Supporting Information

Insights into CO_2 Adsorption and Chemical Fixation Properties of VPI-100 Metal-Organic Frameworks

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Section 1. Structure determination and refinement of Hf-VPI-100 (Cu) and Hf-VPI-100 (Ni)

XRD indexing and Rietveld analysis was performed with TOPAS version 5. Figure 2 shows the XRD profiles of Hf-VPI-100 (Cu) and Hf-VPI-100 (Ni) at room temperature after activation at 100 °C under helium flow. The high similarity of the diffraction patterns suggested the Cu and Ni analogues are isostructural. Indexing of the Hf-VPI-100 (Ni) patterns suggested a body-centered tetragonal lattice with unit cell parameters: a ~ 16.6 Å and c ~ 18.6 Å. For Rietveld refinement, our previously published Zr-VPI-100 structure was used as the initial model, in which Zr atoms were substituted by Hf. Rigid body constraint was applied to the cyclam ligand and the Hf_6 cluster. The final CIFs are included with this submission and the refinement plots are shown as Figure S1 and S2.

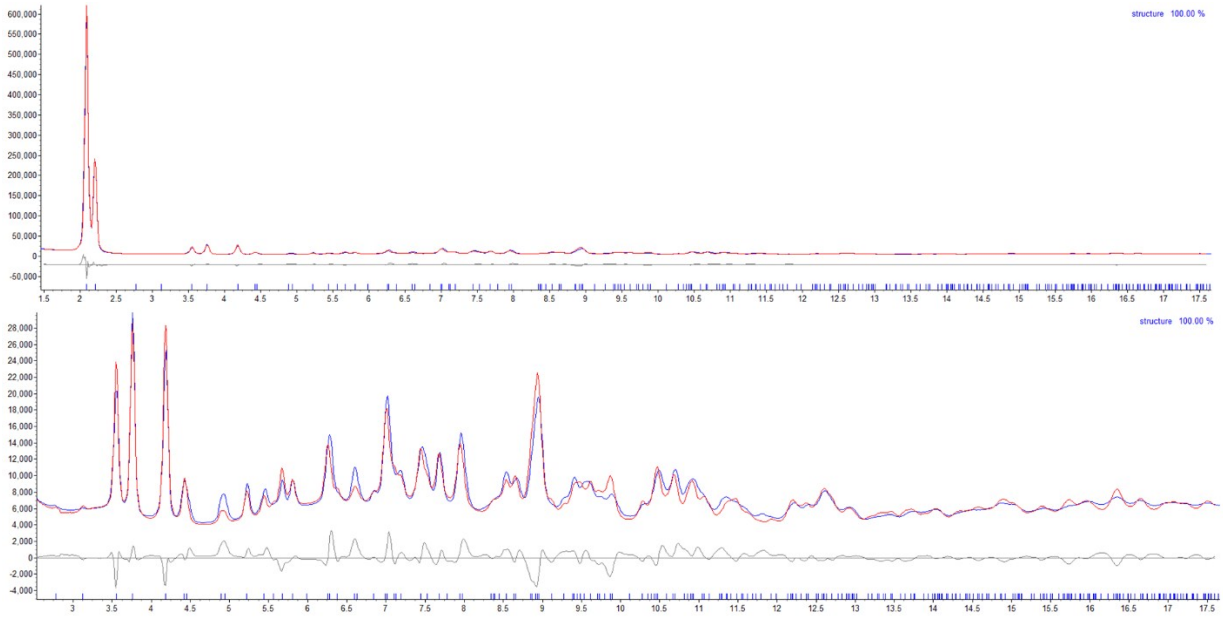


Figure S1. Refinement plots of Hf-VPI-100 (Ni) as synthesized under room temperature. The bottom panel is a zoomed-in view of the low intensity peaks in the top panel. The blue line is the observed curve, the red line is the calculated curve, and the grey line oscillating around 0 is the difference between the observed and the calculated.

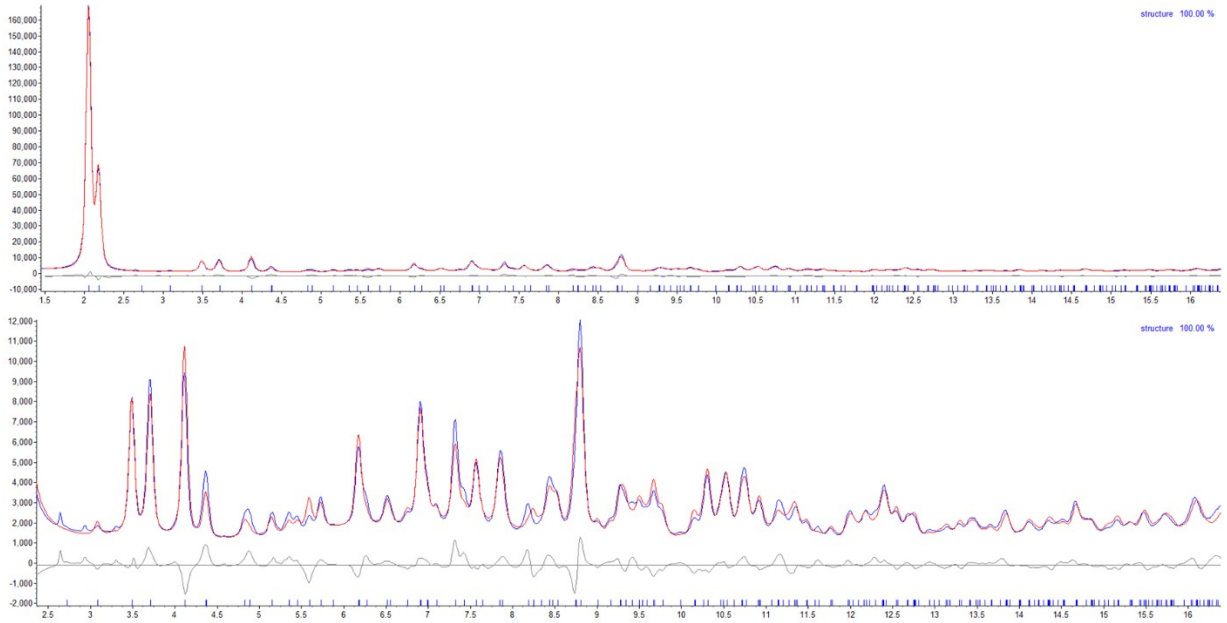


Figure S2. Refinement plots of Hf-VPI-100 (Cu) as synthesized under room temperature. The bottom panel is a zoomed-in view of the low intensity peaks in the top panel. The blue line is the observed curve, the red line is the calculated curve, and the grey line oscillating around 0 is the difference between the observed and the calculated.

Table S1. Crystallographic data for Hf-VPI-100 (Cu) and Hf-VPI-100 (Ni) and refinement statistics

	Hf-VPI-100 (Cu)	**Hf-VPI-100 (Ni)**
Chemical Formula*	C_{24} H_{44} $Cl_{2.68}$ Cu_2 Hf_3 N_8 O_{16}	C_{24} H_{44} $Cl_{1.64}$ Ni_2 Hf_3 N_8 O_{16}
Space group	*I* 4/m	*I* 4/m
***a* (Å)**	16.793(1)	16.594(1)
***c* (Å)**	19.020 (3)	18.661(2)
***V* (Å^3)**	5364(1)	5139(1)
Temperature (K)	298	298
Wavelength (Å)	0.45260(2)	0.45260(2)
2θ range (°)	1.5-16.4	1.5-17.6
R_p	0.0529	0.0537

*Charge balancing chloride and solvent in the MOF pores are not included in the chemical formula

Section 2. Characterization of Hf-VPI-100 (Cu) and Hf-VPI-100 (Ni)

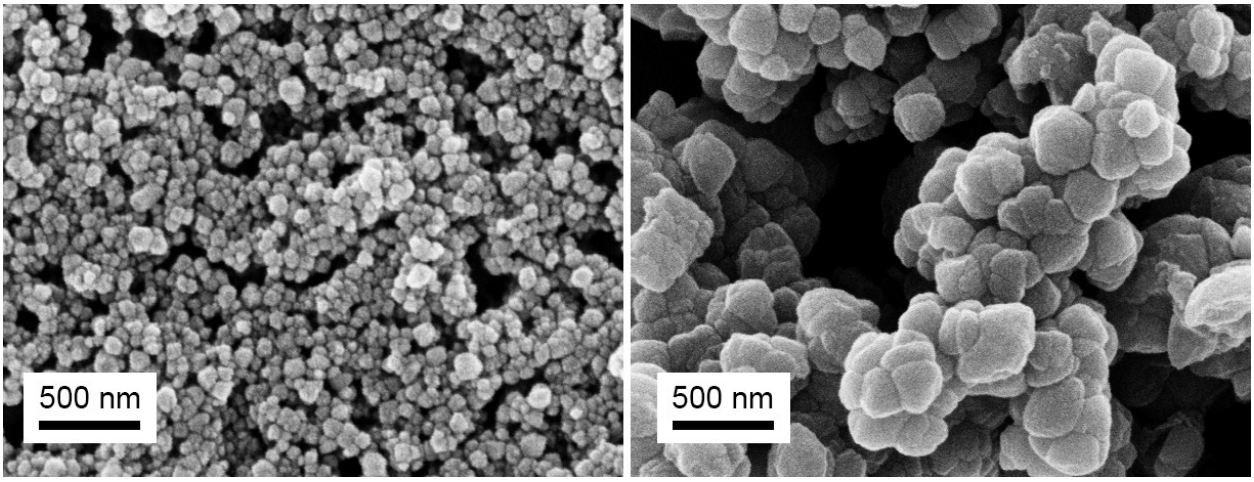


Figure S3. SEM image of the microcrystalline powder of Hf-VPI-100 (Cu) (left) and Hf-VPI-100 (Ni) (right).

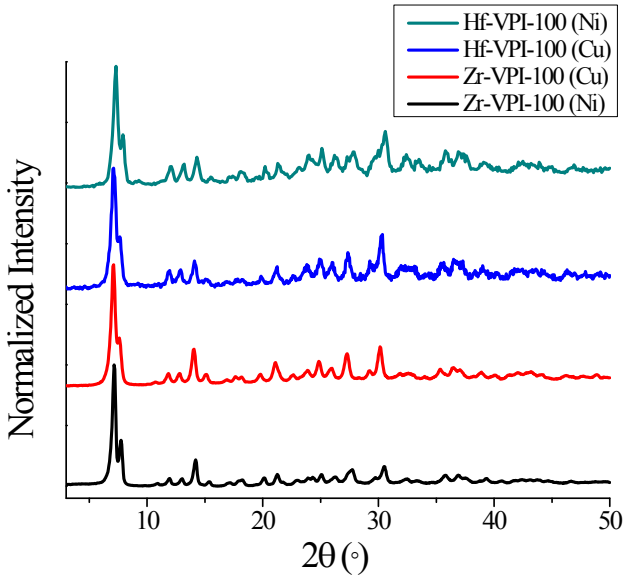


Figure S4. PXRD patterns of as synthesized Hf-VPI-100 and Zr-VPI-100 powders measured at room temperature.

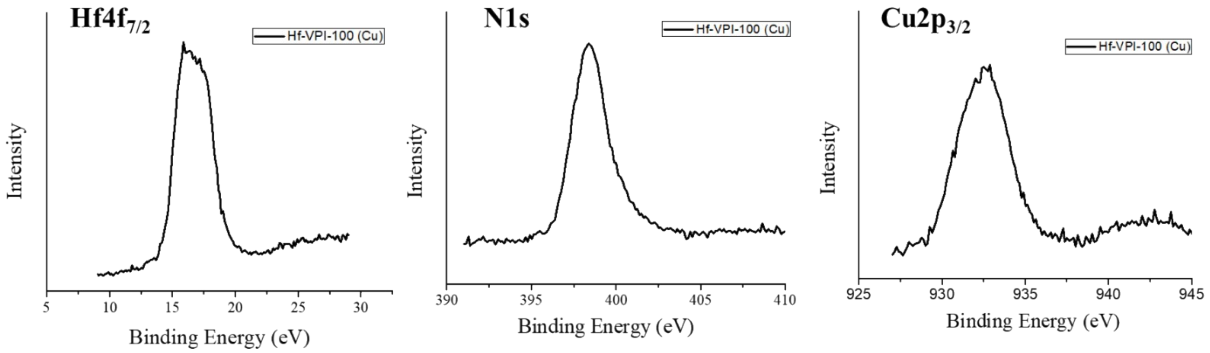


Figure S5. XPS spectrum of Hf-VPI-100 (Cu) powder displaying (left to right) $Hf4f_{7/2}$, N1s and $Cu2p_{3/2}$ binding energy regions.

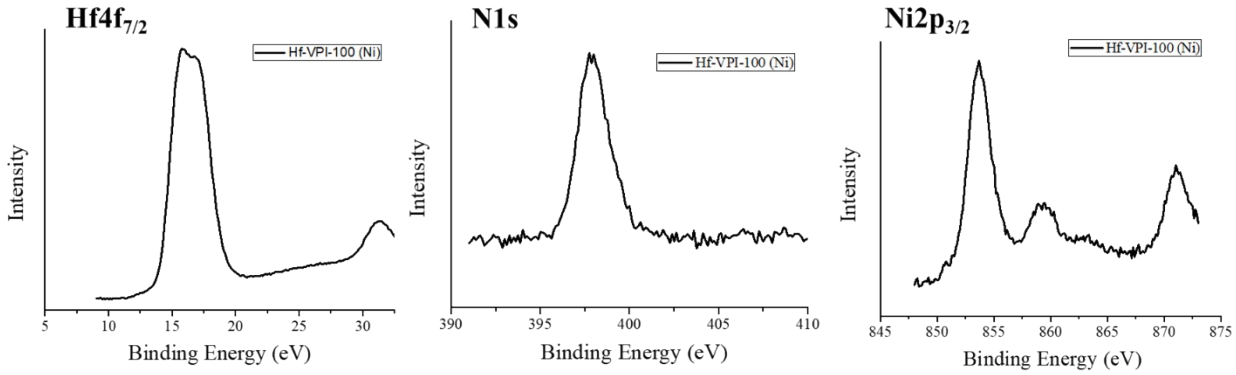


Figure S6. XPS spectrum of Hf-VPI-100 (Ni) powder displaying (left to right) $Hf4f_{7/2}$, N1s and $Ni2p_{3/2}$ binding energy regions.

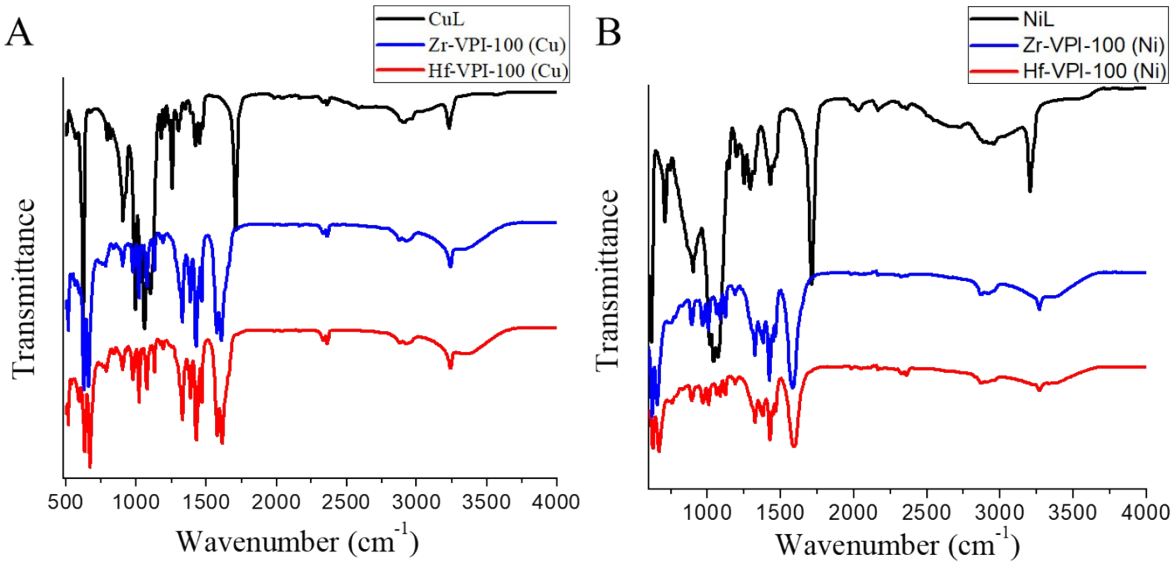


Figure S7. FTIR spectra of metal-cyclam linkers, Zr-VPI-100 MOFs and Hf-VPI-100 MOFs.

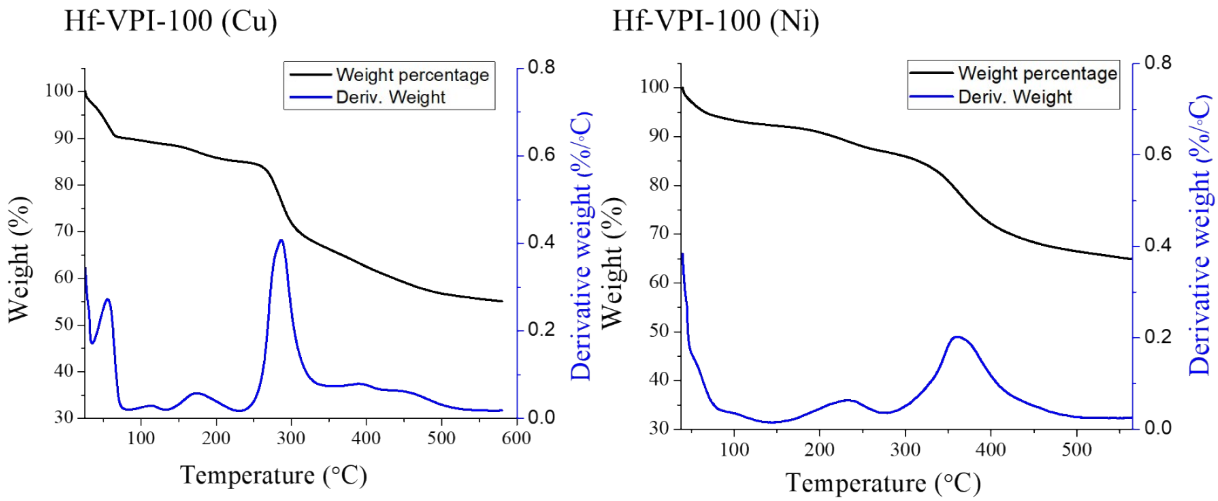


Figure S8. TGA curves of Hf-VPI-100 (Cu) and Hf-VPI-100 (Ni).

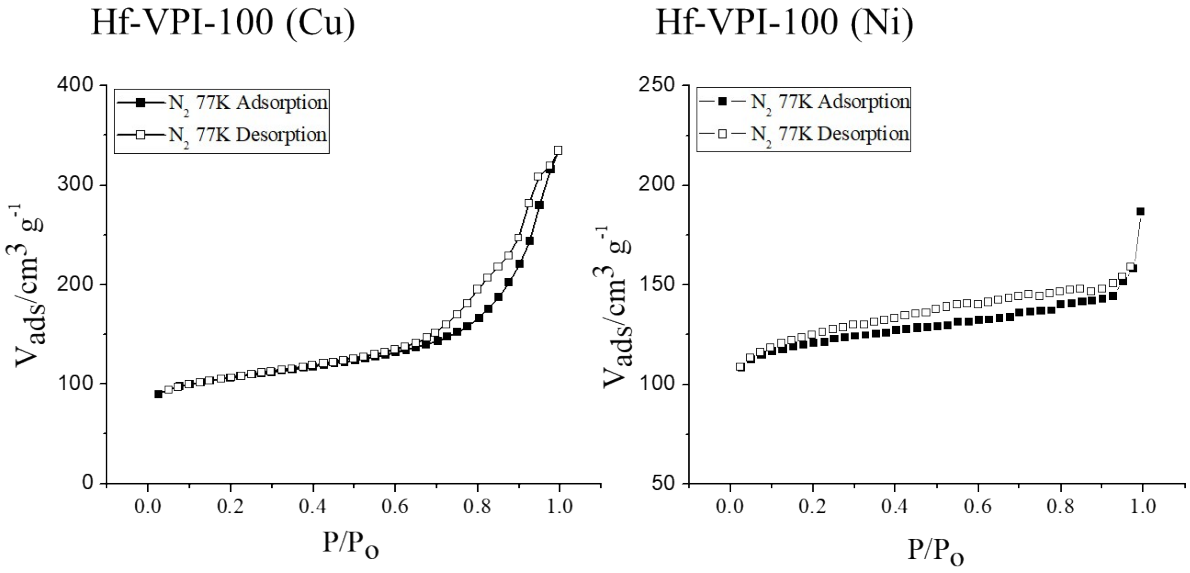


Figure S9. N_2 adsorption isotherms of (A) VPI-100 (Cu) and (B) VPI-100 (Ni) at 77 K, 1 atm after activation at 100 °C for 24 h.

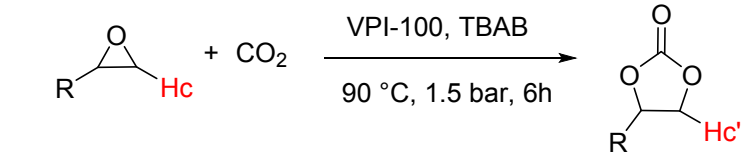
Table S2. The summary of gas sorption properties of VPI-100 and Hf-VPI-100

MOF	**Activation Condition**	**BET surface areas (N_2, 77 K)**	**Pore size**	**CO_2 sorption at 273 K under 1 atm**	
				STP (cm^3/g)	wt. %
VPI-100 (Cu)	373 K	399 m^2/g	6.37 Å	33.85	6.65
VPI-100 (Ni)	373 K	344 m^2/g	5.77 Å	28.2	5.52

Hf- VPI-100 (Cu)	373 K	396 m^2/g	7.7 Å	41.60	8.25
Hf- VPI-100 (Ni)	373 K	399 m^2/g	7.2 Å	46.05	9.13

Section 3. Catalytic studies of cycloaddition of CO_2 to epoxides using Hf-VPI-100

Determination of the catalytic conversion.



R= CH_2Cl (a), C_2H_5 (b)

Scheme S1. Synthesis of cyclic carbonates from CO_2 and epoxides catalyzed by Hf-VPI-100.

For each reaction, conversion was determined by comparison of the ^{1}H NMR integrals of the corresponding proton in the starting material (^{1}Hc) and in the product (^{1}Hc′) according to equation 1 and Table S2.

$$\text{Conversion} = \frac{I_{Hc}'}{(I_{Hc} + I_{Hc}')} \qquad (1)$$

Table S3. Chemical shifts (δ, ppm) for the integrated proton in the epoxides and in the corresponding carbonates (in $CDCl_3$).

Epoxides	**δH ($CDCl_3$)(epoxide, ^{1}Hc)**	**δH ($CDCl_3$)(carbonate, ^{1}Hc′)**
a	2.65	4.35
b	2.45	4.05

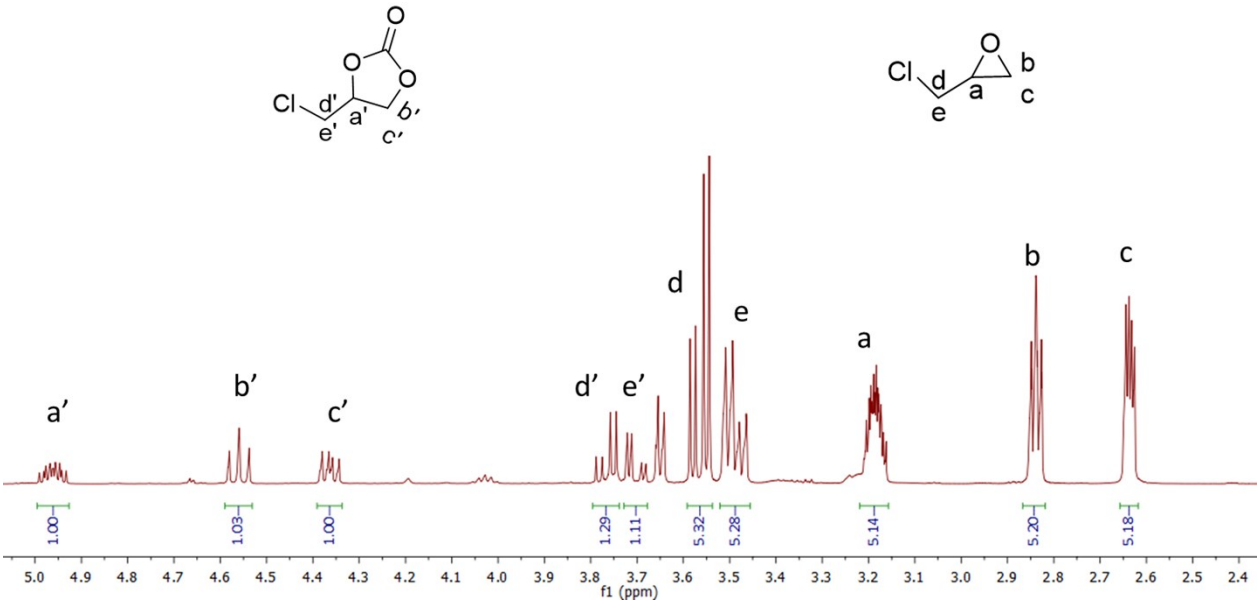


Figure S10. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of reaction mixture in Table 1 entry 1 only using TBAB as catalysts. Conversion = 1/6.18 = 16.2%

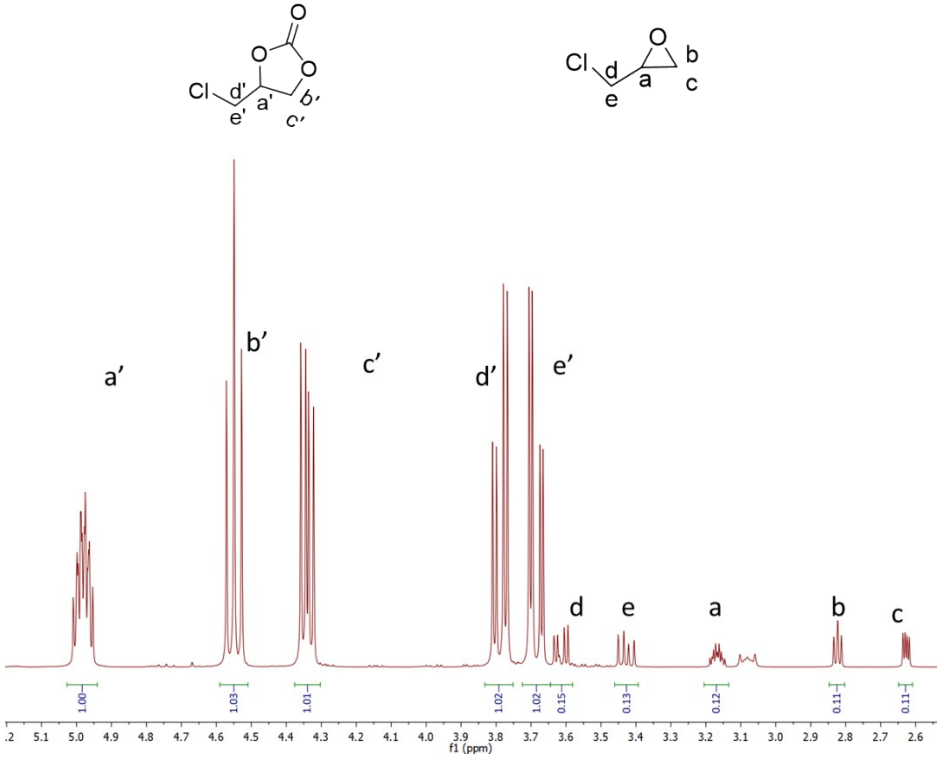


Figure S11. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of reaction mixture in Table 1 entry 2 using $[CuL(ClO_4)_2]$ (1) and TBAB as catalysts. Conversion = 1/2.12, = 90.2%.

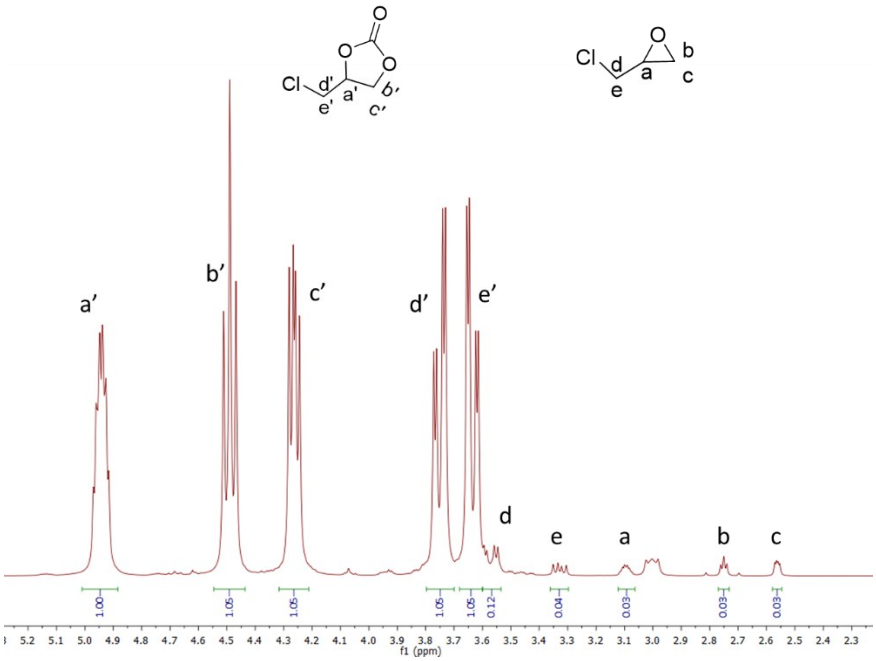


Figure S12. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of reaction mixture in Table 1 entry 3, run 1 using Hf-VPI-100 (Cu) and TBAB as catalysts. Conversion = 1.05/1.08, = 97.2%.

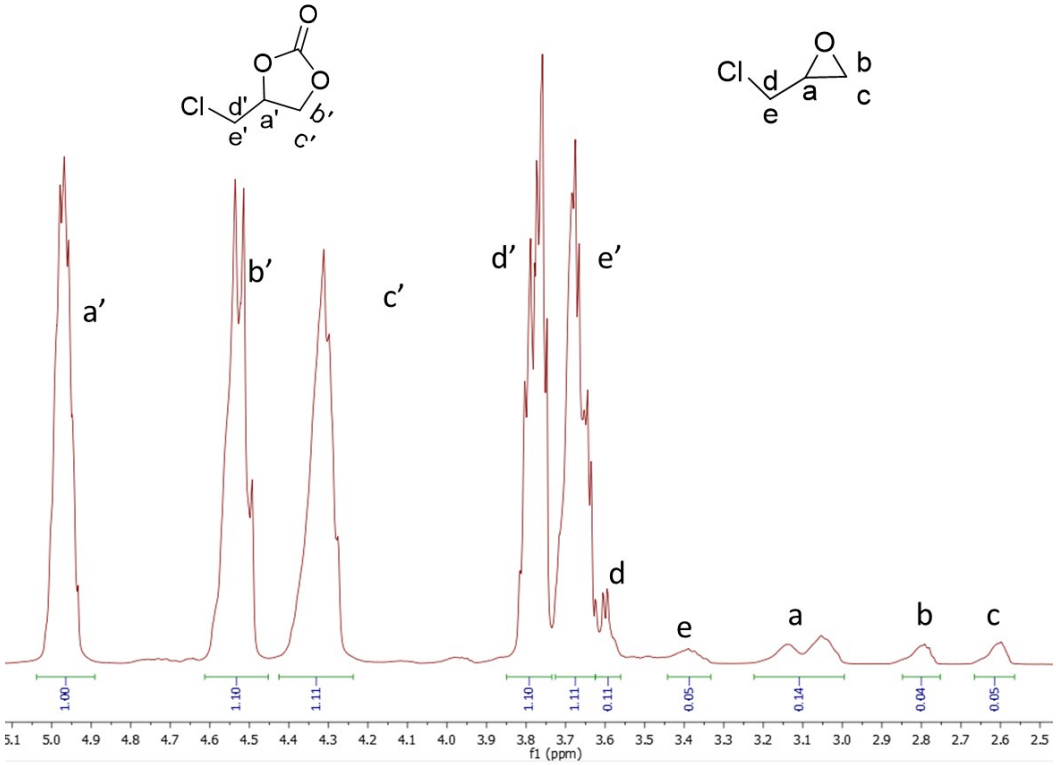


Figure S13. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of reaction mixture in Table 1 entry 4, run 2 using Hf-VPI-100 (Cu) and TBAB as catalysts. Conversion = 1.11/1.16, = 95.6%.

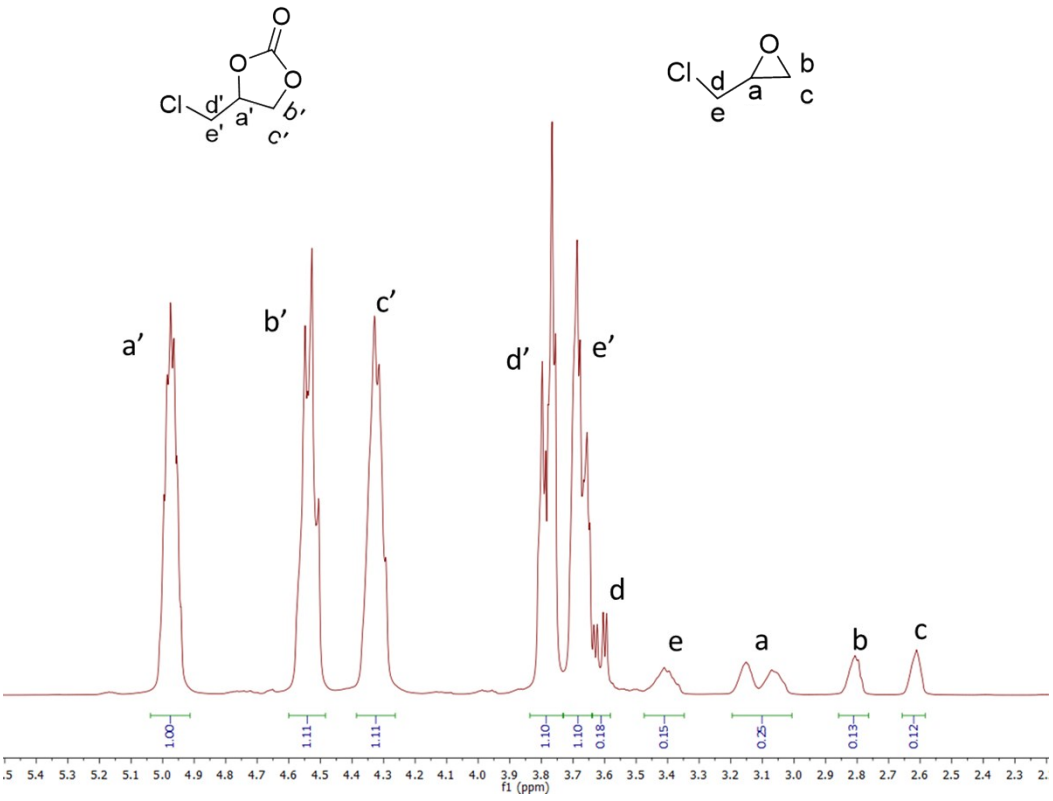


Figure S14. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of reaction mixture in Table 1 entry 5, run 1 using Hf-VPI-100 (Ni) and TBAB as catalysts. Conversion = 1.11/1.23, = 89.5%.

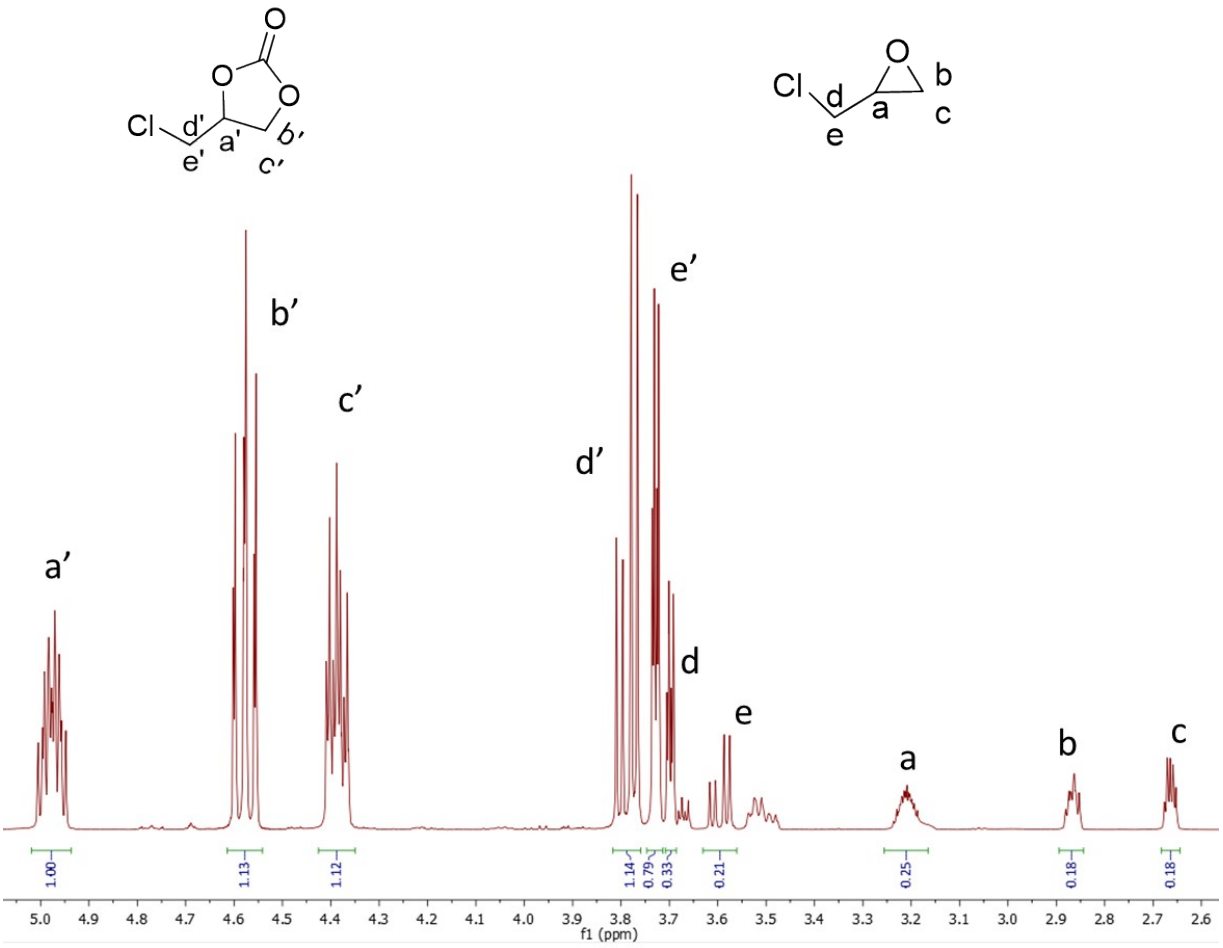


Figure S15. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of reaction mixture in Table 1 entry 6, run 2 using Hf-VPI-100 (Ni) and TBAB as catalysts. Conversion = 1.12/1.3, = 86.2%.

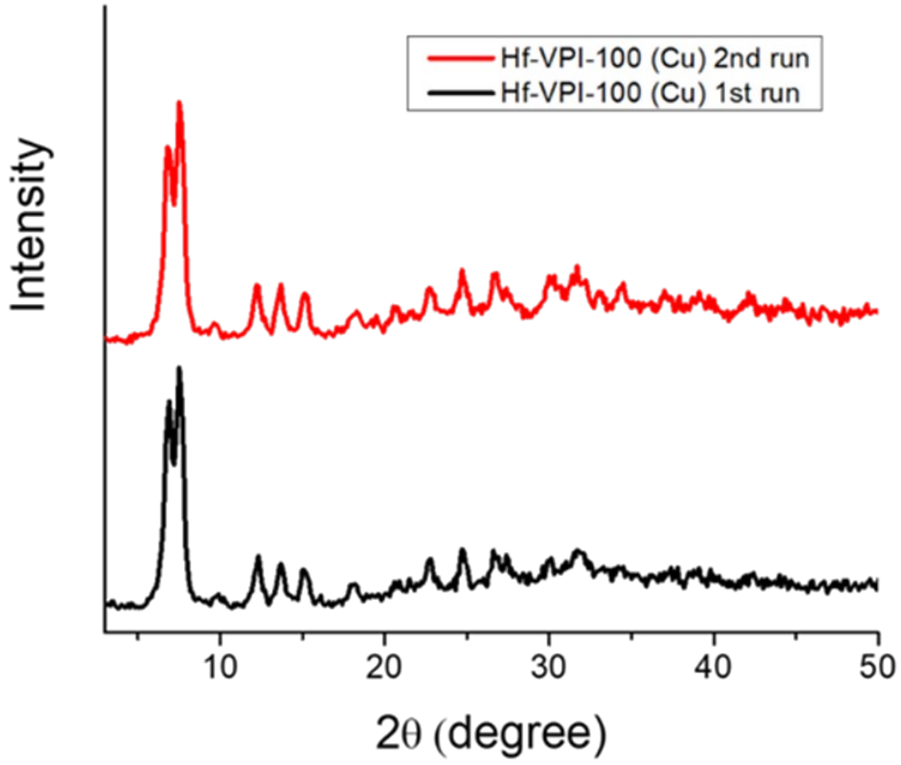


Figure S16. PXRD of Hf-VPI-100 (Cu) after catalysis.

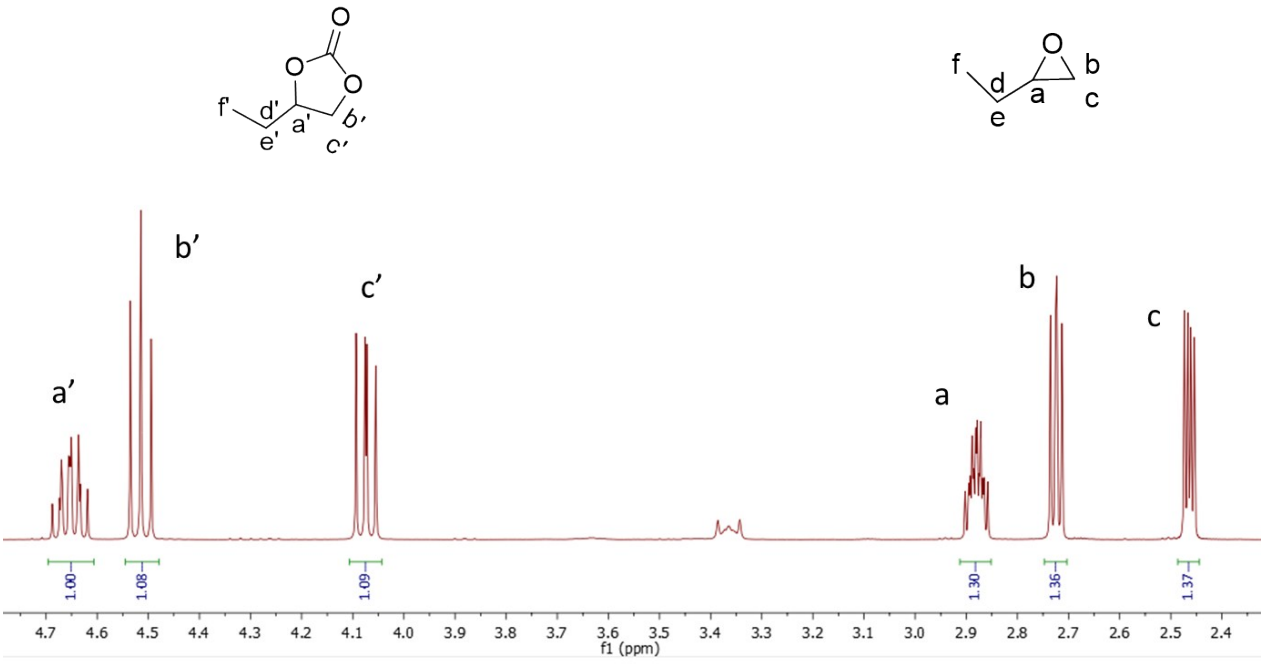


Figure S17. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of reaction mixture in run 1 using Hf-VPI-100 (Cu) and TBAB as catalysts. Conversion = 1.09/2.46, = 43.8%.

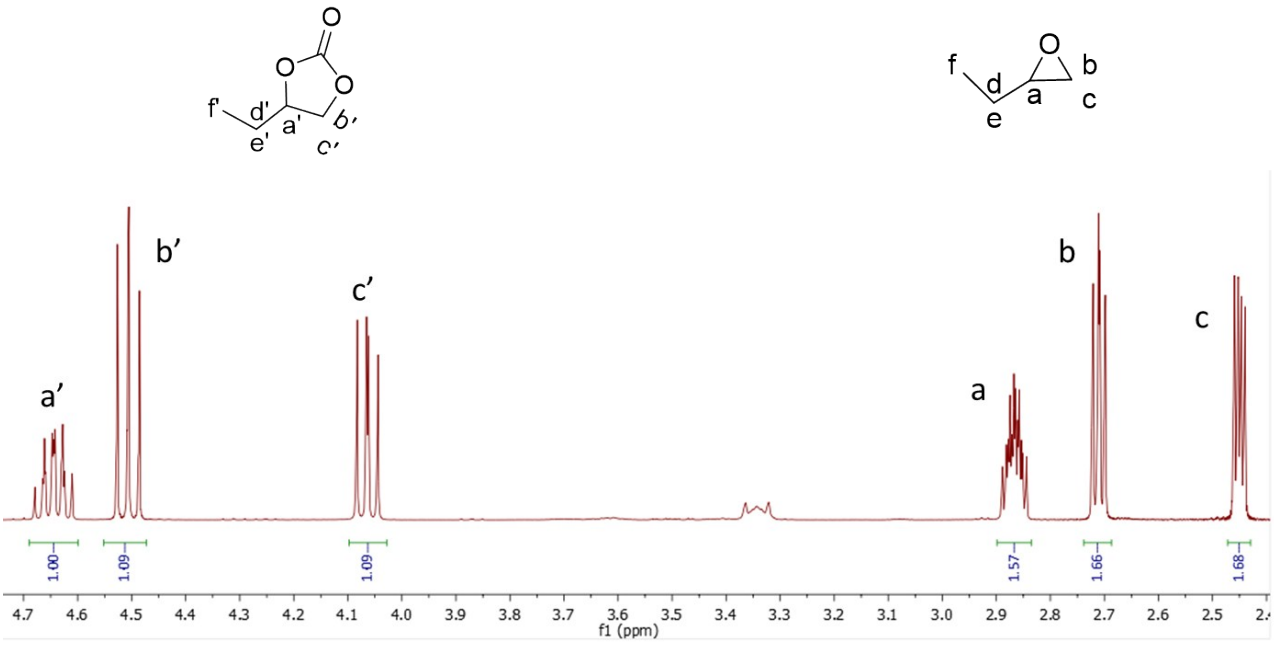


Figure S18. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of reaction mixture in run 1 using Hf-VPI-100 (Ni) and TBAB as catalysts. Conversion = 1.09/2.77, = 39.4%.

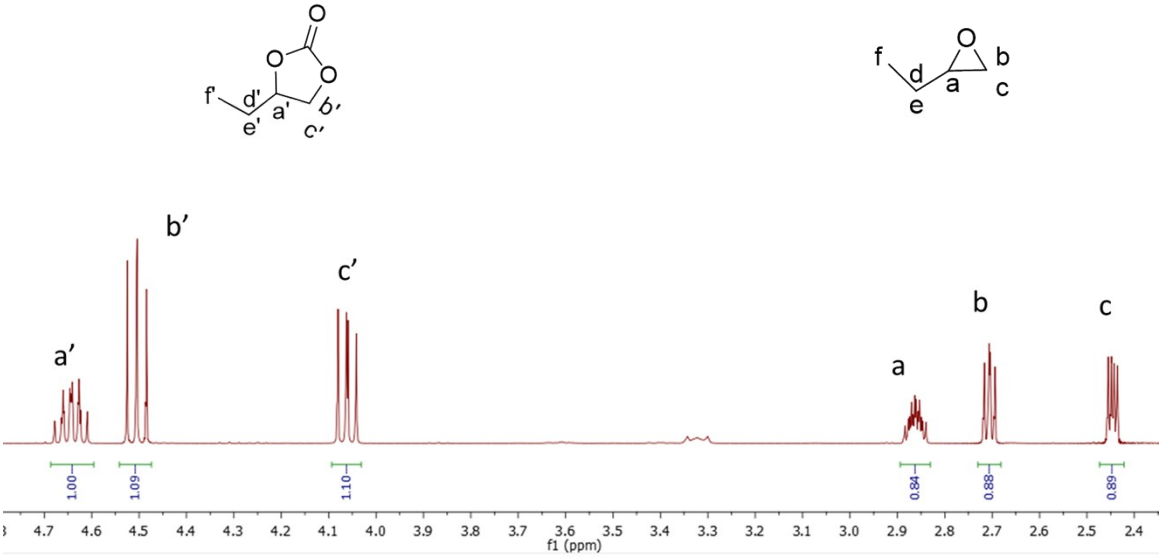


Figure S19. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of reaction mixture in run 1 using Zr-VPI-100 (Cu) and TBAB as catalysts. Conversion = 1.1/1.99, = 55.3%.

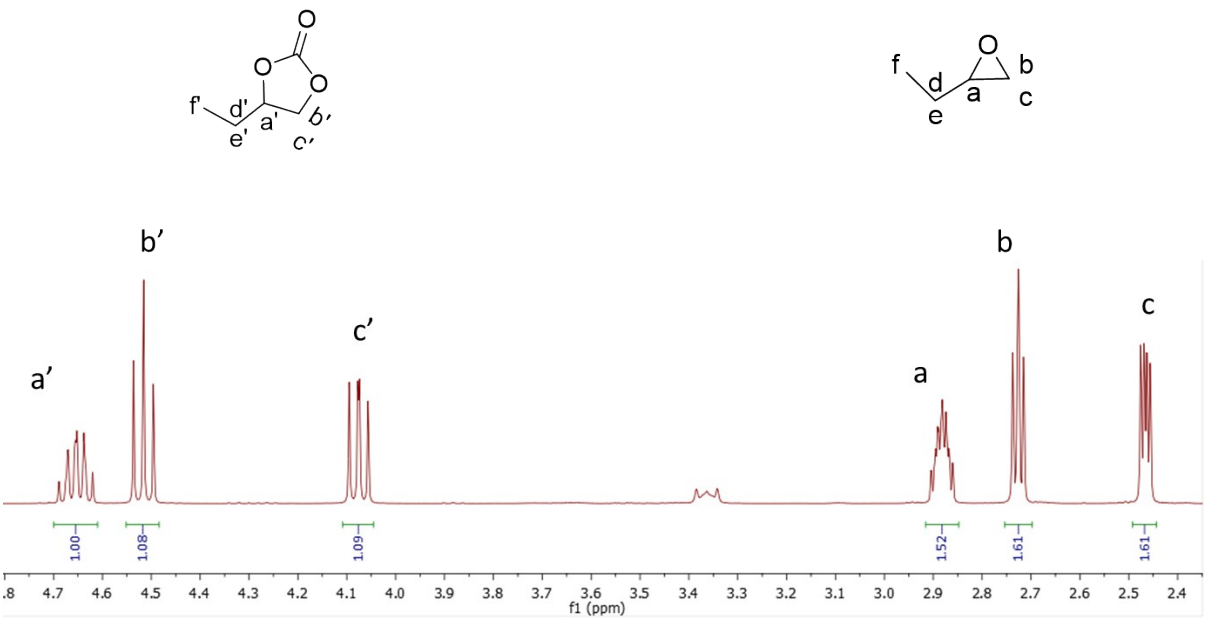


Figure S20. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of reaction mixture in run 1 using Zr-VPI-100 (Ni) and TBAB as catalysts. Conversion = 1.09/2.70, = 40.3%.

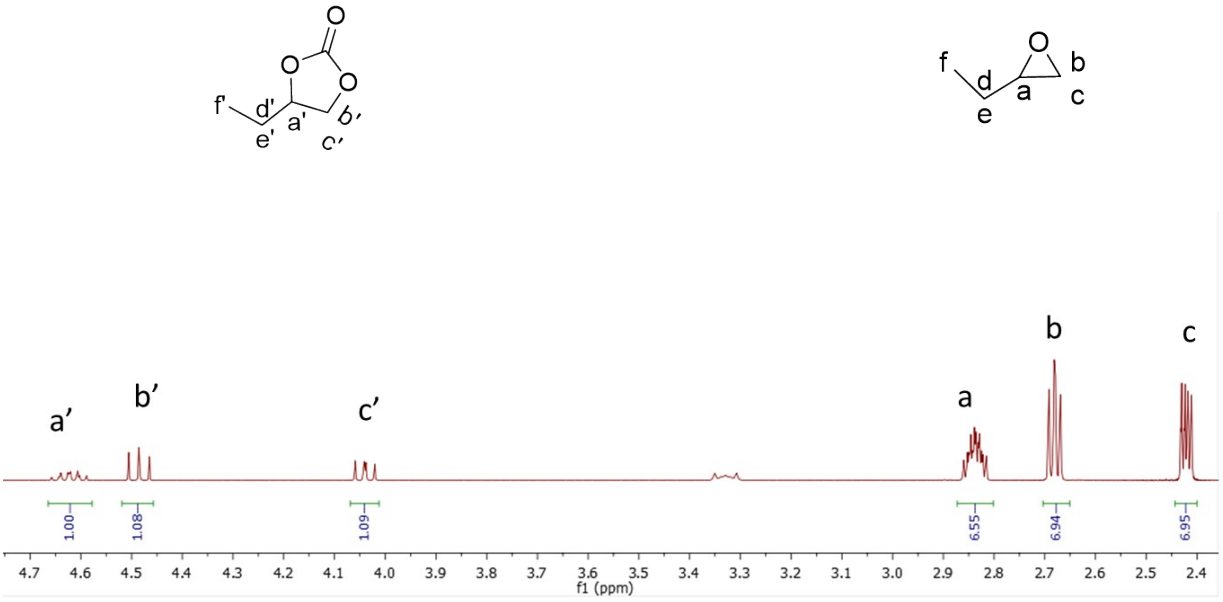


Figure S21. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of reaction mixture using only TBAB as catalysts. Conversion = 1.09/8.04, = 13.5%.

Section 4. The structure of metallo-cyclam ligands

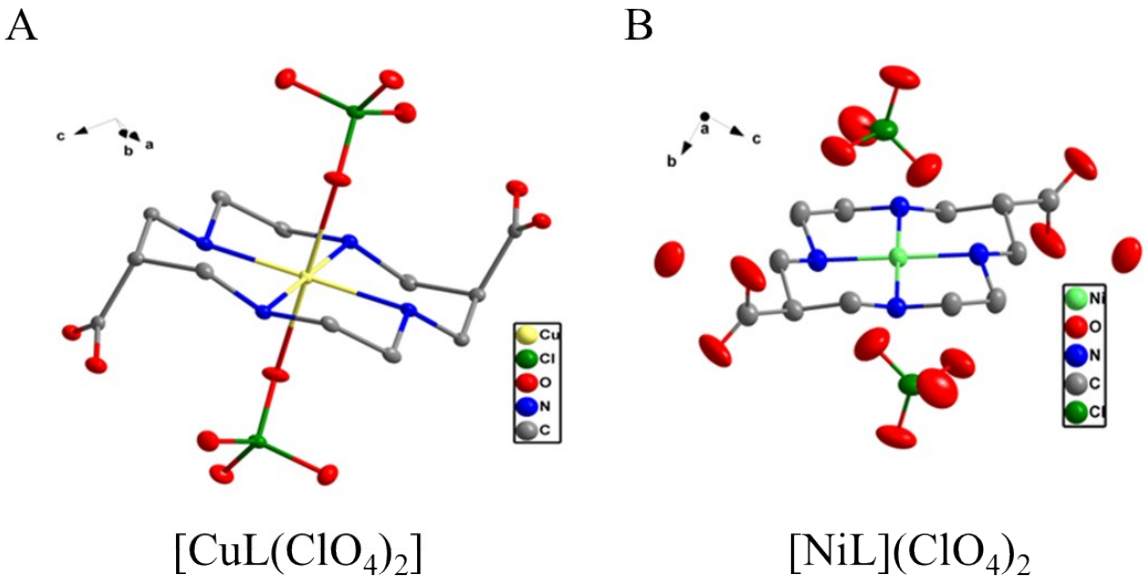


Figure S22. Anisotropic displacement ellipsoid drawings (30%) of (A) $[CuL(ClO_4)_2]$ and (B) $[NiL](ClO_4)_2$. Hydrogen atoms were omitted forclarity. Color scheme: C, gray; O, red; N, blue; Ni, light green; Cu, yellow; Cl, green.

Section 5. Xyz coordinates of optimized structures

M06-L/def2-SVP data in Angstrom.

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Cy(Ni)NH--EPO

  C     -0.238640     2.999911    -0.319202
  N      0.374682     1.873845    -1.018300
  Ni     0.550506     0.113619     0.115019
  Cl    -0.684558    -1.033468    -1.728611
  C     -1.602629     2.655675     0.259661
  C     -1.611915     1.728547     1.465606
  N     -1.267838     0.356333     1.108337
  C     -1.221940    -0.579459     2.229125
  C     -0.619750    -1.891078     1.762557
  N      0.725517    -1.650488     1.242678
  C      1.342095    -2.775694     0.546578
  C      2.711632    -2.431355    -0.019484
  C      2.736417    -1.501450    -1.223240
  N      2.389131    -0.126067    -0.877401
  C      2.330433     0.807686    -2.000687
  C      1.718238     2.117115    -1.540718
```

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H	-0.589305	-0.134630	3.015468
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H	-2.609543	1.763594	1.945153
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H	-0.332590	3.873882	-0.991759
H	0.449325	3.290673	0.491183
H	2.316238	2.540559	-0.716878
H	1.725917	2.856992	-2.361379
H	3.035456	0.233691	-0.170053
H	1.331244	-1.332292	2.003786
H	3.321301	0.983660	-2.457069
H	1.693668	0.347854	-2.774495
H	2.004711	-1.841175	-1.973887
H	3.733654	-1.545774	-1.701162
H	3.352658	-2.020605	0.781970
H	1.431578	-3.651211	1.217727
H	0.660203	-3.064896	-0.269457
H	-1.221654	-2.304263	0.935678
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O	-3.874115	-0.413400	-0.074136
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C	-4.051996	-1.626440	-0.788790
H	-5.160303	0.059252	-1.703359
H	-3.340789	-0.007963	-2.091987
H	-3.136360	-2.210016	-0.941818
H	-4.951757	-2.193426	-0.524189

Cy(Ni)NH--EPO TS

C	0.877021	2.059096	-2.216384
N	0.942487	0.616026	-2.001024
Ni	1.431660	0.030660	-0.044317
Cl	-0.580278	-1.418436	-0.088889
C	-0.045062	2.760572	-1.231100
C	0.450969	2.855808	0.203908
N	0.384699	1.568280	0.886464
C	0.880976	1.590000	2.259039
C	1.022132	0.164726	2.758300
N	1.967862	-0.549687	1.902107
C	2.062738	-1.988843	2.117231
C	3.031790	-2.657239	1.152610
C	2.578440	-2.775373	-0.295097
N	2.561749	-1.489693	-0.983814
C	2.066857	-1.518317	-2.357688
C	1.884418	-0.098395	-2.860079
Cl	3.581991	1.343401	-0.083659
H	3.225555	-3.674266	1.524586

H	-0.213247	3.782084	-1.604171
H	-0.629642	1.329563	0.948643
H	0.011457	0.200825	-2.090652
H	0.211590	2.163822	2.926560
H	1.866366	2.087622	2.269462
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H	-0.158095	3.604616	0.746391
H	-1.040629	2.280673	-1.233900
H	0.556466	2.285191	-3.251911
H	1.903732	2.445494	-2.106390
H	2.844873	0.441131	-2.805514
H	1.573065	-0.101032	-3.920694
H	3.491990	-1.063364	-0.963606
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H	2.731654	-2.083615	-3.036757
H	1.095098	-2.039028	-2.343769
H	1.552717	-3.175953	-0.333758
H	3.229074	-3.497984	-0.825112
H	4.010526	-2.144299	1.195411
H	2.368055	-2.212511	3.157892
H	1.051561	-2.405101	1.981335
H	0.050532	-0.351488	2.679442
H	1.319147	0.144949	3.823193
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H	-2.715550	0.243066	-0.422304
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H	-4.147852	1.073899	2.213770
Br	-5.246093	-0.848513	-0.458341

NU-1000(Hf)--EPO

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C	4.824185	-3.977029	-0.585755
C	5.957662	-4.759453	-0.377283
C	6.850476	-4.478525	0.675624
C	3.285294	-2.106255	0.106873
O	2.528404	-2.358286	-0.874880
Hf	0.402304	-1.721231	-1.439350
O	0.972976	0.072669	-0.546136
Hf	0.200145	1.861585	-1.400675
O	-0.725533	-0.013387	-2.430699
Hf	-2.795971	-0.079170	-1.403347
O	-1.670130	1.442150	-0.567083
Hf	-1.846413	1.717736	1.544487
O	0.311678	2.101215	0.859620
Hf	1.306027	0.067620	1.502311
O	0.466051	-2.027039	0.849055
Hf	-1.715263	-1.871130	1.463453

O	-0.518748	-2.420577	3.400863
C	0.630948	-2.139310	3.821226
O	1.436856	-1.319836	3.303819
O	-4.544316	1.287375	-0.932359
C	-4.689086	2.231693	-0.112952
O	-3.882320	2.572326	0.787135
O	-2.968763	1.319841	-3.163205
C	-2.224530	2.222944	-3.616915
O	-1.086246	2.553939	-3.192383
O	-4.453096	-1.528854	-0.936994
C	-4.589291	-2.420995	-0.062126
O	-3.773351	-2.712430	0.849722
O	-2.863561	-1.510562	-3.162319
C	-2.081851	-2.424559	-3.536291
O	-0.948429	-2.687270	-3.066358
O	-1.559815	-1.510638	-0.574189
O	-3.082294	-0.086591	0.917121
O	-0.730129	-0.012824	1.864889
O	-0.649041	2.502973	3.345236
C	0.514213	2.284381	3.767134
O	1.347132	1.468204	3.291916
O	-1.630712	3.947278	1.062823
O	-3.061173	1.264428	3.197496
O	-2.984085	-1.322469	3.283441
O	-1.389216	-3.918820	1.139109
O	0.107164	-3.950771	-0.980526
O	1.512364	-1.245258	-3.140968
O	3.038425	-1.242299	1.000605
O	2.954062	1.469823	0.980606
C	3.150427	2.315269	0.053203
O	2.351098	2.525615	-0.899488
O	1.476551	1.341821	-3.237218
O	-0.127489	3.907891	-1.042361
C	4.388945	3.143141	0.141637
C	5.299703	2.915753	1.184330
C	6.433191	3.711805	1.317062
C	6.690624	4.766787	0.420541
C	5.784332	4.969497	-0.638873
C	4.653965	4.168827	-0.778046
H	0.841520	2.864793	4.656105
H	0.972832	-2.656215	4.743618
H	-5.527633	-3.014420	-0.101080
H	-2.436882	-3.063037	-4.374257
H	-2.609872	2.787808	-4.492868
H	-5.628141	2.820394	-0.196054
H	5.099775	2.112099	1.894897
H	3.949715	4.339283	-1.595303
H	5.965081	5.771905	-1.358461
H	7.127809	3.522784	2.139517
H	5.209536	-1.759907	1.967020
H	4.134160	-4.205461	-1.401014
H	6.154029	-5.605549	-1.040445
H	7.245582	-3.132922	2.327678
H	7.572879	5.398877	0.534166

H	7.736473	-5.093892	0.840060
H	-0.719346	-0.059731	-3.393825
H	0.751878	2.909229	1.150679
H	-2.566436	-1.616165	4.104891
H	-3.066926	-0.305817	3.354832
H	2.454805	-1.475417	-3.157611
H	-0.488213	-4.053826	-0.157532
H	-2.196084	-4.437789	1.041754
H	-0.362843	-4.385290	-1.705480
H	-3.991942	-0.084324	1.240206
H	0.930251	-2.800910	1.191503
H	-2.797454	1.691259	4.021057
H	1.552540	0.320704	-3.297696
H	1.152655	1.641654	-4.096043
H	-2.494072	4.320833	0.837469
H	-0.506307	4.387732	-1.788139
H	-1.053348	4.049240	0.225699
O	4.303039	-0.672192	-3.320185
C	5.416701	-0.645987	-2.445860
C	4.305671	0.272559	-2.262247
H	6.351048	-0.286306	-2.891656
H	5.524170	-1.517869	-1.790709
H	4.402822	1.320428	-2.569036
H	3.557746	0.092819	-1.477457

NU-1000(Hf)--EPO TS

C	6.197203	-3.388530	1.830918
C	5.072641	-2.608773	1.576687
C	4.223561	-2.912699	0.501194
C	4.532579	-4.009082	-0.318269
C	5.652860	-4.794132	-0.055437
C	6.506122	-4.502793	1.027019
C	2.978610	-2.121019	0.288457
O	2.248537	-2.396413	-0.704840
Hf	0.190643	-1.731933	-1.394295
O	0.701013	0.067856	-0.480804
Hf	-0.020104	1.843192	-1.386521
O	-0.929857	-0.030973	-2.426295
Hf	-3.022234	-0.088473	-1.480830
O	-1.931682	1.446613	-0.619582
Hf	-2.177241	1.737156	1.478207
O	0.000102	2.114311	0.872770
Hf	0.975897	0.083562	1.567586
O	0.140172	-2.014776	0.919423
Hf	-2.051401	-1.845709	1.433383
O	-0.948638	-2.375320	3.435263
C	0.183432	-2.088210	3.898021
O	1.015513	-1.283107	3.405395
O	-4.788200	1.295594	-1.097124
C	-4.957289	2.253195	-0.298570
O	-4.193362	2.594964	0.637568
O	-3.128098	1.292176	-3.266936

C	-2.360070	2.182514	-3.704642
O	-1.243349	2.524359	-3.236824
O	-4.709156	-1.524556	-1.065023
C	-4.885300	-2.398746	-0.179014
O	-4.108541	-2.679291	0.767758
O	-3.035037	-1.539543	-3.220308
C	-2.246345	-2.464037	-3.553734
O	-1.130464	-2.726051	-3.046899
O	-1.827983	-1.514947	-0.595112
O	-3.400046	-0.065730	0.826793
O	-1.082858	0.013968	1.863553
O	-1.052986	2.556448	3.310865
C	0.093368	2.334804	3.777746
O	0.935651	1.505026	3.349510
O	-1.946586	3.969864	0.974015
O	-3.456350	1.307041	3.095952
O	-3.382225	-1.289438	3.221007
O	-1.722860	-3.902895	1.160502
O	-0.151493	-3.967626	-0.922688
O	1.326353	-1.271431	-3.035036
O	2.704695	-1.239132	1.158429
O	2.625874	1.480076	1.107508
C	2.870401	2.299921	0.167935
O	2.107723	2.498672	-0.817730
O	1.299658	1.312189	-3.174497
O	-0.360420	3.899175	-1.063331
C	4.109178	3.122760	0.292396
C	4.977946	2.905607	1.372433
C	6.109893	3.697781	1.537560
C	6.407406	4.738663	0.636972
C	5.543606	4.930881	-0.459256
C	4.415000	4.133985	-0.630633
H	0.391848	2.929027	4.668508
H	0.481443	-2.590662	4.844422
H	-5.827561	-2.985033	-0.243057
H	-2.581196	-3.114165	-4.391998
H	-2.703739	2.727806	-4.610877
H	-5.882795	2.854503	-0.436079
H	4.756040	2.100437	2.073825
H	3.746284	4.292880	-1.479409
H	5.758340	5.719606	-1.184919
H	6.776589	3.509870	2.383171
H	4.841611	-1.746412	2.203773
H	3.875050	-4.241846	-1.158966
H	5.872097	-5.648308	-0.701204
H	6.849558	-3.129919	2.668825
H	7.290989	5.364832	0.772755
H	7.384314	-5.117676	1.231503
H	-0.867828	-0.092130	-3.386415
H	0.435773	2.922395	1.169693
H	-2.943979	-1.559253	4.040235
H	-3.467059	-0.273081	3.270991
H	2.318132	-1.378795	-3.091314
H	-0.769972	-4.051042	-0.118665

H	-2.528632	-4.418229	1.038642
H	-0.624533	-4.375353	-1.661190
H	-4.320540	-0.056704	1.116151
H	0.592953	-2.783123	1.287802
H	-3.206246	1.738012	3.921513
H	1.377442	0.285832	-3.208848
H	0.999394	1.589811	-4.048745
H	-2.803817	4.320570	0.695195
H	-0.707784	4.364994	-1.832829
H	-1.333157	4.053852	0.159504
O	3.913146	-0.958877	-3.347511
C	5.450469	-0.840945	-2.175861
C	4.243159	-0.044801	-2.377221
H	6.219129	-0.784660	-2.944094
H	5.352559	-1.788004	-1.647696
H	4.425245	0.999517	-2.715766
H	3.562380	0.006941	-1.495986
Br	6.918993	0.147670	-0.447571

Cy(Ni)-EPO

C	2.725269	1.369079	0.191798
N	1.299366	1.577029	0.478319
Ni	0.074650	0.007916	-0.193114
N	-1.207106	-1.550097	-0.762411
C	-2.631983	-1.353273	-0.493246
C	-3.166294	-0.059694	-1.086235
H	-4.263347	-0.093757	-1.028769
C	3.263065	0.071820	0.772158
C	2.803290	-1.209257	0.096319
N	1.396309	-1.523673	0.378545
C	0.883365	-2.710068	-0.321056
C	-0.624785	-2.765830	-0.188769
H	4.359406	0.108507	0.699840
C	0.724538	2.771203	-0.156408
C	-0.785037	2.739469	-0.036786
N	-1.296542	1.518714	-0.665204
C	-2.711877	1.232468	-0.427839
O	-0.818951	-0.204807	1.877322
Cl	0.877923	0.112042	-2.463025
H	1.303661	-1.683264	1.384051
H	1.182937	1.663302	1.490897
H	1.344885	-3.641614	0.046779
H	1.161002	-2.605173	-1.381835
H	2.897569	-1.113266	-0.996129
H	3.451709	-2.048140	0.405400
H	3.053768	0.024555	1.856681
H	3.318817	2.220978	0.568505
H	2.831476	1.360717	-0.903849
H	1.013493	2.741126	-1.218869
H	1.130878	3.705123	0.266149
H	-1.128531	1.576651	-1.674062
H	-1.050447	-1.556262	-1.774382

H	-1.226938	3.651278	-0.473199
H	-1.086636	2.728720	1.023883
H	-2.869522	1.180621	0.662208
H	-3.340207	2.068162	-0.785064
H	-2.937657	-0.024300	-2.166064
H	-3.219625	-2.204725	-0.881343
H	-2.767991	-1.357847	0.600506
H	-0.916792	-2.807500	0.873843
H	-1.021052	-3.682085	-0.658496
C	-1.567463	0.329346	2.964548
C	-0.406134	-0.510566	3.206022
H	0.538080	-0.051063	3.519553
H	-0.539828	-1.557345	3.499034
H	-1.487982	1.413085	3.102754
H	-2.574326	-0.086378	3.074255

Cy(Ni)-EPO TS

C	-0.532650	2.667924	1.408575
N	-0.320750	1.226200	1.589285
Ni	-1.097586	0.061299	0.009722
N	-1.899225	-1.115581	-1.542101
C	-1.713168	-2.556917	-1.389531
C	-2.264165	-3.082870	-0.073488
H	-2.279010	-4.180615	-0.133304
C	0.028919	3.195607	0.098178
C	-0.731919	2.820979	-1.163953
N	-0.580825	1.408666	-1.518647
C	-1.373675	0.973190	-2.672252
C	-1.345237	-0.539462	-2.767397
H	0.038678	4.293243	0.163613
C	-0.961115	0.671931	2.789440
C	-0.956923	-0.842743	2.730965
N	-1.650349	-1.287256	1.521950
C	-1.505117	-2.702278	1.188029
O	0.705414	-0.936345	-0.405637
Cl	-3.355616	1.038734	0.255903
H	0.404197	1.211682	-1.708462
H	0.685200	1.053473	1.649178
H	-1.026559	1.429828	-3.615511
H	-2.406835	1.317618	-2.503965
H	-1.808328	3.000823	-1.016301
H	-0.406429	3.468537	-1.998806
H	1.093112	2.913745	-0.000286
H	-0.092925	3.228714	2.253161
H	-1.620317	2.834816	1.440270
H	-2.000316	1.037043	2.794096
H	-0.484878	1.026957	3.719363
H	-2.643378	-1.051874	1.605445
H	-2.894261	-0.883871	-1.482446
H	-1.401812	-1.262316	3.650375
H	0.076810	-1.223322	2.690197
H	-0.430031	-2.910399	1.059307

H	-1.846051	-3.338189	2.026197
H	-3.323875	-2.788027	0.031699
H	-2.186057	-3.102424	-2.227490
H	-0.631324	-2.753719	-1.450539
H	-0.305244	-0.893398	-2.858165
H	-1.879440	-0.879397	-3.672249
C	1.815318	-1.283911	0.363150
C	2.408929	-0.363620	-0.582685
H	2.347602	0.706281	-0.398644
H	2.672373	-0.707649	-1.578903
H	1.809414	-0.961460	1.420578
H	2.119137	-2.342258	0.299703
Br	4.985656	-0.157118	-0.041805

Cy(Cu)-EPO

C	-2.673528	-1.400906	0.477758
N	-1.219319	-1.573665	0.552706
Cu	-0.142509	0.005180	-0.229843
N	1.056614	1.579869	-0.837018
C	2.504995	1.397703	-0.751051
C	2.981040	0.155785	-1.480478
H	4.076168	0.205121	-1.552132
C	-3.153005	-0.143496	1.175466
C	-2.790228	1.157437	0.486389
N	-1.360101	1.471160	0.593068
C	-0.964420	2.699033	-0.111065
C	0.542178	2.777553	-0.166710
H	-4.248480	-0.194603	1.242405
C	-0.725272	-2.754371	-0.167385
C	0.781353	-2.703822	-0.239780
N	1.185714	-1.452346	-0.887343
C	2.619141	-1.168687	-0.836696
O	1.063721	-0.089304	2.035012
Cl	-1.216574	-0.014144	-2.512950
H	-1.113016	1.558238	1.582247
H	-0.925458	-1.623169	1.532369
H	-1.394703	3.598419	0.358712
H	-1.375058	2.629768	-1.130957
H	-3.021094	1.094529	-0.588783
H	-3.387637	1.986672	0.903347
H	-2.802518	-0.131818	2.223214
H	-3.178967	-2.284961	0.904213
H	-2.932273	-1.360840	-0.592285
H	-1.152422	-2.712990	-1.182009
H	-1.070065	-3.692371	0.297666
H	0.862361	-1.456495	-1.861997
H	0.759119	1.588672	-1.819353
H	1.178276	-3.586984	-0.767576
H	1.217565	-2.718333	0.772323
H	2.924719	-1.174791	0.221681
H	3.182419	-1.983438	-1.325158
H	2.623146	0.175738	-2.524514

H	3.021370	2.285415	-1.157303
H	2.770790	1.343765	0.317709
H	0.967730	2.804642	0.849752
H	0.869441	3.702671	-0.669526
C	2.102162	-0.466871	2.930448
C	1.108397	0.516018	3.321720
H	0.296828	0.232180	4.000704
H	1.373349	1.579340	3.329054
H	2.038360	-1.490865	3.313815
H	3.107576	-0.136239	2.646293

Cy(Cu)-EPO TS

C	-1.787430	-2.597444	-1.331181
N	-1.256180	-1.261295	-1.585810
Cu	-1.249515	0.022776	0.032616
N	-1.148050	1.324095	1.642086
C	-0.639032	2.668258	1.384364
C	-1.362622	3.362392	0.245463
H	-1.062479	4.419434	0.251342
C	-1.073368	-3.303275	-0.193633
C	-1.335706	-2.740948	1.190981
N	-0.703375	-1.439064	1.393926
C	-0.940664	-0.840302	2.708415
C	-0.449869	0.588810	2.697811
H	-1.392425	-4.354930	-0.196877
C	-1.930200	-0.529354	-2.658135
C	-1.443234	0.900947	-2.665370
N	-1.698852	1.497902	-1.353220
C	-1.094310	2.810197	-1.142397
O	1.010422	0.012373	-0.467450
Cl	-3.787860	-0.161649	0.501652
H	0.302919	-1.495872	1.212480
H	-0.245213	-1.288656	-1.757001
H	-0.464329	-1.416855	3.519595
H	-2.028762	-0.862640	2.883466
H	-2.417920	-2.597687	1.343194
H	-0.988626	-3.456778	1.957969
H	0.013961	-3.330650	-0.389788
H	-1.727562	-3.212266	-2.247735
H	-2.856334	-2.477308	-1.089760
H	-3.011175	-0.558374	-2.443688
H	-1.777817	-1.002867	-3.643191
H	-2.709798	1.535428	-1.180548
H	-2.153523	1.352927	1.846735
H	-1.917395	1.474543	-3.480098
H	-0.355241	0.932942	-2.840144
H	-0.009278	2.707892	-1.309826
H	-1.459206	3.524856	-1.902226
H	-2.449294	3.368569	0.441253
H	-0.709707	3.285010	2.298544
H	0.435150	2.578986	1.154394
H	0.628866	0.621803	2.470020

H	-0.582664	1.058387	3.687450
C	2.153697	0.779601	-0.617546
C	2.787452	-0.447708	-0.172045
H	2.920948	-1.261708	-0.879709
H	2.781628	-0.685419	0.889260
H	2.390919	1.104963	-1.648847
H	2.257212	1.646005	0.065577
Br	5.356293	-0.125134	-0.060155
