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Environment-friendly, co-catalyst and solvent-free fixation of CO_2 using an ionic Zinc(II)-porphyrin complex immobilized in porous metal-organic framework

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Table S2. Comparison of the catalytic activity of $[Zn(II)NMeTPyP]^{4+}[I^-]_4$@PCN-224 with reported MOF catalyst known for co-catalyst-free cycloaddition of CO_2 with epoxides.

Table S3. Optimized coordinates for structure of $[Zn(II)NMeTPyP]^{4+}[I^-]_4$@PCN-224.

Experimental section

(a) Materials

All reagents and solvents were purchased from commercial sources and used without further purification. $ZrCl_4$ (98 %), $Zn(OAc)_2.6H_2O$, and pyrrole (98 %) were obtained from Sigma-Aldrich Chemicals. Methyl iodide (98 %) and propionic acid (99 %) were received from TCI Chemicals. $[Zn(II)NMeTPyP]^{4+}[I^-]_4$ and H_4TCPP ligands was prepared by following the previously reported literature procedure with modification and characterized by ^1H NMR, UV-Vis. and FTIR spectroscopy.[1] PCN-224 is synthesized based on the reported procedure and the phase purity of the compound was identified by PXRD analysis, UV-Vis and FTIR spectroscopy. [2]

(b) Physical measurements

Powder X-ray powder diffraction (PXRD) patterns were collected on a PANalytical X'PERT PRO diffractometer using Cu Kα radiation (λ =1.542 Å; 40 kV, 20 mA). Elemental analysis (C, H, and N) of the compounds were collected on a Thermo Fischer Flash 2000 elemental analyzer. Fourier transform infrared spectra were recorded on KBr pellets using Bruker IFS66 v/S spectrophotometer. Thermogravimetric analysis (TGA) of MOF1 was recorded in the temperature range of RT−600 °C at a heating rate of 10 °C min^{-1}on a Mettler Toledo thermogravimetric analyzer under N_2 atmosphere with a flow rate of 30 $mLmin^{-1}$. The products of the catalytic reactions were analyzed by ^1H NMR spectra recorded in $CDCl_3$ on a JEOL JNM-ECS-400 spectrometer at 400 MHz.

(c) **Adsorption measurements**

N_2 adsorption measurements of PCN-224 and $[Zn(II)NMeTPyP]^{4+}[I^-]_4$@PCN-224 were carried out at 77K, whereas CO_2 adsorption measurements were conducted at 273 and 298K on Quadrasorb-SI automatic volumetric instrument. Ultrapure (99.995%) N_2, and CO_2 gases were utilized for carrying out the adsorption measurements. Prior to adsorption measurements, the $[Zn(II)NMeTPyP]^{4+}[I^-]_4$@PCN sample (~ 0.1 g) was degassed at 393K under vacuum (18 mTorr) for 16 hours, then the activated sample was connected to the surface area analyzer and the operations were computer controlled. The temperature 77 K was achieved using liquid nitrogen, while 273 and 298K by using water/ethylene glycol (1:1) and the dead volume of the sample cell was determined using Helium gas (99.995%).

(d) **Analysis of gas adsorption isotherms**

Clausius-Clapeyron Equation[3] was used to calculate the enthalpies of CO_2 adsorption. By using Langmuir Freundlich equation[4] an accurate fit was retrieved which gives a precise prediction of hydrogen adsorbed at saturation. A modification of Clausius-Clapeyron equation is used for calculations.

$$\ln\left[\frac{P_1}{P_2}\right] = \Delta H_{ads} \times \left[\frac{T_2 - T_1}{R \times T_2 T_1}\right] \quad \text{------(i)}$$

where, P_1 and P_2 = pressures for isotherm at 273K and 298K respectively.

T_1 and T_2 = temperatures for isotherm at 273K and 298K respectively.

ΔH_{ads} = Enthalpy of adsorption.

R = Universal gas constant = 8.314 J/K/mol.

Pressure is a function of amount of gas adsorbed which was determined by using the Langmuir-Freundlich fit.

$$\frac{Q}{Q_m} = \frac{B \times P^{(1/t)}}{1 + (B \times P^{(1/t)})} \qquad \text{------(ii)}$$

where, Q = moles of gas adsorbed.

Q_m = moles of gas adsorbed at saturation.

B and t = constants.

P = Pressure.

By rearranging equation (ii) we get equation (iii)

$$P = \left[\frac{Q/Q_m}{B - (B \times Q/Q_m)}\right]^t \qquad \text{------(iii)}$$

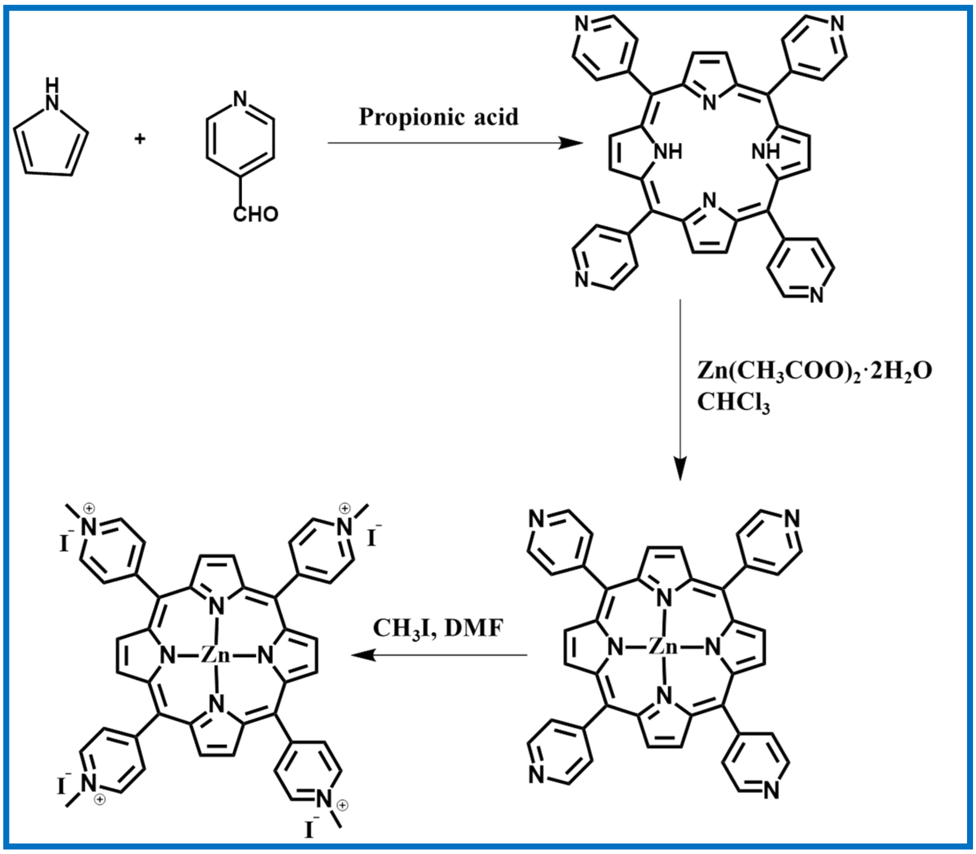
Substituting equation (iii) into equation (i) we get

$$\Delta H_{ads} = \frac{R \times T_1 \times T_2}{T_2 - T_1} \ln \frac{\left[\frac{Q/Q_{m1}}{B - (B \times Q/Q_{m1})}\right]^{t1}}{\left[\frac{Q/Q_{m2}}{B - (B \times Q/Q_{m2})}\right]^{t2}} \qquad \text{------(iv)}$$

In equation (iv), subscript 1 and 2 are representing data corresponding to 273K and 298K in case of carbon dioxide gas.

randomly inside the pores of PCN-224 and then the geometry optimization was carried out.

(e) Synthesis and characterization



Synthesis of Tetrakis(4-pyridyl)porphyrin: In a 250-mL round bottom flask 4-pyridinecarboxaldehyde (5.63 g, 50 mmol) was dissolved in propionic acid (100 mL). Pyrrole was then added dropwise (3.36 g, 50 mmol) and the solution was refluxed at 140 °C for 12h. After the reaction mixture the solvent was removed under reduced pressure and precipitated in DMF at low temerature. The precipitate was filtered and washed with diethyl ether and dried under vacuum to yield purple solid. ^{1}H-NMR (400 MHz, DMSO-d6,) δ 8.94 (d, 8H, δ 8.83 (s, 8H,), δ 8.07 (d, 8H,), -2.83 (s, 2H).

Synthesis of 5, 10, 15, 20-tetrakis (4'-pyridyl) Zn(II) porphyrin, [Zn(II)TPyP]. In a 250-mL round bottom flask TPyP (100 mg, 0.16 mmol) and 1 ml solution of $Zn(CH_3COO)_2·2H_2O$ (88 mg, 0.40 mmol) in methanol were added in 60 mL chloroform and the mixture was stirred for 20 hours at room temperature. The resulting violet product is precipitated by adding methanol to the concentrated reaction mixture, filtered, washed thoroughly with methanol and dried under vacuum. UV-Vis. (λ) 427 (Soret band), 560 nm, 599 nm (Q bands). ^{1}H-NMR (400 MHz, DMSO-d_6,) δ 8.94 (d, 8H, δ 8.83 (s, 8H,), δ 8.07 (d, 8H,).

Synthesis of 5, 10, 15, 20-tetrakis (1-methylpyridinium-4'-yl) Zn(II) porphyrin, $[Zn(II)NMeTPyP]^{4+}[I^-]_4$.

In a 100-mL round bottom flask Zn(II)TPyP (109 mg, 0.16 mmol) and excess of methyl iodide (0.5 mL, 8 mmol) is dissolved in 20 mL DMF and the mixture was stirred for 20 hours at 45 ^oC. After cooling down to room temperature 40 mL of diethyl ether was introduced. The resultant violet solid was filtered and washed with diethyl ether and chloroform and dried under vacuum. UV-Vis. (λ) 450 nm (Soret band), 576 nm, 624 nm (Q bands). ^{1}H NMR (400 MHz, DMSO-d6,) δ 9.43 (d, 8H), δ 9.12 (s, 8H), δ 8.93 (d, 8H), δ 4.73 (s, 12H). FTIR (KBr, cm^{-1}): 2998, 1632, 1498, 1386, 1332, 1258, 1188, 1093, 998, 860, 719, 664. ESI-MS m/z calcd. for $C_{44}H_{36}N_8Zn^{4+}$ ($[M-4I]^+$) 185.06, found 185.03.

Synthesis of 5, 10, 15, 20-Tetrakis (4-methoxycarbonylphenyl) porphyrin (TPPCOOMe)

In a 250-mL round bottom flask, methyl 4-formylbenzoate (6.9 g, 0.042 mol) was added in 100 mL of propionic acid. To this solution 0.043 mol (3.0 mL) pyrrole was added dropwise and the solution was refluxed at 140 °C for 12h. After the reaction mixture was cooled down to room temperature the solid was filtered and washed with methanol and water and dried under vacuum to obtain purple solid (1.8 g, 2.12 mmol, 20% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.82 (s, 8H), 8.43 (d, 8H), 8.29 (d, 8H), 4.10 (s, 12H), -2.83 (s, 2H).

Synthesis of [5, 10, 15, 20-Tetrakis (4-carboxyphenyl) porphyrin] (H_4TCPP)

In a 250-mL round bottom flask 0.75 g of TPPCOOMe was dissolved in 25 mL of THF and 25 mL of MeOH to which an aqueous solution of 2.63 g KOH (0.0469 mol) in 25 mL H_2O was added. This mixture was refluxed for 12h and after being cooled to room temperature the solvent was evaporated. Additional water was added and filtered and the filtrate was acidified with 1M HCl until complete precipitation of the purple solid of the ligand which was collected by filtration, washed with water and dried in vacuum desiccator.

Synthesis of PCN-224

PCN-224 was prepared based on the reported procedure. $ZrCl_4$ (120 mg,), benzoic acid (1.2 g), H_4TCPP ligand (40 mg), acetic acid (0.5 mL) were mixed in 7.5 mL of DMF and the solution was sonicated for 15 min in a 23 mL Teflon vessel. The vessel was sealed in a stainless-steel autoclave which was kept at 120 ºC for 24 h. After cooling to room temperature purple solid was centrifuged and washed with acetone and the phase purity of the compound was identified by PXRD analysis. FTIR (KBr, cm^{-1}): 3314, 1657, 1602 , 1542 , 1412 , 1269, 1180, 1020, 962, 871 , 799 , 771 , 724, 653. UV-Vis. (λ) 439 nm (Soret band), 523 nm, 560 nm, 604 nm and 659 nm (Q bands).

Synthesis of $[Zn(II)NMeTPyP]^{4+}[I^-]_4$@PCN-224

The complex@MOF hybrid was synthesized as follows: In a 100-mL round bottom flask, 30 mg of $[Zn(II)NMeTPyP]^{4+}[I^-]_4$ was dissolved in 20 mL of DMF to this solution, 70 mg of freshly activated PCN-224 was added and the mixture was stirred for 24 h at 60 °C. After cooling to room temperature the brown solid obtained was centrifuged and washed with diethyl ether and acetone. The resulting hybrid material was thoroughly characterized by PXRD, TGA, UV-vis, FT-IR, MP-AES, and SEM-EDS analysis. FT-IR (KBr, cm^{-1}): 3314, 2992, 1657, 1634, 1542, 1498, 1412, 1386, 1332, 1269, 1258, 1188, 1180, 1020, 1093, 998, 962, 871, 860, 799, 771, 724, 719, 653 (Fig. S1). UV-Vis (λ) 433 nm (Soret band), 521 nm, 554 nm, 593 nm and 650 nm (Q bands) (Fig. S2).

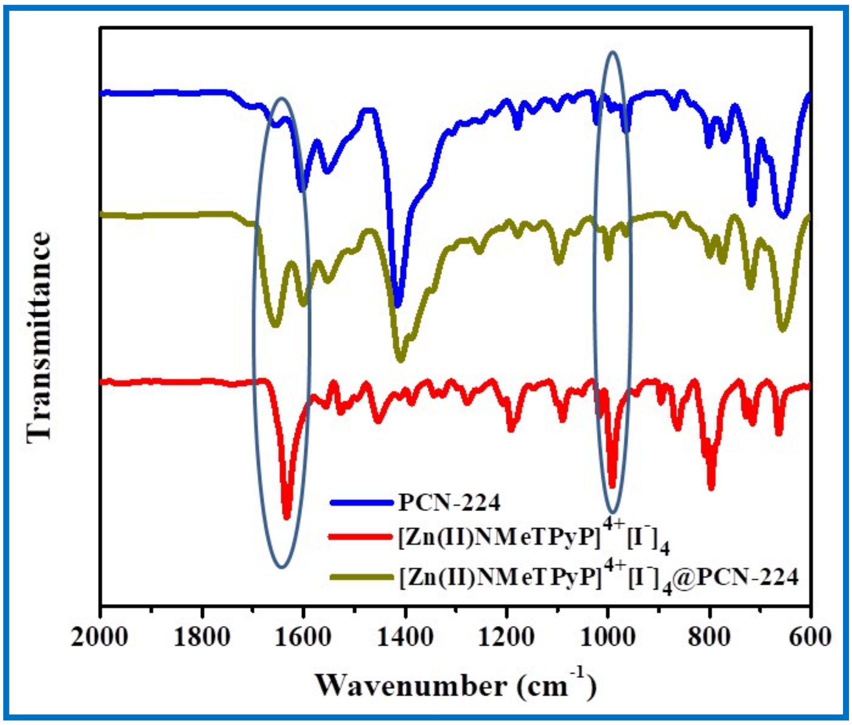


Figure S1: FTIR spectra of [Zn(II)NMeTPyP]$^{4+}$[I$^-$]$_4$, [Zn(II)NMeTPyP]$^{4+}$[I$^-$]$_4$@PCN-224 and PCN-224.

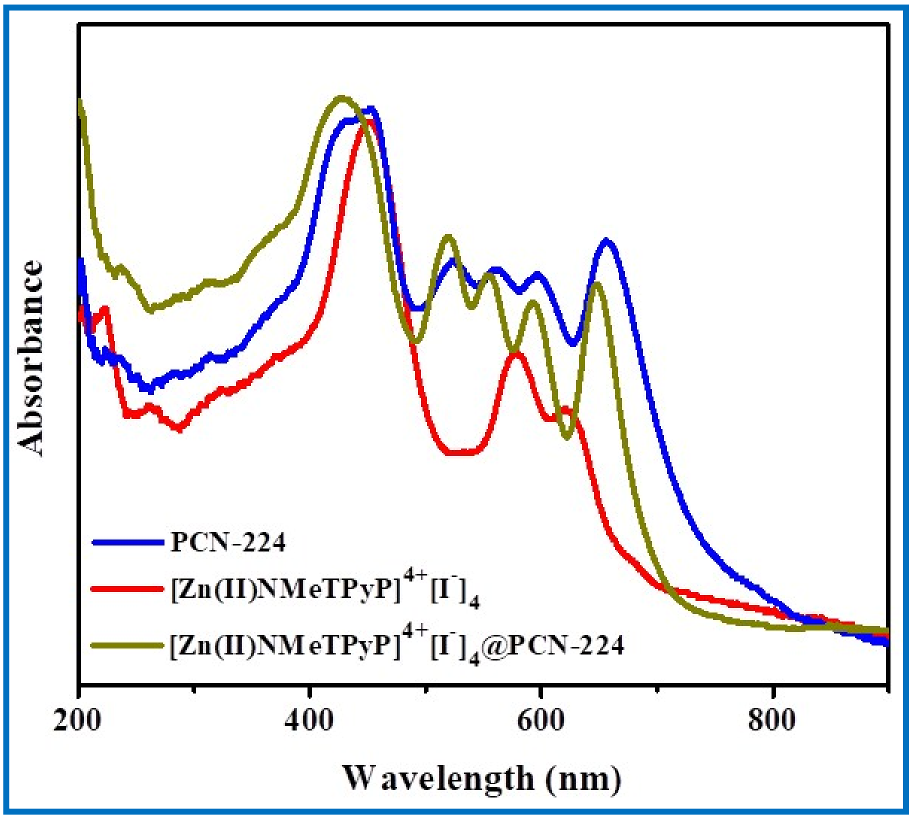


Figure S2. UV-Vis spectra of [Zn(II)NMeTPyP]$^{4+}$[I^{-}]$_4$, [Zn(II)NMeTPyP]$^{4+}$[I^{-}]$_4$@PCN-224 and PCN-224.

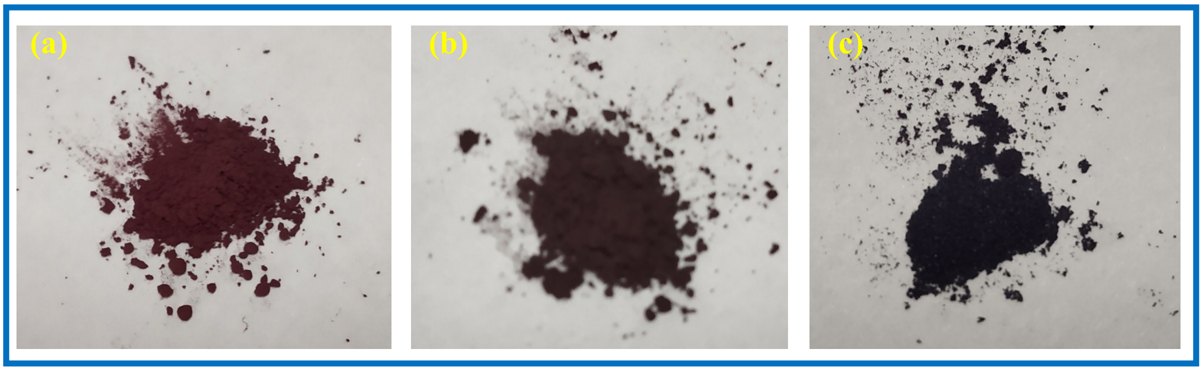


Figure S3: Physical photos of: (a) PCN-224, (b) [Zn(II)NMeTPyP]$^{4+}$[I^{-}]$_4$@PCN-224, [Zn(II)NMeTPyP]$^{4+}$[I^{-}]$_4$.

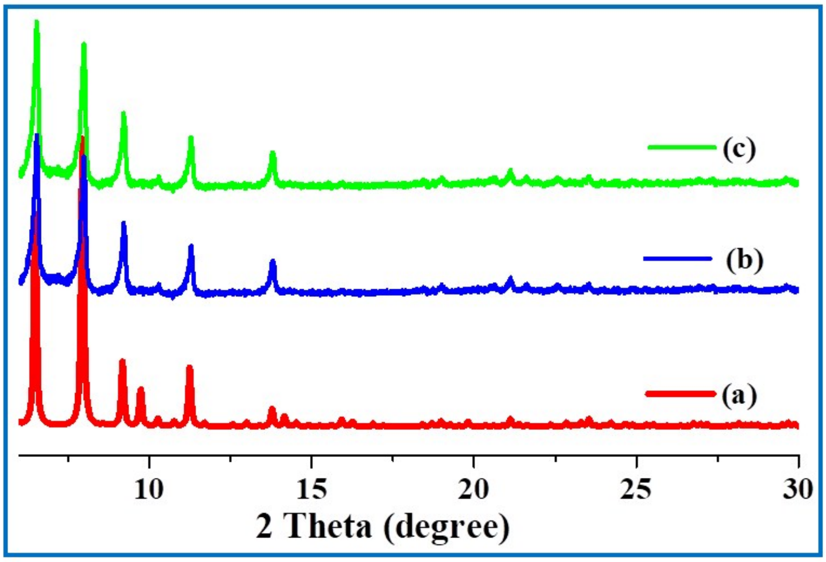


Figure S4. PXRD patterns: (a) pattern calculated from single crystal X-ray data for PCN-224; (b) as-synthesized PCN-224; (c) for $[Zn(II)NMeTPyP]^{4+}[I^{-}]_4$@PCN-224.

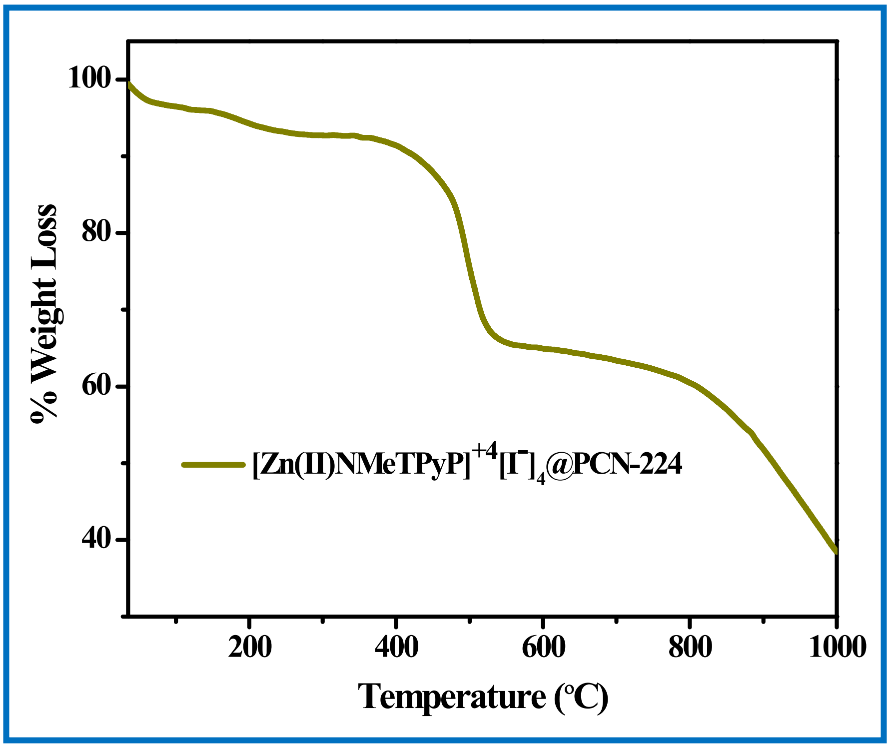


Figure S5. Thermogravimetric analysis of $[Zn(II)NMeTPyP]^{4+}[I^{-}]_4$@PCN-224.

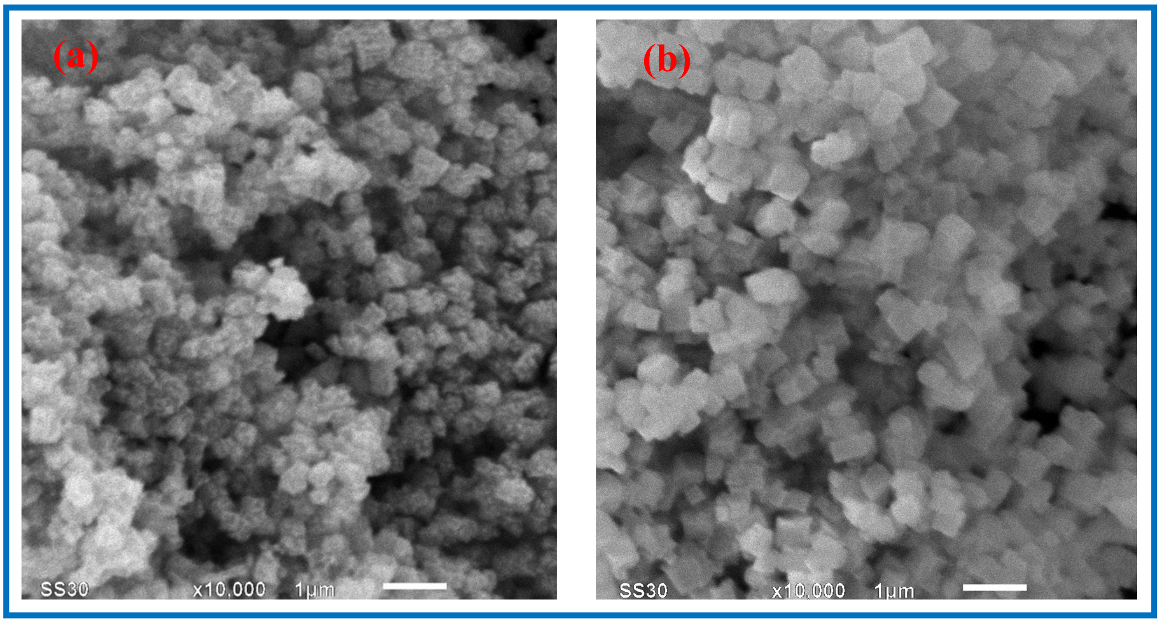


Figure S6: SEM image of: (a) PCN-224 and (b) $[Zn(II)NMeTPyP]^{4+}[I^-]_4$@PCN-224.

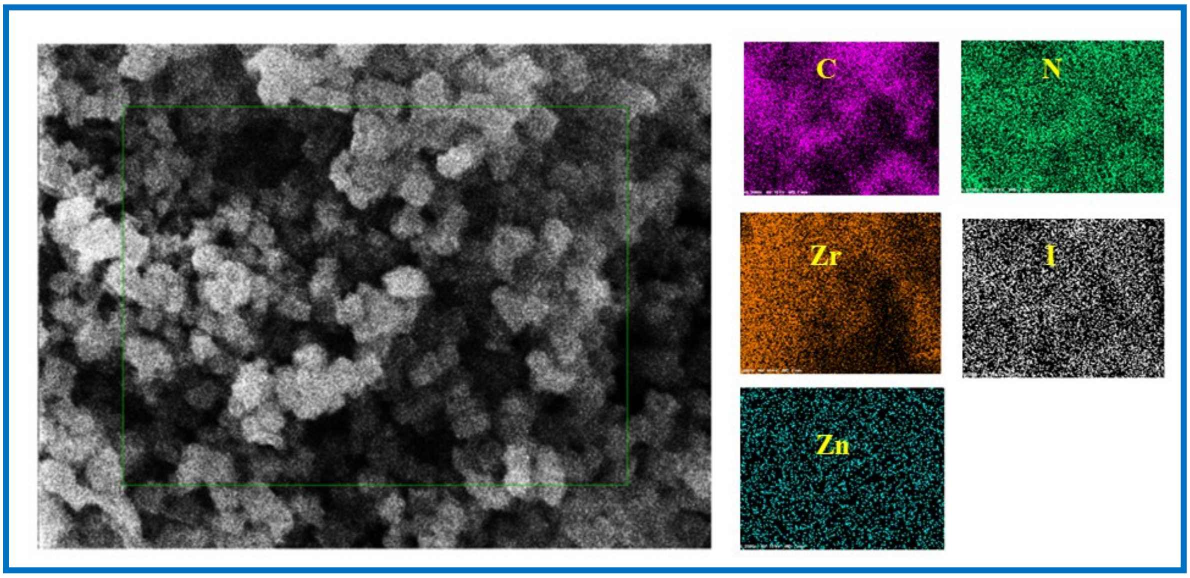


Figure S7: EDS mapping of $[Zn(II)NMeTPyP]^{4+}[I^-]_4$@PCN-224.

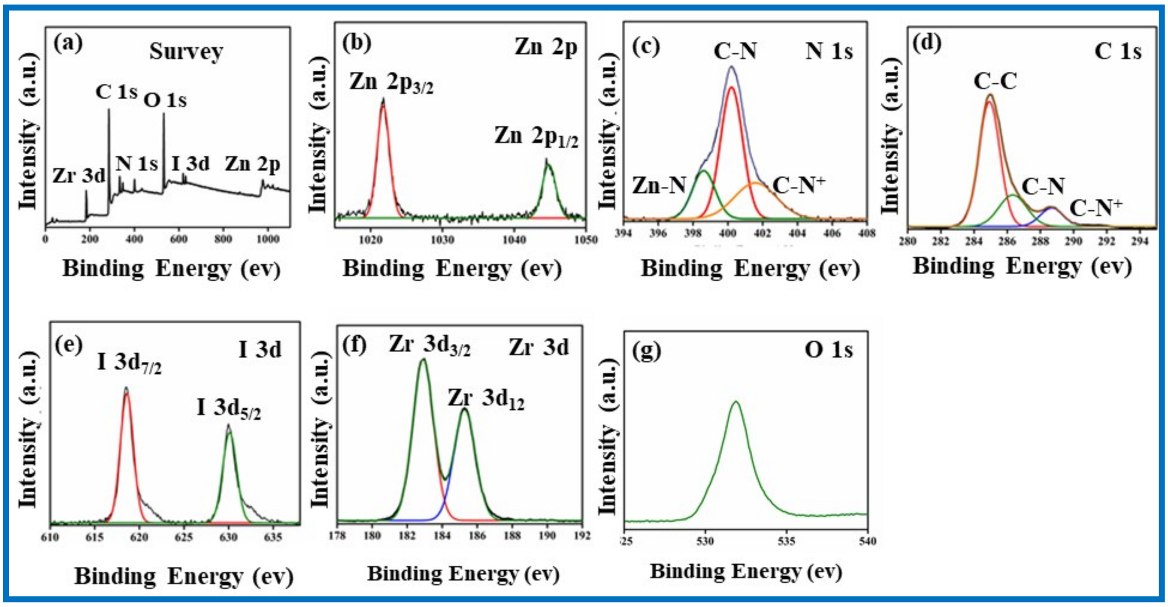


Figure S8. X-ray photoelectron spectroscopy (XPS) analysis of $[Zn(II)NMeTPyP]^{4+}[I^-]_4$@PCN-224: (a) Survey scan, (b) Zn 2p, (c) N 1s, (d) C 1s, (e) I 3d, (f) Zr 3d and (g) O 1s.

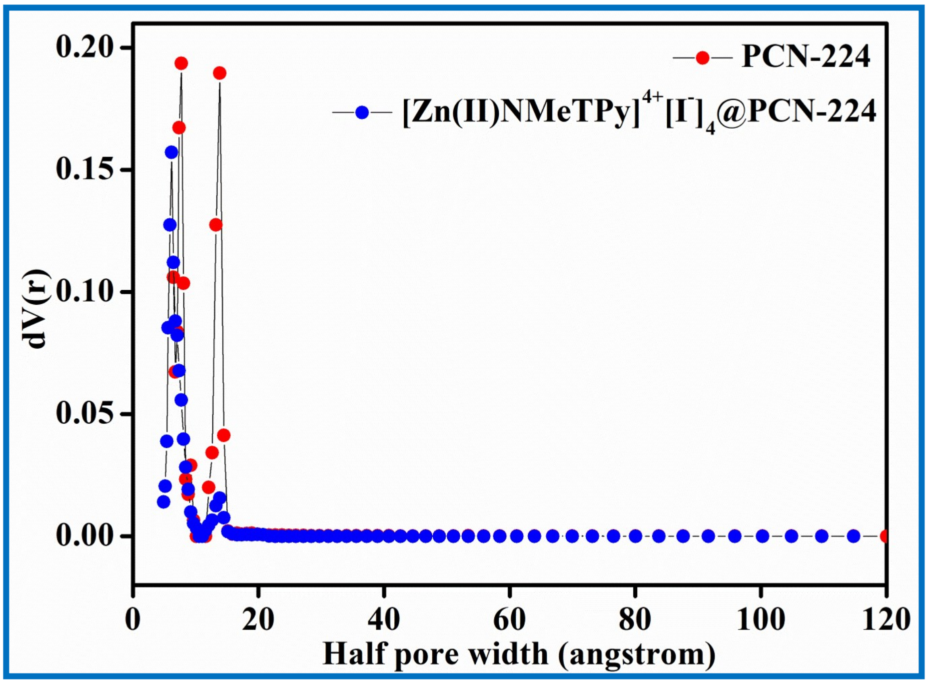


Figure S9. Pore size distribution plots estimated by using QSDFT on N_2 isotherm for $[Zn(II)NMeTPyP]^{4+}[I^-]_4$@PCN-224 and PCN-224.

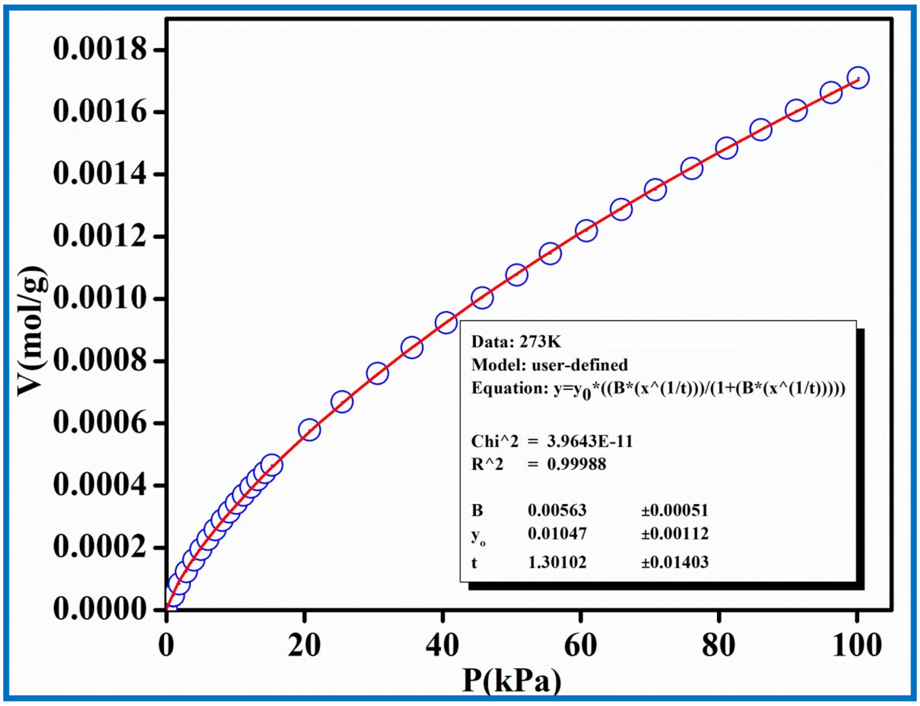


Figure S10. Carbon dioxide adsorption isotherm of **PCN-224** at 273K. The solid line shows the best fit to the data using Langmuir- Freundlich Equation.

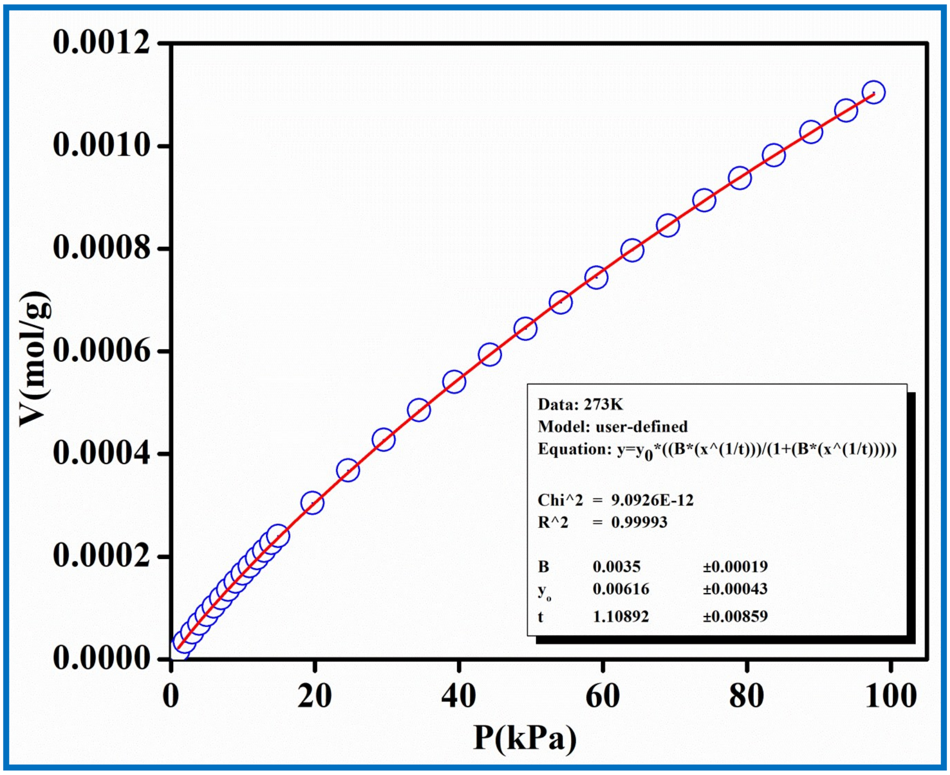


Figure S11. Carbon dioxide adsorption isotherm of **PCN-224** at 298K. The solid line shows the best fit to the data using Langmuir-Freundlich Equation.

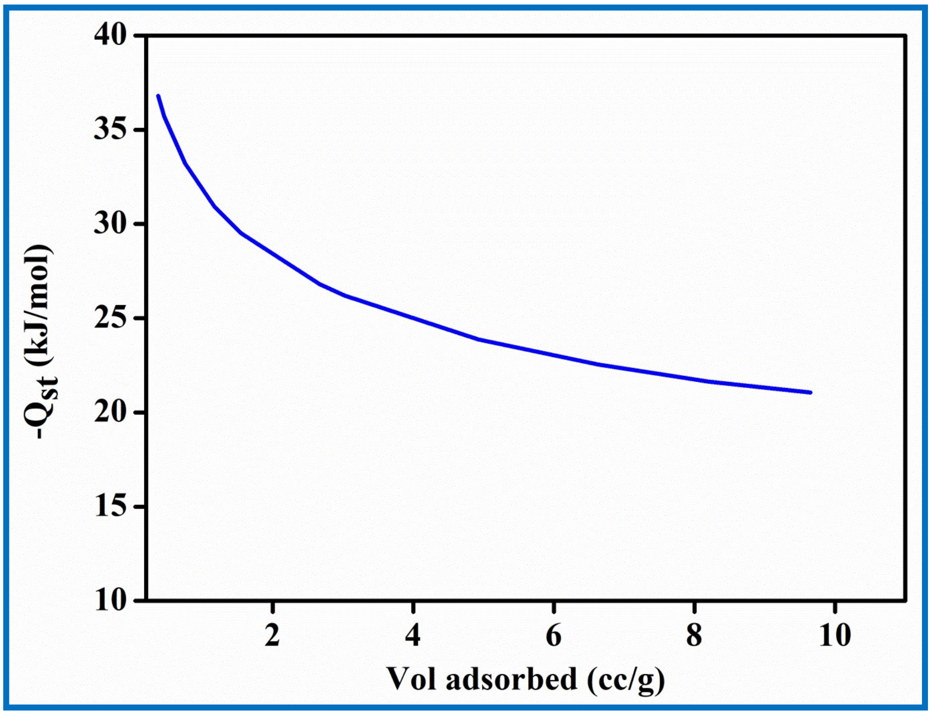


Figure S12. Enthalpy of carbon dioxide adsorption for **PCN-224** calculated using Clausius-Clapeyron equation.

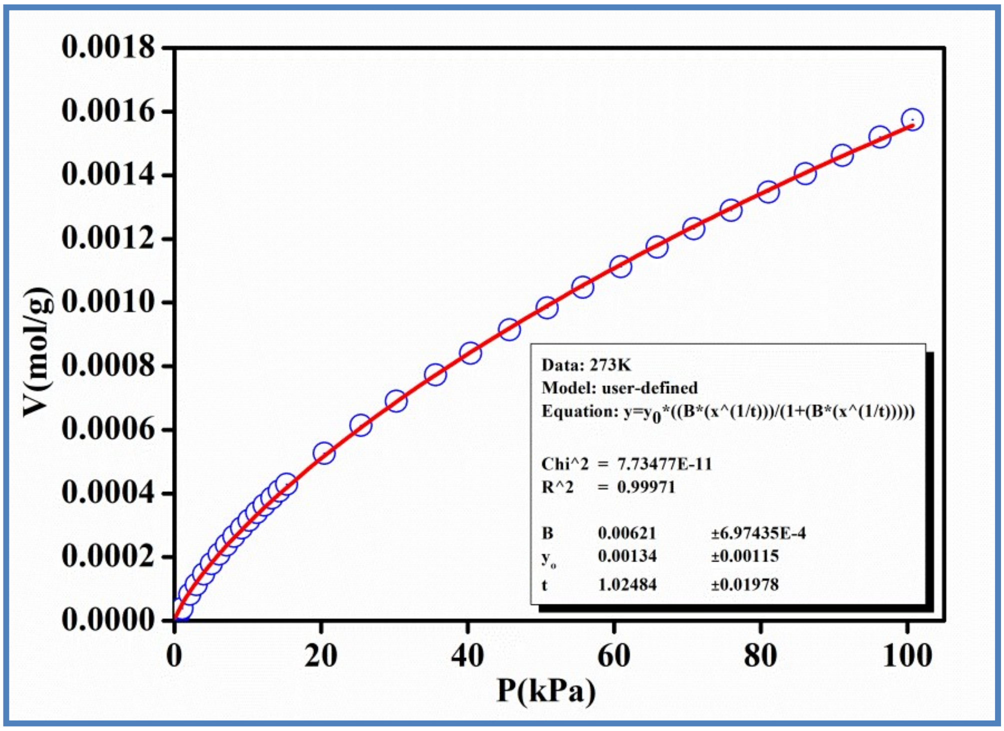


Figure S13. Carbon dioxide adsorption isotherm of $[Zn(II)NMeTPyP]^{4+}[I^-]_4$@PCN-224 at 273K. The solid line shows the best fit to the data using Langmuir-Freundlich Equation.

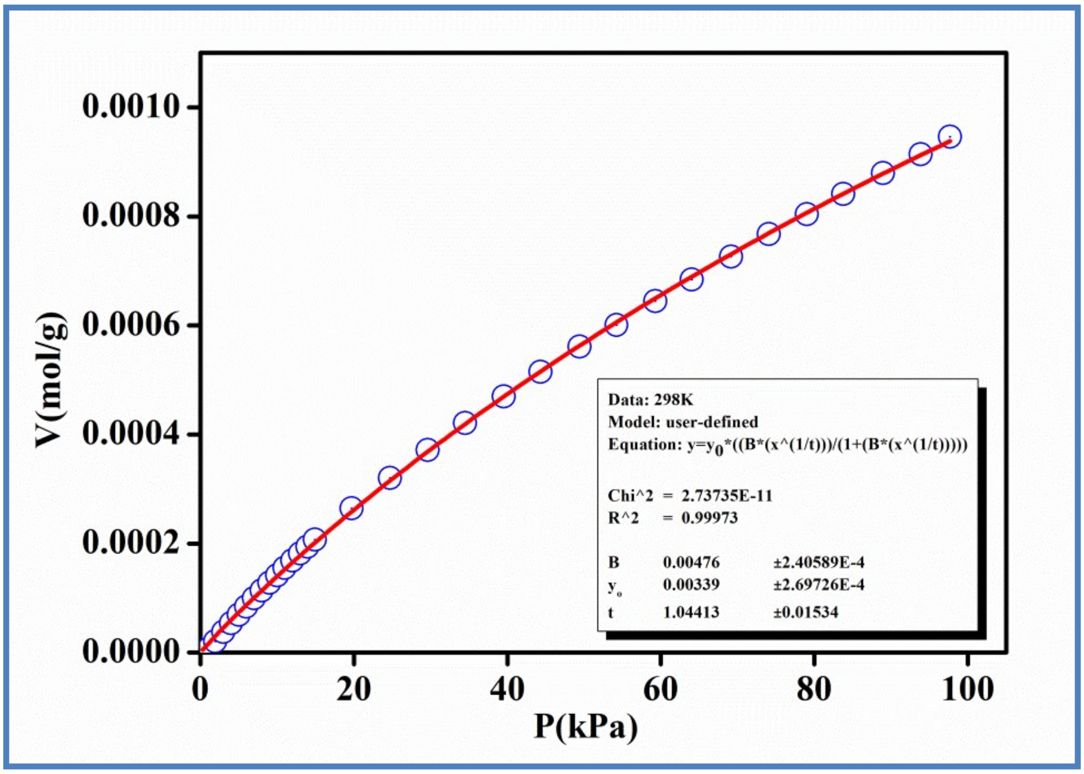


Figure S14. Carbon dioxide adsorption isotherm of $[Zn(II)NMeTPyP]^{4+}[I^-]_4$@PCN-224 at 298K. The solid line shows the best fit to the data using Langmuir-Freundlich Equation.

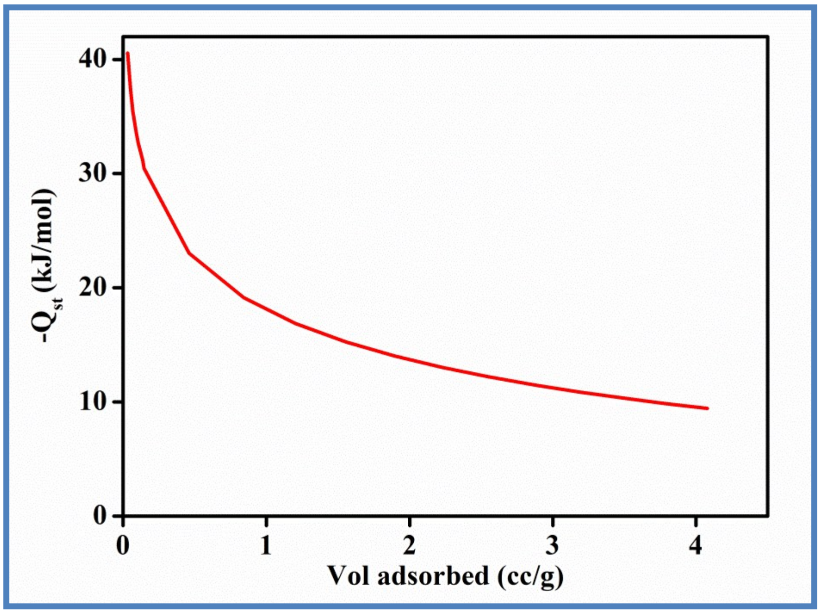


Figure S15. Enthalpy of carbon dioxide adsorption for $[Zn(II)NMeTPyP]^{4+}[I^-]_4$@PCN-224 calculated using Clausius-Clapeyron equation.

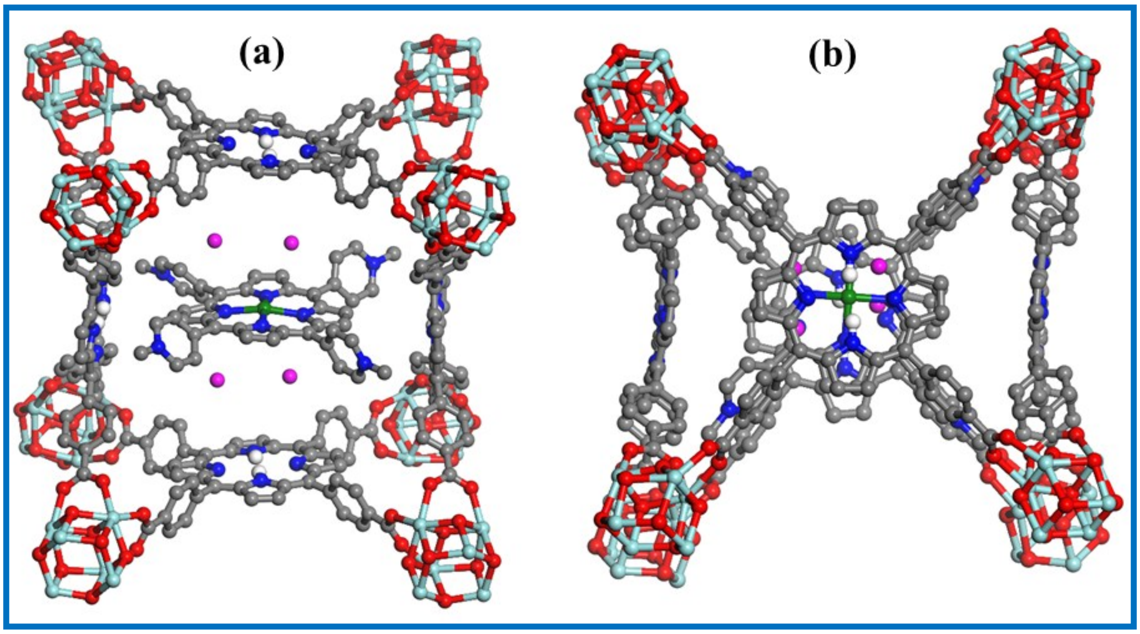
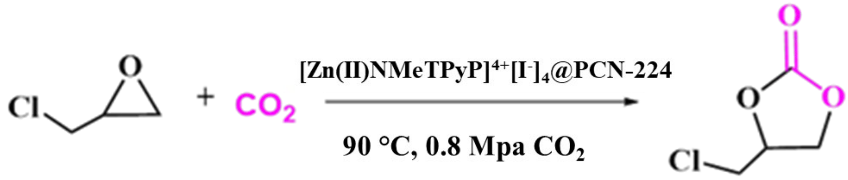


Figure S16. (a) Optimized geometry of $[Zn(II)NMeTPyP]^{4+}[I^-]_4$@PCN-224 (b) View of stacking of porphyrin macrocyclic rings via π-π interactions between the porphyrin rings of PCN-224 and the $[Zn(II)NMeTPyP]^{4+}[I^-]_4$ complex.

Table S1. Optimization of reaction parameters for cycloaddition of CO_2 with ECH.



S. N.	Catalyst	CO_2 pressure (MPa)	Temperature (°C)	Time (h)	Conversion (%)
1	None	None	None	24	0
2	None	None	90	24	0
3	None	0.8	90	24	0
4	[(a)] $[Zn(II)NMeTPyP]^{4+}[I^-]_4$@PCN-224	0.8	90	24	>99
5	$[Zn(II)NMeTPyP]^{4+}[I^-]_4$@PCN-224	None	90	24	0
6	[(b)] PCN-224	0.8	90	24	10
7	PCN-224	None	90	24	0
8	[(c)] $[Zn(II)NMeTPyP]^{4+}[I^-]_4$	0.8	90	24	55.2

Reaction conditions: ECH (10 mmol), catalyst: (a) 50 mg (0.012 mmol) (b) 47.54 mg (c) 2.46 mg.

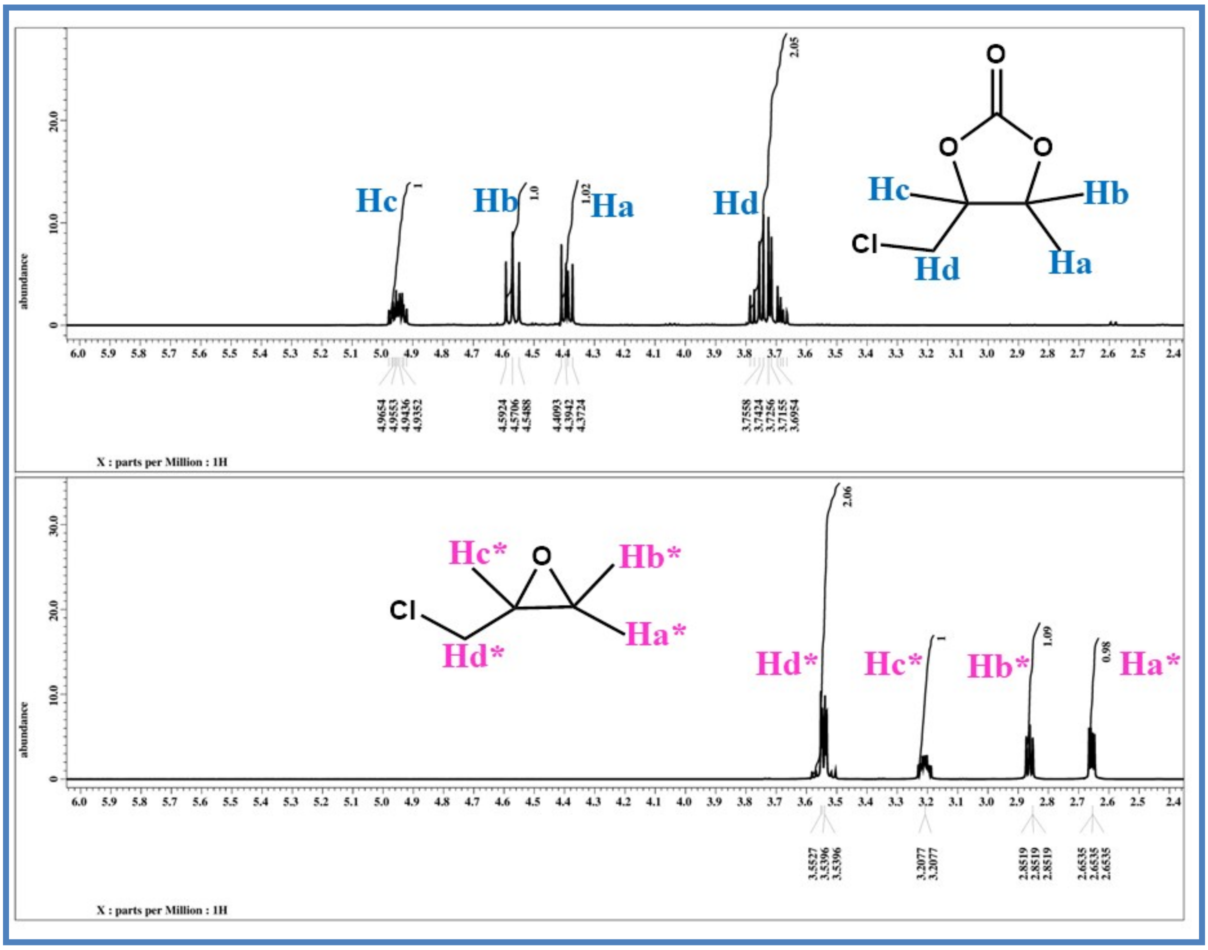


Figure S17. ^1H NMR ($CDCl_3$, 400 MHz) spectra for the cycloaddition reaction of CO_2 with epichlorohydrin catalysed by $[Zn(II)NMeTPyP]^{4+}[I^-]_4$@PCN-224 at 0.8 MPa of CO_2 and 90 ^oC.

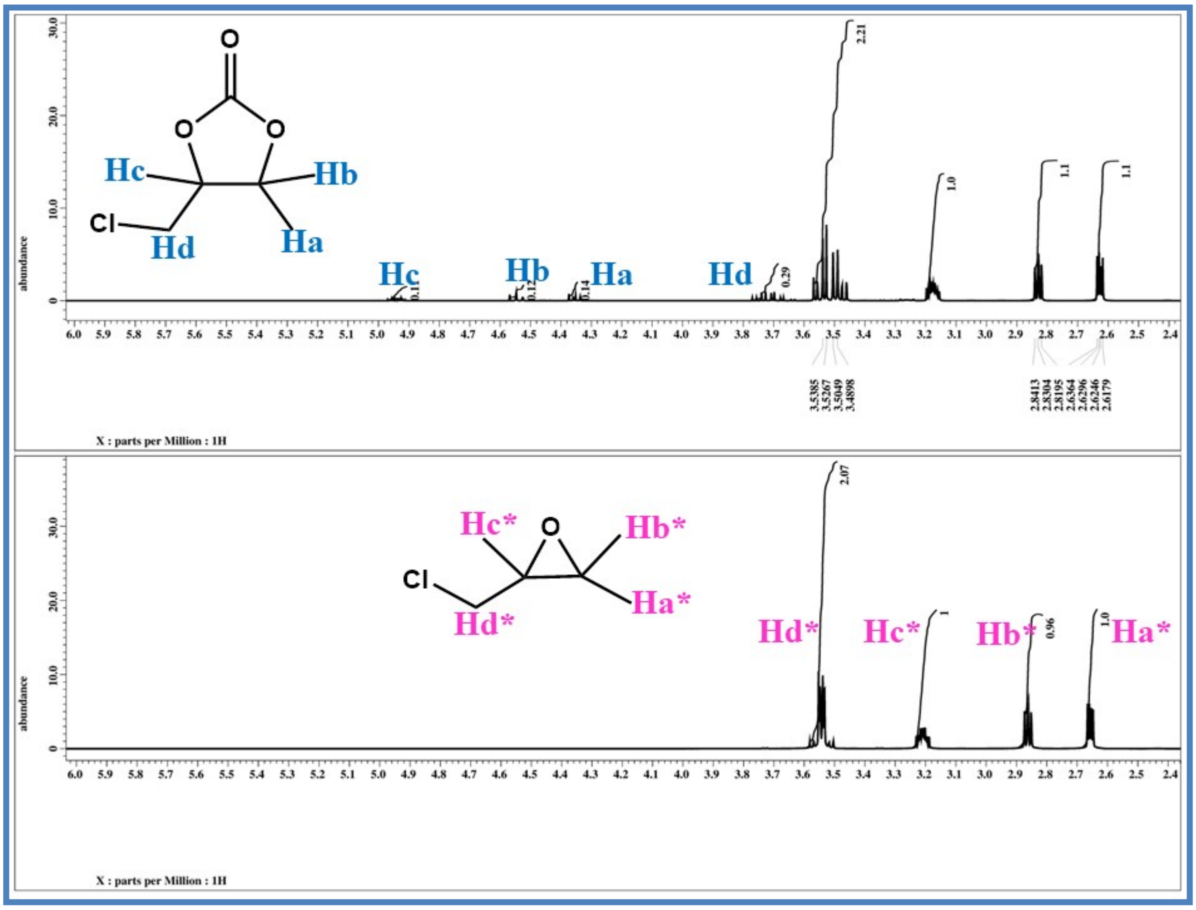


Figure S18. [1]H NMR ($CDCl_3$, 400 MHz) spectra for the cycloaddition reaction of CO_2 with epichlorohydrin catalysed by PCN-224 at 0.8 MPa of CO_2 and 90 ^oC.

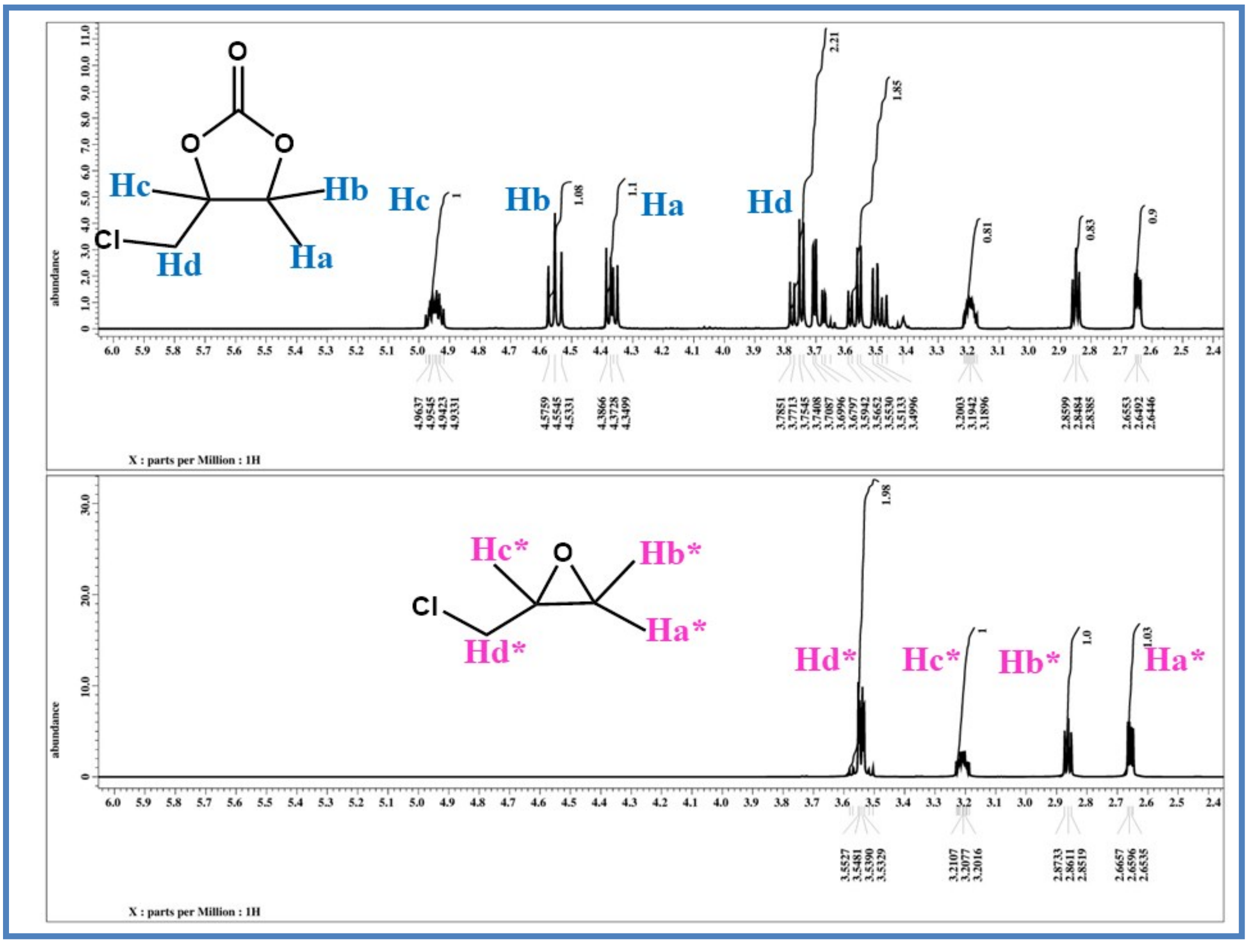


Figure S19. ¹H NMR ($CDCl_3$, 400 MHz) spectra for the cycloaddition reaction of CO_2 with epichlorohydrin catalysed by $[Zn(II)NMeTPyP]^{4+}[I^-]_4$ at 0.8 MPa of CO_2 and 90 ^oC.

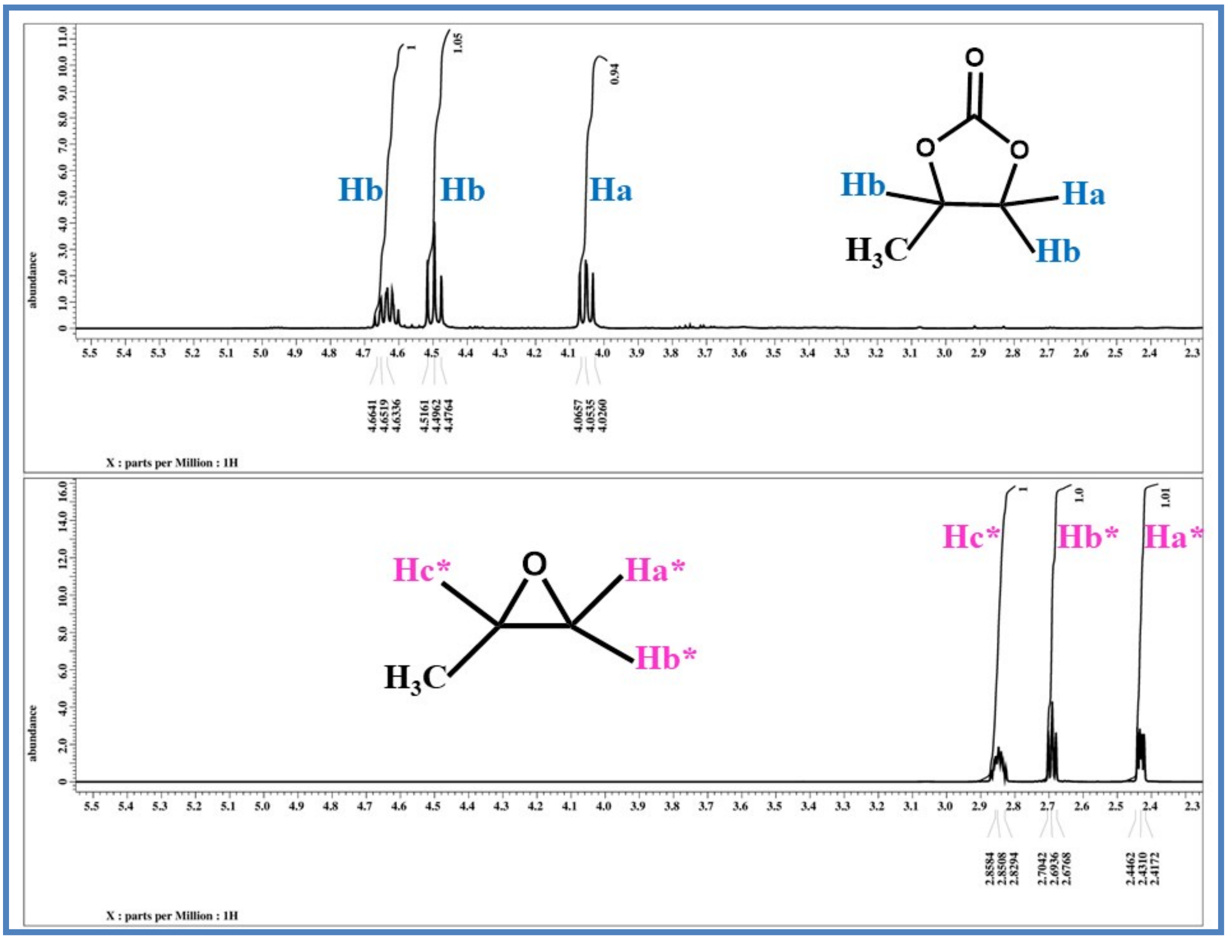


Figure S20. ${}^{1}H$ NMR ($CDCl_3$, 400 MHz) spectra for the cycloaddition reaction of CO_2 with 1,2-epoxypropane catalysed by $[Zn(II)NMeTPyP]^{4+}[I^-]_4$@PCN-224 at 0.8 MPa of CO_2 and 90 ^oC.

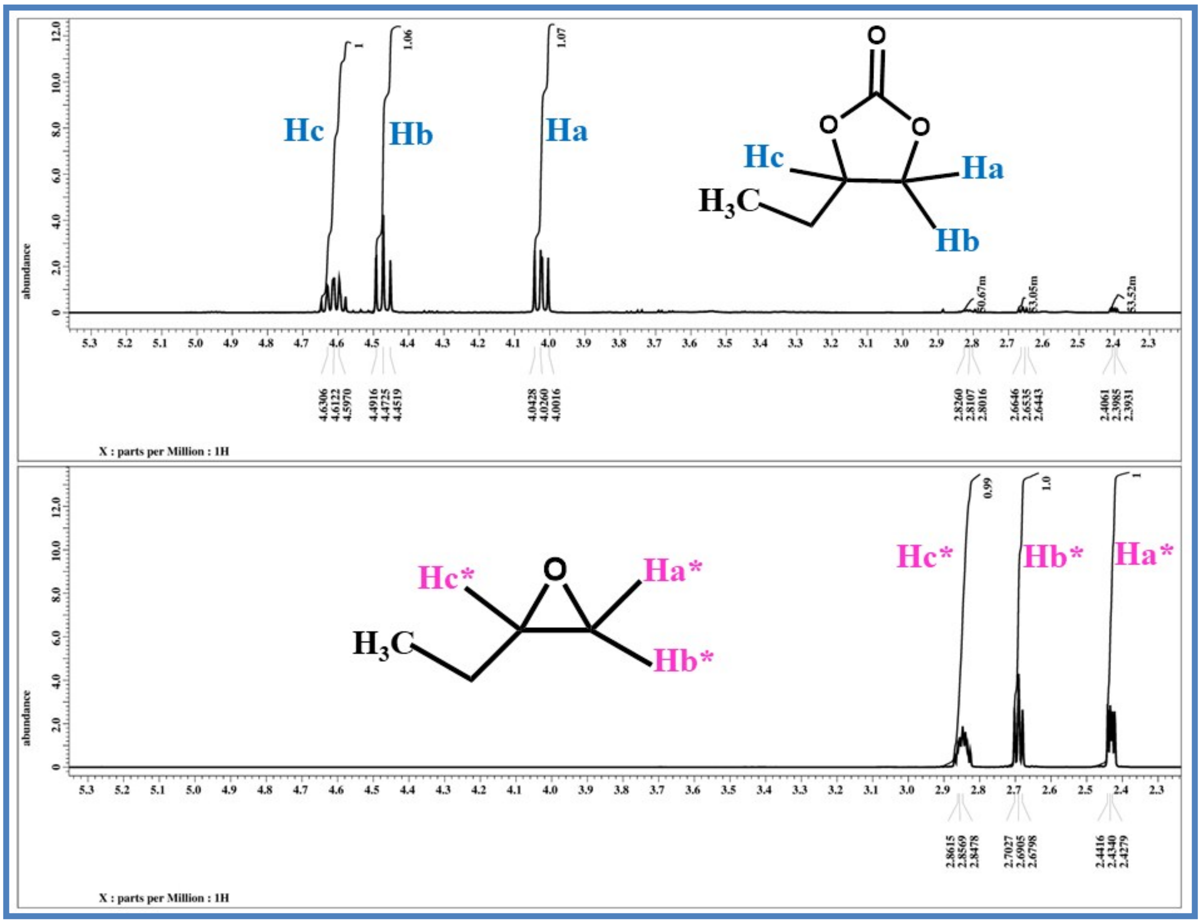


Figure S21. ^{1}H NMR ($CDCl_3$, 400 MHz) spectra for the cycloaddition reaction of CO_2 with 1,2-epoxybutane catalysed by $[Zn(II)NMeTPyP]^{4+}[I^-]_4$@PCN-224 at 0.8 MPa of CO_2 and 90 ^oC.

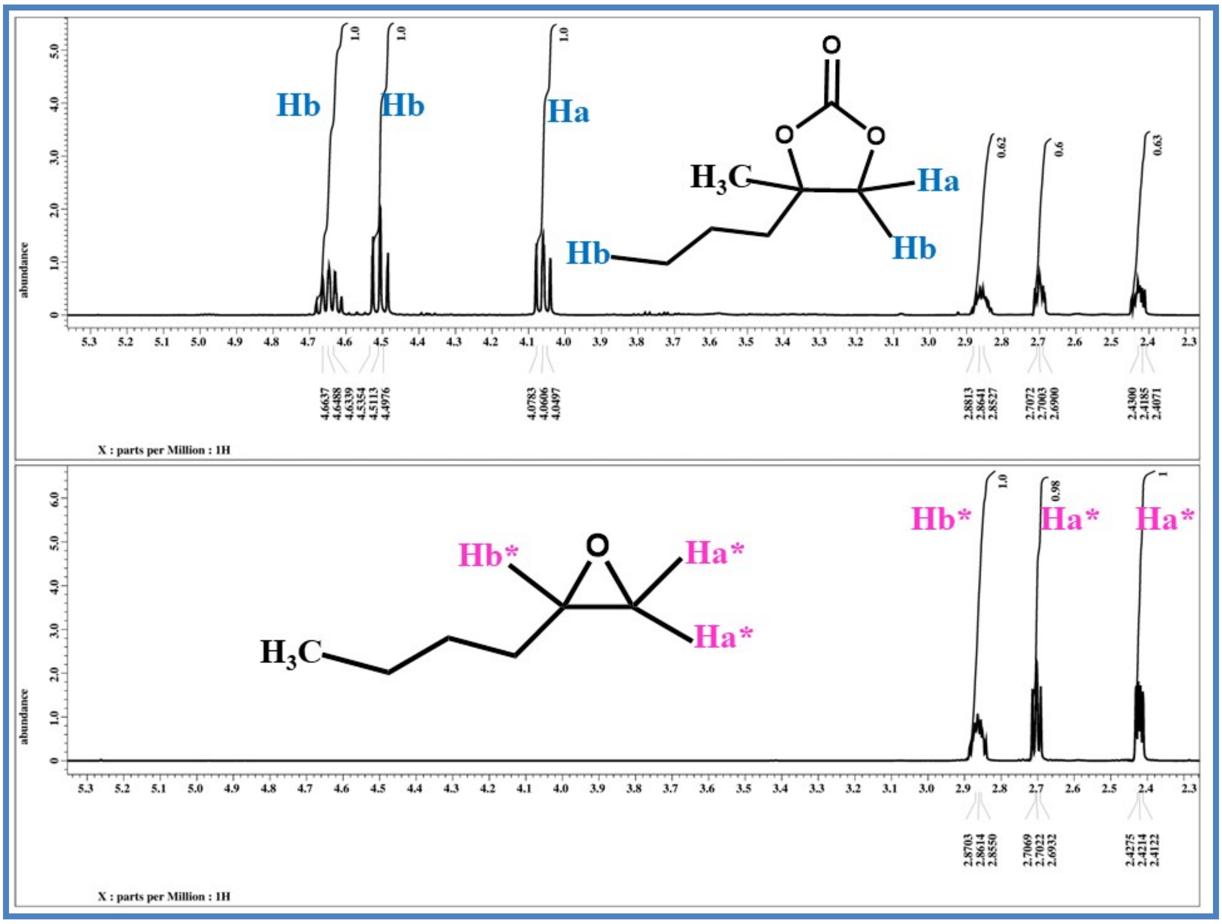


Figure S22. ^{1}H NMR ($CDCl_3$, 400 MHz) spectra for the cycloaddition reaction of CO_2 with 1,2-epoxyhexane catalysed by $[Zn(II)NMeTPyP]^{4+}[I^-]_4$@PCN-224 at 0.8 MPa of CO_2 and 90 ^{o}C.

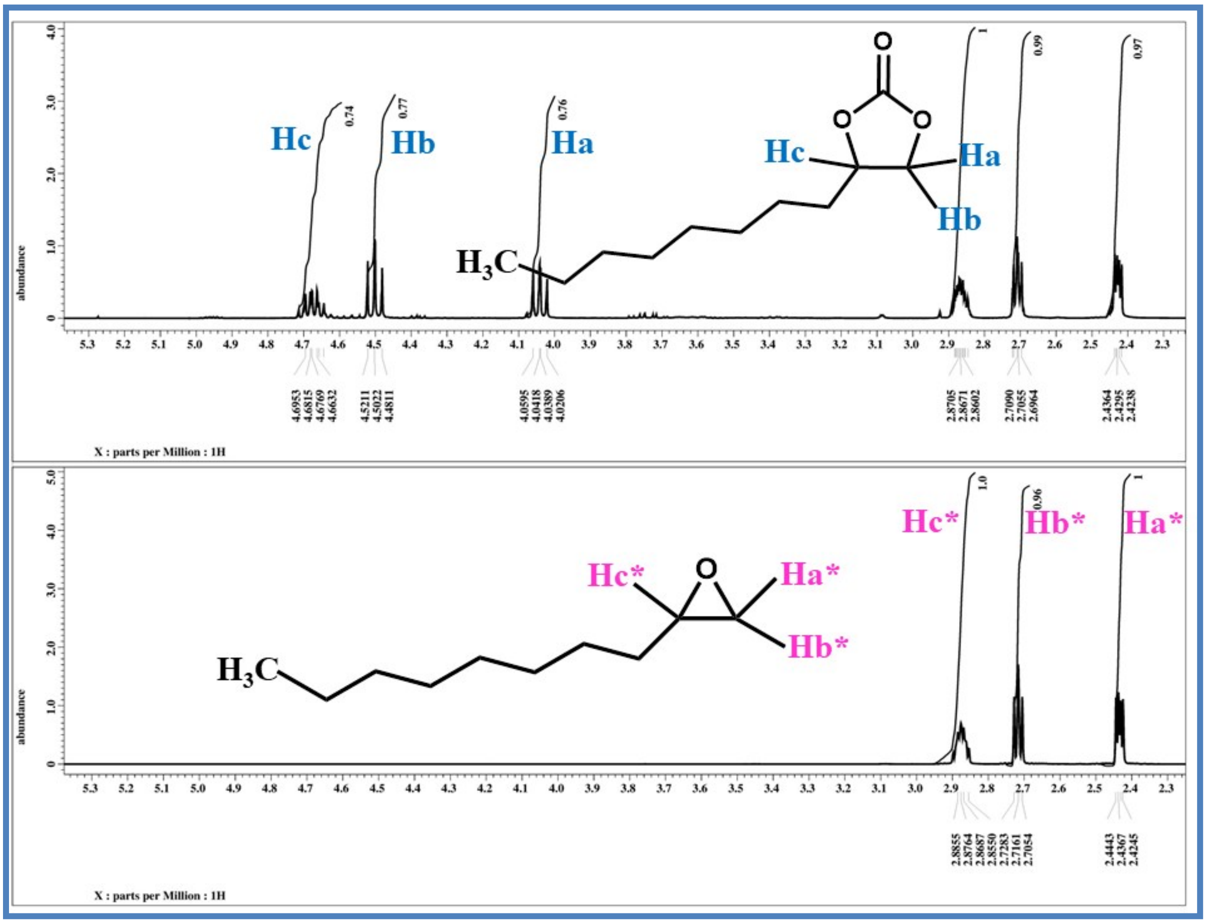


Figure S23. [1]H NMR ($CDCl_3$, 400 MHz) spectra for the cycloaddition reaction of CO_2 with 1,2-epoxydecane catalysed by $[Zn(II)NMeTPyP]^{4+}[I^-]_4$@PCN-224 at 0.8 MPa of CO_2 and 90 ^oC.

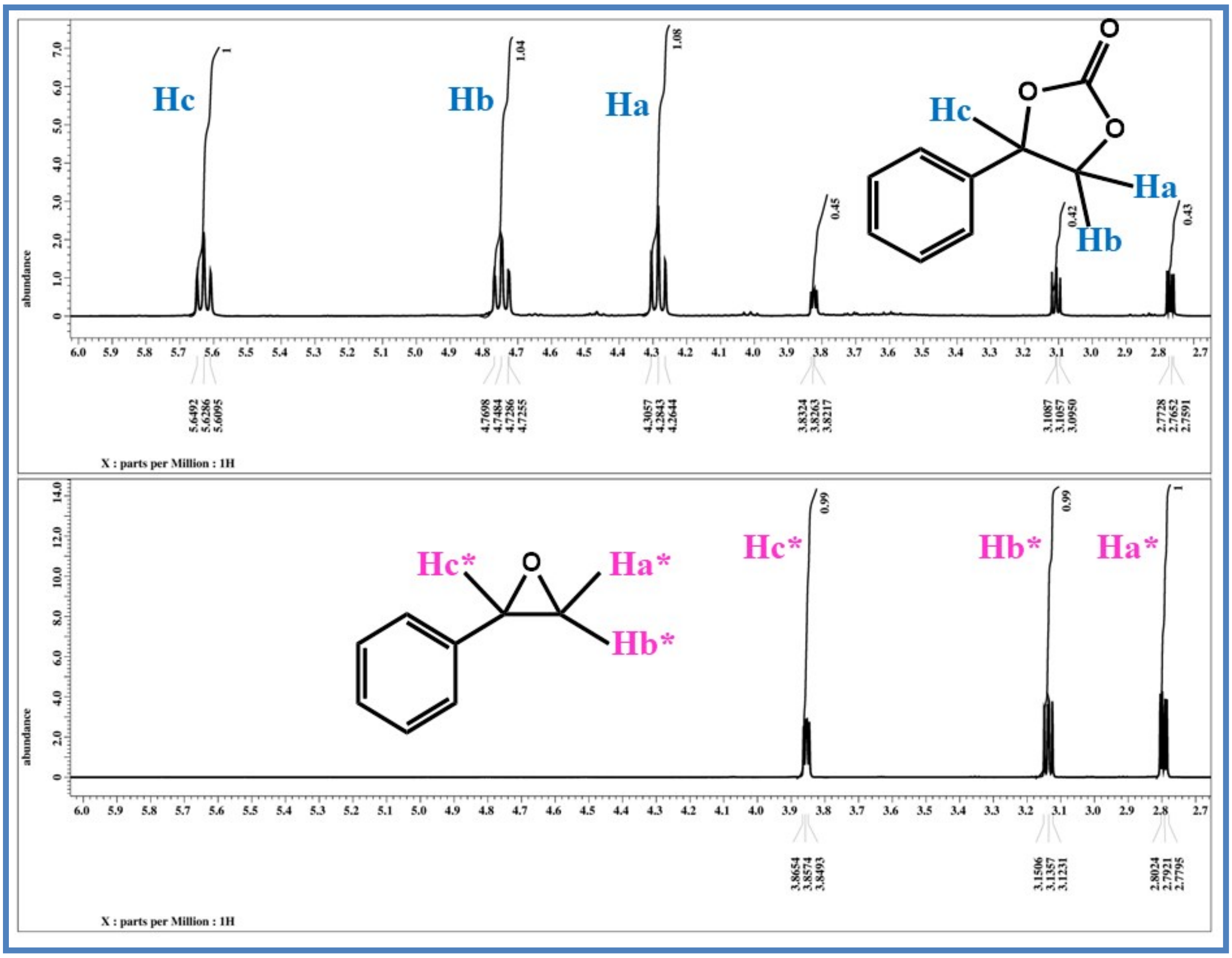


Figure S24. [1]H NMR ($CDCl_3$, 400 MHz) spectra for the cycloaddition reaction of CO_2 with styrene oxide catalysed by $[Zn(II)NMeTPyP]^{4+}[I^-]_4$@PCN-224 at 0.8 MPa of CO_2 and 90 ^oC.

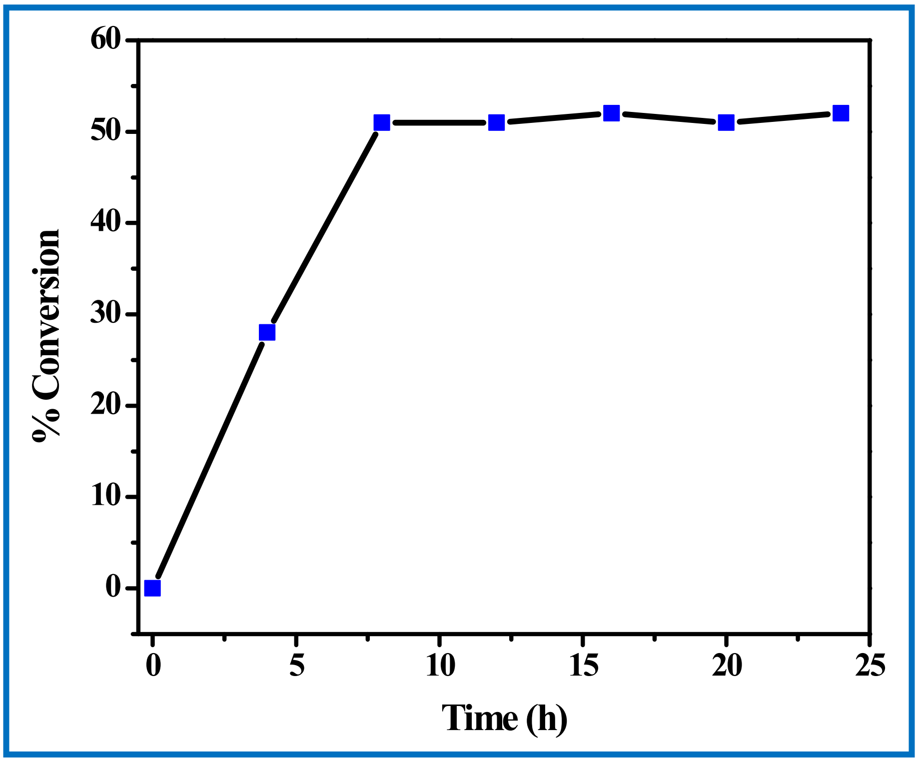


Figure S25. Hot filtration test.

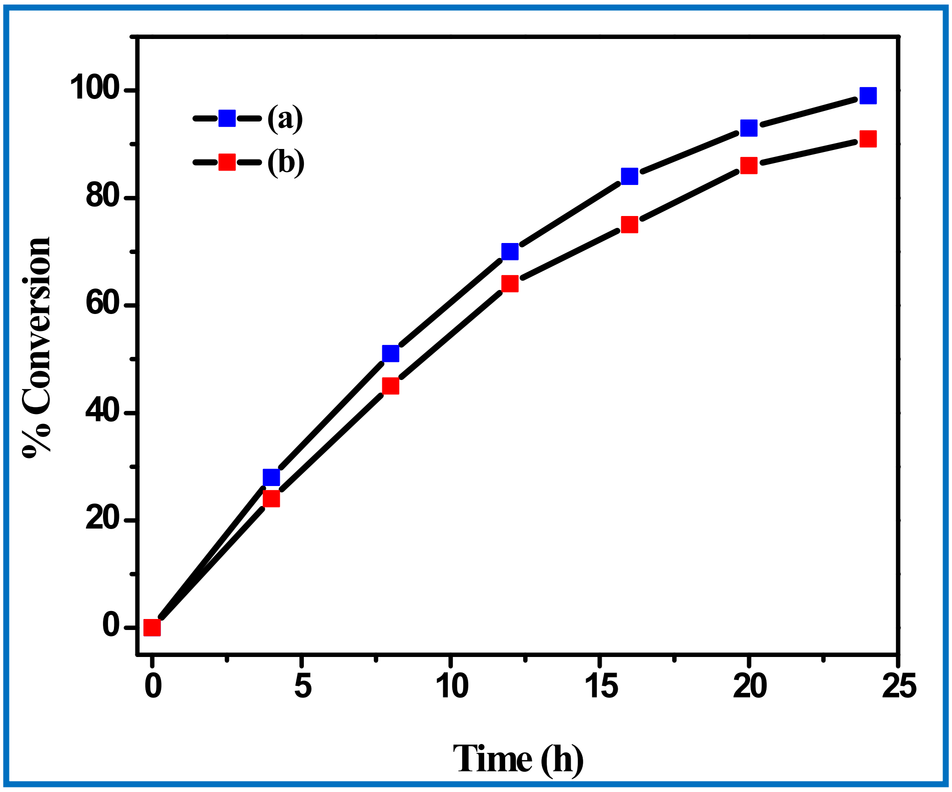


Figure S26. Time-dependent catalytic conversion of epichlorohydrin (ECH) with time: (a) as synthesized and (b) recycled catalyst after five cycles.

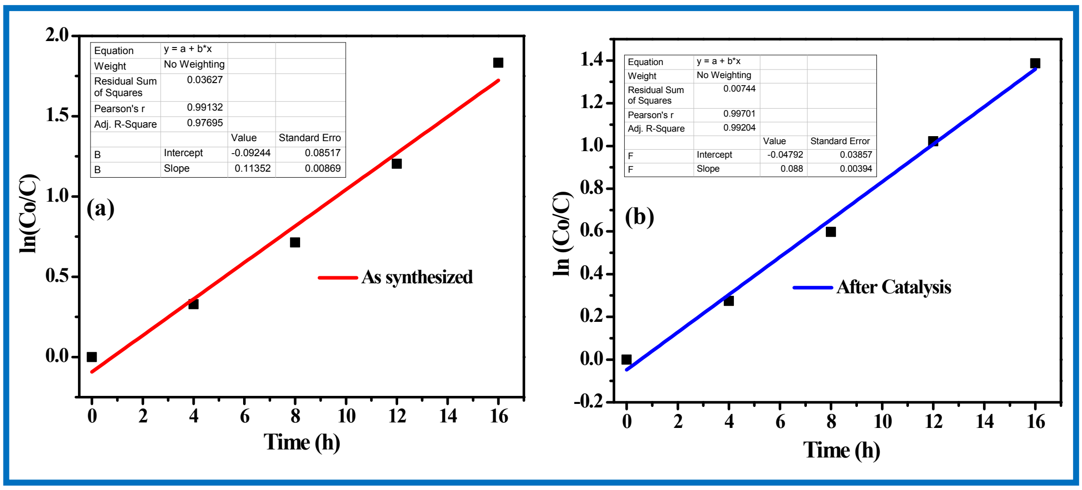


Figure S27. First-order kinetic curves of catalytic conversion of ECH with time for (a) as synthesized and (b) recycled catalyst after five cycles.

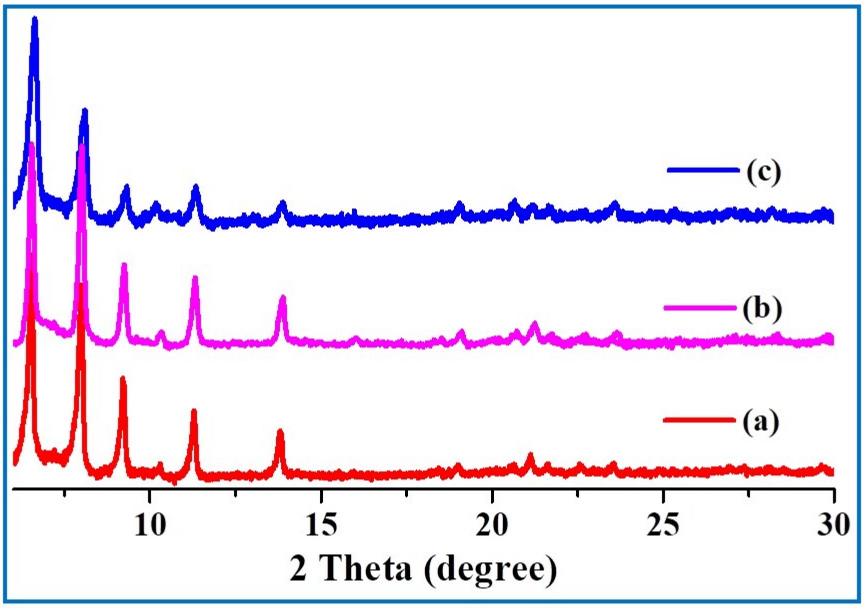


Figure S28. PXRD patterns of $[Zn(II)NMeTPyP]^{4+}[I^-]_4$@PCN-224, (a) as-synthesized sample; (b) for activated sample by heating at 120 ^oC for 12 h; (c) recycled sample after catalysis.

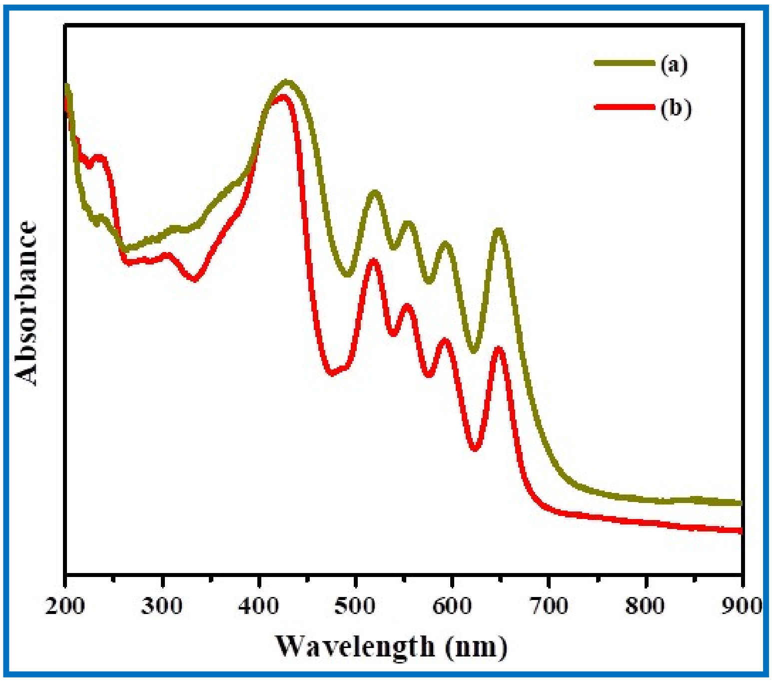


Figure S29. UV-Vis Spectra: (a) as synthesized $[Zn(II)NMeTPyP]^{4+}[I^-]_4$@PCN-224, (b) recycled after catalysis.

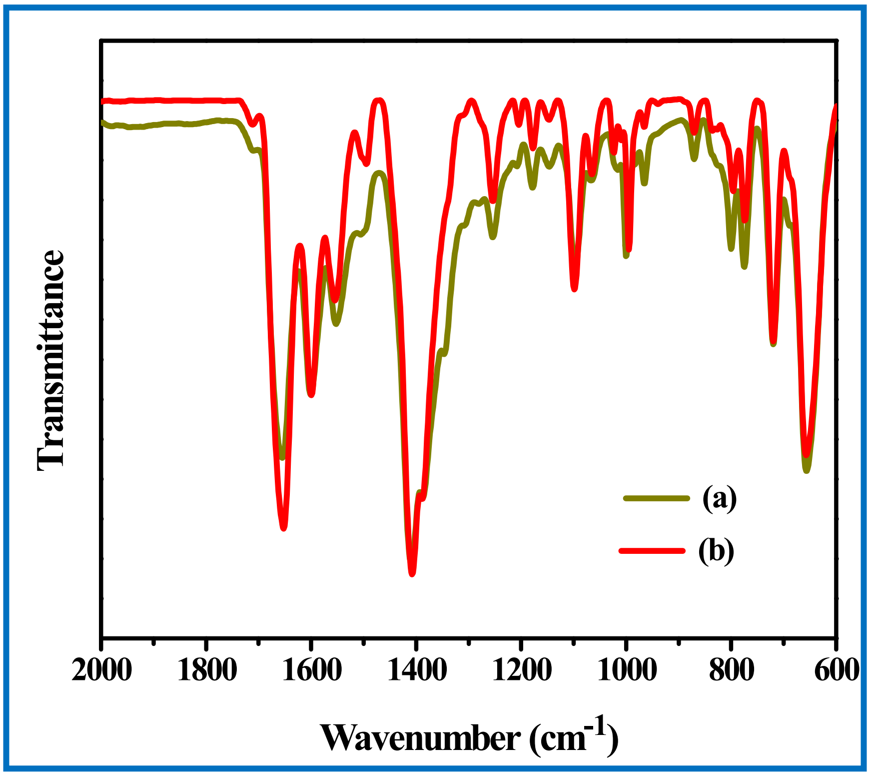
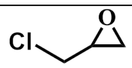
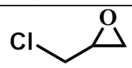
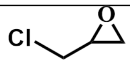
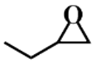
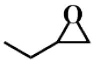
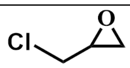
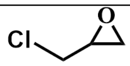
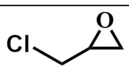
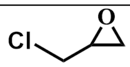
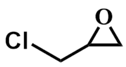
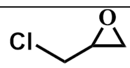
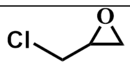
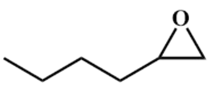
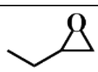


Figure S30. FTIR Spectra: (a) as synthesized $[Zn(II)NMeTPyP]^{4+}[I^-]_4$@PCN-224, (b) recovered after five cycles of catalysis.

Table S2. Comparison of the catalytic activity of $[Zn(II)NMeTPyP]^{4+}[I^-]_4$@PCN-224 with reported MOFs known for co-catalyst-free cycloaddition of CO_2 with epoxides.

S. No.	Substrate	MOF catalyst	Catalyst mol (%)	Reaction Conditions	Conversion (%)	Reference
1.		(I_)Meim-UiO-66	0.52	0.1 MPa, 120 °C, 24 h	100	5a
2.		F-IRMOF-3	-	0.1 Mpa, 120 °C, 3h	89	5b
3.		Zn-TATAB	0.42	0.1 Mpa, 100 °C, 16 h	98	5c
4.		Co-TATAB	0.2	0.1 Mpa, 80 °C, 15h	98	5d
5.		MIL-101-N(n-Bu)$_3$Br	0.9	2 MPa, 80 °C, 8 h	87.5	6a
6.		polyILs@MIL-101	-	0.1 MPa, 45 °C, 48 h	94	6b
7.		IL@MIL-101−SO$_3$H	0.43	0.1 Mpa, 90 °C, 48 h	98	6c
8.		MIL-101-IP	0.298	0.1 Mpa, 50 °C, 68 h	99	6d
9.		Il-ZIF-90	0.49	0.1 Mpa, 120 °C, 3h	94	6e
10.		UiO-67-IL	1.5	0.1 Mpa, 90 °C, 12h	95	6f
11.		F-ZIF-90	0.177	1.17 MPa, 120 °C, 6 h	94	6g
12.		IL/MIL-101-NH$_2$	0.435	1.3 MPa, 120 °C, 1 h	91	6h
13		ZnTCPP⊂(Br⁻)Etim-UiO-66	0.95	0.1 Mpa, 140 °C, 14 h	86.9	6i
14		FJI-C10	0.35	0.1 Mpa, 60 °C, 24 h	87	6j
15		SalenCo(23%)C(Br) Etim-UiO-66	-	0.1 Mpa, 120 °C, 12 h	84	6k
16.		$[Zn(II)NMeTPyP]^{4+}[I^-]_4$@PCN-224	0.116	0.8 MPa, 90 °C, 24 h	95.2	Present work

17.		$[Zn(II)NMeTPyP]^{4+}[I^-]_4$@PCN-224	0.116	0.8 MPa, 90 °C, 24 h	>99	Present work
18.		$[Zn(II)NMeTPyP]^{4+}[I^-]_4$@PCN-224	0.116	0.8 MPa, 90 °C, 24 h	>99	Present work

Table S3: Optimized coordinates for structure of $[Zn(II)NMeTPyP]^{4+}[I^-]_4$@PCN-224

Zr	7.80700000	10.19400000	8.24300000
O	8.21800000	11.93000000	6.77800000
O	7.27300000	9.44200000	10.23000000
O	8.48300000	7.97400000	8.45500000
N	9.92300000	19.03400000	2.00800000
C	9.25800000	12.77300000	6.65700000
C	9.37900000	13.65300000	5.50100000
C	8.32200000	13.81300000	4.54300000
H	7.38700000	13.25900000	4.68900000
C	8.47400000	14.70400000	3.44600000
H	7.64400000	14.86000000	2.74300000
C	9.68900000	15.44400000	3.26800000
C	9.80100000	16.50900000	2.23100000
C	9.75100000	17.83900000	2.74200000
C	9.48300000	18.22600000	4.10600000
H	9.27000000	17.52300000	4.91300000
O	10.25900000	12.76900000	7.55300000
N	10.01600000	17.02600000	-0.23900000
C	10.60900000	14.37200000	5.30400000
H	11.43300000	14.21500000	6.01100000
C	10.76000000	15.24100000	4.19800000
H	11.69800000	15.79400000	4.05400000
C	9.93100000	16.13400000	0.85700000
C	9.95100000	14.76800000	0.37000000
H	9.91300000	13.87400000	0.99800000
O	8.36300000	25.77300000	7.30600000
C	9.51200000	25.11100000	7.07700000
C	9.59700000	24.20000000	5.93700000
C	8.46800000	24.01300000	5.06800000
H	7.53200000	24.53500000	5.30000000
C	8.56400000	23.18600000	3.91800000
H	7.69300000	23.04600000	3.26400000
C	9.78300000	22.49200000	3.61800000
C	9.87900000	21.52600000	2.48400000
C	9.77100000	20.15500000	2.85600000
C	9.49900000	19.64400000	4.17500000
H	9.27800000	20.27000000	5.04000000
O	10.61300000	25.36300000	7.80600000
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H	11.69900000	23.67800000	6.27200000
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H	11.84600000	22.15300000	4.25600000
C	10.08800000	22.01300000	1.15800000
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C	9.70200000	13.89500000	-6.06200000
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H	12.06300000	15.91400000	-4.50200000
C	9.98100000	15.74500000	-3.86900000
C	10.10700000	16.72700000	-2.75300000
C	10.06600000	16.23100000	-1.41200000
C	10.03100000	14.82800000	-1.04400000
H	10.07500000	13.99100000	-1.74600000
O	10.89100000	25.93800000	-7.56300000
C	9.89700000	25.72400000	-6.68300000
C	10.06800000	24.77400000	-5.59400000
C	11.29800000	24.05000000	-5.42900000
H	12.13000000	24.25600000	-6.11400000
C	11.43400000	23.09800000	-4.38500000
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C	10.39200000	21.74000000	-2.48700000
C	10.33000000	22.10500000	-1.10400000

C	10.36500000	23.47000000	-0.60800000	O	8.78700000	11.58600000	9.66900000
H	10.49200000	24.35900000	-1.22900000	Zr	11.14600000	27.47800000	-9.26600000
O	8.43000000	12.24400000	-7.30200000	O	11.77200000	9.45900000	9.69900000
N	10.32500000	19.21000000	-2.26600000	O	9.08900000	26.76700000	-9.59800000
C	8.58400000	14.19200000	-5.21200000	Zr	10.21200000	30.16600000	7.91100000
H	7.62200000	13.70100000	-5.40800000	Zr	7.83400000	30.60700000	10.64600000
C	8.72500000	15.10700000	-4.13700000	Zr	7.78000000	7.28200000	-10.11200000
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C	10.21500000	18.62000000	-4.47500000	Zr	8.32900000	27.33800000	-11.51200000
H	10.12000000	18.01200000	-5.37600000	Zr	11.22000000	7.75400000	-11.10500000
O	8.73300000	26.39300000	-6.77700000	Zr	10.74000000	30.07400000	-11.73200000
C	8.98800000	24.53600000	-4.67800000	Zr	8.72300000	10.31500000	-11.81800000
H	8.04900000	25.08600000	-4.80800000	Zr	8.81700000	27.53300000	11.98400000
C	9.13000000	23.58600000	-3.63900000	Zr	11.19200000	10.85800000	-9.24900000
H	8.29400000	23.38300000	-2.95600000	Zr	11.18400000	27.08700000	9.23100000
C	10.36800000	20.41200000	-3.01200000	Zr	10.93200000	11.41500000	9.24100000
C	10.31100000	20.03500000	-4.40200000	Zr	11.24000000	8.72100000	11.68000000
H	10.29200000	20.74100000	-5.23300000	O	6.48600000	7.67000000	12.27200000
Zr	7.90500000	27.96800000	-8.16300000	O	12.67700000	6.85800000	8.85300000
Zr	7.84300000	10.40500000	-8.49900000	O	11.97900000	8.70200000	-6.43600000
O	6.35000000	11.80500000	-9.56600000	O	6.64200000	9.89000000	13.02200000
O	9.85200000	9.93900000	-7.76800000	O	11.87400000	6.09200000	-7.97900000
O	8.04900000	8.09500000	-8.10500000	O	12.34200000	8.99800000	6.92900000
C	6.18100000	12.17400000	-10.83300000	O	8.86800000	5.98100000	12.28300000
O	6.94900000	11.73900000	-11.84000000	O	12.74000000	28.06400000	-7.74200000
O	6.33800000	26.34300000	-8.68300000	O	7.36800000	28.46200000	10.59400000
C	6.00200000	25.71400000	-9.80600000	O	7.06200000	28.57400000	-10.22200000
O	6.60900000	25.92300000	-10.98100000	O	7.31900000	9.31500000	-10.47000000
O	6.38600000	12.06100000	11.06100000	O	9.96200000	28.63300000	-7.83600000
C	5.69000000	12.16500000	9.93200000	O	11.74700000	8.71800000	-9.26700000
O	7.21500000	25.89300000	11.88000000	O	9.18600000	11.34200000	-9.98300000
C	6.40800000	25.48300000	10.90400000	O	9.21900000	26.59400000	10.04000000
O	6.01900000	11.53900000	8.80400000	O	11.56400000	29.56700000	-9.81800000
O	6.43300000	25.97100000	9.66500000	O	9.09400000	8.86300000	12.10300000
Zr	8.12100000	7.47200000	10.67700000	O	8.03200000	30.29800000	-8.30900000
O	10.26300000	7.31400000	10.25200000	O	10.45000000	27.90300000	-11.59800000
Zr	10.79200000	8.05800000	8.27600000	O	10.55200000	10.92500000	11.47500000
O	9.94500000	10.02000000	7.83000000	Zr	28.36200000	7.95100000	8.04600000
Zr	10.36300000	7.82000000	-7.78000000	O	26.67800000	8.65700000	6.65100000
O	9.79800000	6.76800000	-9.75400000	O	28.94200000	7.11300000	9.97500000
Zr	7.78800000	27.54200000	8.64600000	O	30.61700000	8.39200000	8.42300000
O	9.75200000	28.04300000	7.83800000	N	19.42200000	10.66200000	2.16800000
O	7.97500000	29.84800000	8.46500000	C	25.86300000	9.72300000	6.63900000
Zr	8.24700000	10.83600000	11.65100000	C	24.92200000	9.90100000	5.54400000

C	24.72900000	8.86900000	4.56500000
H	25.30100000	7.93800000	4.65200000
C	23.78300000	9.04100000	3.52100000
H	23.60500000	8.23500000	2.79400000
C	23.01000000	10.24500000	3.42300000
C	21.93800000	10.39500000	2.40400000
C	20.60500000	10.44700000	2.91300000
C	20.20200000	10.29800000	4.29000000
H	20.88700000	10.09900000	5.11500000
O	25.93000000	10.65700000	7.59700000
N	21.43700000	10.50100000	-0.07900000
C	24.17100000	11.12100000	5.43200000
H	24.35200000	11.91900000	6.16200000
C	23.23900000	11.29100000	4.37900000
H	22.66900000	12.22500000	4.29600000
C	22.31900000	10.45800000	1.02600000
C	23.68900000	10.45300000	0.55000000
H	24.57900000	10.44400000	1.18500000
C	12.93300000	10.20100000	6.82400000
C	13.93500000	10.38800000	5.78300000
C	14.21200000	9.30600000	4.88000000
H	13.66200000	8.36500000	4.99500000
C	15.17300000	9.45800000	3.85000000
H	15.37100000	8.63400000	3.15300000
C	15.90600000	10.68200000	3.70700000
C	16.93400000	10.78400000	2.63200000
C	18.29600000	10.65300000	3.02400000
C	18.79000000	10.42400000	4.35800000
H	18.16200000	10.34400000	5.24800000
O	12.59500000	11.20800000	7.64500000
N	17.25900000	10.79100000	0.12000000
C	14.65200000	11.62300000	5.63100000
H	14.42800000	12.45300000	6.31200000
C	15.63200000	11.76200000	4.60900000
H	16.18600000	12.70400000	4.50500000
C	16.45700000	10.86900000	1.28600000
C	15.06300000	10.97900000	0.90800000
H	14.22700000	11.07700000	1.60500000
O	25.81900000	10.81300000	-7.78600000
C	25.49100000	9.77400000	-7.00000000
C	24.54900000	9.96200000	-5.90500000
C	23.95800000	11.24900000	-5.65400000
H	24.22800000	12.09000000	-6.30300000
C	23.06300000	11.42500000	-4.56500000
H	22.60700000	12.40900000	-4.38100000
C	22.74300000	10.33200000	-3.69600000
C	21.75600000	10.48500000	-2.59100000
C	22.24100000	10.49400000	-1.24600000
C	23.64100000	10.47000000	-0.86700000
H	24.48300000	10.47900000	-1.56300000
O	12.62300000	10.69300000	-7.48700000
C	12.74200000	9.81000000	-6.48300000
C	13.69600000	10.06600000	-5.41600000
C	14.42800000	11.30400000	-5.36900000
H	14.22500000	12.06700000	-6.13100000
C	15.38900000	11.53000000	-4.34800000
H	15.94400000	12.47700000	-4.31500000
C	15.65500000	10.52600000	-3.35800000
C	16.74400000	10.68500000	-2.35800000
C	16.37500000	10.81000000	-0.98300000
C	15.01000000	10.94300000	-0.50800000
H	14.12300000	11.00700000	-1.14300000
O	26.09200000	8.57700000	-7.14200000
N	19.26900000	10.67300000	-2.12300000
C	24.23300000	8.86800000	-5.03100000
H	24.69000000	7.88800000	-5.21700000
C	23.35000000	9.05500000	-3.93800000
H	23.10300000	8.21500000	-3.27600000
C	20.38700000	10.54400000	-2.97900000
C	19.87000000	10.44100000	-4.32000000
H	20.48600000	10.32000000	-5.21200000
C	13.92600000	9.07800000	-4.39800000
H	13.37000000	8.13500000	-4.43600000
C	14.89500000	9.30700000	-3.38700000
H	15.09500000	8.53900000	-2.62800000
C	18.07100000	10.62400000	-2.87300000
C	18.45400000	10.47500000	-4.25300000
H	17.75200000	10.38600000	-5.08400000
Zr	27.77500000	7.78500000	-8.43700000
O	26.15600000	6.37600000	-9.32100000
O	28.48500000	9.76700000	-7.83900000
O	30.10500000	7.80600000	-8.28900000
C	25.65500000	6.19400000	-10.53800000
O	26.03800000	6.89900000	-11.61200000
C	12.54200000	5.56600000	-9.00200000
O	12.45600000	6.02500000	-10.25600000
O	26.19100000	6.39700000	10.57300000
C	26.09400000	5.86700000	9.35700000
O	13.05000000	7.39900000	11.10600000
C	13.38400000	6.77800000	9.97800000

O	26.81800000	6.26600000	8.31500000
Zr	30.94600000	7.72100000	10.60500000
O	31.30500000	9.88100000	10.44900000
Zr	30.72300000	10.71600000	8.50900000
O	28.73100000	10.08700000	7.89100000
Zr	30.63100000	10.09200000	-8.06500000
O	31.42600000	9.38100000	-10.10600000
Zr	27.56500000	8.04700000	11.44500000
O	26.97900000	8.88800000	9.51700000
O	29.34200000	11.65700000	9.97000000
Zr	30.69600000	7.41300000	-10.35100000
Zr	30.43000000	10.83900000	-11.41300000
Zr	27.58500000	8.56600000	-11.78100000
Zr	27.54900000	11.14000000	-9.27900000
Zr	27.35000000	11.03900000	9.35000000
Zr	29.91600000	10.80600000	11.91000000
O	30.50800000	5.89900000	11.96400000
O	32.05000000	12.40300000	9.35800000
O	30.03900000	11.81400000	-6.67400000
O	28.27300000	6.18800000	12.62100000
O	32.47400000	11.43200000	-8.49900000
O	29.96700000	12.44300000	7.19300000
O	32.39400000	8.11800000	12.35800000
O	28.60600000	7.11900000	-10.48800000
O	29.71500000	11.50400000	-9.51300000
O	26.80600000	9.16200000	-9.87900000
O	29.56300000	8.64600000	12.07900000
O	10.83800000	9.87800000	-11.48800000
O	27.68600000	10.36300000	11.53800000
Zr	30.48900000	27.57700000	8.16800000
O	29.57700000	26.00700000	6.87000000
O	31.35100000	27.90100000	10.11900000
O	30.67300000	29.82000000	8.40300000
N	27.65300000	19.16900000	2.14400000
C	28.34500000	25.46400000	6.74900000
C	28.10500000	24.56200000	5.63500000
C	29.19200000	24.23600000	4.75400000
H	30.17900000	24.67800000	4.94100000
C	28.99300000	23.35100000	3.66900000
H	29.83300000	23.07800000	3.01500000
C	27.70900000	22.75700000	3.43600000
C	27.61700000	21.69100000	2.40100000
C	27.61400000	20.35900000	2.90400000
C	27.66500000	19.96700000	4.29000000
H	27.68200000	20.66100000	5.13200000
O	27.35300000	25.81200000	7.58100000
N	27.94500000	21.20700000	-0.06700000
C	26.80200000	24.01000000	5.37200000
H	25.96300000	24.30000000	6.01600000
C	26.61100000	23.12300000	4.27800000
H	25.61600000	22.69800000	4.07700000
C	27.71900000	22.07800000	1.02900000
C	27.70100000	23.45200000	0.55800000
H	27.53000000	24.32700000	1.18800000
C	28.77900000	13.05800000	7.06300000
C	28.54500000	13.96000000	5.94300000
C	29.58000000	14.21500000	4.97900000
H	30.56200000	13.74100000	5.10800000
C	29.32900000	15.06600000	3.87400000
H	30.12000000	15.26200000	3.13800000
C	28.05400000	15.70100000	3.69900000
C	27.87600000	16.68500000	2.59700000
C	27.76100000	18.04700000	2.99800000
C	27.76200000	18.55400000	4.34700000
H	27.84900000	17.93700000	5.24300000
O	27.75800000	12.77200000	7.88700000
N	28.06800000	17.03300000	0.09600000
C	27.25600000	14.57300000	5.75600000
H	26.46000000	14.35300000	6.47800000
C	27.01500000	15.43400000	4.65400000
H	26.03300000	15.91200000	4.53100000
C	27.93200000	16.21500000	1.24500000
C	27.92600000	14.82100000	0.84800000
H	27.81400000	13.97400000	1.52900000
O	27.87300000	25.85400000	-7.49500000
C	28.91200000	25.65300000	-6.66600000
C	28.81900000	24.63100000	-5.63500000
C	27.61600000	23.86100000	-5.48800000
H	26.76900000	24.06900000	-6.15200000
C	27.51500000	22.87200000	-4.47700000
H	26.57800000	22.31100000	-4.36600000
C	28.60800000	22.61700000	-3.58400000
C	28.46800000	21.58000000	-2.52000000
C	28.11300000	22.02800000	-1.20900000
C	27.93400000	23.41800000	-0.83800000
H	27.99600000	24.26500000	-1.52500000
O	28.01600000	12.58000000	-7.56800000
C	28.97700000	12.64000000	-6.63400000
C	28.84300000	13.59400000	-5.54000000
C	27.64400000	14.37300000	-5.39500000

H	26.82100000	14.21200000	-6.10300000
C	27.52000000	15.30300000	-4.33300000
H	26.59200000	15.87600000	-4.20600000
C	28.59300000	15.50200000	-3.40100000
C	28.46800000	16.56200000	-2.36000000
C	28.19300000	16.16200000	-1.01400000
C	28.07600000	14.78500000	-0.56300000
H	28.11800000	13.90400000	-1.20800000
O	30.02400000	26.41700000	-6.75400000
N	28.42500000	19.08600000	-2.09000000
C	29.91600000	24.38100000	-4.74100000
H	30.83600000	24.96700000	-4.84500000
C	29.80400000	23.39100000	-3.72800000
H	30.63900000	23.20900000	-3.03600000
C	28.67700000	20.22000000	-2.89900000
C	29.13500000	19.72600000	-4.17300000
H	29.44900000	20.36200000	-5.00200000
C	29.90100000	13.76000000	-4.58500000
H	30.81300000	13.16200000	-4.69000000
C	29.77500000	14.70400000	-3.53100000
H	30.59500000	14.85100000	-2.81400000
C	28.66100000	17.90000000	-2.81900000
C	29.12100000	18.30500000	-4.12500000
H	29.41500000	17.61100000	-4.91400000
Zr	30.61600000	28.13900000	-8.09700000
O	28.56100000	28.64900000	-7.79100000
O	30.38900000	30.39800000	-8.39200000
C	32.94100000	12.01600000	-9.60100000
O	32.34200000	11.93500000	-10.79700000
O	31.42600000	12.52600000	11.62000000
C	32.13300000	12.94200000	10.57300000
Zr	31.26700000	30.07600000	10.62800000
O	29.30200000	31.00300000	10.24700000
Zr	28.44300000	30.55600000	8.27600000
O	28.55000000	28.42000000	7.80000000
Zr	28.06400000	30.69400000	-8.42900000
O	28.89500000	31.14600000	-10.55800000
Zr	29.88600000	27.04100000	11.60900000
O	29.19700000	26.47800000	9.63700000
O	27.09800000	29.56300000	9.72800000
Zr	30.94800000	30.60600000	-10.48400000
Zr	27.59100000	29.86500000	-11.74600000
Zr	30.14400000	27.39400000	-11.46100000
Zr	27.43100000	27.35400000	-9.15500000
Zr	27.20100000	27.41600000	9.23700000
Zr	27.91600000	30.06200000	11.69400000
O	32.81200000	29.16100000	12.10100000
O	27.18500000	32.36300000	8.91600000
O	26.36900000	30.15000000	-7.03600000
O	31.84300000	27.12100000	12.76800000
O	26.60800000	32.26800000	-9.26500000
O	26.59000000	30.22200000	6.91700000
O	31.17200000	31.67200000	12.25500000
O	31.53800000	28.53700000	-10.16800000
O	26.89600000	29.39900000	-9.77300000
O	29.57700000	26.75600000	-9.50900000
O	29.88100000	29.14000000	12.07700000
O	28.24700000	10.65000000	-11.57600000
O	27.74700000	27.74400000	11.46200000
O	11.79000000	29.37600000	6.48900000
O	9.80600000	31.09900000	9.84000000
N	19.27300000	28.65700000	2.10500000
C	12.62300000	28.32500000	6.46100000
C	13.63600000	28.28900000	5.41400000
C	13.77600000	29.42800000	4.54900000
H	13.10600000	30.28500000	4.69100000
C	14.78900000	29.45500000	3.56400000
H	14.90900000	30.33600000	2.91900000
C	15.68300000	28.34700000	3.40200000
C	16.76100000	28.40900000	2.37700000
C	18.08800000	28.56800000	2.87000000
C	18.47800000	28.69400000	4.25100000
H	17.78400000	28.67900000	5.09300000
O	12.55500000	27.36200000	7.39200000
N	17.20200000	28.53100000	-0.12200000
C	14.52100000	27.17000000	5.24700000
H	14.39700000	26.29300000	5.89400000
C	15.52700000	27.19800000	4.24600000
H	16.19900000	26.33900000	4.10600000
C	16.35900000	28.37400000	1.00200000
C	14.98800000	28.20700000	0.55900000
H	14.12900000	28.04500000	1.21500000
C	25.70400000	29.21700000	6.83000000
C	24.71800000	29.17500000	5.75500000
C	24.53600000	30.27400000	4.84900000
H	25.14300000	31.17700000	4.98500000
C	23.57900000	30.19900000	3.80300000
H	23.43400000	31.05500000	3.12800000
C	22.77400000	29.02300000	3.62600000
C	21.75400000	28.93500000	2.54400000

C	20.39100000	28.83400000	2.95300000
C	19.88600000	28.86100000	4.30300000
H	20.50100000	29.00000000	5.19300000
O	25.75500000	28.17500000	7.67600000
N	21.37700000	28.88200000	0.03700000
C	23.91300000	27.99600000	5.57800000
H	24.07000000	27.14100000	6.24700000
C	22.96900000	27.92300000	4.52600000
H	22.37200000	27.01200000	4.38900000
C	22.21000000	28.92100000	1.18500000
C	23.60100000	28.92100000	0.77200000
H	24.46000000	28.92500000	1.44800000
C	12.89900000	29.11100000	-6.91700000
C	13.87100000	29.01200000	-5.83600000
C	14.62000000	27.79600000	-5.66900000
H	14.43700000	26.96200000	-6.35700000
C	15.55800000	27.66800000	-4.61600000
H	16.12900000	26.73800000	-4.49500000
C	15.77800000	28.74500000	-3.69700000
C	16.80300000	28.65100000	-2.62100000
C	16.36600000	28.49600000	-1.26700000
C	14.99200000	28.28900000	-0.85600000
H	14.13800000	28.20000000	-1.53300000
O	25.85400000	27.93000000	-7.58600000
C	25.66400000	29.02200000	-6.82500000
C	24.72200000	28.97400000	-5.71400000
C	24.00600000	27.76400000	-5.41200000
H	24.18600000	26.87200000	-6.02400000
C	23.09300000	27.73000000	-4.32800000
H	22.53500000	26.81200000	-4.10300000
C	22.86900000	28.89400000	-3.51800000
C	21.82100000	28.86100000	-2.46100000
C	22.23400000	28.87100000	-1.09000000
C	23.61500000	28.88900000	-0.64600000
H	24.48900000	28.86600000	-1.30200000
O	12.12500000	30.20800000	-7.03100000
N	19.29700000	28.71200000	-2.18300000
C	14.08300000	30.09000000	-4.91200000
H	13.51300000	31.01800000	-5.03600000
C	15.01700000	29.95100000	-3.85400000
H	15.18500000	30.78100000	-3.15400000
C	18.16400000	28.75200000	-3.03000000
C	18.65600000	28.90100000	-4.37600000
H	18.02400000	28.97600000	-5.26300000
C	24.51700000	30.13300000	-4.89000000
H	25.06900000	31.05200000	-5.12100000
C	23.60300000	30.09200000	-3.80600000
H	23.43200000	30.98600000	-3.19200000
C	20.48000000	28.83600000	-2.94700000
C	20.07400000	28.94400000	-4.32700000
H	20.75800000	29.06900000	-5.16800000
O	11.71900000	32.40000000	-9.16700000
C	12.21500000	32.69900000	-10.36400000
O	11.99000000	31.97000000	-11.46300000
C	26.05600000	32.48400000	-10.45500000
O	26.27700000	31.70500000	-11.52100000
O	12.61300000	31.71400000	10.21600000
C	12.63900000	32.20300000	8.97900000
O	26.74000000	31.97300000	11.18500000
C	26.62300000	32.69600000	10.07500000
O	11.82700000	31.80300000	8.00400000
Zr	11.24300000	30.15500000	11.24500000
O	11.66000000	29.22600000	9.31200000
O	8.44800000	32.45900000	11.89000000
O	10.71200000	32.09500000	12.38700000
O	6.51200000	30.35100000	12.51800000
O	9.46800000	31.29000000	-10.43800000
O	9.27700000	29.67500000	12.05700000
O	28.00900000	27.72100000	-11.50800000
O	11.03900000	27.84300000	11.43300000
C	9.59400000	32.81100000	12.46500000
O	7.25500000	28.34800000	13.48900000
C	6.47700000	29.42700000	13.47200000
C	9.93700000	5.97000000	13.07200000
O	10.89500000	6.89200000	13.03300000
C	6.11200000	8.67100000	13.06600000
C	32.83200000	28.02100000	12.78700000
O	28.96400000	31.60600000	13.05500000
C	30.20600000	32.08100000	13.07600000
C	32.45400000	9.07800000	13.27400000
O	31.63100000	10.12100000	13.31000000
C	29.42700000	5.52600000	12.64300000
Zn	19.17400000	19.33400000	0.67900000
N	19.39700000	19.12100000	-1.36600000
N	25.08100000	19.03800000	-4.48100000
N	18.95600000	19.22700000	2.75600000
C	16.41900000	19.32300000	2.90600000
N	17.10200000	19.06700000	0.48100000
C	21.39300000	19.11500000	3.44900000
N	21.24400000	19.07700000	0.91700000

C	16.96400000	18.98400000	-2.05300000	H	19.98800000	19.62400000	5.95200000
N	24.22000000	19.04800000	6.72700000	H	15.50100000	16.75400000	-2.71800000
N	13.14100000	20.05900000	5.64800000	H	13.87200000	19.05200000	1.48100000
C	20.62300000	19.18100000	-2.08400000	H	21.37300000	17.46300000	5.67000000
C	19.42100000	19.51300000	5.02700000	H	24.17200000	20.71200000	-1.63700000
C	15.33300000	17.59400000	-3.40300000	H	21.09200000	19.38300000	-4.28200000
C	16.04900000	18.82400000	-3.21400000	H	22.28100000	17.27700000	-3.58900000
C	19.99800000	19.26900000	3.72300000	H	24.41800000	18.49600000	-0.10100000
C	14.81400000	19.01900000	0.93300000	H	15.89500000	21.61200000	4.32800000
C	22.20000000	18.18400000	5.67300000	H	24.11600000	18.48200000	2.60900000
C	24.12900000	19.96000000	-2.43500000	H	12.40400000	18.12300000	5.17700000
C	20.34000000	19.28200000	-3.49600000	H	24.13000000	17.34800000	-5.35300000
C	23.04400000	19.02300000	-2.49100000	H	16.31200000	20.85200000	-4.02400000
C	17.73100000	19.39000000	3.46500000	H	18.37200000	19.24100000	-4.58800000
C	23.05800000	18.04800000	-3.54800000	H	14.18800000	18.79100000	-1.21600000
C	23.50300000	18.69500000	0.45800000	H	17.26900000	19.75400000	5.64400000
C	15.29700000	19.55400000	3.85200000	H	13.96600000	21.99900000	5.95800000
C	15.17200000	20.81100000	4.53100000	H	23.60800000	20.75500000	3.81800000
C	21.95400000	18.96400000	2.14400000	H	23.07500000	17.46400000	7.57600000
C	21.92900000	19.06600000	-1.52000000	H	13.84300000	16.53600000	-4.64500000
C	23.34600000	18.68700000	1.86200000	H	25.99400000	20.63200000	-3.41200000
C	13.21600000	18.83100000	4.97300000	H	26.75100000	19.94200000	-5.41600000
C	18.35600000	19.12000000	-2.33500000	H	26.61500000	18.15900000	-5.65900000
C	24.07200000	18.06500000	-4.52500000	H	25.49600000	19.27200000	-6.55000000
C	22.34200000	19.11300000	4.58600000	H	14.33500000	17.58500000	3.59700000
C	15.80000000	19.88900000	-4.14100000	H	12.11900000	21.29800000	7.03000000
C	18.93500000	19.22200000	-3.65400000	H	11.99800000	19.51800000	7.36000000
C	16.39000000	18.94600000	-0.74600000	H	11.05700000	20.26600000	6.00400000
C	14.97500000	18.88800000	-0.46600000	H	14.59700000	20.52900000	-5.88500000
C	18.01800000	19.58400000	4.86700000	H	25.24000000	20.64500000	5.76400000
C	14.10500000	21.05300000	5.42300000	H	24.98600000	18.20400000	8.51400000
N	14.16800000	18.52100000	-5.33400000	H	25.25700000	19.98600000	8.33600000
C	22.20700000	18.96600000	-0.12500000	H	26.23900000	18.81800000	7.35900000
C	23.45500000	20.02300000	4.62100000	H	12.66900000	17.41700000	-6.34500000
C	23.13600000	18.15800000	6.72800000	H	12.37800000	19.19300000	-6.26300000
C	14.41100000	17.45200000	-4.45900000	H	13.63600000	18.53200000	-7.39900000
C	25.13600000	19.95300000	-3.42100000	I	21.83500000	22.70400000	1.88100000
C	16.13200000	19.11800000	1.51800000	I	21.63700000	15.72300000	-0.51200000
C	26.04800000	19.11000000	-5.59900000	I	17.72500000	15.57600000	0.50600000
C	14.28800000	18.56100000	4.09400000	I	17.75800000	22.61600000	1.85900000
C	12.00700000	20.30100000	6.56900000	H	5.18400000	24.97400000	-9.76800000
C	14.86300000	19.73100000	-5.18300000	H	30.45400000	32.85700000	13.82000000
C	24.36900000	19.98300000	5.69100000	H	5.31400000	8.47300000	13.80400000
C	25.23800000	19.01100000	7.80200000	H	5.77400000	29.57600000	14.31200000
C	13.15100000	18.40900000	-6.40700000	H	5.67200000	24.69400000	11.13700000

H	4.78200000	12.79200000	9.93200000
H	33.87700000	12.59500000	-9.52800000
H	33.71100000	27.80300000	13.41800000
H	10.04700000	5.14200000	13.79600000
H	13.22000000	4.71800000	-8.80400000
H	29.49300000	4.61300000	13.26000000
H	33.23200000	8.99700000	14.05600000
H	14.30700000	6.17400000	9.97200000
H	5.37200000	12.88600000	-11.07000000
H	24.87700000	5.42300000	-10.68500000
H	9.62000000	33.75600000	13.03400000
H	26.04000000	33.63100000	10.12000000
H	19.25500000	28.64200000	-1.15600000
H	19.32000000	28.62800000	1.07600000
H	19.31800000	10.73500000	-1.09600000
H	19.37900000	10.76700000	1.14400000
H	10.29300000	19.15700000	-1.23900000
H	10.08800000	19.08900000	0.99300000
H	28.12800000	19.12700000	-1.10500000
H	27.70200000	19.12700000	1.11600000
H	12.85000000	33.59700000	-10.45900000
H	32.82800000	13.78800000	10.72200000
H	25.37900000	33.34800000	-10.57400000
H	25.37000000	5.04800000	9.19900000
H	13.38000000	32.98800000	8.74600000

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