**Supporting Information**

# Visible-light-driven sustainable conversion of carbon dioxide to methanol using a metal-free covalent organic framework as a recyclable photocatalyst

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**Instrumentation:**

*Absorption spectroscopy:*UV-Vis absorption spectra of the catalyst was recorded on SHIMADZU, UV-2600 UV-Vis spectrometer with a standard 1 cm x 1 cm cuvette.

*Gas Chromatography:* Gas Chromatography spectra of the reaction mixture was recorded on VARIAN 430-GC

*IR Spectra:* The FTIR spectra of the materials were recorded from a Perkin-Elmer spectrophotometer (FT-IR 783) on KBr pellets.

*Fluorescence Spectroscopy:* The Fluorescence Emission spectra was recorded by using Horiba Fluoro Max 4 spectrometer.

*PXRD:*ThePXRD analysis was performed by using an X-raydiffractometer (BRUKER, Powder X-Ray eco D8 ADVANCE) equipped with Ni-filtered Cu Kα (λ= 0.15406 nm) radiation.

*SEM:*FESEM images of the catalyst were acquired by using Scanning Electron Microscope (SEM) [JEOL JSM IT 300], was done to know about the morphological information of the sample.

*TEM:* Transmission Electron Microscope (TEM) [JEOL JEM 2100] was used obtain the morphological information of the sample.

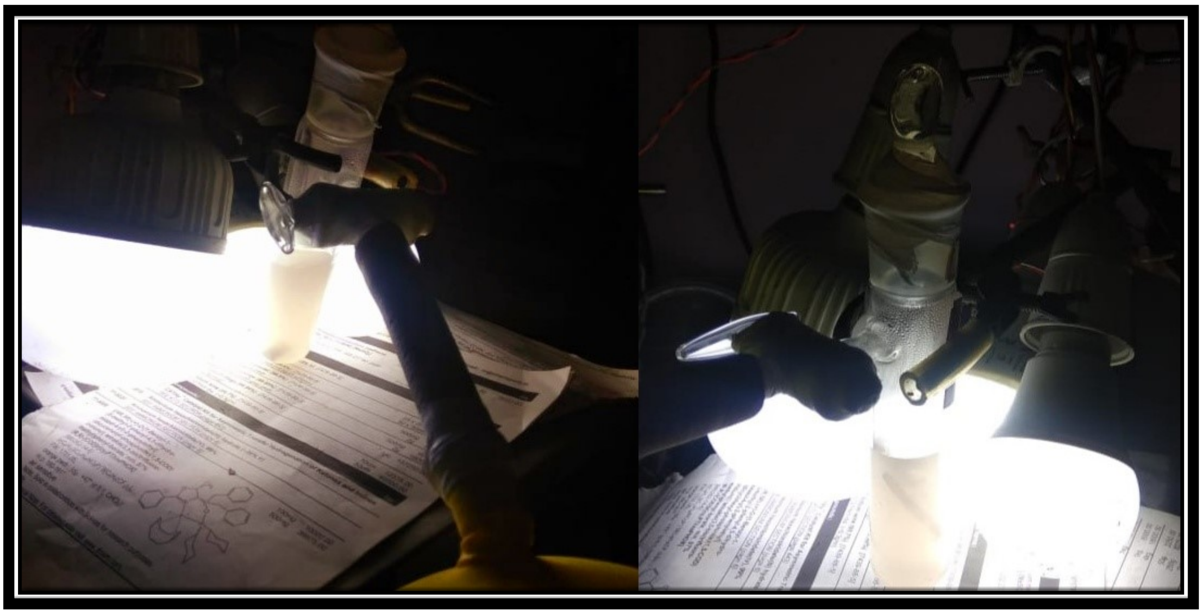
*BET:*The $N_2$ adsorption-desorption analysis of TFPG-DAAQ COF sample was conducted by using a BET Surface Analyzer [QUANTACHROME ASIQCOV602-5].

GC/MS: The detection of methanol in the reaction mixture was conducted by Agilent 7000D Triple Quadrupole GC/MS.

**Chemicals**

4-aminobenzonitrile, p-toluenesulphonic acid (PTSA), and 4-4ʾ-biphenyldicarbaldehyde (BDC) were received from Sigma Aldrich. Trifluoromethanesulfonic acid was also purchased from Sigma-Aldrich. 4,4,4-(1,3,5-Triazine-2,4,6-triyl)-trianiline (TPAT) was prepared by conducting the trimerization reaction of 4-aminobenzonitrile with the assistance of the super acid catalyst, trifluoromethanesulfonic acid. Nickel chloride hexahydrate, hydrazine monohydrate were obtained from Merck, India. Organic solvents such as acetonitrile, acetone, N, N-dimethylacetamide (DMAc) and ethelene glycol were received from Spectrochem, India, and used without further purification. All the reactions were carried out using oven-dried glassware.

**Reaction set up:**



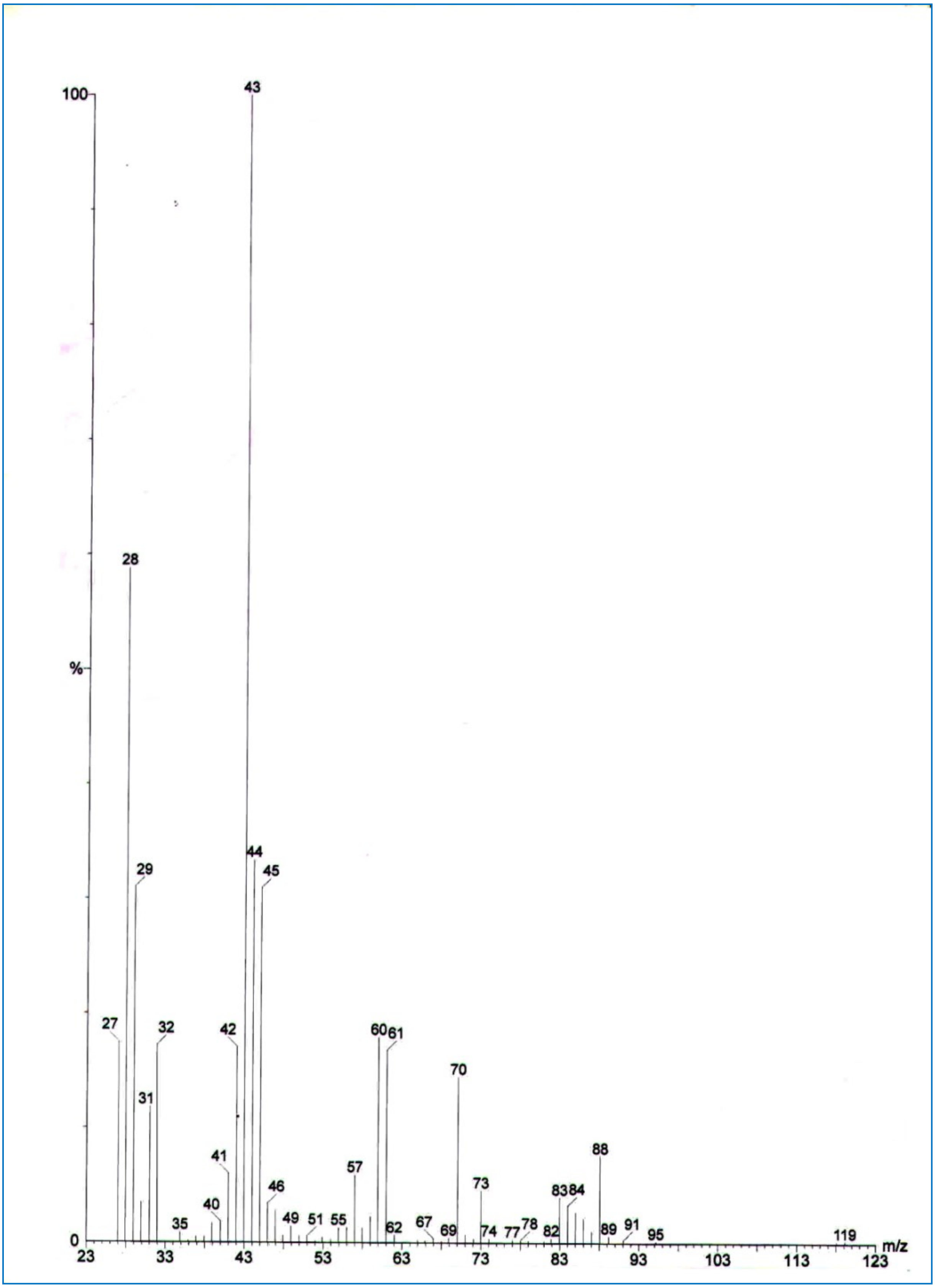
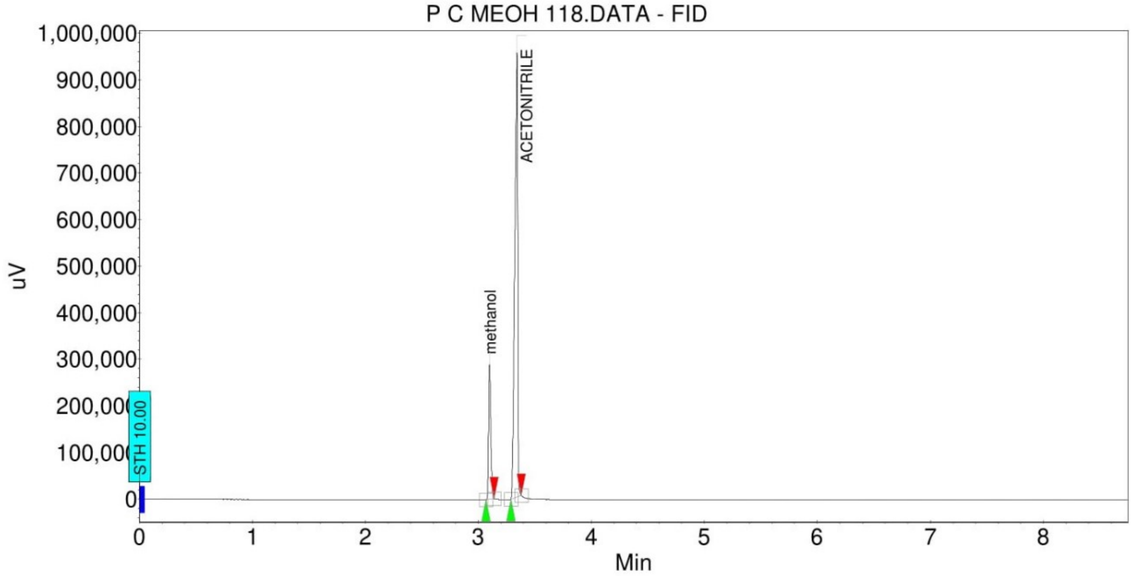



**Figure S1.** GC MS spectra of the reaction mixture.(methanol formation at optimised reaction condition)




**Peak results :**

| Index | Name | Time [Min] | Quantity [M] | Height [uV] | Area [uV.Min] | Area % [%] | Area [uV.Sec] | Quantity [M] |
|---|---|---|---|---|---|---|---|---|
| 1 | methanol | 3.10 | 0.30 | 289159.2 | 6580.8 | 18.727 | 394845.8 | 0.30 |
| 2 | ACETONITRILE | 3.34 | 0.48 | 953322.7 | 28558.8 | 81.273 | 1713529.7 | 0.48 |
| | | | | | | | | |
| Total | | | 0.78 | 1242482.0 | 35139.6 | 100.000 | 2108375.5 | 0.78 |

**Figure S2.** GC spectrum of reaction mixture.(methanol formation at optimised reaction condition)

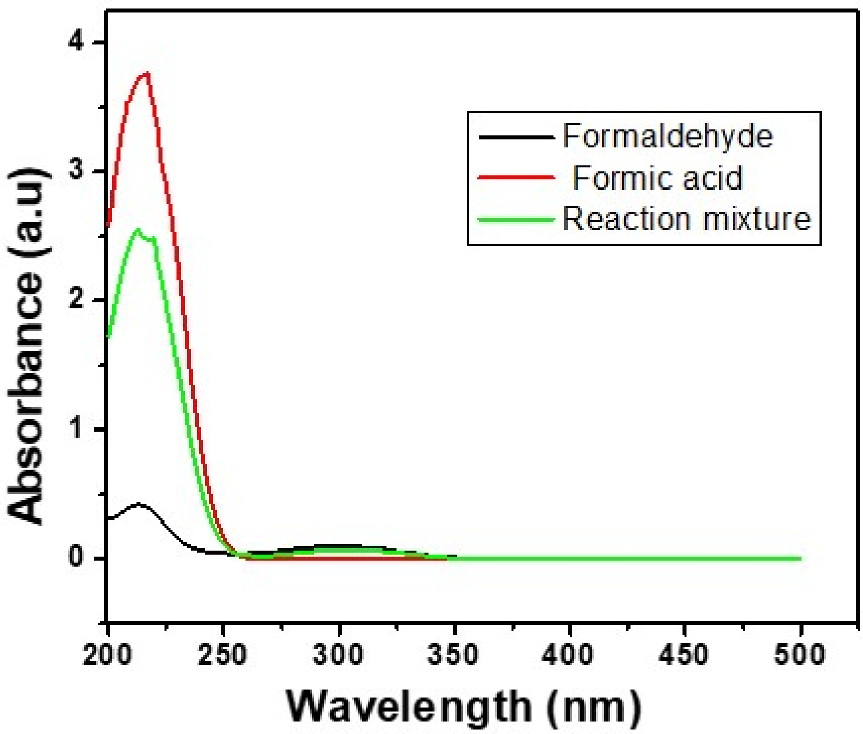



**Figure S3.**UV-vis spectra of reaction mixture, pure formic acid and pure formaldehyde

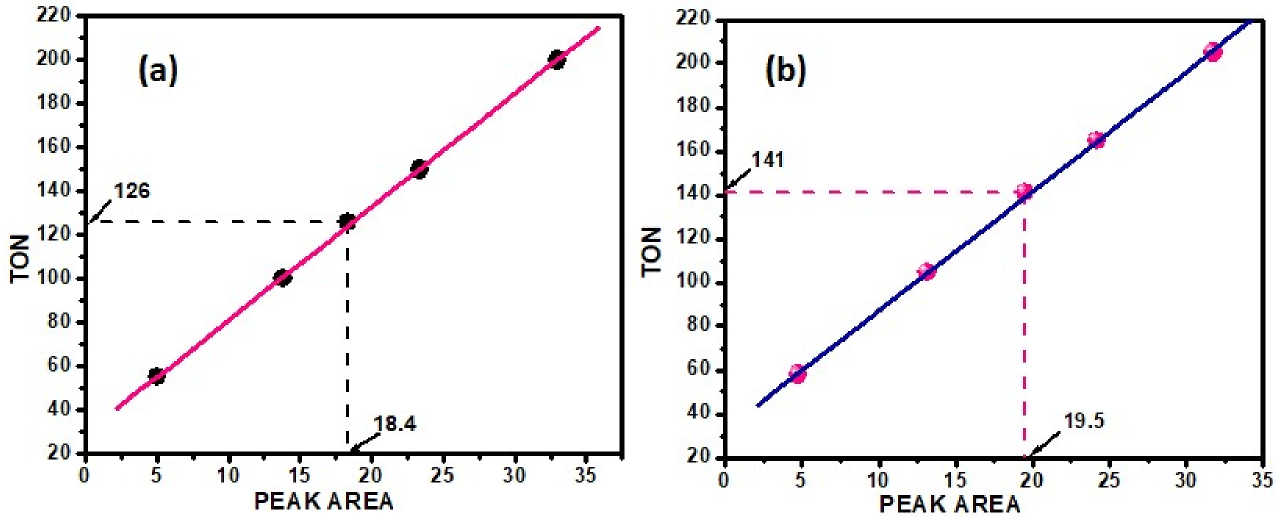



**Figure S4.** Calibration curve of methanol for determination of concentration of methanol produced. (a) Calibration curve of methanol in presence of COF catalyst (TRITER-2 was synthesized through hydrothermal process) (b) Calibration curve of methanol in presence of COF photocatalyst (TRITER-2 was constructed under solvothermal conditions: 6M AcOH in mesitylene:dioxane=9:1)

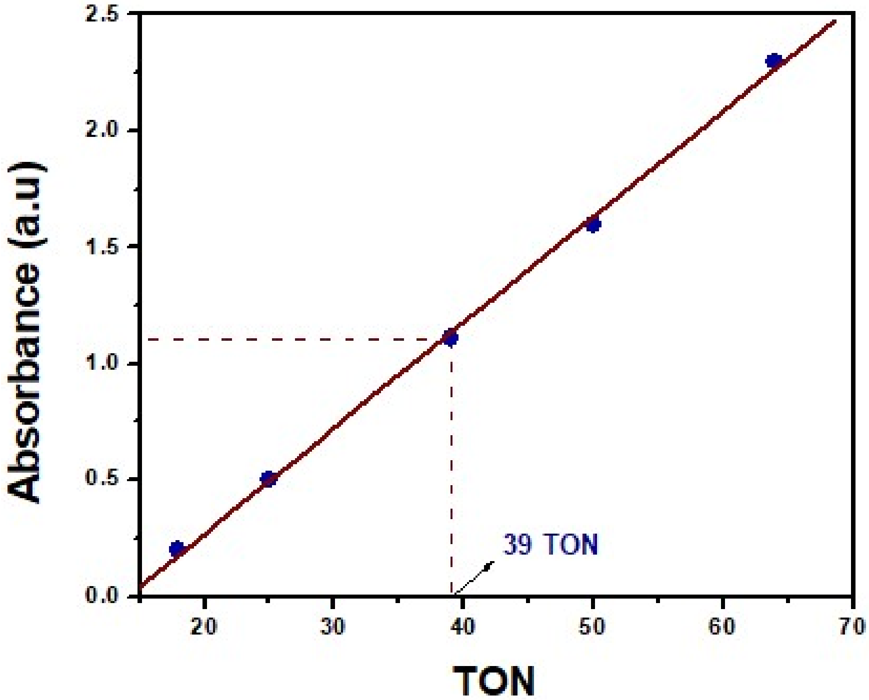



**Figure S5.** Calibration curve of formic acid for determination of concentration of formic acid produced.

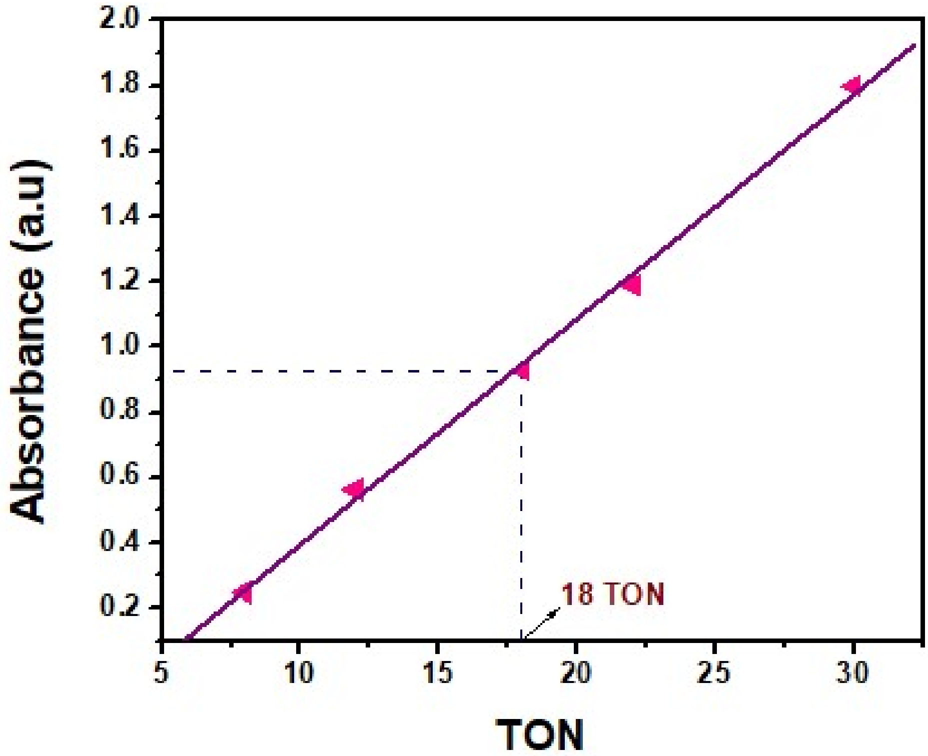



**Figure S6.** Calibration curve of formaldehyde for determination of concentration of formaldehyde formation.

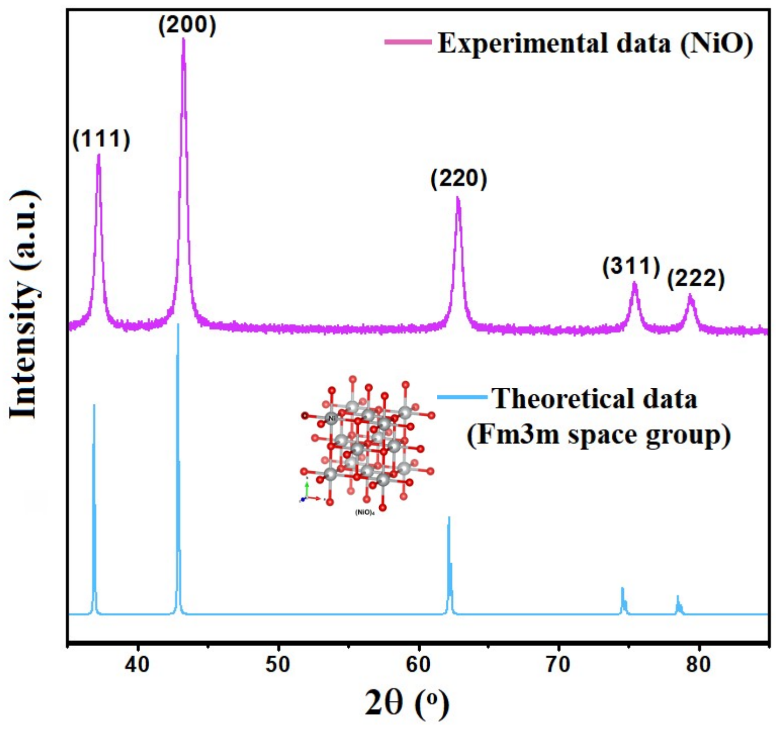



**Figure S7.**PXRD pattern of NiO and B3LYP/6-31G-optimized geometrical structures of $(NiO)_4$. Bond lengths are given in Ǻ and bond angles in degrees. The model of $(NiO)_4$ nanocluster (space group Fm3m) has been selected to simultaneously investigate the performance of NiO and the impact of the COF on NiO.

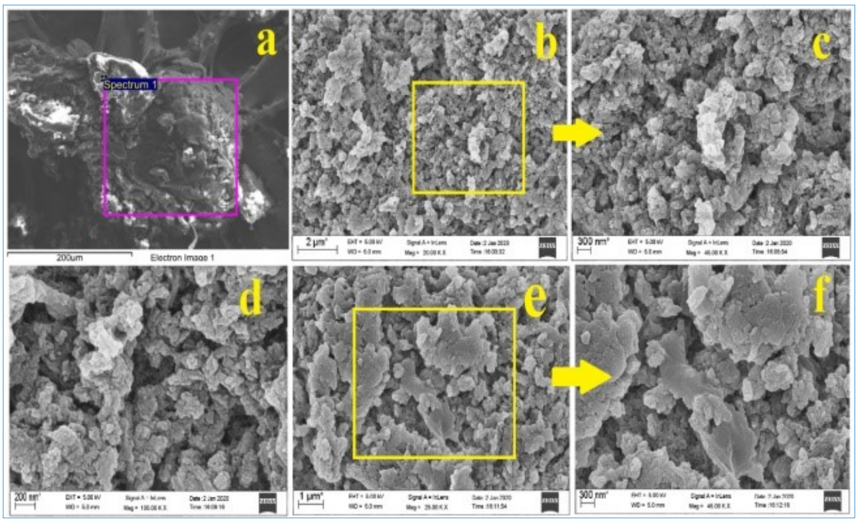



**Figure S8.**a) electron image of TRITER-2, (b-f) FE-SEM images of COF (TRITER-2) at different magnifications.

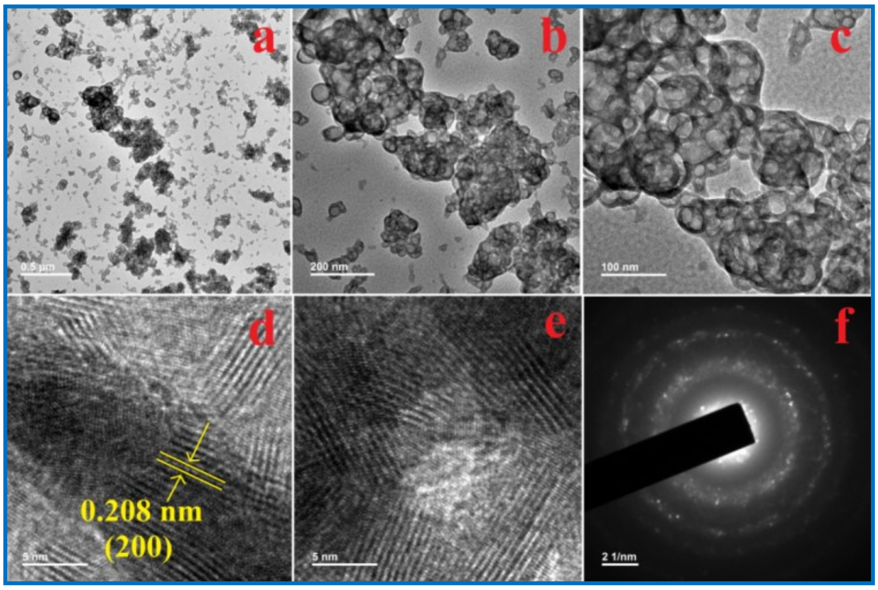



**Figure S9.**The TEM pictures of NiO at several scales (a) 0.5 µm, (b) 200 nm, (c) 100 nm, (d, e) HRTEM image of NiO nanoparticles showcasing the fringe pattern of NiO crystal, and (f) SAED pattern of NiO.

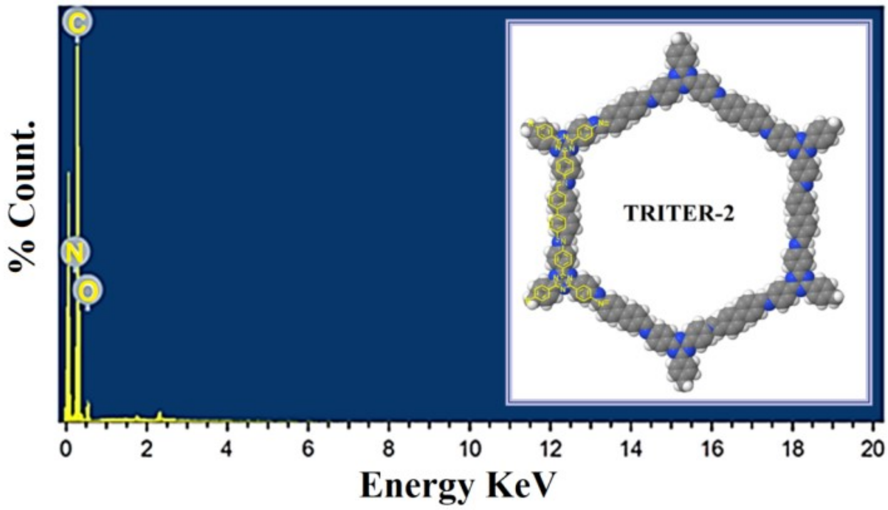



**Figure S10.**The EDAX pattern of the COF (TRITER-2).

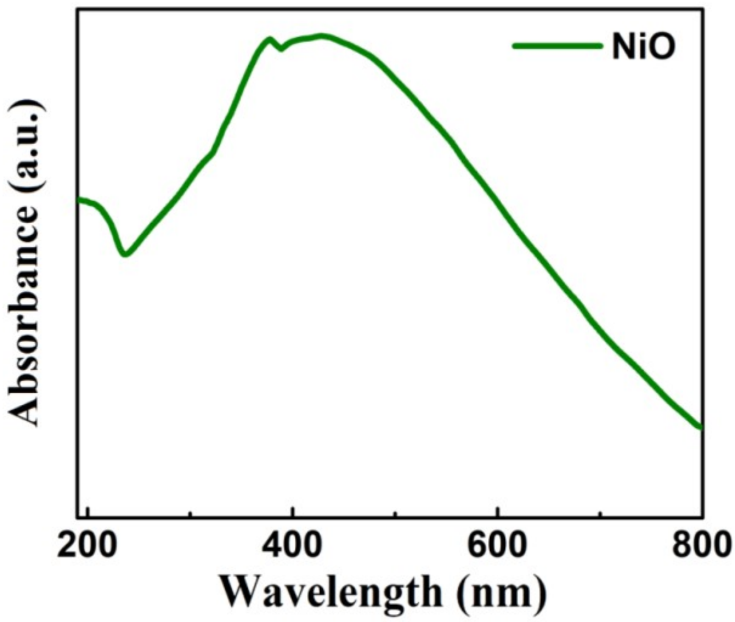



**Figure S11.** UV/Vis spectra of the synthesized NiO NPs.

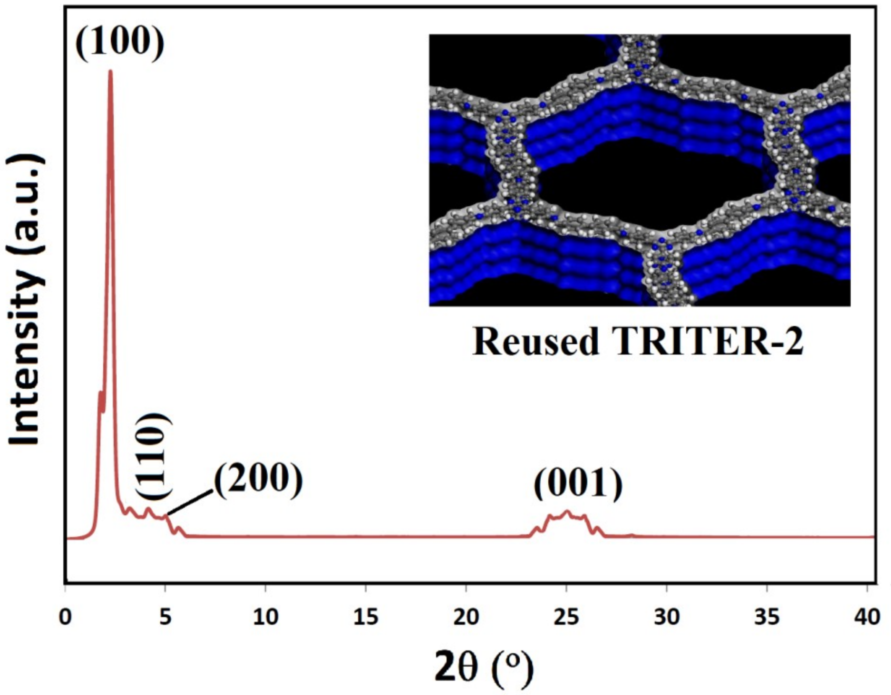



**Figure S12.** PXRD pattern of reused TRITER-2 catalyst after 5$^{th}$ run.

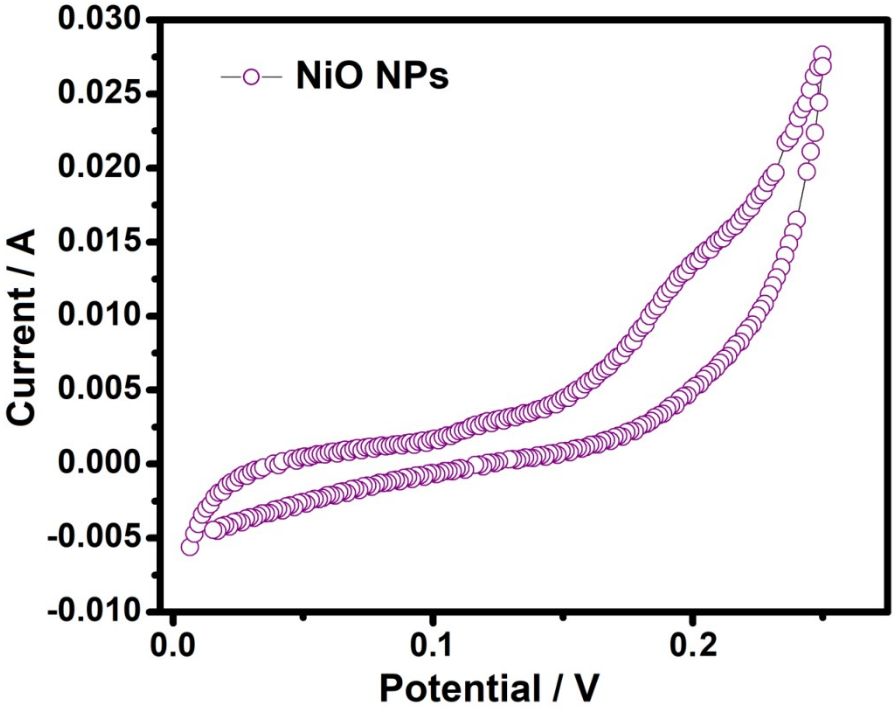



**Figure S13.** Cyclic voltammogram of the synthesized NiO nanoparticles.

The CV study was performed with the scan rate of 1 $mVS^{-1}$ and the potential range of 0 to 0.3 volts. The cyclic voltammogram of the NiO nanoparticles is presented in Figure S13.

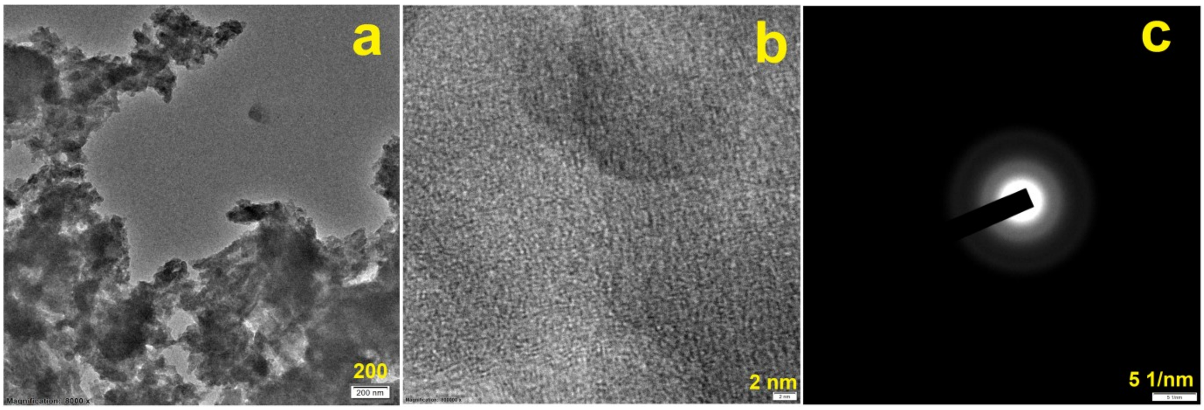



**Figure S14.** TEM pictures of the reused COF (TRITER-2) after 5th run at several scales (a) 200 nm, (b) 2 nm, and (c) SAED pattern of the reused COF (TRITER-2).

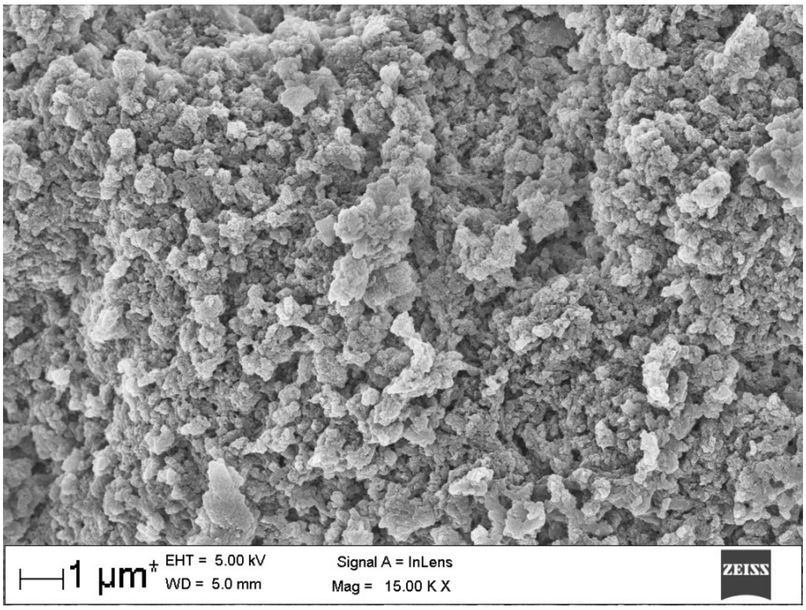



**Figure S15.**FE-SEM image of the reused COF (TRITER-2) after 5th cycle.

**Kinetic curves (TON vs. time):**

The stability of photocatalyst COF TRITER-2 was estimated via recycling and regeneration experiment. After completion of the photocatalytic reaction, COF TRITER-2 was recovered from the reaction mixture by centrifugation and washed multiple times with ethanol. After that, the recovered catalyst was kept in hot oven and dried for the next experiment. Recycling experiment was carried out up to five runs (Fig12). The methanol yield of each recycled run was consistent with the fresh catalyst. Slight reduction in yield after eachruncould be attributed to the crystalline destruction and pore blockage after continuous stirring during photocatalytic experiment and centrifugation for catalyst isolation. It is worth mentioning that the catalytic efficiency dropped upon recycling, owing to pore blockage. Finally, Powder X-ray diffraction pattern of the reused photo-catalyst confirmed that there is no prominent change in the crystallinity of 2D COF (TRITER-2), as shown in Fig. S12.

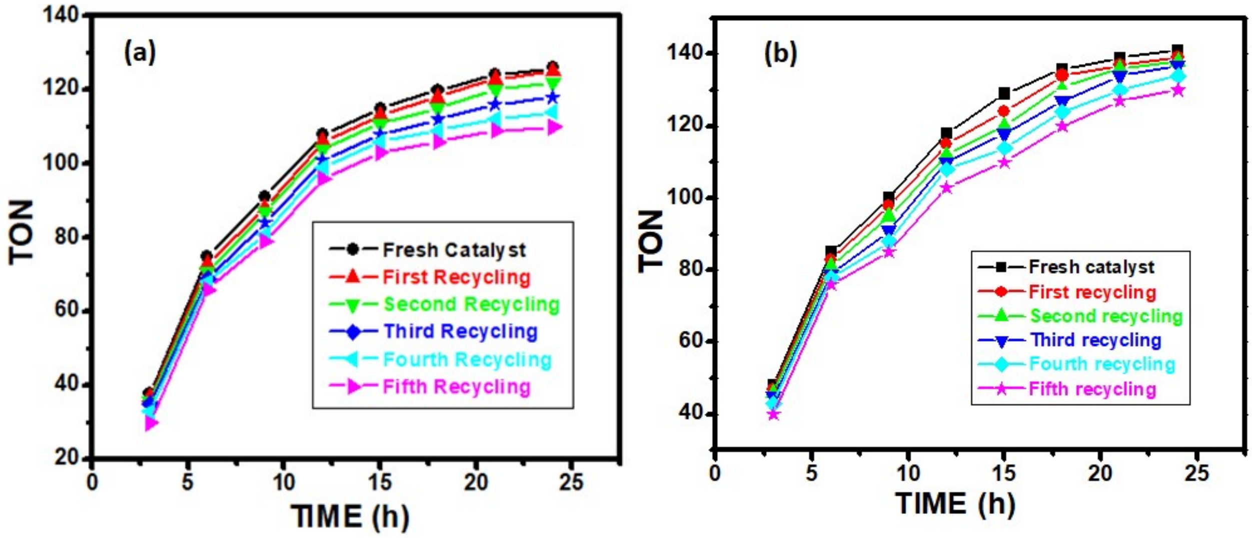
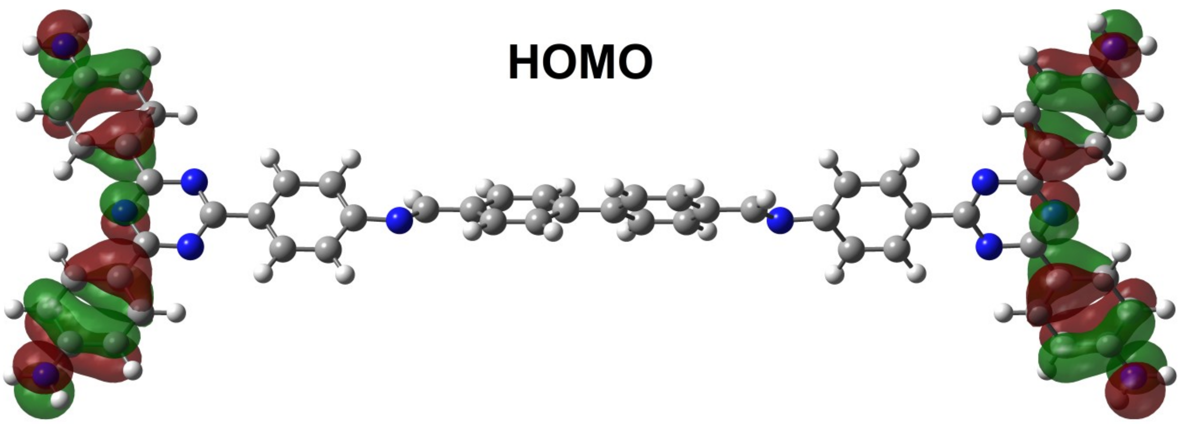



**Figure S16.** Kinetic curve for methanol synthesis and comparison of conversion rates of different recycling runs for methanol synthesis. (a) Kinetic curve for methanol synthesis with COF catalyst (TRITER-2 was synthesized through hydrothermal process); (b Kinetic curve for methanol synthesis with COF photocatalyst (TRITER-2 was constructed under solvothermal conditions: 6M AcOH in mesitylene:dioxane=9:1



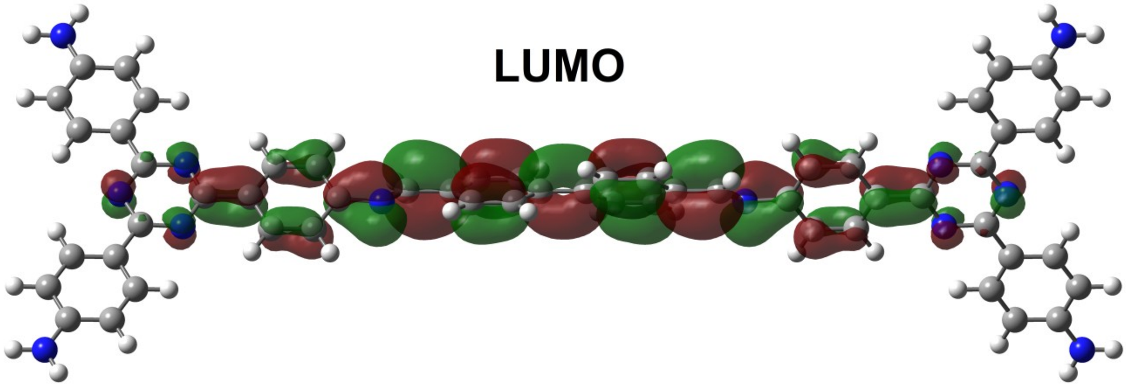



**Figure S17.** HOMO-LUMO of TRITER-2 fragment.

**The comparison of photocatalytic activity with previously reported works and the role of COF in the catalytic process:**

It is worth mentioning that the current COF for $CO_2$ reduction is more active than g-$C_3N_4$ and those coupled with semiconductors reported by others.[1-3] This could be ascribed to a higher adsorption affinity of the azine-based COF to $CO_2$, higher crystallinity (higher degree of structural order) and superior surface area compared to that of g-$C_3N_4$. Yield of $CH_3OH$ over g-$C_3N_4$ is much lower. Thus this triazine-based COF is more competitive than g-$C_3N_4$ and COFs (i.e., ACOF-1 and $N_3$-COF)[4] in the photocatalytic reduction of $CO_2$.

It's well-established that the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) are often invoked to rationalize delocalization of exciton, charge separation, and location of potential charge-transfer sites. Consequently, the density functional theory (DFT) calculations were conducted to investigate the conformational and electronic information based on the optimized geometries of TRITER-2 fragment. It is noteworthy that triazine moiety and phenyl groups in TRITER-2 are coplanar (Fig. S19), revealing a strong conjugation effect. Taking TRITER-2 fragment as an instance for better visibility, the HOMO is localized solely on the triazine linker unit, whereas the LUMO is delocalized across the conjugated π-system of the synthesized COF. The electronic distributions of TRITER-2 at the HOMO and the LUMO have a good electron-separated state and well-overlapped orbital, which is conducive to the intramolecular charge transfer transition. By calculating, the HOMO and LUMO energy levels can be predicted as -5.31 and -2.12 eV for TRITER-2, respectively. In principle, the observed HOMO-LUMO gap (3.19 eV) of TRITER-2 is large enough to enable $CO_2$ reduction through band gap excitation and at the same time small enough to harvest a significant portion of the visible light spectrum. The excited electrons from the LUMO energy level can react with the adsorbed $CO_2$ on the catalyst surface to produce methanol, as shown in Scheme 1. Compared with other reported systems[1-3], the synthesized 2D COF with electron-poor character of triazine building blocks shows more efficient at stabilizing the negative charge generated on the COF, which is important for the photocatalytic process to get a better activity.[5] This is consistent with the results from photocurrent experiments and photocatalytic reactions.

This COF was of great interest owing to the highly conjugated structure, accessible active sites, and accelerated charge transfer. Photocatalytic experiments indicated that the conjugated framework played a vital role in enhancing the photoactivity. Apart from narrowing the band gap, dialdehydes were also considered to possess higher charge carrier mobility and enable the accelerated migration of photogenerated excitons to the surface of the photocatalyst. In addition, electron donors such as tris-(4-aminophenyl)triazine (TAPT) and tris(4-aminophenyl)-benzene (TPB) were employed to construct COFs with tailored band gaps and improved charge separation and transfer.[6,7] TRITER-2 with a narrow band gap and a negative conduction band was found to exhibit promoted visible-light harvesting efficiency and produce more charge carriers. The narrow band gap and facilitated electron transfer in the π-conjugated COF greatly enhanced the photocatalytic performance. Understandably, in the reaction of $CO_2$ photoreduction, the $CO_2$ absorption capability of the catalyst is the key point. In this study, the high surface area of TRITER-2 (1260 $m^2$ $g^{-1}$, see Fig. 2c) with abundant accessible nitrogen sites rendered them with high $CO_2$ absorption, leading to the facilitated photocatalytic reduction of $CO_2$ to $CH_3OH$. Compared with g-$C_3N_4$,[1-3] the synthesized COF (TRITER-2) with electron-poor triazine moieties was able to stabilize the negative charge generated on the COF which was important for the enhanced photocatalytic activity. Activity of the COF outperformed that of other materials such as g-$C_3N_4$.[1-3] Furthermore, the electronic properties and configuration of the COF were calculated with density functional theory (DFT). The results suggested that the potential of their LUMO was enough to drive $CO_2$ reduction. The band gap was suitable for the visible light response. Under visible light irradiation, the excited electrons at the LUMO energy level could reduce the adsorbed $CO_2$ on the catalyst surface to produce methanol (see Fig. 6b).

Photo-catalytic performance of the synthesized 2D COF can be improved following solvothermal method, profiting from the ordered nanoporous structure of the COF. The smooth flow of gas molecules, high efficient adsorption ability of $CO_2$, and the fast and steady transmission of hot electrons can be obtained by the high surface area and three-dimensional transport channels of the COF. The ordered microporous COF exhibits superior material and structure, with a high surface area that offers more catalytically active sites. More importantly, the three-dimensional transport channels ensure the smooth flow of gas molecules, highly efficient $CO_2$ adsorption, and the fast and steady transmission of hot electrons excited, which lead to a further improvement in the photocatalytic performance. These results highlight the possibility of improving the photocatalysis for $CO_2$ reduction under visible light by constructing COF photocatalyst. Keeping these parameters in mind, we have developed the 2D COF (TRITER-2) for enhanced visible-light photocatalytic performance in sustainable metal-free $CO_2$ conversion induced by NiO.

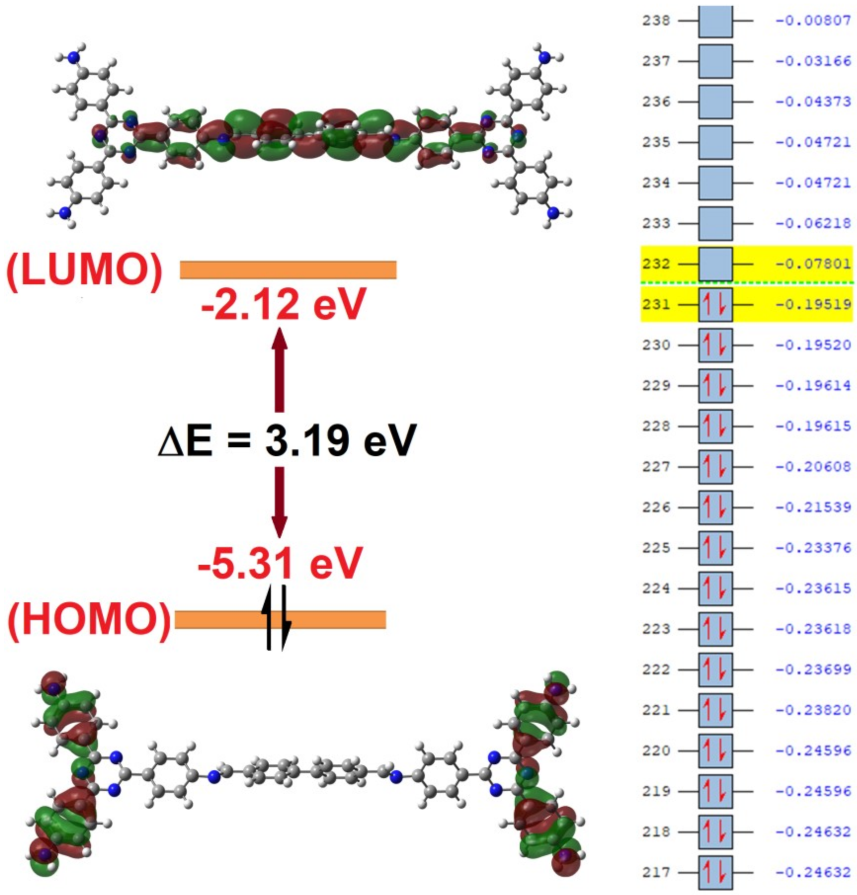



**Figure S18.** Diagram for computed HOMO–LUMO as achieved in the TD-DFT-B3LYP/6-31G.

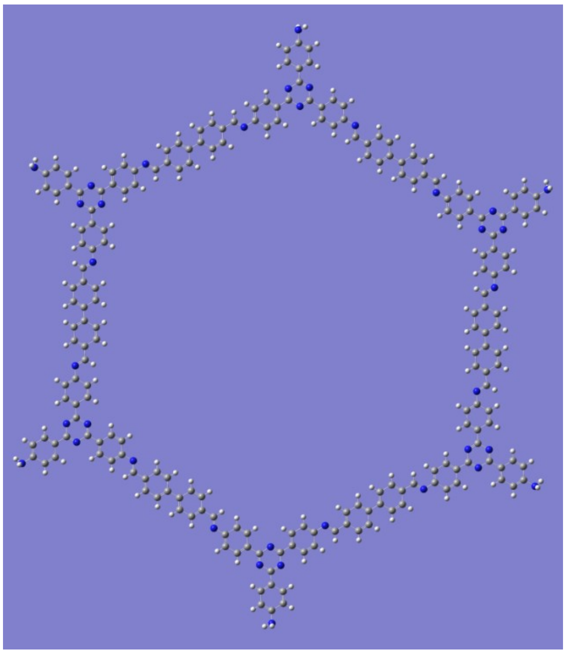


**Figure S19.** Optimized structure of TRITER-2 using DFT-B3LYP/6-31G, revealing that triazine moiety and phenyl groups in TRITER-2 are coplanar.

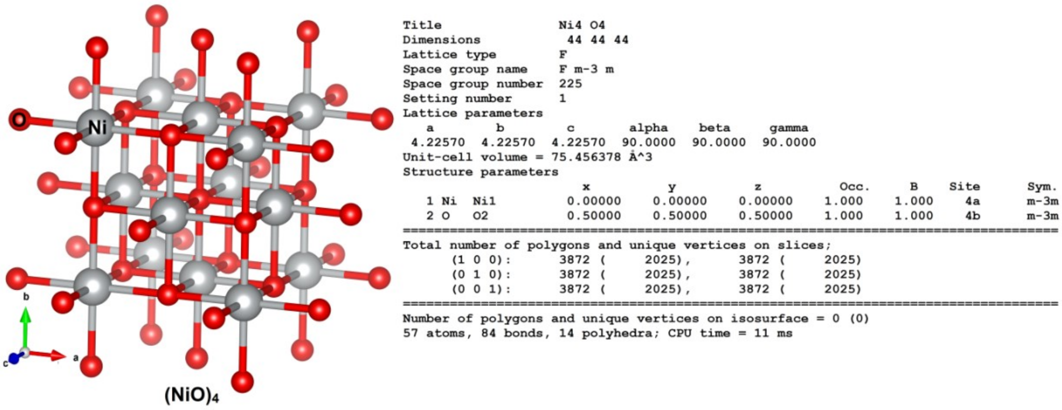



**Figure S20.** The model of $(NiO)_4$ nanocluster (space group Fm3m).

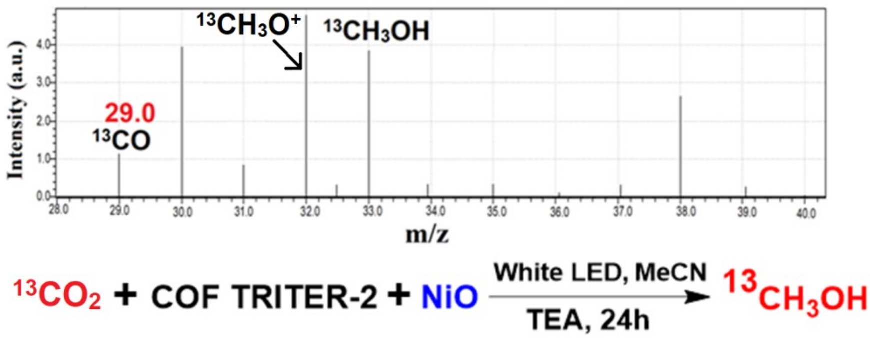
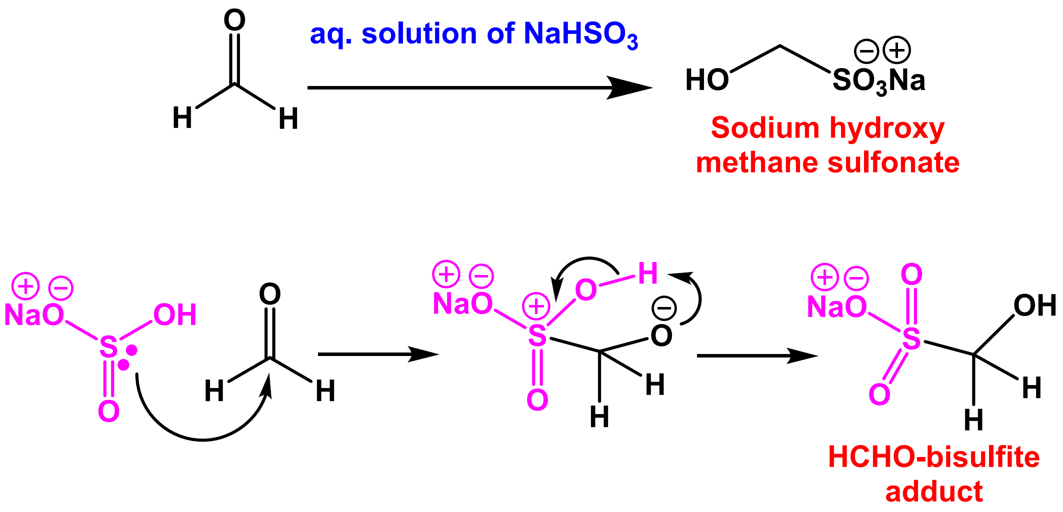



**Figure S21.**Mass spectra of the synthesized methanol employing $^{13}CO_2$ as the carbon source in the photocatalytic reaction. Reaction conditions: TRITER-2 photocatalyst (10 mg), NiO (5 mol%), time: 24 h, 1 atm $^{13}CO_2$ pressure (balloon), Intensity: 20W white LED light, RT.GC-

MS spectrum also showing photogenerated $^{13}CO$ under $^{13}CO_2$atmosphere with TRITER-2 as the photocatalyst.




**Scheme S1:** Reaction between HCHO and $NaHSO_3$.

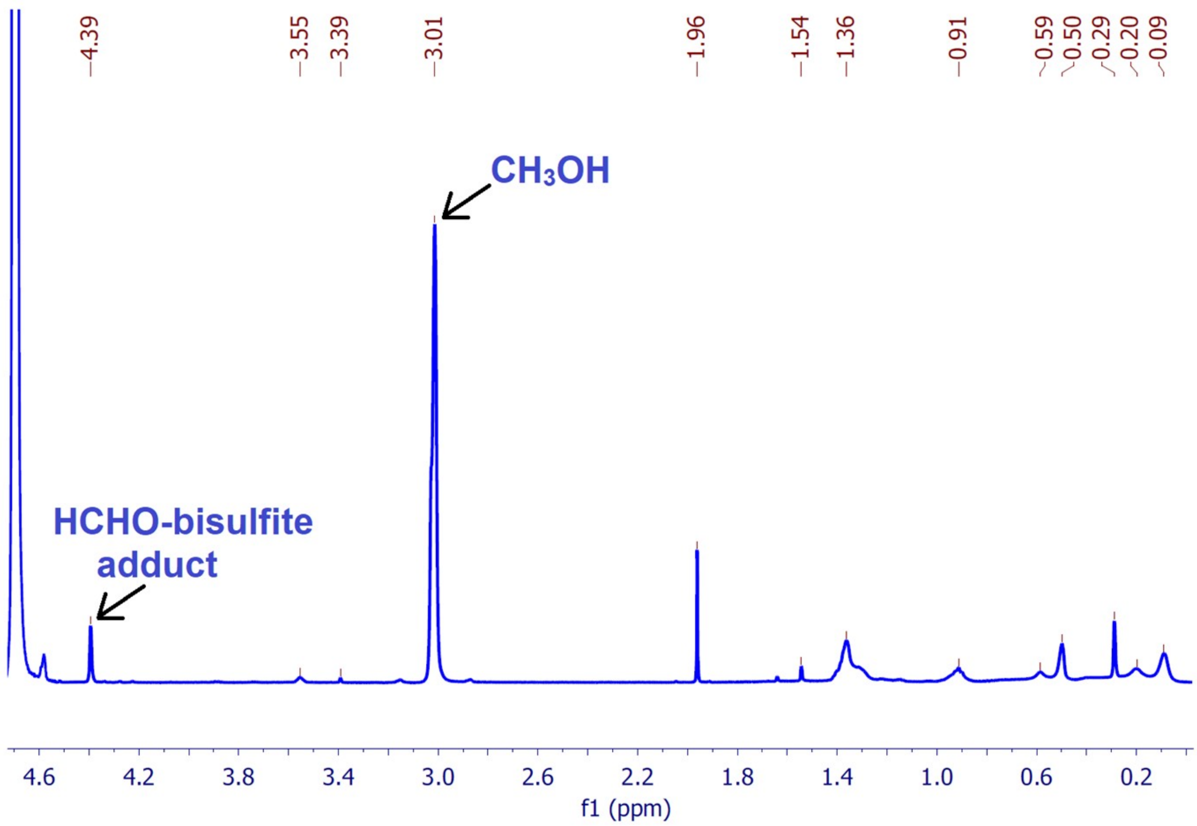



**Figure S22.**$^{1}H$-NMR spectrum of the reaction mixture after photocatalytic $CO_2$reduction (after treatment of the reaction mixture with $NaHSO_3$).

(**Reaction conditions:** TRITER-2 photocatalyst (10 mg), NiO (5 mol%), time: 24 h, 1 atm $CO_2$ pressure (balloon), Intensity: 20W white LED light, RT, solvent: acetonitrile-$d_3$)

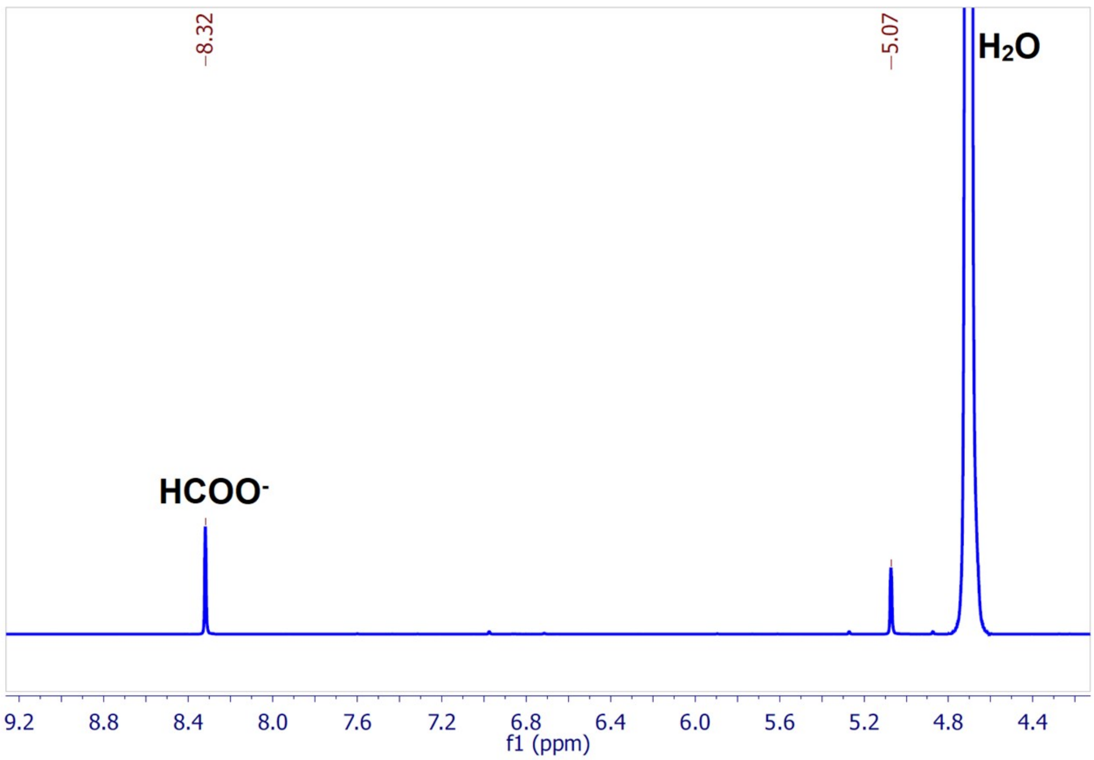
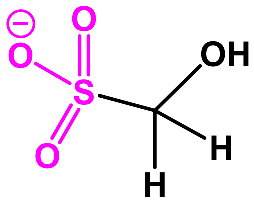



**Figure S23.**[1]H-NMR spectrum of the reaction mixture after $CO_2$ reduction (after treatment of the reaction mixture with excess water due to the presence of formic acid in the form of methyl formate).

(**Reaction conditions:** TRITER-2 photocatalyst (10 mg), NiO (5 mol%), time: 24 h, 1 atm $CO_2$ pressure (balloon), Intensity: 20W white LED light, RT, solvent: acetonitrile-$d_3$)

**ESI-MS spectrum of the reaction mixture (after treatment with $NaHSO_3$):**



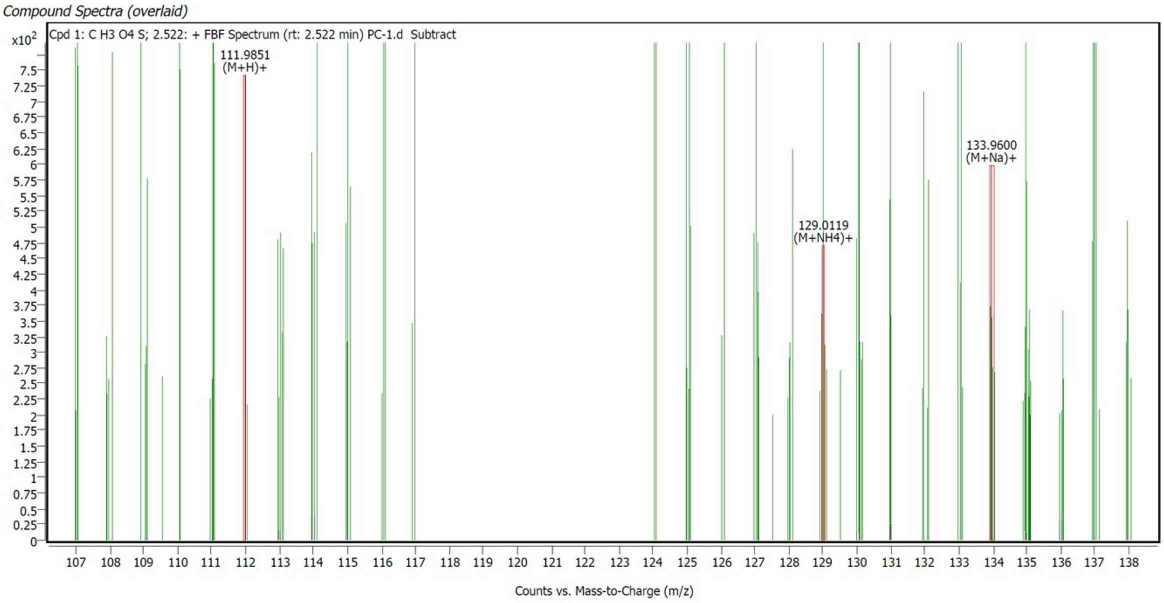

**HCHO-bisulfite adduct**

**Chemical Formula: $CH_3O_4S^-$**

**Compound Details**

**Cpd. 1: C H3 O4 S**

*Compound Spectra (overlaid)*

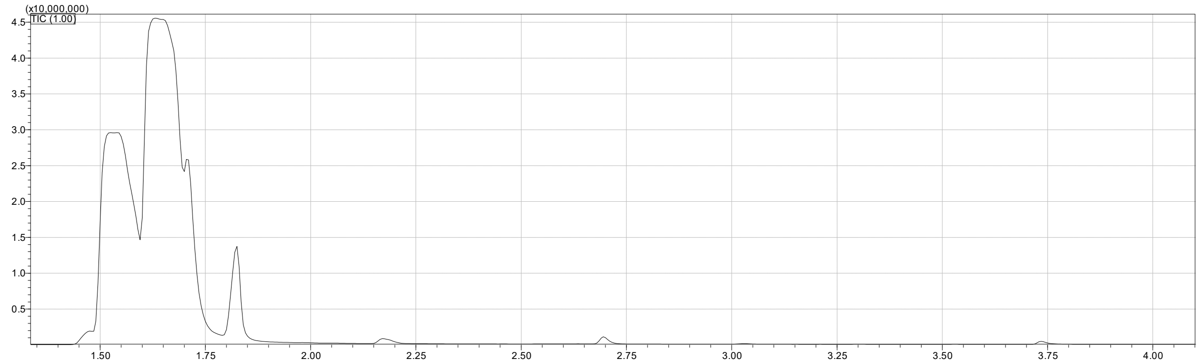



*Compound ID Table*

| Cpd | Formula | Mass (Tgt) | Calc. Mass | Mass | Species | Diff(Tgt.ppm) | mDa |
|---|---|---|---|---|---|---|---|
| 1 | C H3 O4 S | 110.9752 | 110.9756 | 111.9851<br>129.0119<br>133.9600 | (M+H)+<br>(M+NH4)+<br>(M+Na)+ | 3.19 | 0.35 |

**GC-MS spectrum of the reaction mixture:**

## GC-MS spectrum of the reaction mixture (Zoom-in):



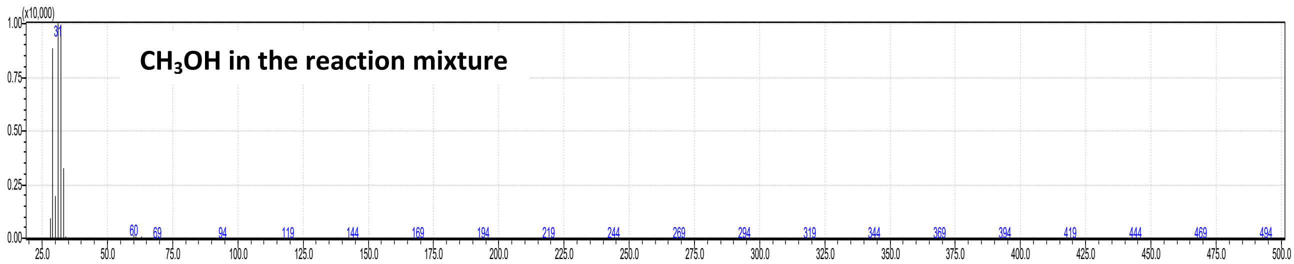
## Qualitative table of the above GC-MS spectrum:

| Peak# | Ret.Time | Start Tm | End Tm | m/z | Area | Area% | Height | Height% | A/H |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 1.470 | 1.430 | 1.485 | TIC | 3575610 | 0.77 | 1766689 | 1.94 | 2.02 |
| 2 | 1.540 | 1.485 | 1.595 | TIC | 151165454 | 32.70 | 29457164 | 32.42 | 5.13 |
| 3 | 1.632 | 1.595 | 1.790 | TIC | 285024314 | 61.65 | 45325997 | 49.89 | 6.29 |
| 4 | 1.823 | 1.790 | 1.885 | TIC | 21146404 | 4.57 | 13306512 | 14.65 | 1.59 |
| 5 | 2.695 | 2.670 | 2.735 | TIC | 1411208 | 0.31 | 991551 | 1.09 | 1.42 |

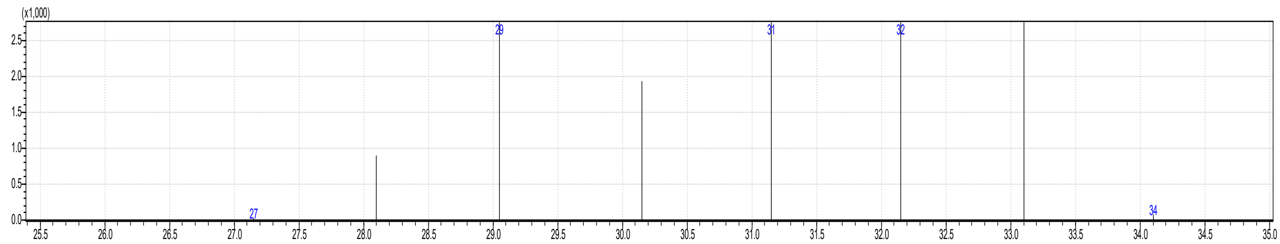
**GC MS data of the reaction mixture:**

**1. Ret. Time: 1.540 (Methanol)**

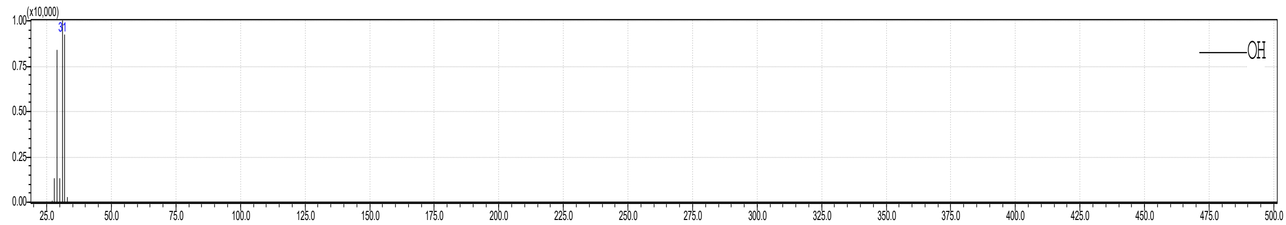
## Mass spectra of the reaction mixture:




## Mass spectra of the reaction mixture (Zoom-in):

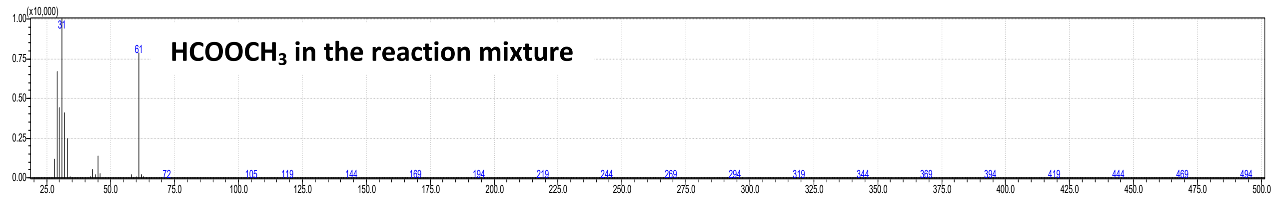


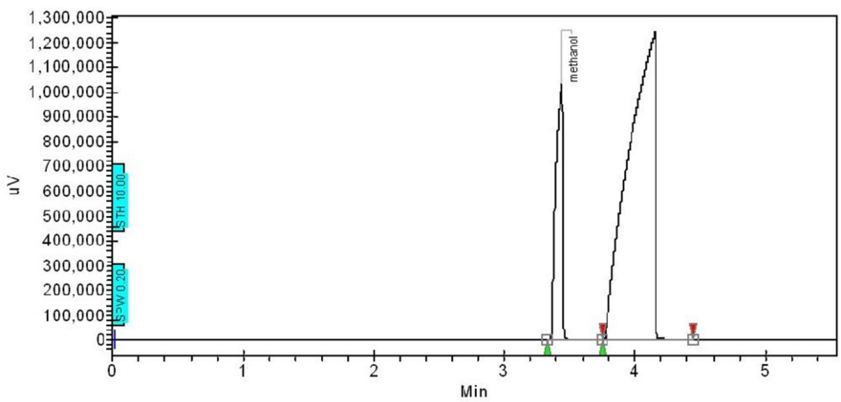
**Standard sample (Pure methanol):**




**2. Ret. Time: 1.823 (Methyl formate)**

**Mass spectra of the reaction mixture:**




Peak results :

| Index | Name | Time [Min] | Quantity [M] | Height [uV] | Area [uV.Min] | Area % [%] | Area [uV.Sec] | Quantity [M] |
|---|---|---|---|---|---|---|---|---|
| 1 | methanol | 3.44 | 12.84 | 1034277.2 | 64324.4 | 18.053 | 3859465.7 | 12.84 |
| 2 | UNKNOWN | 4.16 | 0.00 | 1243405.4 | 291983.7 | 81.947 | 17519020.3 | 0.00 |
| | | | | | | | | |
| Total | | | 12.84 | 2277682.6 | 356308.1 | 100.000 | 21378486.0 | 12.84 |

**Figure S24.** GC spectrum of the reaction mixture.(methanol formation catalyzed by TRITER-2 photocatalyst under optimised conditions).

(**Reaction conditions:** TRITER-2 photocatalyst (10 mg), NiO (5 mol%), time: 24 h, 1 atm $CO_2$ pressure (balloon), Intensity: 20W white LED light, RT.)

## Preparation of g-$C_3N_4$:

Graphitic carbon nitride (g-$C_3N_4$) was synthesized by pyrolysis of urea in a muffle furnace; 20 g urea was put into an alumina crucible with a cover, then heated to 250 °C within 110 min and kept at 250 °C for 1 h. The further treatment was performed at 350 and 550 °C for 2 h, respectively. The heating rate of the whole reaction was 2 °C·min$^{-1}$. The yellow power (g-$C_3N_4$) was collected. The collected amount of the g-$C_3N_4$ was around 1 g.

## Sample characterization

Figure S25 illustrates the XRD pattern of g-$C_3N_4$. Observed from Figure S25, there are two obvious diffraction peaks at around 12.9° and 27.1°, which were assigned to the (100) and (002) planes of g-$C_3N_4$. These two peaks are likely to be attributed to the structure of the tri-s-triazine unit with interplanar spacing and the conjugated aromatic system, respectively.[8]

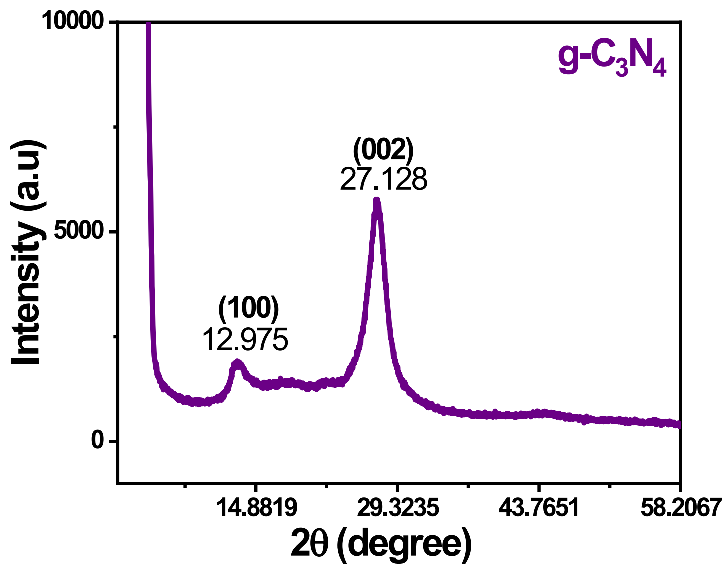
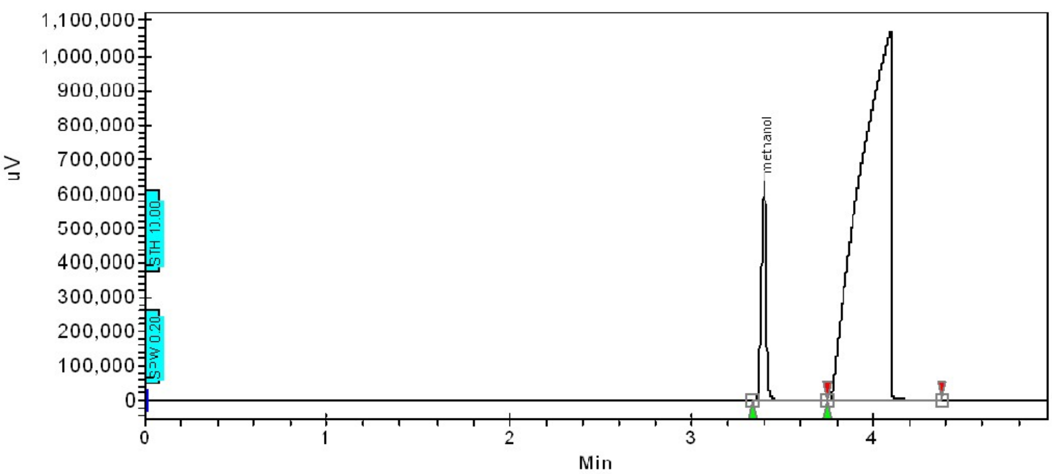



**Figure S25.** PXRD pattern of g-$C_3N_4$.




**Peak results :**

| Index | Name | Time [Min] | Quantity [M] | Height [uV] | Area [uV.Min] | Area % [%] | Area [uV.Sec] | Quantity [M] |
|---|---|---|---|---|---|---|---|---|
| 1 | methanol | 3.40 | 4.25 | 634679.5 | 21268.9 | 9.329 | 1276135.7 | 4.25 |
| 2 | UNKNOWN | 4.09 | 0.00 | 1068951.5 | 206713.7 | 90.671 | 12402822.7 | 0.00 |
| | | | | | | | | |
| Total | | | 4.25 | 1703631.1 | 227982.6 | 100.000 | 13678958.4 | 4.25 |

**Figure S26.** GC spectrum of the reaction mixture.(methanol production catalyzed by g-$C_3N_4$ employing already established reaction conditions).

(**Reaction conditions:** g-$C_3N_4$ photocatalyst (10 mg), NiO (5 mol%), time: 24 h, 1 atm $CO_2$ pressure (balloon), Intensity: 20W white LED light, RT.)

The identification and quantification of the methanol production was carried out using GC-MS using headspace at elevated temperature of 90$^{o}$C. For the observed GC peak areas using the observed peak area of 79.0 for 1.0 M methanol as standard the methanol concentrations were determined. Methanol was analyzed by GC-FID, and a DB-WAX 123-7033 column was used for the detection of methanol. Helium gas was introduced as the shipper gas, and the flow rate was 35 cm/s. The oven temperature was adjusted at 40 °C, and inlet temperature was fixed at 200 °C. The split ratio was

1:50 and the FID temperature was 300 °C. Nitrogen gas was used as the makeup with a flow rate of 30 mL/min at the FID detector. The yield was calculated by using the following equation.

$$\mathbf{Y = (C \times V/W)}$$

Y = yield

C = methanol concentration, μmol/L

V = volume, L

W = mass of catalyst, g

All the relevant original spectra of HCOOH/HCHO were given in SI.

In the case of catalytic TRITER-2, methanol was attained in excellent yield of about 1,14000 μmol. gcat$^{-1}$. In the case of catalytic g-$C_3N_4$, methanol was achieved in poor yield of about 59,000 μmol. gcat$^{-1}$.

**Table S1:** The results of photochemical reduction of $CO_2$ to methanol using TRITER-2 and g-$C_3N_4$as photocatalyst. A 5 mL and 0.01 g (i.e., 10 mg) were used as the volumeand weight of the photocatalyst, respectively. GC standard peak area of 79.0 for 1.0 M Methanol (MeOH) was used.

| Catalyst | Reaction time, t reaction (h) | GC area found for MeOH | Molarity of MeOH formed (M) | Moles of MeOH formed (μ mol.) |
|---|---|---|---|---|
| **TRITER-2** | 24 | 18.053 | 0.228 | 1140 |
| **g-$C_3N_4$** | 24 | 9.329 | 0.118 | 590 |

We have carried out two more experiments with blue LED (450 nm) and green LED (520-555 nm). We observed poor yield with blue LED. Although with the green LED and white LED gave us comparable reaction yield, we have selected the White LED as our reaction source. Since, we observed from the UV-Vis spectra of TRITER-2 (Figure 6a) in the manuscript, the excitation maxima is 520 nm, so we have selected the white LED as the light source which is in between 480-590 nm, which confirms that the reaction proceeds by bad gap excitation of TRITER-2.

| Light source | Wave length (nm) | Yield (TON)/ (μ mol.) |
|---|---|---|
| White LED | 480-590 | 141 TON (conc=0.228M), 1140 μ mol |
| Green LED | 520-530 | 132 TON (conc=0.214M), 1070 μ mol |
| Blue | 450 | 118 TON (conc=0.191M), 955 μ mol |

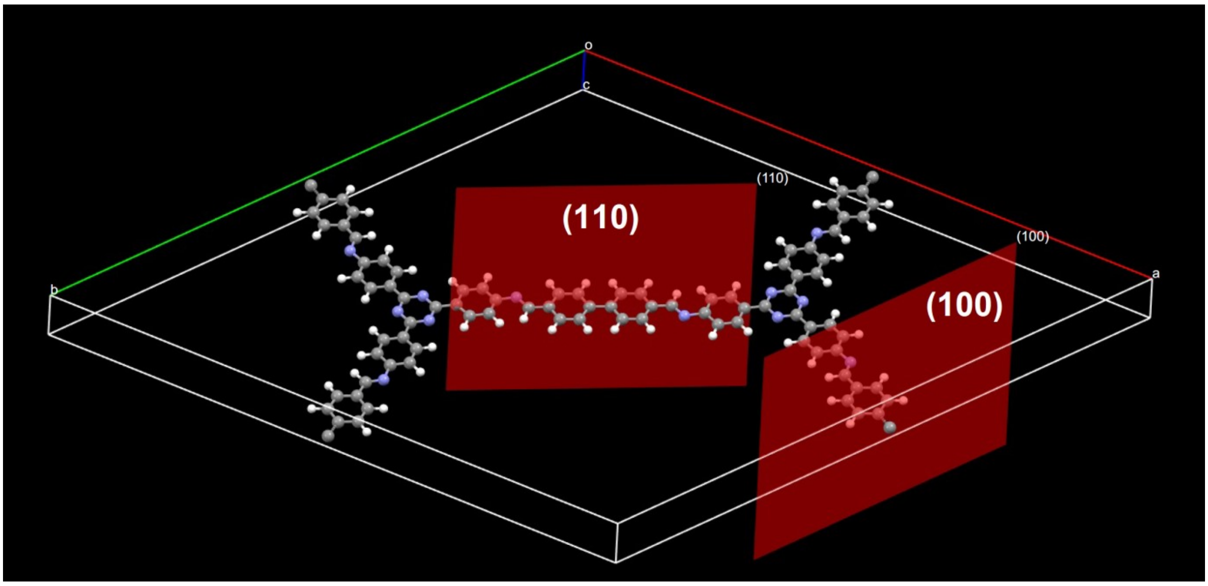



**Figure S27.** 1×1 unit cell of the COF (TRITER-2) showing (100) and (110) plane.

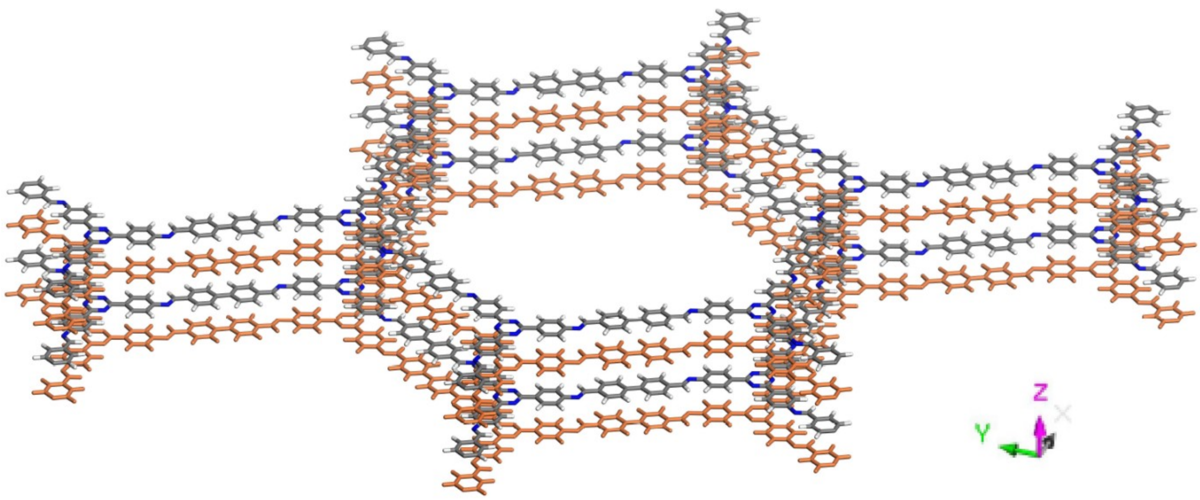



**Figure S28.** 2×2 unit cell of the COF (TRITER-2) displaying π-π stacking between the COF layers.

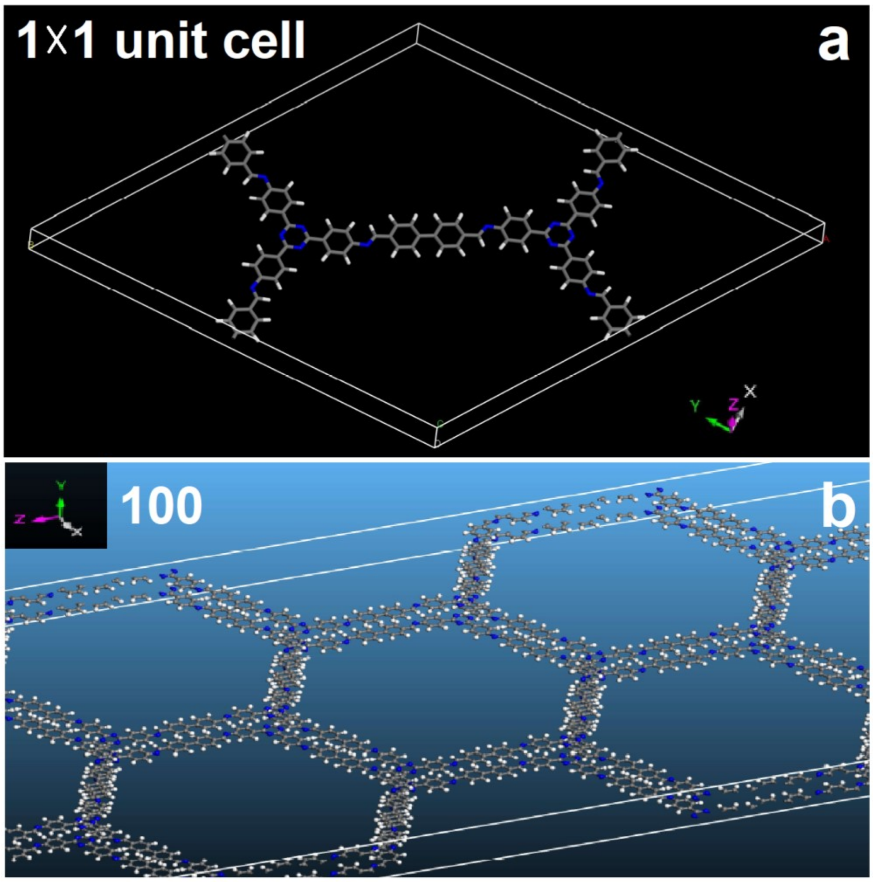



**Figure S29.** 1×1 unit cell of the COF (TRITER-2) (a) and TRITER-2 (100) supercell (b).

**Table S2.** Fractional main atomic coordinates for the unit cell of the COF (TRITER-2) after Pawley refinement.

**Space group symmetry $P_{6/m}$**
**a = b = 42.3348 Å, c = 3.8828 Å,**
**α = β = 90° and γ = 120°**

| No | Label | Charge | SybylType | Xfrac + ESD | Yfrac + ESD | Zfrac + ESD | Symm. op. |
|---|---|---|---|---|---|---|---|
| 1 | N1 | 0 | N.2 | 0.32022 | 0.68798 | 0.50000 | x,y,z |
| 2 | C2 | 0 | C.2 | 0.35481 | 0.70135 | 0.50000 | x,y,z |
| 3 | C3 | 0 | C.2 | 0.37825 | 0.73921 | 0.50000 | x,y,z |
| 4 | C4 | 0 | C.2 | 0.36496 | 0.76174 | 0.50000 | x,y,z |
| 5 | C5 | 0 | C.2 | 0.38706 | 0.79738 | 0.50000 | x,y,z |
| 6 | C6 | 0 | C.2 | 0.42290 | 0.81125 | 0.50000 | x,y,z |
| 7 | C7 | 0 | C.2 | 0.43624 | 0.78887 | 0.50000 | x,y,z |
| 8 | C8 | 0 | C.2 | 0.41417 | 0.75323 | 0.50000 | x,y,z |
| 9 | N9 | 0 | N.2 | 0.44667 | 0.84881 | 0.50000 | x,y,z |
| 10 | C10 | 0 | C.2 | 0.43488 | 0.87005 | 0.50000 | x,y,z |
| 11 | C11 | 0 | C.2 | 0.45454 | 0.90703 | 0.50000 | x,y,z |
| 12 | C12 | 0 | C.2 | 0.49064 | 0.92578 | 0.50000 | x,y,z |
| 13 | C13 | 0 | C.2 | 0.50825 | 0.96178 | 0.50000 | x,y,z |
| 14 | C14 | 0 | C.2 | 0.49047 | 0.98047 | 0.50000 | x,y,z |
| 15 | C15 | 0 | C.2 | 0.45404 | 0.96092 | 0.50000 | x,y,z |
| 16 | C16 | 0 | C.2 | 0.43663 | 0.92496 | 0.50000 | x,y,z |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 17 | H17 | 0 | H | 0.33590 | 0.75070 | 0.50000 | x,y,z |
| 18 | H18 | 0 | H | 0.37602 | 0.81540 | 0.50000 | x,y,z |
| 19 | H19 | 0 | H | 0.46528 | 0.79972 | 0.50000 | x,y,z |
| 20 | H20 | 0 | H | 0.42524 | 0.73523 | 0.50000 | x,y,z |
| 21 | H21 | 0 | H | 0.53759 | 0.97677 | 0.50000 | x,y,z |
| 22 | H22 | 0 | H | 0.50563 | 0.91143 | 0.50000 | x,y,z |
| 23 | H23 | 0 | H | 0.43831 | 0.97451 | 0.50000 | x,y,z |
| 24 | H24 | 0 | H | 0.40730 | 0.90982 | 0.50000 | x,y,z |
| 25 | H25 | 0 | H | 0.40593 | 0.85971 | 0.50000 | x,y,z |
| 26 | N26 | 0 | N.2 | 0.31202 | 0.63224 | 0.50000 | x,y,z |
| 27 | C27 | 0 | C.2 | 0.29865 | 0.65346 | 0.50000 | x,y,z |
| 28 | C28 | 0 | C.2 | 0.26079 | 0.63904 | 0.50000 | x,y,z |
| 29 | C29 | 0 | C.2 | 0.23826 | 0.60322 | 0.50000 | x,y,z |
| 30 | C30 | 0 | C.2 | 0.20262 | 0.58968 | 0.50000 | x,y,z |
| 31 | C31 | 0 | C.2 | 0.18875 | 0.61165 | 0.50000 | x,y,z |
| 32 | C32 | 0 | C.2 | 0.21113 | 0.64737 | 0.50000 | x,y,z |
| 33 | C33 | 0 | C.2 | 0.24677 | 0.66094 | 0.50000 | x,y,z |
| 34 | N34 | 0 | N.2 | 0.15119 | 0.59786 | 0.50000 | x,y,z |
| 35 | C35 | 0 | C.2 | 0.12995 | 0.56483 | 0.50000 | x,y,z |
| 36 | C36 | 0 | C.2 | 0.09297 | 0.54751 | 0.50000 | x,y,z |
| 37 | C37 | 0 | C.2 | 0.07422 | 0.56486 | 0.50000 | x,y,z |
| 38 | C38 | 0 | C.2 | 0.03822 | 0.54647 | 0.50000 | x,y,z |
| 39 | C39 | 0 | C.2 | 0.01953 | 0.51000 | 0.50000 | x,y,z |
| 40 | C40 | 0 | C.2 | 0.03908 | 0.49312 | 0.50000 | x,y,z |
| 41 | C41 | 0 | C.2 | 0.07504 | 0.51167 | 0.50000 | x,y,z |
| 42 | H42 | 0 | H | 0.24930 | 0.58520 | 0.50000 | x,y,z |
| 43 | H43 | 0 | H | 0.18460 | 0.56062 | 0.50000 | x,y,z |
| 44 | H44 | 0 | H | 0.20028 | 0.66556 | 0.50000 | x,y,z |
| 45 | H45 | 0 | H | 0.26477 | 0.69001 | 0.50000 | x,y,z |
| 46 | H46 | 0 | H | 0.02323 | 0.56082 | 0.50000 | x,y,z |
| 47 | H47 | 0 | H | 0.08857 | 0.59420 | 0.50000 | x,y,z |
| 48 | H48 | 0 | H | 0.02549 | 0.46380 | 0.50000 | x,y,z |
| 49 | H49 | 0 | H | 0.09018 | 0.49748 | 0.50000 | x,y,z |
| 50 | H50 | 0 | H | 0.14029 | 0.54622 | 0.50000 | x,y,z |
| 51 | N51 | 0 | N.2 | 0.36776 | 0.67978 | 0.50000 | x,y,z |
| 52 | C52 | 0 | C.2 | 0.34654 | 0.64519 | 0.50000 | x,y,z |
| 53 | C53 | 0 | C.2 | 0.36096 | 0.62175 | 0.50000 | x,y,z |
| 54 | C54 | 0 | C.2 | 0.39678 | 0.63504 | 0.50000 | x,y,z |
| 55 | C55 | 0 | C.2 | 0.41032 | 0.61294 | 0.50000 | x,y,z |
| 56 | C56 | 0 | C.2 | 0.38835 | 0.57710 | 0.50000 | x,y,z |
| 57 | C57 | 0 | C.2 | 0.35263 | 0.56376 | 0.50000 | x,y,z |
| 58 | C58 | 0 | C.2 | 0.33906 | 0.58583 | 0.50000 | x,y,z |
| 59 | N59 | 0 | N.2 | 0.40214 | 0.55333 | 0.50000 | x,y,z |
| 60 | C60 | 0 | C.2 | 0.43517 | 0.56512 | 0.50000 | x,y,z |
| 61 | C61 | 0 | C.2 | 0.45249 | 0.54546 | 0.50000 | x,y,z |
| 62 | C62 | 0 | C.2 | 0.43514 | 0.50936 | 0.50000 | x,y,z |
| 63 | C63 | 0 | C.2 | 0.45353 | 0.49175 | 0.50000 | x,y,z |
| 64 | C64 | 0 | C.2 | 0.49000 | 0.50953 | 0.50000 | x,y,z |
| 65 | C65 | 0 | C.2 | 0.50688 | 0.54596 | 0.50000 | x,y,z |
| 66 | C66 | 0 | C.2 | 0.48833 | 0.56337 | 0.50000 | x,y,z |
| 67 | H67 | 0 | H | 0.41480 | 0.66410 | 0.50000 | x,y,z |
| 68 | H68 | 0 | H | 0.43938 | 0.62398 | 0.50000 | x,y,z |
| 69 | H69 | 0 | H | 0.33444 | 0.53472 | 0.50000 | x,y,z |
| 70 | H70 | 0 | H | 0.30999 | 0.57476 | 0.50000 | x,y,z |
| 71 | H71 | 0 | H | 0.43918 | 0.46241 | 0.50000 | x,y,z |
| 72 | H72 | 0 | H | 0.40580 | 0.49437 | 0.50000 | x,y,z |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 73 | H73 | 0 | H | 0.53620 | 0.56169 | 0.50000 | x,y,z |
| 74 | H74 | 0 | H | 0.50252 | 0.59270 | 0.50000 | x,y,z |
| 75 | H75 | 0 | H | 0.45378 | 0.59407 | 0.50000 | x,y,z |
| 76 | N76 | 0 | N.2 | 0.67978 | 0.31202 | 0.50000 | x,y,z |
| 77 | C77 | 0 | C.2 | 0.64519 | 0.29865 | 0.50000 | x,y,z |
| 78 | C78 | 0 | C.2 | 0.62175 | 0.26079 | 0.50000 | x,y,z |
| 79 | C79 | 0 | C.2 | 0.63504 | 0.23826 | 0.50000 | x,y,z |
| 80 | C80 | 0 | C.2 | 0.61294 | 0.20262 | 0.50000 | x,y,z |
| 81 | C81 | 0 | C.2 | 0.57710 | 0.18875 | 0.50000 | x,y,z |
| 82 | C82 | 0 | C.2 | 0.56376 | 0.21113 | 0.50000 | x,y,z |
| 83 | C83 | 0 | C.2 | 0.58583 | 0.24677 | 0.50000 | x,y,z |
| 84 | N84 | 0 | N.2 | 0.55333 | 0.15119 | 0.50000 | x,y,z |
| 85 | C85 | 0 | C.2 | 0.56512 | 0.12995 | 0.50000 | x,y,z |
| 86 | C86 | 0 | C.2 | 0.54546 | 0.09297 | 0.50000 | x,y,z |
| 87 | C87 | 0 | C.2 | 0.50936 | 0.07422 | 0.50000 | x,y,z |
| 88 | C88 | 0 | C.2 | 0.49175 | 0.03822 | 0.50000 | x,y,z |
| 89 | C89 | 0 | C.2 | 0.50953 | 0.01953 | 0.50000 | x,y,z |
| 90 | C90 | 0 | C.2 | 0.54596 | 0.03908 | 0.50000 | x,y,z |
| 91 | C91 | 0 | C.2 | 0.56337 | 0.07504 | 0.50000 | x,y,z |
| 92 | H92 | 0 | H | 0.66410 | 0.24930 | 0.50000 | x,y,z |
| 93 | H93 | 0 | H | 0.62398 | 0.18460 | 0.50000 | x,y,z |
| 94 | H94 | 0 | H | 0.53472 | 0.20028 | 0.50000 | x,y,z |
| 95 | H95 | 0 | H | 0.57476 | 0.26477 | 0.50000 | x,y,z |
| 96 | H96 | 0 | H | 0.46241 | 0.02323 | 0.50000 | x,y,z |
| 97 | H97 | 0 | H | 0.49437 | 0.08857 | 0.50000 | x,y,z |
| 98 | H98 | 0 | H | 0.56169 | 0.02549 | 0.50000 | x,y,z |
| 99 | H99 | 0 | H | 0.59270 | 0.09018 | 0.50000 | x,y,z |
| 100 | H100 | 0 | H | 0.59407 | 0.14029 | 0.50000 | x,y,z |
| 101 | N101 | 0 | N.2 | 0.68798 | 0.36776 | 0.50000 | x,y,z |
| 102 | C102 | 0 | C.2 | 0.70135 | 0.34654 | 0.50000 | x,y,z |
| 103 | C103 | 0 | C.2 | 0.73921 | 0.36096 | 0.50000 | x,y,z |
| 104 | C104 | 0 | C.2 | 0.76174 | 0.39678 | 0.50000 | x,y,z |
| 105 | C105 | 0 | C.2 | 0.79738 | 0.41032 | 0.50000 | x,y,z |
| 106 | C106 | 0 | C.2 | 0.81125 | 0.38835 | 0.50000 | x,y,z |
| 107 | C107 | 0 | C.2 | 0.78887 | 0.35263 | 0.50000 | x,y,z |
| 108 | C108 | 0 | C.2 | 0.75323 | 0.33906 | 0.50000 | x,y,z |
| 109 | N109 | 0 | N.2 | 0.84881 | 0.40214 | 0.50000 | x,y,z |
| 110 | C110 | 0 | C.2 | 0.87005 | 0.43517 | 0.50000 | x,y,z |
| 111 | C111 | 0 | C.2 | 0.90703 | 0.45249 | 0.50000 | x,y,z |
| 112 | C112 | 0 | C.2 | 0.92578 | 0.43514 | 0.50000 | x,y,z |
| 113 | C113 | 0 | C.2 | 0.96178 | 0.45353 | 0.50000 | x,y,z |
| 114 | C114 | 0 | C.2 | 0.98047 | 0.49000 | 0.50000 | x,y,z |
| 115 | C115 | 0 | C.2 | 0.96092 | 0.50688 | 0.50000 | x,y,z |
| 116 | C116 | 0 | C.2 | 0.92496 | 0.48833 | 0.50000 | x,y,z |
| 117 | H117 | 0 | H | 0.75070 | 0.41480 | 0.50000 | x,y,z |
| 118 | H118 | 0 | H | 0.81540 | 0.43938 | 0.50000 | x,y,z |
| 119 | H119 | 0 | H | 0.79972 | 0.33444 | 0.50000 | x,y,z |
| 120 | H120 | 0 | H | 0.73523 | 0.30999 | 0.50000 | x,y,z |
| 121 | H121 | 0 | H | 0.97677 | 0.43918 | 0.50000 | x,y,z |
| 122 | H122 | 0 | H | 0.91143 | 0.40580 | 0.50000 | x,y,z |
| 123 | H123 | 0 | H | 0.97451 | 0.53620 | 0.50000 | x,y,z |
| 124 | H124 | 0 | H | 0.90982 | 0.50252 | 0.50000 | x,y,z |
| 125 | H125 | 0 | H | 0.85971 | 0.45378 | 0.50000 | x,y,z |
| 126 | N126 | 0 | N.2 | 0.63224 | 0.32022 | 0.50000 | x,y,z |
| 127 | C127 | 0 | C.2 | 0.65346 | 0.35481 | 0.50000 | x,y,z |
| 128 | C128 | 0 | C.2 | 0.63904 | 0.37825 | 0.50000 | x,y,z |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 129 | C129 | 0 | C.2 | 0.60322 | 0.36496 | 0.50000 | x,y,z |
| 130 | C130 | 0 | C.2 | 0.58968 | 0.38706 | 0.50000 | x,y,z |
| 131 | C131 | 0 | C.2 | 0.61165 | 0.42290 | 0.50000 | x,y,z |
| 132 | C132 | 0 | C.2 | 0.64737 | 0.43624 | 0.50000 | x,y,z |
| 133 | C133 | 0 | C.2 | 0.66094 | 0.41417 | 0.50000 | x,y,z |
| 134 | N134 | 0 | N.2 | 0.59786 | 0.44667 | 0.50000 | x,y,z |
| 135 | C135 | 0 | C.2 | 0.56483 | 0.43488 | 0.50000 | x,y,z |
| 136 | C136 | 0 | C.2 | 0.54751 | 0.45454 | 0.50000 | x,y,z |
| 137 | C137 | 0 | C.2 | 0.56486 | 0.49064 | 0.50000 | x,y,z |
| 138 | C138 | 0 | C.2 | 0.54647 | 0.50825 | 0.50000 | x,y,z |
| 139 | C139 | 0 | C.2 | 0.51000 | 0.49047 | 0.50000 | x,y,z |
| 140 | C140 | 0 | C.2 | 0.49312 | 0.45404 | 0.50000 | x,y,z |
| 141 | C141 | 0 | C.2 | 0.51167 | 0.43663 | 0.50000 | x,y,z |
| 142 | H142 | 0 | H | 0.58520 | 0.33590 | 0.50000 | x,y,z |
| 143 | H143 | 0 | H | 0.56062 | 0.37602 | 0.50000 | x,y,z |
| 144 | H144 | 0 | H | 0.66556 | 0.46528 | 0.50000 | x,y,z |
| 145 | H145 | 0 | H | 0.69001 | 0.42524 | 0.50000 | x,y,z |
| 146 | H146 | 0 | H | 0.56082 | 0.53759 | 0.50000 | x,y,z |
| 147 | H147 | 0 | H | 0.59420 | 0.50563 | 0.50000 | x,y,z |
| 148 | H148 | 0 | H | 0.46380 | 0.43831 | 0.50000 | x,y,z |
| 149 | H149 | 0 | H | 0.49748 | 0.40730 | 0.50000 | x,y,z |
| 150 | H150 | 0 | H | 0.54622 | 0.40593 | 0.50000 | x,y,z |
| 151 | C14 | 0 | C.3 | 0.49047 | -0.01953 | 0.50000 | x,-1+y,z |
| 152 | C39 | 0 | C.3 | 1.01953 | 0.51000 | 0.50000 | 1+x,y,z |
| 153 | C89 | 0 | C.3 | 0.50953 | 1.01953 | 0.50000 | x,1+y,z |
| 154 | C114 | 0 | C.3 | -0.01953 | 0.49000 | 0.50000 | -1+x,y,z |

**Table S3.** List of all torsions present in the COF (TRITER-2)

| No | Atom 1 | Atom 2 | Atom 3 | Atom 4 | Torsion |
|---|---|---|---|---|---|
| 1 | C27 | N1 | C2 | C3 | 180.00 |
| 2 | C27 | N1 | C2 | N51 | 0.00 |
| 3 | C2 | N1 | C27 | N26 | 0.00 |
| 4 | C2 | N1 | C27 | C28 | 180.00 |
| 5 | N1 | C2 | C3 | C4 | 0.00 |
| 6 | N1 | C2 | C3 | C8 | 180.00 |
| 7 | N51 | C2 | C3 | C4 | 180.00 |
| 8 | N51 | C2 | C3 | C8 | 0.00 |
| 9 | N1 | C2 | N51 | C52 | 0.00 |
| 10 | C3 | C2 | N51 | C52 | 180.00 |
| 11 | C2 | C3 | C4 | C5 | 180.00 |
| 12 | C2 | C3 | C4 | H17 | 0.00 |
| 13 | C8 | C3 | C4 | C5 | 0.00 |
| 14 | C8 | C3 | C4 | H17 | 180.00 |
| 15 | C2 | C3 | C8 | C7 | 180.00 |
| 16 | C2 | C3 | C8 | H20 | 0.00 |
| 17 | C4 | C3 | C8 | C7 | 0.00 |
| 18 | C4 | C3 | C8 | H20 | 180.00 |
| 19 | C3 | C4 | C5 | C6 | 0.00 |
| 20 | C3 | C4 | C5 | H18 | 180.00 |
| 21 | H17 | C4 | C5 | C6 | 180.00 |
| 22 | H17 | C4 | C5 | H18 | 0.00 |
| 23 | C4 | C5 | C6 | C7 | 0.00 |
| 24 | C4 | C5 | C6 | N9 | 180.00 |

| | | | | | |
|---|---|---|---|---|---|
| 25 | H18 | C5 | C6 | C7 | 180.00 |
| 26 | H18 | C5 | C6 | N9 | 0.00 |
| 27 | C5 | C6 | C7 | C8 | 0.00 |
| 28 | C5 | C6 | C7 | H19 | 180.00 |
| 29 | N9 | C6 | C7 | C8 | 180.00 |
| 30 | N9 | C6 | C7 | H19 | 0.00 |
| 31 | C5 | C6 | N9 | C10 | 0.00 |
| 32 | C7 | C6 | N9 | C10 | 180.00 |
| 33 | C6 | C7 | C8 | C3 | 0.00 |
| 34 | C6 | C7 | C8 | H20 | 180.00 |
| 35 | H19 | C7 | C8 | C3 | 180.00 |
| 36 | H19 | C7 | C8 | H20 | 0.00 |
| 37 | C6 | N9 | C10 | C11 | 180.00 |
| 38 | C6 | N9 | C10 | H25 | 0.00 |
| 39 | N9 | C10 | C11 | C12 | 0.00 |
| 40 | N9 | C10 | C11 | C16 | 180.00 |
| 41 | H25 | C10 | C11 | C12 | 180.00 |
| 42 | H25 | C10 | C11 | C16 | 0.00 |
| 43 | C10 | C11 | C12 | C13 | 180.00 |
| 44 | C10 | C11 | C12 | H22 | 0.00 |
| 45 | C16 | C11 | C12 | C13 | 0.00 |
| 46 | C16 | C11 | C12 | H22 | 180.00 |
| 47 | C10 | C11 | C16 | C15 | 180.00 |
| 48 | C10 | C11 | C16 | H24 | 0.00 |
| 49 | C12 | C11 | C16 | C15 | 0.00 |
| 50 | C12 | C11 | C16 | H24 | 180.00 |
| 51 | C11 | C12 | C13 | C14 | 0.00 |
| 52 | C11 | C12 | C13 | H21 | 180.00 |
| 53 | H22 | C12 | C13 | C14 | 180.00 |
| 54 | H22 | C12 | C13 | H21 | 0.00 |
| 55 | C12 | C13 | C14 | C15 | 0.00 |
| 56 | C12 | C13 | C14 | C89 | 180.00 |
| 57 | H21 | C13 | C14 | C15 | 180.00 |
| 58 | H21 | C13 | C14 | C89 | 0.00 |
| 59 | C13 | C14 | C15 | C16 | 0.00 |
| 60 | C13 | C14 | C15 | H23 | 180.00 |
| 61 | C89 | C14 | C15 | C16 | 180.00 |
| 62 | C89 | C14 | C15 | H23 | 0.00 |
| 63 | C14 | C15 | C16 | C11 | 0.00 |
| 64 | C14 | C15 | C16 | H24 | 180.00 |
| 65 | H23 | C15 | C16 | C11 | 180.00 |
| 66 | H23 | C15 | C16 | H24 | 0.00 |
| 67 | C52 | N26 | C27 | N1 | 0.00 |
| 68 | C52 | N26 | C27 | C28 | 180.00 |
| 69 | C27 | N26 | C52 | N51 | 0.00 |
| 70 | C27 | N26 | C52 | C53 | 180.00 |
| 71 | N1 | C27 | C28 | C29 | 180.00 |
| 72 | N1 | C27 | C28 | C33 | 0.00 |
| 73 | N26 | C27 | C28 | C29 | 0.00 |
| 74 | N26 | C27 | C28 | C33 | 180.00 |
| 75 | C27 | C28 | C29 | C30 | 180.00 |
| 76 | C27 | C28 | C29 | H42 | 0.00 |
| 77 | C33 | C28 | C29 | C30 | 0.00 |
| 78 | C33 | C28 | C29 | H42 | 180.00 |
| 79 | C27 | C28 | C33 | C32 | 180.00 |
| 80 | C27 | C28 | C33 | H45 | 0.00 |

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|---|---|---|---|---|---|
| 81 | C29 | C28 | C33 | C32 | 0.00 |
| 82 | C29 | C28 | C33 | H45 | 180.00 |
| 83 | C28 | C29 | C30 | C31 | 0.00 |
| 84 | C28 | C29 | C30 | H43 | 180.00 |
| 85 | H42 | C29 | C30 | C31 | 180.00 |
| 86 | H42 | C29 | C30 | H43 | 0.00 |
| 87 | C29 | C30 | C31 | C32 | 0.00 |
| 88 | C29 | C30 | C31 | N34 | 180.00 |
| 89 | H43 | C30 | C31 | C32 | 180.00 |
| 90 | H43 | C30 | C31 | N34 | 0.00 |
| 91 | C30 | C31 | C32 | C33 | 0.00 |
| 92 | C30 | C31 | C32 | H44 | 180.00 |
| 93 | N34 | C31 | C32 | C33 | 180.00 |
| 94 | N34 | C31 | C32 | H44 | 0.00 |
| 95 | C30 | C31 | N34 | C35 | 0.00 |
| 96 | C32 | C31 | N34 | C35 | 180.00 |
| 97 | C31 | C32 | C33 | C28 | 0.00 |
| 98 | C31 | C32 | C33 | H45 | 180.00 |
| 99 | H44 | C32 | C33 | C28 | 180.00 |
| 100 | H44 | C32 | C33 | H45 | 0.00 |
| 101 | C31 | N34 | C35 | C36 | 180.00 |
| 102 | C31 | N34 | C35 | H50 | 0.00 |
| 103 | N34 | C35 | C36 | C37 | 0.00 |
| 104 | N34 | C35 | C36 | C41 | 180.00 |
| 105 | H50 | C35 | C36 | C37 | 180.00 |
| 106 | H50 | C35 | C36 | C41 | 0.00 |
| 107 | C35 | C36 | C37 | C38 | 180.00 |
| 108 | C35 | C36 | C37 | H47 | 0.00 |
| 109 | C41 | C36 | C37 | C38 | 0.00 |
| 110 | C41 | C36 | C37 | H47 | 180.00 |
| 111 | C35 | C36 | C41 | C40 | 180.00 |
| 112 | C35 | C36 | C41 | H49 | 0.00 |
| 113 | C37 | C36 | C41 | C40 | 0.00 |
| 114 | C37 | C36 | C41 | H49 | 180.00 |
| 115 | C36 | C37 | C38 | C39 | 0.00 |
| 116 | C36 | C37 | C38 | H46 | 180.00 |
| 117 | H47 | C37 | C38 | C39 | 180.00 |
| 118 | H47 | C37 | C38 | H46 | 0.00 |
| 119 | C37 | C38 | C39 | C40 | 0.00 |
| 120 | C37 | C38 | C39 | C114 | 180.00 |
| 121 | H46 | C38 | C39 | C40 | 180.00 |
| 122 | H46 | C38 | C39 | C114 | 0.00 |
| 123 | C38 | C39 | C40 | C41 | 0.00 |
| 124 | C38 | C39 | C40 | H48 | 180.00 |
| 125 | C114 | C39 | C40 | C41 | 180.00 |
| 126 | C114 | C39 | C40 | H48 | 0.00 |
| 127 | C39 | C40 | C41 | C36 | 0.00 |
| 128 | C39 | C40 | C41 | H49 | 180.00 |
| 129 | H48 | C40 | C41 | C36 | 180.00 |
| 130 | H48 | C40 | C41 | H49 | 0.00 |
| 131 | C2 | N51 | C52 | N26 | 0.00 |
| 132 | C2 | N51 | C52 | C53 | 180.00 |
| 133 | N26 | C52 | C53 | C54 | 180.00 |
| 134 | N26 | C52 | C53 | C58 | 0.00 |
| 135 | N51 | C52 | C53 | C54 | 0.00 |
| 136 | N51 | C52 | C53 | C58 | 180.00 |

| | | | | | |
|---|---|---|---|---|---|
| 137 | C52 | C53 | C54 | C55 | 180.00 |
| 138 | C52 | C53 | C54 | H67 | 0.00 |
| 139 | C58 | C53 | C54 | C55 | 0.00 |
| 140 | C58 | C53 | C54 | H67 | 180.00 |
| 141 | C52 | C53 | C58 | C57 | 180.00 |
| 142 | C52 | C53 | C58 | H70 | 0.00 |
| 143 | C54 | C53 | C58 | C57 | 0.00 |
| 144 | C54 | C53 | C58 | H70 | 180.00 |
| 145 | C53 | C54 | C55 | C56 | 0.00 |
| 146 | C53 | C54 | C55 | H68 | 180.00 |
| 147 | H67 | C54 | C55 | C56 | 180.00 |
| 148 | H67 | C54 | C55 | H68 | 0.00 |
| 149 | C54 | C55 | C56 | C57 | 0.00 |
| 150 | C54 | C55 | C56 | N59 | 180.00 |
| 151 | H68 | C55 | C56 | C57 | 180.00 |
| 152 | H68 | C55 | C56 | N59 | 0.00 |
| 153 | C55 | C56 | C57 | C58 | 0.00 |
| 154 | C55 | C56 | C57 | H69 | 180.00 |
| 155 | N59 | C56 | C57 | C58 | 180.00 |
| 156 | N59 | C56 | C57 | H69 | 0.00 |
| 157 | C55 | C56 | N59 | C60 | 0.00 |
| 158 | C57 | C56 | N59 | C60 | 180.00 |
| 159 | C56 | C57 | C58 | C53 | 0.00 |
| 160 | C56 | C57 | C58 | H70 | 180.00 |
| 161 | H69 | C57 | C58 | C53 | 180.00 |
| 162 | H69 | C57 | C58 | H70 | 0.00 |
| 163 | C56 | N59 | C60 | C61 | 180.00 |
| 164 | C56 | N59 | C60 | H75 | 0.00 |
| 165 | N59 | C60 | C61 | C62 | 0.00 |
| 166 | N59 | C60 | C61 | C66 | 180.00 |
| 167 | H75 | C60 | C61 | C62 | 180.00 |
| 168 | H75 | C60 | C61 | C66 | 0.00 |
| 169 | C60 | C61 | C62 | C63 | 180.00 |
| 170 | C60 | C61 | C62 | H72 | 0.00 |
| 171 | C66 | C61 | C62 | C63 | 0.00 |
| 172 | C66 | C61 | C62 | H72 | 180.00 |
| 173 | C60 | C61 | C66 | C65 | 180.00 |
| 174 | C60 | C61 | C66 | H74 | 0.00 |
| 175 | C62 | C61 | C66 | C65 | 0.00 |
| 176 | C62 | C61 | C66 | H74 | 180.00 |
| 177 | C61 | C62 | C63 | C64 | 0.00 |
| 178 | C61 | C62 | C63 | H71 | 180.00 |
| 179 | H72 | C62 | C63 | C64 | 180.00 |
| 180 | H72 | C62 | C63 | H71 | 0.00 |
| 181 | C62 | C63 | C64 | C65 | 0.00 |
| 182 | C62 | C63 | C64 | C139 | 180.00 |
| 183 | H71 | C63 | C64 | C65 | 180.00 |
| 184 | H71 | C63 | C64 | C139 | 0.00 |
| 185 | C63 | C64 | C65 | C66 | 0.00 |
| 186 | C63 | C64 | C65 | H73 | 180.00 |
| 187 | C139 | C64 | C65 | C66 | 180.00 |
| 188 | C139 | C64 | C65 | H73 | 0.00 |
| 189 | C63 | C64 | C139 | C138 | 180.00 |
| 190 | C63 | C64 | C139 | C140 | 0.00 |
| 191 | C65 | C64 | C139 | C138 | 0.00 |
| 192 | C65 | C64 | C139 | C140 | 180.00 |

| | | | | | |
|---|---|---|---|---|---|
| 193 | C64 | C65 | C66 | C61 | 0.00 |
| 194 | C64 | C65 | C66 | H74 | 180.00 |
| 195 | H73 | C65 | C66 | C61 | 180.00 |
| 196 | H73 | C65 | C66 | H74 | 0.00 |
| 197 | C102 | N76 | C77 | C78 | 180.00 |
| 198 | C102 | N76 | C77 | N126 | 0.00 |
| 199 | C77 | N76 | C102 | N101 | 0.00 |
| 200 | C77 | N76 | C102 | C103 | 180.00 |
| 201 | N76 | C77 | C78 | C79 | 0.00 |
| 202 | N76 | C77 | C78 | C83 | 180.00 |
| 203 | N126 | C77 | C78 | C79 | 180.00 |
| 204 | N126 | C77 | C78 | C83 | 0.00 |
| 205 | N76 | C77 | N126 | C127 | 0.00 |
| 206 | C78 | C77 | N126 | C127 | 180.00 |
| 207 | C77 | C78 | C79 | C80 | 180.00 |
| 208 | C77 | C78 | C79 | H92 | 0.00 |
| 209 | C83 | C78 | C79 | C80 | 0.00 |
| 210 | C83 | C78 | C79 | H92 | 180.00 |
| 211 | C77 | C78 | C83 | C82 | 180.00 |
| 212 | C77 | C78 | C83 | H95 | 0.00 |
| 213 | C79 | C78 | C83 | C82 | 0.00 |
| 214 | C79 | C78 | C83 | H95 | 180.00 |
| 215 | C78 | C79 | C80 | C81 | 0.00 |
| 216 | C78 | C79 | C80 | H93 | 180.00 |
| 217 | H92 | C79 | C80 | C81 | 180.00 |
| 218 | H92 | C79 | C80 | H93 | 0.00 |
| 219 | C79 | C80 | C81 | C82 | 0.00 |
| 220 | C79 | C80 | C81 | N84 | 180.00 |
| 221 | H93 | C80 | C81 | C82 | 180.00 |
| 222 | H93 | C80 | C81 | N84 | 0.00 |
| 223 | C80 | C81 | C82 | C83 | 0.00 |
| 224 | C80 | C81 | C82 | H94 | 180.00 |
| 225 | N84 | C81 | C82 | C83 | 180.00 |
| 226 | N84 | C81 | C82 | H94 | 0.00 |
| 227 | C80 | C81 | N84 | C85 | 0.00 |
| 228 | C82 | C81 | N84 | C85 | 180.00 |
| 229 | C81 | C82 | C83 | C78 | 0.00 |
| 230 | C81 | C82 | C83 | H95 | 180.00 |
| 231 | H94 | C82 | C83 | C78 | 180.00 |
| 232 | H94 | C82 | C83 | H95 | 0.00 |
| 233 | C81 | N84 | C85 | C86 | 180.00 |
| 234 | C81 | N84 | C85 | H100 | 0.00 |
| 235 | N84 | C85 | C86 | C87 | 0.00 |
| 236 | N84 | C85 | C86 | C91 | 180.00 |
| 237 | H100 | C85 | C86 | C87 | 180.00 |
| 238 | H100 | C85 | C86 | C91 | 0.00 |
| 239 | C85 | C86 | C87 | C88 | 180.00 |
| 240 | C85 | C86 | C87 | H97 | 0.00 |
| 241 | C91 | C86 | C87 | C88 | 0.00 |
| 242 | C91 | C86 | C87 | H97 | 180.00 |
| 243 | C85 | C86 | C91 | C90 | 180.00 |
| 244 | C85 | C86 | C91 | H99 | 0.00 |
| 245 | C87 | C86 | C91 | C90 | 0.00 |
| 246 | C87 | C86 | C91 | H99 | 180.00 |
| 247 | C86 | C87 | C88 | C89 | 0.00 |
| 248 | C86 | C87 | C88 | H96 | 180.00 |

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|---|---|---|---|---|---|
| 249 | H97 | C87 | C88 | C89 | 180.00 |
| 250 | H97 | C87 | C88 | H96 | 0.00 |
| 251 | C87 | C88 | C89 | C90 | 0.00 |
| 252 | C87 | C88 | C89 | C14 | 180.00 |
| 253 | H96 | C88 | C89 | C90 | 180.00 |
| 254 | H96 | C88 | C89 | C14 | 0.00 |
| 255 | C88 | C89 | C90 | C91 | 0.00 |
| 256 | C88 | C89 | C90 | H98 | 180.00 |
| 257 | C14 | C89 | C90 | C91 | 180.00 |
| 258 | C14 | C89 | C90 | H98 | 0.00 |
| 259 | C89 | C90 | C91 | C86 | 0.00 |
| 260 | C89 | C90 | C91 | H99 | 180.00 |
| 261 | H98 | C90 | C91 | C86 | 180.00 |
| 262 | H98 | C90 | C91 | H99 | 0.00 |
| 263 | C127 | N101 | C102 | N76 | 0.00 |
| 264 | C127 | N101 | C102 | C103 | 180.00 |
| 265 | C102 | N101 | C127 | N126 | 0.00 |
| 266 | C102 | N101 | C127 | C128 | 180.00 |
| 267 | N76 | C102 | C103 | C104 | 180.00 |
| 268 | N76 | C102 | C103 | C108 | 0.00 |
| 269 | N101 | C102 | C103 | C104 | 0.00 |
| 270 | N101 | C102 | C103 | C108 | 180.00 |
| 271 | C102 | C103 | C104 | C105 | 180.00 |
| 272 | C102 | C103 | C104 | H117 | 0.00 |
| 273 | C108 | C103 | C104 | C105 | 0.00 |
| 274 | C108 | C103 | C104 | H117 | 180.00 |
| 275 | C102 | C103 | C108 | C107 | 180.00 |
| 276 | C102 | C103 | C108 | H120 | 0.00 |
| 277 | C104 | C103 | C108 | C107 | 0.00 |
| 278 | C104 | C103 | C108 | H120 | 180.00 |
| 279 | C103 | C104 | C105 | C106 | 0.00 |
| 280 | C103 | C104 | C105 | H118 | 180.00 |
| 281 | H117 | C104 | C105 | C106 | 180.00 |
| 282 | H117 | C104 | C105 | H118 | 0.00 |
| 283 | C104 | C105 | C106 | C107 | 0.00 |
| 284 | C104 | C105 | C106 | N109 | 180.00 |
| 285 | H118 | C105 | C106 | C107 | 180.00 |
| 286 | H118 | C105 | C106 | N109 | 0.00 |
| 287 | C105 | C106 | C107 | C108 | 0.00 |
| 288 | C105 | C106 | C107 | H119 | 180.00 |
| 289 | N109 | C106 | C107 | C108 | 180.00 |
| 290 | N109 | C106 | C107 | H119 | 0.00 |
| 291 | C105 | C106 | N109 | C110 | 0.00 |
| 292 | C107 | C106 | N109 | C110 | 180.00 |
| 293 | C106 | C107 | C108 | C103 | 0.00 |
| 294 | C106 | C107 | C108 | H120 | 180.00 |
| 295 | H119 | C107 | C108 | C103 | 180.00 |
| 296 | H119 | C107 | C108 | H120 | 0.00 |
| 297 | C106 | N109 | C110 | C111 | 180.00 |
| 298 | C106 | N109 | C110 | H125 | 0.00 |
| 299 | N109 | C110 | C111 | C112 | 0.00 |
| 300 | N109 | C110 | C111 | C116 | 180.00 |
| 301 | H125 | C110 | C111 | C112 | 180.00 |
| 302 | H125 | C110 | C111 | C116 | 0.00 |
| 303 | C110 | C111 | C112 | C113 | 180.00 |
| 304 | C110 | C111 | C112 | H122 | 0.00 |

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|---|---|---|---|---|---|
| 305 | C116 | C111 | C112 | C113 | 0.00 |
| 306 | C116 | C111 | C112 | H122 | 180.00 |
| 307 | C110 | C111 | C116 | C115 | 180.00 |
| 308 | C110 | C111 | C116 | H124 | 0.00 |
| 309 | C112 | C111 | C116 | C115 | 0.00 |
| 310 | C112 | C111 | C116 | H124 | 180.00 |
| 311 | C111 | C112 | C113 | C114 | 0.00 |
| 312 | C111 | C112 | C113 | H121 | 180.00 |
| 313 | H122 | C112 | C113 | C114 | 180.00 |
| 314 | H122 | C112 | C113 | H121 | 0.00 |
| 315 | C112 | C113 | C114 | C115 | 0.00 |
| 316 | C112 | C113 | C114 | C39 | 180.00 |
| 317 | H121 | C113 | C114 | C115 | 180.00 |
| 318 | H121 | C113 | C114 | C39 | 0.00 |
| 319 | C113 | C114 | C115 | C116 | 0.00 |
| 320 | C113 | C114 | C115 | H123 | 180.00 |
| 321 | C39 | C114 | C115 | C116 | 180.00 |
| 322 | C39 | C114 | C115 | H123 | 0.00 |
| 323 | C114 | C115 | C116 | C111 | 0.00 |
| 324 | C114 | C115 | C116 | H124 | 180.00 |
| 325 | H123 | C115 | C116 | C111 | 180.00 |
| 326 | H123 | C115 | C116 | H124 | 0.00 |
| 327 | C77 | N126 | C127 | N101 | 0.00 |
| 328 | C77 | N126 | C127 | C128 | 180.00 |
| 329 | N101 | C127 | C128 | C129 | 180.00 |
| 330 | N101 | C127 | C128 | C133 | 0.00 |
| 331 | N126 | C127 | C128 | C129 | 0.00 |
| 332 | N126 | C127 | C128 | C133 | 180.00 |
| 333 | C127 | C128 | C129 | C130 | 180.00 |
| 334 | C127 | C128 | C129 | H142 | 0.00 |
| 335 | C133 | C128 | C129 | C130 | 0.00 |
| 336 | C133 | C128 | C129 | H142 | 180.00 |
| 337 | C127 | C128 | C133 | C132 | 180.00 |
| 338 | C127 | C128 | C133 | H145 | 0.00 |
| 339 | C129 | C128 | C133 | C132 | 0.00 |
| 340 | C129 | C128 | C133 | H145 | 180.00 |
| 341 | C128 | C129 | C130 | C131 | 0.00 |
| 342 | C128 | C129 | C130 | H143 | 180.00 |
| 343 | H142 | C129 | C130 | C131 | 180.00 |
| 344 | H142 | C129 | C130 | H143 | 0.00 |
| 345 | C129 | C130 | C131 | C132 | 0.00 |
| 346 | C129 | C130 | C131 | N134 | 180.00 |
| 347 | H143 | C130 | C131 | C132 | 180.00 |
| 348 | H143 | C130 | C131 | N134 | 0.00 |
| 349 | C130 | C131 | C132 | C133 | 0.00 |
| 350 | C130 | C131 | C132 | H144 | 180.00 |
| 351 | N134 | C131 | C132 | C133 | 180.00 |
| 352 | N134 | C131 | C132 | H144 | 0.00 |
| 353 | C130 | C131 | N134 | C135 | 0.00 |
| 354 | C132 | C131 | N134 | C135 | 180.00 |
| 355 | C131 | C132 | C133 | C128 | 0.00 |
| 356 | C131 | C132 | C133 | H145 | 180.00 |
| 357 | H144 | C132 | C133 | C128 | 180.00 |
| 358 | H144 | C132 | C133 | H145 | 0.00 |
| 359 | C131 | N134 | C135 | C136 | 180.00 |
| 360 | C131 | N134 | C135 | H150 | 0.00 |

| | | | | | |
|---|---|---|---|---|---|
| 361 | N134 | C135 | C136 | C137 | 0.00 |
| 362 | N134 | C135 | C136 | C141 | 180.00 |
| 363 | H150 | C135 | C136 | C137 | 180.00 |
| 364 | H150 | C135 | C136 | C141 | 0.00 |
| 365 | C135 | C136 | C137 | C138 | 180.00 |
| 366 | C135 | C136 | C137 | H147 | 0.00 |
| 367 | C141 | C136 | C137 | C138 | 0.00 |
| 368 | C141 | C136 | C137 | H147 | 180.00 |
| 369 | C135 | C136 | C141 | C140 | 180.00 |
| 370 | C135 | C136 | C141 | H149 | 0.00 |
| 371 | C137 | C136 | C141 | C140 | 0.00 |
| 372 | C137 | C136 | C141 | H149 | 180.00 |
| 373 | C136 | C137 | C138 | C139 | 0.00 |
| 374 | C136 | C137 | C138 | H146 | 180.00 |
| 375 | H147 | C137 | C138 | C139 | 180.00 |
| 376 | H147 | C137 | C138 | H146 | 0.00 |
| 377 | C137 | C138 | C139 | C64 | 180.00 |
| 378 | C137 | C138 | C139 | C140 | 0.00 |
| 379 | H146 | C138 | C139 | C64 | 0.00 |
| 380 | H146 | C138 | C139 | C140 | 180.00 |
| 381 | C64 | C139 | C140 | C141 | 180.00 |
| 382 | C64 | C139 | C140 | H148 | 0.00 |
| 383 | C138 | C139 | C140 | C141 | 0.00 |
| 384 | C138 | C139 | C140 | H148 | 180.00 |
| 385 | C139 | C140 | C141 | C136 | 0.00 |
| 386 | C139 | C140 | C141 | H149 | 180.00 |
| 387 | H148 | C140 | C141 | C136 | 180.00 |
| 388 | H148 | C140 | C141 | H149 | 0.00 |

**Table S4.** List of all angles present in the COF (TRITER-2)

| No | Atom1 | Atom2 | Atom3 | Angle |
|---|---|---|---|---|
| 1 | C2 | N1 | C27 | 120.74 |
| 2 | N1 | C2 | C3 | 120.37 |
| 3 | N1 | C2 | N51 | 119.26 |
| 4 | C3 | C2 | N51 | 120.37 |
| 5 | C2 | C3 | C4 | 120.64 |
| 6 | C2 | C3 | C8 | 120.61 |
| 7 | C4 | C3 | C8 | 118.75 |
| 8 | C3 | C4 | C5 | 120.58 |
| 9 | C3 | C4 | H17 | 119.42 |
| 10 | C5 | C4 | H17 | 120.00 |
| 11 | C4 | C5 | C6 | 120.46 |
| 12 | C4 | C5 | H18 | 120.00 |
| 13 | C6 | C5 | H18 | 119.54 |
| 14 | C5 | C6 | C7 | 119.12 |

| | | | | |
|---|---|---|---|---|
| 15 | C5 | C6 | N9 | 121.29 |
| 16 | C7 | C6 | N9 | 119.59 |
| 17 | C6 | C7 | C8 | 120.47 |
| 18 | C6 | C7 | H19 | 119.99 |
| 19 | C8 | C7 | H19 | 119.54 |
| 20 | C3 | C8 | C7 | 120.62 |
| 21 | C3 | C8 | H20 | 119.38 |
| 22 | C7 | C8 | H20 | 120.00 |
| 23 | C6 | N9 | C10 | 120.66 |
| 24 | N9 | C10 | C11 | 127.29 |
| 25 | N9 | C10 | H25 | 119.99 |
| 26 | C11 | C10 | H25 | 112.73 |
| 27 | C10 | C11 | C12 | 123.37 |
| 28 | C10 | C11 | C16 | 117.93 |
| 29 | C12 | C11 | C16 | 118.70 |
| 30 | C11 | C12 | C13 | 120.57 |
| 31 | C11 | C12 | H22 | 119.44 |
| 32 | C13 | C12 | H22 | 120.00 |
| 33 | C12 | C13 | C14 | 121.54 |
| 34 | C12 | C13 | H21 | 120.00 |
| 35 | C14 | C13 | H21 | 118.45 |
| 36 | C13 | C14 | C15 | 116.75 |
| 37 | C13 | C14 | C89 | 121.62 |
| 38 | C15 | C14 | C89 | 121.63 |
| 39 | C14 | C15 | C16 | 121.37 |
| 40 | C14 | C15 | H23 | 119.99 |
| 41 | C16 | C15 | H23 | 118.64 |
| 42 | C11 | C16 | C15 | 121.07 |
| 43 | C11 | C16 | H24 | 118.91 |
| 44 | C15 | C16 | H24 | 120.02 |
| 45 | C27 | N26 | C52 | 120.74 |
| 46 | N1 | C27 | N26 | 119.26 |
| 47 | N1 | C27 | C28 | 120.37 |
| 48 | N26 | C27 | C28 | 120.37 |

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| 49 | C27 | C28 | C29 | 120.64 |
| 50 | C27 | C28 | C33 | 120.61 |
| 51 | C29 | C28 | C33 | 118.75 |
| 52 | C28 | C29 | C30 | 120.58 |
| 53 | C28 | C29 | H42 | 119.42 |
| 54 | C30 | C29 | H42 | 120.00 |
| 55 | C29 | C30 | C31 | 120.46 |
| 56 | C29 | C30 | H43 | 120.00 |
| 57 | C31 | C30 | H43 | 119.54 |
| 58 | C30 | C31 | C32 | 119.12 |
| 59 | C30 | C31 | N34 | 121.29 |
| 60 | C32 | C31 | N34 | 119.59 |
| 61 | C31 | C32 | C33 | 120.47 |
| 62 | C31 | C32 | H44 | 119.99 |
| 63 | C33 | C32 | H44 | 119.54 |
| 64 | C28 | C33 | C32 | 120.62 |
| 65 | C28 | C33 | H45 | 119.38 |
| 66 | C32 | C33 | H45 | 120.00 |
| 67 | C31 | N34 | C35 | 120.66 |
| 68 | N34 | C35 | C36 | 127.29 |
| 69 | N34 | C35 | H50 | 119.99 |
| 70 | C36 | C35 | H50 | 112.73 |
| 71 | C35 | C36 | C37 | 123.37 |
| 72 | C35 | C36 | C41 | 117.93 |
| 73 | C37 | C36 | C41 | 118.70 |
| 74 | C36 | C37 | C38 | 120.57 |
| 75 | C36 | C37 | H47 | 119.44 |
| 76 | C38 | C37 | H47 | 120.00 |
| 77 | C37 | C38 | C39 | 121.54 |
| 78 | C37 | C38 | H46 | 120.00 |
| 79 | C39 | C38 | H46 | 118.45 |
| 80 | C38 | C39 | C40 | 116.75 |
| 81 | C38 | C39 | C114 | 121.62 |
| 82 | C40 | C39 | C114 | 121.63 |

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| 83 | C39 | C40 | C41 | 121.37 |
| 84 | C39 | C40 | H48 | 119.99 |
| 85 | C41 | C40 | H48 | 118.64 |
| 86 | C36 | C41 | C40 | 121.07 |
| 87 | C36 | C41 | H49 | 118.91 |
| 88 | C40 | C41 | H49 | 120.02 |
| 89 | C2 | N51 | C52 | 120.74 |
| 90 | N26 | C52 | N51 | 119.26 |
| 91 | N26 | C52 | C53 | 120.37 |
| 92 | N51 | C52 | C53 | 120.37 |
| 93 | C52 | C53 | C54 | 120.64 |
| 94 | C52 | C53 | C58 | 120.61 |
| 95 | C54 | C53 | C58 | 118.75 |
| 96 | C53 | C54 | C55 | 120.58 |
| 97 | C53 | C54 | H67 | 119.42 |
| 98 | C55 | C54 | H67 | 120.00 |
| 99 | C54 | C55 | C56 | 120.46 |
| 100 | C54 | C55 | H68 | 120.00 |
| 101 | C56 | C55 | H68 | 119.54 |
| 102 | C55 | C56 | C57 | 119.12 |
| 103 | C55 | C56 | N59 | 121.29 |
| 104 | C57 | C56 | N59 | 119.59 |
| 105 | C56 | C57 | C58 | 120.47 |
| 106 | C56 | C57 | H69 | 119.99 |
| 107 | C58 | C57 | H69 | 119.54 |
| 108 | C53 | C58 | C57 | 120.62 |
| 109 | C53 | C58 | H70 | 119.38 |
| 110 | C57 | C58 | H70 | 120.00 |
| 111 | C56 | N59 | C60 | 120.66 |
| 112 | N59 | C60 | C61 | 127.29 |
| 113 | N59 | C60 | H75 | 119.99 |
| 114 | C61 | C60 | H75 | 112.73 |
| 115 | C60 | C61 | C62 | 123.37 |
| 116 | C60 | C61 | C66 | 117.93 |

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| 117 | C62 | C61 | C66 | 118.70 |
| 118 | C61 | C62 | C63 | 120.57 |
| 119 | C61 | C62 | H72 | 119.44 |
| 120 | C63 | C62 | H72 | 120.00 |
| 121 | C62 | C63 | C64 | 121.54 |
| 122 | C62 | C63 | H71 | 120.00 |
| 123 | C64 | C63 | H71 | 118.45 |
| 124 | C63 | C64 | C65 | 116.75 |
| 125 | C63 | C64 | C139 | 121.62 |
| 126 | C65 | C64 | C139 | 121.63 |
| 127 | C64 | C65 | C66 | 121.37 |
| 128 | C64 | C65 | H73 | 119.99 |
| 129 | C66 | C65 | H73 | 118.64 |
| 130 | C61 | C66 | C65 | 121.07 |
| 131 | C61 | C66 | H74 | 118.91 |
| 132 | C65 | C66 | H74 | 120.02 |
| 133 | C77 | N76 | C102 | 120.74 |
| 134 | N76 | C77 | C78 | 120.37 |
| 135 | N76 | C77 | N126 | 119.26 |
| 136 | C78 | C77 | N126 | 120.37 |
| 137 | C77 | C78 | C79 | 120.64 |
| 138 | C77 | C78 | C83 | 120.61 |
| 139 | C79 | C78 | C83 | 118.75 |
| 140 | C78 | C79 | C80 | 120.58 |
| 141 | C78 | C79 | H92 | 119.42 |
| 142 | C80 | C79 | H92 | 120.00 |
| 143 | C79 | C80 | C81 | 120.46 |
| 144 | C79 | C80 | H93 | 120.00 |
| 145 | C81 | C80 | H93 | 119.54 |
| 146 | C80 | C81 | C82 | 119.12 |
| 147 | C80 | C81 | N84 | 121.29 |
| 148 | C82 | C81 | N84 | 119.59 |
| 149 | C81 | C82 | C83 | 120.47 |
| 150 | C81 | C82 | H94 | 119.99 |

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| 151 | C83 | C82 | H94 | 119.54 |
| 152 | C78 | C83 | C82 | 120.62 |
| 153 | C78 | C83 | H95 | 119.38 |
| 154 | C82 | C83 | H95 | 120.00 |
| 155 | C81 | N84 | C85 | 120.66 |
| 156 | N84 | C85 | C86 | 127.29 |
| 157 | N84 | C85 | H100 | 119.99 |
| 158 | C86 | C85 | H100 | 112.73 |
| 159 | C85 | C86 | C87 | 123.37 |
| 160 | C85 | C86 | C91 | 117.93 |
| 161 | C87 | C86 | C91 | 118.70 |
| 162 | C86 | C87 | C88 | 120.57 |
| 163 | C86 | C87 | H97 | 119.44 |
| 164 | C88 | C87 | H97 | 120.00 |
| 165 | C87 | C88 | C89 | 121.54 |
| 166 | C87 | C88 | H96 | 120.00 |
| 167 | C89 | C88 | H96 | 118.45 |
| 168 | C88 | C89 | C90 | 116.75 |
| 169 | C88 | C89 | C14 | 121.62 |
| 170 | C90 | C89 | C14 | 121.63 |
| 171 | C89 | C90 | C91 | 121.37 |
| 172 | C89 | C90 | H98 | 119.99 |
| 173 | C91 | C90 | H98 | 118.64 |
| 174 | C86 | C91 | C90 | 121.07 |
| 175 | C86 | C91 | H99 | 118.91 |
| 176 | C90 | C91 | H99 | 120.02 |
| 177 | C102 | N101 | C127 | 120.74 |
| 178 | N76 | C102 | N101 | 119.26 |
| 179 | N76 | C102 | C103 | 120.37 |
| 180 | N101 | C102 | C103 | 120.37 |
| 181 | C102 | C103 | C104 | 120.64 |
| 182 | C102 | C103 | C108 | 120.61 |
| 183 | C104 | C103 | C108 | 118.75 |
| 184 | C103 | C104 | C105 | 120.58 |

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| 185 | C103 | C104 | H117 | 119.42 |
| 186 | C105 | C104 | H117 | 120.00 |
| 187 | C104 | C105 | C106 | 120.46 |
| 188 | C104 | C105 | H118 | 120.00 |
| 189 | C106 | C105 | H118 | 119.54 |
| 190 | C105 | C106 | C107 | 119.12 |
| 191 | C105 | C106 | N109 | 121.29 |
| 192 | C107 | C106 | N109 | 119.59 |
| 193 | C106 | C107 | C108 | 120.47 |
| 194 | C106 | C107 | H119 | 119.99 |
| 195 | C108 | C107 | H119 | 119.54 |
| 196 | C103 | C108 | C107 | 120.62 |
| 197 | C103 | C108 | H120 | 119.38 |
| 198 | C107 | C108 | H120 | 120.00 |
| 199 | C106 | N109 | C110 | 120.66 |
| 200 | N109 | C110 | C111 | 127.29 |
| 201 | N109 | C110 | H125 | 119.99 |
| 202 | C111 | C110 | H125 | 112.73 |
| 203 | C110 | C111 | C112 | 123.37 |
| 204 | C110 | C111 | C116 | 117.93 |
| 205 | C112 | C111 | C116 | 118.70 |
| 206 | C111 | C112 | C113 | 120.57 |
| 207 | C111 | C112 | H122 | 119.44 |
| 208 | C113 | C112 | H122 | 120.00 |
| 209 | C112 | C113 | C114 | 121.54 |
| 210 | C112 | C113 | H121 | 120.00 |
| 211 | C114 | C113 | H121 | 118.45 |
| 212 | C113 | C114 | C115 | 116.75 |
| 213 | C113 | C114 | C39 | 121.62 |
| 214 | C115 | C114 | C39 | 121.63 |
| 215 | C114 | C115 | C116 | 121.37 |
| 216 | C114 | C115 | H123 | 119.99 |
| 217 | C116 | C115 | H123 | 118.64 |
| 218 | C111 | C116 | C115 | 121.07 |

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| 219 | C111 | C116 | H124 | 118.91 |
| 220 | C115 | C116 | H124 | 120.02 |
| 221 | C77 | N126 | C127 | 120.74 |
| 222 | N101 | C127 | N126 | 119.26 |
| 223 | N101 | C127 | C128 | 120.37 |
| 224 | N126 | C127 | C128 | 120.37 |
| 225 | C127 | C128 | C129 | 120.64 |
| 226 | C127 | C128 | C133 | 120.61 |
| 227 | C129 | C128 | C133 | 118.75 |
| 228 | C128 | C129 | C130 | 120.58 |
| 229 | C128 | C129 | H142 | 119.42 |
| 230 | C130 | C129 | H142 | 120.00 |
| 231 | C129 | C130 | C131 | 120.46 |
| 232 | C129 | C130 | H143 | 120.00 |
| 233 | C131 | C130 | H143 | 119.54 |
| 234 | C130 | C131 | C132 | 119.12 |
| 235 | C130 | C131 | N134 | 121.29 |
| 236 | C132 | C131 | N134 | 119.59 |
| 237 | C131 | C132 | C133 | 120.47 |
| 238 | C131 | C132 | H144 | 119.99 |
| 239 | C133 | C132 | H144 | 119.54 |
| 240 | C128 | C133 | C132 | 120.62 |
| 241 | C128 | C133 | H145 | 119.38 |
| 242 | C132 | C133 | H145 | 120.00 |
| 243 | C131 | N134 | C135 | 120.66 |
| 244 | N134 | C135 | C136 | 127.29 |
| 245 | N134 | C135 | H150 | 119.99 |
| 246 | C136 | C135 | H150 | 112.73 |
| 247 | C135 | C136 | C137 | 123.37 |
| 248 | C135 | C136 | C141 | 117.93 |
| 249 | C137 | C136 | C141 | 118.70 |
| 250 | C136 | C137 | C138 | 120.57 |
| 251 | C136 | C137 | H147 | 119.44 |
| 252 | C138 | C137 | H147 | 120.00 |

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| 253 | C137 | C138 | C139 | 121.54 |
| 254 | C137 | C138 | H146 | 120.00 |
| 255 | C139 | C138 | H146 | 118.45 |
| 256 | C64 | C139 | C138 | 121.62 |
| 257 | C64 | C139 | C140 | 121.63 |
| 258 | C138 | C139 | C140 | 116.75 |
| 259 | C139 | C140 | C141 | 121.37 |
| 260 | C139 | C140 | H148 | 119.99 |
| 261 | C141 | C140 | H148 | 118.64 |
| 262 | C136 | C141 | C140 | 121.07 |
| 263 | C136 | C141 | H149 | 118.91 |
| 264 | C140 | C141 | H149 | 120.02 |

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