Electronic Supplementary Material (ESI) for Materials Chemistry Frontiers.


# Supporting Information

# Exploring Multifunctional Applications of a Luminescent Covalent Triazine Polymer in Acid Vapour Sensing, $CO_2$ Capture, Dye Removal, and Turn-off Fluorescence Sensing of Dichromate Ions

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**Chemical & Reagents:** 4-Cyanobenzylbromide, triflic acid, and NaH were purchased from Sigma-Aldrich. p-xylylenediol was purchased from TCI India. Dry *N*, *N*-dimethylformamide (DMF), Hydrochloric acid, and methanol were purchased from Finar Chemicals. Potassium dichromate was purchased from Merck Life Science Pvt. Ltd. Methyl Orange (MO), Methylene Blue (MB), and Malachite Green oxalate were purchased from AVRA Chemicals.

**Characterization Techniques:** Fourier-transform infrared (FTIR) analysis was carried out on a PerkinElmer's spectrum II spectrometer. NMR spectra were obtained by an AVANCE III 500 Ascend Bruker Biospin machine at an ambient temperature using $CDCl_3$. $^{13}C$ CP/MAS NMR was carried out by an ECZR series 600 MHz NMR by JEOL. Morphological data of the polymer were recorded using a JEOL JSM-7400F field emission scanning electron microscope (FE-SEM). A Quantachrome, Autosorb iQ2 Brunauer–Emmett–Teller (BET) surface area analyzer was used to collect the data of the surface area, pore volume, and pore size. Powder X-ray diffraction (PXRD) of the polymer was done on an Empyrean, Malvern Panalytical, with Cu Kα radiation with a 2θ range from 20 to 60° and a step size of 0.02°. UV-DRS spectra were obtained from a Cary 5000 UV–vis NIR Spectrometer.

**Computational Methods:** The ground-state structures of SMCOP-2 were optimized without symmetry constraints using the hybrid density functional B3LYP[1] involving Grimme's dispersion correction (D3)[2], in combination with the 6-31G(d) basis set. Harmonic frequency analysis revealed no imaginary frequencies, signifying true minimum geometry. Excitation energies of 100 states of SMCOP-2 were computed using the time-dependent variant of B3LYP (TD-B3LYP) using the same basis set to obtain the absorption spectrum. Excitation energies of SMCOP-2 were computed in the gas phase to match the solid-state absorption spectrum obtained experimentally. Gaussian 16 software was used for all computations[3]. The binding energy between $CO_2$ and SMCOP-2 is calculated using the following equation:

$$\textbf{Binding energy} = E_{SMCOP\text{-}2\text{-}CO2} - (E_{SMCOP\text{-}2} + E_{CO2})$$

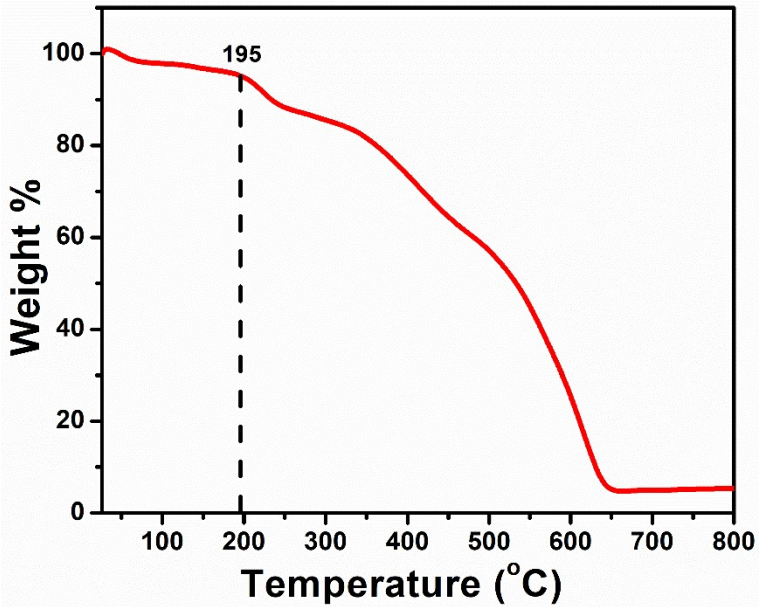


**Figure S1:** TGA of SMCOP-2

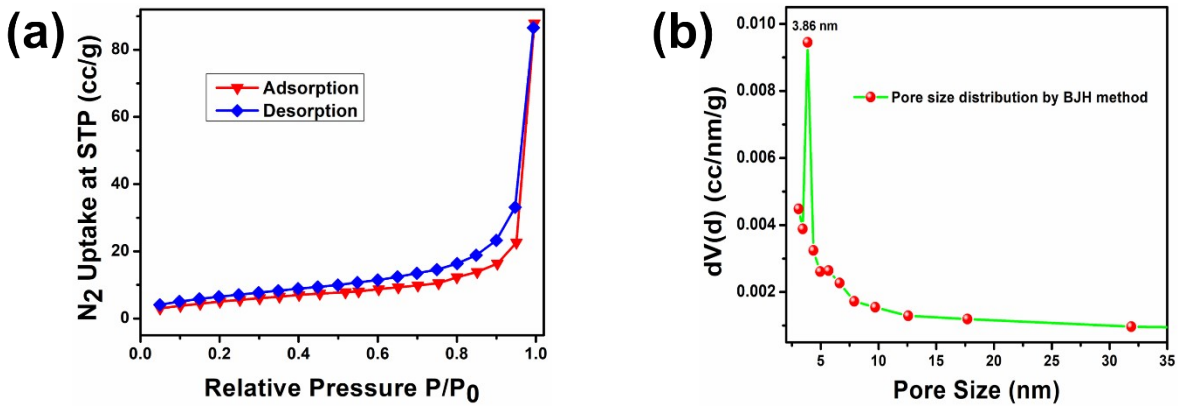


**Figure S2:** (a) BET isotherm of SMCOP-2. (b) Porosity distribution by BJH method.

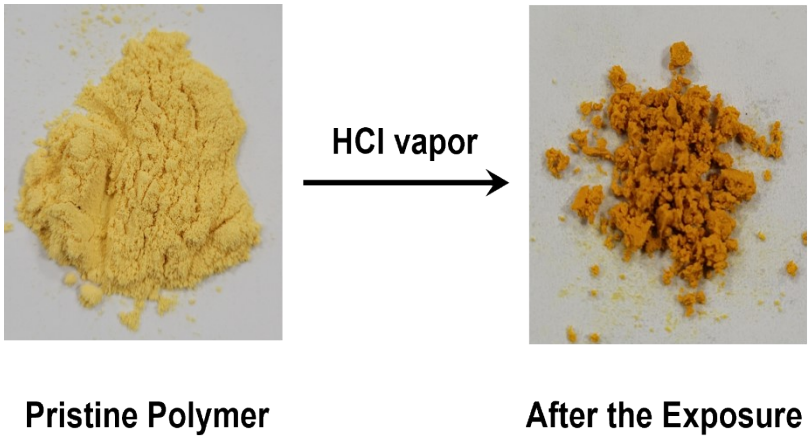


**Figure S3.** Change in color when exposed to acid vapor.

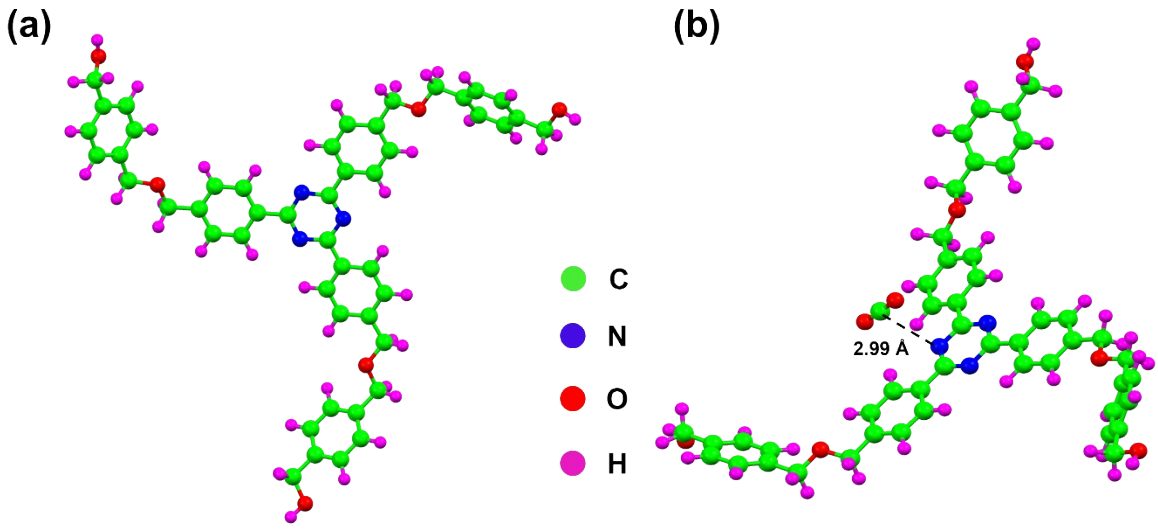


**Figure S4.** Geometry optimized structure of (a) Truncated SMCOP-2. (b) SMCOP-2@$CO_2$.

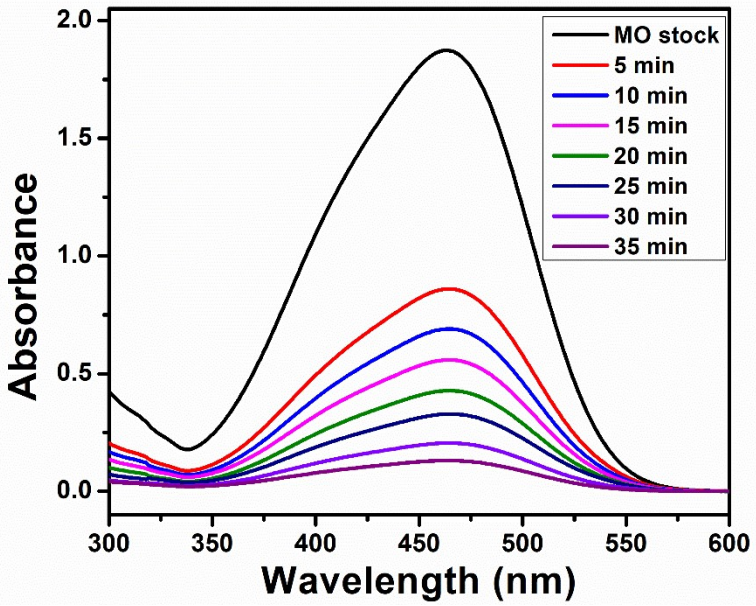


**Figure S5.** Time-dependent UV-vis spectra of MO adsorption.

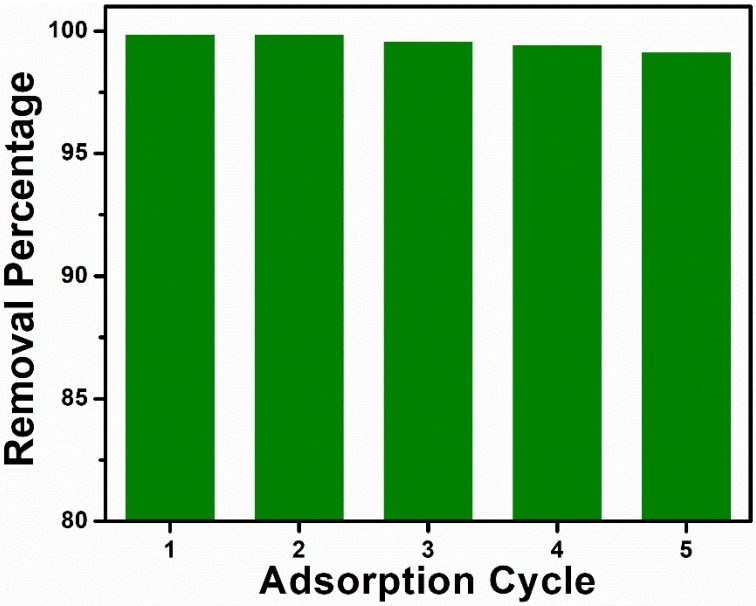


**Figure S6.** Consecutive MO adsorption cycle.

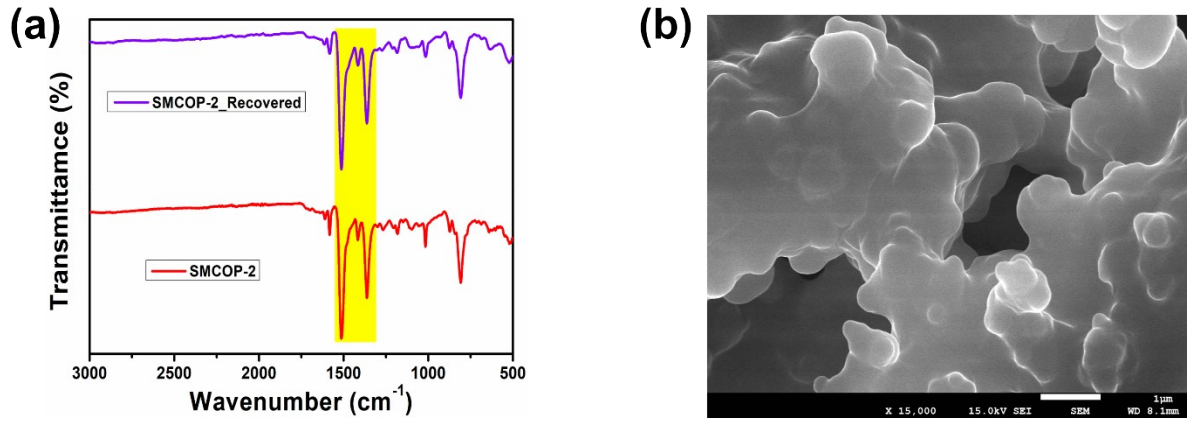


**Figure S7.** (a) Comparative FT-IR spectra. (b) FE-SEM image of recovered SMCOP-2 after the 5$^{th}$ cycle.

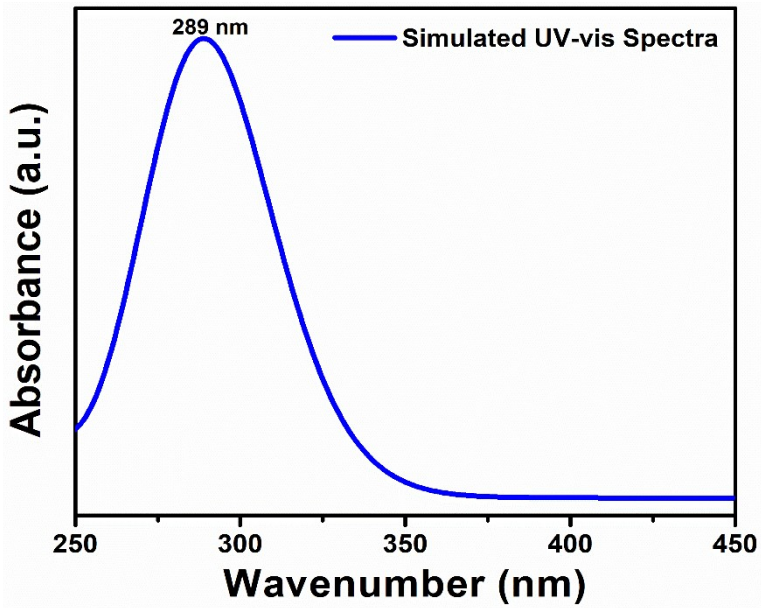


**Figure S8.** Simulated UV-vis spectra of SMCOP-2.

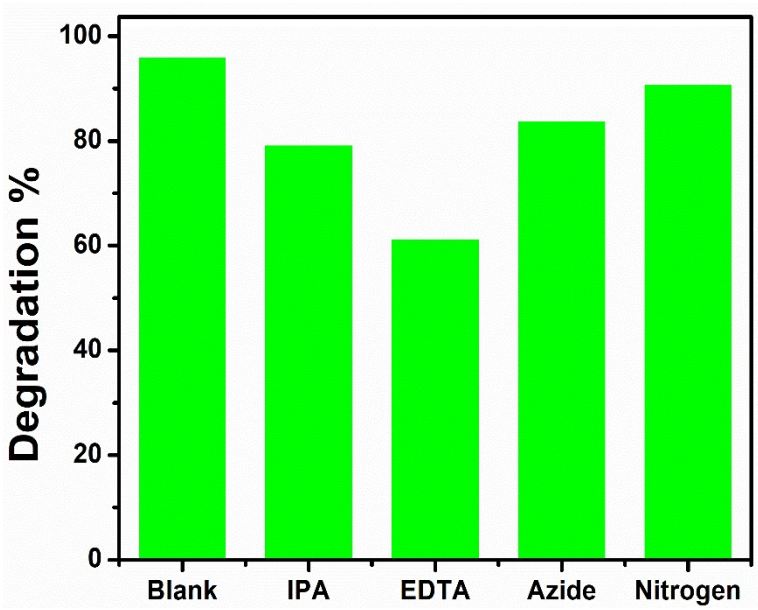


**Figure S9.** Control photocatalytic reactions.

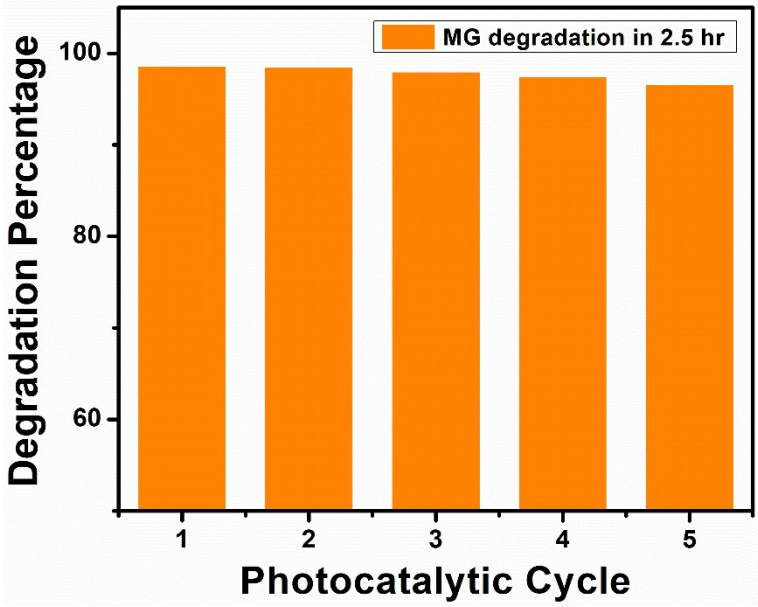


**Figure S10.** Consecutive MG degradation cycles.

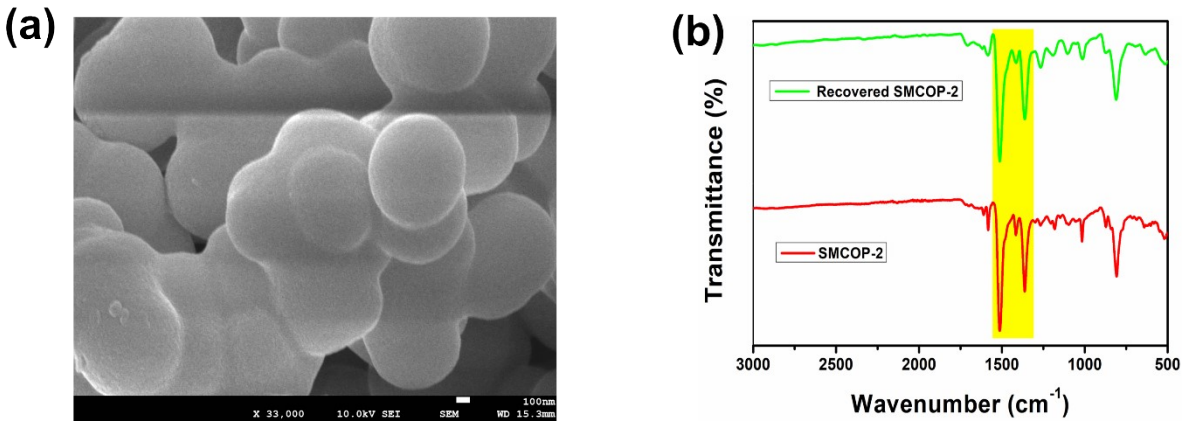


**Figure S11.** (a) FE-SEM image of the recovered photocatalyst. (b) Comparative FT-IR spectra of the recovered photocatalyst with the pristine polymer.

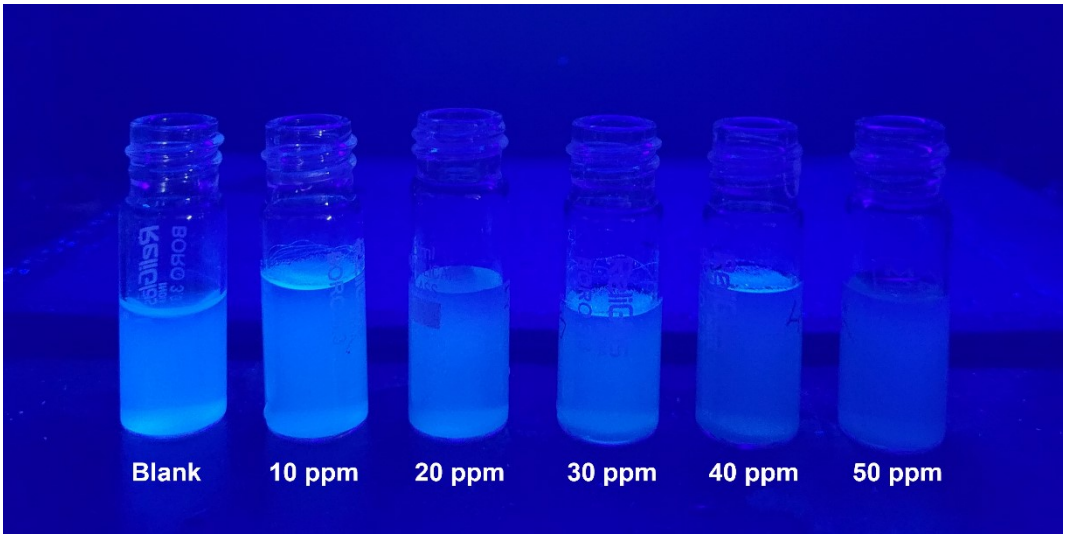


**Figure S12.** Fluorescence quenching of SMCOP-2 with the gradual increase in dichromate concentration.

**Table S1.** Calculation of Standard Deviation.

| Entry No. | FL Intensity |
|---|---|
| 1 | 231325.3 |
| 2 | 231339.7 |
| 3 | 231347.8 |
| 4 | 231333.2 |
| 5 | 231350.5 |
| Standard Deviation | 9.28 |

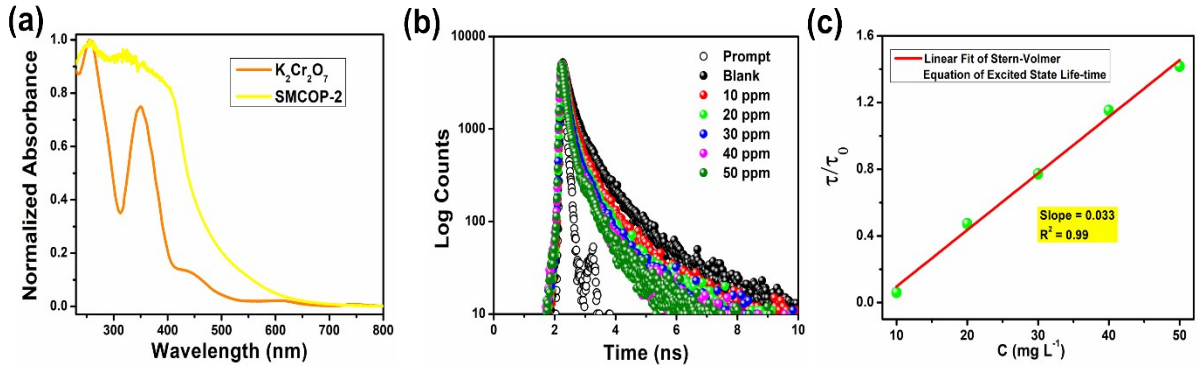


**Figure S13.** (a) UV-vis spectra of SMCOP-2 and $K_2Cr_2O_7$. (b) TCSPC Lifetime. (c) Stern-Volmer plot of lifetime vs quencher concentration.

**Table S2.** Coordinates of truncated SMCOP-2.

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Energy: -2471.8930631 Hartree

| | | | |
|---|---|---|---|
| C | 1.218700 | 0.476890 | -0.634310 |
| N | 0.171940 | 1.317770 | -0.632600 |
| C | -1.041370 | 0.743450 | -0.597730 |

| | | | |
|---|---|---|---|
| C | -0.141480 | -1.347050 | -0.572060 |
| N | 1.109790 | -0.861110 | -0.604560 |
| N | -1.245890 | -0.583240 | -0.567730 |
| C | 2.578700 | 1.061530 | -0.670800 |
| C | 3.713100 | 0.233750 | -0.686660 |
| C | 2.758210 | 2.454960 | -0.685260 |
| C | 4.991380 | 0.783520 | -0.720980 |
| H | 3.581760 | -0.842490 | -0.673130 |
| C | 4.037840 | 2.999850 | -0.711370 |
| H | 1.888100 | 3.101510 | -0.666560 |
| C | 5.169120 | 2.172830 | -0.733140 |
| H | 5.862680 | 0.137760 | -0.728520 |
| H | 4.160390 | 4.080300 | -0.712050 |
| C | -0.313850 | -2.817210 | -0.538020 |
| C | 0.804650 | -3.668120 | -0.528210 |
| C | -1.596610 | -3.387360 | -0.510400 |
| C | 0.638780 | -5.048190 | -0.488200 |
| H | 1.798980 | -3.236140 | -0.544000 |
| C | -1.757980 | -4.769960 | -0.478660 |
| H | -2.464220 | -2.736930 | -0.514920 |
| C | -0.642630 | -5.616460 | -0.466180 |
| H | 1.514170 | -5.693120 | -0.471450 |
| H | -2.752170 | -5.202180 | -0.454250 |
| C | -2.228100 | 1.628920 | -0.591210 |

| | | | |
|---|---|---|---|
| C | -2.079870 | 3.024710 | -0.633010 |
| C | -3.523780 | 1.087830 | -0.537190 |
| C | -3.195840 | 3.856920 | -0.624940 |
| H | -1.082760 | 3.449000 | -0.672670 |
| C | -4.635490 | 1.923410 | -0.521070 |
| H | -3.647170 | 0.011370 | -0.498920 |
| C | -4.486570 | 3.316390 | -0.567530 |
| H | -3.072960 | 4.934030 | -0.653390 |
| H | -5.631320 | 1.489760 | -0.468690 |
| C | -0.793790 | -7.119470 | -0.470900 |
| H | -0.642850 | -7.500850 | -1.496620 |
| H | -0.009760 | -7.580010 | 0.152690 |
| C | 6.547740 | 2.784540 | -0.813750 |
| H | 6.786210 | 3.016890 | -1.867140 |
| H | 6.571120 | 3.742060 | -0.268110 |
| C | -5.710440 | 4.201050 | -0.597240 |
| H | -6.103750 | 4.251350 | -1.628360 |
| H | -6.509980 | 3.762080 | 0.022010 |
| O | 7.506290 | 1.882930 | -0.287030 |
| O | -2.081750 | -7.478940 | -0.003350 |
| O | -5.378560 | 5.500760 | -0.140300 |
| C | -6.468950 | 6.414670 | -0.235680 |
| H | -7.292740 | 6.100450 | 0.423940 |
| H | -6.859790 | 6.412010 | -1.267430 |

| | | | |
|---|---|---|---|
| C | 8.845490 | 2.348120 | -0.439670 |
| H | 9.029460 | 2.593300 | -1.499580 |
| H | 8.999810 | 3.272580 | 0.138330 |
| C | -2.326280 | -8.881210 | -0.078910 |
| H | -2.124690 | -9.233440 | -1.104970 |
| H | -1.643760 | -9.427390 | 0.590740 |
| C | -5.981790 | 7.792060 | 0.137590 |
| C | -4.867540 | 8.340490 | -0.511500 |
| C | -6.632010 | 8.553770 | 1.113460 |
| C | -4.420040 | 9.620890 | -0.192120 |
| H | -4.353820 | 7.757810 | -1.271240 |
| C | -6.183510 | 9.836500 | 1.434670 |
| H | -7.495700 | 8.141290 | 1.629990 |
| C | -5.071240 | 10.384100 | 0.786520 |
| H | -3.558830 | 10.034910 | -0.711940 |
| H | -6.697800 | 10.421430 | 2.190420 |
| C | 9.790310 | 1.266660 | 0.020770 |
| C | 9.685760 | -0.027020 | -0.507810 |
| C | 10.793180 | 1.528600 | 0.959320 |
| C | 10.566150 | -1.029950 | -0.107080 |
| H | 8.910500 | -0.242990 | -1.237890 |
| C | 11.675340 | 0.523780 | 1.361850 |
| H | 10.885750 | 2.526100 | 1.382810 |
| C | 11.570720 | -0.767700 | 0.834550 |

| | | | |
|---|---|---|---|
| H | 10.475850 | -2.026550 | -0.533710 |
| H | 12.452920 | 0.738850 | 2.087720 |
| C | -3.764260 | -9.145040 | 0.291910 |
| C | -4.793800 | -8.435000 | -0.342860 |
| C | -4.102850 | -10.108100 | 1.246000 |
| C | -6.126960 | -8.679730 | -0.024690 |
| H | -4.540120 | -7.681000 | -1.082980 |
| C | -5.441620 | -10.366350 | 1.552550 |
| H | -3.318210 | -10.668390 | 1.748930 |
| C | -6.467630 | -9.651950 | 0.927230 |
| H | -6.918210 | -8.127750 | -0.522500 |
| H | -5.686190 | -11.127800 | 2.289590 |
| C | -4.548260 | 11.750770 | 1.165700 |
| H | -3.853030 | 11.649460 | 2.014850 |
| H | -3.969140 | 12.170810 | 0.328650 |
| C | 12.486950 | -1.874520 | 1.304380 |
| H | 12.054260 | -2.345900 | 2.201760 |
| H | 12.547890 | -2.657170 | 0.532210 |
| C | -7.913080 | -9.887210 | 1.300380 |
| H | -8.016240 | -10.868370 | 1.788890 |
| H | -8.226810 | -9.128760 | 2.035740 |
| O | -5.640880 | 12.601240 | 1.515940 |
| H | -5.268660 | 13.386760 | 1.945930 |
| O | 13.777160 | -1.337170 | 1.597630 |

| | | | |
|---|---|---|---|
| H | 14.270500 | -2.018880 | 2.079690 |
| O | -8.724660 | -9.805920 | 0.126660 |
| H | -9.648300 | -9.753120 | 0.417780 |

**Table S3.** Coordinates of $CO_2$.

3

Energy: -188.5835366 Hartree

| | | | |
|---|---|---|---|
| C | 0.00000 | 0.00000 | 0.00000 |
| O | -0.00000 | -0.00000 | 1.16921 |
| O | 0.00000 | -0.00000 | -1.16921 |

**Table S4.** Coordinates of SMCOP-2@$CO_2$

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Energy: -2660.4856291 Hartree

| | | | |
|---|---|---|---|
| C | 1.33628 | 0.73366 | -0.61975 |
| N | 0.19193 | 1.43148 | -0.71083 |
| C | -0.93339 | 0.70441 | -0.77992 |
| C | 0.22544 | -1.25283 | -0.66534 |
| N | 1.40003 | -0.60755 | -0.59351 |
| N | -0.96450 | -0.63814 | -0.76495 |
| C | 2.60592 | 1.49012 | -0.54282 |
| C | 3.83577 | 0.81783 | -0.46792 |

| | | | |
|---|---|---|---|
| C | 2.60274 | 2.89613 | -0.54074 |
| C | 5.03118 | 1.52923 | -0.39762 |
| H | 3.84603 | -0.26647 | -0.46682 |
| C | 3.79756 | 3.60204 | -0.46416 |
| H | 1.65740 | 3.42419 | -0.59404 |
| C | 5.02600 | 2.92882 | -0.39467 |
| H | 5.97629 | 1.00154 | -0.33861 |
| H | 3.77852 | 4.68940 | -0.45713 |
| C | 0.24003 | -2.73227 | -0.62048 |
| C | 1.45302 | -3.43107 | -0.49885 |
| C | -0.95774 | -3.46283 | -0.68692 |
| C | 1.46209 | -4.82065 | -0.44062 |
| H | 2.38151 | -2.87433 | -0.44074 |
| C | -0.94260 | -4.85378 | -0.63454 |
| H | -1.89874 | -2.93283 | -0.77454 |
| C | 0.26662 | -5.54922 | -0.51009 |
| H | 2.40807 | -5.34662 | -0.33627 |
| H | -1.87240 | -5.41012 | -0.67958 |
| C | -2.22358 | 1.42497 | -0.86696 |
| C | -2.27454 | 2.82022 | -0.71945 |
| C | -3.42137 | 0.72411 | -1.09010 |
| C | -3.48921 | 3.49682 | -0.79063 |
| H | -1.35477 | 3.36718 | -0.54420 |
| C | -4.63296 | 1.40392 | -1.15488 |

| | | | |
|---|---|---|---|
| H | -3.39404 | -0.35315 | -1.20414 |
| C | -4.68247 | 2.79699 | -1.00878 |
| H | -3.52080 | 4.57365 | -0.66673 |
| H | -5.55159 | 0.84626 | -1.32058 |
| C | 0.30449 | -7.05907 | -0.49330 |
| H | 0.52487 | -7.43274 | -1.50924 |
| H | 1.12379 | -7.41089 | 0.15497 |
| C | 6.30670 | 3.72926 | -0.34850 |
| H | 6.47738 | 4.20572 | -1.33020 |
| H | 6.20967 | 4.54904 | 0.38314 |
| C | -6.00517 | 3.51581 | -1.13302 |
| H | -6.25802 | 3.63619 | -2.20159 |
| H | -6.80980 | 2.90800 | -0.68732 |
| O | 7.39616 | 2.88962 | -0.01643 |
| O | -0.94133 | -7.56761 | -0.04873 |
| O | -5.92831 | 4.78369 | -0.50611 |
| C | -7.10588 | 5.56414 | -0.68931 |
| H | -7.96685 | 5.08341 | -0.19890 |
| H | -7.34102 | 5.62594 | -1.76583 |
| C | 8.64693 | 3.57089 | -0.03001 |
| H | 8.77313 | 4.08715 | -0.99717 |
| H | 8.67297 | 4.34410 | 0.75379 |
| C | -1.01674 | -8.98932 | -0.12062 |
| H | -0.75821 | -9.31881 | -1.14143 |

| | | | |
|---|---|---|---|
| H | -0.28584 | -9.44871 | 0.56292 |
| C | -6.87398 | 6.94421 | -0.12544 |
| C | -5.70107 | 7.64459 | -0.43563 |
| C | -7.83205 | 7.56405 | 0.68376 |
| C | -5.49623 | 8.93458 | 0.05147 |
| H | -4.94987 | 7.17333 | -1.06292 |
| C | -7.62718 | 8.85595 | 1.17083 |
| H | -8.74608 | 7.03236 | 0.93837 |
| C | -6.45540 | 9.55585 | 0.86181 |
| H | -4.58300 | 9.46697 | -0.20516 |
| H | -8.37908 | 9.33006 | 1.79380 |
| C | 9.75383 | 2.56634 | 0.17433 |
| C | 9.77191 | 1.37832 | -0.56792 |
| C | 10.79452 | 2.81028 | 1.07644 |
| C | 10.80876 | 0.46018 | -0.41048 |
| H | 8.96808 | 1.17786 | -1.27042 |
| C | 11.83320 | 1.89098 | 1.23371 |
| H | 10.79336 | 3.72537 | 1.66429 |
| C | 11.85120 | 0.70370 | 0.49340 |
| H | 10.81077 | -0.45408 | -0.99990 |
| H | 12.63847 | 2.09171 | 1.93319 |
| C | -2.41955 | -9.41882 | 0.22913 |
| C | -3.51423 | -8.84531 | -0.43439 |
| C | -2.65906 | -10.40079 | 1.19373 |

| | | | |
|---|---|---|---|
| C | -4.81453 | -9.24177 | -0.13407 |
| H | -3.33814 | -8.07743 | -1.18282 |
| C | -3.96335 | -10.81132 | 1.48278 |
| H | -1.82295 | -10.85619 | 1.71911 |
| C | -5.05510 | -10.23300 | 0.82895 |
| H | -5.65613 | -8.79463 | -0.65409 |
| H | -4.12967 | -11.58515 | 2.22869 |
| C | -6.20714 | 10.93445 | 1.42924 |
| H | -5.78788 | 10.83972 | 2.44401 |
| H | -5.45281 | 11.45589 | 0.81985 |
| C | 12.94458 | -0.31950 | 0.69862 |
| H | 12.67795 | -0.97060 | 1.54695 |
| H | 13.01772 | -0.96677 | -0.18911 |
| C | -6.46903 | -10.63157 | 1.18320 |
| H | -6.46288 | -11.60329 | 1.70050 |
| H | -6.88811 | -9.89578 | 1.88840 |
| O | -7.43572 | 11.66299 | 1.46548 |
| H | -7.28768 | 12.45003 | 2.01251 |
| O | 14.18118 | 0.34846 | 0.95432 |
| H | 14.80890 | -0.31878 | 1.27267 |
| O | -7.25917 | -10.68403 | -0.00679 |
| H | -8.18801 | -10.74106 | 0.26660 |
| C | -2.72779 | -1.20028 | 1.58613 |
| O | -3.49373 | -1.90151 | 1.04853 |

O -1.97374 -0.50208 2.14262

**References:**

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