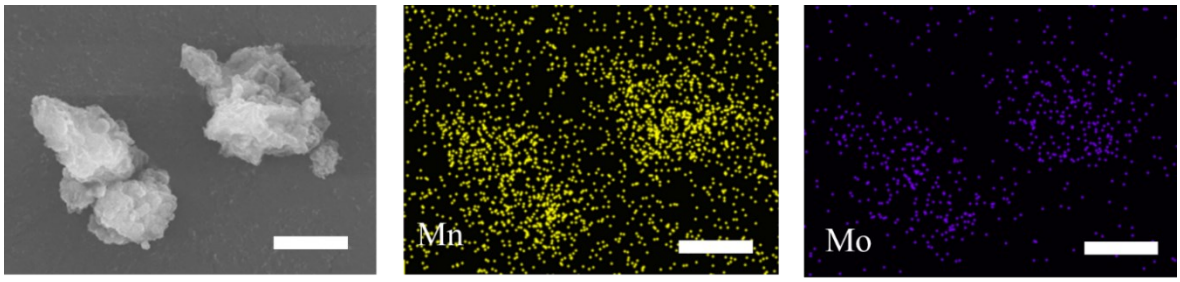

Fig. S23 | SEM mapping images of **NKPOM-OF-2(Mn),** Scale bar 10 μm.

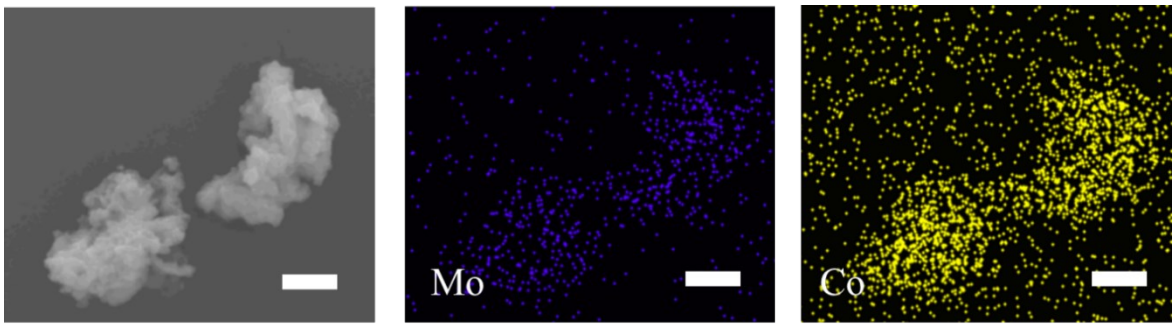

Fig. S24 | SEM mapping images of **NKPOM-OF-2(Co)**, Scale bar 10 μm.

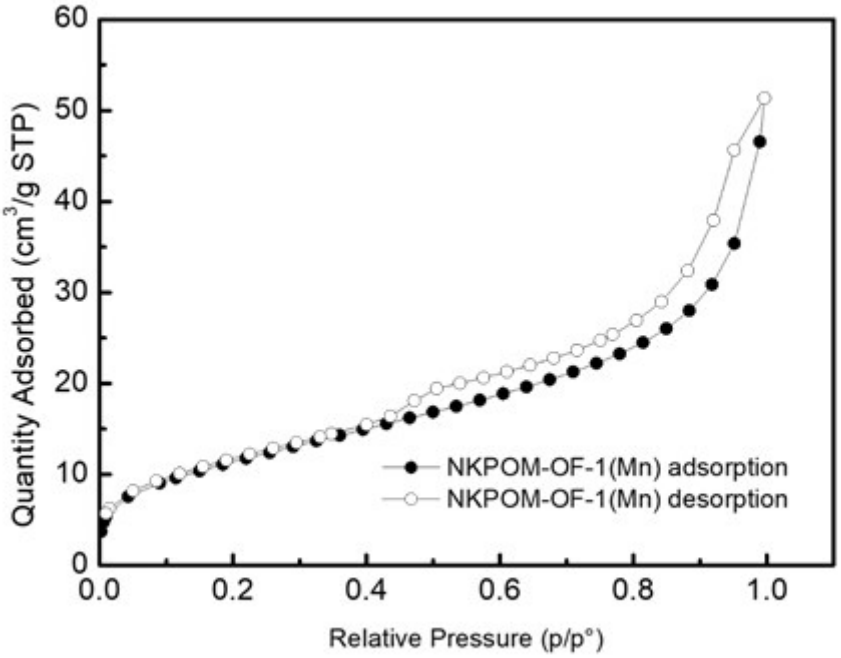

Fig. S25 | N_2 sorption isotherm at 77 K of **NKPOM-OF-1(Mn)**. The inset is the pore size distributions of **NKPOM-OF-1(Mn)**.

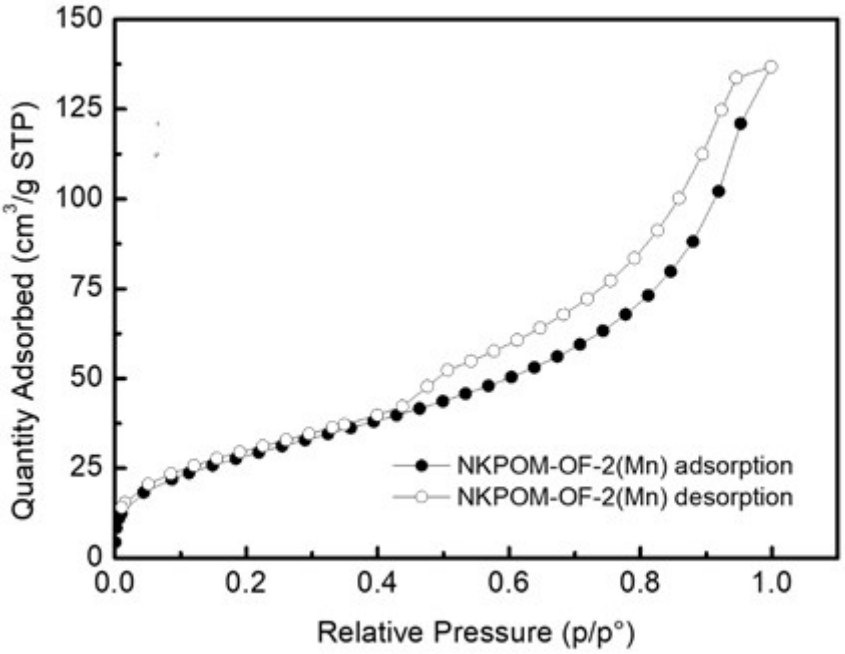

Fig. S26 | N_2 sorption isotherm at 77 K of **NKPOM-OF-2(Mn)**. The inset is the pore size distributions of **NKPOM-OF-2(Mn)**.

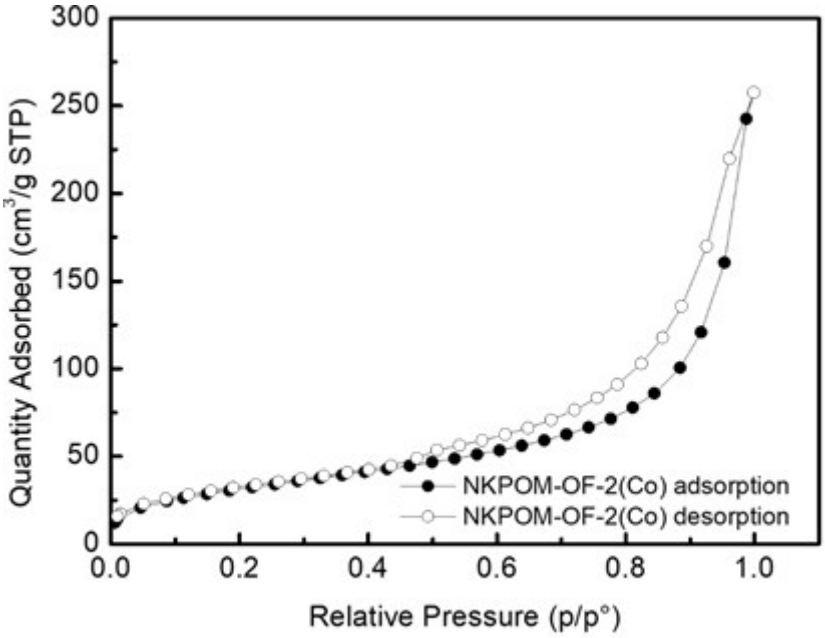

Fig. S27 | N_2 adsorption isotherm at 77 K of **NKPOM-OF-2(Co)**. The inset is the pore size distributions of **NKPOM-OF-2(Co)**.

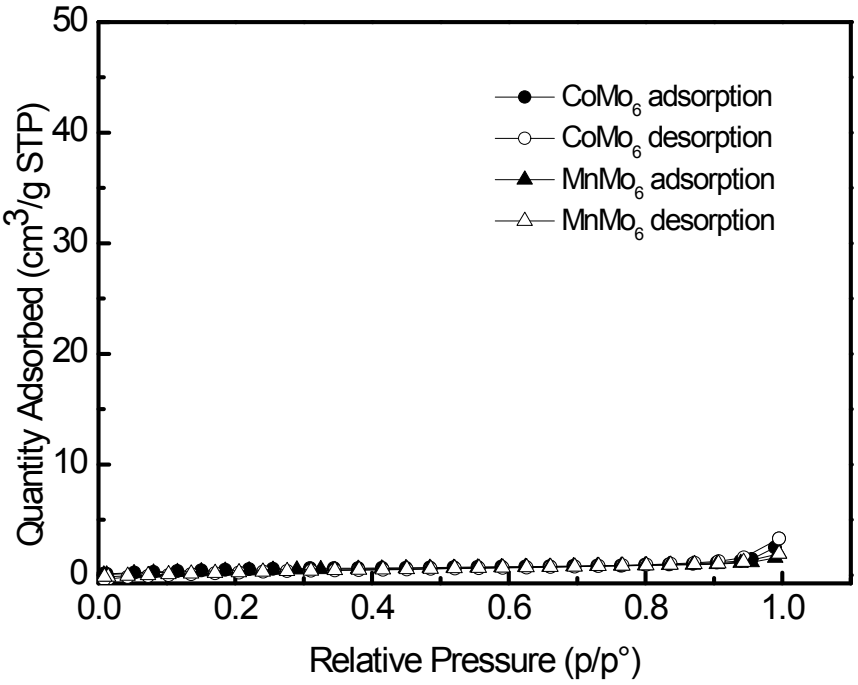

Fig. S28 | N_2 adsorption isotherm at 77 K of **$CoMo_6$** and **$MnMo_6$**.

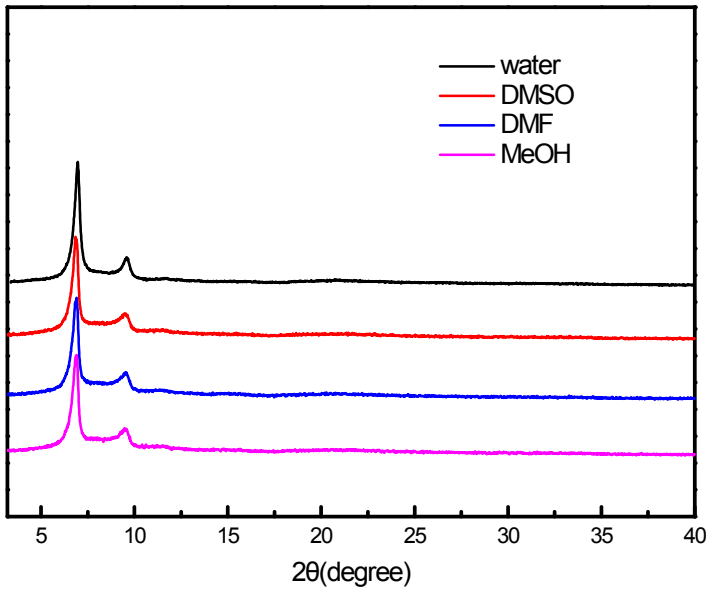

Fig. S29 | Powder X-ray diffraction (PXRD) pattern of **NKPOM-OF-1(Mn)** after the treatment in various solvents for 48 h.

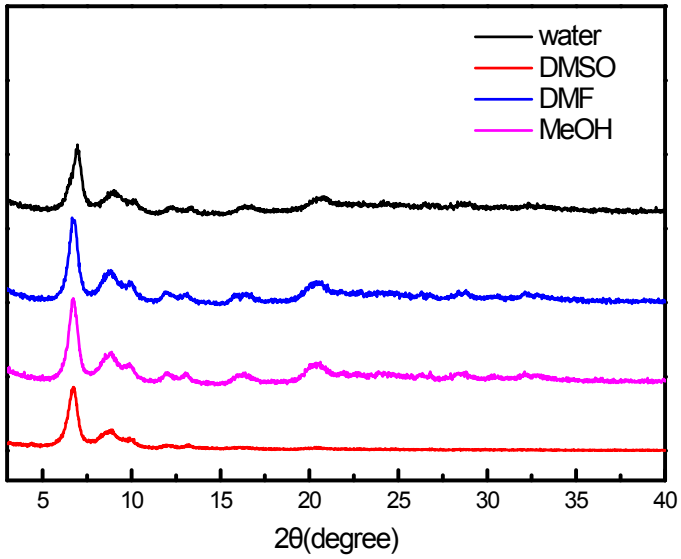

Fig. S30 | Powder X-ray diffraction (PXRD) pattern of **NKPOM-OF-2(Co)** after the treatment in various solvents for 48 h.

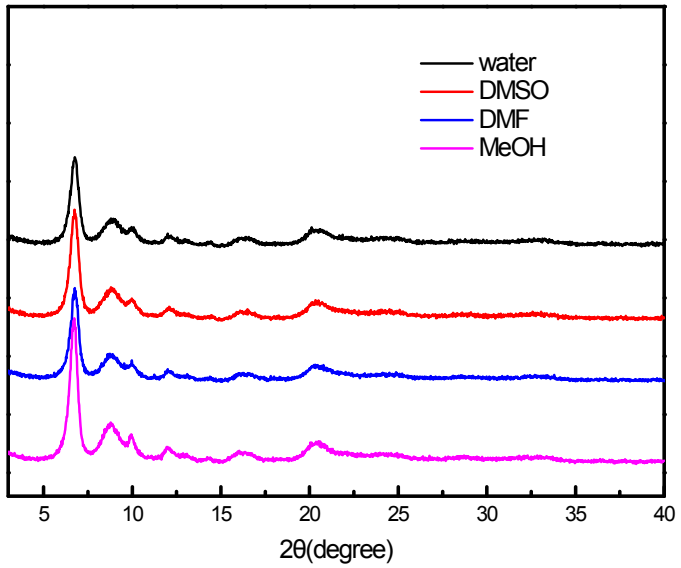

Fig. S31 | Powder X-ray diffraction (PXRD) pattern of **NKPOM-OF-2(Mn)** after the treatment in various solvents for 48 h.

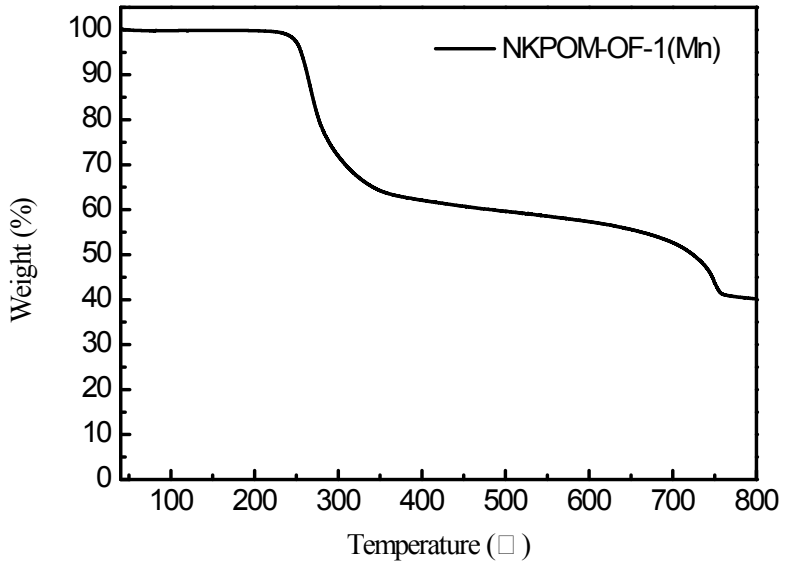

Fig. S32 | TGA curve of **NKPOM-OF-1(Mn)**.

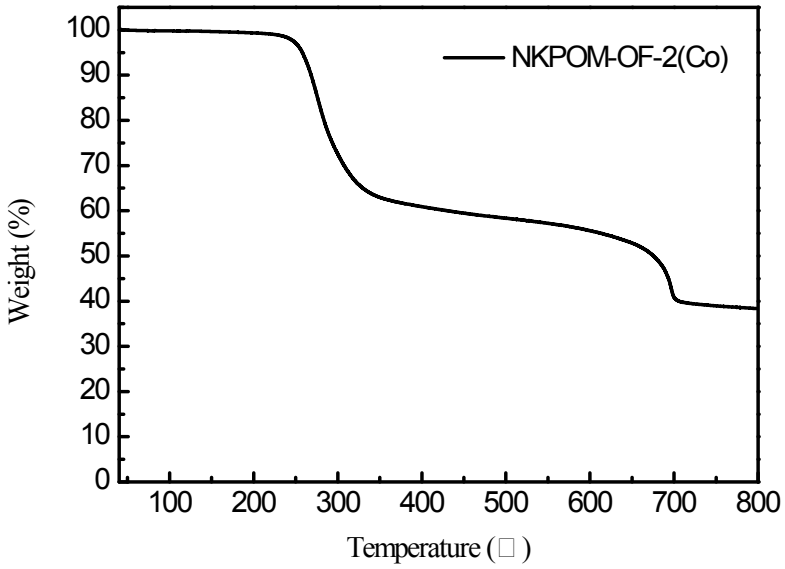

Fig. S33 | TGA curve of **NKPOM-OF-2(Co)**.

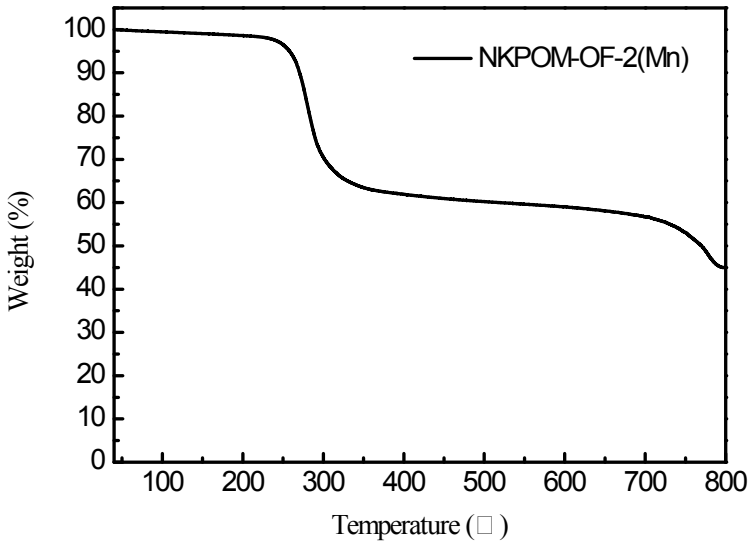

Fig. S34 | TGA curve of **NKPOM-OF-2(Mn)**.

SI-7. Sulfite Oxidase activity of NKMOP-OFs

As synthesized NKPOM-OFs were washed thoroughly by acetonitrile and methanol to remove unreacted POM and organic monomers. The samples were dried using supercritical carbon dioxide to remove residual solvent.

The catalytic reaction was performed in distilled water in a 10 mL centrifuge tube. The water was degassed under Argon flue in order to eliminate the influence of different amount of oxygen dissolved in water. 5 mg NKPOM-OF was put in 5 mL 6.6 mM sodium sulfite. The system was shaken with 80 r/min. After reaction, the catalyst was filtered off. The SO_4^{2-} was precipitated by adding excess $BaCl_2$. Excess diluted HCl was added subsequently to remove unreacted SO_3^{2-}. The precipitation was collected by centrifugation, washed by distilled water and dried under 100 ℃. The yield was calculated based on the mass of $BaSO_4$. The blank experiment was performed under the same condition in the absence of NKPOM-OFs.

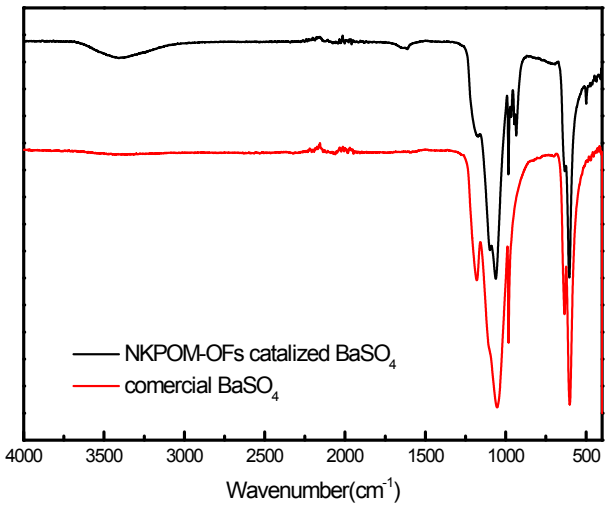

Fig. S35 | FT-IR spectra of obtained $BaSO_4$ product and commercially available $BaSO_4$.

Table S2 | Turnover frequency (TOF) of **NKPOM-OF-1(Co)**, sulfite oxidase and MoO_3 nanoparticle.

	NKPOM-OF-1(Co)	Sulfite oxidase[3]	MoO_3 nanoparticle[4]
TOF	1.4 min^{-1}	25 s^{-1}	2.78 s^{-1}

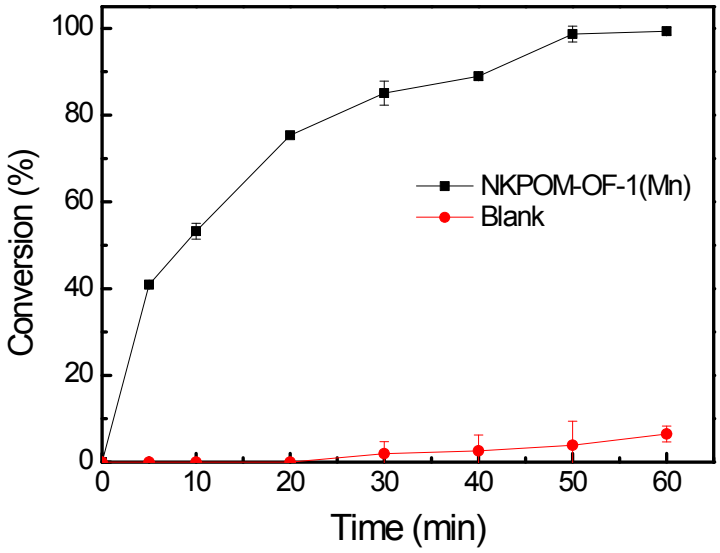

Fig. S36 | Conversion of sulfite to sulfate catalyzed by **NKPOM-OF-1(Mn)**.

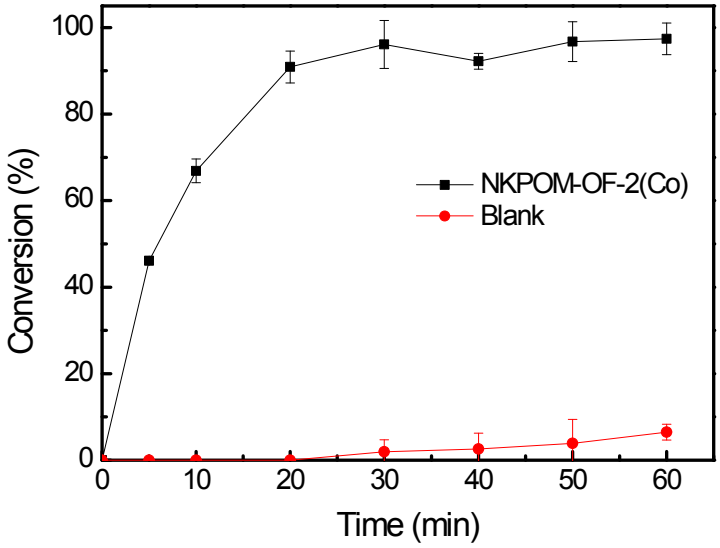

Fig. S37 | Conversion of sulfite to sulfate catalyzed by **NKPOM-OF-2(Co)**.

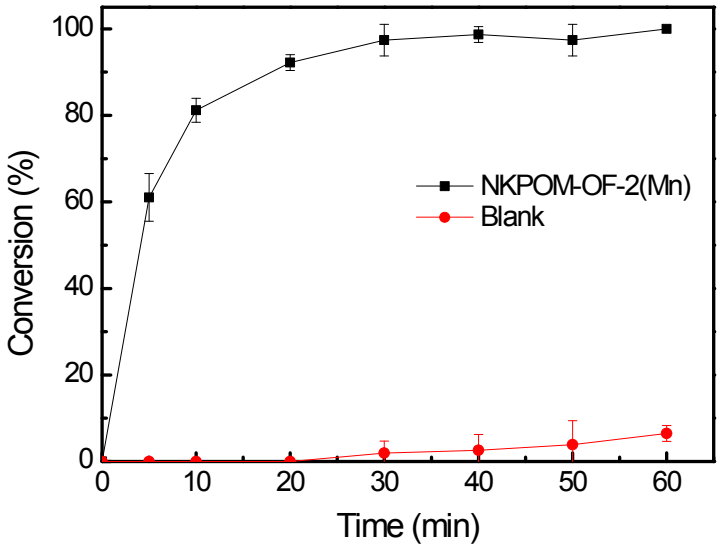

Fig. S38 | Conversion of sulfite to sulfate catalyzed by **NKPOM-OF-2(Mn)**.

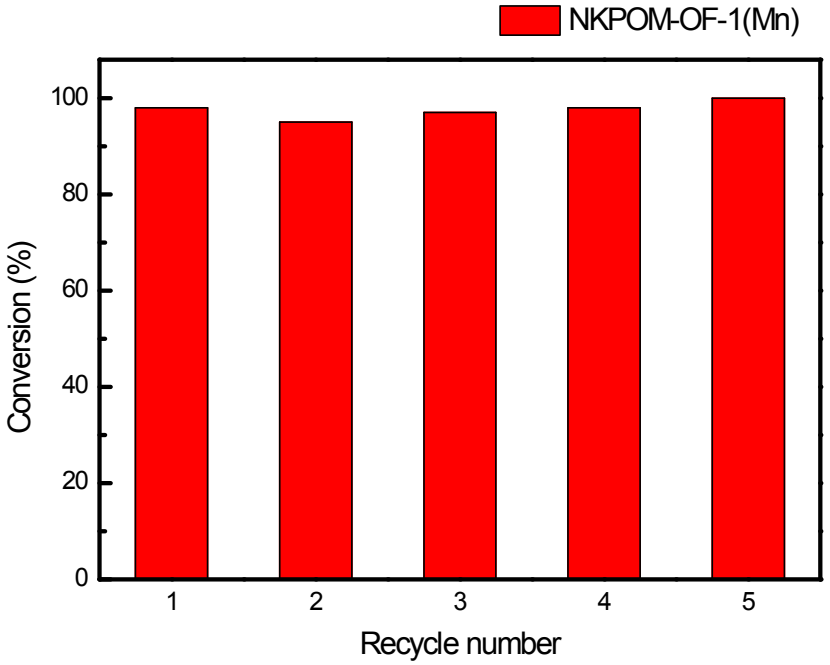

Fig. S39 | **NKPOM-OF-1(Mn)** recycled for 5 times.

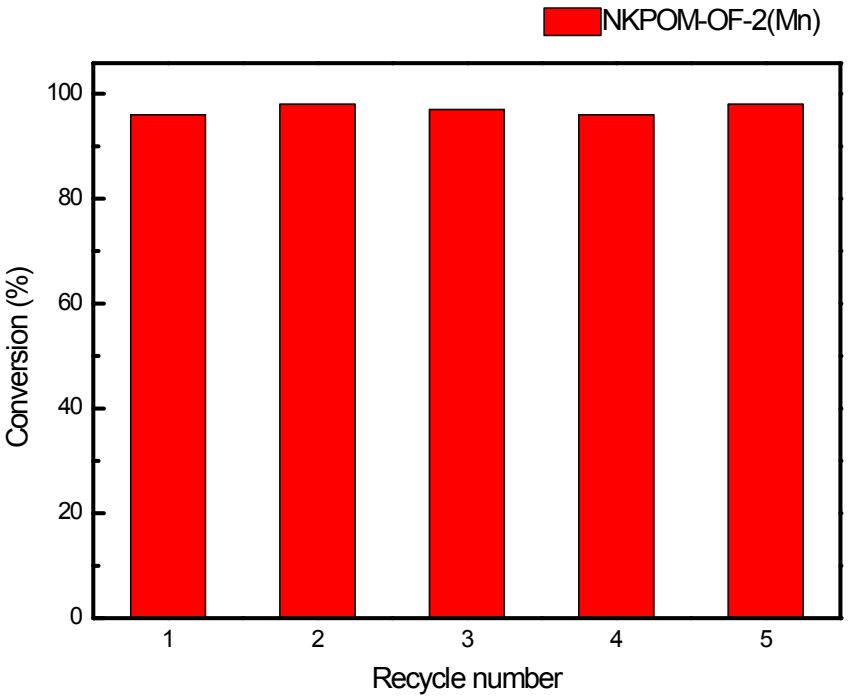

Fig. S40 | **NKPOM-OF-2(Mn)** recycled for 5 times.

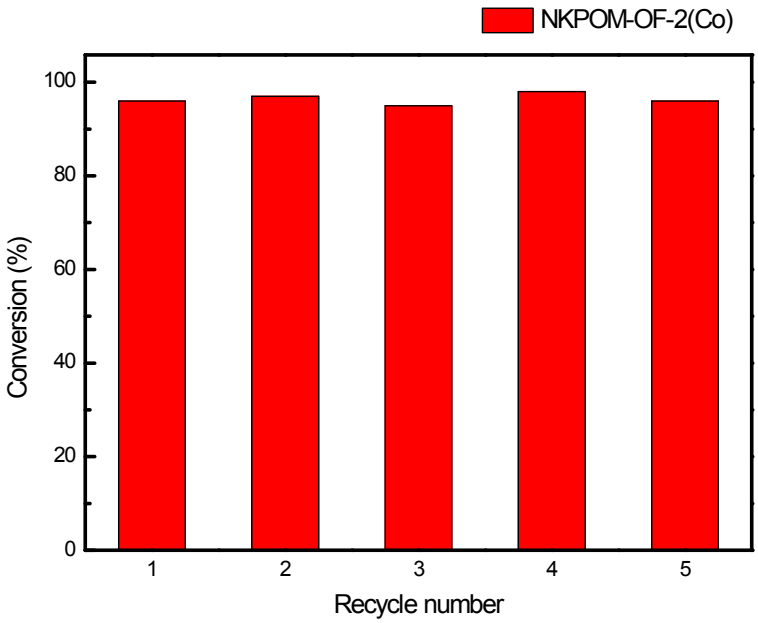

Fig. S41 | **NKPOM-OF-2(Co)** recycled for 5 times.

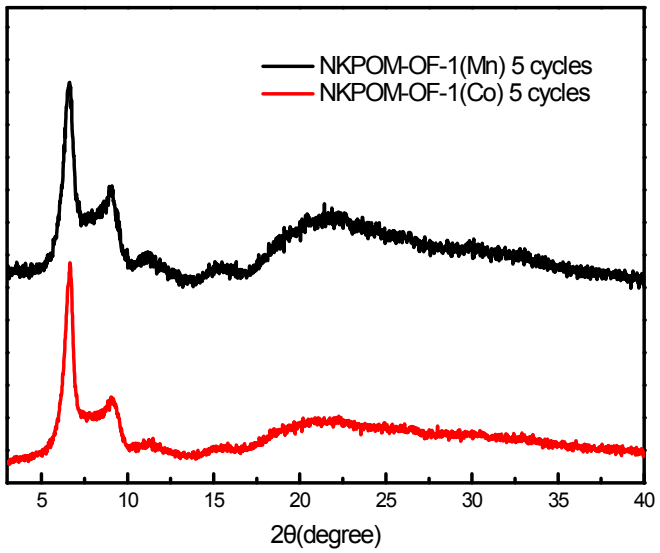

Fig. S42 | PXRD patterns of **NKPOM-OF-1(Mn)** and **NKPOM-OF-1(Co)** after 5 cycles.

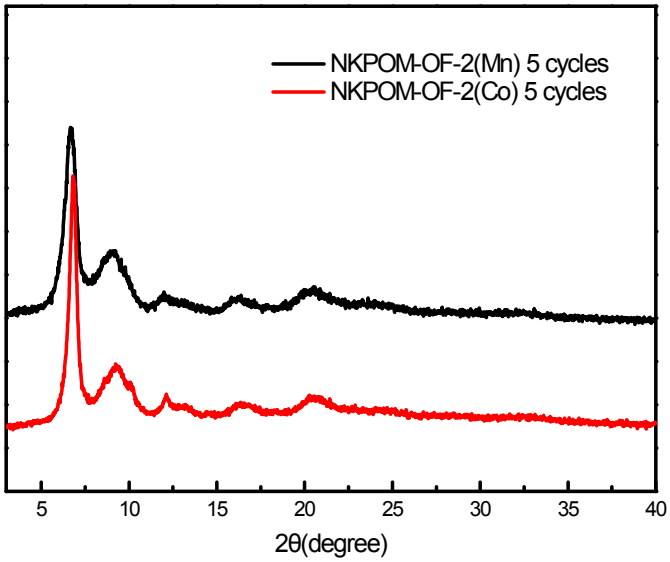

Fig. S43 | PXRD patterns of **NKPOM-OF-2(Mn)** and **NKPOM-OF-2(Co)** after 5 cycles.

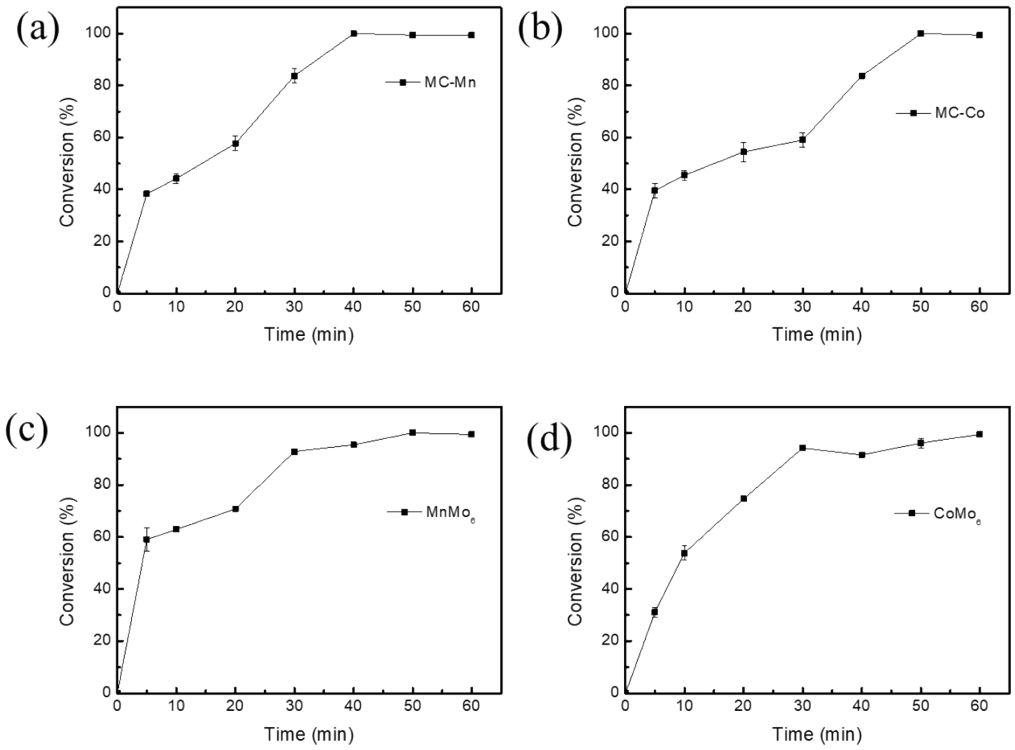

Fig. S44 | Conversion of sulfite to sulfate catalyzed by (a) **MC-Mn**, (b) **MC-Co**, (c) **$MnMo_6$**, (d) **$CoMo_6$**.

The catalytic reaction was also performed under O_2 and Ar to explore whether O_2

play a role in the catalytic reaction. The water was degassed under O_2 and Argon flue, respectively. 5 mg **NKPOM-OF-1(Co)** was added in a 25 mL round bottom flask and the system was filled with O_2 and Ar, respectively. 5 mL 6.6 mM sodium sulfite was added subsequently. The system was shaken with 80 r/min. After reaction, the catalyst was filtered off. The SO_4^{2-} was precipitated by adding excess $BaCl_2$. Excess diluted HCl was added subsequently to remove unreacted SO_3^{2-}. The precipitation was collected by centrifugation, washed by distilled water and dried under 100 ℃. The yield was calculated based on the mass of $BaSO_4$.

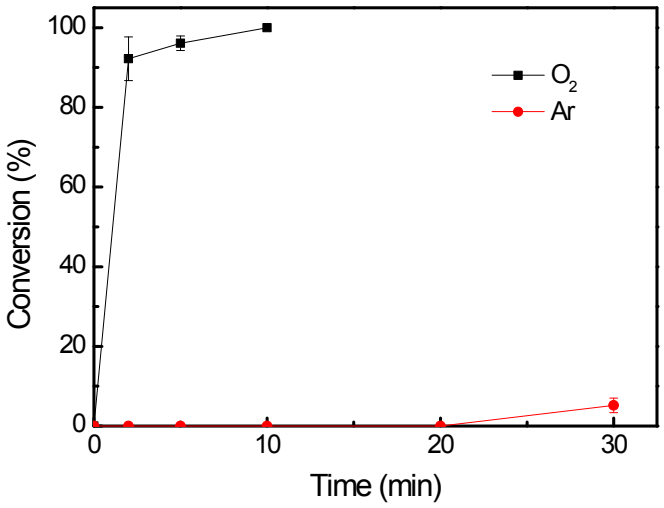

Fig. S45 | Conversion of sulfite to sulfate catalyzed by **NKPOM-OF-1(Co)** under O_2 and Ar.

SI-8. Exfoliation of NKPOM-OFs

Sonication-assisted liquid-phase exfoliation of NKPOM-OFs was performed in ethanol. 50 mg NKPOM-OF was added to 50 mL ethanol and exfoliated under sonication for 2 h. The system was set aside for 24 h. After the sedimentation of bulk NKPOM-OF, the NKPOM-OF-e ('e' represents exfoliation) was collected by centrifugation at 9000 rpm and dried under ambient condition.

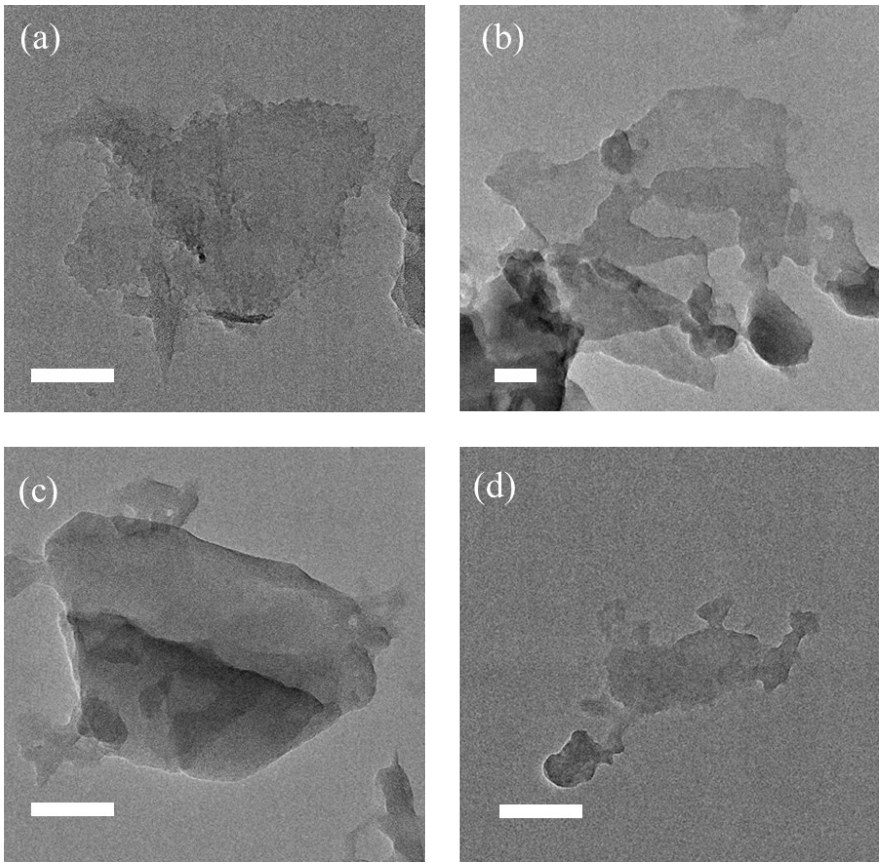

Fig. S46 | HR-TEM images of (a) **NKPOM-OF-1(Mn)-e**, (b)**NKPOM-OF-1(Co)-e**, (c) **NKPOM-OF-2(Mn)-e**, (d) **NKPOM-OF-2(Co)-e**. Scale bar 100 nm.

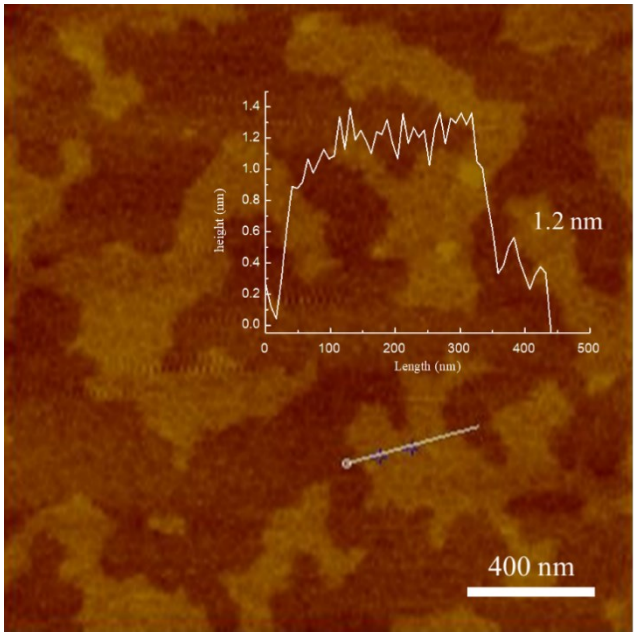

Fig. S47 | AFM image of **NKPOM-OF-1(Mn)-e**. The thickness is about 1.2 nm.

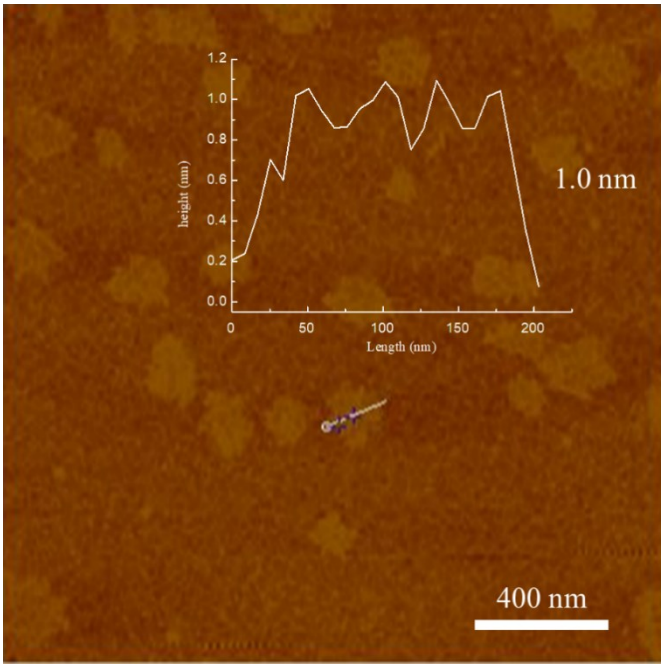

Fig. S48 | AFM image of **NKPOM-OF-2(Co)-e**. The thickness is about 1.0 nm.

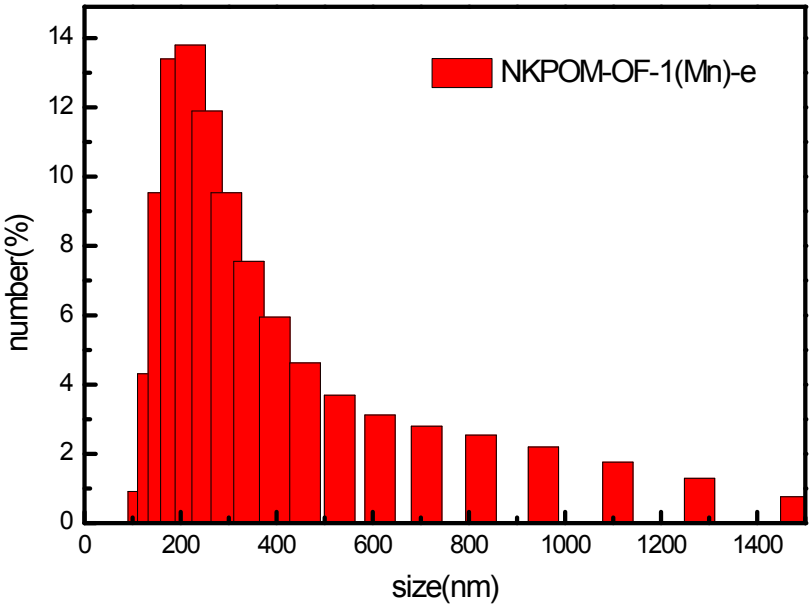

Fig. S49 | Particle size distribution of **NKPOM-OF-1(Mn)-e**.

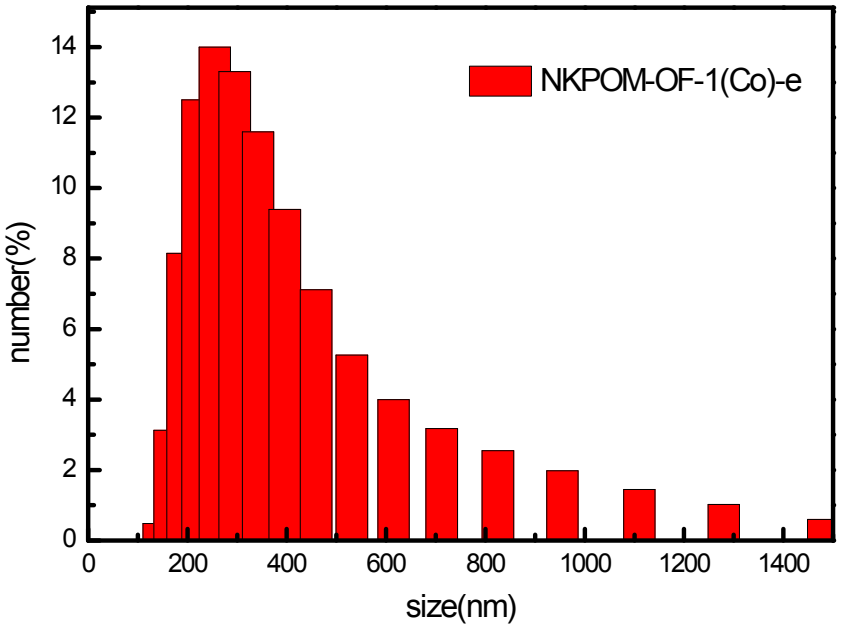

Fig. S50 | Particle size distribution of **NKPOM-OF-1(Co)-e**.

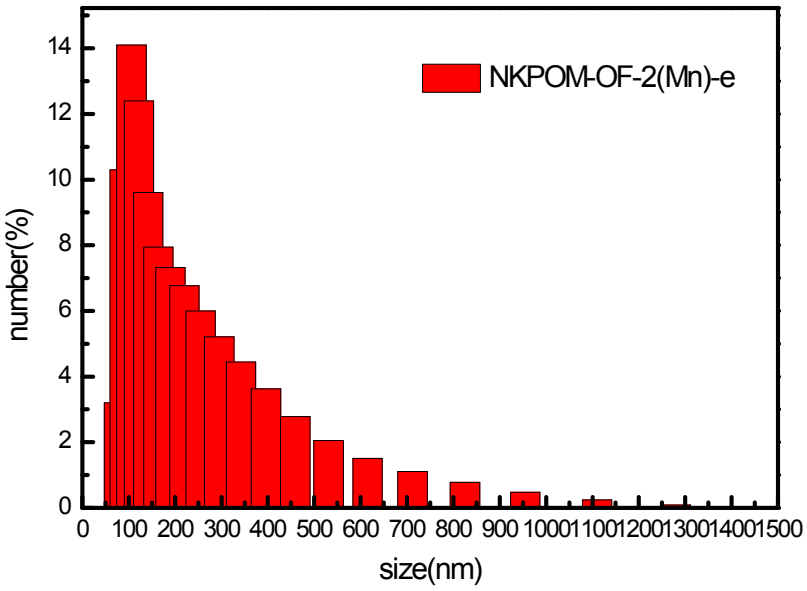

Fig. S51 | Particle size distribution of **NKPOM-OF-2(Mn)-e**.

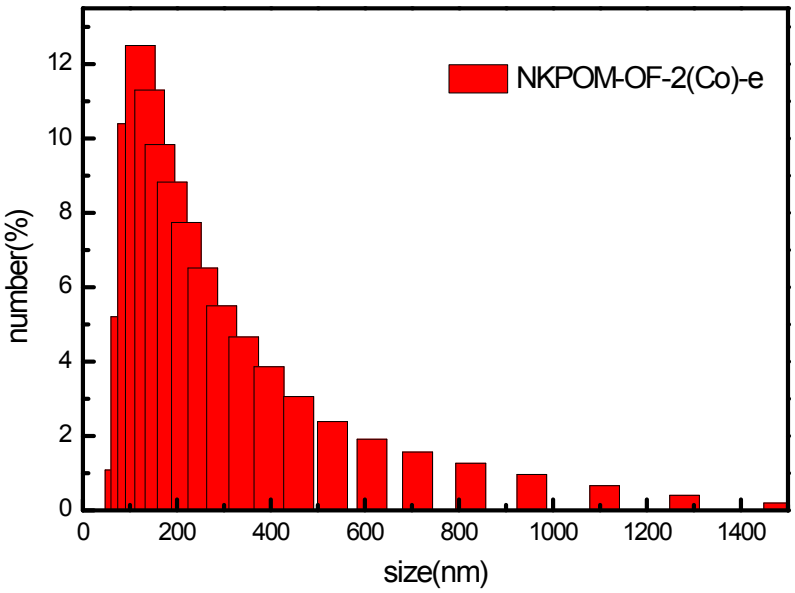

Fig. S52 | Particle size distribution of **NKPOM-OF-2(Co)-e**.

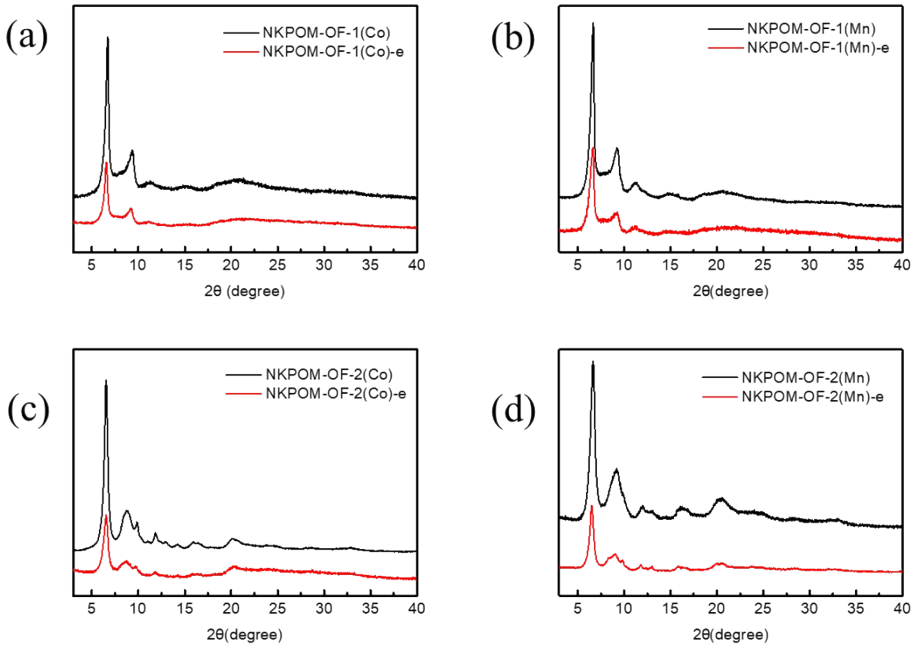

Fig. S53 | PXRD patterns of (a) **NKPOM-OF-1(Co),** (b) **NKPOM-OF-1(Mn)**, (c) **NKPOM-OF-2(Co)**, (d) **NKPOM-OF-2(Mn)** before and after exfoliation.

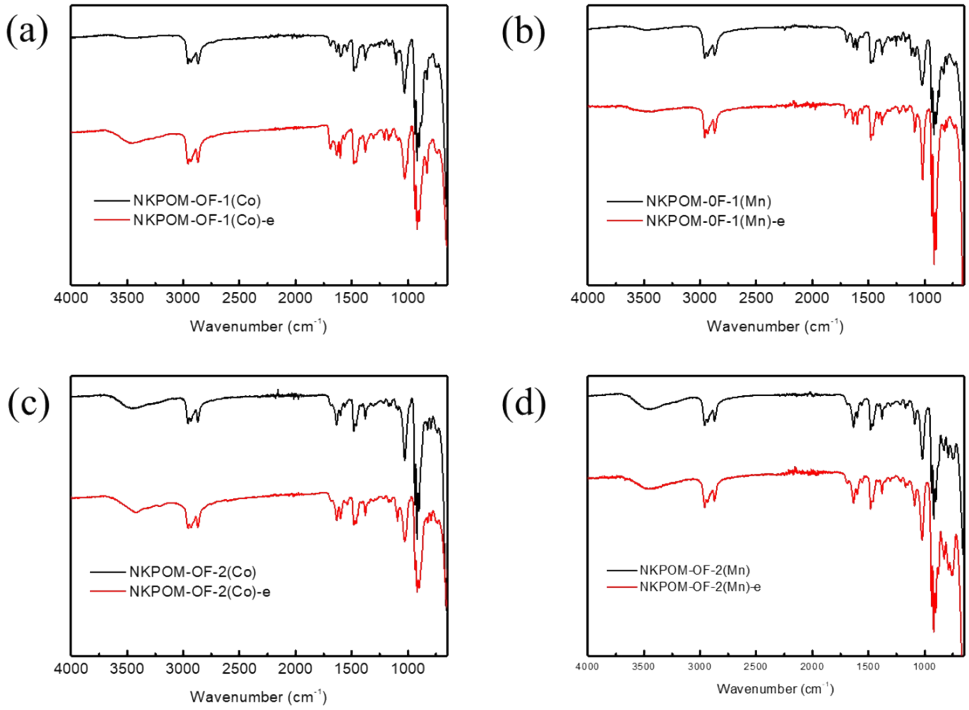

Fig. S54 | FT-IR spectra of (a) **NKPOM-OF-1(Co),** (b) **NKPOM-OF-1(Mn)**, (c) **NKPOM-OF-2(Co)**, (d) **NKPOM-OF-2(Mn)** before and after exfoliation.

The catalytic reaction of NKPOM-OF-e was performed under the same condition of bulk NKPOM-OF. The catalytic reaction was performed in distilled water in a 10 mL centrifuge tube. The water was degassed under Argon flue in order to eliminate the influence of different amount of oxygen dissolved in water. 5 mg NKPOM-OF-e were added in 5 mL 6.6 mM sodium sulfite. The system was shaken with 80 r/min. After reaction, the catalyst was filtered off. The SO_4^{2-} was precipitated by adding excess $BaCl_2$. Excess diluted HCl was added subsequently to remove unreacted SO_3^{2-}. The precipitation was collected by centrifugation, washed by distilled water and dried under 100 ℃. The yield was calculated based on the mass of $BaSO_4$.

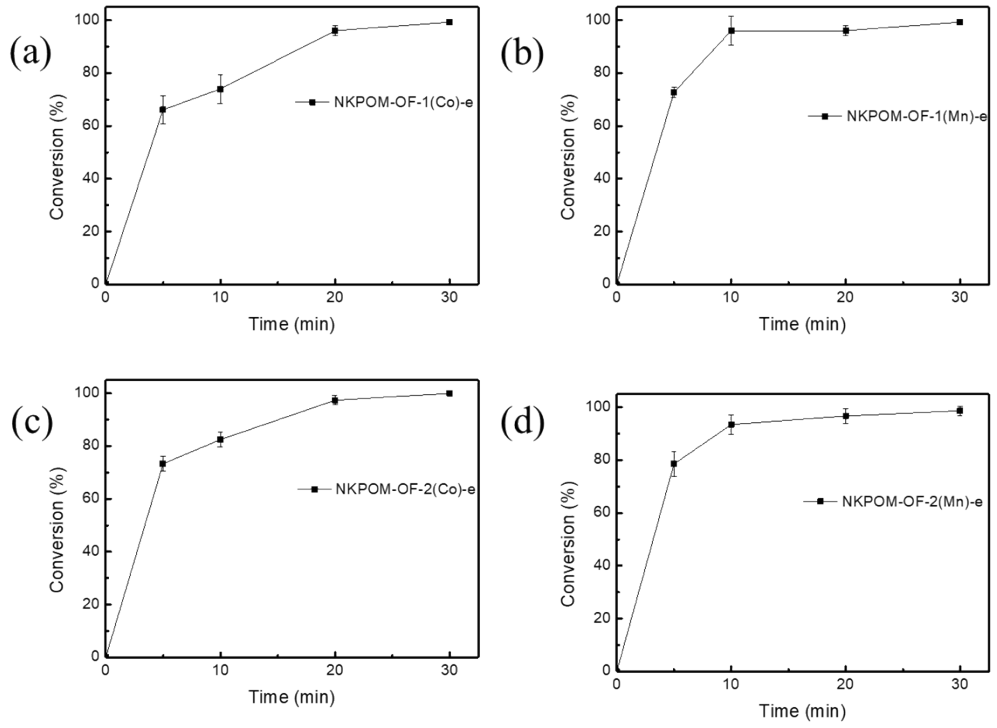

Fig.S55 | Conversion of sulfite to sulfate catalyzed by (a) **NKPOM-OF-1(Co)-e,** (b) **NKPOM-OF-1(Mn)-e**, (c) **NKPOM-OF-2(Co)-e**, (d) **NKPOM-OF-2(Mn)-e**.

Table S3. Crystal data and structure refinement of MC-Co and MC-Mn.

	MC-Co	**MC-Mn**
Formula sum	$C_{74}H_{140}CoMo_6N_7O_{24}$	$C_4H_{6.30}Mn_{0.10}Mo_{0.60}N_{0.40}O_{2.40}$
Formula weight	2146.50	161.45
Temperature/K	293	293
Crystal system	monoclinic	monoclinic
Space-group	P21/c	P21/c
a/ Å	18.0770(3)	15.4385(5)
b/ Å	20.9593(2)	24.0709(8)
c/ Å	25.0897(3)	25.3004(8)
α/°	90.00	90.00
β/°	106.497(2)	100.116(3)
γ/°	90.00	90
Cell volume/ Å^3	9114.7(2)	9255.9(5)
Z	4	40
Calc. density	1.564	1.159
F (000)	4416	3200
R (int)	0.0364	0.0450
GOF on F^2	1.089	1.110
$R_1/wR_2[I>2\sigma(I)]$	0.0384/0.0864	0.0465/0.1367
R_1/wR_2[all data)	0.0560/0.0947	0.0641/0.1432
CCDC number	1997411	1997412

Table S4. Fractional atomic coordinates of NKPOM-OF-1(Co).

Simulated: hexagonal P1; a=26.4 Å, b=39.0 Å, c=19.0 Å, α=γ=90.0°, β=88.2°.

Atom	*x*/*a*	*y*/*b*	*z*/*c*
N1	0.30342	0.35493	0.14458
N2	0.1522	0.16716	0.15812
C3	0.3398	0.36165	0.10002
C4	0.36609	0.39336	0.10807
C5	0.40996	0.39957	0.06776
C6	0.43873	0.42823	0.08256
C7	0.42348	0.44989	0.13799
C8	0.37889	0.44408	0.17699
C9	0.35036	0.41563	0.16226
C10	0.45178	0.48046	0.15106
C11	0.11591	0.16044	0.20284
C12	0.08981	0.12863	0.19514
C13	0.04598	0.12239	0.23551
C14	0.0174	0.0936	0.22101
C15	0.03283	0.07185	0.16583
C16	0.0774	0.07767	0.12682
C17	0.10573	0.10625	0.14126
C18	0.00456	0.04128	0.15269
Mo19	0.15404	0.28705	0.04951
Mo20	0.13432	0.29634	0.20307
Mo21	0.24728	0.2518	-0.00211
O22	0.12063	0.33231	0.26015
O23	0.15815	0.25934	0.13743
O24	0.08719	0.28135	0.03707
O25	0.13861	0.32585	0.11645
O26	0.15734	0.31503	-0.02597
O27	0.06748	0.29056	0.19079
O28	0.22764	0.28736	0.06903
O29	0.1724	0.24724	-0.01276
O30	0.25041	0.27981	-0.07746
O31	0.26098	0.21582	-0.05911
O32	0.24634	0.22588	0.08858
O33	0.32158	0.25676	0.01521
C34	0.13736	0.22678	0.14096
C35	0.21851	0.19586	0.09652
C36	0.17815	0.19934	0.15685
C37	0.25357	0.31821	0.07256

Mo38	0.30156	0.23503	0.25305
Mo39	0.32126	0.22574	0.09949
Mo40	0.20831	0.27028	0.30467
O41	0.33495	0.18976	0.04242
O42	0.29744	0.26274	0.16513
O43	0.3684	0.24073	0.26547
O44	0.31697	0.19623	0.18611
O45	0.29825	0.20706	0.32853
O46	0.3881	0.23151	0.11177
O47	0.22796	0.23473	0.23353
O48	0.28319	0.27484	0.31532
O49	0.20518	0.24227	0.38002
O50	0.19459	0.30626	0.36168
O51	0.20925	0.2962	0.21398
O52	0.13401	0.26531	0.28735
C53	0.31822	0.29529	0.16161
C54	0.23706	0.32622	0.20605
C55	0.27744	0.32274	0.14574
C56	0.20205	0.20389	0.23001
Co57	0.22779	0.26104	0.15128
N58	0.65206	0.66736	0.14422
N59	0.80324	0.85489	0.15864
C60	0.61788	0.66053	0.09941
C61	0.59149	0.62871	0.10731
C62	0.54948	0.62231	0.06698
C63	0.52033	0.59352	0.08172
C64	0.53334	0.57193	0.13707
C65	0.57613	0.57792	0.17606
C66	0.60503	0.60649	0.16139
C67	0.50457	0.54135	0.15045
C68	0.83744	0.86169	0.20343
C69	0.86407	0.89341	0.19538
C70	0.90607	0.89971	0.23578
C71	0.93551	0.92835	0.2209
C72	0.92279	0.94989	0.16533
C73	0.88003	0.944	0.12622
C74	0.85085	0.91556	0.14103
C75	0.95169	0.98043	0.15215
Mo76	0.80628	0.73484	0.0504
Mo77	0.81837	0.72571	0.20411
Mo78	0.71574	0.77021	-0.00207
O79	0.8291	0.68978	0.26135
O80	0.79795	0.76267	0.13821
O81	0.87375	0.74038	0.03854

O82	0.81822	0.69609	0.11753
O83	0.80655	0.70676	-0.02503
O84	0.88583	0.73133	0.1924
O85	0.73173	0.73471	0.06928
O86	0.79116	0.7746	-0.01209
O87	0.71621	0.74211	-0.07738
O88	0.70501	0.80615	-0.05925
O89	0.71233	0.79624	0.08855
O90	0.64059	0.76541	0.01461
C91	0.81869	0.7952	0.14184
C92	0.73987	0.82622	0.09666
C93	0.77725	0.82274	0.15733
C94	0.70549	0.70393	0.07263
Mo95	0.64898	0.78741	0.25253
Mo96	0.63688	0.79654	0.09881
Mo97	0.73952	0.75204	0.30499
O98	0.62616	0.83247	0.04157
O99	0.6573	0.75958	0.16472
O100	0.58151	0.78187	0.2644
O101	0.63703	0.82616	0.1854
O102	0.64871	0.81549	0.32796
O103	0.56943	0.79092	0.11052
O104	0.72354	0.78754	0.23365
O105	0.66411	0.74765	0.31502
O106	0.73905	0.78014	0.3803
O107	0.75025	0.7161	0.36216
O108	0.74293	0.72602	0.21437
O109	0.81467	0.75683	0.28832
C110	0.63656	0.72705	0.16107
C111	0.71538	0.69604	0.20626
C112	0.67801	0.69952	0.14557
C113	0.74977	0.81833	0.23029
Co114	0.72763	0.76113	0.15146
N115	0.65313	0.355	0.15934
N116	0.80405	0.16715	0.14354
C117	0.61672	0.36155	0.20401
C118	0.59041	0.39328	0.1967
C119	0.54663	0.39933	0.23734
C120	0.51784	0.42806	0.2233
C121	0.53299	0.44994	0.16829
C122	0.57749	0.44429	0.12895
C123	0.60604	0.41577	0.14294
C124	0.50456	0.4805	0.15575
C125	0.84047	0.16059	0.09892

C126	0.86661	0.12878	0.10617
C127	0.91043	0.12266	0.06567
C128	0.939	0.09382	0.07967
C129	0.92357	0.0719	0.13448
C130	0.87902	0.07762	0.17365
C131	0.8507	0.10625	0.15971
C132	0.95185	0.04129	0.14715
Mo133	0.80208	0.2867	0.25413
Mo134	0.8223	0.29644	0.10082
Mo135	0.7086	0.25139	0.30458
O136	0.83627	0.33257	0.04441
O137	0.79819	0.25927	0.16572
O138	0.86886	0.28089	0.2669
O139	0.8178	0.32569	0.18791
O140	0.79858	0.31445	0.33005
O141	0.88908	0.29056	0.11345
O142	0.72856	0.28714	0.23413
O143	0.78342	0.24672	0.31565
O144	0.70528	0.27918	0.38037
O145	0.69462	0.21526	0.36095
O146	0.70978	0.22574	0.21348
O147	0.63438	0.25648	0.28687
C148	0.81891	0.22671	0.1618
C149	0.73757	0.19571	0.20523
C150	0.77814	0.19935	0.14519
C151	0.70273	0.31802	0.23095
Mo152	0.65514	0.23545	0.04878
Mo153	0.63491	0.22571	0.20208
Mo154	0.74861	0.27077	-0.00168
O155	0.62094	0.18958	0.25849
O156	0.65903	0.26289	0.13718
O157	0.58835	0.24126	0.03602
O158	0.63942	0.19646	0.115
O159	0.65863	0.2077	-0.02714
O160	0.56813	0.23159	0.18946
O161	0.72865	0.23502	0.06877
O162	0.67379	0.27543	-0.01274
O163	0.75194	0.24297	-0.07746
O164	0.76259	0.3069	-0.05805
O165	0.74743	0.29642	0.08942
O166	0.82283	0.26568	0.01604
C167	0.6383	0.29545	0.1411
C168	0.71964	0.32645	0.09767
C169	0.67907	0.32281	0.15771

C170	0.75448	0.20414	0.07195
Co171	0.72861	0.26108	0.15145
N172	0.30398	0.66728	0.159
N173	0.15313	0.85487	0.14279
C174	0.33819	0.66071	0.2039
C175	0.36463	0.62888	0.19672
C176	0.40652	0.62273	0.2374
C177	0.43569	0.59386	0.22348
C178	0.42278	0.57193	0.16858
C179	0.38012	0.57768	0.1292
C180	0.3512	0.60634	0.14306
C181	0.45163	0.54132	0.15594
C182	0.11883	0.86147	0.09803
C183	0.0922	0.8932	0.10564
C184	0.05024	0.89934	0.06509
C185	0.02083	0.92806	0.07947
C186	0.03355	0.94984	0.13473
C187	0.07626	0.94409	0.17402
C188	0.10541	0.91558	0.15969
C189	0.00466	0.98043	0.14749
Mo190	0.15017	0.73526	0.25274
Mo191	0.13755	0.72554	0.09925
Mo192	0.24099	0.77075	0.30414
O193	0.12652	0.6894	0.04257
O194	0.15828	0.76274	0.16452
O195	0.08275	0.74091	0.26495
O196	0.1379	0.69626	0.18621
O197	0.15007	0.70748	0.32853
O198	0.07014	0.73127	0.11132
O199	0.22466	0.735	0.23338
O200	0.16561	0.77526	0.31459
O201	0.24071	0.74294	0.3798
O202	0.25203	0.8069	0.36077
O203	0.24417	0.79642	0.21316
O204	0.31608	0.76582	0.28704
C205	0.13762	0.79527	0.16056
C206	0.21667	0.8264	0.20482
C207	0.17908	0.82271	0.14444
C208	0.25079	0.70418	0.23029
Mo209	0.30696	0.78689	0.04892
Mo210	0.31959	0.79661	0.20241
Mo211	0.21615	0.7514	-0.00248
O212	0.33063	0.83274	0.2591
O213	0.29885	0.75941	0.13714

O214	0.37439	0.78124	0.0367
O215	0.31924	0.82588	0.11545
O216	0.30707	0.81467	-0.02687
O217	0.387	0.79087	0.19034
O218	0.23247	0.78716	0.06828
O219	0.29152	0.7469	-0.01293
O220	0.21643	0.77921	-0.07814
O221	0.20512	0.71525	-0.0591
O222	0.21298	0.72572	0.0885
O223	0.14106	0.75633	0.01462
C224	0.31952	0.72688	0.14111
C225	0.24048	0.69575	0.09685
C226	0.27806	0.69945	0.15725
C227	0.20633	0.81799	0.07138
Co228	0.22857	0.76108	0.15083
C229	0.42539	0.51087	0.15368
C230	0.53088	0.51095	0.15294
C231	0.03092	0.01085	0.15029
C232	0.92546	0.01086	0.14943
N233	0.29459	0.59938	0.63486
N234	0.14337	0.41161	0.64837
C235	0.33091	0.6061	0.59019
C236	0.35699	0.63792	0.59791
C237	0.40088	0.64415	0.55767
C238	0.42941	0.67297	0.57219
C239	0.41386	0.69475	0.62727
C240	0.36923	0.68892	0.66615
C241	0.34095	0.66032	0.65169
C242	0.44207	0.72535	0.64043
C243	0.10702	0.40489	0.69297
C244	0.0807	0.37319	0.68493
C245	0.03689	0.36697	0.72536
C246	0.00807	0.33833	0.71057
C247	0.0232	0.31671	0.65502
C248	0.06774	0.32252	0.6159
C249	0.09632	0.35095	0.63063
C250	-0.00517	0.28617	0.64195
Mo251	0.14524	0.53151	0.53992
Mo252	0.12553	0.5408	0.69349
Mo253	0.23848	0.49626	0.48829
O254	0.11185	0.57678	0.75056
O255	0.14935	0.5038	0.62784
O256	0.07839	0.52582	0.5275
O257	0.12982	0.57031	0.60687

O258	0.14854	0.55949	0.46445
O259	0.05869	0.53503	0.6812
O260	0.21883	0.53181	0.55944
O261	0.1636	0.4917	0.47765
O262	0.24161	0.52428	0.41294
O263	0.25219	0.46029	0.43127
O264	0.23754	0.47034	0.57897
O265	0.31278	0.50123	0.50561
C266	0.12857	0.47124	0.63134
C267	0.20973	0.44031	0.5869
C268	0.16935	0.44379	0.64721
C269	0.24475	0.56265	0.56296
Mo270	0.29276	0.47948	0.74345
Mo271	0.31247	0.4702	0.58988
Mo272	0.19951	0.51473	0.79507
O273	0.32616	0.43423	0.5328
O274	0.28864	0.5072	0.65553
O275	0.3596	0.48518	0.75588
O276	0.30818	0.44069	0.67649
O277	0.28945	0.4515	0.81892
O278	0.37931	0.47598	0.60217
O279	0.21916	0.47918	0.72393
O280	0.27439	0.51929	0.80572
O281	0.19638	0.48672	0.87042
O282	0.18581	0.55071	0.85208
O283	0.20046	0.54065	0.70439
O284	0.12521	0.50978	0.77776
C285	0.30943	0.53975	0.652
C286	0.22828	0.57068	0.69645
C287	0.26865	0.56719	0.63612
C288	0.19323	0.44833	0.72039
Co289	0.21899	0.50549	0.64168
N290	0.6432	0.91186	0.6349
N291	0.79438	1.09938	0.64929
C292	0.60899	0.90505	0.59012
C293	0.58235	0.87334	0.59815
C294	0.54044	0.867	0.55762
C295	0.51104	0.83833	0.57238
C296	0.5237	0.8168	0.62799
C297	0.56637	0.82273	0.66726
C298	0.59552	0.85119	0.65256
C299	0.49483	0.78623	0.64108
C300	0.82856	1.10622	0.6941
C301	0.85495	1.13803	0.68617

C302	0.89704	1.1444	0.72634
C303	0.92623	1.17316	0.71148
C304	0.91316	1.19475	0.65616
C305	0.87028	1.18881	0.61734
C306	0.84135	1.16026	0.63214
C307	0.94195	1.22532	0.64267
Mo308	0.79746	0.97933	0.54099
Mo309	0.80956	0.9702	0.69471
Mo310	0.70693	1.01469	0.48852
O311	0.82029	0.93428	0.75196
O312	0.78914	1.00717	0.6288
O313	0.86494	0.98487	0.52912
O314	0.80942	0.94058	0.60813
O315	0.79774	0.95125	0.46556
O316	0.87702	0.97582	0.68299
O317	0.72291	0.97919	0.55987
O318	0.78234	1.01909	0.47849
O319	0.70739	0.98659	0.41321
O320	0.6962	1.05063	0.43135
O321	0.70352	1.04072	0.57914
O322	0.63178	1.0099	0.5052
C323	0.80989	1.03969	0.63245
C324	0.73106	1.0707	0.58726
C325	0.76844	1.06722	0.64794
C326	0.69667	0.94841	0.56324
Mo327	0.64017	1.03191	0.74312
Mo328	0.62808	1.04103	0.5894
Mo329	0.7307	0.99653	0.79559
O330	0.61736	1.07696	0.53215
O331	0.64849	1.00407	0.65531
O332	0.5727	1.02637	0.75497
O333	0.62823	1.07065	0.67598
O334	0.6399	1.05998	0.81854
O335	0.56062	1.03542	0.60111
O336	0.71472	1.03203	0.72424
O337	0.65529	0.99214	0.80561
O338	0.73024	1.02464	0.87089
O339	0.74144	0.9606	0.85277
O340	0.73412	0.97051	0.70497
O341	0.80586	1.00133	0.77891
C342	0.62775	0.97154	0.65168
C343	0.70658	0.94052	0.69687
C344	0.66919	0.944	0.6362
C345	0.74095	1.06281	0.72089

Co346	0.71882	1.00561	0.64205
N347	0.64251	0.59952	0.65018
N348	0.79342	0.41167	0.63436
C349	0.6061	0.60611	0.69482
C350	0.58001	0.63793	0.68757
C351	0.53609	0.64403	0.72786
C352	0.50752	0.67285	0.71375
C353	0.52306	0.6948	0.65903
C354	0.56773	0.68911	0.6201
C355	0.59604	0.66049	0.63415
C356	0.49476	0.72538	0.64619
C357	0.82984	0.40515	0.58969
C358	0.8562	0.37344	0.59698
C359	0.89987	0.36736	0.55614
C360	0.92867	0.33862	0.57004
C361	0.91364	0.31675	0.62513
C362	0.86926	0.32243	0.66471
C363	0.8407	0.35097	0.65086
C364	0.94205	0.28616	0.63748
Mo365	0.7914	0.53121	0.74492
Mo366	0.81163	0.54096	0.59161
Mo367	0.69792	0.4959	0.79538
O368	0.82559	0.57709	0.5352
O369	0.7875	0.50378	0.65651
O370	0.85818	0.52541	0.75767
O371	0.80711	0.57021	0.6787
O372	0.7879	0.55896	0.82083
O373	0.8784	0.53508	0.60424
O374	0.71788	0.53164	0.72493
O375	0.77274	0.49124	0.80644
O376	0.6946	0.52369	0.87116
O377	0.68394	0.45977	0.85174
O378	0.6991	0.47025	0.70427
O379	0.62371	0.50099	0.77766
C380	0.80823	0.47123	0.6526
C381	0.72689	0.44022	0.69602
C382	0.76747	0.44386	0.63598
C383	0.69206	0.56252	0.72175
Mo384	0.64445	0.47997	0.53956
Mo385	0.62423	0.47023	0.69287
Mo386	0.73793	0.51528	0.48911
O387	0.61026	0.4341	0.74928
O388	0.64834	0.50741	0.62797
O389	0.57767	0.48578	0.52679

O390	0.62873	0.44098	0.60579
O391	0.64794	0.45223	0.46364
O392	0.55745	0.47612	0.68025
O393	0.71797	0.47953	0.55956
O394	0.66311	0.51995	0.47805
O395	0.74125	0.4875	0.41333
O396	0.75191	0.55142	0.43275
O397	0.73675	0.54093	0.58022
O398	0.81215	0.51019	0.50683
C399	0.62762	0.53997	0.63191
C400	0.70896	0.57096	0.58848
C401	0.6684	0.56732	0.64852
C402	0.7438	0.44865	0.56275
Co403	0.71792	0.50559	0.64224
N404	0.29332	0.91174	0.65
N405	0.14248	1.09933	0.63376
C406	0.32759	0.90514	0.69479
C407	0.35423	0.8734	0.68722
C408	0.39614	0.86726	0.72787
C409	0.42556	0.83855	0.71355
C410	0.41291	0.81677	0.65826
C411	0.37024	0.82252	0.61888
C412	0.34107	0.85103	0.63314
C413	0.44185	0.7862	0.64553
C414	0.10824	1.10589	0.5889
C415	0.0818	1.13772	0.59609
C416	0.03987	1.14386	0.5555
C417	0.01071	1.17274	0.56946
C418	0.02369	1.19468	0.62431
C419	0.06639	1.18893	0.66361
C420	0.09528	1.16027	0.64971
C421	-0.00511	1.22531	0.63697
Mo422	0.1395	0.97973	0.74388
Mo423	0.12687	0.97001	0.59038
Mo424	0.23031	1.01522	0.79526
O425	0.11583	0.93387	0.5337
O426	0.14761	1.00721	0.65565
O427	0.07208	0.98538	0.7561
O428	0.12722	0.94073	0.67735
O429	0.1394	0.95195	0.81967
O430	0.05946	0.97575	0.60246
O431	0.21399	0.97945	0.72451
O432	0.15494	1.01972	0.80572
O433	0.23004	0.98741	0.87093

O434	0.24135	1.05137	0.85188
O435	0.23349	1.04089	0.70428
O436	0.30541	1.01029	0.77817
C437	0.12694	1.03973	0.65168
C438	0.20598	1.07087	0.69592
C439	0.1684	1.06717	0.63553
C440	0.24013	0.94863	0.72141
Mo441	0.29629	1.03135	0.54004
Mo442	0.30892	1.04108	0.69353
Mo443	0.20547	0.99586	0.48865
O444	0.31995	1.07722	0.75021
O445	0.28818	1.00387	0.62827
O446	0.36372	1.0257	0.52783
O447	0.30856	1.07035	0.60656
O448	0.29639	1.05912	0.46425
O449	0.37632	1.03534	0.68146
O450	0.2218	1.03162	0.55941
O451	0.28085	0.99135	0.4782
O452	0.20575	1.02367	0.41299
O453	0.19443	0.95971	0.43203
O454	0.20229	0.97019	0.57963
O455	0.13038	1.0008	0.50575
C456	0.30884	0.97134	0.63223
C457	0.22979	0.94021	0.58798
C458	0.26738	0.9439	0.64835
C459	0.19567	1.06244	0.56249
Co460	0.21789	1.00554	0.64196
C461	0.41565	0.75576	0.64267
C462	0.5211	0.75583	0.64395
C463	0.02118	1.25574	0.63918
C464	0.91568	1.25573	0.64033
H465	0.34993	0.3426	0.05626
H466	0.42168	0.38122	0.02345
H467	0.47455	0.43404	0.04966
H468	0.36652	0.46278	0.22036
H469	0.31394	0.41015	0.19409
H470	0.10573	0.17955	0.24644
H471	0.03414	0.14082	0.27963
H472	-0.0184	0.08778	0.25394
H473	0.08991	0.05889	0.08368
H474	0.14215	0.11175	0.10943
H475	0.1196	0.22048	0.08858
H476	0.10679	0.22592	0.18464
H477	0.24521	0.17385	0.10889

H478	0.19856	0.18998	0.04554
H479	0.22616	0.34022	0.06332
H480	0.28509	0.31877	0.03019
H481	0.34905	0.29592	0.11827
H482	0.33568	0.30185	0.21408
H483	0.25667	0.33211	0.25729
H484	0.21054	0.34826	0.19323
H485	0.22946	0.18188	0.23923
H486	0.17086	0.20357	0.27287
H487	0.60973	0.67954	0.05566
H488	0.53957	0.64061	0.02272
H489	0.48601	0.58757	0.04885
H490	0.58673	0.55927	0.21937
H491	0.63999	0.61211	0.1932
H492	0.84544	0.84272	0.24733
H493	0.91575	0.88146	0.28022
H494	0.96981	0.93423	0.25385
H495	0.86968	0.9626	0.08271
H496	0.81591	0.91001	0.10912
H497	0.83906	0.8014	0.08961
H498	0.84712	0.79606	0.18576
H499	0.71266	0.84829	0.10875
H500	0.76234	0.83199	0.04584
H501	0.73324	0.68185	0.06364
H502	0.67605	0.70339	0.03
H503	0.60787	0.72643	0.11746
H504	0.61649	0.72058	0.21338
H505	0.69321	0.69026	0.25732
H506	0.74243	0.67393	0.19373
H507	0.72203	0.84041	0.23927
H508	0.77887	0.81863	0.27338
H509	0.60655	0.34232	0.24735
H510	0.535	0.3808	0.28131
H511	0.48209	0.43371	0.25647
H512	0.58977	0.46317	0.08592
H513	0.64239	0.41042	0.11084
H514	0.85078	0.17985	0.05569
H515	0.92227	0.14121	0.02185
H516	0.97479	0.0881	0.04663
H517	0.86652	0.05872	0.21651
H518	0.81431	0.11166	0.19167
H519	0.83648	0.22023	0.21421
H520	0.84963	0.22596	0.11831
H521	0.71087	0.17376	0.19234

H522	0.75734	0.18967	0.25625
H523	0.73016	0.33997	0.24069
H524	0.67109	0.31848	0.27315
H525	0.60733	0.29596	0.18426
H526	0.62104	0.30219	0.08862
H527	0.70019	0.3325	0.0464
H528	0.74616	0.34843	0.11099
H529	0.72705	0.18218	0.06221
H530	0.7858	0.20393	0.02927
H531	0.34639	0.67997	0.24726
H532	0.41633	0.6413	0.28131
H533	0.46991	0.58813	0.25666
H534	0.36962	0.55878	0.08624
H535	0.31634	0.61177	0.11094
H536	0.11072	0.8423	0.05447
H537	0.04055	0.8809	0.02091
H538	-0.01344	0.9338	0.04639
H539	0.08661	0.96286	0.21729
H540	0.1403	0.91015	0.19176
H541	0.11744	0.80169	0.21284
H542	0.10904	0.79597	0.11682
H543	0.24391	0.8484	0.19226
H544	0.19437	0.83239	0.25569
H545	0.223	0.68216	0.23973
H546	0.28036	0.70378	0.27274
H547	0.34836	0.72642	0.18453
H548	0.3394	0.72019	0.08877
H549	0.26248	0.68975	0.04574
H550	0.21341	0.67371	0.10983
H551	0.23411	0.84001	0.06193
H552	0.1771	0.81814	0.02846
H553	0.3822	0.51068	0.15395
H554	0.57407	0.51115	0.15266
H555	0.07409	0.01102	0.15064
H556	0.88229	0.01102	0.14907
H557	0.34115	0.58698	0.54663
H558	0.41281	0.62571	0.51363
H559	0.46526	0.67879	0.53937
H560	0.35662	0.70772	0.7092
H561	0.30449	0.65483	0.68341
H562	0.09694	0.42392	0.73677
H563	0.02526	0.38529	0.76976
H564	-0.02771	0.33252	0.74356
H565	0.08001	0.30385	0.57243

H566	0.13269	0.35644	0.5987
H567	0.1108	0.46495	0.57896
H568	0.098	0.47037	0.67502
H569	0.23643	0.41831	0.59927
H570	0.18979	0.43444	0.5359
H571	0.21735	0.58466	0.55373
H572	0.27627	0.56321	0.52057
H573	0.34025	0.54037	0.60865
H574	0.32689	0.54631	0.70446
H575	0.24791	0.57656	0.74768
H576	0.20177	0.59272	0.68365
H577	0.22063	0.42631	0.72962
H578	0.16203	0.448	0.76324
H579	0.60098	0.92403	0.54623
H580	0.5308	0.88525	0.51314
H581	0.4768	0.83243	0.53932
H582	0.57668	0.80415	0.71082
H583	0.63039	0.85678	0.6846
H584	0.8367	1.08721	0.73787
H585	0.907	1.12611	0.77059
H586	0.96062	1.1791	0.74423
H587	0.85963	1.20746	0.57407
H588	0.80631	1.15467	0.60047
H589	0.83025	1.0459	0.58022
H590	0.83831	1.04055	0.67638
H591	0.70386	1.09278	0.59934
H592	0.75355	1.07647	0.53644
H593	0.72441	0.92632	0.55426
H594	0.66722	0.94787	0.52062
H595	0.59906	0.97092	0.60808
H596	0.60769	0.96509	0.704
H597	0.68441	0.93474	0.74794
H598	0.73363	0.91841	0.68434
H599	0.71321	1.08489	0.72987
H600	0.77005	1.06311	0.76398
H601	0.59577	0.58685	0.73804
H602	0.52415	0.62545	0.77162
H603	0.47165	0.67855	0.74663
H604	0.58033	0.70804	0.57734
H605	0.63253	0.65512	0.60238
H606	0.83999	0.42438	0.54635
H607	0.91141	0.38588	0.5121
H608	0.96434	0.33295	0.5367
H609	0.85709	0.30358	0.70783

H610	0.80445	0.35635	0.68315
H611	0.82579	0.46475	0.70501
H612	0.83895	0.47048	0.60911
H613	0.70019	0.41827	0.68313
H614	0.74666	0.43418	0.74704
H615	0.71949	0.58448	0.7315
H616	0.66041	0.56298	0.76396
H617	0.59666	0.54048	0.67507
H618	0.61036	0.54671	0.57944
H619	0.68951	0.57701	0.53722
H620	0.73548	0.59294	0.60179
H621	0.71637	0.4267	0.55301
H622	0.77511	0.44844	0.52006
H623	0.33568	0.9243	0.73837
H624	0.40576	0.8857	0.77208
H625	0.45979	0.83281	0.74671
H626	0.35994	0.80374	0.57558
H627	0.30622	0.85645	0.60101
H628	0.10003	1.08663	0.54555
H629	0.03	1.12529	0.51163
H630	-0.02355	1.17847	0.53635
H631	0.07694	1.20784	0.70653
H632	0.13018	1.15484	0.68176
H633	0.10677	1.04616	0.70395
H634	0.09836	1.04043	0.60794
H635	0.23322	1.09287	0.68337
H636	0.18368	1.07686	0.74678
H637	0.21234	0.92661	0.73086
H638	0.26972	0.94823	0.76385
H639	0.33768	0.97088	0.67565
H640	0.32872	0.96466	0.57988
H641	0.25177	0.93421	0.53686
H642	0.20271	0.91817	0.60097
H643	0.22346	1.08445	0.55304
H644	0.16645	1.06258	0.51955
H645	0.37249	0.75556	0.64214
H646	0.56427	0.75603	0.64446
H647	0.06437	1.25557	0.63869
H648	0.87249	1.25556	0.64077

Table S5. Fractional atomic coordinates of NKPOM-OF-1(Mn).

Simulated: hexagonal P1; a=26.4 Å, b=39.0 Å, c=19.0 Å, α=90.1°, β=88.2°,γ=90.0°.

	x/*a*	*y*/*b*	*z*/*c*
N1	0.30342	0.35493	0.14458
N2	0.1522	0.16716	0.15812
C3	0.3398	0.36165	0.10002
C4	0.36609	0.39336	0.10807
C5	0.40996	0.39957	0.06776
C6	0.43873	0.42823	0.08256
C7	0.42348	0.44989	0.13799
C8	0.37889	0.44408	0.17699
C9	0.35036	0.41563	0.16226
C10	0.45178	0.48046	0.15106
C11	0.11591	0.16044	0.20284
C12	0.08981	0.12863	0.19514
C13	0.04598	0.12239	0.23551
C14	0.0174	0.0936	0.22101
C15	0.03283	0.07185	0.16583
C16	0.0774	0.07767	0.12682
C17	0.10573	0.10625	0.14126
C18	0.00456	0.04128	0.15269
Mo19	0.15404	0.28705	0.04951
Mo20	0.13432	0.29634	0.20307
Mo21	0.24728	0.2518	-0.00211
O22	0.12063	0.33231	0.26015
O23	0.15815	0.25934	0.13743
O24	0.08719	0.28135	0.03707
O25	0.13861	0.32585	0.11645
O26	0.15734	0.31503	-0.02597
O27	0.06748	0.29056	0.19079
O28	0.22764	0.28736	0.06903
O29	0.1724	0.24724	-0.01276
O30	0.25041	0.27981	-0.07746
O31	0.26098	0.21582	-0.05911
O32	0.24634	0.22588	0.08858
O33	0.32158	0.25676	0.01521
C34	0.13736	0.22678	0.14096
C35	0.21851	0.19586	0.09652
C36	0.17815	0.19934	0.15685
C37	0.25357	0.31821	0.07256
Mo38	0.30156	0.23503	0.25305

Mo39	0.32126	0.22574	0.09949
Mo40	0.20831	0.27028	0.30467
O41	0.33495	0.18976	0.04242
O42	0.29744	0.26274	0.16513
O43	0.3684	0.24073	0.26547
O44	0.31697	0.19623	0.18611
O45	0.29825	0.20706	0.32853
O46	0.3881	0.23151	0.11177
O47	0.22796	0.23473	0.23353
O48	0.28319	0.27484	0.31532
O49	0.20518	0.24227	0.38002
O50	0.19459	0.30626	0.36168
O51	0.20925	0.2962	0.21398
O52	0.13401	0.26531	0.28735
C53	0.31822	0.29529	0.16161
C54	0.23706	0.32622	0.20605
C55	0.27744	0.32274	0.14574
C56	0.20205	0.20389	0.23001
Mn57	0.22779	0.26104	0.15128
N58	0.65206	0.66736	0.14422
N59	0.80324	0.85489	0.15864
C60	0.61788	0.66053	0.09941
C61	0.59149	0.62871	0.10731
C62	0.54948	0.62231	0.06698
C63	0.52033	0.59352	0.08172
C64	0.53334	0.57193	0.13707
C65	0.57613	0.57792	0.17606
C66	0.60503	0.60649	0.16139
C67	0.50457	0.54135	0.15045
C68	0.83744	0.86169	0.20343
C69	0.86407	0.89341	0.19538
C70	0.90607	0.89971	0.23578
C71	0.93551	0.92835	0.2209
C72	0.92279	0.94989	0.16533
C73	0.88003	0.944	0.12622
C74	0.85085	0.91556	0.14103
C75	0.95169	0.98043	0.15215
Mo76	0.80628	0.73484	0.0504
Mo77	0.81837	0.72571	0.20411
Mo78	0.71574	0.77021	-0.00207
O79	0.8291	0.68978	0.26135
O80	0.79795	0.76267	0.13821
O81	0.87375	0.74038	0.03854
O82	0.81822	0.69609	0.11753

O83	0.80655	0.70676	-0.02503
O84	0.88583	0.73133	0.1924
O85	0.73173	0.73471	0.06928
O86	0.79116	0.7746	-0.01209
O87	0.71621	0.74211	-0.07738
O88	0.70501	0.80615	-0.05925
O89	0.71233	0.79624	0.08855
O90	0.64059	0.76541	0.01461
C91	0.81869	0.7952	0.14184
C92	0.73987	0.82622	0.09666
C93	0.77725	0.82274	0.15733
C94	0.70549	0.70393	0.07263
Mo95	0.64898	0.78741	0.25253
Mo96	0.63688	0.79654	0.09881
Mo97	0.73952	0.75204	0.30499
O98	0.62616	0.83247	0.04157
O99	0.6573	0.75958	0.16472
O100	0.58151	0.78187	0.2644
O101	0.63703	0.82616	0.1854
O102	0.64871	0.81549	0.32796
O103	0.56943	0.79092	0.11052
O104	0.72354	0.78754	0.23365
O105	0.66411	0.74765	0.31502
O106	0.73905	0.78014	0.3803
O107	0.75025	0.7161	0.36216
O108	0.74293	0.72602	0.21437
O109	0.81467	0.75683	0.28832
C110	0.63656	0.72705	0.16107
C111	0.71538	0.69604	0.20626
C112	0.67801	0.69952	0.14557
C113	0.74977	0.81833	0.23029
Mn114	0.72763	0.76113	0.15146
N115	0.65313	0.355	0.15934
N116	0.80405	0.16715	0.14354
C117	0.61672	0.36155	0.20401
C118	0.59041	0.39328	0.1967
C119	0.54663	0.39933	0.23734
C120	0.51784	0.42806	0.2233
C121	0.53299	0.44994	0.16829
C122	0.57749	0.44429	0.12895
C123	0.60604	0.41577	0.14294
C124	0.50456	0.4805	0.15575
C125	0.84047	0.16059	0.09892
C126	0.86661	0.12878	0.10617

C127	0.91043	0.12266	0.06567
C128	0.939	0.09382	0.07967
C129	0.92357	0.0719	0.13448
C130	0.87902	0.07762	0.17365
C131	0.8507	0.10625	0.15971
C132	0.95185	0.04129	0.14715
Mo133	0.80208	0.2867	0.25413
Mo134	0.8223	0.29644	0.10082
Mo135	0.7086	0.25139	0.30458
O136	0.83627	0.33257	0.04441
O137	0.79819	0.25927	0.16572
O138	0.86886	0.28089	0.2669
O139	0.8178	0.32569	0.18791
O140	0.79858	0.31445	0.33005
O141	0.88908	0.29056	0.11345
O142	0.72856	0.28714	0.23413
O143	0.78342	0.24672	0.31565
O144	0.70528	0.27918	0.38037
O145	0.69462	0.21526	0.36095
O146	0.70978	0.22574	0.21348
O147	0.63438	0.25648	0.28687
C148	0.81891	0.22671	0.1618
C149	0.73757	0.19571	0.20523
C150	0.77814	0.19935	0.14519
C151	0.70273	0.31802	0.23095
Mo152	0.65514	0.23545	0.04878
Mo153	0.63491	0.22571	0.20208
Mo154	0.74861	0.27077	-0.00168
O155	0.62094	0.18958	0.25849
O156	0.65903	0.26289	0.13718
O157	0.58835	0.24126	0.03602
O158	0.63942	0.19646	0.115
O159	0.65863	0.2077	-0.02714
O160	0.56813	0.23159	0.18946
O161	0.72865	0.23502	0.06877
O162	0.67379	0.27543	-0.01274
O163	0.75194	0.24297	-0.07746
O164	0.76259	0.3069	-0.05805
O165	0.74743	0.29642	0.08942
O166	0.82283	0.26568	0.01604
C167	0.6383	0.29545	0.1411
C168	0.71964	0.32645	0.09767
C169	0.67907	0.32281	0.15771
C170	0.75448	0.20414	0.07195

Mn171	0.72861	0.26108	0.15145
N172	0.30398	0.66728	0.159
N173	0.15313	0.85487	0.14279
C174	0.33819	0.66071	0.2039
C175	0.36463	0.62888	0.19672
C176	0.40652	0.62273	0.2374
C177	0.43569	0.59386	0.22348
C178	0.42278	0.57193	0.16858
C179	0.38012	0.57768	0.1292
C180	0.3512	0.60634	0.14306
C181	0.45163	0.54132	0.15594
C182	0.11883	0.86147	0.09803
C183	0.0922	0.8932	0.10564
C184	0.05024	0.89934	0.06509
C185	0.02083	0.92806	0.07947
C186	0.03355	0.94984	0.13473
C187	0.07626	0.94409	0.17402
C188	0.10541	0.91558	0.15969
C189	0.00466	0.98043	0.14749
Mo190	0.15017	0.73526	0.25274
Mo191	0.13755	0.72554	0.09925
Mo192	0.24099	0.77075	0.30414
O193	0.12652	0.6894	0.04257
O194	0.15828	0.76274	0.16452
O195	0.08275	0.74091	0.26495
O196	0.1379	0.69626	0.18621
O197	0.15007	0.70748	0.32853
O198	0.07014	0.73127	0.11132
O199	0.22466	0.735	0.23338
O200	0.16561	0.77526	0.31459
O201	0.24071	0.74294	0.3798
O202	0.25203	0.8069	0.36077
O203	0.24417	0.79642	0.21316
O204	0.31608	0.76582	0.28704
C205	0.13762	0.79527	0.16056
C206	0.21667	0.8264	0.20482
C207	0.17908	0.82271	0.14444
C208	0.25079	0.70418	0.23029
Mo209	0.30696	0.78689	0.04892
Mo210	0.31959	0.79661	0.20241
Mo211	0.21615	0.7514	-0.00248
O212	0.33063	0.83274	0.2591
O213	0.29885	0.75941	0.13714
O214	0.37439	0.78124	0.0367

O215	0.31924	0.82588	0.11545
O216	0.30707	0.81467	-0.02687
O217	0.387	0.79087	0.19034
O218	0.23247	0.78716	0.06828
O219	0.29152	0.7469	-0.01293
O220	0.21643	0.77921	-0.07814
O221	0.20512	0.71525	-0.0591
O222	0.21298	0.72572	0.0885
O223	0.14106	0.75633	0.01462
C224	0.31952	0.72688	0.14111
C225	0.24048	0.69575	0.09685
C226	0.27806	0.69945	0.15725
C227	0.20633	0.81799	0.07138
Mn228	0.22857	0.76108	0.15083
C229	0.42539	0.51087	0.15368
C230	0.53088	0.51095	0.15294
C231	0.03092	0.01085	0.15029
C232	0.92546	0.01086	0.14943
N233	0.29459	0.59938	0.63486
N234	0.14337	0.41161	0.64837
C235	0.33091	0.6061	0.59019
C236	0.35699	0.63792	0.59791
C237	0.40088	0.64415	0.55767
C238	0.42941	0.67297	0.57219
C239	0.41386	0.69475	0.62727
C240	0.36923	0.68892	0.66615
C241	0.34095	0.66032	0.65169
C242	0.44207	0.72535	0.64043
C243	0.10702	0.40489	0.69297
C244	0.0807	0.37319	0.68493
C245	0.03689	0.36697	0.72536
C246	0.00807	0.33833	0.71057
C247	0.0232	0.31671	0.65502
C248	0.06774	0.32252	0.6159
C249	0.09632	0.35095	0.63063
C250	-0.00517	0.28617	0.64195
Mo251	0.14524	0.53151	0.53992
Mo252	0.12553	0.5408	0.69349
Mo253	0.23848	0.49626	0.48829
O254	0.11185	0.57678	0.75056
O255	0.14935	0.5038	0.62784
O256	0.07839	0.52582	0.5275
O257	0.12982	0.57031	0.60687
O258	0.14854	0.55949	0.46445

O259	0.05869	0.53503	0.6812
O260	0.21883	0.53181	0.55944
O261	0.1636	0.4917	0.47765
O262	0.24161	0.52428	0.41294
O263	0.25219	0.46029	0.43127
O264	0.23754	0.47034	0.57897
O265	0.31278	0.50123	0.50561
C266	0.12857	0.47124	0.63134
C267	0.20973	0.44031	0.5869
C268	0.16935	0.44379	0.64721
C269	0.24475	0.56265	0.56296
Mo270	0.29276	0.47948	0.74345
Mo271	0.31247	0.4702	0.58988
Mo272	0.19951	0.51473	0.79507
O273	0.32616	0.43423	0.5328
O274	0.28864	0.5072	0.65553
O275	0.3596	0.48518	0.75588
O276	0.30818	0.44069	0.67649
O277	0.28945	0.4515	0.81892
O278	0.37931	0.47598	0.60217
O279	0.21916	0.47918	0.72393
O280	0.27439	0.51929	0.80572
O281	0.19638	0.48672	0.87042
O282	0.18581	0.55071	0.85208
O283	0.20046	0.54065	0.70439
O284	0.12521	0.50978	0.77776
C285	0.30943	0.53975	0.652
C286	0.22828	0.57068	0.69645
C287	0.26865	0.56719	0.63612
C288	0.19323	0.44833	0.72039
Mn289	0.21899	0.50549	0.64168
N290	0.6432	0.91186	0.6349
N291	0.79438	1.09938	0.64929
C292	0.60899	0.90505	0.59012
C293	0.58235	0.87334	0.59815
C294	0.54044	0.867	0.55762
C295	0.51104	0.83833	0.57238
C296	0.5237	0.8168	0.62799
C297	0.56637	0.82273	0.66726
C298	0.59552	0.85119	0.65256
C299	0.49483	0.78623	0.64108
C300	0.82856	1.10622	0.6941
C301	0.85495	1.13803	0.68617
C302	0.89704	1.1444	0.72634

C303	0.92623	1.17316	0.71148
C304	0.91316	1.19475	0.65616
C305	0.87028	1.18881	0.61734
C306	0.84135	1.16026	0.63214
C307	0.94195	1.22532	0.64267
Mo308	0.79746	0.97933	0.54099
Mo309	0.80956	0.9702	0.69471
Mo310	0.70693	1.01469	0.48852
O311	0.82029	0.93428	0.75196
O312	0.78914	1.00717	0.6288
O313	0.86494	0.98487	0.52912
O314	0.80942	0.94058	0.60813
O315	0.79774	0.95125	0.46556
O316	0.87702	0.97582	0.68299
O317	0.72291	0.97919	0.55987
O318	0.78234	1.01909	0.47849
O319	0.70739	0.98659	0.41321
O320	0.6962	1.05063	0.43135
O321	0.70352	1.04072	0.57914
O322	0.63178	1.0099	0.5052
C323	0.80989	1.03969	0.63245
C324	0.73106	1.0707	0.58726
C325	0.76844	1.06722	0.64794
C326	0.69667	0.94841	0.56324
Mo327	0.64017	1.03191	0.74312
Mo328	0.62808	1.04103	0.5894
Mo329	0.7307	0.99653	0.79559
O330	0.61736	1.07696	0.53215
O331	0.64849	1.00407	0.65531
O332	0.5727	1.02637	0.75497
O333	0.62823	1.07065	0.67598
O334	0.6399	1.05998	0.81854
O335	0.56062	1.03542	0.60111
O336	0.71472	1.03203	0.72424
O337	0.65529	0.99214	0.80561
O338	0.73024	1.02464	0.87089
O339	0.74144	0.9606	0.85277
O340	0.73412	0.97051	0.70497
O341	0.80586	1.00133	0.77891
C342	0.62775	0.97154	0.65168
C343	0.70658	0.94052	0.69687
C344	0.66919	0.944	0.6362
C345	0.74095	1.06281	0.72089
Mn346	0.71882	1.00561	0.64205

N347	0.64251	0.59952	0.65018
N348	0.79342	0.41167	0.63436
C349	0.6061	0.60611	0.69482
C350	0.58001	0.63793	0.68757
C351	0.53609	0.64403	0.72786
C352	0.50752	0.67285	0.71375
C353	0.52306	0.6948	0.65903
C354	0.56773	0.68911	0.6201
C355	0.59604	0.66049	0.63415
C356	0.49476	0.72538	0.64619
C357	0.82984	0.40515	0.58969
C358	0.8562	0.37344	0.59698
C359	0.89987	0.36736	0.55614
C360	0.92867	0.33862	0.57004
C361	0.91364	0.31675	0.62513
C362	0.86926	0.32243	0.66471
C363	0.8407	0.35097	0.65086
C364	0.94205	0.28616	0.63748
Mo365	0.7914	0.53121	0.74492
Mo366	0.81163	0.54096	0.59161
Mo367	0.69792	0.4959	0.79538
O368	0.82559	0.57709	0.5352
O369	0.7875	0.50378	0.65651
O370	0.85818	0.52541	0.75767
O371	0.80711	0.57021	0.6787
O372	0.7879	0.55896	0.82083
O373	0.8784	0.53508	0.60424
O374	0.71788	0.53164	0.72493
O375	0.77274	0.49124	0.80644
O376	0.6946	0.52369	0.87116
O377	0.68394	0.45977	0.85174
O378	0.6991	0.47025	0.70427
O379	0.62371	0.50099	0.77766
C380	0.80823	0.47123	0.6526
C381	0.72689	0.44022	0.69602
C382	0.76747	0.44386	0.63598
C383	0.69206	0.56252	0.72175
Mo384	0.64445	0.47997	0.53956
Mo385	0.62423	0.47023	0.69287
Mo386	0.73793	0.51528	0.48911
O387	0.61026	0.4341	0.74928
O388	0.64834	0.50741	0.62797
O389	0.57767	0.48578	0.52679
O390	0.62873	0.44098	0.60579

O391	0.64794	0.45223	0.46364
O392	0.55745	0.47612	0.68025
O393	0.71797	0.47953	0.55956
O394	0.66311	0.51995	0.47805
O395	0.74125	0.4875	0.41333
O396	0.75191	0.55142	0.43275
O397	0.73675	0.54093	0.58022
O398	0.81215	0.51019	0.50683
C399	0.62762	0.53997	0.63191
C400	0.70896	0.57096	0.58848
C401	0.6684	0.56732	0.64852
C402	0.7438	0.44865	0.56275
Mn403	0.71792	0.50559	0.64224
N404	0.29332	0.91174	0.65
N405	0.14248	1.09933	0.63376
C406	0.32759	0.90514	0.69479
C407	0.35423	0.8734	0.68722
C408	0.39614	0.86726	0.72787
C409	0.42556	0.83855	0.71355
C410	0.41291	0.81677	0.65826
C411	0.37024	0.82252	0.61888
C412	0.34107	0.85103	0.63314
C413	0.44185	0.7862	0.64553
C414	0.10824	1.10589	0.5889
C415	0.0818	1.13772	0.59609
C416	0.03987	1.14386	0.5555
C417	0.01071	1.17274	0.56946
C418	0.02369	1.19468	0.62431
C419	0.06639	1.18893	0.66361
C420	0.09528	1.16027	0.64971
C421	-0.00511	1.22531	0.63697
Mo422	0.1395	0.97973	0.74388
Mo423	0.12687	0.97001	0.59038
Mo424	0.23031	1.01522	0.79526
O425	0.11583	0.93387	0.5337
O426	0.14761	1.00721	0.65565
O427	0.07208	0.98538	0.7561
O428	0.12722	0.94073	0.67735
O429	0.1394	0.95195	0.81967
O430	0.05946	0.97575	0.60246
O431	0.21399	0.97945	0.72451
O432	0.15494	1.01972	0.80572
O433	0.23004	0.98741	0.87093
O434	0.24135	1.05137	0.85188

O435	0.23349	1.04089	0.70428
O436	0.30541	1.01029	0.77817
C437	0.12694	1.03973	0.65168
C438	0.20598	1.07087	0.69592
C439	0.1684	1.06717	0.63553
C440	0.24013	0.94863	0.72141
Mo441	0.29629	1.03135	0.54004
Mo442	0.30892	1.04108	0.69353
Mo443	0.20547	0.99586	0.48865
O444	0.31995	1.07722	0.75021
O445	0.28818	1.00387	0.62827
O446	0.36372	1.0257	0.52783
O447	0.30856	1.07035	0.60656
O448	0.29639	1.05912	0.46425
O449	0.37632	1.03534	0.68146
O450	0.2218	1.03162	0.55941
O451	0.28085	0.99135	0.4782
O452	0.20575	1.02367	0.41299
O453	0.19443	0.95971	0.43203
O454	0.20229	0.97019	0.57963
O455	0.13038	1.0008	0.50575
C456	0.30884	0.97134	0.63223
C457	0.22979	0.94021	0.58798
C458	0.26738	0.9439	0.64835
C459	0.19567	1.06244	0.56249
Mn460	0.21789	1.00554	0.64196
C461	0.41565	0.75576	0.64267
C462	0.5211	0.75583	0.64395
C463	0.02118	1.25574	0.63918
C464	0.91568	1.25573	0.64033
H465	0.34993	0.3426	0.05626
H466	0.42168	0.38122	0.02345
H467	0.47455	0.43404	0.04966
H468	0.36652	0.46278	0.22036
H469	0.31394	0.41015	0.19409
H470	0.10573	0.17955	0.24644
H471	0.03414	0.14082	0.27963
H472	-0.0184	0.08778	0.25394
H473	0.08991	0.05889	0.08368
H474	0.14215	0.11175	0.10943
H475	0.1196	0.22048	0.08858
H476	0.10679	0.22592	0.18464
H477	0.24521	0.17385	0.10889
H478	0.19856	0.18998	0.04554

H479	0.22616	0.34022	0.06332
H480	0.28509	0.31877	0.03019
H481	0.34905	0.29592	0.11827
H482	0.33568	0.30185	0.21408
H483	0.25667	0.33211	0.25729
H484	0.21054	0.34826	0.19323
H485	0.22946	0.18188	0.23923
H486	0.17086	0.20357	0.27287
H487	0.60973	0.67954	0.05566
H488	0.53957	0.64061	0.02272
H489	0.48601	0.58757	0.04885
H490	0.58673	0.55927	0.21937
H491	0.63999	0.61211	0.1932
H492	0.84544	0.84272	0.24733
H493	0.91575	0.88146	0.28022
H494	0.96981	0.93423	0.25385
H495	0.86968	0.9626	0.08271
H496	0.81591	0.91001	0.10912
H497	0.83906	0.8014	0.08961
H498	0.84712	0.79606	0.18576
H499	0.71266	0.84829	0.10875
H500	0.76234	0.83199	0.04584
H501	0.73324	0.68185	0.06364
H502	0.67605	0.70339	0.03
H503	0.60787	0.72643	0.11746
H504	0.61649	0.72058	0.21338
H505	0.69321	0.69026	0.25732
H506	0.74243	0.67393	0.19373
H507	0.72203	0.84041	0.23927
H508	0.77887	0.81863	0.27338
H509	0.60655	0.34232	0.24735
H510	0.535	0.3808	0.28131
H511	0.48209	0.43371	0.25647
H512	0.58977	0.46317	0.08592
H513	0.64239	0.41042	0.11084
H514	0.85078	0.17985	0.05569
H515	0.92227	0.14121	0.02185
H516	0.97479	0.0881	0.04663
H517	0.86652	0.05872	0.21651
H518	0.81431	0.11166	0.19167
H519	0.83648	0.22023	0.21421
H520	0.84963	0.22596	0.11831
H521	0.71087	0.17376	0.19234
H522	0.75734	0.18967	0.25625

H523	0.73016	0.33997	0.24069
H524	0.67109	0.31848	0.27315
H525	0.60733	0.29596	0.18426
H526	0.62104	0.30219	0.08862
H527	0.70019	0.3325	0.0464
H528	0.74616	0.34843	0.11099
H529	0.72705	0.18218	0.06221
H530	0.7858	0.20393	0.02927
H531	0.34639	0.67997	0.24726
H532	0.41633	0.6413	0.28131
H533	0.46991	0.58813	0.25666
H534	0.36962	0.55878	0.08624
H535	0.31634	0.61177	0.11094
H536	0.11072	0.8423	0.05447
H537	0.04055	0.8809	0.02091
H538	-0.01344	0.9338	0.04639
H539	0.08661	0.96286	0.21729
H540	0.1403	0.91015	0.19176
H541	0.11744	0.80169	0.21284
H542	0.10904	0.79597	0.11682
H543	0.24391	0.8484	0.19226
H544	0.19437	0.83239	0.25569
H545	0.223	0.68216	0.23973
H546	0.28036	0.70378	0.27274
H547	0.34836	0.72642	0.18453
H548	0.3394	0.72019	0.08877
H549	0.26248	0.68975	0.04574
H550	0.21341	0.67371	0.10983
H551	0.23411	0.84001	0.06193
H552	0.1771	0.81814	0.02846
H553	0.3822	0.51068	0.15395
H554	0.57407	0.51115	0.15266
H555	0.07409	0.01102	0.15064
H556	0.88229	0.01102	0.14907
H557	0.34115	0.58698	0.54663
H558	0.41281	0.62571	0.51363
H559	0.46526	0.67879	0.53937
H560	0.35662	0.70772	0.7092
H561	0.30449	0.65483	0.68341
H562	0.09694	0.42392	0.73677
H563	0.02526	0.38529	0.76976
H564	-0.02771	0.33252	0.74356
H565	0.08001	0.30385	0.57243
H566	0.13269	0.35644	0.5987

H567	0.1108	0.46495	0.57896
H568	0.098	0.47037	0.67502
H569	0.23643	0.41831	0.59927
H570	0.18979	0.43444	0.5359
H571	0.21735	0.58466	0.55373
H572	0.27627	0.56321	0.52057
H573	0.34025	0.54037	0.60865
H574	0.32689	0.54631	0.70446
H575	0.24791	0.57656	0.74768
H576	0.20177	0.59272	0.68365
H577	0.22063	0.42631	0.72962
H578	0.16203	0.448	0.76324
H579	0.60098	0.92403	0.54623
H580	0.5308	0.88525	0.51314
H581	0.4768	0.83243	0.53932
H582	0.57668	0.80415	0.71082
H583	0.63039	0.85678	0.6846
H584	0.8367	1.08721	0.73787
H585	0.907	1.12611	0.77059
H586	0.96062	1.1791	0.74423
H587	0.85963	1.20746	0.57407
H588	0.80631	1.15467	0.60047
H589	0.83025	1.0459	0.58022
H590	0.83831	1.04055	0.67638
H591	0.70386	1.09278	0.59934
H592	0.75355	1.07647	0.53644
H593	0.72441	0.92632	0.55426
H594	0.66722	0.94787	0.52062
H595	0.59906	0.97092	0.60808
H596	0.60769	0.96509	0.704
H597	0.68441	0.93474	0.74794
H598	0.73363	0.91841	0.68434
H599	0.71321	1.08489	0.72987
H600	0.77005	1.06311	0.76398
H601	0.59577	0.58685	0.73804
H602	0.52415	0.62545	0.77162
H603	0.47165	0.67855	0.74663
H604	0.58033	0.70804	0.57734
H605	0.63253	0.65512	0.60238
H606	0.83999	0.42438	0.54635
H607	0.91141	0.38588	0.5121
H608	0.96434	0.33295	0.5367
H609	0.85709	0.30358	0.70783
H610	0.80445	0.35635	0.68315

H611	0.82579	0.46475	0.70501
H612	0.83895	0.47048	0.60911
H613	0.70019	0.41827	0.68313
H614	0.74666	0.43418	0.74704
H615	0.71949	0.58448	0.7315
H616	0.66041	0.56298	0.76396
H617	0.59666	0.54048	0.67507
H618	0.61036	0.54671	0.57944
H619	0.68951	0.57701	0.53722
H620	0.73548	0.59294	0.60179
H621	0.71637	0.4267	0.55301
H622	0.77511	0.44844	0.52006
H623	0.33568	0.9243	0.73837
H624	0.40576	0.8857	0.77208
H625	0.45979	0.83281	0.74671
H626	0.35994	0.80374	0.57558
H627	0.30622	0.85645	0.60101
H628	0.10003	1.08663	0.54555
H629	0.03	1.12529	0.51163
H630	-0.02355	1.17847	0.53635
H631	0.07694	1.20784	0.70653
H632	0.13018	1.15484	0.68176
H633	0.10677	1.04616	0.70395
H634	0.09836	1.04043	0.60794
H635	0.23322	1.09287	0.68337
H636	0.18368	1.07686	0.74678
H637	0.21234	0.92661	0.73086
H638	0.26972	0.94823	0.76385
H639	0.33768	0.97088	0.67565
H640	0.32872	0.96466	0.57988
H641	0.25177	0.93421	0.53686
H642	0.20271	0.91817	0.60097
H643	0.22346	1.08445	0.55304
H644	0.16645	1.06258	0.51955
H645	0.37249	0.75556	0.64214
H646	0.56427	0.75603	0.64446
H647	0.06437	1.25557	0.63869
H648	0.87249	1.25556	0.64077

Table S5. Fractional atomic coordinates of NKPOM-OF-2(Co).

Simulated: hexagonal P2; a=35.0 Å, b=28.3 Å, c=19.0 Å, α=γ=90.0°, β=87.4°.

Atom	*x*/*a*	*y*/*b*	*z*/*c*
N1	0.27381	0.83774	0.25492
C2	0.26799	0.87869	0.27988
C3	0.48153	0.63125	0.24268
C4	0.59081	0.5528	0.25529
C5	0.55655	0.5308	0.29288
C6	0.51839	0.55439	0.29236
C7	0.51415	0.59993	0.25339
C8	0.54814	0.62193	0.21535
C9	0.58638	0.5985	0.21638
C10	0.23286	0.90429	0.27164
C11	0.23109	0.94687	0.23785
C12	0.19694	0.9691	0.23143
C13	0.16399	0.94909	0.2587
C14	0.16561	0.90665	0.29246
C15	0.19975	0.88441	0.2989
Mo16	0.33553	0.69148	0.39568
Mo17	0.36547	0.72465	0.09658
Mo18	0.32614	0.6617	0.22666
O19	0.33353	0.74005	0.20755
O20	0.37526	0.69041	0.29245
O21	0.30056	0.70531	0.45403
O22	0.30642	0.68449	0.31498
O23	0.39863	0.70735	0.03586
O24	0.363	0.67014	0.15299
O25	0.33601	0.60622	0.24806
O26	0.3463	0.6361	0.4138
O27	0.32507	0.72228	0.05389
O28	0.28623	0.65972	0.18151
C29	0.41123	0.66863	0.2913
C30	0.30209	0.77139	0.20899
Mo31	0.38426	0.78454	0.43434
Mo32	0.4142	0.81771	0.13523
Mo33	0.4235	0.84763	0.3039
O34	0.37459	0.81847	0.24012
O35	0.41625	0.76869	0.32496
O36	0.35145	0.80249	0.4944
O37	0.38712	0.83862	0.37901
O38	0.44895	0.80345	0.07577

O39	0.44363	0.82414	0.21696
O40	0.46372	0.8501	0.34937
O41	0.42524	0.78685	0.47642
O42	0.4038	0.87263	0.11635
O43	0.41337	0.90253	0.28237
C44	0.44742	0.73773	0.32
C45	0.3387	0.8413	0.23803
Co46	0.37507	0.75435	0.26586
O47	0.34099	0.76537	0.35131
O48	0.40946	0.74312	0.18023
O49	0.3781	0.71982	0.4337
O50	0.37065	0.78985	0.09883
N51	0.47697	0.67179	0.26976
C52	0.44331	0.6992	0.26774
C53	0.44154	0.71537	0.19063
C54	0.30664	0.80978	0.26331
C55	0.30861	0.79392	0.33801
N56	0.48152	0.33774	0.25159
N57	0.27841	0.17183	0.23676
C58	0.48734	0.37869	0.22663
C59	0.52338	0.40234	0.23428
C60	0.2738	0.13125	0.26384
C61	0.52871	0.4459	0.20457
C62	0.56241	0.4691	0.21127
C63	0.59135	0.44909	0.24782
C64	0.58617	0.40565	0.2775
C65	0.55248	0.38245	0.27081
C66	0.16452	0.0528	0.25123
C67	0.19801	0.03146	0.28699
C68	0.23484	0.05781	0.29058
C69	0.23826	0.106	0.25917
C70	0.20489	0.12765	0.22384
C71	0.16814	0.10111	0.21975
Mo72	0.38777	0.22376	0.41163
Mo73	0.4195	0.19314	0.1124
Mo74	0.42821	0.16213	0.28075
O75	0.37938	0.19112	0.21658
O76	0.42015	0.24081	0.3031
O77	0.35483	0.20495	0.47079
O78	0.3914	0.17012	0.35538
O79	0.45441	0.20828	0.05382
O80	0.44857	0.1865	0.19457
O81	0.4682	0.15984	0.32693
O82	0.42854	0.22166	0.45444

O83	0.40969	0.13823	0.09234
O84	0.41869	0.10726	0.25805
C85	0.45105	0.2722	0.29926
C86	0.34373	0.16784	0.21342
Mo87	0.33842	0.31646	0.37373
Mo88	0.37015	0.28585	0.0745
Mo89	0.32962	0.34734	0.20502
O90	0.3378	0.26923	0.18464
O91	0.37864	0.31879	0.27121
O92	0.3033	0.30176	0.43121
O93	0.30967	0.32366	0.2926
O94	0.40345	0.30401	0.01468
O95	0.36691	0.3399	0.13185
O96	0.33888	0.40279	0.2276
O97	0.3486	0.37184	0.39303
O98	0.32997	0.288	0.0311
O99	0.28994	0.34913	0.15916
C100	0.41441	0.34104	0.27111
C101	0.30666	0.23748	0.18494
Co102	0.37917	0.25505	0.24348
O103	0.34477	0.24297	0.32813
O104	0.41386	0.26734	0.15865
O105	0.38103	0.28839	0.41203
O106	0.3759	0.22071	0.07568
C107	0.44686	0.31105	0.24759
C108	0.44563	0.29542	0.17014
C109	0.31128	0.19876	0.23868
C110	0.31272	0.21411	0.31372
N111	0.98152	0.83774	0.25159
C112	0.98734	0.87869	0.22663
C113	0.7738	0.63125	0.26384
C114	0.66452	0.5528	0.25123
C115	0.69878	0.5308	0.21364
C116	0.73694	0.55439	0.21415
C117	0.74119	0.59993	0.25312
C118	0.70719	0.62193	0.29117
C119	0.66895	0.5985	0.29013
C120	1.02248	0.90429	0.23488
C121	1.02424	0.94687	0.26866
C122	1.05839	0.9691	0.27509
C123	1.09135	0.94909	0.24782
C124	1.08972	0.90665	0.21405
C125	1.05558	0.88441	0.20761
Mo126	0.9198	0.69148	0.11084

Mo127	0.88986	0.72465	0.40994
Mo128	0.92919	0.6617	0.27985
O129	0.92181	0.74005	0.29897
O130	0.88007	0.69041	0.21407
O131	0.95477	0.70531	0.05249
O132	0.94891	0.68449	0.19154
O133	0.8567	0.70735	0.47066
O134	0.89233	0.67014	0.35353
O135	0.91932	0.60622	0.25845
O136	0.90903	0.6361	0.09272
O137	0.93026	0.72228	0.45263
O138	0.9691	0.65972	0.32501
C139	0.8441	0.66863	0.21522
C140	0.95324	0.77139	0.29753
Mo141	0.87107	0.78454	0.07218
Mo142	0.84114	0.81771	0.37128
Mo143	0.83183	0.84763	0.20262
O144	0.88075	0.81847	0.26639
O145	0.83908	0.76869	0.18155
O146	0.90389	0.80249	0.01212
O147	0.86821	0.83862	0.12751
O148	0.80638	0.80345	0.43074
O149	0.8117	0.82414	0.28956
O150	0.79161	0.8501	0.15715
O151	0.83009	0.78685	0.0301
O152	0.85153	0.87263	0.39017
O153	0.84196	0.90253	0.22415
C154	0.80791	0.73773	0.18651
C155	0.91663	0.8413	0.26849
Co156	0.88026	0.75435	0.24065
O157	0.91434	0.76537	0.15521
O158	0.84587	0.74312	0.32629
O159	0.87723	0.71982	0.07282
O160	0.88468	0.78985	0.40769
N161	0.77836	0.67179	0.23676
C162	0.81202	0.6992	0.23878
C163	0.81379	0.71537	0.31589
C164	0.94869	0.80978	0.24321
C165	0.94672	0.79392	0.16851
N166	0.77381	0.33774	0.25492
N167	0.97692	0.17183	0.26975
C168	0.76799	0.37869	0.27988
C169	0.73195	0.40234	0.27224
C170	0.98153	0.13125	0.24268

C171	0.72662	0.4459	0.30195
C172	0.69292	0.4691	0.29525
C173	0.66399	0.44909	0.2587
C174	0.66916	0.40565	0.22901
C175	0.70285	0.38245	0.23571
C176	1.09081	0.0528	0.25529
C177	1.05732	0.03146	0.21953
C178	1.02049	0.05781	0.21593
C179	1.01707	0.106	0.24734
C180	1.05044	0.12765	0.28267
C181	1.08719	0.10111	0.28677
Mo182	0.86756	0.22376	0.09489
Mo183	0.83583	0.19314	0.39411
Mo184	0.82712	0.16213	0.22577
O185	0.87595	0.19112	0.28994
O186	0.83518	0.24081	0.20342
O187	0.9005	0.20495	0.03573
O188	0.86394	0.17012	0.15114
O189	0.80092	0.20828	0.4527
O190	0.80676	0.1865	0.31194
O191	0.78713	0.15984	0.17958
O192	0.82679	0.22166	0.05208
O193	0.84564	0.13823	0.41417
O194	0.83664	0.10726	0.24846
C195	0.80428	0.2722	0.20726
C196	0.9116	0.16784	0.2931
Mo197	0.91691	0.31646	0.13279
Mo198	0.88518	0.28585	0.43202
Mo199	0.92571	0.34734	0.3015
O200	0.91753	0.26923	0.32188
O201	0.87669	0.31879	0.2353
O202	0.95203	0.30176	0.07531
O203	0.94566	0.32366	0.21392
O204	0.85188	0.30401	0.49184
O205	0.88842	0.3399	0.37467
O206	0.91645	0.40279	0.27892
O207	0.90673	0.37184	0.11348
O208	0.92536	0.288	0.47542
O209	0.96539	0.34913	0.34736
C210	0.84092	0.34104	0.2354
C211	0.94867	0.23748	0.32157
Co212	0.87616	0.25505	0.26304
O213	0.91056	0.24297	0.17839
O214	0.84147	0.26734	0.34787

O215	0.8743	0.28839	0.09448
O216	0.87943	0.22071	0.43083
C217	0.80847	0.31105	0.25892
C218	0.8097	0.29542	0.33638
C219	0.94405	0.19876	0.26784
C220	0.94261	0.21411	0.1928
C221	0.12767	0.97358	0.25326
C222	0.12767	0.02642	0.25326
C223	0.62767	0.52642	0.25326
C224	0.62767	0.47358	0.25326
H225	0.29111	0.89696	0.31048
H226	0.45766	0.61961	0.20751
H227	0.55988	0.49591	0.32187
H228	0.49269	0.53772	0.32153
H229	0.54481	0.65654	0.18563
H230	0.61215	0.61531	0.18765
H231	0.25845	0.9637	0.21503
H232	0.19571	1.00455	0.20322
H233	0.13831	0.88971	0.31537
H234	0.20097	0.84898	0.32714
H235	0.41055	0.63664	0.25499
H236	0.41762	0.65603	0.34657
H237	0.27477	0.7508	0.22221
H238	0.29984	0.78858	0.15507
H239	0.45147	0.72132	0.37397
H240	0.47436	0.75822	0.3037
H241	0.33367	0.85262	0.18158
H242	0.33869	0.87391	0.27316
H243	0.44061	0.683	0.1551
H244	0.4681	0.73699	0.17566
H245	0.28161	0.77308	0.3528
H246	0.30996	0.82605	0.37393
H247	0.46387	0.39744	0.19757
H248	0.29806	0.11394	0.29265
H249	0.50487	0.4628	0.17415
H250	0.56679	0.50543	0.18645
H251	0.61004	0.3888	0.30789
H252	0.54811	0.34611	0.29559
H253	0.19507	-0.00515	0.31146
H254	0.26011	0.04111	0.31719
H255	0.20751	0.16448	0.19999
H256	0.14295	0.11767	0.1927
H257	0.47814	0.25156	0.28443
H258	0.45454	0.28925	0.35296

H259	0.34418	0.13475	0.24752
H260	0.33872	0.15722	0.15667
H261	0.41954	0.35401	0.32673
H262	0.41441	0.3728	0.23428
H263	0.30482	0.22104	0.13042
H264	0.27905	0.25738	0.19852
H265	0.47267	0.27464	0.15544
H266	0.44425	0.32787	0.13488
H267	0.31339	0.1814	0.34858
H268	0.28598	0.23537	0.32873
H269	0.96422	0.89696	0.19604
H270	0.79767	0.61961	0.299
H271	0.69545	0.49591	0.18465
H272	0.76264	0.53772	0.18498
H273	0.71052	0.65654	0.32088
H274	0.64318	0.61531	0.31887
H275	0.99688	0.9637	0.29148
H276	1.05962	1.00455	0.30329
H277	1.11702	0.88971	0.19114
H278	1.05436	0.84898	0.17937
H279	0.84478	0.63664	0.25153
H280	0.83772	0.65603	0.15994
H281	0.98056	0.7508	0.2843
H282	0.95549	0.78858	0.35145
H283	0.80386	0.72132	0.13255
H284	0.78097	0.75822	0.20282
H285	0.92166	0.85262	0.32494
H286	0.91665	0.87391	0.23335
H287	0.81472	0.683	0.35142
H288	0.78723	0.73699	0.33085
H289	0.97372	0.77308	0.15372
H290	0.94537	0.82605	0.13259
H291	0.79146	0.39744	0.30895
H292	0.95727	0.11394	0.21387
H293	0.75046	0.4628	0.33237
H294	0.68854	0.50543	0.32006
H295	0.64529	0.3888	0.19862
H296	0.70722	0.34611	0.21093
H297	1.06026	-0.00515	0.19505
H298	0.99522	0.04111	0.18933
H299	1.04782	0.16448	0.30653
H300	1.11238	0.11767	0.31382
H301	0.77719	0.25156	0.22209
H302	0.80079	0.28925	0.15355

H303	0.91115	0.13475	0.259
H304	0.91661	0.15722	0.34985
H305	0.83579	0.35401	0.17979
H306	0.84092	0.3728	0.27223
H307	0.95051	0.22104	0.37609
H308	0.97628	0.25738	0.308
H309	0.78266	0.27464	0.35108
H310	0.81109	0.32787	0.37164
H311	0.94194	0.1814	0.15794
H312	0.96935	0.23537	0.17778
H313	0.13162	0.97358	0.1934
H314	0.12802	0.02642	0.19324

Table S6. Fractional atomic coordinates of NKPOM-OF-2(Mn)

Simulated: hexagonal P2; a=35.0 Å, b=28.3 Å, c=19.0 Å, α=γ=90.0°, β=87.6°.

Atom	*x*/*a*	*y*/*b*	*z*/*c*
N1	0.27381	0.83774	0.25492
C2	0.26799	0.87869	0.27988
C3	0.48153	0.63125	0.24268
C4	0.59081	0.5528	0.25529
C5	0.55655	0.5308	0.29288
C6	0.51839	0.55439	0.29236
C7	0.51415	0.59993	0.25339
C8	0.54814	0.62193	0.21535
C9	0.58638	0.5985	0.21638
C10	0.23286	0.90429	0.27164
C11	0.23109	0.94687	0.23785
C12	0.19694	0.9691	0.23143
C13	0.16399	0.94909	0.2587
C14	0.16561	0.90665	0.29246
C15	0.19975	0.88441	0.2989
Mo16	0.33553	0.69148	0.39568
Mo17	0.36547	0.72465	0.09658
Mo18	0.32614	0.6617	0.22666
O19	0.33353	0.74005	0.20755
O20	0.37526	0.69041	0.29245
O21	0.30056	0.70531	0.45403
O22	0.30642	0.68449	0.31498
O23	0.39863	0.70735	0.03586
O24	0.363	0.67014	0.15299
O25	0.33601	0.60622	0.24806
O26	0.3463	0.6361	0.4138
O27	0.32507	0.72228	0.05389
O28	0.28623	0.65972	0.18151
C29	0.41123	0.66863	0.2913
C30	0.30209	0.77139	0.20899
Mo31	0.38426	0.78454	0.43434
Mo32	0.4142	0.81771	0.13523
Mo33	0.4235	0.84763	0.3039
O34	0.37459	0.81847	0.24012
O35	0.41625	0.76869	0.32496
O36	0.35145	0.80249	0.4944
O37	0.38712	0.83862	0.37901
O38	0.44895	0.80345	0.07577

O39	0.44363	0.82414	0.21696
O40	0.46372	0.8501	0.34937
O41	0.42524	0.78685	0.47642
O42	0.4038	0.87263	0.11635
O43	0.41337	0.90253	0.28237
C44	0.44742	0.73773	0.32
C45	0.3387	0.8413	0.23803
Mn46	0.37507	0.75435	0.26586
O47	0.34099	0.76537	0.35131
O48	0.40946	0.74312	0.18023
O49	0.3781	0.71982	0.4337
O50	0.37065	0.78985	0.09883
N51	0.47697	0.67179	0.26976
C52	0.44331	0.6992	0.26774
C53	0.44154	0.71537	0.19063
C54	0.30664	0.80978	0.26331
C55	0.30861	0.79392	0.33801
N56	0.48152	0.33774	0.25159
N57	0.27841	0.17183	0.23676
C58	0.48734	0.37869	0.22663
C59	0.52338	0.40234	0.23428
C60	0.2738	0.13125	0.26384
C61	0.52871	0.4459	0.20457
C62	0.56241	0.4691	0.21127
C63	0.59135	0.44909	0.24782
C64	0.58617	0.40565	0.2775
C65	0.55248	0.38245	0.27081
C66	0.16452	0.0528	0.25123
C67	0.19801	0.03146	0.28699
C68	0.23484	0.05781	0.29058
C69	0.23826	0.106	0.25917
C70	0.20489	0.12765	0.22384
C71	0.16814	0.10111	0.21975
Mo72	0.38777	0.22376	0.41163
Mo73	0.4195	0.19314	0.1124
Mo74	0.42821	0.16213	0.28075
O75	0.37938	0.19112	0.21658
O76	0.42015	0.24081	0.3031
O77	0.35483	0.20495	0.47079
O78	0.3914	0.17012	0.35538
O79	0.45441	0.20828	0.05382
O80	0.44857	0.1865	0.19457
O81	0.4682	0.15984	0.32693
O82	0.42854	0.22166	0.45444

O83	0.40969	0.13823	0.09234
O84	0.41869	0.10726	0.25805
C85	0.45105	0.2722	0.29926
C86	0.34373	0.16784	0.21342
Mo87	0.33842	0.31646	0.37373
Mo88	0.37015	0.28585	0.0745
Mo89	0.32962	0.34734	0.20502
O90	0.3378	0.26923	0.18464
O91	0.37864	0.31879	0.27121
O92	0.3033	0.30176	0.43121
O93	0.30967	0.32366	0.2926
O94	0.40345	0.30401	0.01468
O95	0.36691	0.3399	0.13185
O96	0.33888	0.40279	0.2276
O97	0.3486	0.37184	0.39303
O98	0.32997	0.288	0.0311
O99	0.28994	0.34913	0.15916
C100	0.41441	0.34104	0.27111
C101	0.30666	0.23748	0.18494
Mn102	0.37917	0.25505	0.24348
O103	0.34477	0.24297	0.32813
O104	0.41386	0.26734	0.15865
O105	0.38103	0.28839	0.41203
O106	0.3759	0.22071	0.07568
C107	0.44686	0.31105	0.24759
C108	0.44563	0.29542	0.17014
C109	0.31128	0.19876	0.23868
C110	0.31272	0.21411	0.31372
N111	0.98152	0.83774	0.25159
C112	0.98734	0.87869	0.22663
C113	0.7738	0.63125	0.26384
C114	0.66452	0.5528	0.25123
C115	0.69878	0.5308	0.21364
C116	0.73694	0.55439	0.21415
C117	0.74119	0.59993	0.25312
C118	0.70719	0.62193	0.29117
C119	0.66895	0.5985	0.29013
C120	1.02248	0.90429	0.23488
C121	1.02424	0.94687	0.26866
C122	1.05839	0.9691	0.27509
C123	1.09135	0.94909	0.24782
C124	1.08972	0.90665	0.21405
C125	1.05558	0.88441	0.20761
Mo126	0.9198	0.69148	0.11084

Mo127	0.88986	0.72465	0.40994
Mo128	0.92919	0.6617	0.27985
O129	0.92181	0.74005	0.29897
O130	0.88007	0.69041	0.21407
O131	0.95477	0.70531	0.05249
O132	0.94891	0.68449	0.19154
O133	0.8567	0.70735	0.47066
O134	0.89233	0.67014	0.35353
O135	0.91932	0.60622	0.25845
O136	0.90903	0.6361	0.09272
O137	0.93026	0.72228	0.45263
O138	0.9691	0.65972	0.32501
C139	0.8441	0.66863	0.21522
C140	0.95324	0.77139	0.29753
Mo141	0.87107	0.78454	0.07218
Mo142	0.84114	0.81771	0.37128
Mo143	0.83183	0.84763	0.20262
O144	0.88075	0.81847	0.26639
O145	0.83908	0.76869	0.18155
O146	0.90389	0.80249	0.01212
O147	0.86821	0.83862	0.12751
O148	0.80638	0.80345	0.43074
O149	0.8117	0.82414	0.28956
O150	0.79161	0.8501	0.15715
O151	0.83009	0.78685	0.0301
O152	0.85153	0.87263	0.39017
O153	0.84196	0.90253	0.22415
C154	0.80791	0.73773	0.18651
C155	0.91663	0.8413	0.26849
Mn156	0.88026	0.75435	0.24065
O157	0.91434	0.76537	0.15521
O158	0.84587	0.74312	0.32629
O159	0.87723	0.71982	0.07282
O160	0.88468	0.78985	0.40769
N161	0.77836	0.67179	0.23676
C162	0.81202	0.6992	0.23878
C163	0.81379	0.71537	0.31589
C164	0.94869	0.80978	0.24321
C165	0.94672	0.79392	0.16851
N166	0.77381	0.33774	0.25492
N167	0.97692	0.17183	0.26975
C168	0.76799	0.37869	0.27988
C169	0.73195	0.40234	0.27224
C170	0.98153	0.13125	0.24268

C171	0.72662	0.4459	0.30195
C172	0.69292	0.4691	0.29525
C173	0.66399	0.44909	0.2587
C174	0.66916	0.40565	0.22901
C175	0.70285	0.38245	0.23571
C176	1.09081	0.0528	0.25529
C177	1.05732	0.03146	0.21953
C178	1.02049	0.05781	0.21593
C179	1.01707	0.106	0.24734
C180	1.05044	0.12765	0.28267
C181	1.08719	0.10111	0.28677
Mo182	0.86756	0.22376	0.09489
Mo183	0.83583	0.19314	0.39411
Mo184	0.82712	0.16213	0.22577
O185	0.87595	0.19112	0.28994
O186	0.83518	0.24081	0.20342
O187	0.9005	0.20495	0.03573
O188	0.86394	0.17012	0.15114
O189	0.80092	0.20828	0.4527
O190	0.80676	0.1865	0.31194
O191	0.78713	0.15984	0.17958
O192	0.82679	0.22166	0.05208
O193	0.84564	0.13823	0.41417
O194	0.83664	0.10726	0.24846
C195	0.80428	0.2722	0.20726
C196	0.9116	0.16784	0.2931
Mo197	0.91691	0.31646	0.13279
Mo198	0.88518	0.28585	0.43202
Mo199	0.92571	0.34734	0.3015
O200	0.91753	0.26923	0.32188
O201	0.87669	0.31879	0.2353
O202	0.95203	0.30176	0.07531
O203	0.94566	0.32366	0.21392
O204	0.85188	0.30401	0.49184
O205	0.88842	0.3399	0.37467
O206	0.91645	0.40279	0.27892
O207	0.90673	0.37184	0.11348
O208	0.92536	0.288	0.47542
O209	0.96539	0.34913	0.34736
C210	0.84092	0.34104	0.2354
C211	0.94867	0.23748	0.32157
Mn212	0.87616	0.25505	0.26304
O213	0.91056	0.24297	0.17839
O214	0.84147	0.26734	0.34787

O215	0.8743	0.28839	0.09448
O216	0.87943	0.22071	0.43083
C217	0.80847	0.31105	0.25892
C218	0.8097	0.29542	0.33638
C219	0.94405	0.19876	0.26784
C220	0.94261	0.21411	0.1928
C221	0.12767	0.97358	0.25326
C222	0.12767	0.02642	0.25326
C223	0.62767	0.52642	0.25326
C224	0.62767	0.47358	0.25326
H225	0.29111	0.89696	0.31048
H226	0.45766	0.61961	0.20751
H227	0.55988	0.49591	0.32187
H228	0.49269	0.53772	0.32153
H229	0.54481	0.65654	0.18563
H230	0.61215	0.61531	0.18765
H231	0.25845	0.9637	0.21503
H232	0.19571	1.00455	0.20322
H233	0.13831	0.88971	0.31537
H234	0.20097	0.84898	0.32714
H235	0.41055	0.63664	0.25499
H236	0.41762	0.65603	0.34657
H237	0.27477	0.7508	0.22221
H238	0.29984	0.78858	0.15507
H239	0.45147	0.72132	0.37397
H240	0.47436	0.75822	0.3037
H241	0.33367	0.85262	0.18158
H242	0.33869	0.87391	0.27316
H243	0.44061	0.683	0.1551
H244	0.4681	0.73699	0.17566
H245	0.28161	0.77308	0.3528
H246	0.30996	0.82605	0.37393
H247	0.46387	0.39744	0.19757
H248	0.29806	0.11394	0.29265
H249	0.50487	0.4628	0.17415
H250	0.56679	0.50543	0.18645
H251	0.61004	0.3888	0.30789
H252	0.54811	0.34611	0.29559
H253	0.19507	-0.00515	0.31146
H254	0.26011	0.04111	0.31719
H255	0.20751	0.16448	0.19999
H256	0.14295	0.11767	0.1927
H257	0.47814	0.25156	0.28443
H258	0.45454	0.28925	0.35296

H259	0.34418	0.13475	0.24752
H260	0.33872	0.15722	0.15667
H261	0.41954	0.35401	0.32673
H262	0.41441	0.3728	0.23428
H263	0.30482	0.22104	0.13042
H264	0.27905	0.25738	0.19852
H265	0.47267	0.27464	0.15544
H266	0.44425	0.32787	0.13488
H267	0.31339	0.1814	0.34858
H268	0.28598	0.23537	0.32873
H269	0.96422	0.89696	0.19604
H270	0.79767	0.61961	0.299
H271	0.69545	0.49591	0.18465
H272	0.76264	0.53772	0.18498
H273	0.71052	0.65654	0.32088
H274	0.64318	0.61531	0.31887
H275	0.99688	0.9637	0.29148
H276	1.05962	1.00455	0.30329
H277	1.11702	0.88971	0.19114
H278	1.05436	0.84898	0.17937
H279	0.84478	0.63664	0.25153
H280	0.83772	0.65603	0.15994
H281	0.98056	0.7508	0.2843
H282	0.95549	0.78858	0.35145
H283	0.80386	0.72132	0.13255
H284	0.78097	0.75822	0.20282
H285	0.92166	0.85262	0.32494
H286	0.91665	0.87391	0.23335
H287	0.81472	0.683	0.35142
H288	0.78723	0.73699	0.33085
H289	0.97372	0.77308	0.15372
H290	0.94537	0.82605	0.13259
H291	0.79146	0.39744	0.30895
H292	0.95727	0.11394	0.21387
H293	0.75046	0.4628	0.33237
H294	0.68854	0.50543	0.32006
H295	0.64529	0.3888	0.19862
H296	0.70722	0.34611	0.21093
H297	1.06026	-0.00515	0.19505
H298	0.99522	0.04111	0.18933
H299	1.04782	0.16448	0.30653
H300	1.11238	0.11767	0.31382
H301	0.77719	0.25156	0.22209
H302	0.80079	0.28925	0.15355

H303	0.91115	0.13475	0.259
H304	0.91661	0.15722	0.34985
H305	0.83579	0.35401	0.17979
H306	0.84092	0.3728	0.27223
H307	0.95051	0.22104	0.37609
H308	0.97628	0.25738	0.308
H309	0.78266	0.27464	0.35108
H310	0.81109	0.32787	0.37164
H311	0.94194	0.1814	0.15794
H312	0.96935	0.23537	0.17778
H313	0.13162	0.97358	0.1934
H314	0.12802	0.02642	0.19324

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