Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Highly Efficient Visible-Light-Driven Reduction of Cr(VI) from Water by Porphyrin-Based Metal−Organic Frameworks: Effect of Band Gap Engineering on the Photocatalytic Activity

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Experimental section

Materials

All reagents and solvents were purchased from commercial sources and used without further purification. $ZrCl_4.8H_2O$ (98%), and pyrrole (98%) were obtained from Sigma-Aldrich Chemicals. Propionic acid (99%) was received from TCI Chemicals. H_2TCPP ligand was prepared by following the previously reported literature procedure with modification and characterized.[1] PCN-222 was synthesized following the reported procedure[2] and the phase purity of the compound was identified by PXRD analysis, UV-Vis and FTIR spectroscopy.

Physical measurements

Powder X-ray powder diffraction (PXRD) patterns were collected on a PANalytical X'PERT PRO diffractometer using Cu-K_α radiation (λ =1.542 Å; 40 kV, 20 mA). pH of the solutions were measured using Mettler Toledo pH meter. UV-vis spectra were recorded on Shimadzu UV-2600 240 V spectrophotometer. Fluorescence spectra of the samples dispersed in water were recorded on a Perkin Elmer LS55 fluorescence spectrophotometer at room temperature.

Time resolved fluorescence measurements of all samples dispersed in water were recorded on Flurocube; Horiba Jobin-Yvin, NJ at room temperature.

Photoelectrochemical studies

The photoelectrochemical measurements were performed in a three-electrode photoelectrochemical (PEC) cell, a scanning potentiostat (Metrohom, Autolab). For this 2.5 mg of the photocatalyst was dispersed in 500 μL ethanol and 20 μL of Nafion (0.25%) solution was added for preparing the working electrode. The mixture was sonicated for 10 minutes and drop-casted on to an indium doped tin oxide (ITO) glass substrate with 2 X 3.5 cm^2 area. A calomel electrode and a platinum wire were used as reference and counter electrodes, respectively. In addition to this, 0.1 M Na_2SO_4 solution was prepared and the pH of solution was adjusted to 1 by adding few drops of H_2SO_4 used as electrolyte. A visible light emitting CFL bulb (45 W) was used as the incident light source and placed at 10 cm distance from the electrochemical cell. The photoelectrochemical (PEC) studies of the photocatalysts were performed by measuring photocurrent density in dark and under visible light irradiation. All the samples were quite stable in 0.1 M Na_2SO_4 electrolytic solution at pH 1.

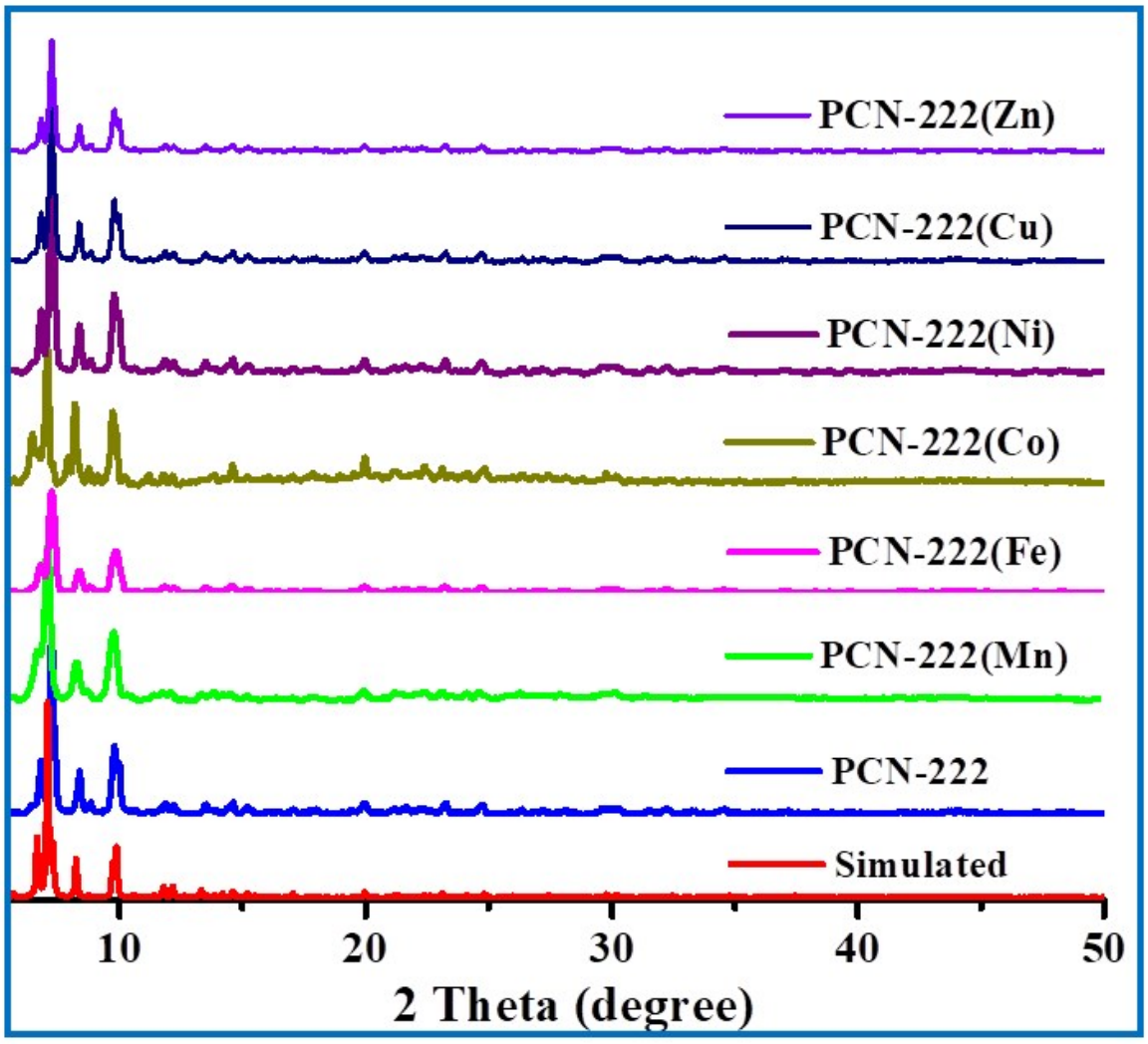

Fig. S1 Powder X-ray diffraction pattern of as-synthesized PCN-222 and PCN-222(M) (Zn^{II}, Cu^{II}, Ni^{II}, Co^{II}, $Fe^{III}Cl$, and $Mn^{III}Cl$).

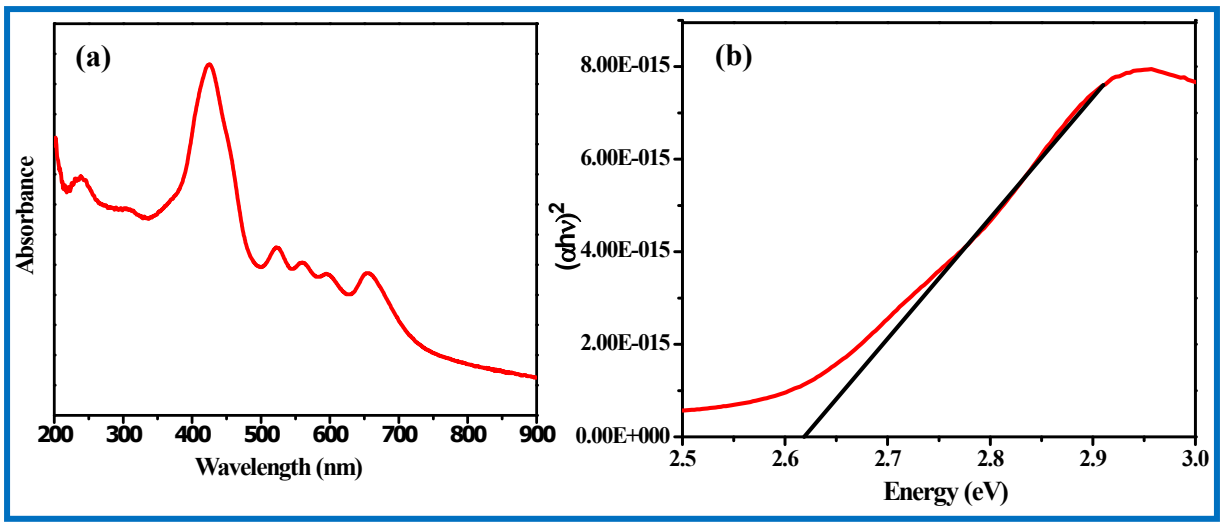

Fig. S2 (a) Solid state UV-Vis absorption spectrum and (b) band gap plot for PCN-222.

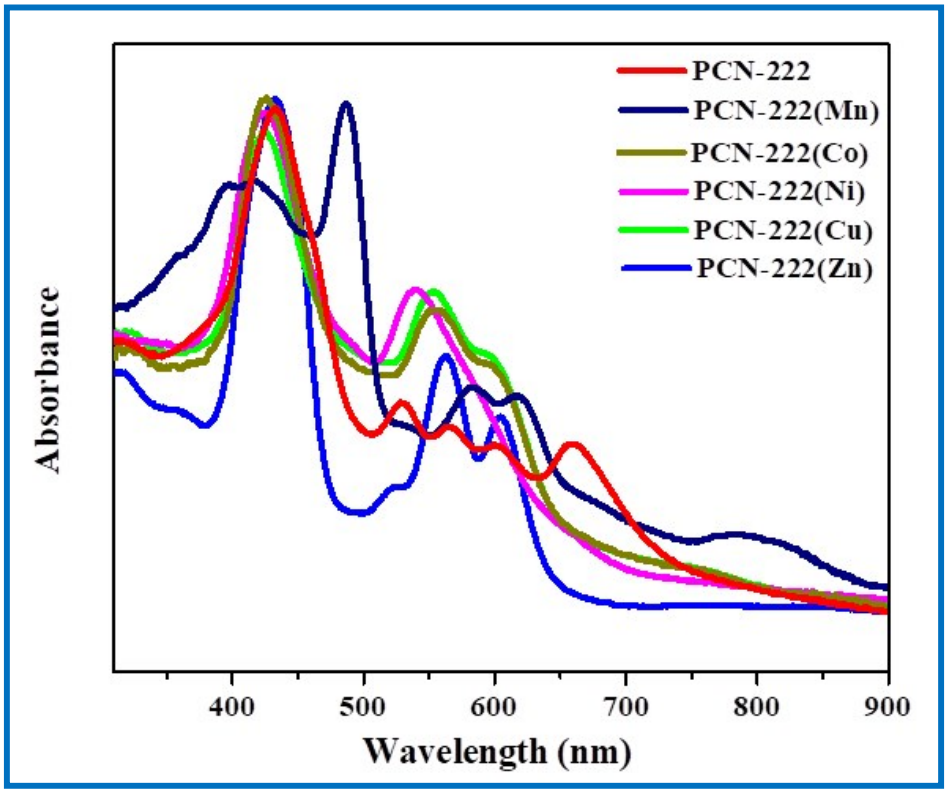

Fig. S3 UV-Vis spectra of PCN-222 and PCN-222(M) (Zn^{II}, Cu^{II}, Ni^{II}, Co^{II}, and $Mn^{III}Cl$) MOFs.

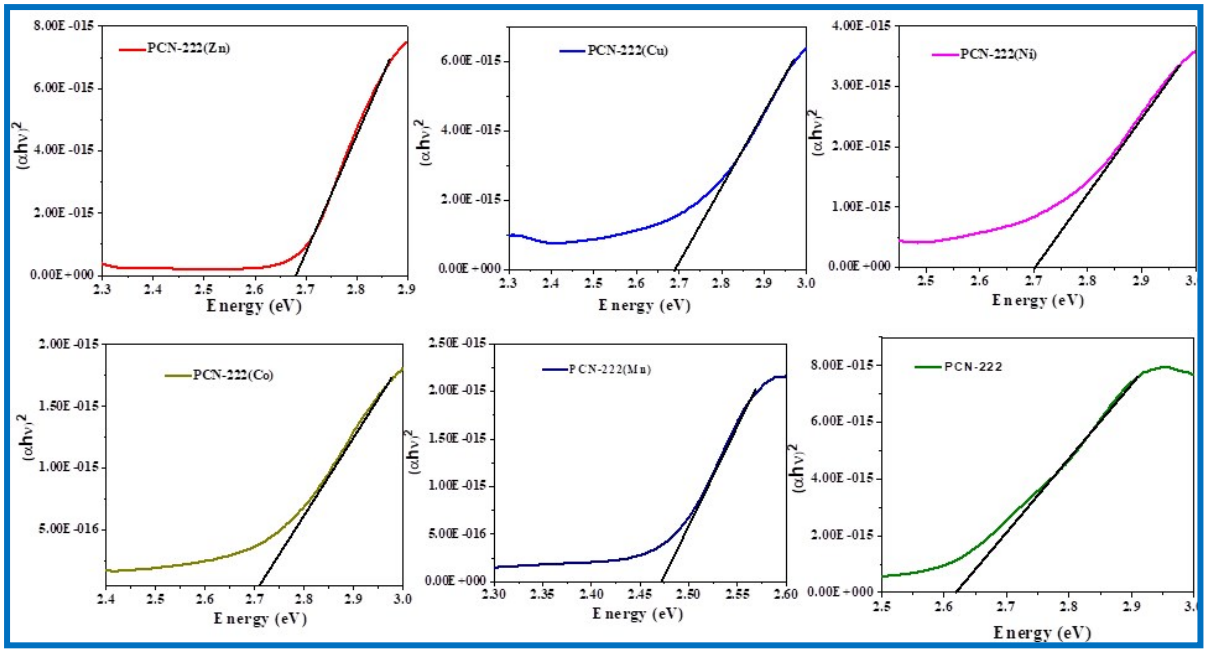

Fig. S4 Bandgap plots for PCN-222 and PCN-222(M) (Zn^{II}, Cu^{II}, Ni^{II}, Co^{II} and $Mn^{III}Cl$) MOFs.

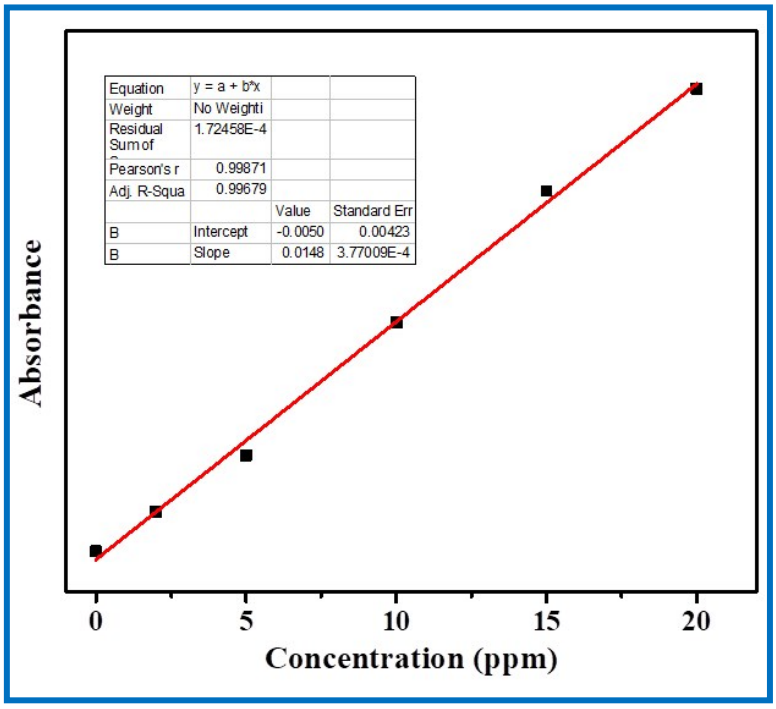

Fig. S5 Calibration curve of Cr(VI)-diphenylcarbazide solution.

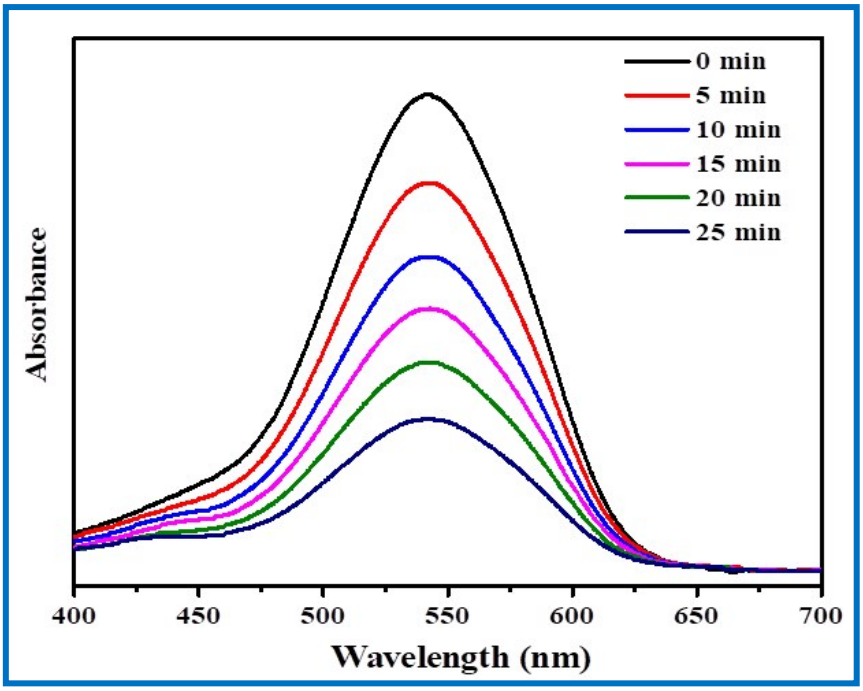

Fig. S6 Absorption spectra for photocatalytic reduction of Cr(VI) to Cr(III) catalysed by PCN-222 in the absence of methanol.

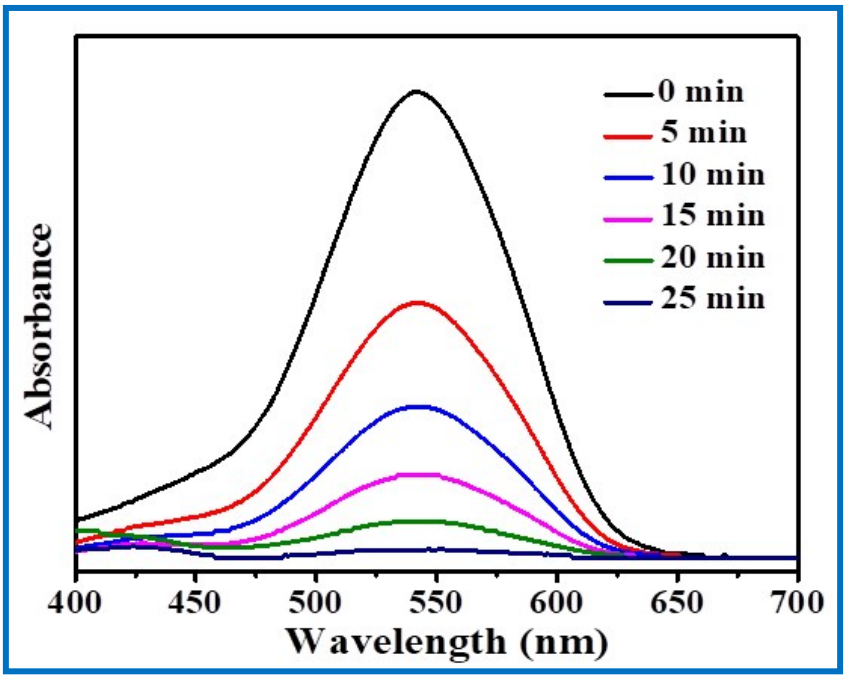

Fig. S7 Absorption spectra for photocatalytic reduction of Cr(VI) to Cr(III) catalysed by PCN-222 in the presence of methanol.

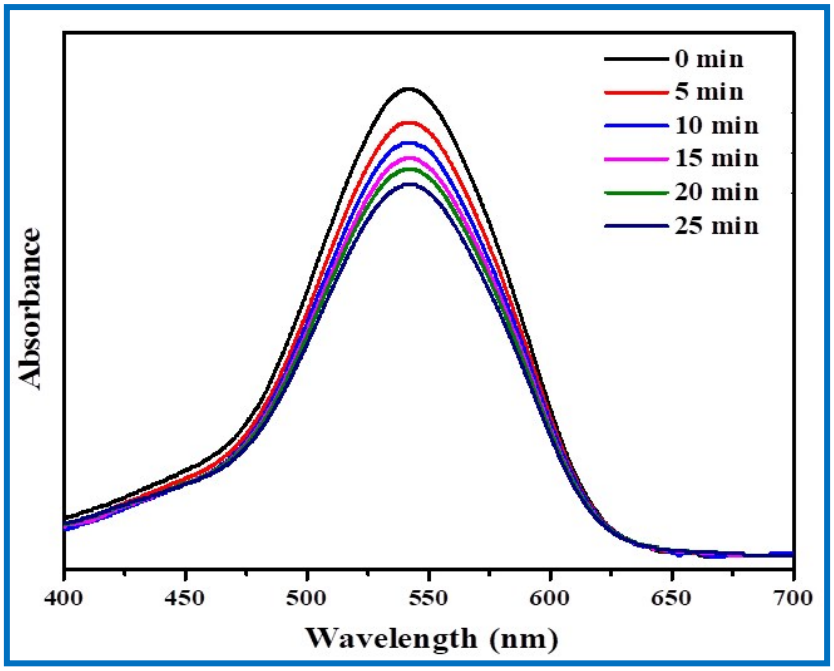

Fig. S8 Absorption spectra for photocatalytic reduction of Cr(VI) to Cr(III) catalysed by PCN-222 in the absence of acid.

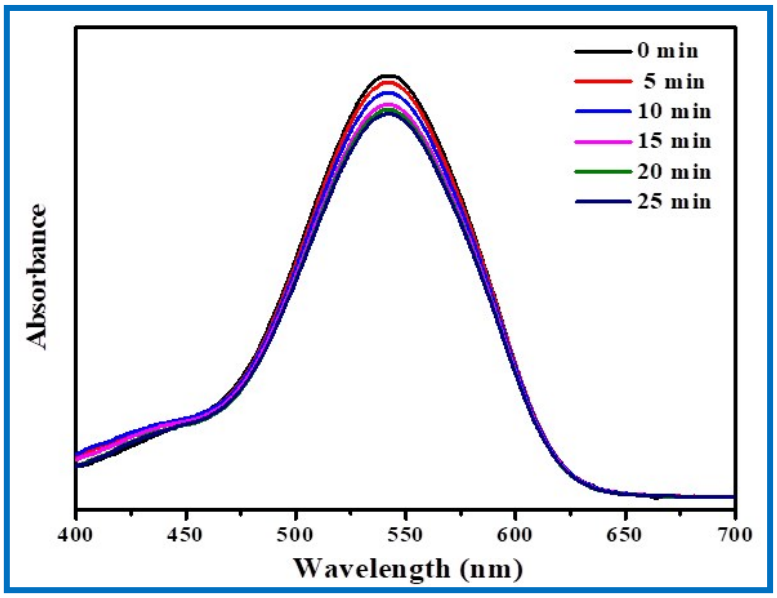

Fig. S9 Absorption spectra for photocatalytic reduction of Cr(VI) to Cr(III) catalysed by PCN-222 in the absence of light.

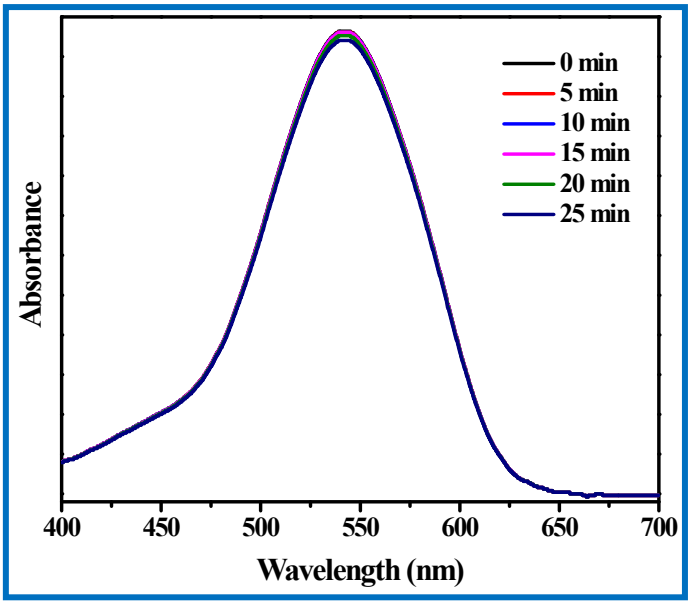

Fig. S10 Absorption spectra for photocatalytic reduction of Cr(VI) to Cr(III) in the absence of PCN-222 catalyst.

Table S1. Comparison of catalytic efficiency for reduction of Cr(VI) to Cr(III) reported for various MOFs[3]

S.No.	Catalysts	Catalyst amount (mg)	Cr(VI) concentration (ppm)	Efficiency	pH	*k* (min^{-1})	References
1	Pd@UiO-66(NH_2)	20	10	99 % in 90 min	2	-	3a
2	UiO-66(NH_2)	20	10	97 % in 80 min	2	-	3b
3	g-C_3N_4/MIL-53(Fe)	20	10	100 % in 180 min	2	0.0191	3c
4	NNU-36	15	10	95.3% in 60 min	2.17	0.0471	3d
5	NH_2-Fe(III)MIL-88B	20	8	100 % in 45 min	2	-	3e
6	$[Cd(4Hptz)_2\cdot(H_2O)_2Cl_2]_n$	7	10	100 % in 50 min	3	0.0481	3f
7	$[Cu(btx)_2(ClO_4)_2]_n$	7	10	92.17 % in 70 min	3	0.0295	3f
8	$[Cu(btx)(ClO_4)]_n$	7	10	82.92 % in 60 min	3	0.0217	3f
9	$[Cu_2I_2(BPEA)](DMF)_4$	15	10	95 % in 10 min	2.23	-	3g
10	**PCN-222**	**5**	**10**	**93 % in 30 min**	**2**	**0.0941**	**Present work**
11	**PCN-222**	**5**	**20**	**97.75 % in 60 min**	**2**	**0.0598**	**Present work**
12	**PCN-222**	**5**	**20**	**100% in 25 min**	**1**	**0.1289**	**Present work**

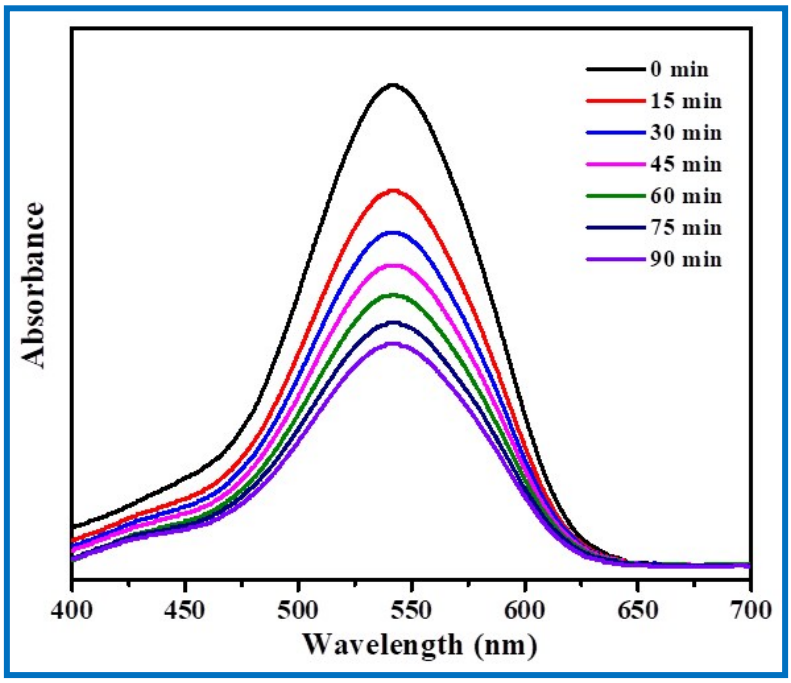

Fig. S11 Absorption spectra for photocatalytic reduction of Cr(VI) to Cr(III) catalysed by PCN-222(Mn).

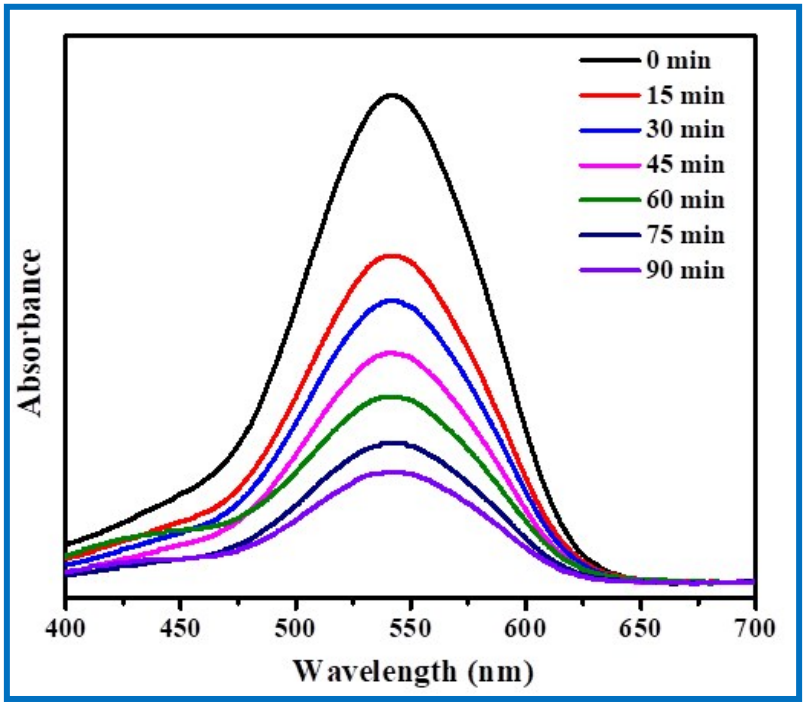

Fig. S12 Absorption spectra for photocatalytic reduction of Cr(VI) to Cr(III) catalysed by PCN-222(Fe).

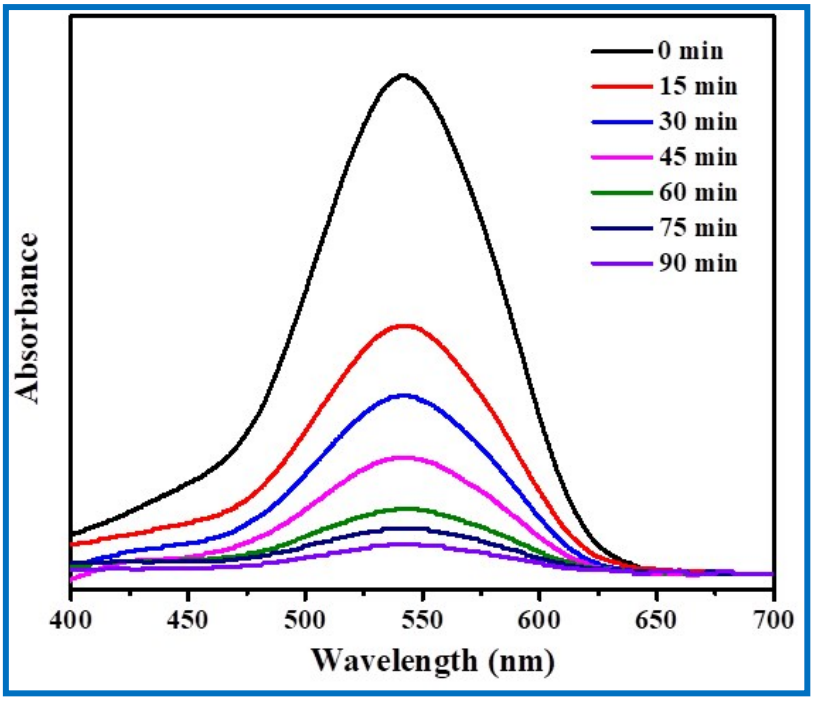

Fig. S13 Absorption spectra for photocatalytic reduction of Cr(VI) to Cr(III) catalysed by PCN-222(Ni).

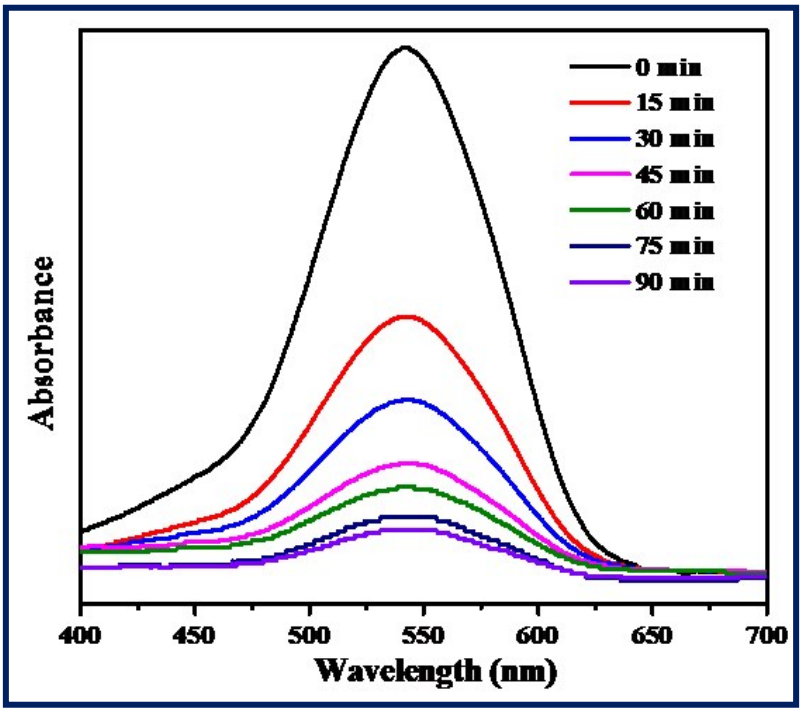

Fig. S14 Absorption spectra for photocatalytic reduction of Cr(VI) to Cr(III) catalysed by PCN-222(Co).

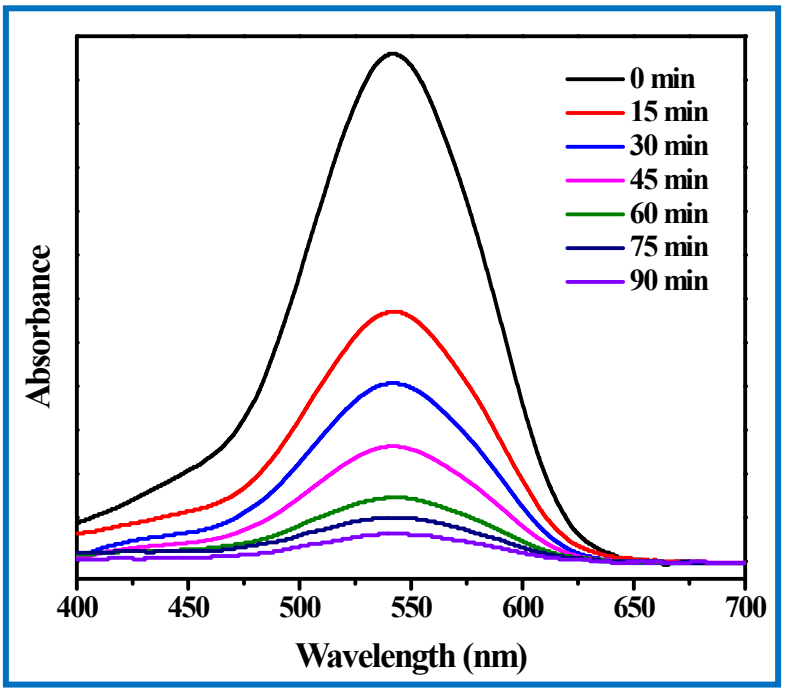

Fig. S15 Absorption spectra for photocatalytic reduction of Cr(VI) to Cr(III) catalysed by PCN-222(Cu).

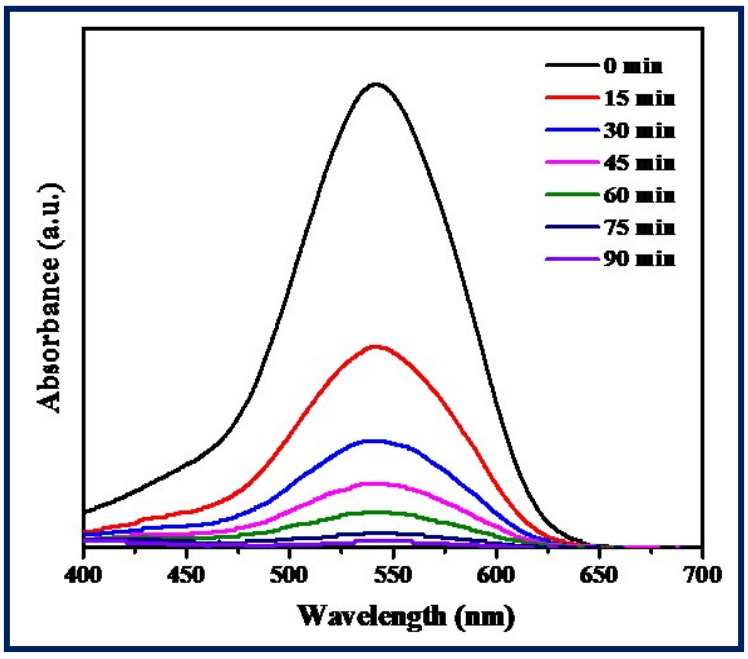

Fig. S16 Absorption spectra for photocatalytic reduction of Cr(VI) to Cr(III) catalysed by PCN-222(Zn).

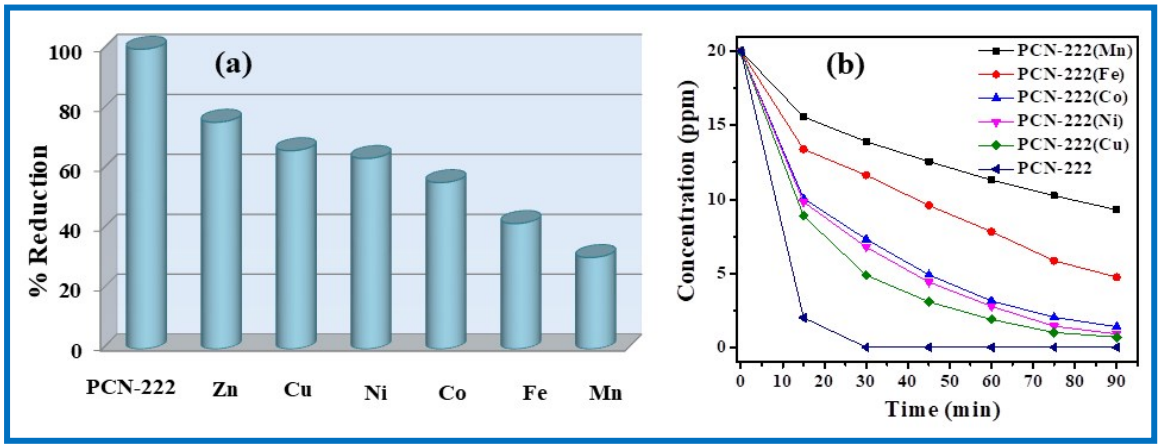

Fig. S17 (a) Histogram showing photocatalytic reduction of Cr(VI) catalysed by PCN-222 and PCN-222(M) (M = Zn^{II}, Cu^{II}, Ni^{II}, Co^{II}, $Fe^{III}Cl$, and $Mn^{III}Cl$) within 30 min at pH 1, (b) Time-dependent plot for photocatalytic reduction of Cr(VI).

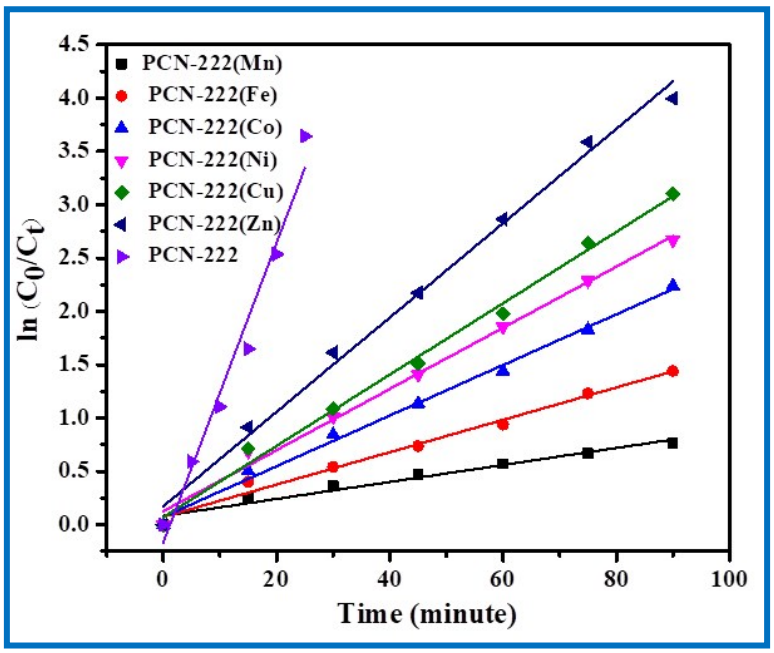

Fig. S18 Kinetics of photocatalytic reduction of Cr(VI) catalysed by PCN-222 and PCN-222(M) (M = Zn^{II}, Cu^{II}, Ni^{II}, Co^{II}, $Fe^{III}Cl$, and $Mn^{III}Cl$).

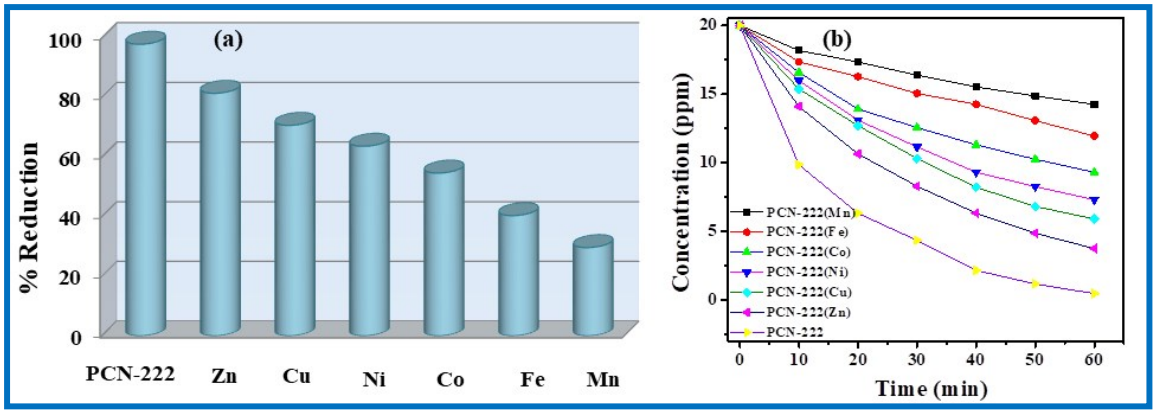

Fig. S19 (a) Histograms showing % reduction of Cr(VI) catalysed by PCN-222 and PCN-222(M) (M = Zn^{II}, Cu^{II}, Ni^{II}, Co^{II}, $Fe^{III}Cl$, and $Mn^{III}Cl$) at pH 2, (b) time-dependent plot for photocatalytic reduction of Cr(VI).

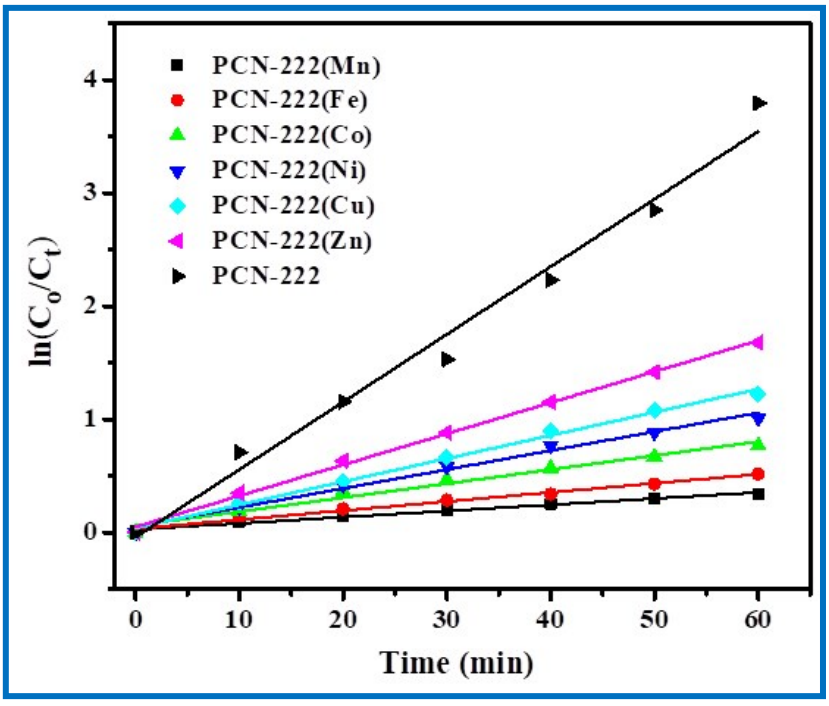

Fig. S20 Kinetic plots for photo-reduction of Cr(VI) catalysed by PCN-MOFs at pH 2.

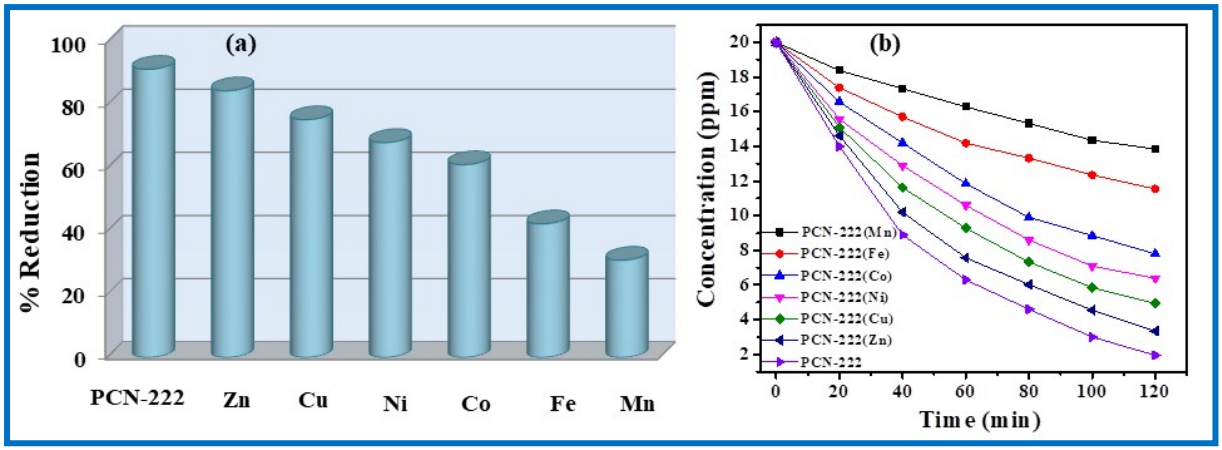

Fig. S21 (a) Histograms showing % reduction of Cr(VI) catalysed by PCN-222 and PCN-222(M) (M = Zn^{II}, Cu^{II}, Ni^{II}, Co^{II}, $Fe^{III}Cl$, and $Mn^{III}Cl$) at pH 3, (b) time-dependent plot for photocatalytic reduction of Cr(VI).

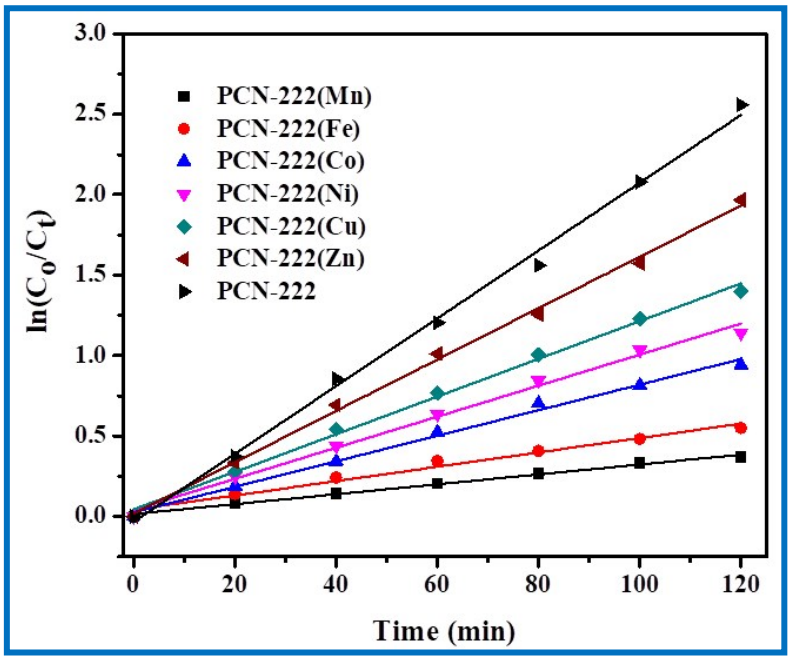

Fig. S22 Kinetic plots for photo-reduction of Cr(VI) catalysed by PCN-MOFs at pH 3.

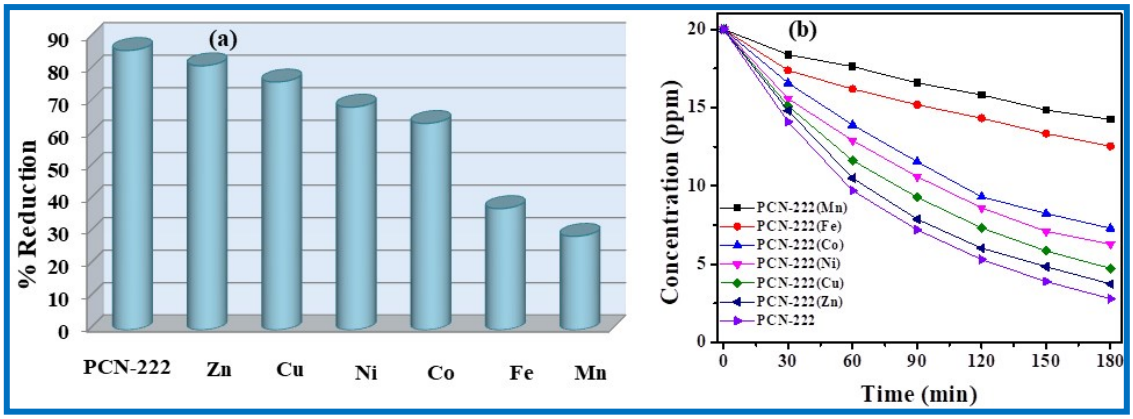

Fig. S23 (a) Histograms showing % reduction of Cr(VI) catalysed by PCN-222 and PCN-222(M) (M = Zn^{II}, Cu^{II}, Ni^{II}, Co^{II}, $Fe^{III}Cl$, and $Mn^{III}Cl$) at pH 4, (b) time-dependent plot for photocatalytic reduction of Cr(VI) catalysed by PCN-MOFs at pH 4.

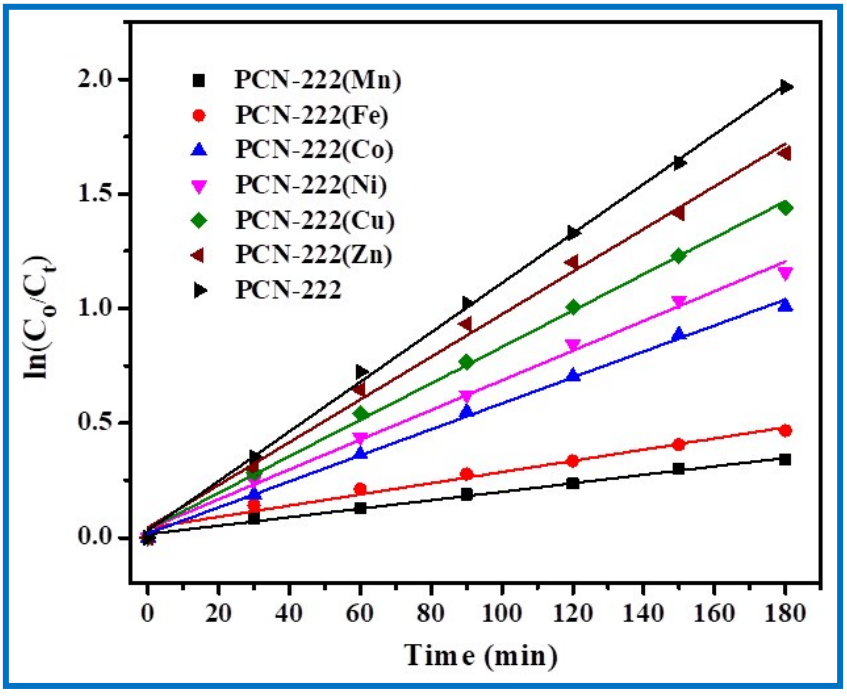

Fig. S24 Kinetic plots for photoreduction of Cr(VI) catalysed by PCN-MOFs at pH 4.

Table S2. Comparison of catalytic reduction of Cr(VI) to Cr(III) using PCN-222 frameworks.

S. No.	MOF	pH	Time (min)	% Reduction	k (min^{-1})
1.	PCN-222	1	30	100	0.1289
2.	PCN-222(Zn)	1	30	76	0.0442
3.	PCN-222(Cu)	1	30	66	0.0335
4.	PCN-222(Ni)	1	30	64	0.0288
5.	PCN-222(Co)	1	30	56	0.0237
6.	PCN-222(Fe)	1	30	42	0.0151
7.	PCN-222(Mn)	1	30	31	0.0079
8.	PCN-222	2	60	98	0.0598
9.	PCN-222(Zn)	2	60	81	0.0274
10.	PCN-222(Cu)	2	60	71	0.0205
11.	PCN-222(Ni)	2	60	63	0.0167
12.	PCN-222(Co)	2	60	55	0.0123
13.	PCN-222(Fe)	2	60	40.	0.0080
14.	PCN-222(Mn)	2	60	29	0.0054
15.	PCN-222	3	120	91	0.0206
16.	PCN-222(Zn)	3	120	84	0.0159
17.	PCN-222(Cu)	3	120	75	0.0117
18.	PCN-222(Ni)	3	120	68	0.0096
19.	PCN-222(Co)	3	120	61	0.0079
20.	PCN-222(Fe)	3	120	42	0.0045
21.	PCN-222(Mn)	3	120	31	0.0033
22.	PCN-222	4	180	86	0.0108
23.	PCN-222(Zn)	4	180	82	0.0093
24.	PCN-222(Cu)	4	180	76	0.0081
25.	PCN-222(Ni)	4	180	68	0.0064
26.	PCN-222(Co)	4	180	63	0.0056
27.	PCN-222(Fe)	4	180	37	0.0025
28.	PCN-222(Mn)	4	180	29	0.0018

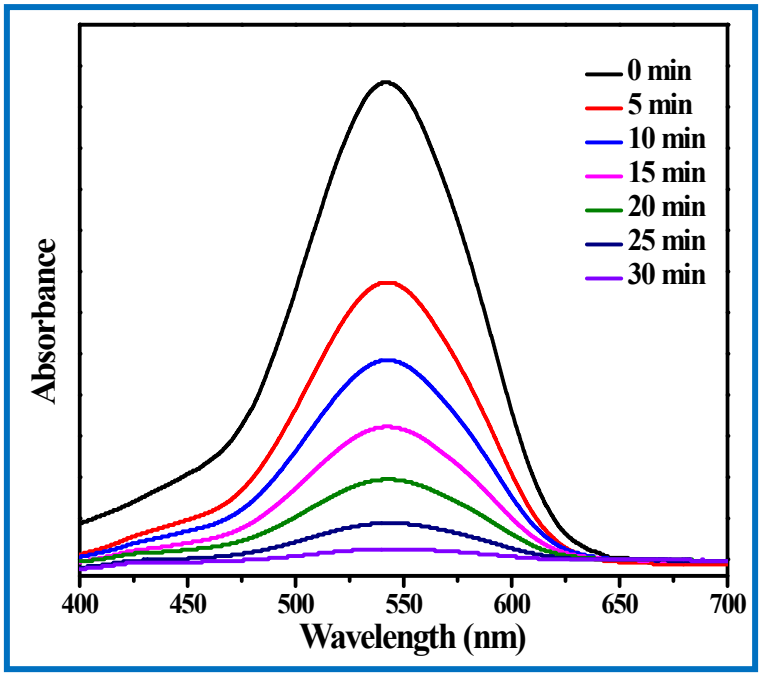

Fig. S25 Absorption spectra for photocatalytic reduction of Cr(VI) to Cr(III) catalysed by PCN-222 in tap water.

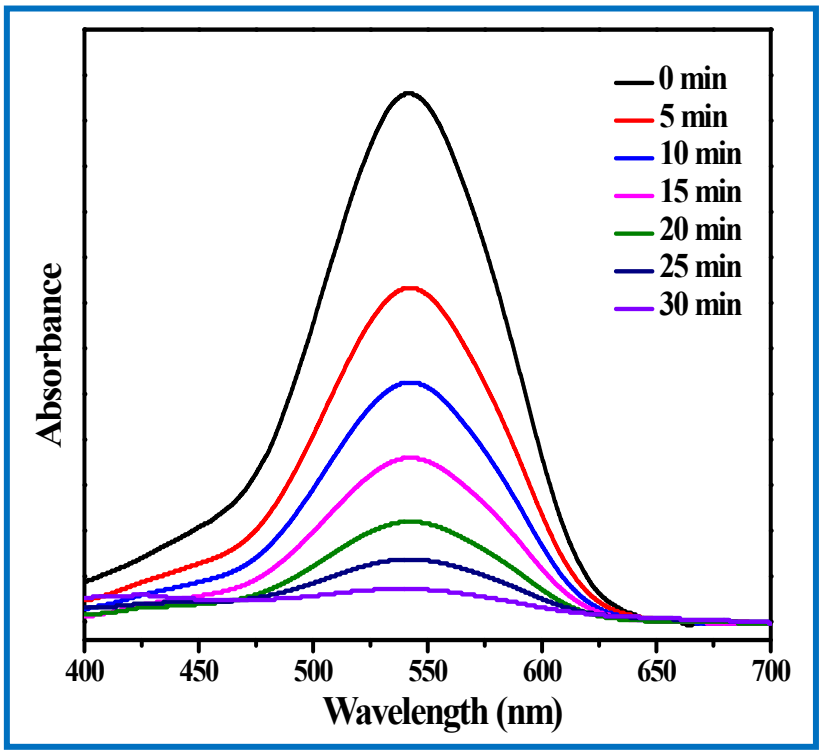

Fig. S26 Absorption spectra for photocatalytic reduction of Cr(VI) to Cr(III) catalysed by PCN-222 in river water.

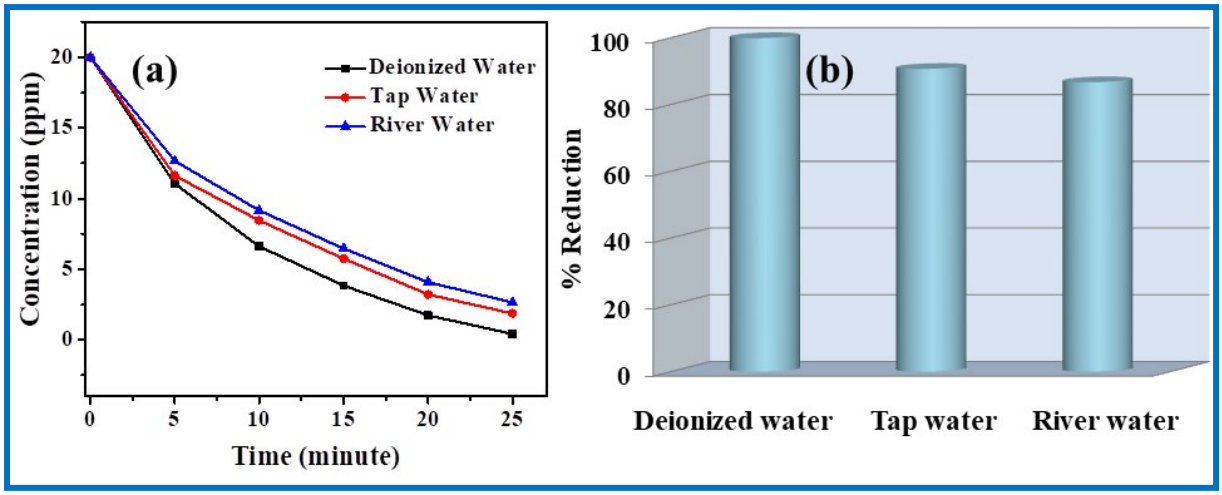

Fig. S27 (a) Photocatalytic reduction of Cr(VI) to Cr(III) carried out in deionized, tap, and river water, (b) the percentage photocatalytic reduction of Cr(VI) within 25 min.

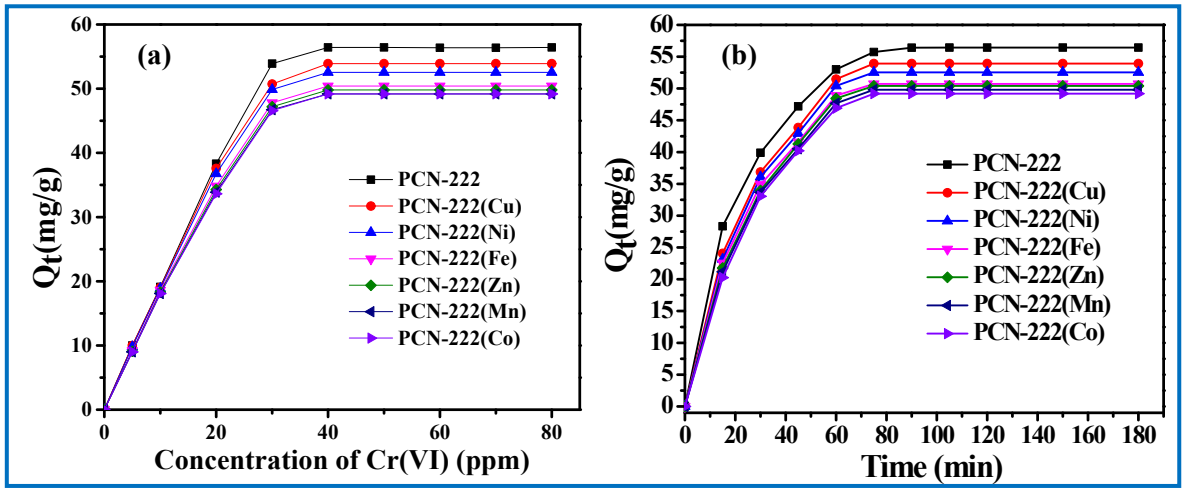

Fig. S28 (a) Concentration-dependent adsorption of Cr(VI) by PCN-222 and PCN-222(M) (M = Zn^{II}, Cu^{II}, Ni^{II}, Co^{II}, $Fe^{III}Cl$, and $Mn^{III}Cl$) carried out under dark conditions, (b) time-dependent adsorption of Cr(VI) carried out with 40 ppm concentration of Cr(VI).

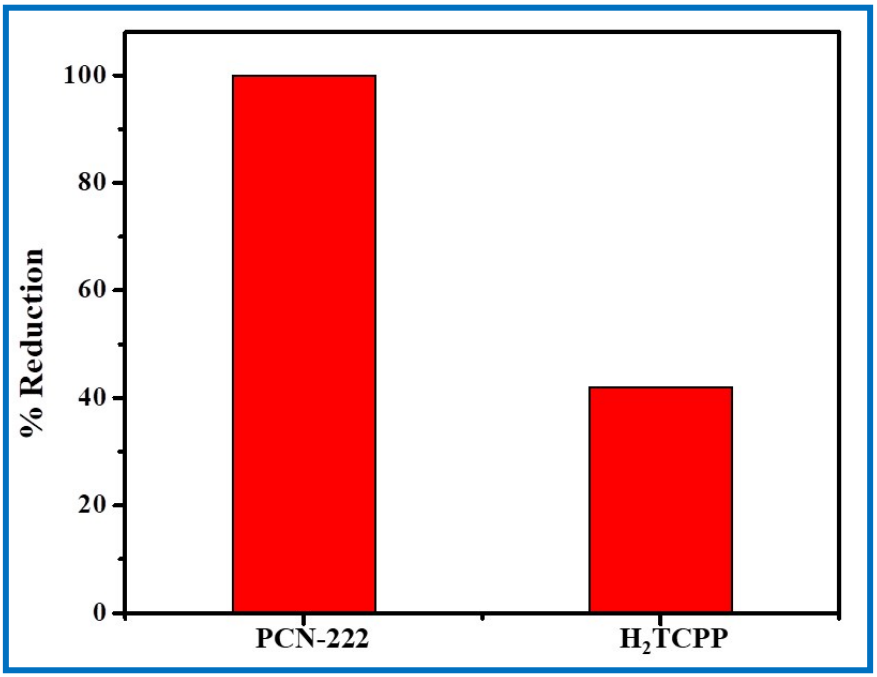

Fig. S29 Percentage photo-reduction of Cr(VI) catalysed by PCN-222 and H_2TCPP ligand

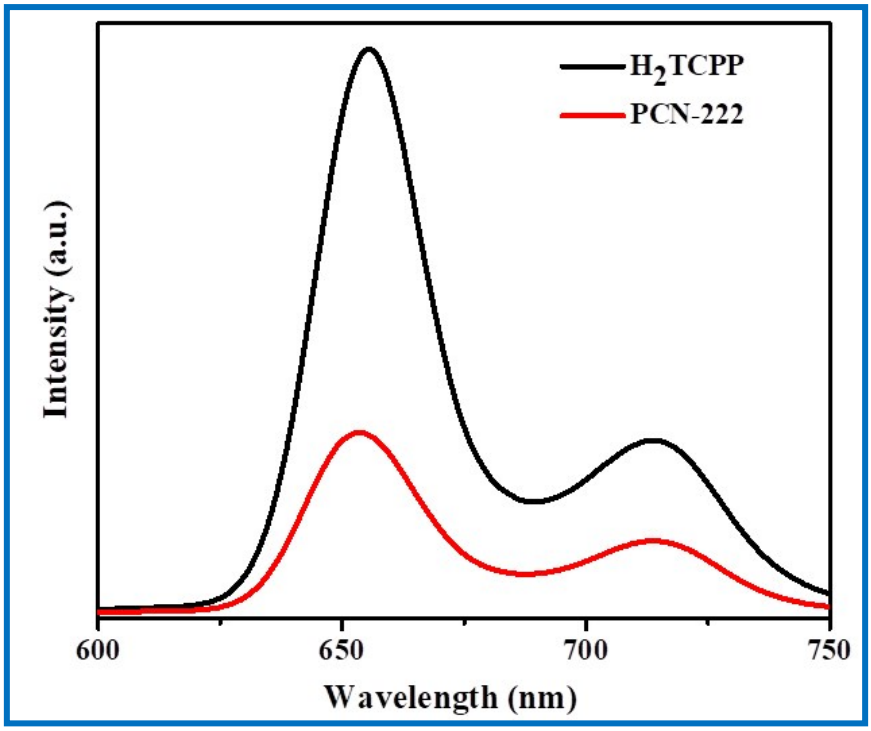

Fig. S30 Fluorescence spectra of H_2TCPP ligand and PCN-222 MOF.

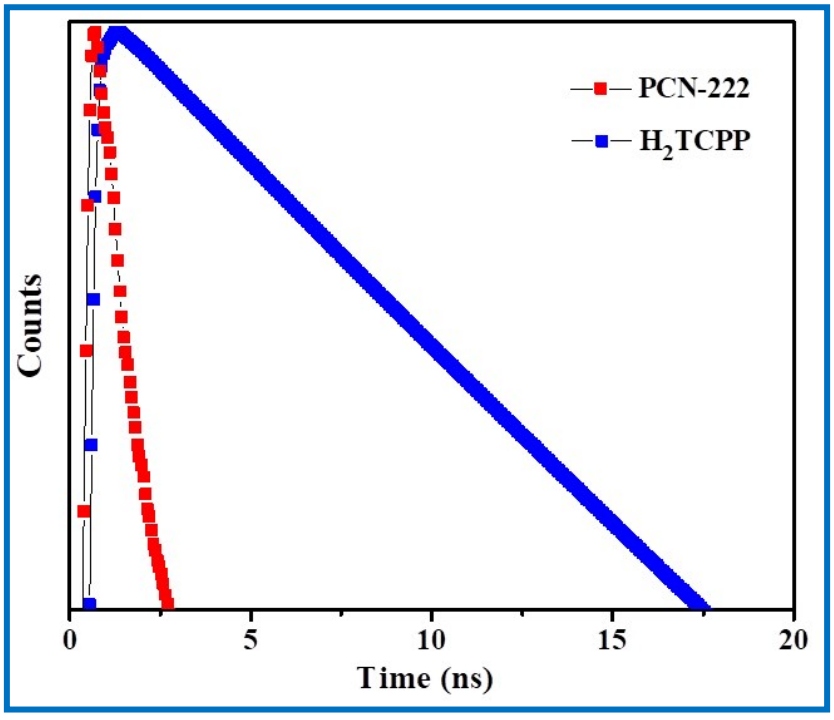

Fig. S31 Time-resolved fluorescence spectra for H_2TCPPligand and PCN-222 MOF recorded with excitation wavelength of 440 nm in water.

Table S3. Decay parameters of samples recorded in water with excitation wavelength of 440 nm.

S. No.	Sample	τ_1 (ns)	τ_2 (ns)	τ (ns)
1	PCN-222	0.067 (92.35 %)	0.961 (7.65 %)	0.14
2	PCN-222(Zn)	0.062 (97.2 %)	1.68 (2.8 %)	0.11
3.	PCN-222(Cu)	0.057 (96.28 %)	0.82 (3.72 %)	0.09

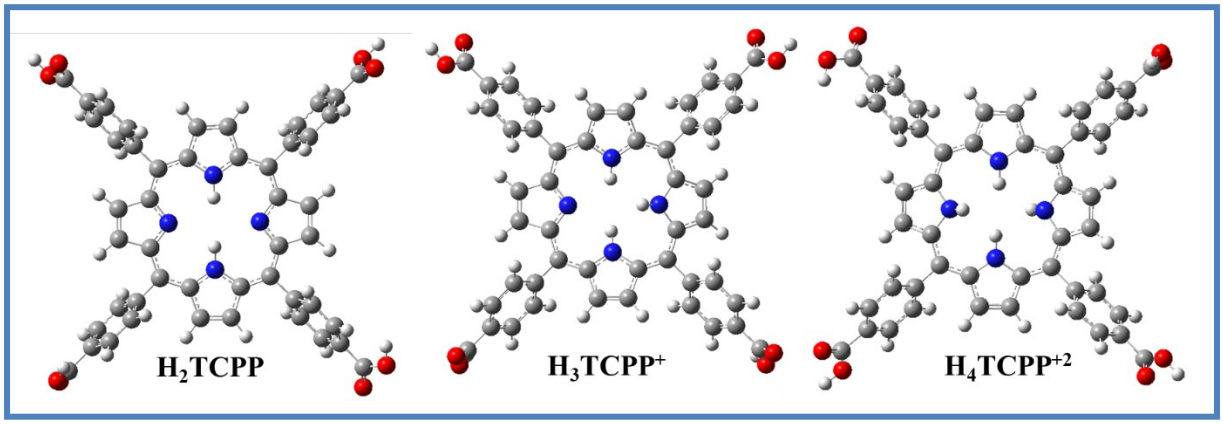

Fig. S32 Optimized structure of H_2TCPP, H_3TCPP^+, and H_4TCPP^{+2}. Here, white: hydrogen, grey: carbon, blue: nitrogen, red: oxygen.

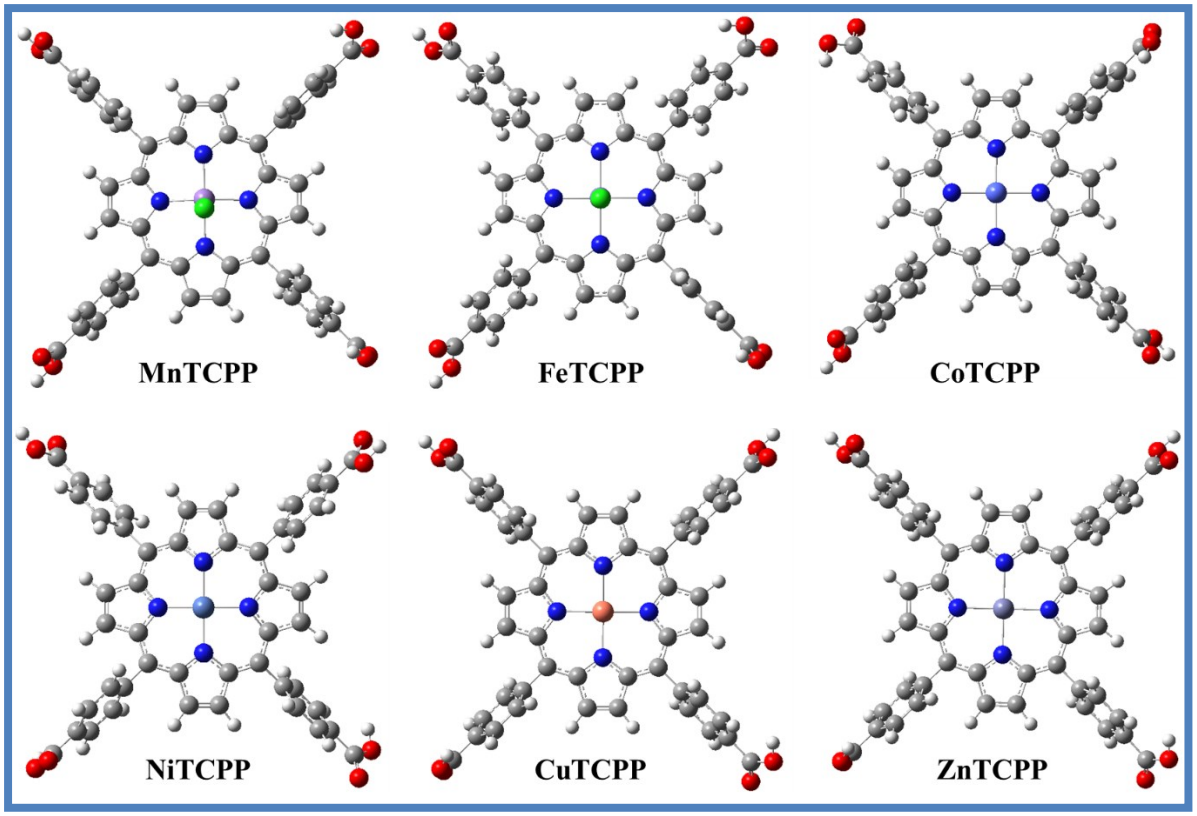

Fig. S33 Optimized structures of porphyrin metal complexes.

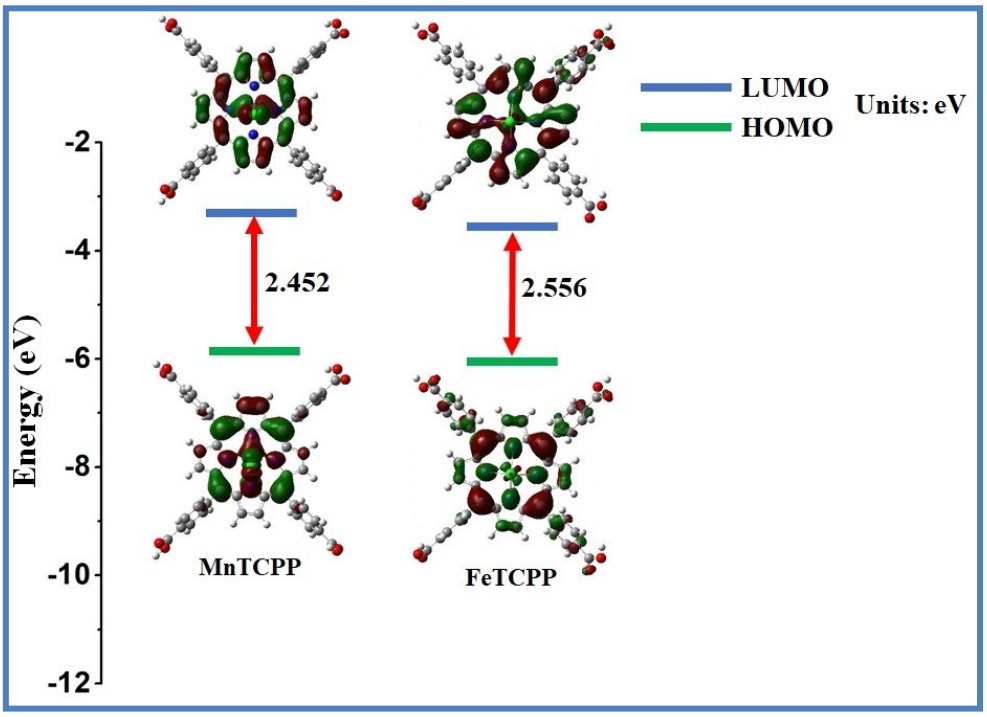

Fig. S34 Bandgaps of optimized FeCl-TCPP and MnCl-TCPP structures.

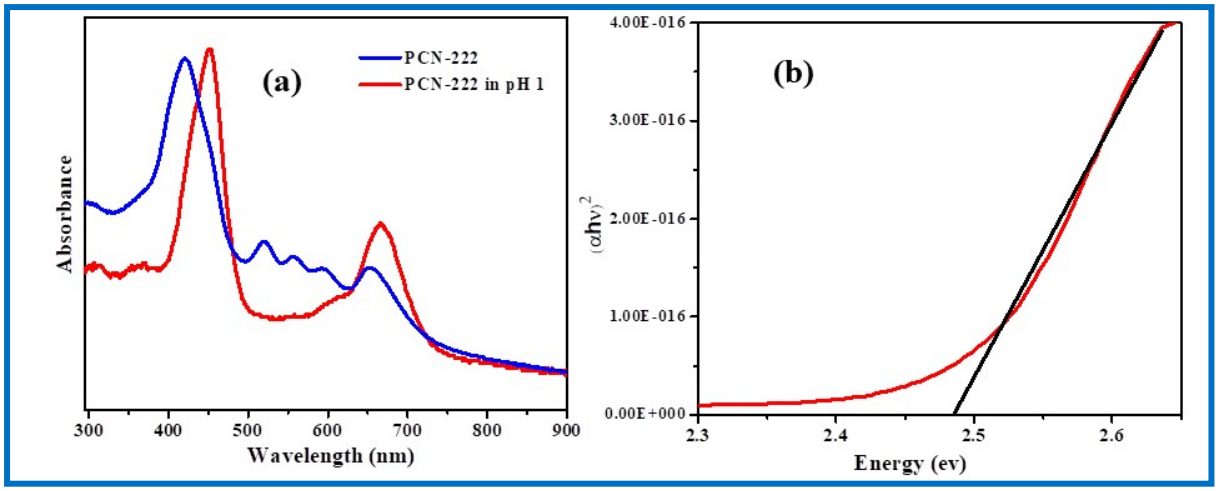

Fig. S35 (a) Solid state UV-Vis absorption spectra of as synthesized PCN-222 and the isolated sample after soaking in dilute H_2SO_4(pH 1), (b) band gap plot for protonated PCN-222 after treated at pH 1.

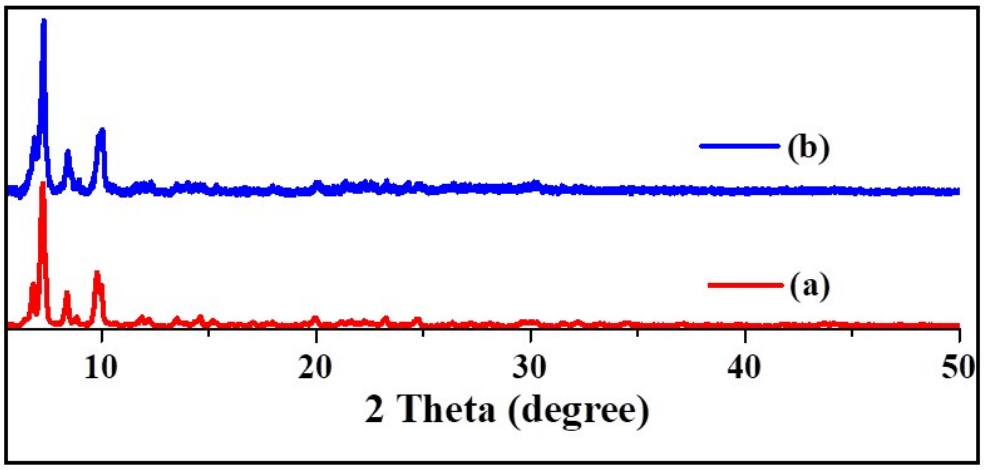

Fig. S36 PXRD patterns of PCN-222, (a) as-synthesized sample (b) recycled sample after catalysis.

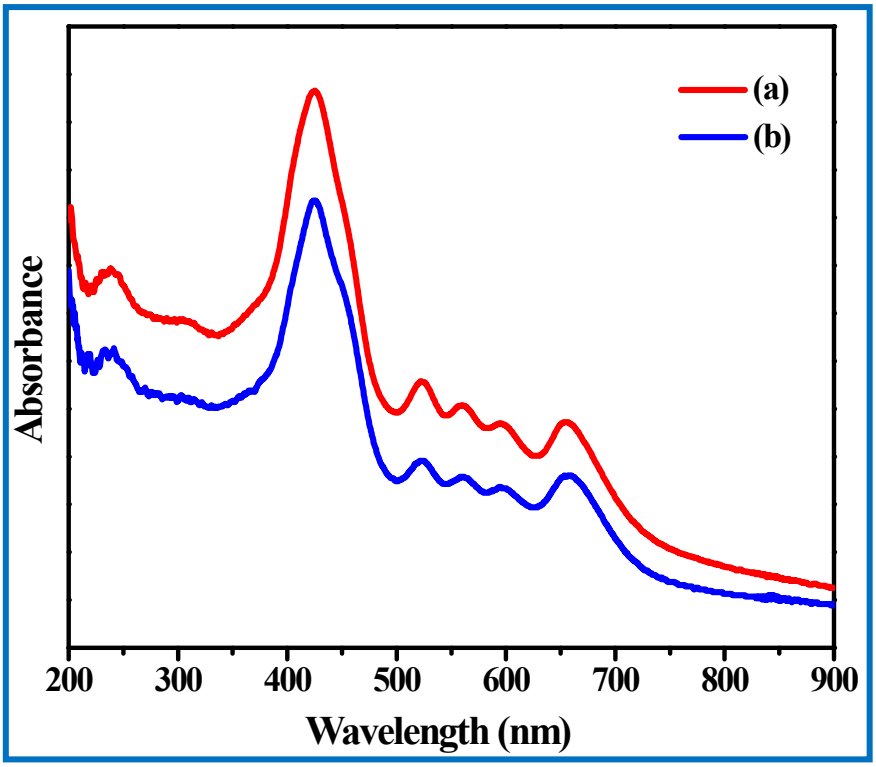

Fig. S37 UV-Vis Spectra of (a) as synthesized PCN-222 and (b) recycled sample after catalysis.

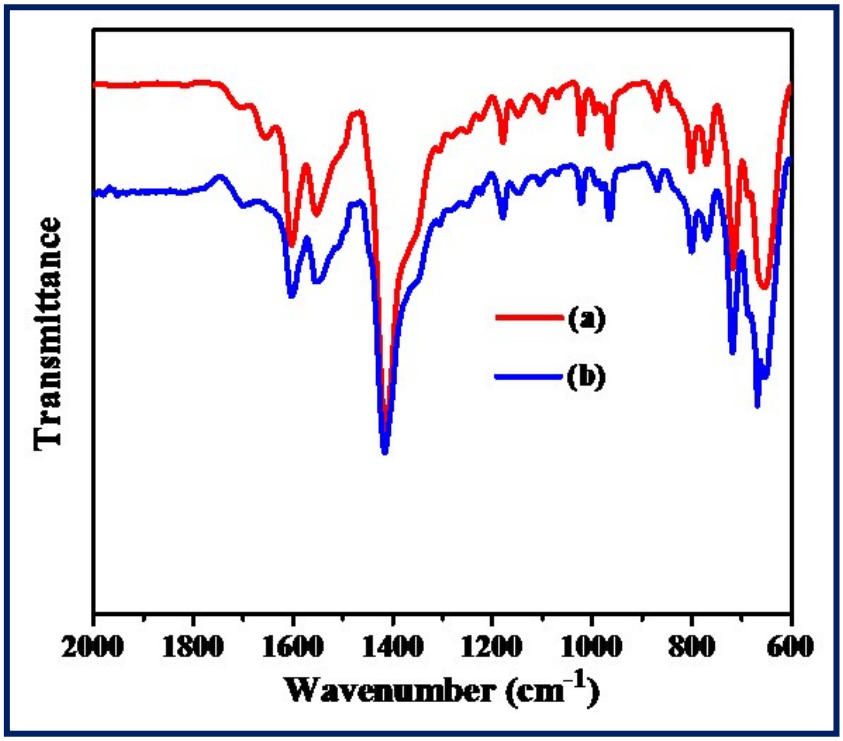

Fig. S38 FT-IR Spectra of (a) as synthesized PCN-222 and (b) recycled sample after catalysis.

Coordinates of optimized structure of H_2TCPP:

O	-6.64595100	7.34237500	1.07135500	C	-3.67209600	4.32686000	1.17711500
N	-2.03788400	0.04116200	-0.03552300	H	-3.09578500	4.12456200	2.07354200
O	7.41623800	6.57635400	1.01942600	C	-6.41212200	6.66445300	0.09942500
C	4.87948500	5.11557100	-1.15247700	O	-7.16728800	-6.81913000	-1.06028200
H	5.08365400	5.68766200	-2.04890100	O	6.89273600	7.00855400	-1.11933500
C	2.51326900	2.37550500	0.00829200	C	6.73044300	6.34638700	0.05211300
C	5.37830100	4.59030200	1.15235400	O	6.34830500	-7.60253500	-0.93932500
H	5.97240600	4.77396200	2.03990500	C	6.40640800	-6.71192600	-0.13709400
O	-7.07905800	6.82712200	-1.06924600	C	-1.06392000	2.90724700	0.01364600
N	2.04173100	-0.05113700	0.03963200	C	-0.58631900	4.25852900	0.01382000
N	-0.04496600	-2.11089200	-0.00733900	H	-1.21769600	5.13259800	0.00859000
H	-0.02219900	-1.09938800	-0.00077900	C	0.77999300	4.22774000	0.02109500
N	0.04866000	2.10088700	0.00937800	H	1.44961800	5.07281100	0.03378300
H	0.02577800	1.08943700	0.00468300	C	1.19648200	2.85635500	0.01083100
O	7.41916300	-6.67544000	0.77033000	C	2.88854200	1.01774100	0.00536700
C	5.64033300	5.33740600	-0.00017400	C	2.84065400	-1.15510000	-0.00724600
C	1.06790200	-2.91712800	-0.01823000	C	2.40477900	-2.49500000	-0.01841200
O	-7.26307500	-6.78040300	1.15722700	C	-1.19307900	-2.86625600	-0.00725900
C	-6.74727900	-6.36620000	-0.03139400	C	-0.77627700	-4.23755800	-0.02435800
C	-5.65460200	-5.34012600	0.03410600	H	-1.44446700	-5.08370900	-0.04156500
C	-5.39219500	-4.59300100	-1.11868200	C	0.59005100	-4.26842100	-0.02175100
H	-5.98820800	-4.77993900	-2.00411000	H	1.21987000	-5.14365700	-0.02275500
C	-4.38661700	-3.63557600	-1.12502500	C	3.66205000	-4.34650000	-1.18514400
H	-4.19802000	-3.05704400	-2.02286000	H	3.07544500	-4.15105500	-2.07635800
C	-3.59764800	-3.41409500	0.01232900	C	4.21415200	-3.83925400	1.10208000
C	-3.84516300	-4.18267900	1.15541300	H	4.04155000	-3.26732000	2.00722200
H	-3.23768400	-4.03229300	2.04124500	C	5.18206200	-4.83861500	1.08944000
C	-4.86266000	-5.13173600	1.16869300	H	5.72443000	-5.04393300	2.00841000
H	-4.99792500	-5.73067600	2.06515700	C	5.40290100	-5.59915400	-0.06435500
C	-2.50948100	-2.38454600	0.00083700	C	4.24737100	-0.77389900	-0.08325800
C	-2.88524500	-1.02642100	0.00176100	H	5.08569000	-1.44968100	-0.15572800
C	-4.27374100	-0.58390900	0.07969200	C	4.27707300	0.57671500	-0.07477800
H	-5.14152300	-1.22239500	0.14270500	H	5.14330700	1.21734400	-0.13720900
C	-4.24340500	0.76663800	0.08167700	C	4.62065900	-5.35118300	-1.19667600
H	-5.08091500	1.44409800	0.14695800	H	4.78142600	-5.95659300	-2.08089000
C	-2.83645800	1.14636800	0.00599800	C	3.44455300	-3.57327900	-0.03629400
C	-2.40114600	2.48602600	0.01248900	C	4.37109800	3.63426800	1.15242200
C	-3.44128500	3.56458900	0.02376800	H	4.16986900	3.06028100	2.05047700
C	-4.20254300	3.83093100	-1.12157500	C	3.86897600	4.16024100	-1.14590300
H	-4.02908100	3.25097400	-2.02159200	H	3.28616800	3.98607300	-2.04405200
C	-5.16794400	4.83156600	-1.11906500	C	3.60099300	3.40620700	0.00375900
H	-5.74714700	5.03303900	-2.01151500	H	7.43100600	-5.83196600	1.23937600
C	-5.39223800	5.58502200	0.03771000	H	7.61861700	7.63617100	-0.98627700
C	-4.63830500	5.32451900	1.18603200	H	-7.71457200	7.54486800	-0.92974300
H	-4.82528900	5.91126600	2.07777800	H	-6.95025800	-6.22453800	1.88160200

Coordinates of optimized structure of H_3TCPP^+:

O	6.47912700	7.53753200	-0.83973000	C	3.44991300	4.59606600	-0.92517200
N	2.10677600	0.02345200	0.10244200	H	2.66417300	4.61497300	-1.67235900
O	-6.70569500	7.32372200	-0.83250100	C	6.48292800	6.63880200	-0.03697200
C	-5.53619900	4.39102100	0.98433600	O	7.28752000	-6.67253400	1.11458000
H	-6.27876000	4.37773300	1.77203500	O	-7.51163300	6.31951500	1.00997800
C	-2.48232100	2.41404200	-0.09316500	C	-6.63498600	6.44632900	-0.00901400
C	-4.61916400	5.41009500	-1.00626100	O	-7.05075500	-6.81725600	1.25307400
H	-4.67341900	6.18439100	-1.76233500	C	-6.54427900	-6.55226600	0.19987900
O	7.42423800	6.50729400	0.92115900	C	1.09481600	2.90166400	0.15802400
N	-2.00390600	-0.01900800	-0.16223500	C	0.61989100	4.20754500	0.49991000
N	0.01829000	-2.12202700	-0.04799100	H	1.25494700	5.03583300	0.77021500
H	-0.04961000	-1.17849500	-0.39982800	C	-0.74802600	4.19487500	0.45922500
N	-0.02820700	2.12466300	-0.04475100	H	-1.41335400	5.01195300	0.68785200
H	-0.07573800	1.17904200	-0.39412000	C	-1.17077500	2.87906500	0.09472800
O	-6.90489500	-7.21232300	-0.92759400	C	-2.83885500	1.05954400	-0.27380800
C	-5.58329000	5.38727000	0.00488900	C	-2.81520400	-1.11508100	-0.27008300
C	-1.10859800	-2.89950300	0.09683800	C	-2.42853800	-2.46122900	-0.08795800
O	6.93912100	-7.18556500	-1.01747300	C	1.15803200	-2.87522100	0.15139300
C	6.67725600	-6.47138600	0.10322700	C	0.71096600	-4.19023200	0.49746800
C	5.58754800	-5.43499400	0.01094900	H	1.36312100	-5.00404200	0.77140400
C	5.58397200	-4.41794600	0.97080400	C	-0.65701700	-4.20576000	0.46207600
H	6.36307200	-4.41348300	1.72359100	H	-1.30394600	-5.03525700	0.69911600
C	4.59464400	-3.44521200	0.96256800	C	-4.43829500	-3.52263000	0.99059000

H	4.60329800	-2.66463600	1.71545600	H	-4.39561700	-2.76486800	1.76525400
C	3.56108300	-3.48349200	0.01357600	C	-3.54744000	-4.51284900	-1.02040000
C	3.55346400	-4.51813300	-0.93116300	H	-2.82045000	-4.52235400	-1.82528000
H	2.76428800	-4.56429100	-1.67340100	C	-4.53886300	-5.48898700	-0.97633000
C	4.55940600	-5.47925700	-0.93596200	H	-4.53596200	-6.26478000	-1.73611800
H	4.50465000	-6.28088500	-1.66633600	C	-5.48247500	-5.49437300	0.05533500
C	2.49065700	-2.44476700	0.01995300	C	-4.19331700	-0.71796100	-0.53730400
C	2.89274000	-1.10747000	-0.12836000	H	-5.02220500	-1.38666700	-0.70801900
C	4.15514300	-0.63823300	-0.58410200	C	-4.20780600	0.63146300	-0.54142500
H	4.95516600	-1.27535600	-0.92645000	H	-5.04988600	1.28199400	-0.71712500
C	4.14030000	0.73391700	-0.58041000	C	-5.40944400	-4.51232600	1.04838700
H	4.92541900	1.39094000	-0.91966100	H	-6.12155100	-4.54600500	1.86423000
C	2.86802500	1.17299500	-0.12215400	C	-3.49131700	-3.51098600	-0.04437100
C	2.43747300	2.50062900	0.03044900	C	-3.61461200	4.45168700	-1.03618900
C	3.48390900	3.56275800	0.02421300	H	-2.87690000	4.46959400	-1.83117900
C	4.52335300	3.54093500	0.96573400	C	-4.53719500	3.42474100	0.94637900
H	4.55237400	2.75802200	1.71574200	H	-4.50009100	2.65977700	1.71423600
C	5.50001700	4.53018500	0.96624000	C	-3.56382700	3.44360200	-0.06233800
H	6.29174900	4.51582100	1.70445100	H	-6.55098200	-6.78658600	-1.71840500
C	5.45901300	5.55277100	0.01433200	H	-8.15619500	7.03916800	0.93020000
C	4.43112700	5.57789200	-0.93236400	H	8.04550000	7.24512700	0.82368400
H	4.41973600	6.37235600	-1.66907700	H	6.49977900	-6.81272800	-1.79187300
				H	1.36750800	0.01344000	0.79269400

Coordinates of optimized structure of H_4TCPP^{+2}:

O	5.87633500	-7.95832100	1.07622800	H	2.40196400	-4.65552400	1.86999300
N	2.08009800	-0.23274000	-0.28570400	C	5.87498900	-7.17899100	0.15966500
O	-8.30114500	-5.52839100	0.82983500	O	7.91827200	5.90610800	-1.14061700
C	-5.25532200	-4.84914100	-1.04631300	O	-7.49062600	-6.46768800	-1.05028100
H	-5.39338800	-5.55550600	-1.85502300	C	-7.45063600	-5.60793000	-0.01727300
C	-2.76770200	-2.21127500	0.07033800	O	-5.45648100	8.21519600	-0.81171800
C	-6.05554200	-3.82645100	0.99483400	C	-5.77040800	7.27791800	-0.13651700
H	-6.81089400	-3.77108900	1.76973500	C	0.77006600	-3.04724000	-0.08146000
O	6.71703100	-7.24183000	-0.88674700	C	0.17270600	-4.34636200	-0.02420400
N	-2.09356500	0.21166500	0.31549800	H	0.72015700	-5.27407700	-0.05737400
N	0.26504200	2.12224400	0.05554700	C	-1.18243600	-4.19852000	0.09427400
H	0.17980800	1.12932900	0.17396100	H	-1.91241300	-4.98472000	0.19842700
N	-0.27673100	-2.14460800	-0.02494700	C	-1.48884500	-2.80288000	0.06800000
H	-0.19025800	-1.15072400	-0.13408900	C	-3.01546000	-0.82329500	0.04099000
O	-6.90628400	7.28636500	0.59135700	C	-2.73351900	1.44610500	0.07006500
C	-6.21966200	-4.75223600	-0.03866600	C	-2.16005000	2.73322500	0.11036800
C	-0.78256400	3.02444100	0.10315800	C	1.47720000	2.78040500	-0.04395600
O	7.84573800	6.23454100	1.05518200	C	1.16922100	4.17612200	-0.08319300
C	7.39837800	5.67417300	-0.08783500	H	1.89759900	4.96240700	-0.19800400
C	6.20002300	4.75787900	0.01437700	C	-0.18552900	4.32405400	0.03297400
C	6.01151200	3.83818200	-1.02255100	H	-0.73296700	5.25223000	0.05417100
H	6.73477200	3.81051500	-1.82869800	C	-3.11342500	4.75884100	-1.05159200
C	4.91173400	2.99361800	-1.02333700	H	-2.43565500	4.59270900	-1.88220200
H	4.77874200	2.29002300	-1.83818200	C	-4.02183600	4.09498800	1.08881600
C	3.94535800	3.08189600	-0.00670800	H	-4.01946800	3.44197300	1.95506900
C	4.12545200	4.01801000	1.02181300	C	-4.90169400	5.17327100	1.04541100
H	3.40129900	4.09100200	1.82595100	H	-5.55374700	5.34352600	1.89627100
C	5.24804700	4.84012500	1.03549000	C	-4.89984000	6.04519700	-0.04668000
H	5.34745200	5.56689300	1.83548800	C	-4.03807400	1.15356700	-0.39648300
C	2.75470100	2.18922500	-0.04405300	H	-4.73627000	1.89221500	-0.75768100
C	3.00290200	0.80107400	-0.01222000	C	-4.20690900	-0.21185500	-0.41556400
C	4.19494500	0.18939900	0.44100500	H	-5.06237800	-0.74969700	-0.79321100
H	5.05273700	0.72615600	0.81483800	C	-3.99382100	5.82979400	-1.09121800
C	4.02525400	-1.17609800	0.42264600	H	-3.99132500	6.52064300	-1.92584100
H	4.72413600	-1.91556800	0.78082500	C	-3.11213200	3.88129100	0.04512600
C	2.72028500	-1.46786900	-0.04317200	C	-4.94100700	-3.00034700	1.02183800
C	2.14852200	-2.75611900	-0.08767400	H	-4.81519200	-2.29645300	1.83752600
C	3.10448800	-3.89885100	-0.03127300	C	-4.12925800	-4.03487900	-1.01270100
C	4.04372700	-4.07204300	-1.05926600	H	-3.39913000	-4.10030600	-1.81217600
H	4.05425200	-3.39254300	-1.90488400	C	-3.95810300	-3.10153500	0.02249700
C	4.94186100	-5.13322300	-1.02124000	H	-7.12393600	6.41675900	0.94977900
H	5.65269300	-5.27514600	-1.82531700	H	-8.30608300	-6.98875100	-0.98068100
C	4.92731000	-6.02186400	0.05669800	H	7.29858700	-8.00850200	-0.76317900
C	4.00618700	-5.84403200	1.09305600	H	7.45744100	5.83302500	1.84269600
H	4.02222500	-6.53442200	1.92812800	H	1.51964300	-0.14484300	-1.12682600
C	3.09686900	-4.79651900	1.04904700	H	-1.53478400	0.12522600	1.15781200

Coordinates of optimized structure of CoTCPP:

O	6.30027800	-7.75565300	-0.28956300	H	3.10019400	-4.47301300	1.48544000
N	1.96752900	-0.16769100	-0.01517000	C	5.95552900	-6.95246300	-1.16380400
O	-7.61472300	-5.93346200	2.38767300	O	7.48621400	6.56250800	0.34017200
C	-5.28225000	-4.87900900	-0.23735400	O	-7.39216700	-6.60411000	0.21612300
H	-5.64555000	-5.51423000	-1.03074500	C	-7.02476600	-5.83621300	1.30566800
C	-2.60761600	-2.22517600	0.33482900	O	-5.63014300	7.80431400	-2.33645300
C	-5.43052200	-4.10262600	2.05479000	C	-5.82404100	7.01673500	-1.41643900
H	-5.91004800	-4.15552700	3.02180500	C	0.86104400	-2.91389100	-0.16695300
O	6.45538100	-7.03342000	-2.45031000	C	0.32594400	-4.25398300	-0.09766500
N	-1.96863500	0.15228900	0.01402800	H	0.90031800	-5.15424100	-0.21797900
N	0.15849900	1.95622400	-0.00327600	C	-1.00314700	-4.14472700	0.16465600
N	-0.16024100	-1.98053600	0.01257700	H	-1.71317500	-4.93928300	0.30347400
O	-6.94113300	7.18970700	-0.60809700	C	-1.31769900	-2.73528600	0.20585300
C	-5.89538700	-4.93183500	1.02329700	C	-2.89973900	-0.86984200	0.19152300
C	-0.85933200	2.88751600	-0.20449400	C	-2.72434500	1.30474100	-0.20494900
O	7.40777900	6.13421900	2.55264100	C	-2.21439200	2.59361800	-0.34695000
C	6.95318400	5.94148700	1.25363900	C	1.31324100	2.71141500	0.19809600
C	5.83767600	4.97489200	1.06418200	C	1.00262400	4.12064300	0.13241300
C	5.64426300	4.43335500	-0.21515000	H	1.71638100	4.91548600	0.25245600
H	6.31205600	4.73286700	-1.01004900	C	-0.32649000	4.22846100	-0.13226000
C	4.60793400	3.53435600	-0.45135500	H	-0.90219100	5.12822800	-0.25196700
H	4.46905600	3.11999300	-1.44028500	C	-3.19715100	4.35217000	-1.86156500
C	3.72619900	3.16660000	0.57928700	H	-2.54072800	4.00112900	-2.64562700
C	3.90649300	3.73204200	1.85095900	C	-4.01645600	4.19907600	0.40490200
H	3.22395500	3.47248400	2.64828800	H	-3.97966000	3.74751700	1.38654200
C	4.95023300	4.62436600	2.09326100	C	-4.89147900	5.25651900	0.16050300
H	5.03663100	5.06760700	3.07765200	H	-5.50108100	5.62476100	0.97645200
C	2.60377800	2.20369900	0.33159800	C	-4.93309800	5.86689300	-1.10285000
C	2.90006400	0.85030700	0.18597800	C	-4.13262800	0.98307200	-0.19047000
C	4.23924600	0.30949400	0.15291500	H	-4.92781900	1.68485600	-0.36381000
H	5.13864700	0.87851800	0.30255400	C	-4.24063200	-0.34500600	0.07883300
C	4.13072200	-1.02075000	-0.10504400	H	-5.13887400	-0.92925600	0.16321700
H	4.92327900	-1.74076300	-0.19906800	C	-4.06518300	5.41249300	-2.10640900
C	2.72159900	-1.32660600	-0.19307100	H	-4.08594900	5.90245200	-3.06918700
C	2.21496200	-2.61917500	-0.31270400	C	-3.16237100	3.72583600	-0.60390600
C	3.18159400	-3.74319400	-0.53887600	C	-4.36816500	-3.23225700	1.82792200
C	3.76138400	-3.93390000	-1.80383200	H	-4.01057500	-2.59670500	2.62619700
H	3.49642100	-3.26744200	-2.61304000	C	-4.21760400	-4.00742300	-0.45799200
C	4.66409500	-4.97214400	-2.02667400	H	-3.75210800	-3.96250800	-1.43289300
H	5.10332000	-5.11808800	-3.00170500	C	-3.74504900	-3.17376600	0.56949500
C	5.00588200	-5.84008400	-0.97928100	H	-7.11173500	6.43809900	-0.01368800
C	4.43442600	-5.65475100	0.28856300	H	-8.14103800	-7.18279100	0.45451000
H	4.71071100	-6.32771100	1.08773700	H	7.07586000	-7.78357000	-2.51936000
C	3.53221400	-4.61715400	0.50481100	H	7.05291800	5.48836000	3.18856000
				Co	-0.00073600	-0.01048900	0.00194000

Coordinates of optimized structure of CuTCPP:

O	-6.29143900	7.62444400	1.07571600	C	-6.05925800	6.96434700	0.09118000
N	-2.00929700	0.13442500	-0.02379600	O	-7.42541000	-6.51713400	-1.04255500
O	7.64692700	6.27302100	1.05481500	O	7.21277900	6.65766900	-1.11277100
C	5.11949400	4.85303500	-1.15498100	C	6.98288400	6.04199300	0.07262700
H	5.37705800	5.38679200	-2.06124700	O	5.98181900	-7.86571700	-0.98788300
C	2.59846600	2.25808600	0.00942800	C	6.05069700	-7.00993400	-0.14941400
C	5.51882400	4.38400100	1.18115000	C	-0.89820600	2.90754000	0.00774400
H	6.09110100	4.57133600	2.08218700	C	-0.38409300	4.25503600	0.00607800
O	-6.67840600	7.19480200	-1.09237000	H	-0.98420400	5.15141900	-0.00019800
N	2.01186400	-0.14316900	0.02203100	C	0.96817700	4.16181400	0.01309000
N	-0.13765200	-2.01537000	-0.00986900	H	1.68503400	4.96791200	0.02405000
N	0.14024300	2.00646300	0.00427100	C	1.29266200	2.75644400	0.00534700
O	7.02606800	-7.05892500	0.79756300	C	2.91234300	0.89597300	0.00854400
C	5.85141200	5.07998700	0.01498000	C	2.76157200	-1.29507200	-0.00739700
C	0.90111600	-2.91616700	-0.02600400	C	2.26299900	-2.60091400	-0.02291100
O	-7.55039800	-6.42829400	1.17202600	C	-1.29015600	-2.76530300	-0.00750400
C	-6.99980000	-6.06222500	-0.01679900	C	-0.96529200	-4.17051600	-0.02897600
C	-5.86464500	-5.08309300	0.04440600	H	-1.68063300	-4.97786300	-0.04557400
C	-5.55123600	-4.37533200	-1.12032200	C	0.38705200	-4.26365900	-0.03209500
H	-6.13993100	-4.55765100	-2.01160800	H	0.98562400	-5.16110900	-0.03848700
C	-4.50497300	-3.46237700	-1.13075700	C	3.46993100	-4.47153200	-1.20884100
H	-4.27607000	-2.91486100	-2.03872100	H	2.92579400	-4.21674600	-2.11193000
C	-3.72663100	-3.24756200	0.01489200	C	3.95659500	-4.07535000	1.11455700

C	-4.02641200	-3.97702900	1.17080500	H	3.77706500	-3.52826100	2.03370700
H	-3.42557800	-3.83383300	2.06232200	C	4.87352100	-5.12191100	1.10058100
C	-5.08321000	-4.88197000	1.18761600	H	5.36845700	-5.38746500	2.03085000
H	-5.25781600	-5.45441100	2.09456800	C	5.10108200	-5.85099400	-0.07199300
C	-2.59583200	-2.26614500	0.00134300	C	4.16614500	-0.96965700	-0.04903400
C	-2.91013700	-0.90365000	0.00048900	H	4.97202500	-1.68528700	-0.09704000
C	-4.25646900	-0.38877100	0.05167800	C	4.25914300	0.38273400	-0.03845000
H	-5.15272000	-0.98748500	0.09634900	H	5.15421300	0.98383000	-0.07470400
C	-4.16282100	0.96353900	0.05012600	C	4.37640800	-5.52351800	-1.22232200
H	-4.96752800	1.68074600	0.09339200	H	4.53973800	-6.10585400	-2.12144800
C	-2.75838400	1.28744700	0.00015100	C	3.24688300	-3.72993000	-0.04072500
C	-2.26033700	2.59331300	0.00490600	C	4.47026300	3.47334000	1.17711600
C	-3.24472300	3.72240200	0.01414000	H	4.21378300	2.93964700	2.08598600
C	-3.95251500	4.06038400	-1.14601300	C	4.06856100	3.94231100	-1.15273300
H	-3.77742500	3.49950800	-2.05783700	H	3.50599200	3.76571700	-2.06321600
C	-4.86722100	5.10781000	-1.14346500	C	3.72942200	3.24038600	0.01066100
H	-5.40550100	5.36447100	-2.04730800	H	7.05915800	-6.23560300	1.30017200
C	-5.09261000	5.83709700	0.02839200	H	7.96104400	7.25723600	-0.97458300
C	-4.39093100	5.50554600	1.19149400	H	-7.28103300	7.93996900	-0.95081400
H	-4.57698900	6.07583200	2.09405200	H	-7.22246200	-5.87258000	1.88977900
C	-3.47612400	4.46058300	1.18263800	H	-2.93793200	4.20513400	2.08912700
				Cu	0.00125100	-0.00417700	-0.00203900

Coordinates of optimized structure of FeTCPP:

O	-7.90715400	6.01156800	0.78348500	C	-7.29577800	5.65500400	-0.22958500
N	-1.98581400	-0.26235000	-0.12100500	O	-5.62633700	-8.22547700	-0.65549600
O	6.24929300	7.61878100	1.34334500	O	5.84370700	7.96608600	-0.87704700
C	4.14108100	5.79549300	-1.03811000	C	5.67150500	7.27296400	0.30691300
H	4.34365900	6.39401100	-1.91309800	O	7.42185400	-6.54251600	-1.26824200
C	2.11260400	2.72639500	-0.05662800	C	7.28851100	-5.70543700	-0.38155500
C	4.49809800	5.34773200	1.31846000	C	-1.46211100	2.65360100	-0.19717300
H	4.97432500	5.61578200	2.25078100	C	-1.21496000	4.06933500	-0.16639100
O	-7.66129900	6.10513700	-1.48485900	H	-1.97962400	4.82449300	-0.16446600
N	1.98678500	0.25362000	-0.10657300	C	0.13366400	4.24590900	-0.10782400
N	0.25255600	-1.95703400	-0.23493300	H	0.67250500	5.17367800	-0.04655400
N	-0.24933600	1.95092700	-0.19401100	C	0.73945200	2.94143800	-0.12543600
O	8.25359800	-5.62183100	0.61477400	C	2.68475200	1.45916700	-0.06610000
C	4.75469600	6.12525800	0.17949400	C	2.97071800	-0.73150900	-0.16250600
C	1.46495800	-2.65904700	-0.24886700	C	2.73988800	-2.09933700	-0.22970300
O	-6.54567200	-7.42017900	1.24035400	C	-0.73764400	-2.94912200	-0.17651600
C	-5.64443000	-7.33326900	0.18608900	C	-0.13042600	-4.25310800	-0.17947800
C	-4.75348300	-6.14141100	0.15408500	H	-0.66686500	-5.18271900	-0.13349600
C	-4.14710500	-5.80438500	-1.06527600	C	1.21807400	-4.07514000	-0.22842300
H	-4.35662200	-6.41342400	-1.93273700	H	1.98192000	-4.83093400	-0.23257000
C	-3.29750200	-4.70471700	-1.15086400	C	4.30492300	-3.66550600	-1.44536500
H	-2.84767200	-4.44494300	-2.09912000	H	3.74310800	-3.48498500	-2.35136400
C	-3.02096500	-3.92299900	-0.01696500	C	4.65482300	-3.27251900	0.91352500
C	-3.60926400	-4.27689400	1.20700400	H	4.35395400	-2.80423400	1.84046400
H	-3.38286900	-3.69845600	2.09173600	C	5.75421000	-4.12986000	0.89233200
C	-4.46428300	-5.37447800	1.29322800	H	6.26990400	-4.33358800	1.82261400
H	-4.86456800	-5.64403900	2.26264900	C	6.14374500	-4.75714300	-0.30133100
C	-2.11050900	-2.73448100	-0.10129200	C	4.28437400	-0.12875100	-0.16494600
C	-2.68420200	-1.46549100	-0.09418800	H	5.21107700	-0.67015200	-0.22062700
C	-4.10894000	-1.21921800	-0.12409500	C	4.10850300	1.21629500	-0.10319400
H	-4.86407400	-1.98339700	-0.12954400	H	4.86156000	1.98286100	-0.09942000
C	-4.28225700	0.12669900	-0.17203600	C	5.39902100	-4.52607900	-1.46719200
H	-5.20650500	0.67330000	-0.21857100	H	5.69170100	-5.03050200	-2.37679300
C	-2.96719900	0.72508700	-0.15859900	C	3.92062700	-3.02418000	-0.25606900
C	-2.73586000	2.09397900	-0.19355000	C	3.64250900	4.25221100	1.23997300
C	-3.91909900	3.01884700	-0.21404200	H	3.44371300	3.65601800	2.11970100
C	-4.39188800	3.54149900	-1.42773000	C	3.28271600	4.69970600	-1.11097700
H	-3.89788400	3.27247400	-2.35138400	H	2.81657600	4.44311700	-2.05245600
C	-5.49063400	4.39902100	-1.45174300	C	3.02391200	3.91496000	0.02435200
H	-5.85560900	4.79936900	-2.38516600	H	8.16152000	-4.83558900	1.18121300
C	-6.13259300	4.74864200	-0.25454900	H	6.45885900	8.71119000	-0.73907700
C	-5.66387400	4.23030800	0.96193200	H	-8.42921200	6.70327100	-1.41286200
H	-6.16693600	4.50999700	1.87659800	H	-6.60679800	-6.60547200	1.76934300
C	-4.56687100	3.37270200	0.98045300	Fe	0.00548200	-0.00490500	0.04516600
H	-4.20513700	2.97430600	1.91824200	Cl	-0.04016000	-0.04362700	2.28468000

Coordinates of optimized structure of MnTCPP:

O	-6.94277400	-7.06646800	0.97484800	C	-6.28782200	-6.75292000	-0.02515300
N	0.09105000	-2.01632400	-0.04396500	O	7.37767700	-6.59637700	-1.20168100
O	-7.23169100	6.81985400	0.93829400	O	-7.39040100	6.46478200	-1.31218100
C	-5.33565400	4.61762400	-1.29695500	C	-6.82882300	6.23116100	-0.07094500
H	-5.82987000	4.87293100	-2.22187900	O	7.08462600	6.90625800	-1.20846800
C	-2.53006700	2.35800200	-0.06164800	C	6.31004100	6.78270500	-0.26555300
C	-5.09692800	4.91176000	1.09835600	C	-2.74876700	-1.22948500	-0.20793400
H	-5.42146400	5.39384700	2.00939400	C	-4.12837800	-0.85385900	-0.31781100
O	-6.46165700	-7.40419200	-1.23196900	H	-4.95028000	-1.54382700	-0.37540200
N	-0.08661000	2.03594200	0.09736600	C	-4.18563400	0.50840400	-0.30350000
N	1.94131500	0.09291800	-0.19891700	H	-5.06393100	1.12642600	-0.33768600
N	-1.93887700	-0.07687900	-0.17009600	C	-2.84067800	1.00109300	-0.20066400
O	6.38983700	7.67951200	0.79163500	C	-1.23349600	2.83348300	0.08250900
C	-5.73985900	5.23716900	-0.10513600	C	0.98540300	2.93031100	0.06308500
C	2.74368200	1.24596400	-0.24786900	C	2.31592800	2.56938300	-0.10212100
O	7.30643700	-6.72751300	1.04761700	C	2.84854200	-0.98414100	-0.24746100
C	6.85473100	-6.21314000	-0.16049700	C	4.18753400	-0.48873400	-0.38623800
C	5.74647700	-5.22041800	-0.10429200	H	5.06614700	-1.10281400	-0.46353200
C	5.00152100	-5.00099800	-1.27213500	C	4.12473500	0.87334200	-0.37700900
H	5.25477200	-5.56215100	-2.16000800	H	4.94498600	1.56526900	-0.43382800
C	3.96206200	-4.07474900	-1.28210300	C	3.93126600	4.06679100	-1.34361000
H	3.38840400	-3.91787900	-2.18515400	H	3.63201200	3.58783100	-2.26572200
C	3.65415000	-3.33131900	-0.13094800	C	3.74617900	4.28950100	1.05532700
C	4.41608100	-3.53522400	1.02949900	H	3.32104700	3.96771700	1.99591100
H	4.19608200	-2.95957100	1.91775300	C	4.69830900	5.30814000	1.03424800
C	5.45070900	-4.46997600	1.04410600	H	5.01578300	5.74015300	1.97520500
H	6.04108200	-4.57536300	1.94583700	C	5.26984200	5.72109000	-0.17913200
C	2.53244800	-2.33460400	-0.13607400	C	0.49484800	4.28998800	0.09243500
C	1.22754200	-2.80819300	-0.02649000	H	1.11433900	5.16811200	0.06977100
C	0.86644600	-4.20962400	0.05849000	C	-0.86277700	4.23079900	0.10371100
H	1.56345000	-5.02669200	0.10167400	H	-1.55687900	5.05135900	0.09288700
C	-0.48990900	-4.26887800	0.06387500	C	4.88656300	5.07917300	-1.36592500
H	-1.11444500	-5.14229900	0.11258100	H	5.34775100	5.38792900	-2.29291700
C	-0.97211200	-2.90448500	-0.01603600	C	3.34620200	3.65937600	-0.13302200
C	-2.31461000	-2.54780000	-0.10978100	C	-4.06273300	3.97983700	1.11007300
C	-3.34484700	-3.63947200	-0.10275400	H	-3.57347900	3.72597000	2.04024300
C	-3.61564300	-4.37499000	-1.26762900	C	-4.30073300	3.68441500	-1.27990800
H	-3.07856200	-4.14558000	-2.17778100	H	-3.98587700	3.21260100	-2.20062000
C	-4.57053300	-5.39044600	-1.26192600	C	-3.65145200	3.35413800	-0.07903100
H	-4.77992700	-5.95269400	-2.15912800	H	5.64570400	7.61655800	1.41584100
C	-5.26943100	-5.68752100	-0.08273500	H	-8.10295900	7.12739100	-1.23630100
C	-5.00189000	-4.95817400	1.08530100	H	-7.14257900	-8.09751900	-1.14144200
H	-5.54550700	-5.20075400	1.98714500	H	6.73943400	-6.50178500	1.80586700
C	-4.04904900	-3.94307600	1.07430000	Mn	0.00193000	0.06202900	0.23582200
H	-3.84109800	-3.38524200	1.97676400	Cl	0.04273800	-0.35797900	2.43892600

Coordinates of optimized structure of NiTCPP:

O	6.77591800	7.10307800	1.28331600	H	3.41448400	4.36250600	-0.98593500
N	1.92314000	-0.00701600	-0.01092000	C	6.36243900	6.24867600	2.03027700
O	-6.24319200	6.89620500	-3.18625300	O	6.59990500	-7.26649000	-1.29006500
C	-5.30774600	4.77261600	-0.37528900	O	-7.13682200	6.69794200	-1.13750400
H	-6.05950300	5.09941900	0.33226000	C	-6.23496900	6.37534900	-2.09656400
C	-2.38703300	2.34224800	-0.53484900	O	-6.60940600	-6.53318700	3.22177200
C	-4.28889600	4.91894700	-2.56088700	C	-6.41850400	-6.26325800	2.06820500
H	-4.26892500	5.36252900	-3.54944700	C	1.02736500	2.75946100	0.32409700
O	6.81349700	6.12457600	3.30229900	C	0.59516400	4.13222600	0.29293800
N	-1.94929700	-0.01960700	0.00125300	H	1.20746800	4.98334300	0.54598200
N	-0.00314300	-1.95672300	0.00864300	C	-0.69209300	4.12936600	-0.13093200
N	-0.01517000	1.92199900	-0.01064400	H	-1.34306300	4.97635800	-0.28172200
O	-7.15795800	-6.86193300	1.09592700	C	-1.07661600	2.75128900	-0.29099000
C	-5.26835300	5.33625400	-1.65481000	C	-2.78678400	1.02369700	-0.33138900
C	-1.05134000	-2.79390600	0.32248200	C	-2.77851800	-1.08165300	0.27979300
O	7.13305700	-6.09026800	-3.09572100	C	-2.36999500	-2.39216600	0.52047900
C	6.40321800	-6.29471300	-1.96615200	C	1.05748100	-2.78807800	-0.27708000
C	5.37170200	-5.25566700	-1.63845400	C	0.66075900	-4.16642400	-0.15422400
C	4.91107400	-5.18862500	-0.31955100	H	1.29892100	-5.01678100	-0.33697100
H	5.32596900	-5.87410400	0.40999000	C	-0.62724500	-4.16882900	0.26737200
C	3.94627600	-4.25836700	0.04388200	H	-1.24656600	-5.02178100	0.49620000
H	3.61154800	-4.20184000	1.07406300	C	-3.94862000	-3.41511700	2.18352200
C	3.39891000	-3.38416300	-0.90515500	H	-3.59909100	-2.69153600	2.91206500

C	3.84653500	-3.46793300	-2.22778500	C	-3.86194700	-4.35241500	-0.03187400
H	3.41818400	-2.81197000	-2.97782900	H	-3.44857600	-4.36241500	-1.03446000
C	4.82150500	-4.39189600	-2.59167000	C	-4.84107600	-5.27565900	0.32135400
H	5.10744800	-4.45581100	-3.63795300	H	-5.14099100	-6.01674000	-0.41453300
C	2.36306500	-2.37331400	-0.52717000	C	-5.38460200	-5.27665500	1.61093600
C	2.75915500	-1.05239400	-0.33217700	C	-4.15668000	-0.69650900	0.12156900
C	4.13485700	-0.63433900	-0.25989900	H	-5.00422700	-1.34659800	0.27363200
H	4.98663400	-1.26254800	-0.46979700	C	-4.15968400	0.59104500	-0.30106600
C	4.13215100	0.65419000	0.16051900	H	-5.01081700	1.20354600	-0.55329500
H	4.98023900	1.29639800	0.34019200	C	-4.91434800	-4.34620500	2.54275800
C	2.75359900	1.04906600	0.28863400	H	-5.31802500	-4.36970600	3.54807600
C	2.34500200	2.35890000	0.53271600	C	-3.40532500	-3.40515800	0.89176300
C	3.37512500	3.36907400	0.92377800	C	-3.36301800	3.95116000	-2.19365700
C	3.92725100	3.34384500	2.21079700	H	-2.60686600	3.62971900	-2.90174100
H	3.58892500	2.59569000	2.91956600	C	-4.38069400	3.80182400	-0.01343200
C	4.89377200	4.26865100	2.59037600	H	-4.40724700	3.37677100	0.98405300
H	5.30953100	4.24419700	3.58987900	C	-3.39806600	3.37478000	-0.91652400
C	5.33120500	5.23682800	1.68115300	H	-7.01066300	-6.43898300	0.24094200
C	4.78998800	5.26531400	0.39207000	H	-7.71583600	7.37591400	-1.51643400
H	5.14275900	6.01540800	-0.30607600	H	7.47398300	6.82115600	3.43289000
C	3.82239400	4.34190900	0.01882700	H	6.98337200	-5.20413100	-3.44779500
				Ni	-0.01160100	-0.01562900	-0.00309300

Coordinates of optimized structure of ZnTCPP:

O	-6.33059500	7.60335900	1.09177600	H	-2.92489000	4.22872300	2.08002800
N	-2.04295400	0.12197000	-0.03578900	C	-6.11674500	6.92837200	0.11315300
O	7.64000700	6.30868100	1.01456700	O	-7.40720900	-6.55271200	-1.05976100
C	5.06237900	4.92378900	-1.15931300	O	7.14440000	6.74171100	-1.13057100
H	5.29189100	5.48058100	-2.05925200	C	6.95094600	6.09612800	0.04547900
C	2.59014100	2.28283600	0.00949500	O	6.03025600	-7.84745200	-0.95568700
C	5.52869700	4.40114000	1.15264800	C	6.11132000	-6.97310600	-0.13765500
H	6.12388400	4.57090600	2.04226200	C	-0.92198200	2.92459700	0.01147100
O	-6.76683300	7.13348400	-1.05851100	C	-0.41388000	4.27687200	0.01098400
N	2.04568800	-0.13144100	0.03645600	H	-1.01539300	5.17250400	0.00522500
N	-0.12540200	-2.04942100	-0.00736800	C	0.94141200	4.19306900	0.01633800
N	0.12809700	2.03988500	0.00630900	H	1.64807300	5.00828800	0.02852500
O	7.10875800	-6.99411100	0.78721500	C	1.27928400	2.78844800	0.00678200
C	5.82474900	5.12776400	-0.00465500	C	2.92958000	0.91938000	0.01150100
C	0.92499600	-2.93395400	-0.01865700	C	2.79374900	-1.28207400	0.00081200
O	-7.49945700	-6.50815900	1.15773400	C	2.28818100	-2.59302100	-0.01338400
C	-6.96937100	-6.11475100	-0.03173200	C	-1.27672100	-2.79789600	-0.00854300
C	-5.83933900	-5.13007200	0.03192500	C	-0.93847600	-4.20244100	-0.02670800
C	-5.54741800	-4.39768200	-1.12312500	H	-1.64360300	-5.01887900	-0.04576100
H	-6.14811100	-4.56633800	-2.00908400	C	0.41686200	-4.28623200	-0.02426300
C	-4.50703300	-3.47814100	-1.13108900	H	1.01683300	-5.18295800	-0.02562100
H	-4.29512500	-2.91201800	-2.03171900	C	3.48201100	-4.48107700	-1.18755300
C	-3.71199800	-3.28070100	0.00649500	H	2.91451800	-4.25072700	-2.08277600
C	-3.99075200	-4.03489800	1.15210000	C	4.02275600	-4.02896200	1.11319900
H	-3.37835200	-3.90504300	2.03774700	H	3.86126100	-3.46348700	2.02451600
C	-5.04197400	-4.94624600	1.16703500	C	4.94796000	-5.06809000	1.09961700
H	-5.19984100	-5.53678200	2.06544000	H	5.46761500	-5.30895200	2.02314500
C	-2.58737600	-2.29154700	-0.00521700	C	5.15325200	-5.82120700	-0.06183700
C	-2.92727200	-0.92772700	-0.00740500	C	4.19714500	-0.94329600	-0.05482100
C	-4.27812200	-0.41903600	0.05322100	H	5.01152000	-1.64886400	-0.11134000
H	-5.17313900	-1.01945800	0.10376000	C	4.28069300	0.41207100	-0.04796700
C	-4.19389600	0.93623400	0.05546100	H	5.17438500	1.01464000	-0.09656600
H	-5.00728400	1.64319600	0.10800400	C	4.39748900	-5.52512100	-1.20062100
C	-2.79046900	1.27367300	-0.00259800	H	4.54440000	-6.12518300	-2.09088600
C	-2.28541100	2.58458100	0.00725800	C	3.28077400	-3.71483700	-0.03108400
C	-3.27828800	3.70660200	0.02188200	C	4.48668400	3.48311700	1.15480800
C	-4.01852500	4.01904500	-1.12549900	H	4.25884100	2.92628600	2.05739100
H	-3.86181400	3.44403800	-2.03183200	C	4.01762700	4.00620500	-1.15043300
C	-4.94093200	5.05953700	-1.11836500	H	3.43219900	3.84752000	-2.04971300
H	-5.50326200	5.29641600	-2.01293000	C	3.71454100	3.27306300	0.00405300
C	-5.14296600	5.80773600	0.04581500	H	7.14578900	-6.16027100	1.27186100
C	-4.40972800	5.50181900	1.19641600	H	7.89219100	7.34315600	-0.99815100
H	-4.57817400	6.08590400	2.09360300	H	-7.37195800	7.87616600	-0.91462500
C	-3.48676400	4.46421900	1.18256200	H	-7.16394200	-5.96477700	1.88138800
				Zn	0.00140500	-0.00430100	-0.00073000

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