Electronic Supplementary Material (ESI) for ChemComm.


# Imidazolium salts modified porous hypercrosslinked polymers for a synergistic $CO_2$ capture and conversion

**Jinquan Wang, Waihong Sng, Guangshun Yi and Yugen Zhang***

*Institute of Bioengineering and Nanotechnology, 31 Biopolis Way, The Nanos, Singapore 138669*

*Email: ygzhang@ibn.a-star.edu.sg*

**Supporting information**

1. *General information* *S2*
2. *Synthesis* *S3*
3. *Characterization of cyclic carbonates* *S4-S6*
4. *Supporting Figures* *S7-S35*
5. *Supporting Tables* *S36-S37*
6. *Cartesian coordinates for all the optimized geometries* *S38-S60*

## 1. General information

The 1-Methylimidazole, 1, 4-bis (chloromethyl) benzene, 1, 2-bis (chloromethyl) benzene and iron chloride were provided by Sigma-Aldrich. The chloromethyl polystyrene was purchased from Fluka, and the epoxides were purchased from the VWR international. GC-MS were measured on SHIMADZU-QP2010. GC analyses were performed on an Agilent GC-6890 using a flame ionization detector. NMR spectra were recorded on a Bruker 400. $N_2$ sorption analysis and $CO_2$ sorption analysis were performed on a Micromeritics Tristar 3000 (77 and 273 K, respectively). TEM experiments were conducted on a FEI Tecnai $G^2$ F20 electron microscope (200 kV). TGA was performed on a Perkin–Elmer Pyris-1 thermogravimetric analyzer. Elemental analysis (CHNS) was performed on an Elementarvario MICRO cube. FT-IR experiments were performed on a Perkin Elmer Spectrum 100. Solid-$^{13}C$ NMR experiments were conducted at a Bruker Avance 400 (DRX400) with CP/MAS.

The calculations were carried out by performing DFT by use of the B3PW91functional with the 6-31++G (d, p) basis set as implemented in Gaussian 03 program package. The solvent effect uses the Conductor Polarizable Continuum Model (CPCM) in each case. Vibrational frequency calculations, from which the zero-point energies were derived, have been performed for each optimized stucture at the same level to indentify the natures of all the stationary points. All the bond lengths are in angstroms (Å). Structures were generated using CYLview.[1]

1. CYLview, 1.0b; C. Y. Legault, Université de Sherbrooke, 2009 (http://www.cylview.org).

The $CO_2$ experiments were performed on a Belsorp-mimiII at 273 and 298 K. Before each measurement, the samples were heated at 150 $^oC$ in vacuum for 24 h. TGA gas capture experiments were conducted on a on a Perkin-Elmer Pyris-1 thermogravimetric analyzer. Porous carbons (5 mg) were subjected to the following gas capture and cycling experiment at 25 $^oC$: $CO_2$ (99.8%) gas flow at 20 mL $min^{-1}$ for 30 min, followed by $N_2$ (99.9995%) gas flow at 20 mL $min^{-1}$ for 45 min. Changes in weight were recorded by using TGA. Prior to the cyclic treatment, the sample was first purged under $N_2$ gas flow at 200 $^oC$ for 60 min, followed by cooling to room temperature. Change in buoyancy effects arising from the switching of gases was recorded by using an empty sample pan, and the buoyancy effects were corrected for in the TGA results. For the adsorption kinetics analysis, the porous carbon was first purged under Ar gas flow (20 mL $min^{-1}$) at 200 $^oC$ for 60 min, followed by cooling to room temperature. The gas was then switched from Ar to $CO_2$ or $N_2$ (20 mL $min^{-1}$). The selectivity of $CO_2$ over $N_2$ is calculated by the saturated absorption according to reported work by Fuertes.[2]

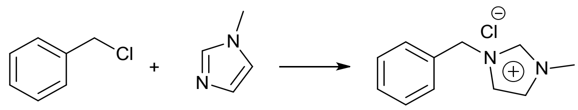
2. M. Sevilla and A. B. Fuertes, Energy Environ. Sci., 2011, 4, 1765;

## 2. *Synthesis*

### 2.1 Material synthesis

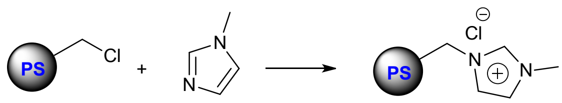
The benzyl halide-functionalized organic polymers were synthesized according to the reported method.[10] Typically, iron (III) chloride (120 mmol) was added to a solution of benzyl halide compound (60 mmol) in anhydrous dichloroethane (80 ml). The resulting mixture was heated at 80 °C for 24 h. When the reaction was completed, the solid product was centrifuged and washed with methanol (3×20 ml). The product was further purified by Soxhlet extraction in methanol for 20 h and dried in vacuum at 60 °C for 24 h. The polymers were obtained in quantitative yields. The content of chloride or bromide in the obtained polymers was determined by elemental analysis (Table S2). The polymers were further reacted with N-methylimidazole (molar ratio of Cl : *N*-methylimidazole = 1 : 2) in 20 ml toluene at 80 °C for 24 h, the resultant supported imidazolium salts were washed with methanol (3×20 ml) and dried in *vacuum* at 60 °C for 24 h. From elemental analysis results, the modification was not completed for most of samples (ESI).

### 2.2 *Synthesis imidazolium salt*



a mixture of benzyl chloride (12 mmol), 1-methylimidazole (10 mmol) and toluene (10 mL) was heated at 80 °C for 24 h in a 25 mL flask with vigorous stirring. After cooled down to room temperature, the solid residue washed with benzene (3×5 mL) and ethyl acetate (3×5 mL). Then, the solid was dried under vacuum at 60 °C for 12 h and the imidazolium salt was obtained. $^1$H NMR ($CDCl_3$, TMS, 400 MHz): δ 10.05 (S, 1H), 7.46 (s, 1H), 7.29 (m, 3H), 7.09 (m, 3H), 5.35 (s, 2H), 3.70 (s, 3H); $^{13}$C NMR ($CDCl_3$, TMS, 100.4 MHz): δ 137.36, 133.58, 129.17, 128.79, 124.00, 122.22, 52.76, 36.29.

### 2.3 *Synthesis of polystyrene resin supported imidazolium salt*




Polystyrene resin supported imidazolium salt was according to reported method[2]: a mixture of chloromethyl polystyrene (1.0 g, 5.5 mmol Cl content), 1-methylimidazole (16.5 mmol) and toluene (10 mL) was heated at 80 °C for 24 h in a 25 mL flask with vigorous stirring. After cooled down to room temperature, the solid residue was collected by filtration and washed with methanol(3×5 mL). Then, the solid was dried under vacuum at 60 °C for 12 h and polystyrene resin supported imidazolium salt was obtained. The loading of imidazolium salt attached on the PS was 3.6 mmol/g determined by nitrogen content from elementary analysis.

2. J. Sun, W. G. Cheng, W. Fan, Y. H. Wang, Z. Y. Meng, and S. J. Zhang, *Catal. Today,* 2009, **148**, 361-367.

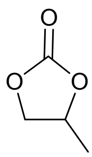
**2.4 $CO_2$ capture**

Imidazolium salt-modified porous hypercrosslinked polymers were subjected to the following gas capture and cycling experiment at 25 $^{o}$C: $CO_2$ (99.8%) gas flow at 20 ml/min for 30 min, followed by $N_2$ (99.9995%) gas flow at 20 ml/min for 45 min. Changes in weight were recorded by TGA. Prior to the cyclic treatment, the sample was first purged under $N_2$ gas flow at 100 $^{o}$C for 60 min, followed by cooling to room temperature. Change in buoyancy effects arising from the switching of gases was recorded by using an empty sample pan, and the buoyancy effects were corrected. For the adsorption kinetics analysis of $CO_2$ and $N_2$, the porous supported imidazolium salt was first purged under Ar gas flow (20 ml/min) at 100 $^{o}$C for 60 min, followed by cooling to room temperature. The gas was then switched from Ar to $CO_2$ or $N_2$ (20 ml/min).

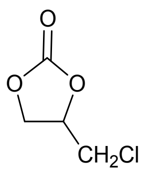
**2.5 $CO_2$ conversion**

$CO_2$ conversion reactions were conducted in a 50 ml stainless steel reactor equipped with a magnetic stirrer and automatic temperature control system. Typically, an appropriate volume of $CO_2$ (1.0 MPa) was added to a mixture of PO (0.1 ml), ethanol (2 ml), porous supported imidazolium salt (5 mmol% based on contents of the imidazolium salt) in the reactor at room temperature. The temperature was then raised to 120 $^{o}$C. After the reaction was preceded for 4 h, the reactor was cooled to 0 $^{o}$C in an ice water bath, and the remaining $CO_2$ was slowly removed. The product was then analyzed by GC and NMR. The porous supported imidazolium salts could be easily separated by centrifugation, and used in the next run without further purification.

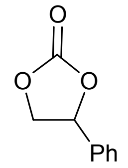
***3. Characterization of cyclic carbonates***



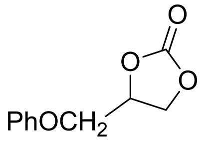
$^{1}$H NMR ($CDCl_3$, TMS, 400 MHz): $\delta$ 4.86-4.94 (m, 1H), 4.60 (t, *J*=8.0 Hz, 1H), 4.05 (t, *J*=8.8 Hz, 1H), 1.49 (d, *J*=6.0 Hz, 3H); $^{13}$C NMR ($CDCl_3$, TMS, 100.4 MHz): $\delta$ 154.95 (C=O), 73.51, 70.46, 18.95.



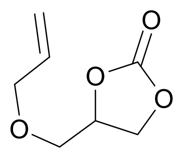

$^{1}$H NMR ($CDCl_3$, TMS, 400 MHz): $\delta$ 4.98 (m, 1H), 4.58 (t, 1H, *J*=8.4 Hz), 4.39 (dd, 1H, *J*=6.0 Hz), 3.80 (dd, 1H, *J*=5.2 Hz), 3.71 (dd, 1H, *J*=3.2 Hz); $^{13}$C NMR ($CDCl_3$, TMS, 100.4 MHz): $\delta$ 154.95 (C=O), 73.51, 70.46, 43.83.



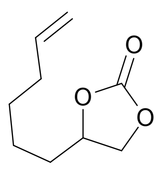
$^{1}$H NMR ($CDCl_3$, TMS, 400 MHz): δ 7.35-7.44 (m, 5H), 5.68 (t, 1H, *J*=8.0 Hz), 4.80 (t, 1H, *J*=8.4 Hz), 4.34 (t, 1H, *J*=8.4 Hz); $^{13}$C NMR ($CDCl_3$, TMS, 100.4 MHz): δ 154.81 (C=O), 135.70, 129.63, 129.12, 125.81, 77.92, 71.10.



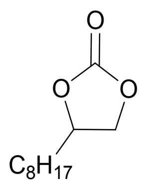
1H NMR ($CDCl_3$, 400 MHz): δ 7.31 (t, $^{3}$J= 8.0 Hz, 2H), 7.02 (t, $^{3}$J = 7.4 Hz, 1H), 6.91 [d, $^{3}$J= 8.0 Hz, 2H], 5.03 [m, 1H], 4.62 [t, $^{3}J$= 8.4 Hz, 1H], 4.55 (dd, $^{3}J$= 8.4 Hz), 4.24 (dd, $^{3}J$ = 3.6 Hz, 1H), 4.15 (dd, $^{3}J$ = 4.4 Hz, 1H), $^{13}$C NMR ($CDCl_3$, TMS, 100.4 MHz): δ 157.71. 154.65, 129.62, 121.92, 114.57, 74.11, 68.84, 66.17.



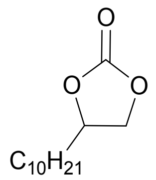
$^{1}$H NMR ($CDCl_3$, 400MHz): δ 5.8 – 6.0 (t, 1H), 5.0-5.2 (d, 2H), 4.4-4.7 (3H), 4.0-4.1 (m, 2H), 3.5-3.8 (d, 2H). $^{13}$C NMR ($CDCl_3$, TMS, 100.4 MHz): δ 155.90, 133.88, 117.47, 72.05, 72.30, 68.92, 66.24.



$^{1}$H NMR ($CDCl_3$, TMS, 400 MHz): δ δ 5.8 – 6.0 (t, 1H), 5.0-5.2 (d, 2H), 4.7 (m, 1H), 4.5 (dd, 1H), 4.04 (dd, 1H, *J*=8.4 Hz), 2.4-2.7 (m, 2H), 2.1 (m, 2H), 1.43-1.55 (m, 4H); $^{13}$C NMR ($CDCl_3$, TMS, 100.4 MHz): δ 155.2 (C=O), 139.2,115.6, 70.4, 66.3, 36.5, 33.8, 29.6, 25.3.



$^{1}$H NMR ($CDCl_3$, TMS, 400 MHz): δ 4.6-4.8 (m, 1H), 4.50 (dd, 1H, *J*=8.4 Hz), 4.04 (dd, 1H, *J*=8.4 Hz), 1.6-1.9 (m, 2H), 1.1-1.6 (m, 12H), 0.86 (t, 2H); $^{13}$C NMR ($CDCl_3$, TMS, 100.4 MHz): δ 155.2 (C=O), 77.1, 69.5, 34.0, 31.9, 29.4, 29.2, 29.2, 24.5, 22.7, 14.2.




$^{1}$H NMR ($CDCl_3$, TMS, 400 MHz): $\delta$ 4.67-4.72 (m, 1H), 4.52 (dd, 1H), 4.07 (dd, 1H), 1.77-1.89 (m, 1H), 1.67-1.69 (m, 1H), 1.42-1.50 (m, 1H), 1.22-1.36 (m, 15H), 0.86 (t, 3H); $^{13}$C NMR ($CDCl_3$, TMS, 100.4 MHz): $\delta$ 155.6 (C=O), 76.7, 69.4, 33.9, 31.8, 29.5, 29.4, 29.3, 29.2, 29.1, 24.3, 22.6, 14.1.

## *4. Supported Figures*

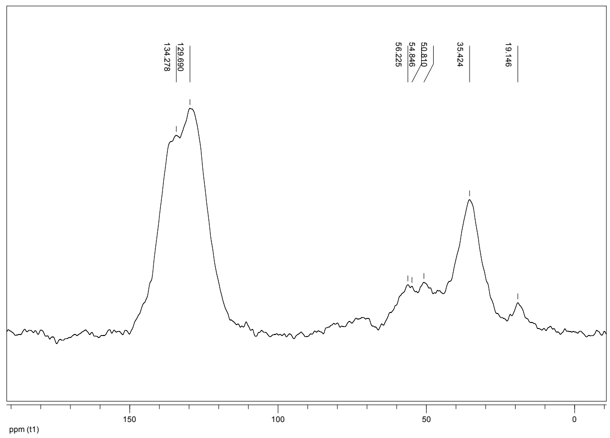



**Fig. S1** Solid-13C NMR spectrum for POM1-IM

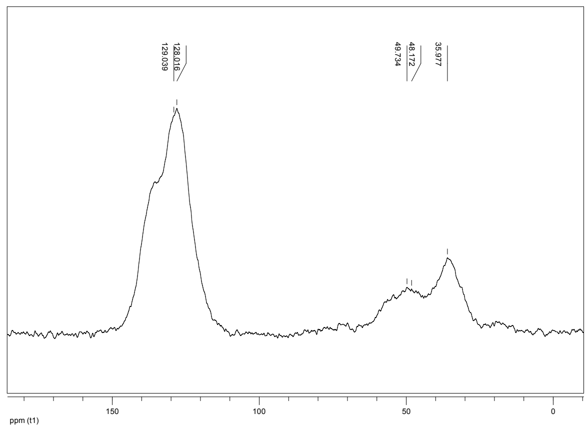



**Fig. S2** Solid-13C NMR spectrum for POM2-IM

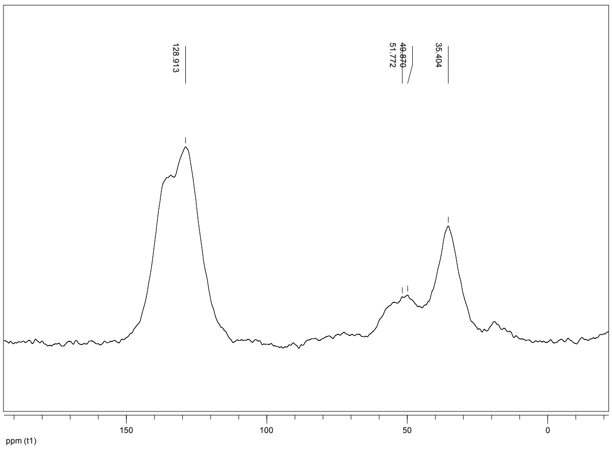



**Fig. S3** Solid-13C NMR spectrum for POM3-IM

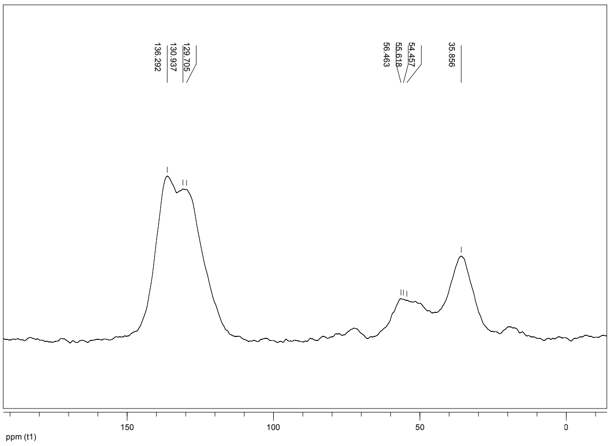



**Fig. S4** Solid-13C NMR spectrum for POM4-IM

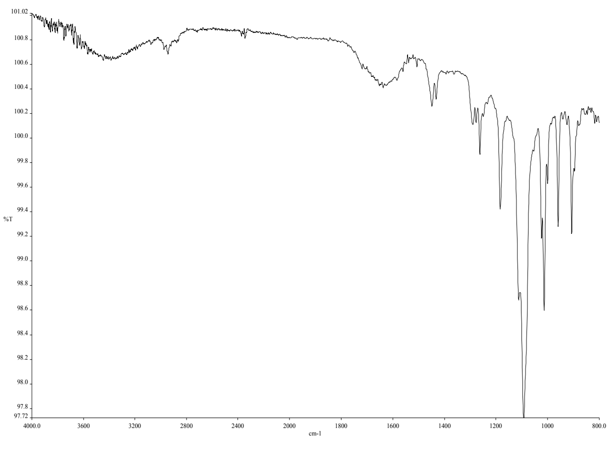



**Fig. S5** FT-IR spectrum for POM1

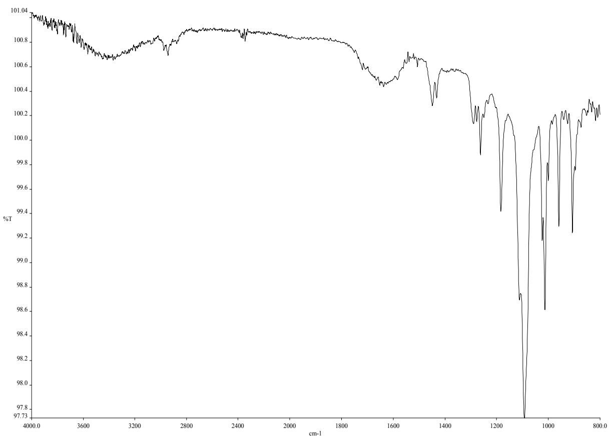


**Fig. S6** FT-IR spectrum for POM2

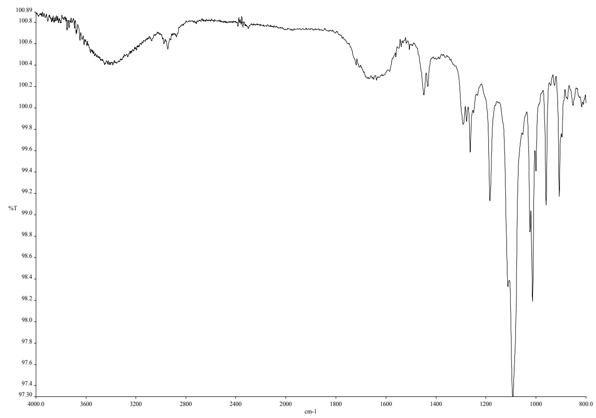


**Fig. S7** FT-IR spectrum for POM3

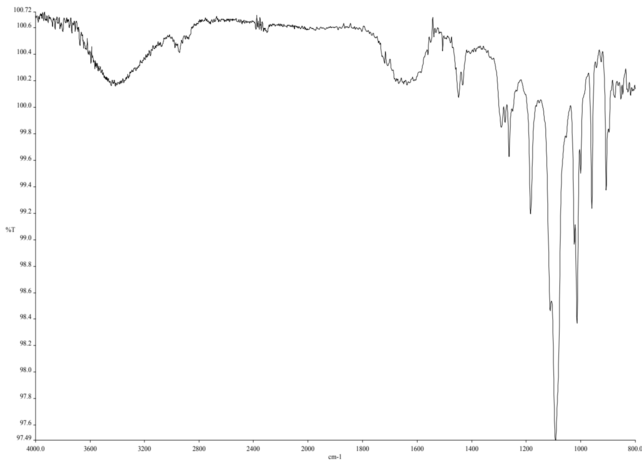


**Fig. S8** FT-IR spectrum for POM4

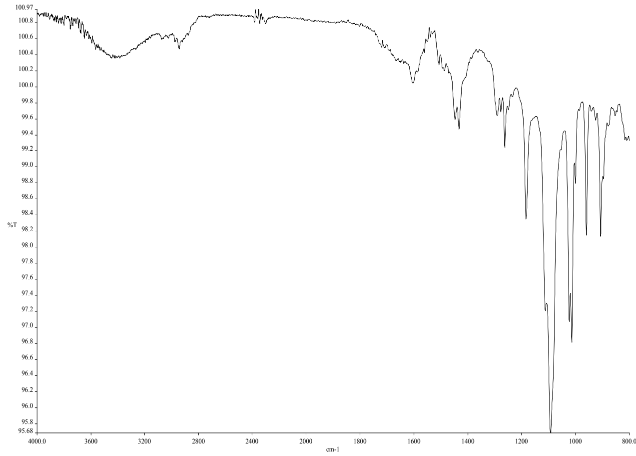


**Fig. S9** FT-IR spectrum for POM5

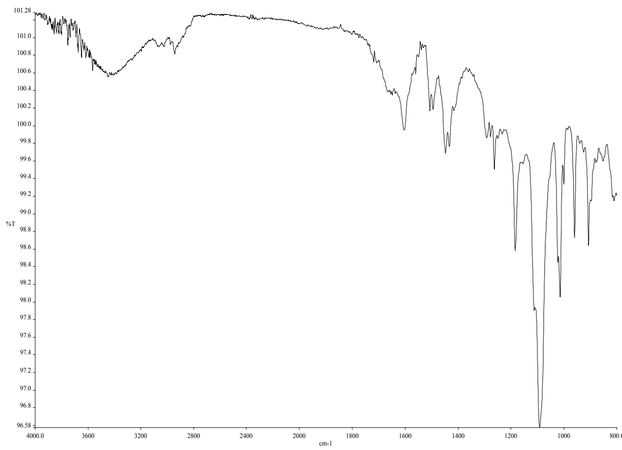


**Fig. S10** FT-IR spectrum for POM6

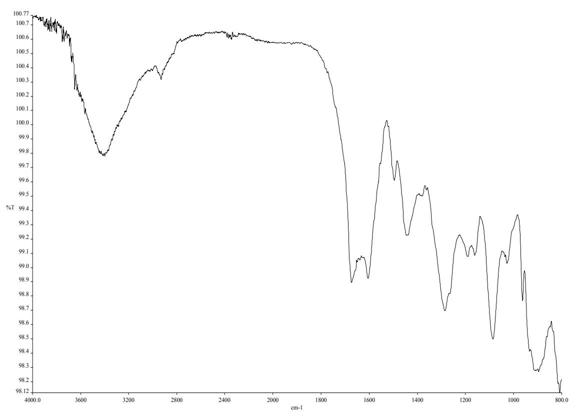


**Fig. S11** FT-IR spectrum for POM1-IM

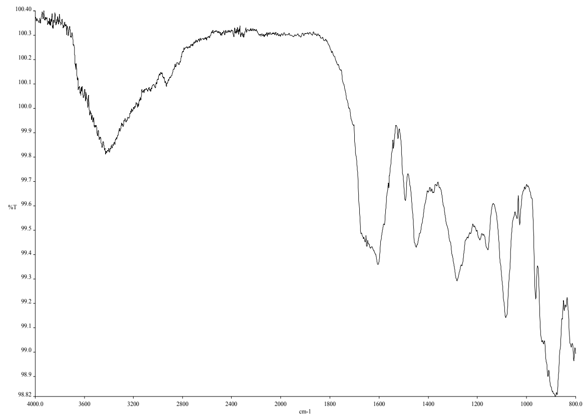


**Fig. S12** FT-IR spectrum for POM2-IM

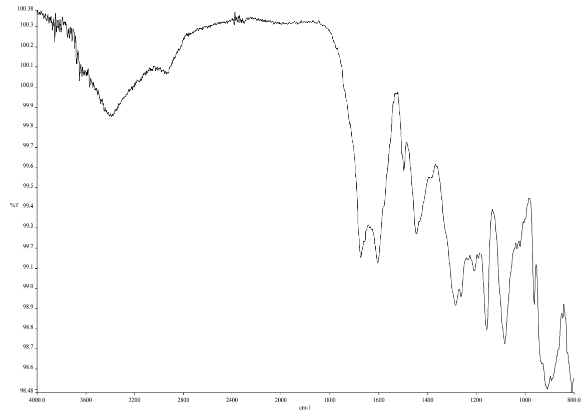


**Fig. S13** FT-IR spectrum for POM3-IM

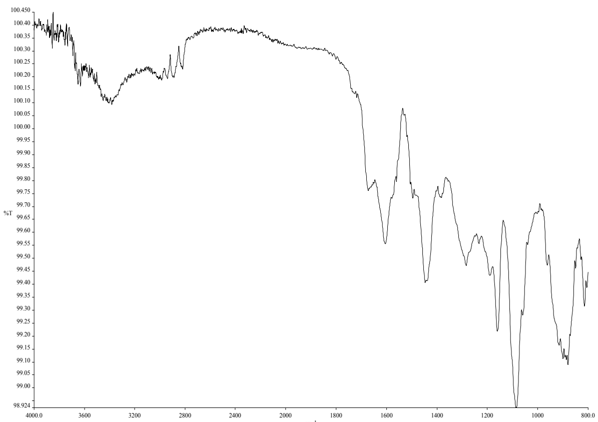


**Fig. S14** FT-IR spectrum for POM4-IM

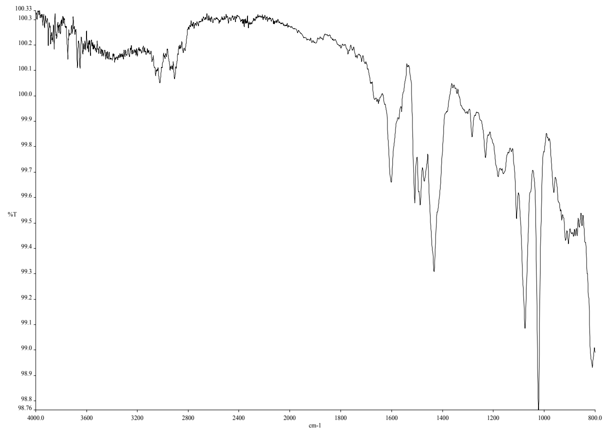


**Fig. S15** FT-IR spectrum for POM5-IM

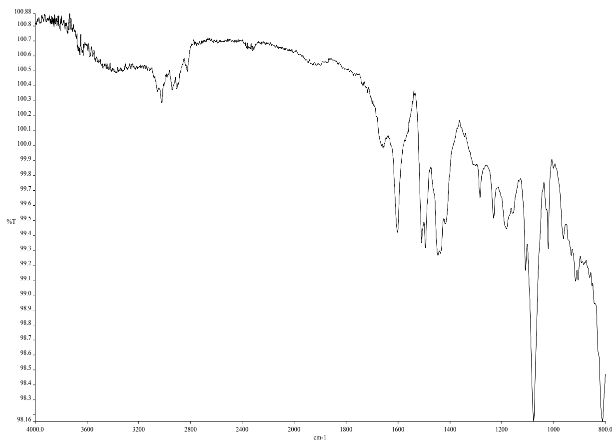


**Fig. S16** FT-IR spectrum for POM6-IM

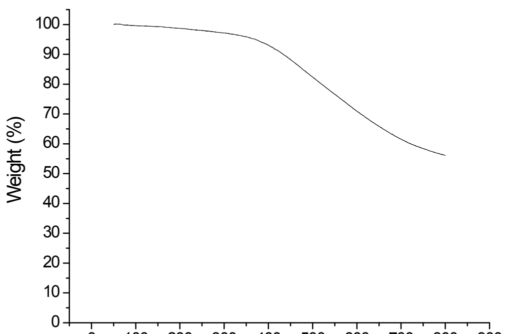



**Fig. S17** The thermogram of POM1 by TGA.

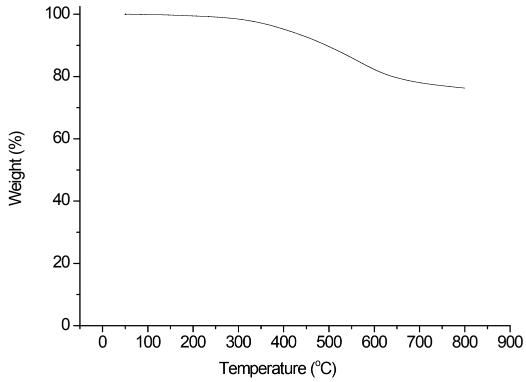



**Fig. S18** The thermogram of POM2 by TGA.

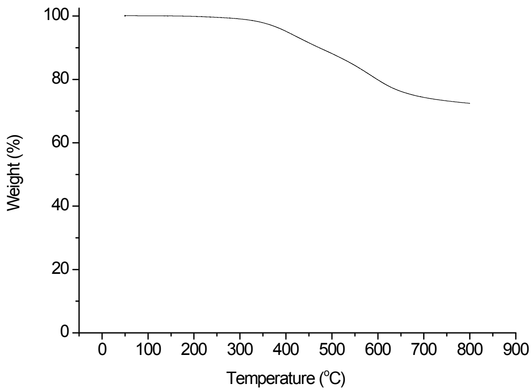



**Fig. S19** The thermogram of POM3 by TGA.

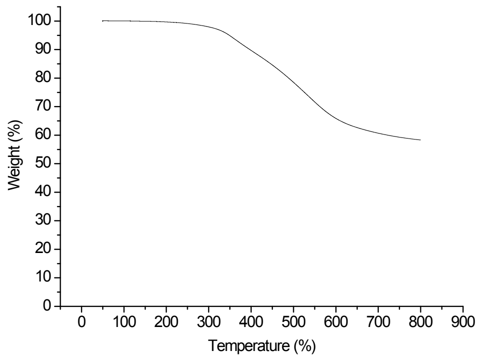



**Fig. S20** The thermogram of POM4 by TGA.

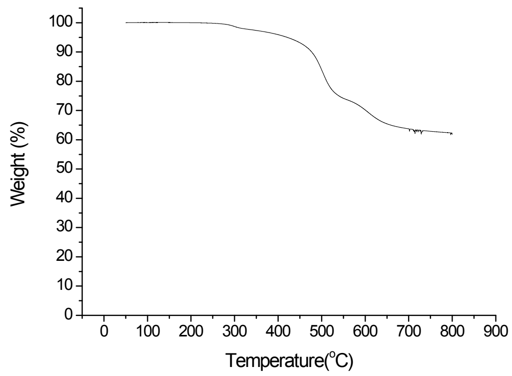



**Fig. S21** The thermogram of POM5 by TGA.

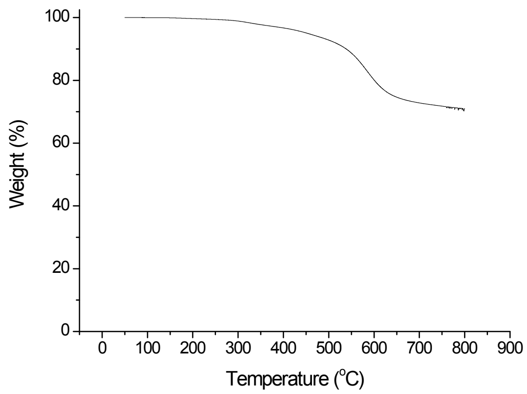



**Fig. S22** The thermogram of POM6 by TGA.

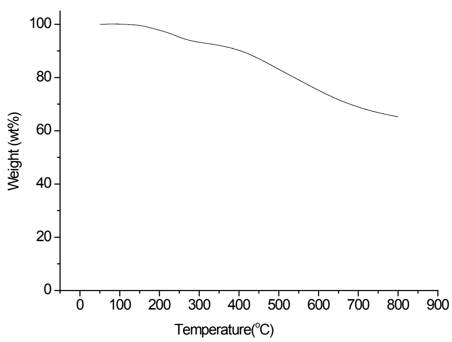



**Fig. S23** The thermogram of POM1-IM by TGA.

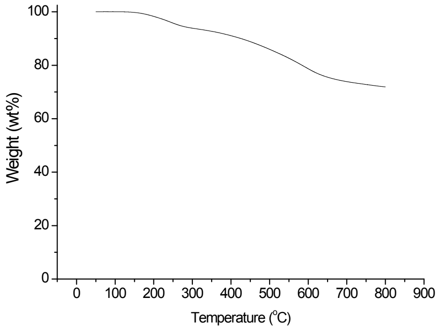



**Fig. S24** The thermogram of POM2-IM by TGA.

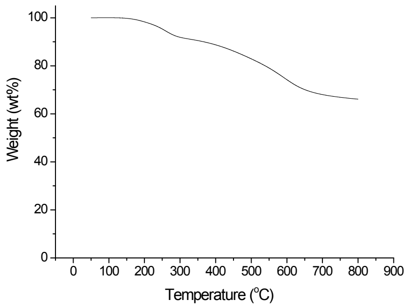



**Fig. S25** The thermogram of POM3-IM by TGA.

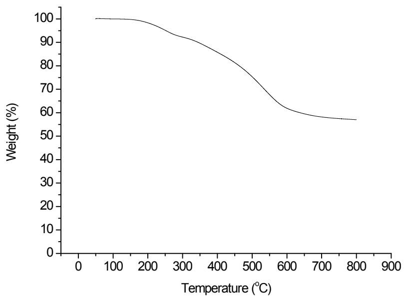



**Fig. S26** The thermogram of POM4-IM by TGA.

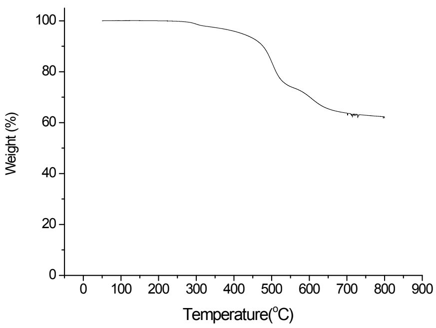



**Fig. S27** The thermogram of POM5-IM by TGA.

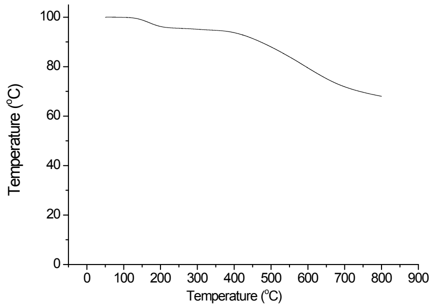



**Fig. S28** The thermogram of POM6-IM by TGA.

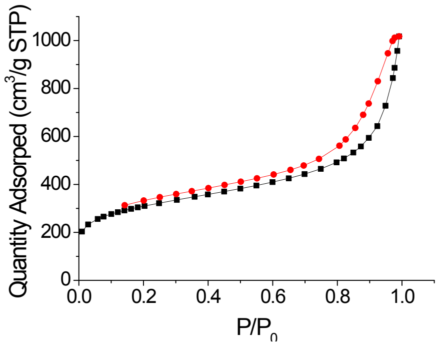



**Fig. S29** Nitrogen adsorption isotherms for POM1 measured at 77K.

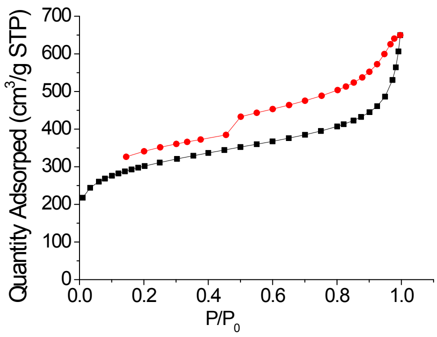



**Fig. S30** Nitrogen adsorption isotherms for POM2 measured at 77K.

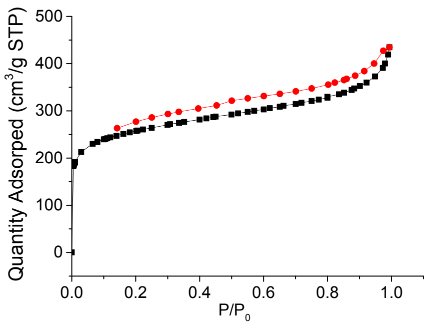



**Fig. S31** Nitrogen adsorption isotherms for POM3 measured at 77K.

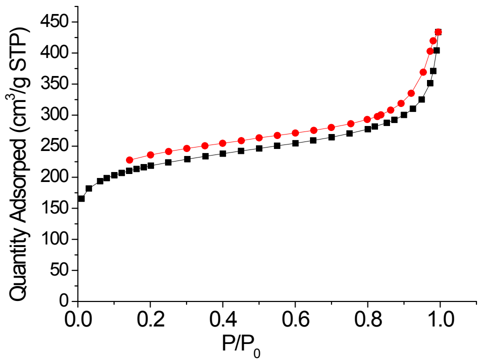



**Fig. S32** Nitrogen adsorption isotherms for POM4 measured at 77K.

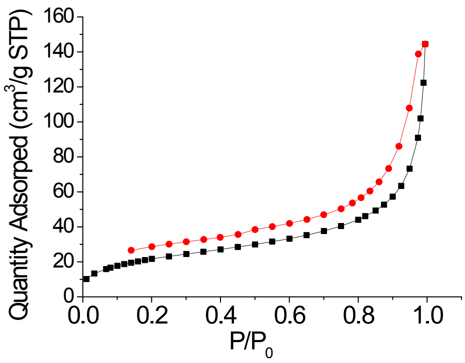



**Fig. S33** Nitrogen adsorption isotherms for POM5 measured at 77K.

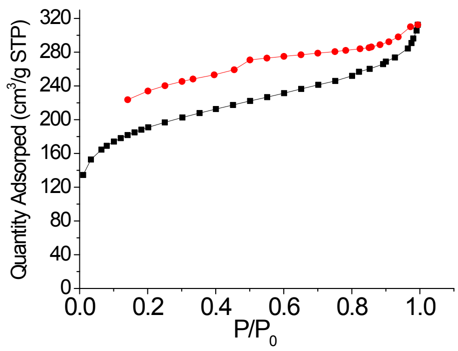



**Fig. S34** Nitrogen adsorption isotherms for POM6 measured at 77K.

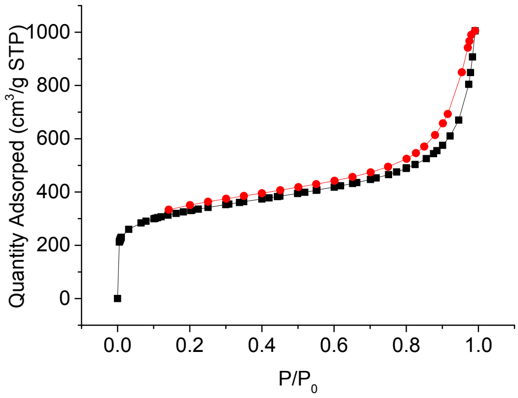



**Fig. S35** Nitrogen adsorption isotherms for POM1-IM measured at 77K.

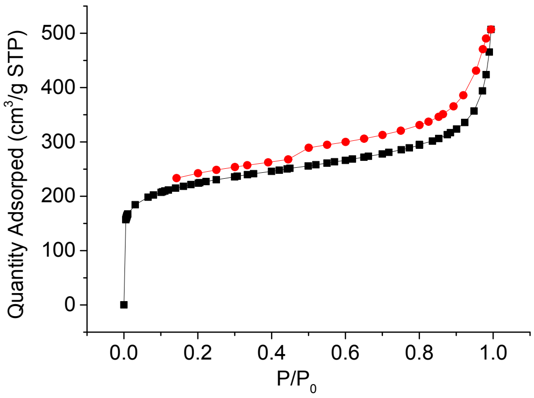



**Fig. S36** Nitrogen adsorption isotherms for POM2-IM measured at 77K.

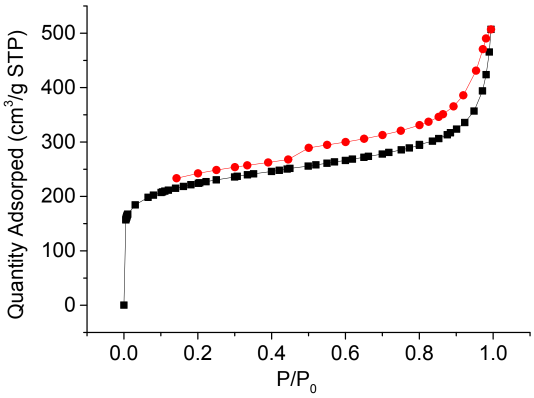



**Fig. S37** Nitrogen adsorption isotherms for POM3-IM measured at 77K.

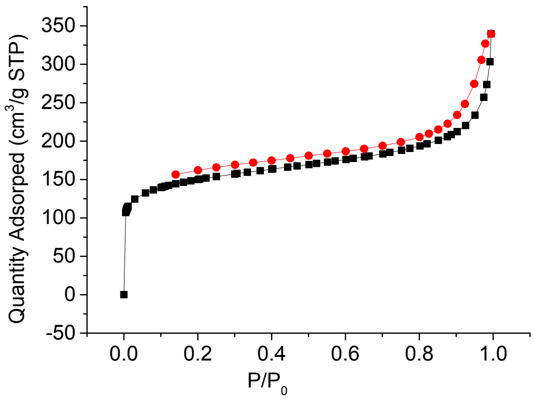



**Fig. S38** Nitrogen adsorption isotherms for POM4-IM measured at 77K.

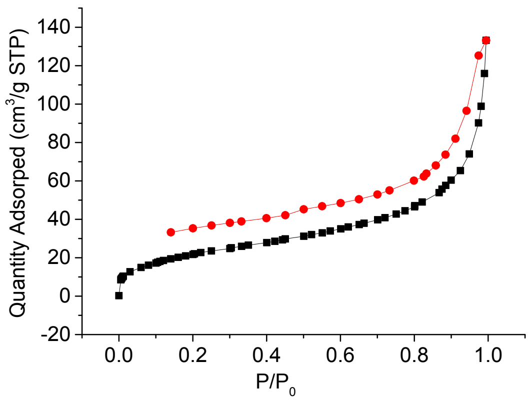



**Fig. S39** Nitrogen adsorption isotherms for POM5-IM measured at 77K.

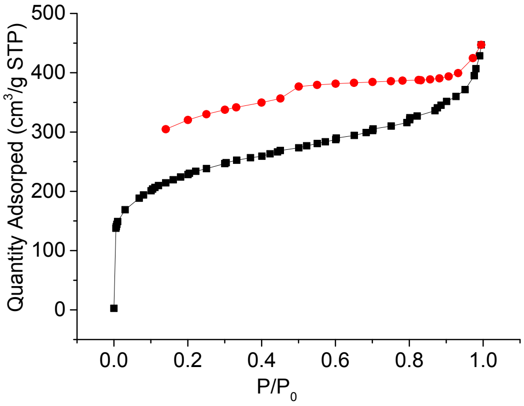



**Fig. S40** Nitrogen adsorption isotherms for POM6-IM measured at 77K.

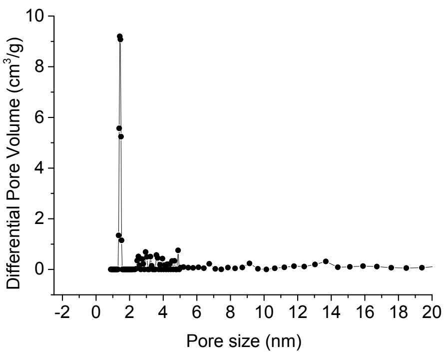



**Fig. S41** Pore size distribution for POM1 calculated using NLDFT.

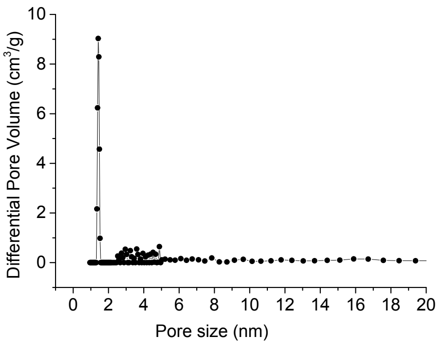



**Fig. S42** Pore size distribution for POM2 calculated using NLDFT.

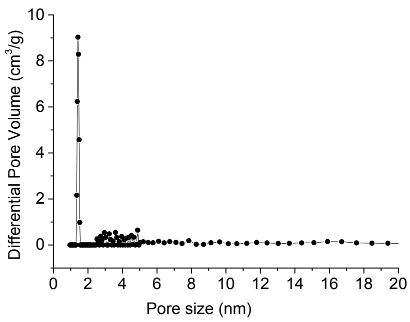



**Fig. S43** Pore size distribution for POM3 calculated using NLDFT.

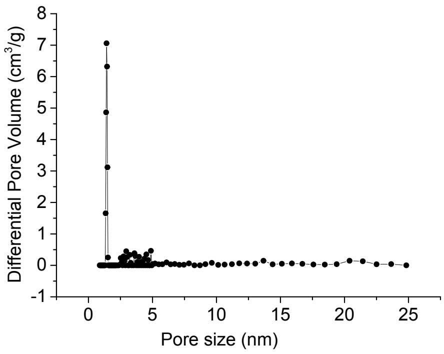



**Fig. S44** Pore size distribution for POM4 calculated using NLDFT.

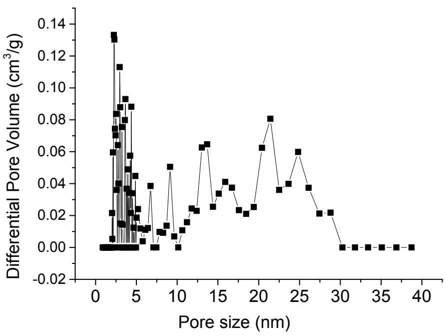



**Fig. S45** Pore size distribution for POM5 calculated using NLDFT.

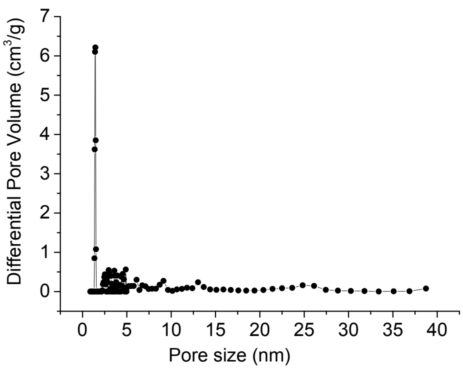



**Fig. S46** Pore size distribution for POM6 calculated using NLDFT.

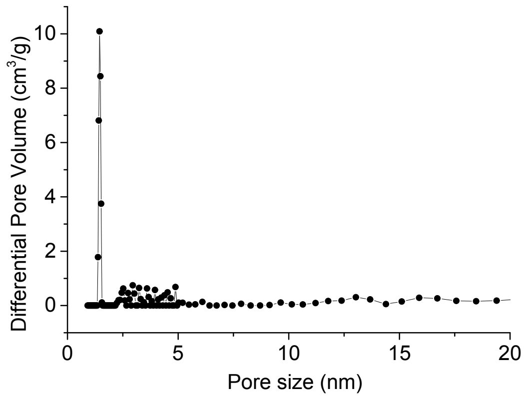



**Fig. S47** Pore size distribution for POM1-IM calculated using NLDFT.

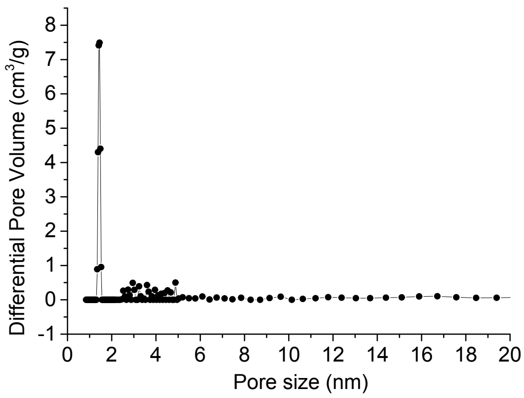



**Fig. S48** Pore size distribution for POM2-IM calculated using NLDFT.

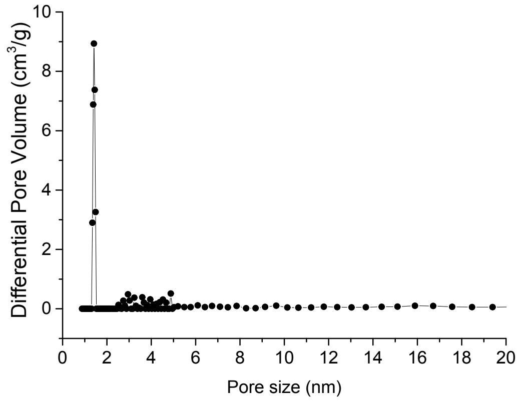



**Fig. S49** Pore size distribution for POM3-IM calculated using NLDFT.

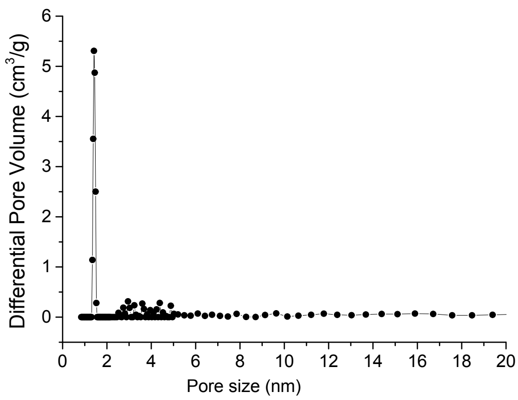



**Fig. S50** Pore size distribution for POM4-IM calculated using NLDFT.

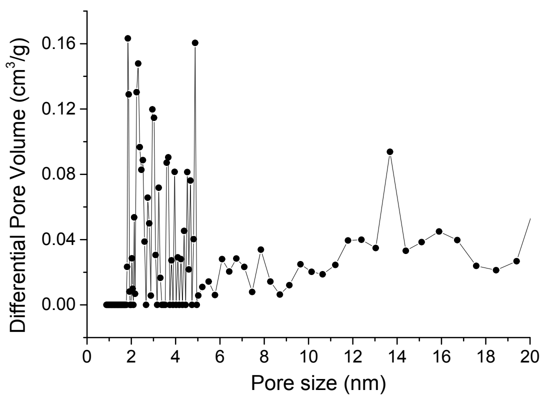



**Fig. S51** Pore size distribution for POM5-IM calculated using NLDFT.

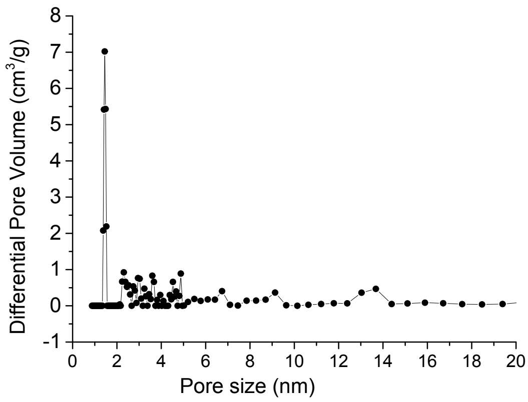



**Fig. S52** Pore size distribution for POM6-IM calculated using NLDFT.

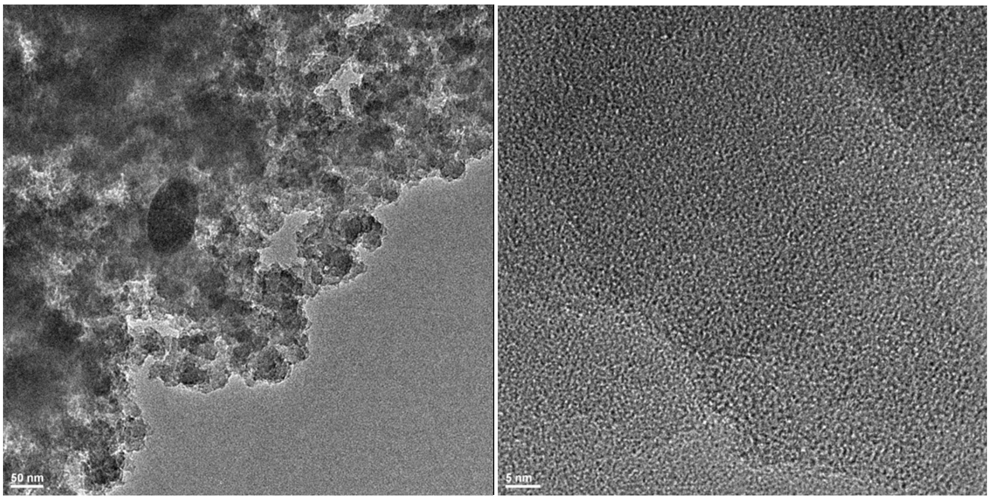



**Fig. S53** Morphological structures of POM1-IM

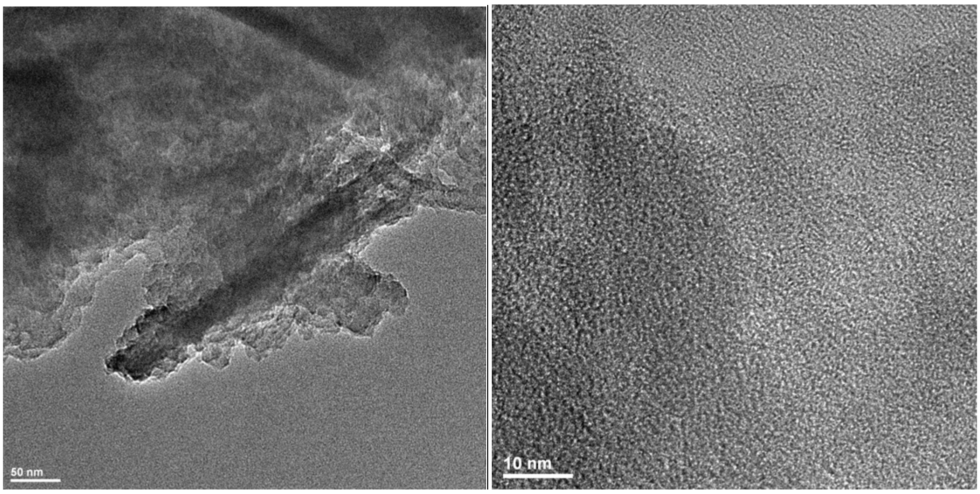



**Fig. S54** Morphological structures of POM2-IM

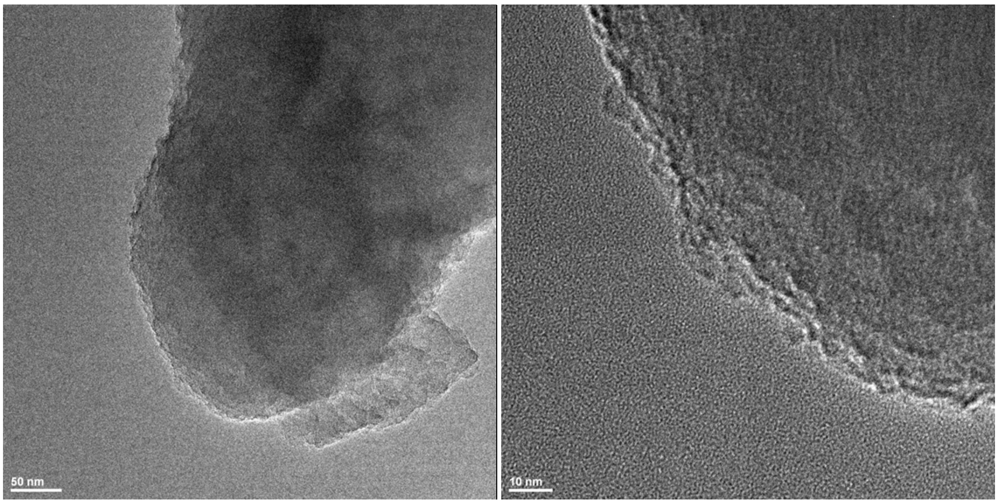



**Fig. S55** Morphological structures of POM3-IM

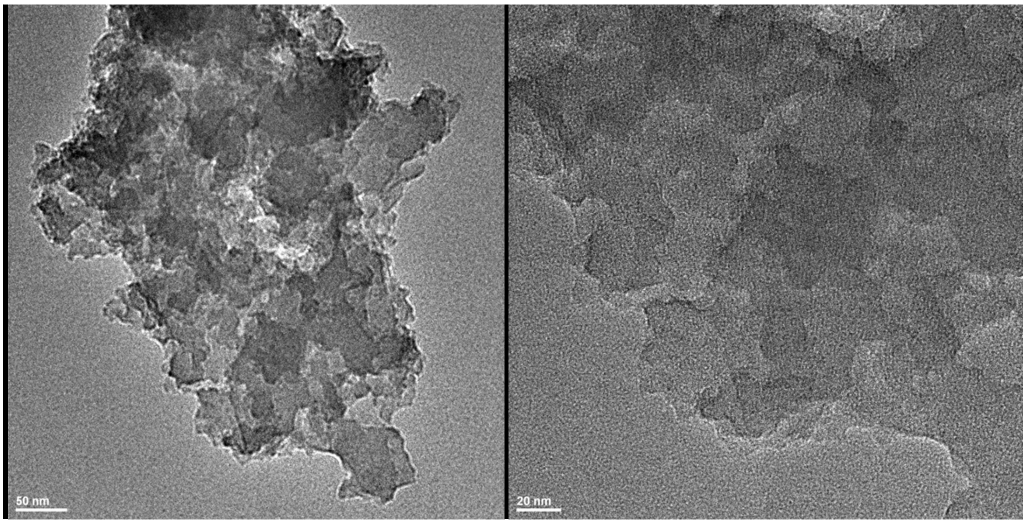



**Fig. S56** Morphological structures of POM4-IM

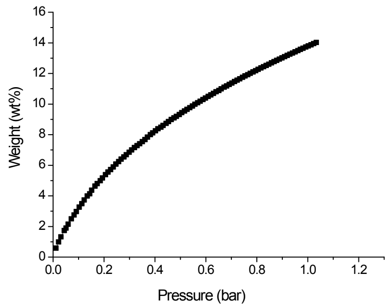



**Fig. S57** $CO_2$ capture isotherms for POM1at 273K.

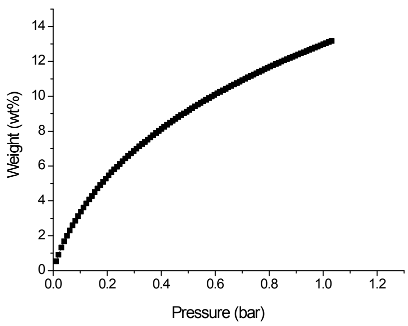



**Fig. S58** $CO_2$ capture isotherms for POM2at 273K.

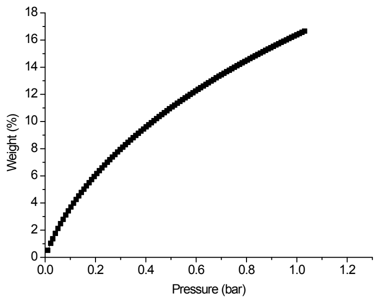



**Fig. S59** $CO_2$ capture isotherms for POM3 at 273K.

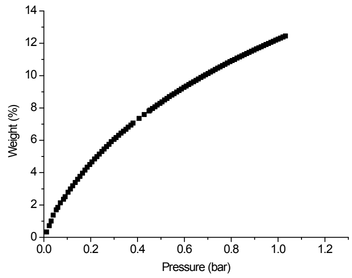



**Fig. S60** $CO_2$ capture isotherms for POM4 at 273K.

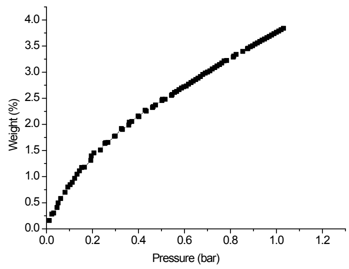



**Fig. S61** $CO_2$ capture isotherms for POM5 at 273K.

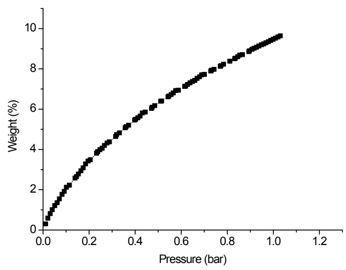



**Fig. S62** $CO_2$ capture isotherms for POM6 at 273K.

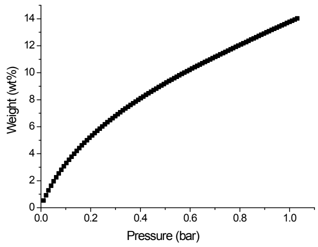



**Fig. S63** $CO_2$ capture isotherms for POM1-IM at 273K.

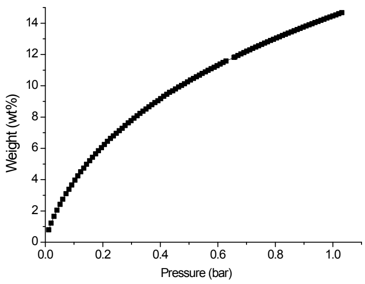



**Fig. S64** $CO_2$ capture isotherms for POM2-IM at 273K.

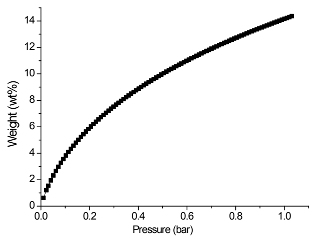



**Fig. S65** $CO_2$ capture isotherms for POM3-IM at 273K.

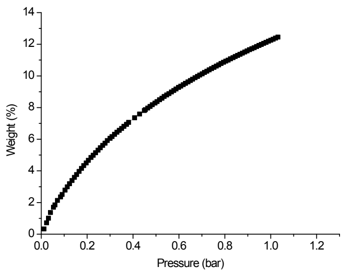



**Fig. S66** $CO_2$ capture isotherms for POM4-IM at 273K.

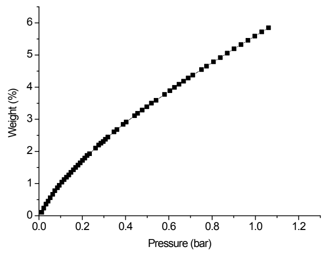



**Fig. S67** $CO_2$ capture isotherms for POM5-IM at 273K.

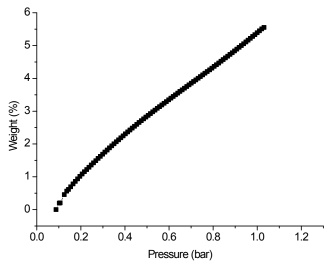



**Fig. S68** $CO_2$ capture isotherms for POM6-IM at 273K.

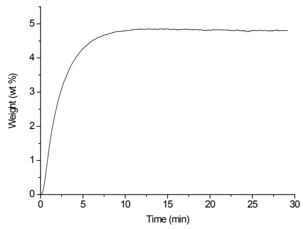



**Fig. S69** $CO_2$ capture by TGA for POM1-IM at 298K.

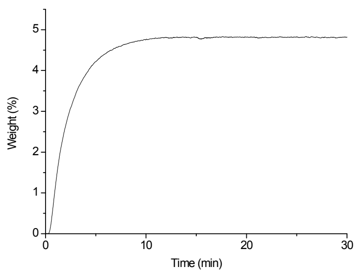
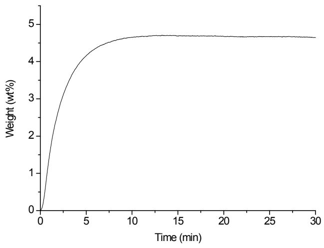
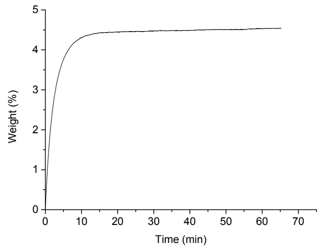


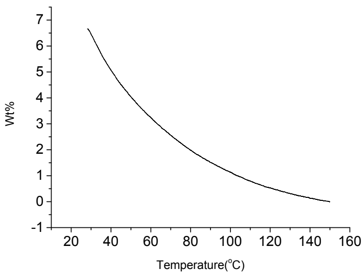

**Fig. S70** $CO_2$ capture by TGA for POM2-IM at 298K.




(a) Fresh polymer




(b) After heated in water at 80 $^{o}C$ and 18 h




(c) $CO_2$ capture under different temperature

**Fig. S71** $CO_2$ capture by TGA for POM3-IM at 298K (a) and (b); at different temperature (c).

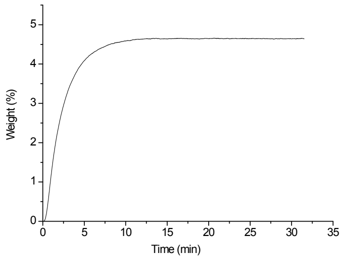



**Fig. S72** $CO_2$ capture by TGA for POM4-IM at 298K.

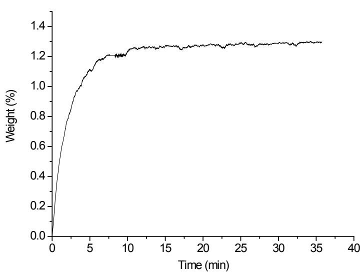



**Fig. S73** $CO_2$ capture by TGA for POM5-IM at 298K.

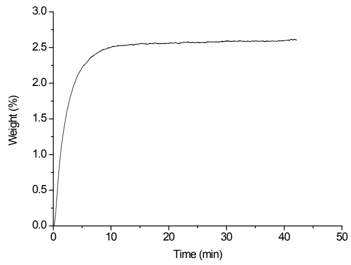



**Fig. S74** $CO_2$ capture by TGA for POM6-IM at 298K.

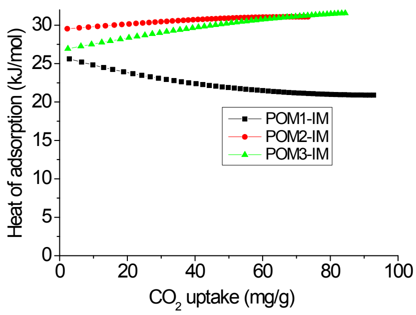



**Fig. S75** Heat of adsorption (Qst) for $CO_2$ catpure

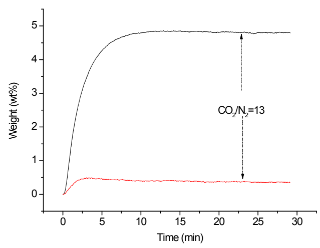



**Fig. S76** Adsorption kinetics of $CO_2$ and $N_2$ obtained for POM-IM2 at 298K by TGA.

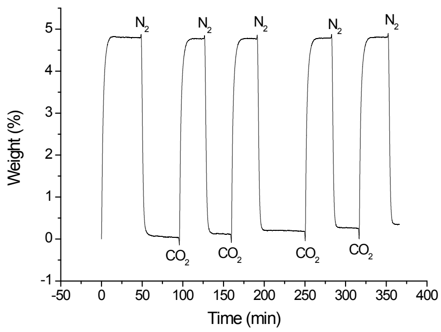



**Fig. S77** $CO_2$ adsorption-desorption cycles obtained for POM-IM2 at 298K by TGA.

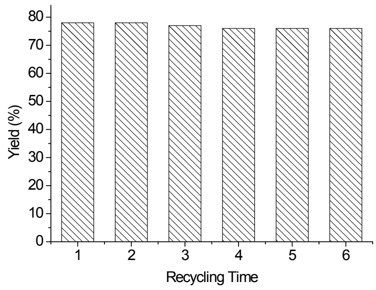



**Fig. S78** Catalyst recycling. Reaction conditions: PO (1.43 mmol), POM3-IM (5 mmol% based on the imidazolium salt), Ethanol (2 ml), CO2 pressure (1 MPa), Temperature (120 oC), Time (4 h).

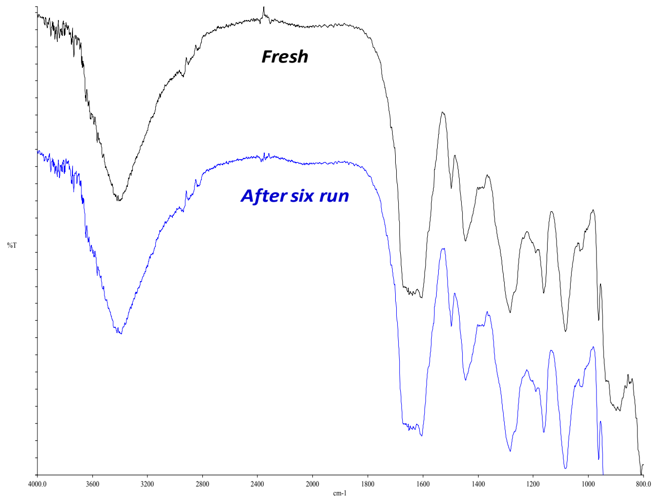



**Fig. S79** FT-IR of POM-IM3 in Scheme 1: fresh and after sixth run: Reaction conditions: Reaction condition: PO (0.1 mL), Catalyst (100 mg, 5 mmol% based on the imidazolium salt), $CO_2$ pressure (1 MPa), reaction time (4.0 h), temperature (120 $^oC$).

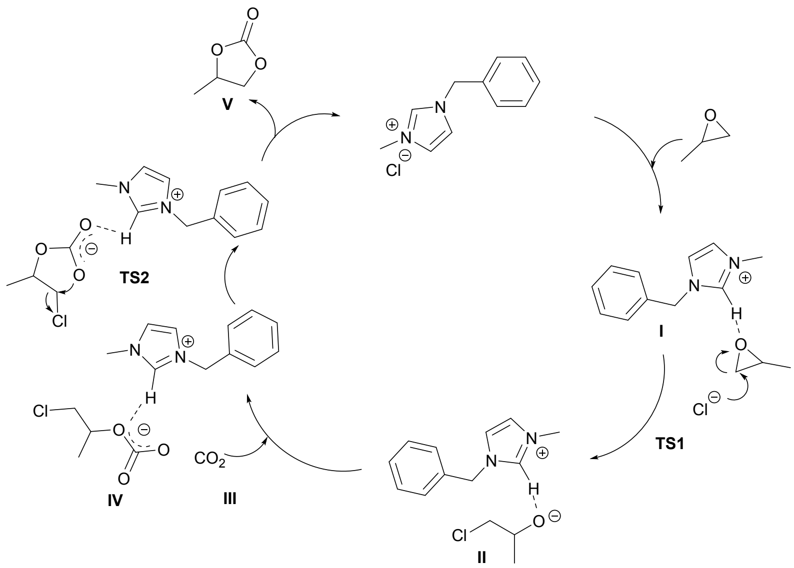



**Fig. S80** Mechanistic hypothesis of the catalytic reaction.

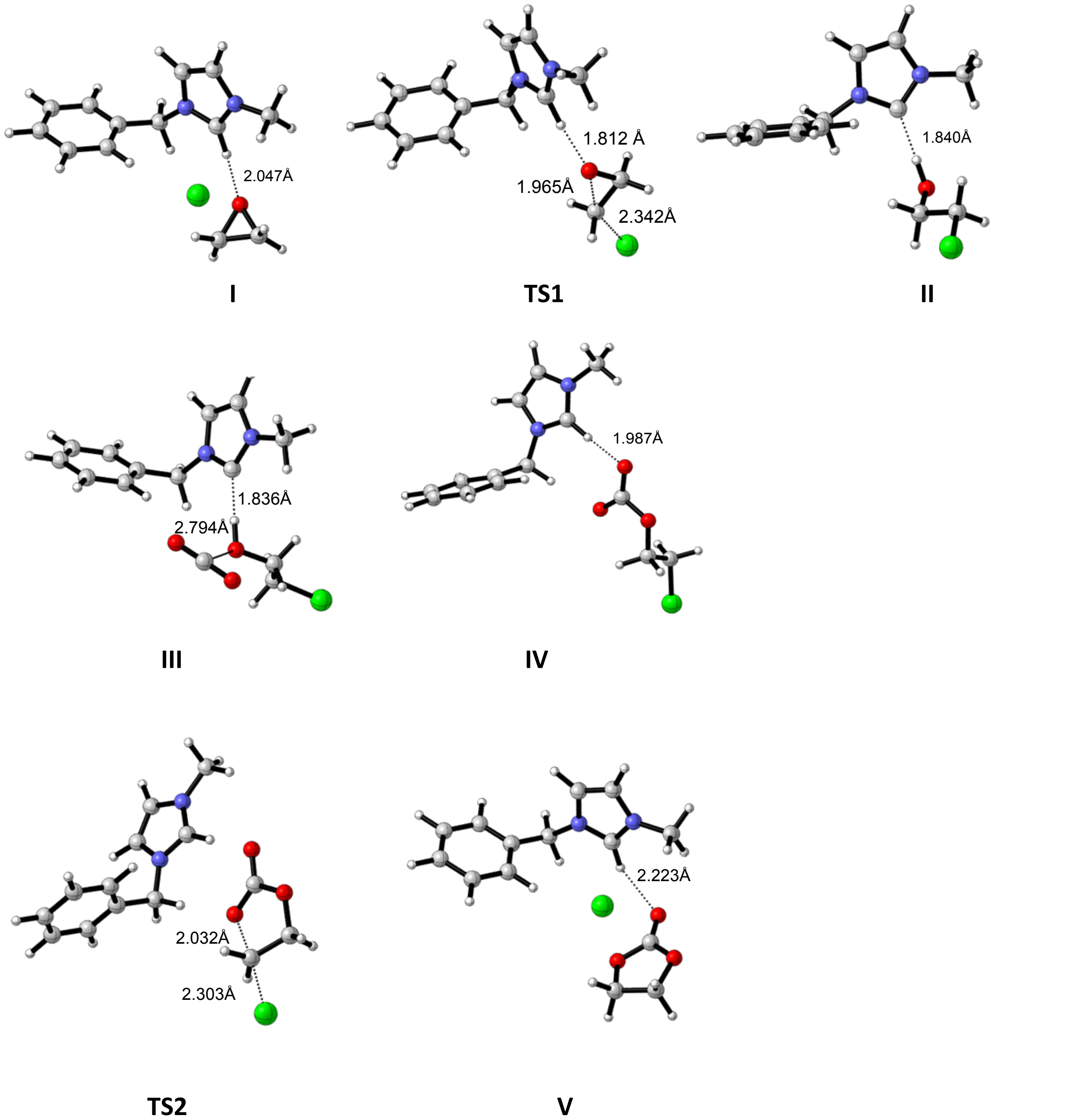



**Fig. S81** Optimized geometries for the intermediates and transition states. H: white, C: gray, N: blue, O: red, Cl: green. Bond lengths and distances are in Å.

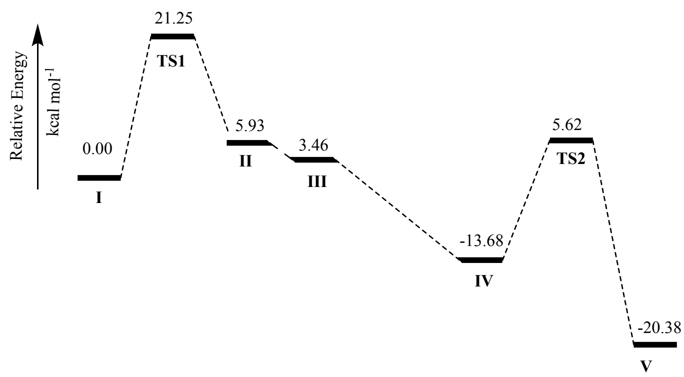



**Fig. S82** Relative energies for fixation of $CO_2$ with PO catalyzed by 1-benzyl-3-methylimidazolium chloride in ethanol, relative energies at the B3PW91/6-311++G (d, p) level.

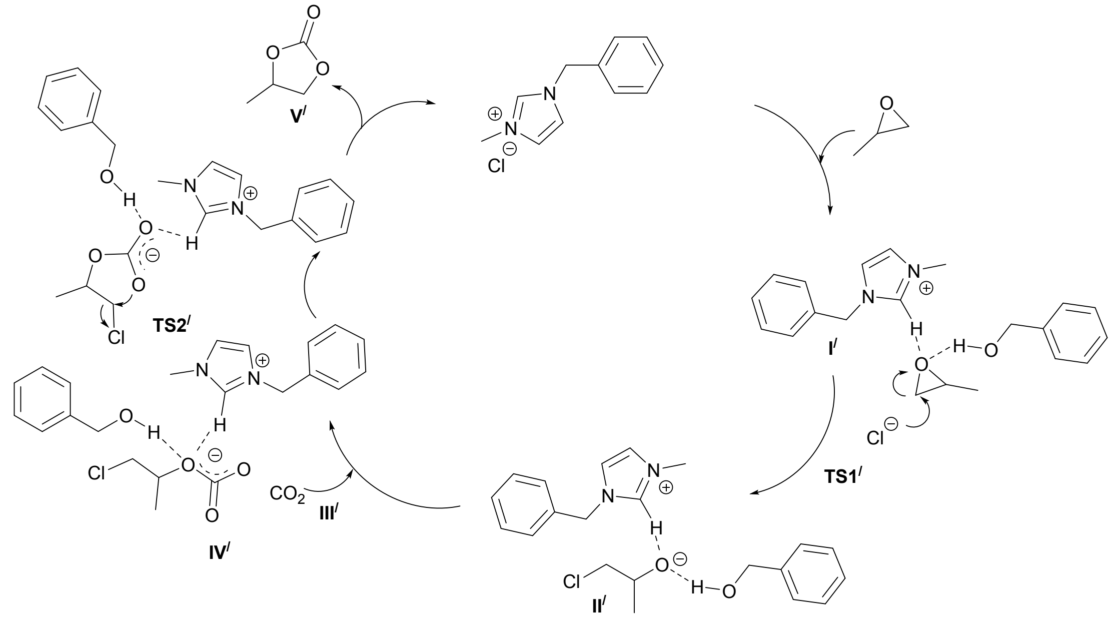


**Fig. S83** Mechanistic hypothesis of the catalytic reaction.

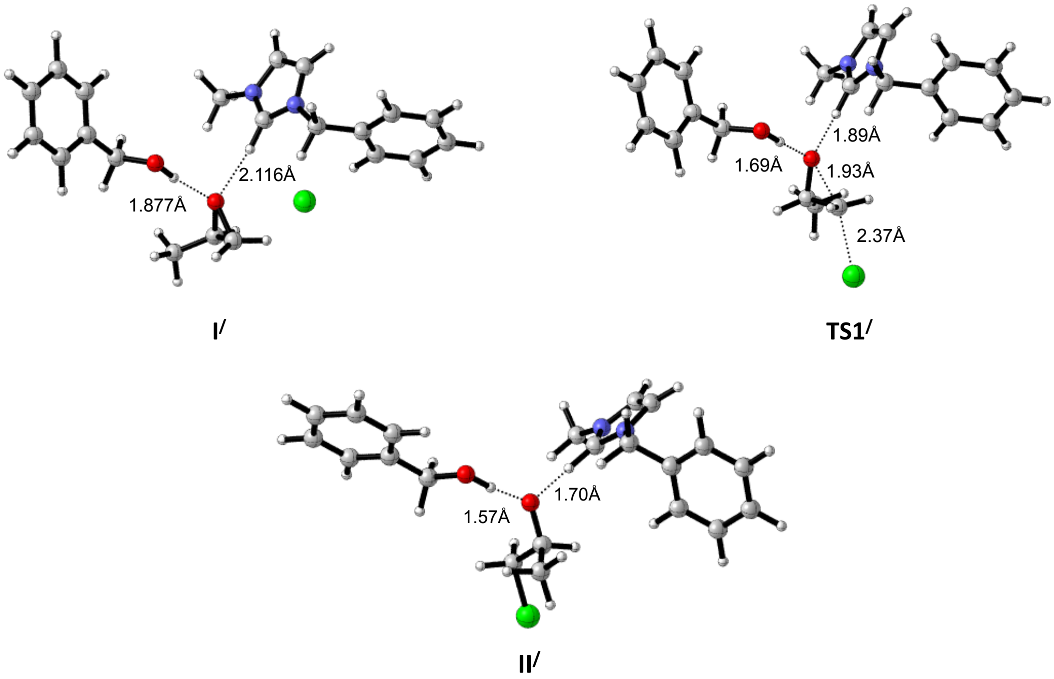



**Fig. S84** Optimized geometries for the intermediates and transition states. H: white, C: gray, N: blue, O: red, Cl: green. Bond lengths and distances are in Å.

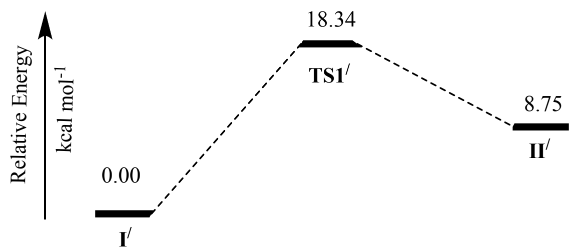



**Fig. S85** Relative energies of ring opening step for fixation of $CO_2$ with PO catalyzed by 1-benzyl-3-methylimidazolium chloride and benzyl alcohol in ethanol, relative energies at the B3PW91/6-311++G (d, p) level.

## *5. Supporting Tables*

**Table S1** Elemental analysis results for POM1~6-IM

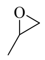
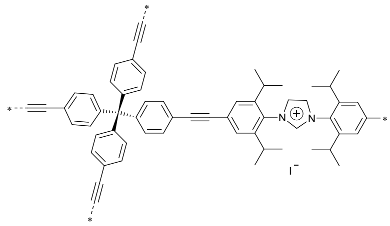
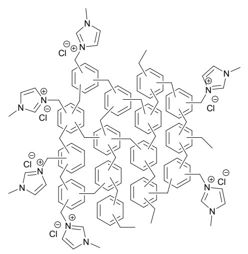
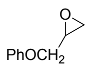
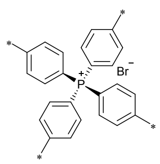
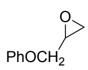
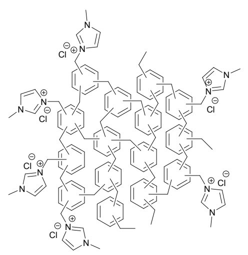
| POM | C (wt%) | H (wt%) | N (wt%) | Degree of halogen substitution (%) |
|---|---|---|---|---|
| POM1-IM | 74.36 | 4.85 | 2.01 | 21% |
| POM2-IM | 75.41 | 4.69 | 2.01 | 23% |
| POM3-IM | 72.11 | 5.06 | 2.84 | 57% |
| POM4-IM | 68.04 | 4.44 | 1.85 | 34 |
| POM5-IM | 80.74 | 5.13 | 1.19 | >99% |
| POM6-IM | 71.89 | 4.63 | <0.50 | - |
| POM3-IM[a] | 72.22 | 5.04 | 2.82 | |

[a]After six runs

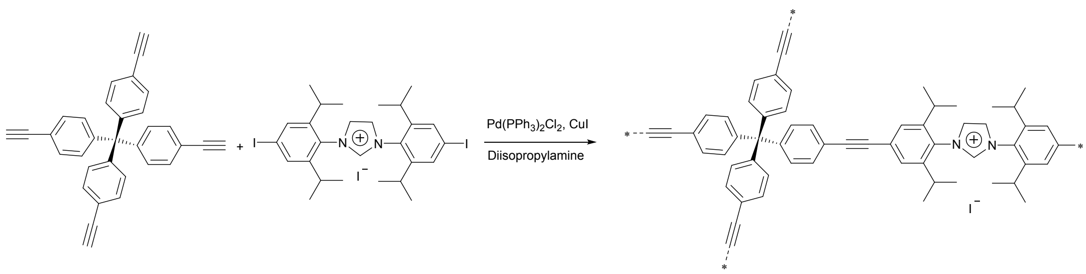
**Table S2** Elemental analysis results for POM1~6

| POM | C (wt%) | H (wt%) | Cl (wt%) | Br (wt%) |
|---|---|---|---|---|
| POM1 | 74.53 | 4.56 | 24.13 | / |
| POM2 | 74.71 | 4.42 | 10.70 | / |
| POM3 | 76.81 | 4.76 | 5.61 | / |
| POM4 | 71.43 | 3.92 | / | 6.8 |
| POM5 | 71.91 | 4.35 | / | 1.5 |
| POM6 | 87.42 | 5.05 | <0.5 | / |

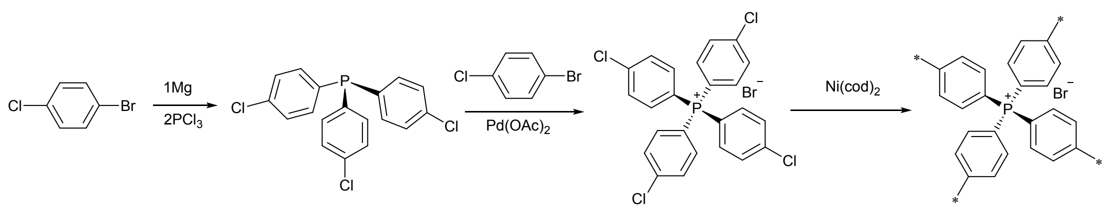
**Table S3** Comparison with the other reported functionalized porous organic materials

| Epoxide | Catalyst | mol% | P(MPa) | Temp. (°C) | Time (h) | Yield (%) | Ref |
|---|---|---|---|---|---|---|---|
|  |  | 0.065 | 1 | 150 | 10 | 87 | 3a[a] |
|  |  | 5 | 1 | 120 | 8 | 92 | This work |
|  |  | 2 | 0.1 | 140 | 20 | 98 | 3h[b] |
|  |  | 5 | 1 | 120 | 12 | 91 | This work |

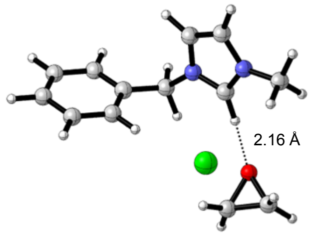
[a] the synthetic method of catalyst:




[b] the synthetic method of catalyst:



## *6. Cartesian coordinates for all the optimized geometries*

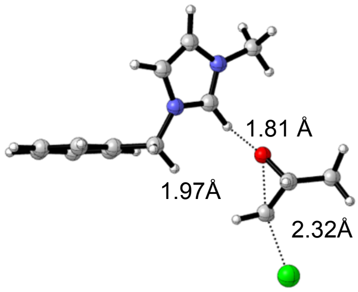



I

| | | | |
|---|---|---|---|
| C | 3.15234700 | -2.20329900 | -0.78958600 |
| C | 2.58302700 | -2.34474800 | 0.55409700 |
| H | 3.87486300 | -1.40271500 | -0.93457900 |
| H | 2.89674400 | -1.67181600 | 1.34689000 |
| H | 2.19138400 | -3.31058000 | 0.86093500 |
| O | 1.82204600 | -1.70310600 | -0.50082000 |
| C | 2.05688100 | 3.13556700 | -0.33963600 |
| H | 2.57538900 | 2.51343300 | 0.39043100 |
| H | 2.66939800 | 3.27850400 | -1.22983600 |
| H | 1.82348800 | 4.10063100 | 0.10578500 |
| H | -0.40743000 | 4.17986100 | -1.25191200 |
| C | -0.34781400 | 3.10975900 | -1.15774400 |
| C | -1.26737100 | 2.14149300 | -1.41501900 |
| H | -2.28115700 | 2.21039900 | -1.76827400 |
| C | 0.57920800 | 1.15943600 | -0.69703600 |
| N | -0.66827900 | 0.93046100 | -1.12268100 |
| N | 0.79603100 | 2.47743000 | -0.70793300 |
| H | -0.50099600 | -1.12952700 | -1.05839400 |
| C | -1.29785800 | -0.40596200 | -1.23274300 |
| H | -1.64268900 | -0.51882400 | -2.26060500 |
| H | 1.28155100 | 0.38801500 | -0.41092200 |
| Cl | 3.26427600 | 0.96528000 | 2.47791000 |
| C | -2.44157400 | -0.58948300 | -0.25819100 |
| C | -3.75619600 | -0.67582200 | -0.72317300 |
| C | -2.19558500 | -0.68709400 | 1.11659300 |
| C | -4.81297400 | -0.85306800 | 0.17121700 |
| H | -3.95650700 | -0.60783400 | -1.78726300 |
| C | -3.24945900 | -0.85971200 | 2.01010700 |
| H | -1.17924200 | -0.62918200 | 1.49142100 |
| C | -4.56127400 | -0.94238600 | 1.53876600 |
| H | -5.82861800 | -0.91978500 | -0.20165900 |
| H | -3.04779600 | -0.93438800 | 3.07254600 |
| H | -5.38082100 | -1.07905700 | 2.23504500 |
| C | 3.24511900 | -3.34912300 | -1.75839200 |

| | | | |
|---|---|---|---|
| H | 3.10767900 | -2.99946300 | -2.78542900 |
| H | 4.23326300 | -3.81383000 | -1.69149300 |
| H | 2.48931000 | -4.10734300 | -1.54186200 |

1 2 1.0 3 1.0 6 1.0 34 1.0
2 4 1.0 5 1.0 6 1.0
3
4
5
6
7 8 1.0 9 1.0 10 1.0 17 1.0
8
9
10
11 12 1.0
12 13 2.0 17 1.0
13 14 1.0 16 1.0
14
15 16 1.5 17 1.5 21 1.0
16 19 1.0
17
18 19 1.0
19 20 1.0 23 1.0
20
21
22
23 24 1.5 25 1.5
24 26 1.5 27 1.0
25 28 1.5 29 1.0
26 30 1.5 31 1.0
27
28 30 1.5 32 1.0
29
30 33 1.0
31
32
33
34 35 1.0 36 1.0 37 1.0
35
36
37

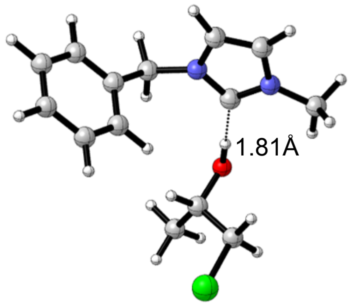



**TS1**

| | | | |
|---|---|---|---|
| C | 3.24736500 | -1.19413000 | 0.47826000 |
| C | 3.43926400 | 0.16697300 | -0.05759400 |
| H | 3.61918500 | -1.38677200 | 1.47363600 |
| H | 2.37044000 | -1.73639000 | 0.16292400 |
| H | 3.16679400 | 0.24050400 | -1.12288200 |
| O | 2.41522500 | 0.56557600 | 0.80623600 |
| C | 0.62021400 | 3.82479800 | 0.78305000 |
| H | 0.17581200 | 4.23629400 | 1.68859700 |
| H | 1.50953900 | 3.25114700 | 1.03510800 |
| H | 0.88036200 | 4.63110800 | 0.09831800 |
| H | -1.97343300 | 4.26909700 | -0.26928000 |
| C | -1.59007500 | 3.26594800 | -0.33801700 |
| C | -2.14258200 | 2.13653900 | -0.85396900 |
| H | -3.09999000 | 1.97055600 | -1.31556800 |
| C | -0.12763200 | 1.61910100 | -0.08493900 |
| N | -1.21571300 | 1.12208200 | -0.68663300 |
| N | -0.33690000 | 2.92160000 | 0.13528400 |
| H | -0.44379100 | -0.78605300 | -0.89307200 |
| C | -1.38964600 | -0.28719900 | -1.10303000 |
| H | -1.54344400 | -0.29549400 | -2.18227300 |
| H | 0.79732500 | 1.08034400 | 0.18792700 |
| Cl | 4.66145400 | -2.75164100 | -0.49790900 |
| C | -2.53835200 | -0.96629000 | -0.38973300 |
| C | -3.70976800 | -1.28362200 | -1.08178800 |
| C | -2.43717800 | -1.29152400 | 0.96801200 |
| C | -4.76993600 | -1.91192000 | -0.42658700 |
| H | -3.79462200 | -1.04388300 | -2.13646700 |
| C | -3.49522200 | -1.91596200 | 1.62331800 |
| H | -1.52838700 | -1.05984900 | 1.51362600 |
| C | -4.66502700 | -2.22650700 | 0.92672600 |
| H | -5.67340800 | -2.15471100 | -0.97412200 |
| H | -3.40591100 | -2.16583700 | 2.67432400 |
| H | -5.48718400 | -2.71524800 | 1.43693400 |
| C | 4.78661000 | 0.83062100 | 0.18326500 |
| H | 5.56213800 | 0.39312200 | -0.45192700 |

| | | | |
|---|---|---|---|
| H | 4.71656700 | 1.89860800 | -0.04359800 |
| H | 5.08556700 | 0.72001000 | 1.22994700 |

1 2 1.0 3 1.0 4 1.0
2 5 1.0 6 1.0 34 1.0
3
4
5
6
7 8 1.0 9 1.0 10 1.0 17 1.0
8
9
10
11 12 1.0
12 13 2.0 17 1.0
13 14 1.0 16 1.0
14
15 16 1.5 17 1.5 21 1.0
16 19 1.0
17
18 19 1.0
19 20 1.0 23 1.0
20
21
22
23 24 1.5 25 1.5
24 26 1.5 27 1.0
25 28 1.5 29 1.0
26 30 1.5 31 1.0
27
28 30 1.5 32 1.0
29
30 33 1.0
31
32
33
34 35 1.0 36 1.0 37 1.0
35
36
37

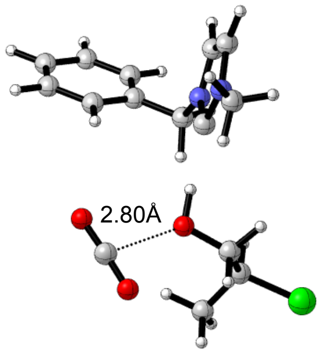



II

| | | | |
|---|---|---|---|
| C | -3.45495300 | -0.52498400 | -0.36554900 |
| C | -2.65336200 | -0.73568700 | 0.92374300 |
| H | -4.46978200 | -0.19172800 | -0.15411000 |
| H | -2.95580700 | 0.18599700 | -1.01901900 |
| H | -1.68618500 | -1.18190900 | 0.65705100 |
| O | -2.45501400 | 0.54648200 | 1.50488900 |
| C | -1.36515100 | 3.58947700 | -0.97861600 |
| H | -1.42172300 | 3.53854100 | -2.06759300 |
| H | -2.23160800 | 3.09226400 | -0.54899700 |
| H | -1.36021500 | 4.63607300 | -0.66890900 |
| H | 1.33728100 | 4.16320500 | -1.44813900 |
| C | 1.12757800 | 3.31514200 | -0.81789800 |
| C | 1.96269500 | 2.45285400 | -0.18899200 |
| H | 3.03833100 | 2.40335400 | -0.17074300 |
| C | -0.17320300 | 1.82273200 | 0.31475900 |
| N | 1.15195900 | 1.55411900 | 0.49294000 |
| N | -0.16310000 | 2.91418800 | -0.49855900 |
| H | 0.78511000 | 0.00634000 | 1.79324400 |
| C | 1.65940900 | 0.45587200 | 1.32091300 |
| H | 2.28594600 | 0.87153500 | 2.11320500 |
| H | -1.66508500 | 0.98897000 | 1.06766000 |
| Cl | -3.61726700 | -2.06449300 | -1.35359000 |
| C | 2.44011800 | -0.58316400 | 0.53879900 |
| C | 3.74182100 | -0.91934600 | 0.91858300 |
| C | 1.86208500 | -1.24157700 | -0.55332600 |
| C | 4.45594800 | -1.89812200 | 0.22440400 |
| H | 4.20180800 | -0.41327400 | 1.76122600 |
| C | 2.57319200 | -2.21569000 | -1.24978200 |
| H | 0.85328800 | -0.98785000 | -0.86113300 |
| C | 3.87314000 | -2.54789500 | -0.86158500 |
| H | 5.46577000 | -2.14724500 | 0.53064400 |
| H | 2.11350400 | -2.71869500 | -2.09323700 |
| H | 4.42595400 | -3.30668500 | -1.40383100 |
| C | -3.36322800 | -1.62805700 | 1.93293500 |

| | | | |
|---|---|---|---|
| H | -4.31882900 | -1.18167100 | 2.22471600 |
| H | -3.55508100 | -2.62087700 | 1.52075600 |
| H | -2.74757700 | -1.73928500 | 2.82813500 |

1 2 1.0 3 1.0 4 1.0 22 1.0
2 5 1.0 6 1.0 34 1.0
3
4
5
6 21 1.0
7 8 1.0 9 1.0 10 1.0 17 1.0
8
9
10
11 12 1.0
12 13 2.0 17 1.0
13 14 1.0 16 1.0
14
15 16 1.5 17 1.5
16 19 1.0
17
18 19 1.0
19 20 1.0 23 1.0
20
21
22
23 24 1.5 25 1.5
24 26 1.5 27 1.0
25 28 1.5 29 1.0
26 30 1.5 31 1.0
27
28 30 1.5 32 1.0
29
30 33 1.0
31
32
33
34 35 1.0 36 1.0 37 1.0
35
36
37



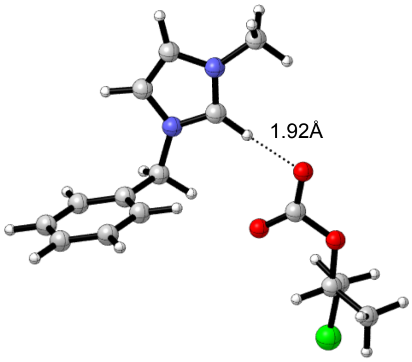

III

| | | | |
|---|---|---|---|
| C | 2.98289400 | -0.75348700 | -1.50622700 |
| C | 2.96980000 | 0.06213700 | -0.20830100 |
| H | 2.08183600 | -0.54932100 | -2.08350400 |
| H | 2.91020600 | 1.12868500 | -0.45338300 |
| H | 3.90566500 | -0.11038300 | 0.33383600 |
| O | 1.88778800 | -0.32950200 | 0.61313600 |
| C | 0.62793400 | 3.37996500 | 1.54335400 |
| H | 0.16876500 | 3.66690600 | 2.49095600 |
| H | 1.42013900 | 2.65921600 | 1.73197800 |
| H | 1.05133300 | 4.26641300 | 1.06724800 |
| H | -1.79634400 | 4.38117800 | 0.55377500 |
| C | -1.53118500 | 3.38045200 | 0.25594200 |
| C | -2.17703300 | 2.49355900 | -0.53987300 |
| H | -3.11512200 | 2.57165300 | -1.06309600 |
| C | -0.24432600 | 1.50085800 | 0.15841000 |
| N | -1.37729400 | 1.35850000 | -0.58606000 |
| N | -0.36164900 | 2.75641500 | 0.66978800 |
| H | -0.82968900 | -0.48984300 | -1.29970000 |
| C | -1.71595800 | 0.14449400 | -1.33571400 |
| H | -1.88996300 | 0.41413400 | -2.37959500 |
| H | 1.11310800 | 0.29345700 | 0.44262700 |
| C | 2.31979600 | -1.29298600 | 3.20259000 |
| O | 1.18271100 | -1.29271100 | 3.43737300 |
| O | 3.46674200 | -1.31455200 | 3.02327300 |
| Cl | 4.34832900 | -0.08289100 | -2.57158800 |
| C | -2.92207800 | -0.59124600 | -0.78318500 |
| C | -4.03184100 | -0.83875200 | -1.59467300 |
| C | -2.93159200 | -1.05518600 | 0.53786900 |
| C | -5.13406900 | -1.53861300 | -1.09935300 |
| H | -4.03654500 | -0.48331700 | -2.62001700 |
| C | -4.03109600 | -1.74991600 | 1.03571400 |
| H | -2.07583400 | -0.86900400 | 1.17817800 |
| C | -5.13639500 | -1.99440900 | 0.21723700 |
| H | -5.98835700 | -1.72263800 | -1.74117000 |

| | | | |
|---|---|---|---|
| H | -4.02575900 | -2.10411700 | 2.06053900 |
| H | -5.99152800 | -2.53631600 | 0.60516400 |
| C | 3.18467900 | -2.24238900 | -1.30720100 |
| H | 4.13313100 | -2.44525700 | -0.80359300 |
| H | 2.37344300 | -2.62211600 | -0.68101500 |
| H | 3.16741300 | -2.77735700 | -2.25810500 |

1 2 1.0 3 1.0 25 1.0 37 1.0
2 4 1.0 5 1.0 6 1.0
3
4
5
6 21 1.0
7 8 1.0 9 1.0 10 1.0 17 1.0
8
9
10
11 12 1.0
12 13 2.0 17 1.0
13 14 1.0 16 1.0
14
15 16 1.5 17 1.5
16 19 1.0
17
18 19 1.0
19 20 1.0 26 1.0
20
21
22 23 2.0 24 2.0
23
24
25
26 27 1.5 28 1.5
27 29 1.5 30 1.0
28 31 1.5 32 1.0
29 33 1.5 34 1.0
30
31 33 1.5 35 1.0
32
33 36 1.0
34
35
36
37 38 1.0 39 1.0 40 1.0

38
39
40




**IV**

| | | | |
|---|---|---|---|
| C | -2.28064200 | 4.25009100 | 0.55416600 |
| H | -2.89698300 | 4.40857000 | 1.43831900 |
| H | -1.22997700 | 4.26082800 | 0.83376300 |
| H | -2.47273300 | 5.03395700 | -0.17736600 |
| H | -4.67287700 | 3.21905100 | -0.54285300 |
| C | -3.82270800 | 2.55937300 | -0.54077700 |
| C | -3.68620300 | 1.28175100 | -0.98416200 |
| H | -4.39743900 | 0.61719000 | -1.44208800 |
| C | -1.73253300 | 1.92965300 | -0.16736500 |
| N | -2.37658100 | 0.90781000 | -0.74279600 |
| N | -2.59404800 | 2.94438700 | -0.03521600 |
| H | -0.70644000 | -0.31606800 | -0.81607100 |
| C | -1.76616400 | -0.40271400 | -1.07085600 |
| H | -1.85345700 | -0.53957300 | -2.14933800 |
| H | -0.68211300 | 1.93733300 | 0.14123200 |
| C | 4.59213200 | 0.14208300 | -0.71953900 |
| C | 3.93944100 | -0.14093300 | 0.63386100 |
| H | 3.83703000 | 0.33777800 | -1.47531400 |
| H | 5.29862200 | 0.96835500 | -0.66159200 |
| H | 3.32216100 | -1.03637000 | 0.54757100 |
| O | 3.09338400 | 0.98403400 | 0.92967300 |
| C | 1.77715100 | 0.99051400 | 0.41295900 |
| O | 1.14367200 | 2.01887000 | 0.73591700 |
| O | 1.41125300 | 0.01611100 | -0.26948000 |
| Cl | 5.54155100 | -1.29913200 | -1.33147900 |
| C | -2.42723700 | -1.54570600 | -0.33220300 |
| C | -3.23606600 | -2.45746200 | -1.01585900 |

| | | | |
|---|---|---|---|
| C | -2.22539100 | -1.71306400 | 1.04325700 |
| C | -3.83957900 | -3.51784400 | -0.33800400 |
| H | -3.39267200 | -2.34185900 | -2.08329900 |
| C | -2.83010500 | -2.76805700 | 1.72198800 |
| H | -1.58988200 | -1.01986900 | 1.58415500 |
| C | -3.63958500 | -3.67314800 | 1.03229300 |
| H | -4.46298700 | -4.21921100 | -0.88079900 |
| H | -2.66486200 | -2.88905500 | 2.78657400 |
| H | -4.10697600 | -4.49615100 | 1.56090600 |
| C | 4.93297100 | -0.27345200 | 1.77804800 |
| H | 5.61430600 | -1.10816500 | 1.60162600 |
| H | 5.52386300 | 0.64051400 | 1.88551200 |
| H | 4.40209200 | -0.45602100 | 2.71457800 |

1 2 1.0 3 1.0 4 1.0 11 1.0
2
3
4
5 6 1.0
6 7 2.0 11 1.0
7 8 1.0 10 1.0
8
9 10 1.5 11 1.5 15 1.0
10 13 1.0
11
12 13 1.0
13 14 1.0 26 1.0
14
15
16 17 1.0 18 1.0 19 1.0 25 1.0
17 20 1.0 21 1.0 37 1.0
18
19
20
21 22 1.0
22 23 2.0 24 2.0
23
24
25
26 27 1.5 28 1.5
27 29 1.5 30 1.0
28 31 1.5 32 1.0
29 33 1.5 34 1.0
30

31 33 1.5 35 1.0

32

33 36 1.0

34

35

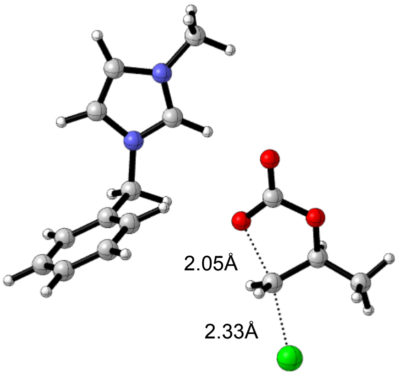
36

37 38 1.0 39 1.0 40 1.0

38

39

40



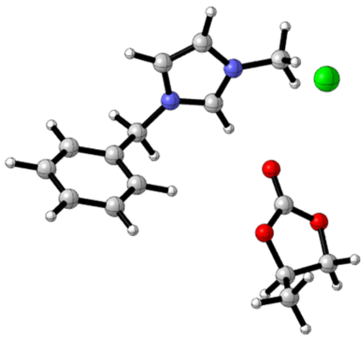

**TS2**

| | | | |
|---|---|---|---|
| C | 3.03057100 | -3.97300800 | 0.59465900 |
| H | 3.67815100 | -4.00053700 | 1.46988200 |
| H | 2.00571200 | -4.18185100 | 0.89145400 |
| H | 3.35882200 | -4.71291700 | -0.13410800 |
| H | 5.17560600 | -2.50261300 | -0.50911400 |
| C | 4.21209200 | -2.02354700 | -0.51744200 |
| C | 3.82868000 | -0.80394200 | -0.97938900 |
| H | 4.39742400 | -0.01890700 | -1.44587700 |
| C | 2.03888000 | -1.81393000 | -0.15843100 |
| N | 2.46977800 | -0.69282300 | -0.74735800 |
| N | 3.08159200 | -2.63718100 | -0.00896300 |
| H | 0.58745000 | 0.15988700 | -0.91179800 |
| C | 1.61939100 | 0.47272400 | -1.08329300 |
| H | 1.74422400 | 0.66720900 | -2.14866700 |
| H | 1.01280500 | -2.01680800 | 0.14732700 |
| C | -3.36015000 | 0.31759900 | -0.47174100 |
| C | -3.98436000 | -1.01375300 | -0.06320000 |
| H | -2.94273000 | 0.96308800 | 0.28227100 |
| H | -3.18764300 | 0.55120000 | -1.50308700 |
| H | -4.19096600 | -1.58234300 | -0.97504500 |
| O | -3.00122000 | -1.76109400 | 0.70096400 |

| | | | |
|---|---|---|---|
| C | -1.70596000 | -1.58684900 | 0.26947100 |
| O | -0.84676300 | -2.33517100 | 0.74523400 |
| O | -1.55431800 | -0.64545200 | -0.57187700 |
| Cl | -5.14993000 | 1.79573000 | -0.66945800 |
| C | 1.97097700 | 1.70014000 | -0.27046400 |
| C | 2.53699300 | 2.81743100 | -0.88945500 |
| C | 1.71509200 | 1.73939500 | 1.10548400 |
| C | 2.84723500 | 3.95764600 | -0.14656900 |
| H | 2.73334800 | 2.79957100 | -1.95637700 |
| C | 2.02857000 | 2.87443000 | 1.84878900 |
| H | 1.26650600 | 0.88281300 | 1.59773300 |
| C | 2.59574200 | 3.98689300 | 1.22359500 |
| H | 3.28439800 | 4.81876600 | -0.63897300 |
| H | 1.82454100 | 2.89452000 | 2.91327100 |
| H | 2.83614300 | 4.87142200 | 1.80237300 |
| C | -5.22376300 | -0.97544200 | 0.81871100 |
| H | -6.07800100 | -0.58497000 | 0.27156000 |
| H | -5.44347800 | -1.99431800 | 1.14461200 |
| H | -5.05461300 | -0.35156600 | 1.69867200 |

1 2 1.0 3 1.0 4 1.0 11 1.0
2
3
4
5 6 1.0
6 7 2.0 11 1.0
7 8 1.0 10 1.0
8
9 10 1.5 11 1.5 15 1.0
10 13 1.0
11
12 13 1.0
13 14 1.0 26 1.0
14
15
16 17 1.0 18 1.0 19 1.0
17 20 1.0 21 1.0 37 1.0
18
19
20
21 22 1.0
22 23 2.0 24 2.0
23
24

25
26 27 1.5 28 1.5
27 29 1.5 30 1.0
28 31 1.5 32 1.0
29 33 1.5 34 1.0
30
31 33 1.5 35 1.0
32
33 36 1.0
34
35
36
37 38 1.0 39 1.0 40 1.0
38
39
40



**V**

| | | | |
|---|---|---|---|
| C | 0.59585100 | 3.39381300 | -0.98797000 |
| H | 0.68084400 | 3.73771800 | 0.04492100 |
| H | 1.48949500 | 2.84217800 | -1.27111200 |
| H | 0.45917300 | 4.23855900 | -1.66170000 |
| H | -2.17846600 | 3.87298300 | -0.74557000 |
| C | -1.88521200 | 2.85894200 | -0.95395600 |
| C | -2.63008300 | 1.73283100 | -1.11608200 |
| H | -3.69452300 | 1.58226700 | -1.07594200 |
| C | -0.50172700 | 1.18524700 | -1.35352400 |
| N | -1.74766900 | 0.69761000 | -1.36508400 |
| N | -0.56067300 | 2.49586300 | -1.10749400 |
| H | -1.18428600 | -1.23351300 | -1.85536300 |
| C | -2.11233300 | -0.71543900 | -1.61326700 |
| H | -2.74970000 | -0.73972900 | -2.49733100 |
| H | 0.40686600 | 0.61983800 | -1.51314100 |
| C | 3.67598600 | -2.42047500 | 0.39841900 |

| | | | |
|---|---|---|---|
| C | 4.91120800 | -1.64539300 | -0.07403700 |
| H | 3.59909500 | -3.38354300 | -0.11033300 |
| H | 5.70262300 | -2.28213700 | -0.46118400 |
| H | 5.30274800 | -0.97394200 | 0.69194400 |
| O | 4.40093400 | -0.83532700 | -1.16372200 |
| C | 3.06219000 | -0.77472900 | -1.08001100 |
| O | 2.37661700 | -0.06952600 | -1.77651800 |
| O | 2.58750400 | -1.59302700 | -0.13161700 |
| Cl | 0.81498600 | 4.25539200 | 2.70519600 |
| C | -2.80851300 | -1.35442900 | -0.43132000 |
| C | -4.14911700 | -1.73443900 | -0.52987300 |
| C | -2.11828600 | -1.58566600 | 0.76451000 |
| C | -4.79558900 | -2.33491400 | 0.55153800 |
| H | -4.69086500 | -1.56349700 | -1.45418300 |
| C | -2.76380500 | -2.18042700 | 1.84529200 |
| H | -1.07502400 | -1.30141500 | 0.85364700 |
| C | -4.10461200 | -2.55653600 | 1.74081700 |
| H | -5.83584500 | -2.62629000 | 0.46274600 |
| H | -2.22079800 | -2.35470600 | 2.76709800 |
| H | -4.60519800 | -3.02145800 | 2.58243900 |
| C | 3.53395100 | -2.57728300 | 1.89444200 |
| H | 2.60361300 | -3.09107600 | 2.14155200 |
| H | 4.36456200 | -3.17722300 | 2.27533600 |
| H | 3.54943200 | -1.60458500 | 2.39088100 |

1 2 1.0 3 1.0 4 1.0 11 1.0
2
3
4
5 6 1.0
6 7 2.0 11 1.0
7 8 1.0 10 1.0
8
9 10 1.5 11 1.5 15 1.0
10 13 1.0
11
12 13 1.0
13 14 1.0 26 1.0
14
15
16 17 1.0 18 1.0 24 1.0 37 1.0
17 19 1.0 20 1.0 21 1.0
18
19

20

21 22 1.5

22 23 2.0 24 1.5

23

24

25

26 27 1.5 28 1.5

27 29 1.5 30 1.0

28 31 1.5 32 1.0

29 33 1.5 34 1.0

30

31 33 1.5 35 1.0

32

33 36 1.0

34

35

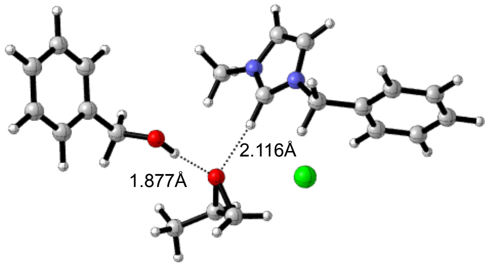
36

37 38 1.0 39 1.0 40 1.0

38

39

40



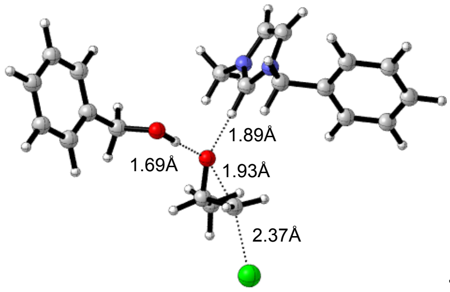

**I/**

| | | | |
|---|---|---|---|
| C | -0.34752900 | 3.23345200 | -0.84817800 |
| C | -0.09171300 | 2.40495000 | -2.02895900 |
| H | 0.51968500 | 3.51380300 | -0.25459900 |
| H | 0.92592500 | 2.13333700 | -2.28962300 |
| H | -0.80933700 | 2.40366500 | -2.84382200 |
| O | -0.58007800 | 1.79062400 | -0.80631800 |
| C | 0.12760100 | 0.63005700 | 3.24873100 |
| H | -0.31689700 | 1.39149900 | 2.61320200 |
| H | -0.65661600 | 0.07576900 | 3.76244800 |
| H | 0.78827600 | 1.10165700 | 3.97452100 |
| H | 1.66996300 | -1.64017700 | 3.90615800 |
| C | 1.62903200 | -1.37636800 | 2.86372500 |
| C | 2.20586200 | -1.95306000 | 1.77664100 |
| H | 2.84674400 | -2.81307500 | 1.69348900 |
| C | 1.03837300 | -0.20724300 | 1.08387200 |
| N | 1.82467200 | -1.20847300 | 0.67484600 |
| N | 0.90417100 | -0.28938000 | 2.41011400 |
| H | 1.72424700 | -0.70425700 | -1.32913600 |
| C | 2.20261400 | -1.47918100 | -0.72990600 |
| H | 1.76496900 | -2.43739100 | -1.01112900 |
| H | 0.57816700 | 0.53686500 | 0.44508100 |
| Cl | 3.10811300 | 3.18144500 | 0.98176700 |
| C | 3.70092300 | -1.49084600 | -0.94223200 |
| C | 4.32698100 | -2.64562800 | -1.41767600 |
| C | 4.46839100 | -0.34605500 | -0.69382700 |
| C | 5.70390000 | -2.66063600 | -1.64599400 |
| H | 3.73876700 | -3.53621500 | -1.61242700 |
| C | 5.84307600 | -0.36414000 | -0.91620200 |
| H | 3.99803400 | 0.55999900 | -0.32309000 |
| C | 6.46377100 | -1.52035800 | -1.39415600 |
| H | 6.17862500 | -3.56199500 | -2.01646000 |
| H | 6.43001300 | 0.52604600 | -0.72066100 |
| H | 7.53364900 | -1.52996200 | -1.56887600 |
| C | -1.55838300 | 4.11402600 | -0.72773800 |
| H | -1.90119800 | 4.16171300 | 0.30923100 |
| H | -1.30322700 | 5.13012600 | -1.04260200 |
| H | -2.37649400 | 3.75238500 | -1.35450600 |

| | | | |
|---|---|---|---|
| C | -7.23817400 | -2.18108200 | -0.34537900 |
| C | -7.14320800 | -1.12583700 | -1.25352600 |
| C | -6.09708400 | -0.20941700 | -1.15156100 |
| C | -5.13288700 | -0.33373700 | -0.14506200 |
| C | -5.23886000 | -1.39467600 | 0.76070500 |
| C | -6.28379100 | -2.31353200 | 0.66362600 |
| H | -8.05301500 | -2.89244600 | -0.42074500 |
| H | -7.88488400 | -1.01476700 | -2.03677600 |
| H | -6.02950800 | 0.61223300 | -1.85746700 |
| H | -4.50046300 | -1.49976200 | 1.54921900 |
| H | -6.35478000 | -3.12872700 | 1.37519500 |
| C | -3.98174200 | 0.63671900 | -0.06177200 |
| H | -4.30611000 | 1.62774100 | -0.40075700 |
| H | -3.64652700 | 0.72715600 | 0.97833500 |
| O | -2.90857400 | 0.16003400 | -0.88709700 |
| H | -2.17154300 | 0.79548100 | -0.83243600 |

1 2 1.0 3 1.0 6 1.0 34 1.0
2 4 1.0 5 1.0 6 1.0
3
4
5
6
7 8 1.0 9 1.0 10 1.0 17 1.0
8
9
10
11 12 1.0
12 13 2.0 17 1.0
13 14 1.0 16 1.0
14
15 16 1.5 17 1.5 21 1.0
16 19 1.0
17
18 19 1.0
19 20 1.0 23 1.0
20
21
22
23 24 1.5 25 1.5
24 26 1.5 27 1.0
25 28 1.5 29 1.0
26 30 1.5 31 1.0
27

28 30 1.5 32 1.0
29
30 33 1.0
31
32
33
34 35 1.0 36 1.0 37 1.0
35
36
37
38 39 1.5 43 1.5 44 1.0
39 40 1.5 45 1.0
40 41 1.5 46 1.0
41 42 1.5 49 1.0
42 43 1.5 47 1.0
43 48 1.0
44
45
46
47
48
49 50 1.0 51 1.0 52 1.0
50
51
52 53 1.0
53




**TS1/**

| | | | |
|---|---|---|---|
| C | 0.29382100 | 2.90310800 | -0.27541700 |
| C | -0.45830000 | 2.79461700 | 0.98168900 |
| H | 1.35661600 | 2.72048300 | -0.24412400 |
| H | -0.22663400 | 2.71617200 | -1.20019700 |
| H | -1.49355500 | 3.14896500 | 0.89645800 |
| O | -0.33307300 | 1.40636800 | 0.76539400 |

| | | | |
|---|---|---|---|
| C | 1.14540900 | -0.90977400 | 4.20240000 |
| H | 2.01502200 | -0.65763200 | 4.80801200 |
| H | 0.54192000 | -0.02014400 | 4.04022200 |
| H | 0.54889000 | -1.66870000 | 4.70673600 |
| H | 2.65710700 | -3.19219900 | 3.51028400 |
| C | 2.33517900 | -2.56671700 | 2.69596900 |
| C | 2.53263400 | -2.67922300 | 1.35588100 |
| H | 3.06196600 | -3.42022000 | 0.78329200 |
| C | 1.33293000 | -0.85225900 | 1.71772000 |
| N | 1.90018200 | -1.60054200 | 0.76444900 |
| N | 1.58545000 | -1.42192400 | 2.90050500 |
| H | 1.24081800 | -0.39899500 | -0.78110000 |
| C | 1.82573200 | -1.31428600 | -0.68699700 |
| H | 1.26647100 | -2.12459900 | -1.15518000 |
| H | 0.75922200 | 0.06131600 | 1.53491200 |
| Cl | 0.63253900 | 5.16933100 | -0.89570400 |
| C | 3.19151500 | -1.16763200 | -1.32054000 |
| C | 3.65556900 | -2.12716500 | -2.22372500 |
| C | 3.99938500 | -0.06416200 | -1.02110500 |
| C | 4.91106000 | -1.99038400 | -2.81821200 |
| H | 3.03402100 | -2.98231800 | -2.46752400 |
| C | 5.25337700 | 0.07152200 | -1.61074400 |
| H | 3.64711100 | 0.69253900 | -0.32802100 |
| C | 5.71208800 | -0.89259500 | -2.51088300 |
| H | 5.25949900 | -2.74032200 | -3.51906100 |
| H | 5.87001900 | 0.93107400 | -1.37410700 |
| H | 6.68720300 | -0.78454600 | -2.97197400 |
| C | 0.18778300 | 3.30896300 | 2.25419800 |
| H | 0.15129300 | 4.40077300 | 2.29444800 |
| H | -0.34384500 | 2.91375400 | 3.12448600 |
| H | 1.23273800 | 2.99118800 | 2.31219200 |
| C | -5.50800200 | 0.14467600 | -1.06718300 |
| C | -4.66049700 | -0.56302100 | -0.20693500 |
| C | -4.89263200 | -1.92834100 | -0.01013900 |
| C | -5.94547500 | -2.57500800 | -0.65848900 |
| C | -6.78157800 | -1.85983000 | -1.51596200 |
| C | -6.56082800 | -0.49651200 | -1.71880500 |
| H | -5.34226000 | 1.20567400 | -1.22508500 |
| H | -4.24557500 | -2.48822300 | 0.65777100 |
| H | -6.11413800 | -3.63341900 | -0.49276000 |
| H | -7.60182200 | -2.35951000 | -2.01927200 |
| H | -7.21051800 | 0.06635800 | -2.38001200 |
| C | -3.49775800 | 0.12744200 | 0.46354700 |
| H | -3.78310400 | 1.15480200 | 0.72567800 |

| | | | |
|---|---|---|---|
| H | -3.24890000 | -0.39692500 | 1.39558200 |
| O | -2.37547400 | 0.13572400 | -0.42027200 |
| H | -1.63228300 | 0.62603700 | 0.02207500 |

1 2 1.0 3 1.0 4 1.0
2 5 1.0 6 1.0 34 1.0
3
4
5
6
7 8 1.0 9 1.0 10 1.0 17 1.0
8
9
10
11 12 1.0
12 13 2.0 17 1.0
13 14 1.0 16 1.0
14
15 16 1.5 17 1.5 21 1.0
16 19 1.0
17
18 19 1.0
19 20 1.0 23 1.0
20
21
22
23 24 1.5 25 1.5
24 26 1.5 27 1.0
25 28 1.5 29 1.0
26 30 1.5 31 1.0
27
28 30 1.5 32 1.0
29
30 33 1.0
31
32
33
34 35 1.0 36 1.0 37 1.0
35
36
37
38 39 1.5 43 1.5 44 1.0
39 40 1.5 49 1.0
40 41 1.5 45 1.0

41 42 1.5 46 1.0

42 43 1.5 47 1.0

43 48 1.0

44

45

46

47

48

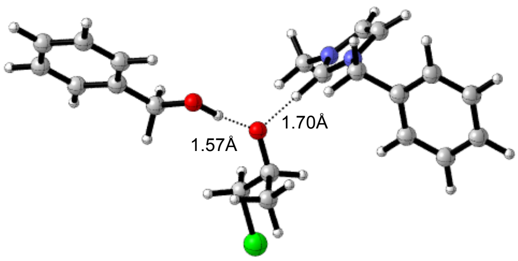
49 50 1.0 51 1.0 52 1.0

50

51

52 53 1.0

53




II/

| | | | |
|---|---|---|---|
| C | -0.81688000 | 3.21058700 | 0.09489100 |
| C | 0.02402300 | 2.06935000 | -0.49653700 |
| H | -1.84927600 | 3.16791100 | -0.25013800 |
| H | -0.77944700 | 3.18890400 | 1.18097300 |
| H | 1.07859600 | 2.27154100 | -0.21457500 |
| O | -0.43014500 | 0.89704000 | 0.09005400 |
| C | 1.07053800 | 0.65183300 | 3.88846200 |
| H | 1.76717600 | 1.38026500 | 4.30234300 |
| H | 0.29320700 | 1.16583000 | 3.32831900 |
| H | 0.61958200 | 0.07287300 | 4.69355000 |
| H | 3.19385100 | -1.15418700 | 4.33770600 |
| C | 2.82429200 | -1.08961700 | 3.32905300 |
| C | 3.20768900 | -1.73912600 | 2.19913000 |
| H | 3.97713400 | -2.47334700 | 2.03720100 |
| C | 1.53336400 | -0.37614400 | 1.66760300 |
| N | 2.39279600 | -1.28100400 | 1.17847400 |
| N | 1.78357700 | -0.24761300 | 2.97692700 |
| H | 1.61056200 | -1.21039000 | -0.72960400 |
| C | 2.44173600 | -1.71312000 | -0.23492300 |
| H | 2.25321300 | -2.78677900 | -0.26136300 |

| | | | |
|---|---|---|---|
| H | 0.74148400 | 0.15602000 | 1.07574100 |
| Cl | -0.21898700 | 4.90982300 | -0.36542700 |
| C | 3.76079300 | -1.38490900 | -0.90042000 |
| C | 4.64597700 | -2.40691100 | -1.25246900 |
| C | 4.10421800 | -0.05748600 | -1.18364900 |
| C | 5.85940500 | -2.10988000 | -1.87504800 |
| H | 4.38599000 | -3.43943800 | -1.04401500 |
| C | 5.31618700 | 0.24065600 | -1.80113500 |
| H | 3.42160200 | 0.74544000 | -0.92529600 |
| C | 6.19711900 | -0.78593400 | -2.14804200 |
| H | 6.53674300 | -2.91200900 | -2.14499000 |
| H | 5.57123100 | 1.27176500 | -2.01783000 |
| H | 7.13886900 | -0.55311500 | -2.63185800 |
| C | -0.04604300 | 2.03725600 | -2.03067500 |
| H | -1.08045900 | 1.89015500 | -2.35883600 |
| H | 0.33315200 | 2.95910000 | -2.48203900 |
| H | 0.55063500 | 1.20155000 | -2.40611000 |
| C | -4.84370800 | -1.95568600 | -0.90025200 |
| C | -5.99514700 | -2.72391700 | -1.09410800 |
| C | -7.22929200 | -2.27379600 | -0.62945600 |
| C | -7.30628200 | -1.04517500 | 0.03200400 |
| C | -6.15758300 | -0.28132900 | 0.22299500 |
| C | -4.91177600 | -0.72734100 | -0.23912100 |
| H | -3.88430700 | -2.30323300 | -1.26167200 |
| H | -5.92471700 | -3.67556400 | -1.61034300 |
| H | -8.12244700 | -2.86996700 | -0.78005700 |
| H | -8.26154500 | -0.68335200 | 0.39689200 |
| H | -6.22794400 | 0.67327800 | 0.73675300 |
| C | -3.68079100 | 0.12543000 | -0.00717200 |
| H | -3.87675200 | 1.13102000 | -0.41290100 |
| H | -3.54877600 | 0.25451600 | 1.07908100 |
| O | -2.53114600 | -0.44170200 | -0.59017100 |
| H | -1.72589000 | 0.13339400 | -0.35832800 |

1 2 1.0 3 1.0 4 1.0 22 1.0
2 5 1.0 6 1.0 34 1.0
3
4
5
6
7 8 1.0 9 1.0 10 1.0 17 1.0
8
9
10

11 12 1.0
12 13 2.0 17 1.0
13 14 1.0 16 1.0
14
15 16 1.5 17 1.5 21 1.0
16 19 1.0
17
18 19 1.0
19 20 1.0 23 1.0
20
21
22
23 24 1.5 25 1.5
24 26 1.5 27 1.0
25 28 1.5 29 1.0
26 30 1.5 31 1.0
27
28 30 1.5 32 1.0
29
30 33 1.0
31
32
33
34 35 1.0 36 1.0 37 1.0
35
36
37
38 39 1.5 43 1.5 44 1.0
39 40 1.5 45 1.0
40 41 1.5 46 1.0
41 42 1.5 47 1.0
42 43 1.5 48 1.0
43 49 1.0
44
45
46
47
48
49 50 1.0 51 1.0 52 1.0
50
51
52 53 1.0
53