Supporting Information

Atomically Dispersed Co^{2+} in a Redox-Active COF for Electrochemical CO_2 Reduction to Ethanol: Unravelling Mechanistic Insight through Operando Studies

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Experimental Section

Physical Measurements

Infrared (IR) spectroscopy measurements were performed in Bruker FT-IR spectrometer and samples were prepared by making KBr pellets. Thermal stability of the materials was studied using Mettler Toledo TGA 850 instrument in the temperature range of 30-800 °C with a heating rate of 5 °C/min in N_2 atmosphere. Elemental analysis was performed using Thermo Scientific Flash 2000 CHN analyser. Powder X-ray diffraction experiment was performed in Bruker D8 discover instrument using Cu-Kα radiation. Field Emission Scanning Electron Microscope (FESEM) images were collected using Lica-S440I FESEM instrument. Samples were prepared on silicon wafers for FESEM studies, and a high vacuum with 100 kV accelerating voltage was used for FESEM analysis. Transmission Electron Microscopic (TEM) images were captured using JEOL JEM-3010 TEM with an accelerating voltage of 300 kV. The EDS elemental mapping images were recorded in a JEOL JEM-F200 TEM. The polymer was dispersed in ethanol and drop cast over carbon-coated copper grid prior to TEM analysis. Solid-state ^{13}C NMR was performed on a Varian infinity plus 300WB spectrometer at a MAS rate of 5 kHz and a CP contact time of 1.4 ns. The gas adsorption studies (N_2 adsorption at 77 K) were performed using QUANTACHROME QUADRASORD-SI analyzer. Samples were activated at 150 °C under $1x10^{-1}$ Pa vacuum for 12 h prior to measurement of the adsorption isotherm. Electron paramagnetic resonance (EPR) study was carried out at room temperature in the solid-state using Bruker EMX 1444 EPR spectrometer. All the electrochemical experiments were performed using the three-electrode system in Autolab Nova 2.1.3 potentiostat/galvanostat instrument assembled with a Metrohm RDE-2 rotator and CHI 760E potentiostat instrument. HADAAF-STEM experiment was performed in 60 – 300 kV low base Titan® Themis™ instrument. ATR-FTIR spectra were recorded in the FT-IR spectrophotometer (BRUKER, VERTEX 70B). XAS experiments at 300 K were performed at PETRA III, beamline P65, of DESY, Germany. Measurements of Co-K edge at ambient pressure were performed in fluorescence as well as transmission mode using gas ionization chambers to monitor the incident and transmitted X-ray intensities. Monochromatic X-rays were obtained using a Si (111) double crystal monochromator which was calibrated by defining the inflection point (first derivative maxima) of Co foil as 7709 eV. The beam was focused by employing a Kirkpatrick-Baez (K-B) mirror optic. Rhodium-coated X-ray mirror was used to suppress higher-order harmonics. A CCD detector was used to record the transmitted signals. Pellets for the *ex-situ* measurements were made by

homogeneously mixing the sample with an inert Boron nitride matrix to obtain an X-ray absorption edge jump close to one. X-ray absorption near edge spectra (XANES) of the XAS spectra were obtained by subtracting the pre-edge background from the overall absorption and normalizing it to the spline fit using ATHENA software package. The k^2 -weighted extended X-ray absorption fine structure (EXAFS) was Fourier transformed over the limited range of k from 3 to 14 $Å^{-1}$.

The normalized, energy-calibrated Co K-edge XANES spectra were obtained using standard data reduction techniques with Athena and Artemis software. The EXAFS oscillations $\chi(k)$ as a function of photoelectron wave number k was extracted by following standard procedures. The theoretical paths were generated using FEFF and the models were completed in a conventional way using a fitting program named Artemis5. The theoretical phase and amplitude functions of Co-N and Co-O and Co-Cl were calculated with FEFF. CIF file was obtained for Co-TAPA-OPE COF from the modeled structure of OPE-TAPA-COF from Materials Studio 2020. The values for the amplitude reduction factor (S_0^2) and the mean square disorder (σ^2) were determined by fitting the corresponding CIF with FEFF. The EXAFS parameters were obtained by a least-squares fit in the R-space of the k^2-weighted Fourier transform (FT) data.

Materials and method

The reagents and chemicals used for the synthesis of the organic linker (OPE-pyr) were purchased from Sigma-Aldrich Chemical Co. Ltd and used as such. KBr pellets were made for recording the FT-IR spectra.

Computational Details

The models of the COF were built using the Forcite module of the Accelrys Materials Studio software package. For the modeling, we applied the space group with the highest possible symmetry, taking into account the rotation of the phenyl group w.r.t the basic plane of TAPA unit. The lattice models were geometry optimized using the MS Forcite molecular dynamics module (Universal force fields). Structure refinements using the Pawley method were then carried out as implemented in the Reflex module of the Materials Studio software. Pseudo-Voigt peak profiles were used, and peak asymmetry was corrected using the Berar-Baldinozzi method. The unit cell parameters *a*, *b*, *c*, crystallite size along *a*, *b*, *c*, FWHM parameters, U, V, W, profile parameters NA, NB, and zero-point were refined based on previous studies.[1-4] As for the AB stacked COF model, in addition to the above

parameters, alpha, beta, and gamma parameters were also refined. The background was refined with 20th-order polynomial. The eclipsed (AA-stacked) model with $P\bar{3}$ space group was refined to give lattice parameters, $a = b = 55.932229$ Å, $c = 4.121883$ Å and $\alpha = \beta = 90^{\circ}$, $\gamma = 120^{\circ}$ with a weighted-profile R factor $R_{wp} = 4.09\%$ and unweighted-profile R factor $R_p = 3.14\%$ (Fig. S3-S4, Table S2). However, the staggered (AB-stacked) model (space group symmetry $P1$, $a = 55.837446$ Å, $b = 55.826763$ Å, $c = 9.348897$ Å and $\alpha = 90.18597^{\circ}$, $\beta = 90.04859^{\circ}$, $\gamma = 119.66183^{\circ}$) showed better agreement with the experimental PXRD pattern with $R_{wp} = 3.73\%$ and $R_p = 2.83\%$. Thus, the staggered model is likely to be the model for TAPA-OPE COF.

Furthermore, the computational studies were carried out for repeating units of TAPA-OPE and Co-TAPA-OPE. Density functional theoretical (DFT) calculations have been carried out using the Gaussian16 program package utilizing structural units of TAPA-OPE and Co-TAPA-OPE as the model systems.[5] The calculations were performed utilizing B3LYP exchange-correlation functional along with 6-31+G(d) basis set for all atoms except for Co atom, for which LANL2DZ, which utilizes a widely used effective core potential (ECP)- type basis set, was used.[6-13] The calculations were performed in absence of any solvent. Grimme's d3 dispersion was also used to tackle weak interactions. The harmonic vibrational frequency analysis of the optimized geometries was performed to confirm the nature of stationary points. All the optimized intermediates revealed the absence of any imaginary vibrational mode, indicating the optimized geometries as minima on the potential energy surface (PES). All thermochemical data were obtained with the ideal gas-rigid rotor-simple harmonic oscillator approximations at 298.15 K and 1 atm. Zero point-energy corrections were included in the Gibbs free energy values along with entropy effect and enthalpy effect. The pictures of the optimized structures were taken from Gauss View 6.0.16.

Electrochemical Experiment

All electrochemical experiments were done in a three-electrode cell configuration with a glassy carbon (GC) electrode as the working electrode (WE), platinum as a counter electrode (CE), and Ag/AgCl as a reference electrode (RE). An electro-chemical ink was prepared by making a dispersion of a mixture of COF (2 mg) and Vulcan carbon (2 mg) in the solvent mixture of isopropanol (500 µL) and water (500 µl). Further, Nafion (13 µL) was added as a binder to the electrochemical ink. Upon sonication for 30 minutes, a well-dispersed ink (3.5

μL) was drop casted over the GC electrode and allowed to dry for 3 h under ambient conditions. This was done thrice, and therefore cumulatively, 10.5 μL ink was drop-cast. LSVs were performed with the scan rate of 5 mV/s. The potentials are reported with respect to reversible hydrogen electrode (RHE). All current densities were calculated using the geometric surface area of the electrode. All potentials were rescaled to the pH-independent reversible hydrogen electrode (RHE) and reported without iR compensation.

Electrolysis in H-type cell

Carbon fibre paper (CFP) (Global Nanotech, thickness ~ 270 μm) was used as received and cut into 1 cm^2 as the working electrode while performing controlled potential electrolysis in an H-type cell (Fig. S15). The two compartments were separated using Nafion 117 membrane. The cathodic compartment was comprised of CFP as working electrode and Ag/AgCl as reference electrode, whereas Pt plate was used as counter electrode in anodic compartment. An aliquot of 100 μL of the catalyst ink was drop-casted onto a CFP and allowed to dry in air overnight, resulting in the catalyst loading of 0.2 mg cm^{-2}.

0.2 M $KHCO_3$ electrolyte was used for both chambers. The total volume of the working electrode chamber is 85.0 mL. 40.0 mL of electrolyte was added to this chamber. A CO_2-saturated electrolyte was prepared by purging CO_2 (99.99%) into aqueous solution of $KHCO_3$ for 30 min, and a flow of 10 sccm CO_2 was maintained over the electrolyte throughout the electrochemical measurements. At first, 20 cycles of CV sweep between -0.07 V and -0.47 V vs. RHE were conducted to generate stable CV curves. Chronoamperometry was performed for 2 h at each potential for CO_2 reduction tests in the H-type cell.

Electrolysis in flow cell

The flow cell uses a three-electrode system with an electrochemical workstation as a potentiostat. In the flow cell, 1 M $KHCO_3$ was used for the electrolyte. Using a peristaltic pump, 30 mL of cathode was circulated through the cathode chamber at a constant rate of 20 mL min^{-1}. An additional 30 mL of anode fluid was circulated through the anode chamber at the same rate. Carbon dioxide gas was used to flow at 30 standard cubic centimeters per minute (sccm) on the back of the GDE, controlled by a mass flowmeter. The 400 μL catalyst ink was sprayed on GDL to prepare the GDEs with a load of ~1mg cm^{-2}, which was further dried at room temperature for use.

The partial current density of the products was calculated according to:

$$j_{\text{partial}} = j_{\text{tot}} \cdot \text{FE}_{\text{product}}$$

Calculation of overpotential

The overpotential η is the difference between the actual electrode reduction potential and the thermodynamic potential, defined by the following equation:

Overpotential (η) = E (RHE) – $E^{0}_{CO_2/EtOH}$ (RHE)

In the equation, E is the applied potential (vs. RHE) and $E^{0}_{CO_2/EtOH}$ is the standard electrode for CO_2 to ethanol conversion, which is 0.09 V (vs. RHE).*n*

Synthesis

OPE-pyr aldehyde synthesis

The synthesis and characterization of 1,4-diethynyl-2,5-bis(pentyloxy)benzene (**D**) (Scheme S1) was reported previously by our group. Further, details about synthetic procedure and characterization data for newly synthesized 5,5'-((2,5-bis(pentyloxy)-1,4-phenylene)bis(ethyne-2,1-diyl))dipicolinaldehyde (OPE-pyr) is given below. We have characterized OPE-pyr organic linker using various experimental techniques like ^{1}H-NMR, IR and Mass spectrometry.

The compound 5,5'-((2,5-bis(pentyloxy)-1,4-phenylene)bis(ethyne-2,1-diyl)) dipicolinaldehyde (OPE-pyr) was synthesized by the Sonogashira-Hagihara coupling reaction. The earlier reported 1,4-diethynyl-2,5-bis(pentyloxy)benzene (**D**) (2.3 mmol, 1 equiv.) and 5-bromopicolinaldehyde (4.6 mmol, 2 equiv.) were taken together in mixed of dried solvent tetrahydrofuron (THF) (40 mL) and triethyl amine (20 mL) followed by addition of Cu(I) (20 mol%) which acts as co-catalyst. The N_2 gas was purged into the reaction mixture for 30 minutes to ensure the removal of dissolved oxygen from the solvents. In the last, 10 mol% of Palladium catalyst [Pd (0)] was added and again, the reaction mixture was degassed for 20 minutes by N_2 purging. Subsequently, the reaction mixture (R.M.) was stirred under an inert atmosphere at 75 ˚C for 48 hrs. Reaction progress was monitored by

TLC analysis. Once the reactant was finished, then the R.M. was cooled to room temperature and the solvent was evaporated under reduced pressure. The solid product was dissolved in ethyl acetate and washed thrice using water, 2 N HCL and saturated brine solution. The organic layer was dried over anhydrous sodium sulphate. The solvent was evaporated in a rotary evaporator that yielded a crude product of OPE-pyr. The crude product was further purified separately by column chromatography packed in silica gel (60-120 mess size) using hexane: ethyl acetate solvent system. The yield of column purified OPE-pyr product is found to be 58%. Characterization data for OPE-pyr is given as follows.

5,5'-((2,5-bis(pentyloxy)-1,4-phenylene)bis(ethyne-2,1-diyl))dipicolinaldehyde (OPE-pyr)

R_f: 0.5 (7% ethyl acetate: hexane), IR (KBr) ν_{max}/cm^{-1} = 2936, 2862, 2819, 2205, 2035, 1960, 1709, 1574, 1503, 1393, 1294, 1219, 1015, 836, 761, 723, 618, 530. ^{1}H NMR ($CDCl_3$, 600 MHz): δ 0.92-0.95 (t, 6H, -2CH_3), 1.39-1.45 (m, 4H, -2CH_2), 1.50-1.55 (m, 4H, -2CH_2), 1.85-1.90 (pentate, 4H, -2CH_2), 4.04-4.06 (t, 4H, -2OCH_2), 7.06 (s, 2H, 2ArH), 7.96 (broad, 4H, 4ArH), 8.89 (s, 2H, 2ArH), 10.08 (s, 2H, 2CHO).^{13}C NMR ($CDCl_3$, 150 MHz): 14.1, 22.4, 28.2, 28.9, 69.6, 91.3, 92.8, 113.7, 116.7, 121.1, 124.9, 139.1, 150.9, 152.4, 153.9, 192.5. ESI-MS+ m/z Calcd. for $C_{32}H_{32}N_2O_4$: 509.2440 $[M+H]^+$, found 509.2437.

Synthesis of TAPA-OPE

The linker, 4,4'-(2,5-bis(pentyloxy)-1,4-phenylene)bis(ethyne-2,1-diyl)dipicolinaldehyde (OPE-5) was synthesized through Sonogashira-Hagihara coupling reaction by adapting a reported procedure (Scheme S1 and Fig. S1-S2). Next, the COF, namely, **TAPA-OPE**, was synthesized by the Schiff base condensation between OPE-5 and commercially available *tris*-(4-aminophenyl) amine (TAPA). In brief, OPE-5 (15 mg, 0.03 mmol) and TAPA (6 mg, 0.02 mmol) were mixed together in a Pyrex tube, followed by adding 1 mL of a binary solvent system comprising of *n*-butanol and *o*-dichlorobenzene in a volume ratio of 3:7 (Fig. 1a & S2). The reaction mixture was sonicated for 15 minutes to homogenize, followed by the addition of the catalytic amount of 6 M acetic acid (100 µL). The reaction mixture was degassed by flash-frozen in liquid nitrogen upon applying high vacuum through three freeze pump-thaw cycles. The degassed sample was sealed under a high vacuum and kept at 120 °C for 72 h. An orange-colored material was obtained, which was washed thrice with fresh n-butanol (30 mL), tetrahydrofuran (THF) (30 mL), and hot DMF (150 mL) to remove oligomeric species. Purified COF (TAPA-OPE) was washed with acetone (50 mL) and dried at 150 °C for 12 h. The yield of COF was found to be 60-65%.

Covalent integration of Co^{II} in TAPA-OPE (Co-TAPA-OPE)

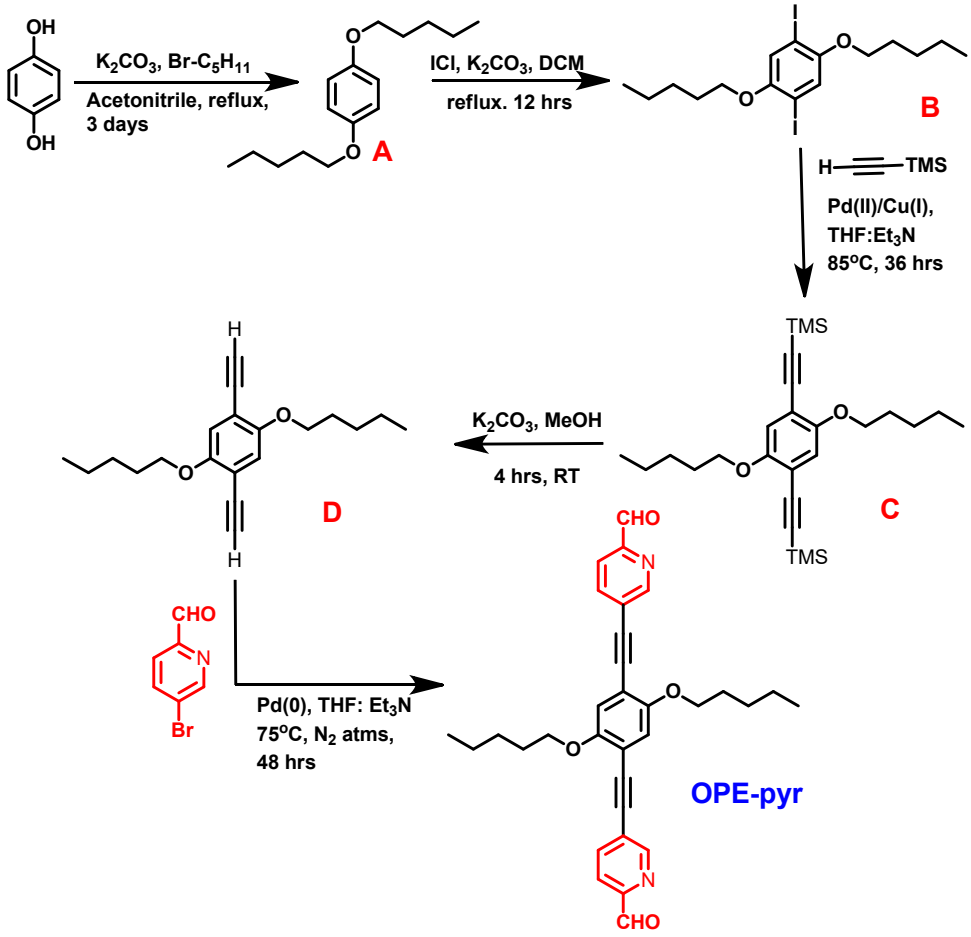
Prior to cobalt complexation, TAPA-OPE (20 mg) was activated at 150 °C for 12 h (Fig. 3a). Now, activated TAPA-OPE COF was dispersed in acetonitrile (10 mL). A solution of $CoCl_2.6H_2O$ (5 mg) in acetonitrile (5 mL) was slowly added to the dispersed solution of TAPA-OPE and allowed to stir at reflux conditions for 4 h. This has resulted in Co^{II} coordinated TAPA-OPE (**Co-TAPA-OPE**). The Co-TAPA-OPE was isolated by centrifugation and washed with fresh acetonitrile (10 mL) multiple times to remove unreacted cobalt salt and then dried at 120 °C overnight for further use.

Electrical conductivity

A fine dispersion of 2 mg of TAPA-OPE in 0.2 mL THF was made upon sonication and subsequently spin-coated on the glass surface at 1200 rpm for 60 seconds. A thin coating of TAPA-OPE on the glass surface was dried at 60 °C for 1 hr. Next, aluminium metal (Al) was deposited under vacuum by physical vapor deposition (PVD) method on TAPA-OPE coated glass by masking the polymer layer using Teflon tape. Electrical conductivity was then measured for the Al deposited thin film of TAPA-OPE. The conductivity for TAPA-OPE was calculated by the following formula;

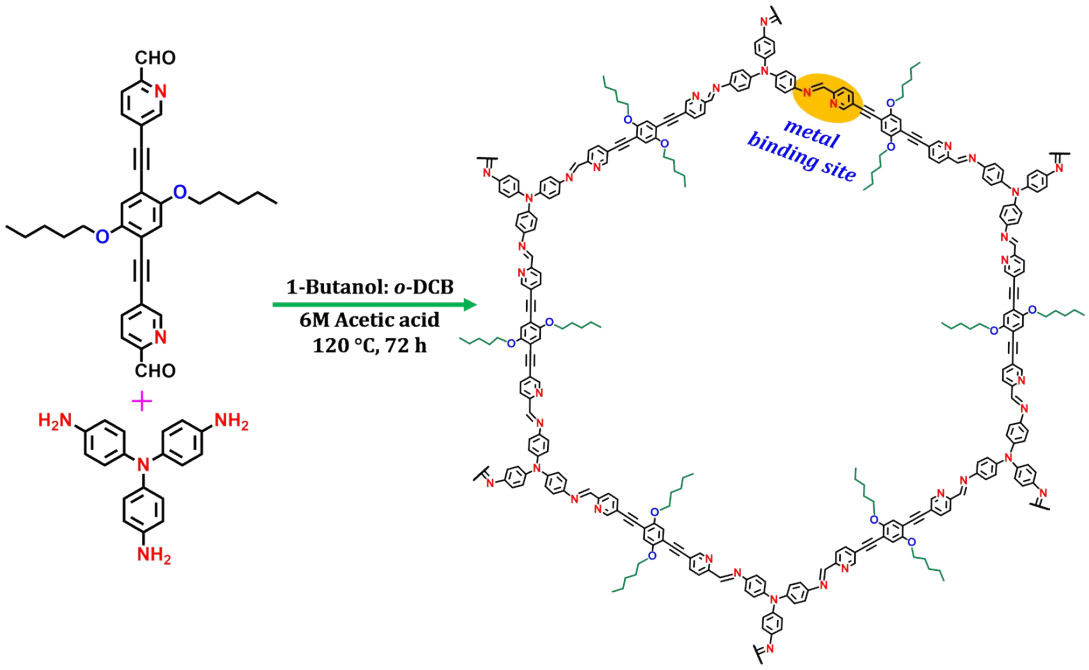
Conductivity = Slope × (WT/L)

Where L= length of the coated surface (1 cm), W= width of the coated surface (1 cm), T= Film Thickness (T = 345 nm).



Scheme S1. Synthetic scheme for OPE-pyr organic linker.

Scheme for COF synthesis (TAPA-OPE):



Scheme S2. Synthetic scheme for TAPA-OPE COF.

NMR spectra for organic linker (OPE-pyr):

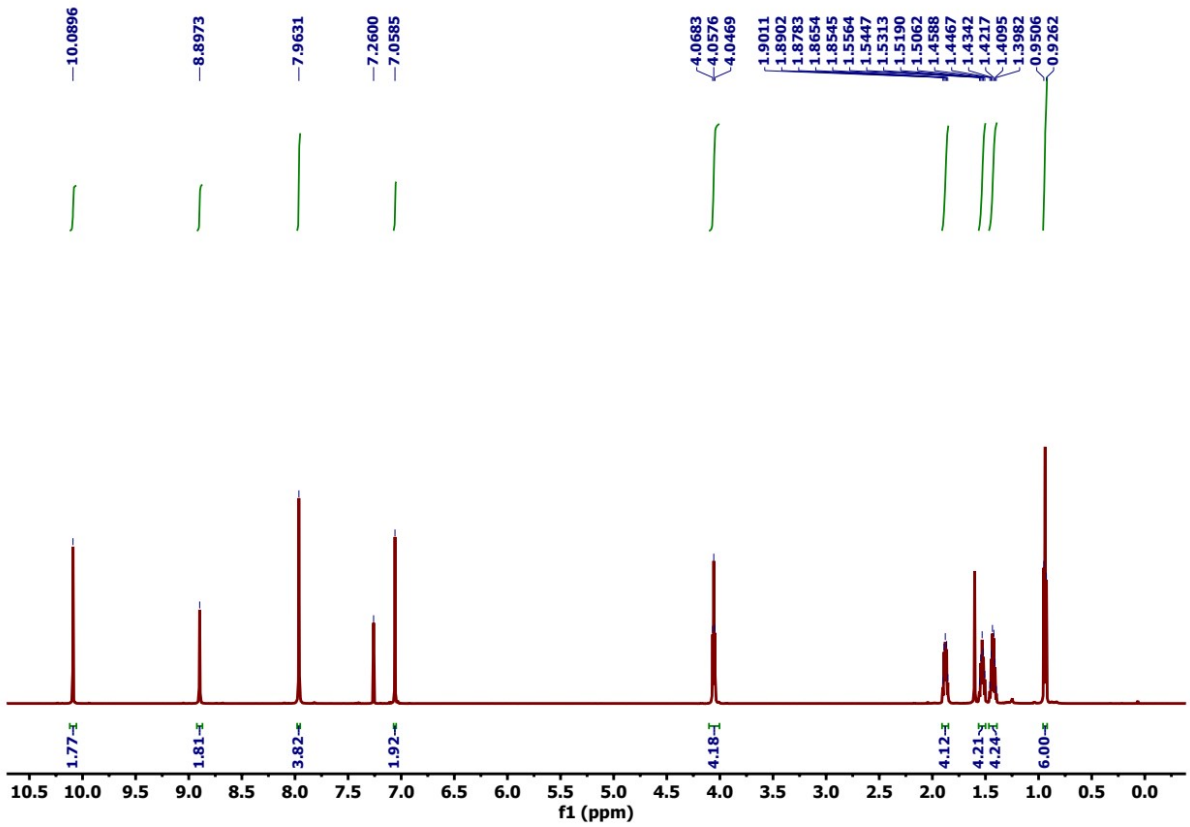


Fig. S1. ^{1}H-NMR spectrum for OPE-pyr recorded in $CDCl_3$.

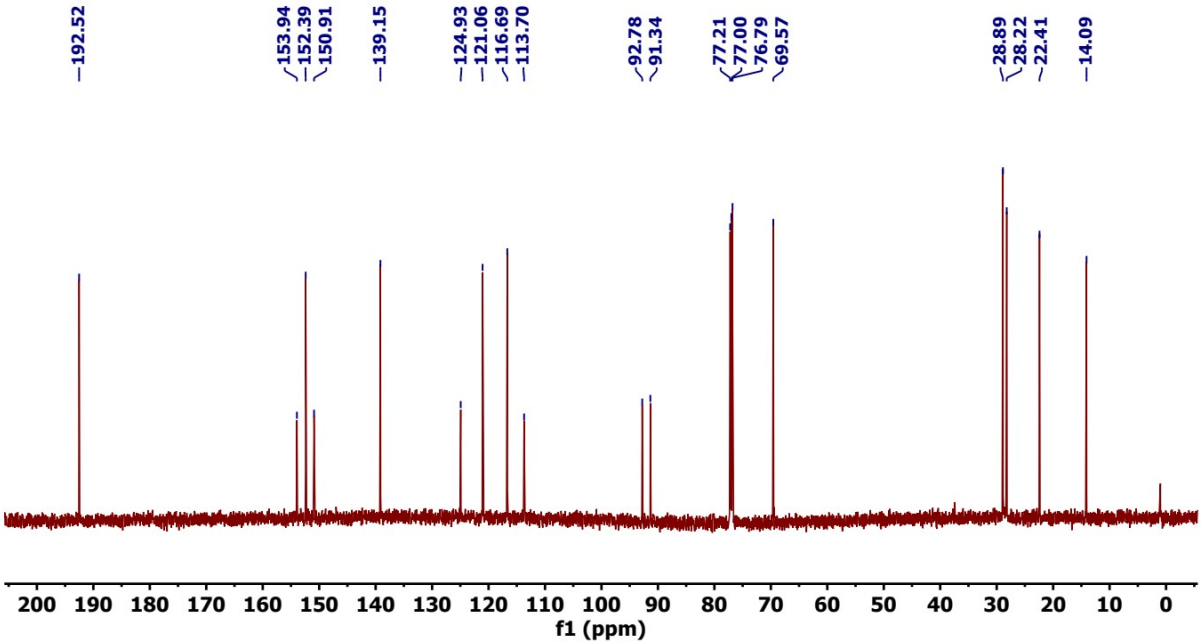


Fig. S2. ^{13}C-NMR spectrum for OPE-pyr recorded in $CDCl_3$.

Characterization of TAPA-OPE:

PXRD for eclipsed model of TAPA-OPE:

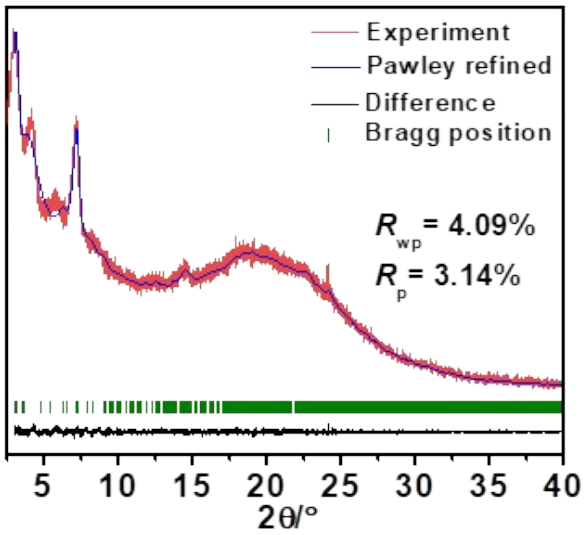


Fig. S3. Experimental and simulated PXRD for the eclipsed model of TAPA-OPE COF.

Modelled structure for eclipsed conformation of TAPA-OPE:

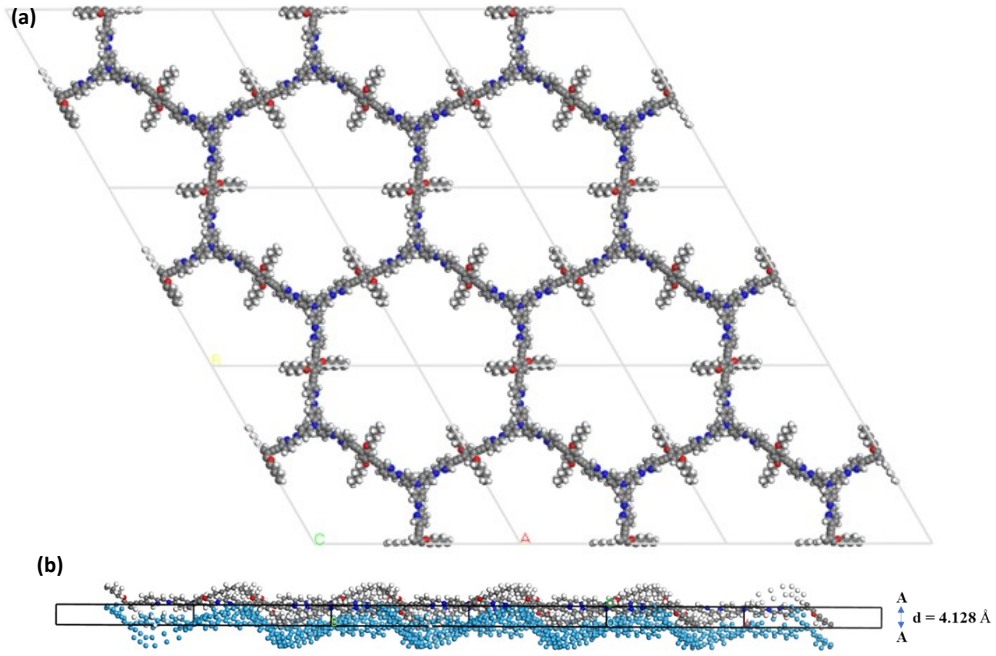


Fig. S4. Simulated structure of TAPA-OPE in eclipsed conformation, and extended 2D structure.

IR-Spectrum for TAPA-OPE:

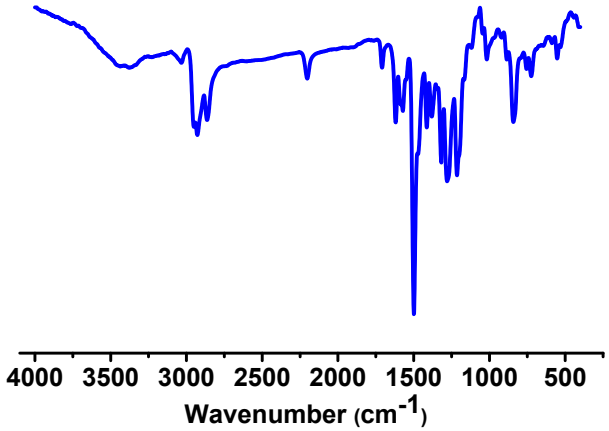


Fig. S5. IR-spectrum for TAPA-OPE.

TGA plot:

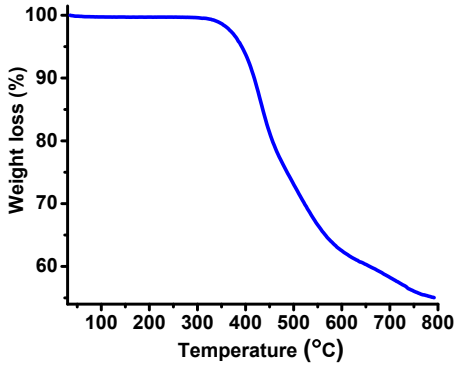


Fig. S6. TGA graph for TAPA-OPE under N_2 atmosphere.

Pore size distribution in TAPA-OPE:

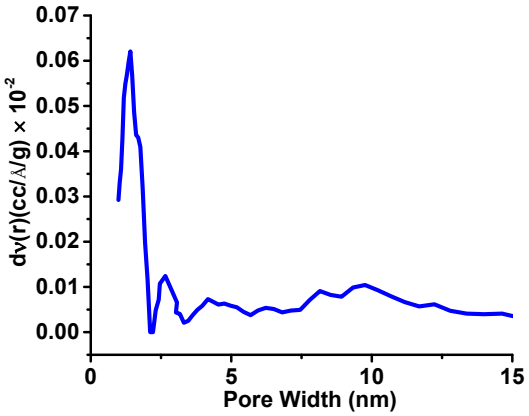


Fig. S7. Pore size distribution (from N_2 adsorption data) for TAPA-OPE.

Electrochemical band gap for TAPA-OPE:

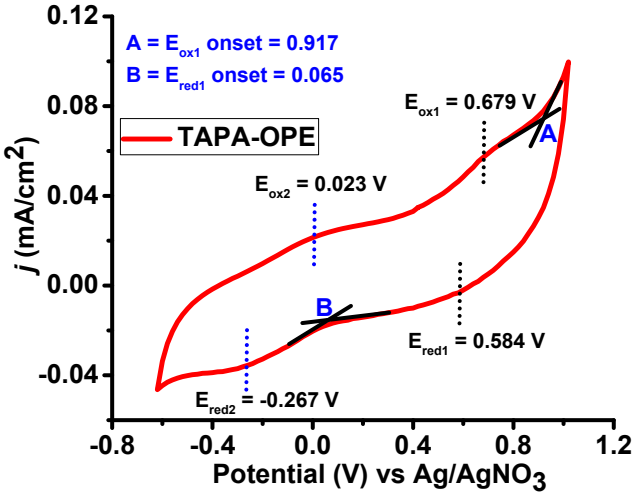


Fig. S8. CV for electrochemical band gap for TAPA-OPE.

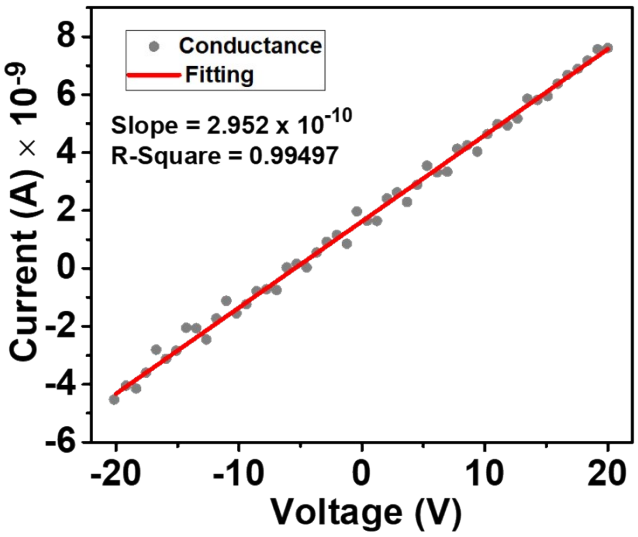


Fig. S9. Electrical Conductivity for TAPA-OPE COF.

Characterization of Co-TAPA-OPE:

ATR-FTIR spectra:

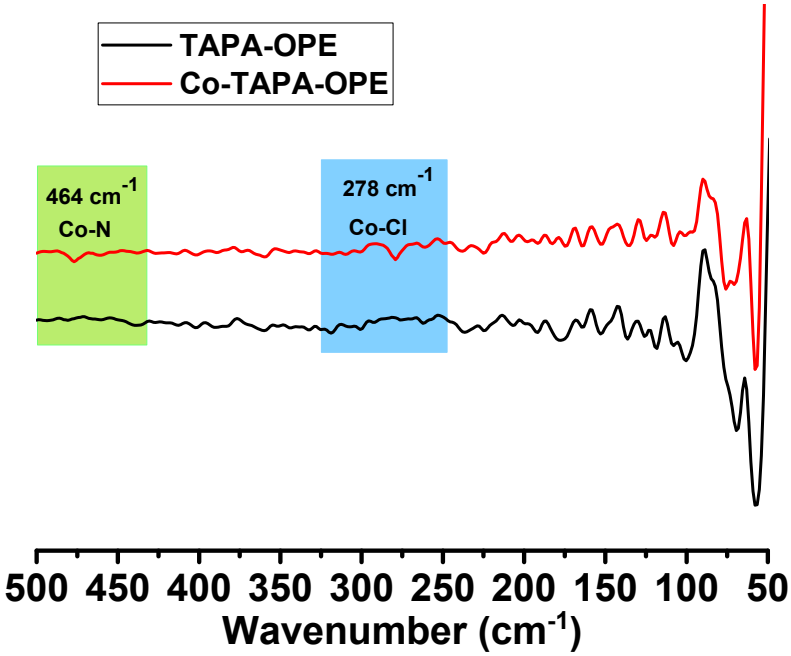


Fig. S10. ATR-FTIR spectra for as-synthesized COF and metalated COF.

TGA-Mass analysis for Co-TAPA-OPE:

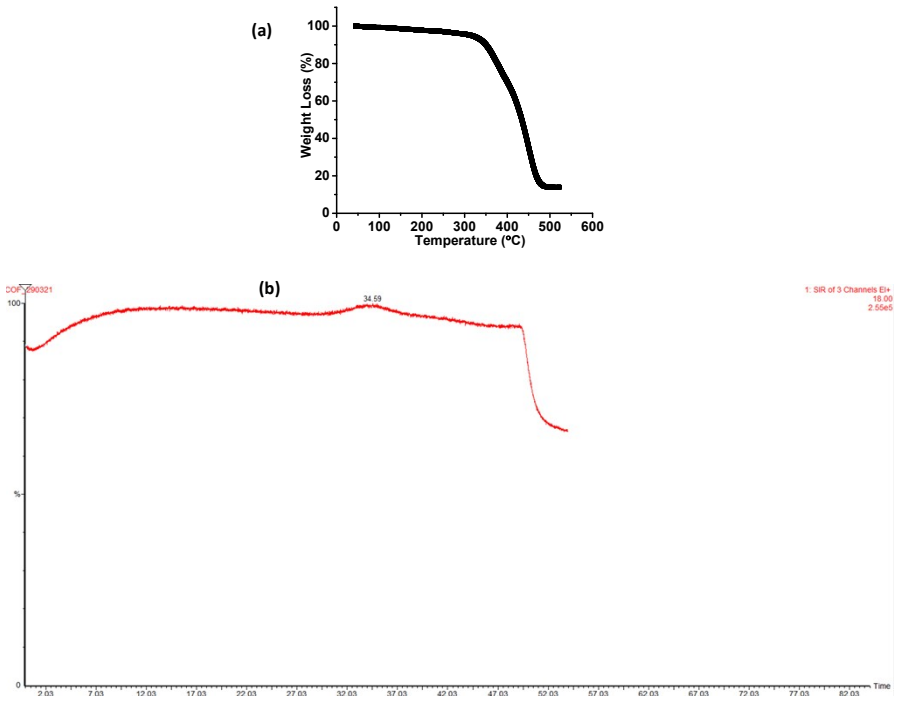


Fig. S11. TGA-Mass analysis for Co-TAPA-OPE. (a) TGA plot under Ar atmosphere. (b) Weight loss observed for water molecule in the TGA-Mass spectrometry.

PXRD pattern for Co-TAPA-OPE:

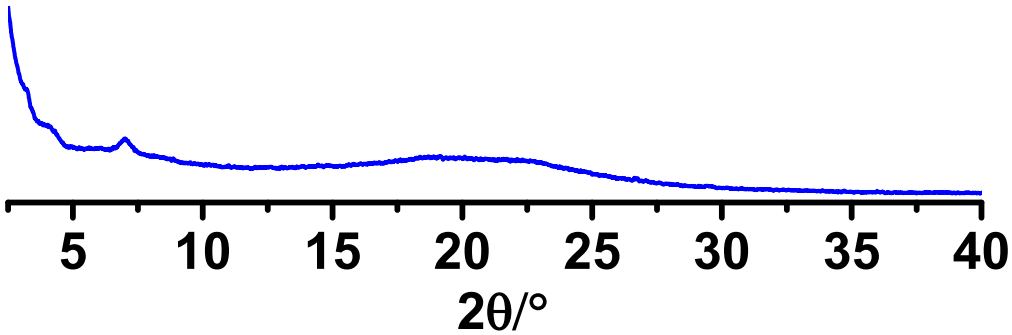
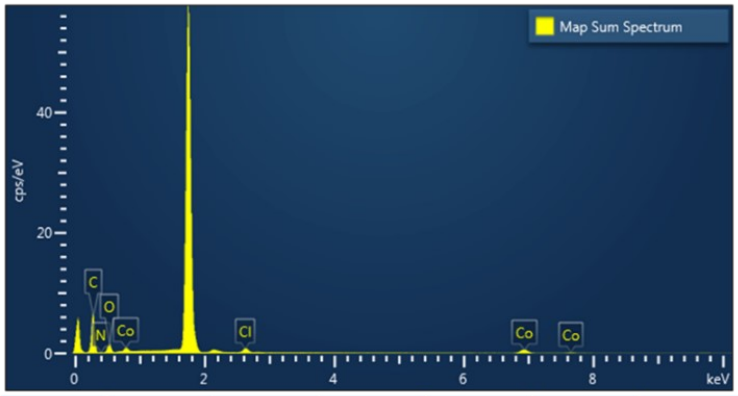


Fig. S12. PXRD pattern for Co-TAPA-OPE.

EDX analysis for Co-TAPA-OPE:



Element	Line Type	Apparent Concentration	k Ratio	Wt%	Wt% Sigma	Standard Label
C	K series	2.71	0.02713	69.87	0.97	C Vit
N	K series	0.00	0.00000	4.08	3.61	BN
O	K series	0.75	0.00253	22.21	0.95	SiO2
Cl	K series	0.07	0.00065	1.07	0.16	NaCl
Co	K series	0.29	0.00290	2.81	0.47	Co
Total:				100.00		

Fig. S13. EDX analysis for Co-TAPA-OPE.

Co K-edge EXAFS experiment for Co-TAPA-OPE:

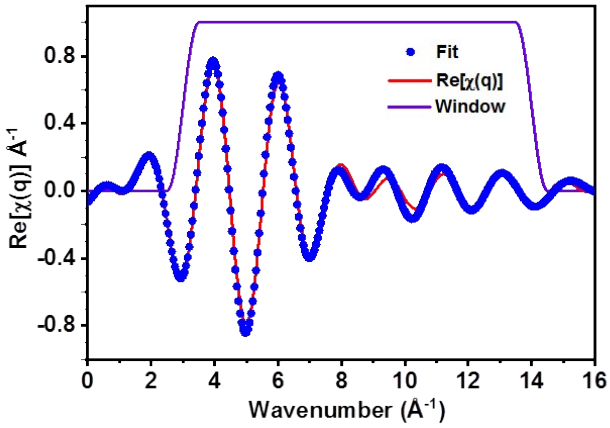


Fig. S14. Co K-edge EXAFS experimental data for Co-TAPA-OPE and corresponding fitting in Fourier transformed back into the wavevector space (q -space).

Table S1. CN, coordination number; R, the distance between absorber and backscatter atoms; σ^2, Debye-Waller factor (a measure of thermal and static disorder in absorber-scatterer distances); R factor is used to value the goodness of the fitting; S_0^2= 1

Sample	Path	CN	R(Å)	$\sigma^2(10^{-3}Å^2)$	R factor
Co-TAPA-OPE COF	Co-N	2.004	1.96	5.9	0.0014
	Co-O	2.006	2.1	7.3	
	Co-Cl	1.98	2.16	10.06	

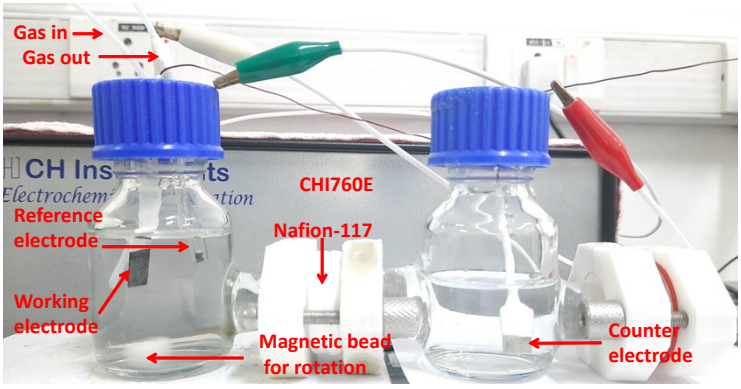


Fig. S15. Photograph of the used H-type cell during electrochemical CO_2RR.

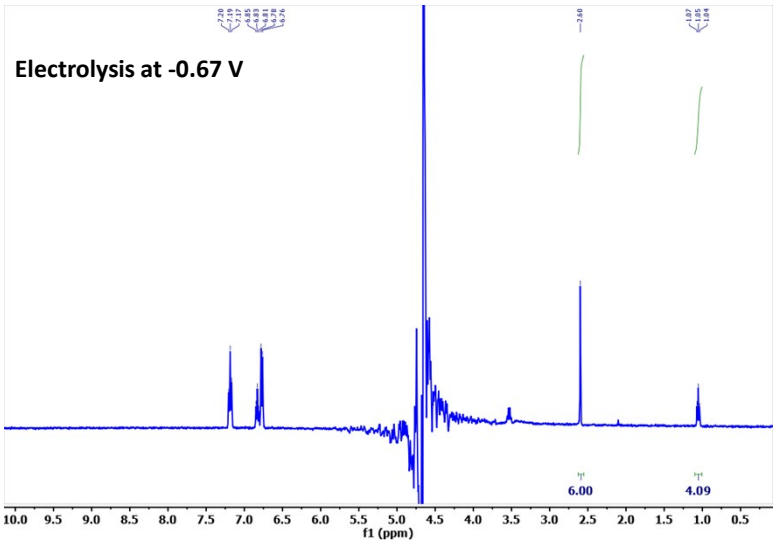


Fig. S16. ^{1}H-NMR spectra of electrolyte solution after controlled potential electrolysis at -0.67 V for 2h with the integration value of ethanol.

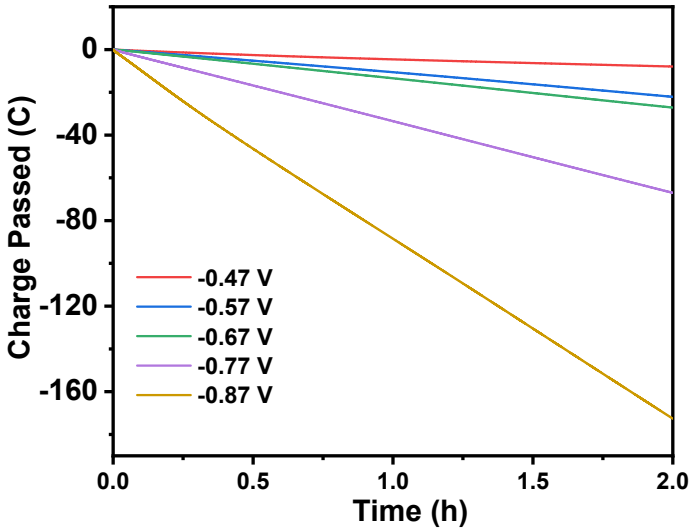


Fig. S17. Total charge passed (Q) during controlled potential electrolysis in CO_2RR which was used for the calculation of FE.

Calculation of Faradaic efficiency for liquid product

The Faradaic efficiency of liquid product was calculated using the following equation[14]:

$$FE = \frac{z.n.F}{Q}$$

Where, z= the number of electron exchanged (here in case of CO_2 reduction to ethanol, z=12)

N= Number of moles of product

F= Faraday's constant (F=96485 C/mol)

Q= Total charge passed (C)

From Fig. S16, the ratio of [DMSO] and [EtOH] was obtained using integration value.

[DMSO]/[EtOH] = [6/6]/[4.09/3] = 0.733

[EtOH] = [DMSO]/0.733 ----------(1)

Now, during NMR sample preparation 600 µL aliquot was taken along with 50 µL D_2O and 50 µL external standard.

So effective strength of DMSO in the NMR tube is 0.286 mM;

From equation 1, we found [EtOH] = 0.39 mM

The amount of EtOH in 0.6 mL = 0.234 µmol

In a total of 40 mL solution, the amount of EtOH = 15.6 µmol

From Fig. S17, we found the total amount of charge passed during 2 h to be 27 C.

$$\text{So, FE\%} = \frac{15.6 \times 10^{-6}\, mol \times 12 \times 96485\, C\, mol^{-1}}{27\, C} \times 100\% = \mathbf{66.8}\ \%$$

Calculation of Faradaic efficiency for gaseous products

Faradaic efficiencies for the formation of gas products were calculated as follows[14]:

$$\text{FE\%} = \frac{n.F.V.\nu.P^{0}}{R.T.i} \times 100\%$$

Where, n is the number of electrons required for products (for CO formation it is 2), V (vol %) is the volume concentration of gas in the gasbag from electrochemical cell, ν (mL min^{-1} at room temperature and ambient pressure) is the gas flow rate, i (mA) is the steady-state cell current, P = 1.01 x 10^5 Pa, T = 273.15 K, F = 96485 C mol^{-1}, and R = 8.314 J mol^{-1} K^{-1}.

Table S2: Product distribution table at different applied potentials.

Potential vs. RHE	FE%(H_2)	FE% (CO)	FE% (HCOOH)	FE% (CH_4)	FE% (C_2H_5OH)	Total FE%
-0.47 V	28.1	13.02	26.2	N.D.	30.8	98.12
-0.57 V	22.02	18.1	8.5	N.D.	47	95.6
-0.67 V	20.1	8.2	N.D.	4.32	66.8	99
-0.77 V	44.8	15.5	N.D.	6.17	31.8	98.1
-0.87 V	52.9	18.7	N.D.	15.2	12.8	99.6

N.D- not detected

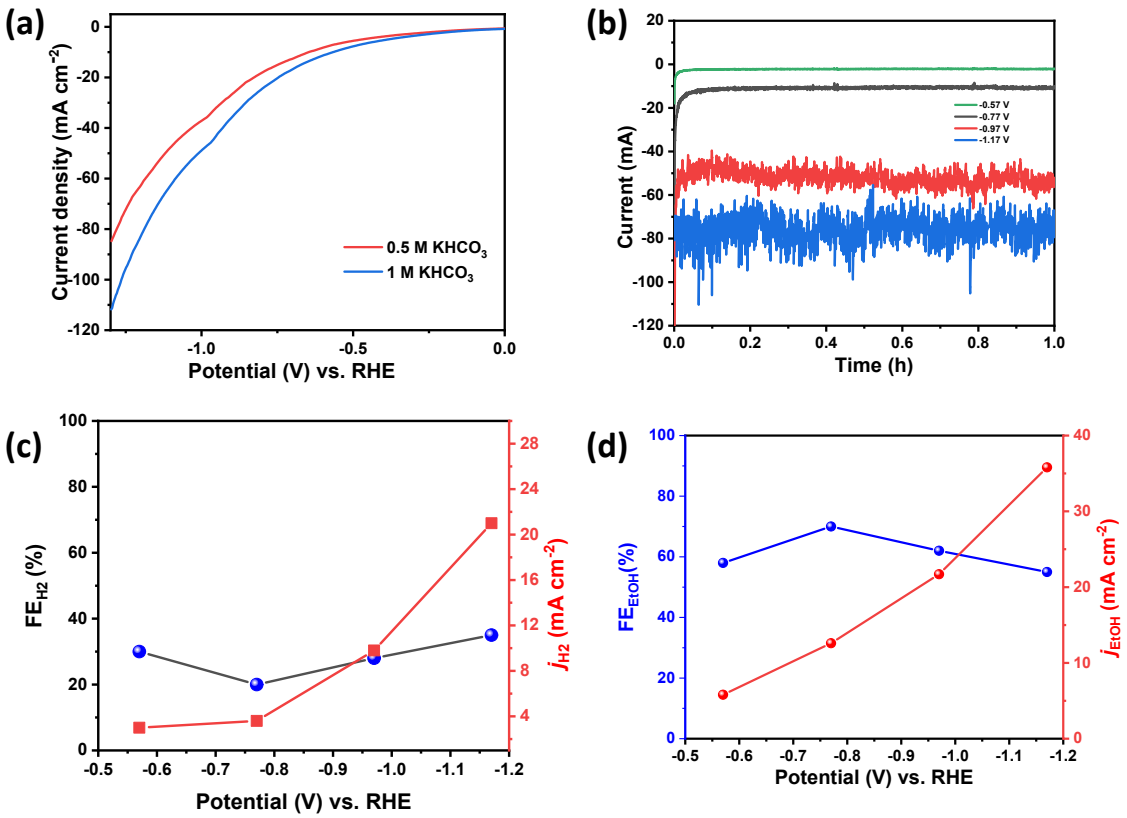


Fig. S18. (a) LSV plot in flow cell under CO_2. (b) i-t plots at different applied potential in 1M $KHCO_3$ solution. (c) FE% and partial current density of ethanol. (d) FE% and partial current density of H_2.

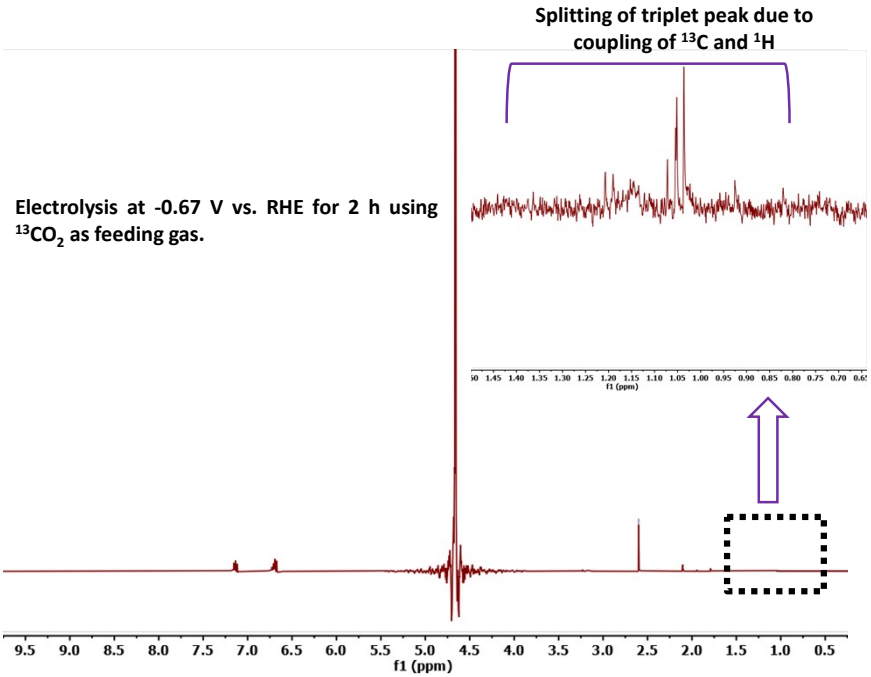


Fig. S19. ^{1}H-NMR spectra of the electrolytes containing $^{13}CH_3{}^{13}CH_2OH$ while using $^{13}CO_2$ as feeding gas at -0.67 V vs. RHE.

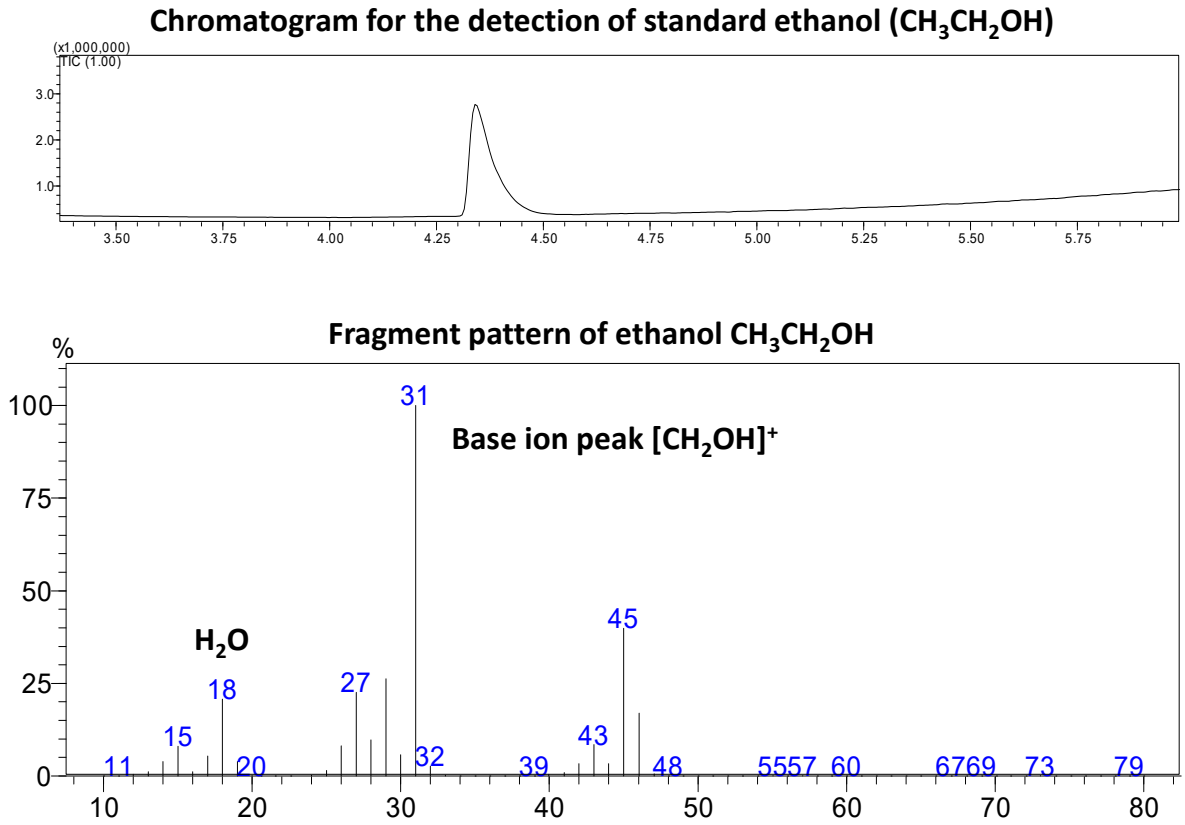


Fig. S20a. GC-MS chromatogram and corresponding mass spectrum of standard ethanol sample using Stabilwax®-DA column **(**30 m; 0.18 mm ID; 0.18µm**).**

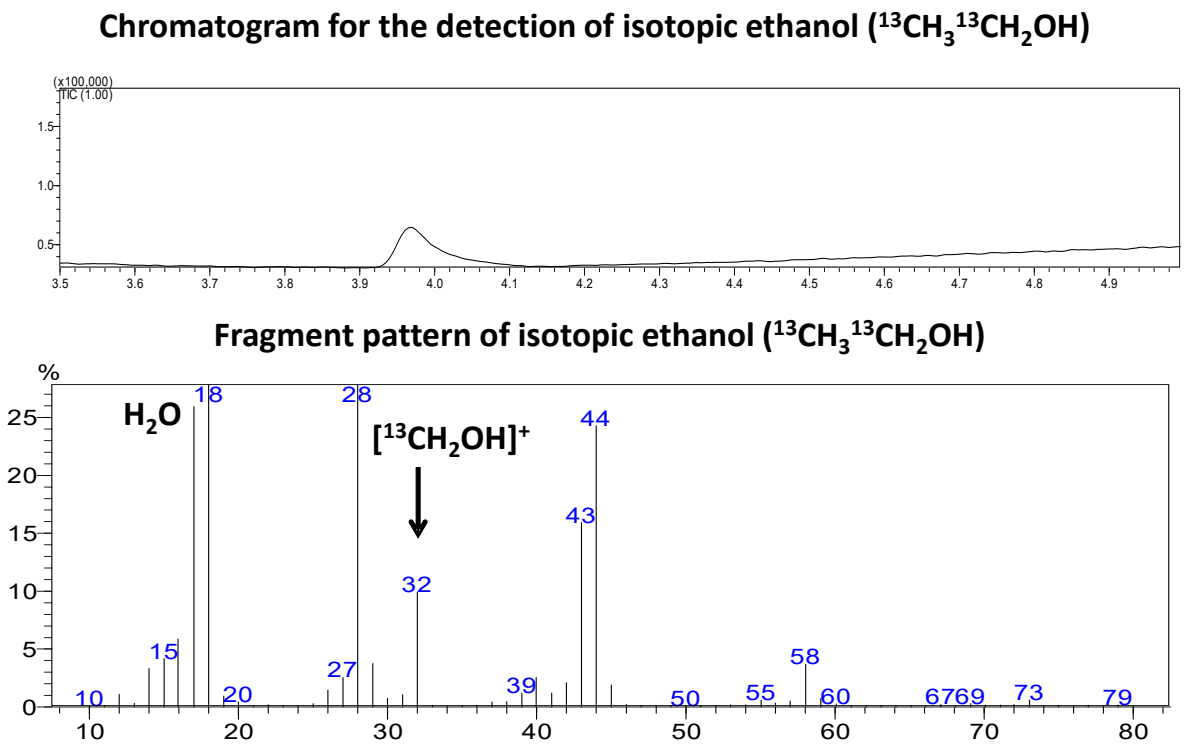


Fig. S20b. GC-MS chromatogram and corresponding mass spectrum of the sample using $^{13}CO_2$ as feeding gas during controlled potential electrolysis at -0.67 V vs. RHE. The electrolyte solution was directly injected to GC-MS and acquired spectra using Stabilwax®-DA column **(**30 m; 0.18 mm ID; 0.18µm**).**

Electrochemical double layer capacitance determination:

Electrochemical double layer capacitance (EDLC) measurement was performed on Co-TAPA-OPE electrode before and after electrolysis. Cyclic voltammetry (CV) curves were then taken between 0 and 0.2 V vs. Ag/AgCl (1 M KCl) at various scan rate (mV/s) while keeping the solution still. Then, currents were extracted at 0.1 V vs. Ag/AgCl (1 M KCl) as a function of the scan rate, leading to a slope for each sample before and after electrolysis. The slope of the plot equals the capacitance of measured samples.

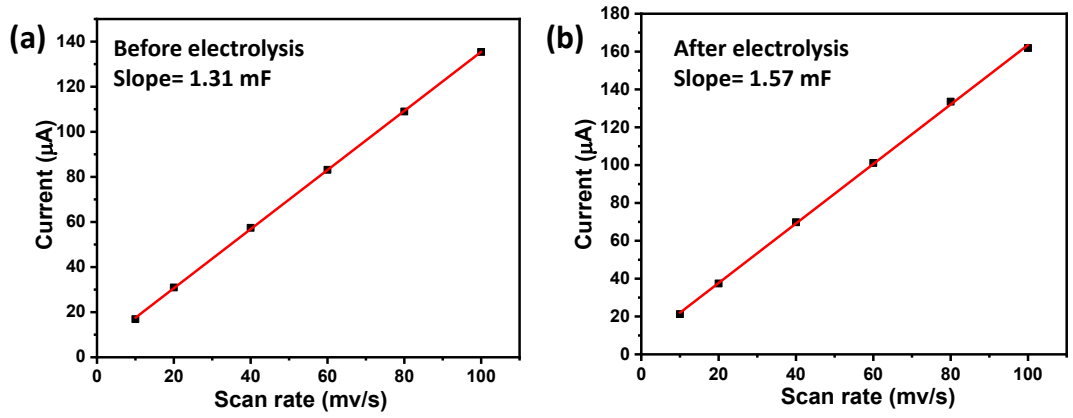


Fig. S21. Electrochemical double-layer capacitance with the CV curves acquired at different scanning rates from 10, 20 40, 60, 80, 100, mV s^{-1}. Current densities ($j = j_{anode} - j_{cathode}$) as a function of scanning rates of with the corresponding slope being twice that of the C_{dl} values (a) before and (b) after electrolysis.

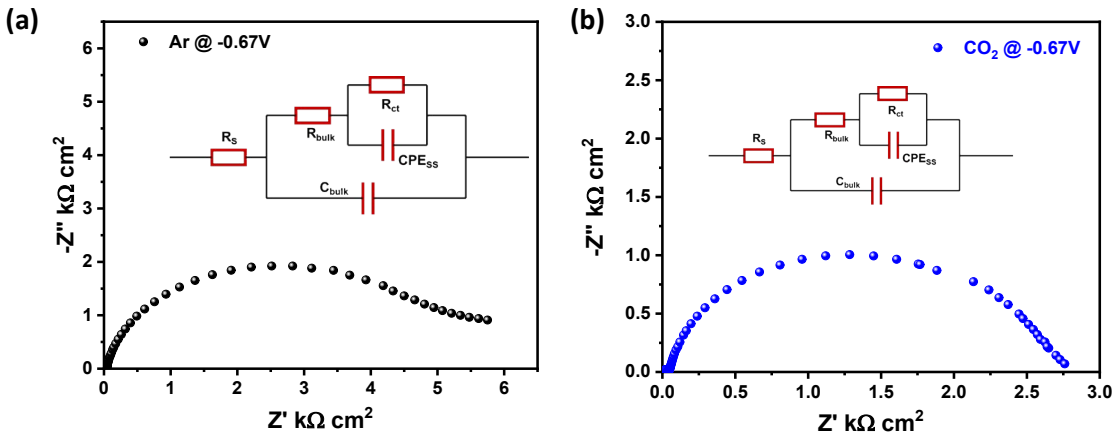


Fig. S22. Impedance spectra showing charge transfer resistance (R_{ct}) in (a) Ar and, (b) CO_2 at -0.67 V.

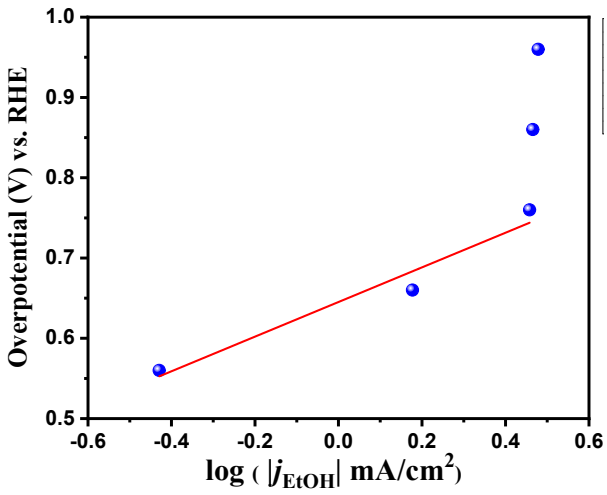


Fig. S23. Tafel plots of polarization overpotential (η) versus ethanol partial current density.

FE-SEM image of Co-TAPA-OPE after CO_2RR measurement:

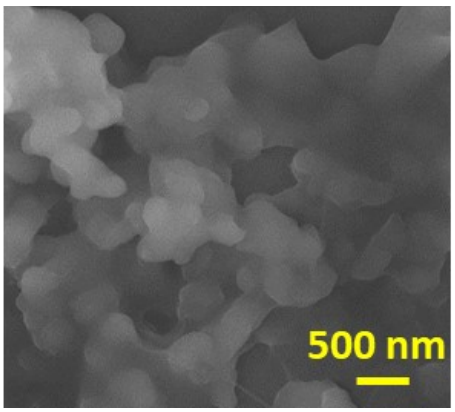


Fig. S24a. FE-SEM image for Co-TAPA-OPE after CO_2RR measurement. The sample for SEM was collected by scratching the carbon paper after electrolysis.

Elemental mapping of Co-TAPA-OPE after CO_2RR:

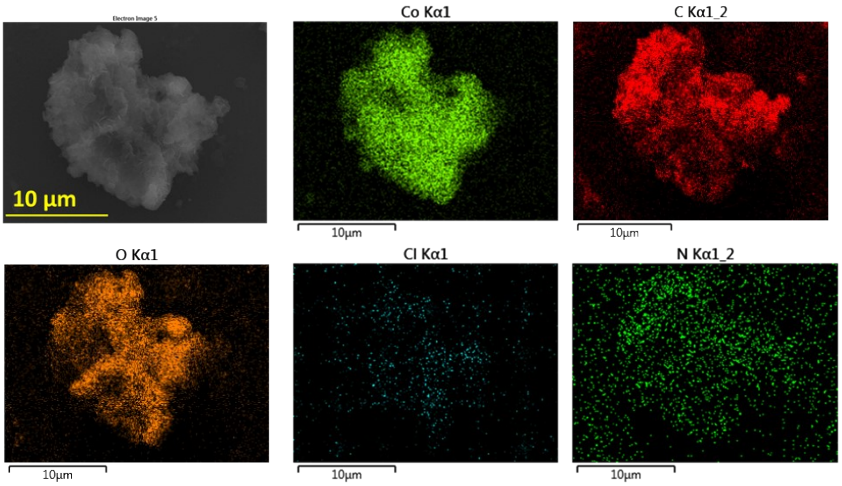
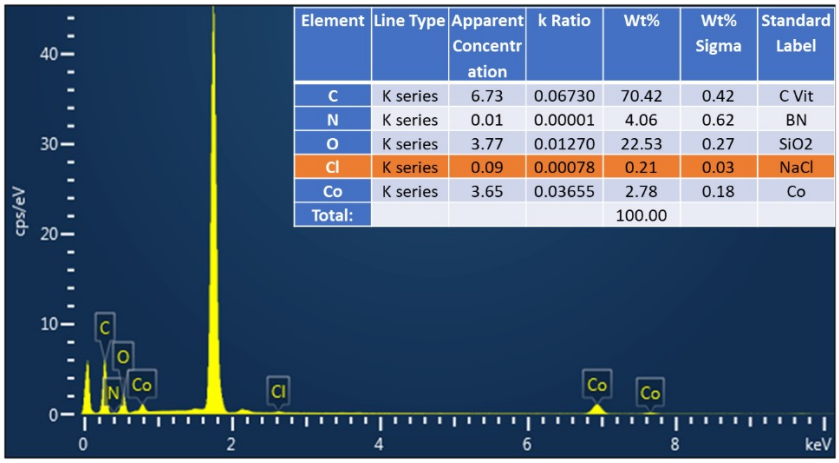


Fig. S24b. Elemental mapping for Co-TAPA-OPE after CO_2RR.

EDAX analysis for Co-TAPA-OPE after electrocatalytic CO_2RR:



Element	Line Type	Apparent Concentration	k Ratio	Wt%	Wt% Sigma	Standard Label
C	K series	6.73	0.06730	70.42	0.42	C Vit
N	K series	0.01	0.00001	4.06	0.62	BN
O	K series	3.77	0.01270	22.53	0.27	SiO2
Cl	K series	0.09	0.00078	0.21	0.03	NaCl
Co	K series	3.65	0.03655	2.78	0.18	Co
Total:				100.00		

Fig. S24c. EDAX analysis for Co-TAPA-OPE after CO_2RR.

Table S3. Comparison of electrochemical CO_2 reduction to ethanol performance with state-of-art single atom-based catalysts in H-type cell in aqueous medium.

Sl. No.	Catalysts	Potential (V) vs. RHE	Partial Current density (mA cm^{-2})	FE (%) for Ethanol	Electrolyte	Ref.
1.	Cu/C-0.4 (Cu single atom)	-0.7 V	1.23	91	0.1 M $KHCO_3$	*Nat. Energy* 2020, **5**, 623.
2.	Cu-N-C	-1.2 V	16*	55	0.1 M $CsHCO_3$	*Angew. Chem., Int. Ed.* 2019, **58**, 15098
3.	Co-Corrole	-0.8 V	-2.5	48	0.1 M $NaClO_4$	*Nat. Commun., 2019,* **10**, *3864*
4.	Co-TAPA-OPE COF (Co single atom)	-0.67 V	2.9	66.8	0.2 M $KHCO_3$	**This work**

* Total current density

Table S4. Comparison of electrochemical CO_2 reduction performance with COF-based catalysts in H-type cell.

Sl. No.	Catalysts	Potential (V) vs. RHE	Main product	FE (%)	Electrolyte	Ref.
1.	COF-366-Co	-1.05 V	CO	91	0.5 M $KHCO_3$	*Science* 2015, **349**, 1208.
2.	COF-366-F-Co	-0.67 V	CO	87	0.5 M $KHCO_3$	*J. Am. Chem. Soc.* 2018, **140**, 1116
3.	TT-Por (Co)-COF	-0.9 V	CO	93.2	0.5 M $KHCO_3$	*ACS Energy Lett.* 2021, **6**, 3496

4.	TTF-Por (Co)-COF	-0.7 V	CO	95	0.5 M $KHCO_3$	*ACS Energy Lett.* 2020, **5**, 1005
5.	Co-TTCOF	-0.7 V	CO	91.3	0.5 M $KHCO_3$	*Nat. Commun.* 2020, **11**, 497.
6.	CoPc-PDQ-COF	-0.66 V	CO	96	0.5 M $KHCO_3$	*Angew. Chem. Int. Ed.* 2020, **59**, 16587.
7.	CoPc-PI-COF-1	-0.8 V	CO	97	0.5 M $KHCO_3$	*J. Am. Chem. Soc 2021,* **143**, 7104
8.	Cu-Tph-COF-Dct	-0.9 V	CH_4	80	1 M KOH	*Angew. Chem. Int. Ed.* 2022, **61**, e202114648
9.	FN-CTF-400	-0.9 V	CH_4	99.3	0.1 M $KHCO_3$	*Angew. Chem. Int. Ed.* 2018, **57**, 13120
10.	**Co-TAPA-OPE COF**	**-0.67 V**	**Ethanol**	**66.8**	**0.2 M $KHCO_3$**	**This work**

Electrocatalytic CO_2RR using TAPA-OPE COF:

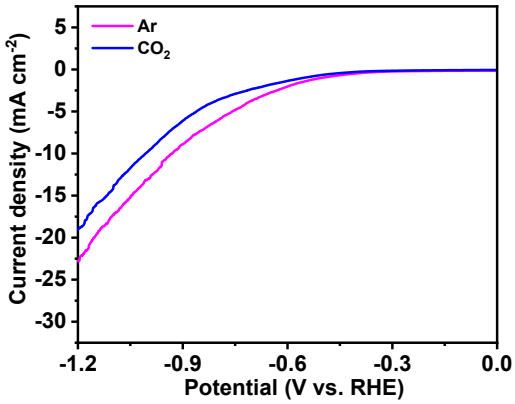


Fig. S25. LSV plot showing the current density in Ar and CO_2 atmosphere using TAPA-OPE COF.

Chronoamperometric curve for TAPA-OPE COF:

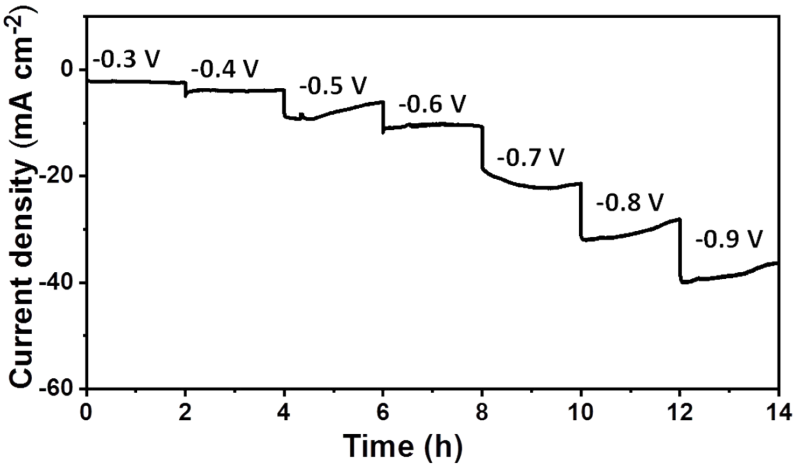


Fig. S26. Typical chronoamperometric curve of TAPA-OPE COF under bias from -0.3 V to -0.9 V in CO_2 saturated 0.2 M $KHCO_3$ solution.

^{1}H-NMR spectra for TAPA-OPE COF:

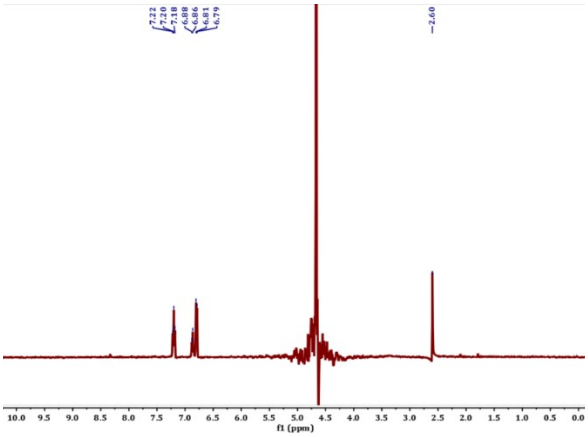


Fig. S27. ^{1}H-NMR spectra of the solution after performing chronoamperometric measurement with TAPA-OPE COF using bias from -0.3 V to -0.9 V through solvent presaturation method.

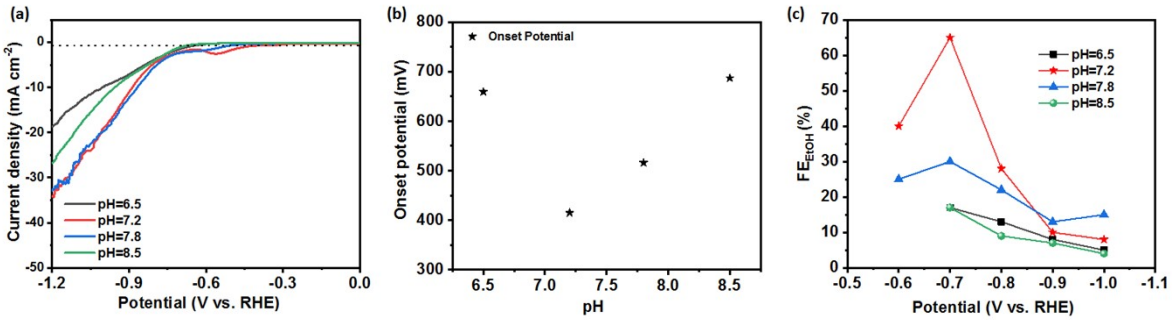


Fig. S28. (a) LSV plot at different pH in CO_2 (b) Onset potential at 1 mA cm^2 (c) FE_{EtOH} calculated over potential range from -0.6 to -1 V at different pH.

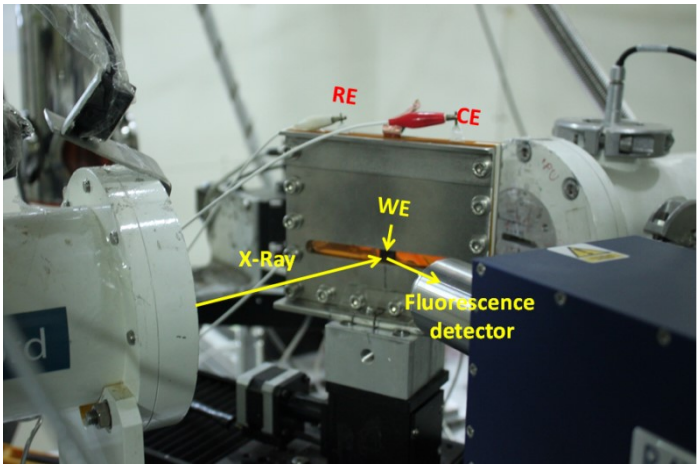


Fig. S29. Photograph of real time *in-situ* XAS set-up for electrochemical CO_2RR. (b) EXAFS fitting in k space (c) After catalysis Co K-edge EXAFS experimental data for Co TAPA-OPE COF and corresponding fitting in Fourier transformed back into the wavevector space (q - space).

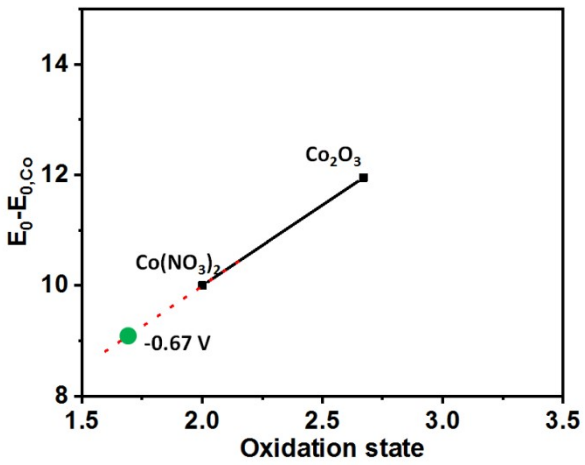


Fig. S30. Oxidation-state analysis by edge position fitting of XANES of Co-TAPA-OPE COF during electrolysis.

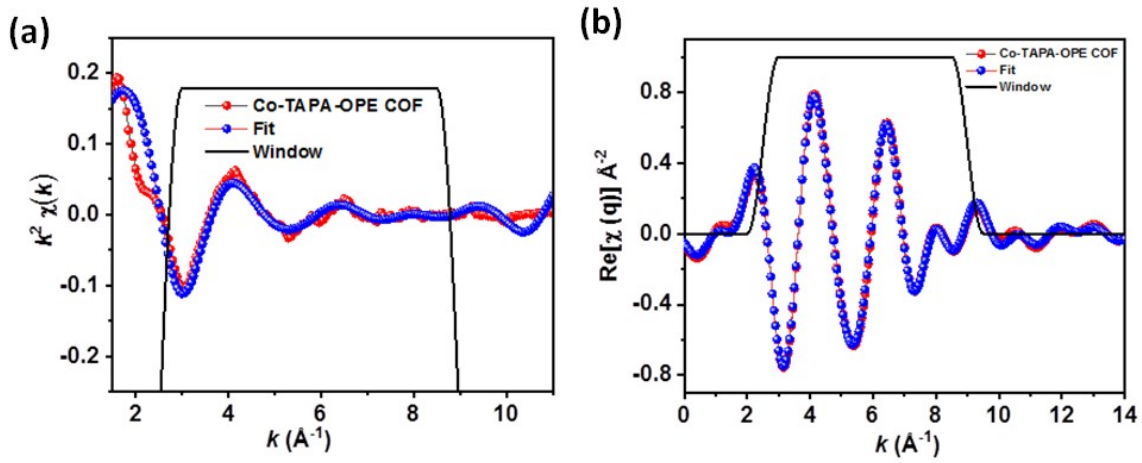


Fig. S31. (a) EXAFS fitting in k space (b) After catalysis Co K-edge EXAFS experimental data for Co-TAPA-OPE COF and corresponding fitting in Fourier transformed back into the wavevector space (q -space).

Table S5. CN, coordination number; R, the distance between absorber and backscatter atoms; σ^2, Debye-Waller factor (a measure of thermal and static disorder in absorber-scatterer distances); R factor is used to value the goodness of the fitting; $S_0^2 = 1$

Sample	Path	CN	R(Å)	$\sigma^2(10^{-3}Å^2)$	R factor
Co-TAPA-OPE COF (After catalysis)	Co-N	2.002	2.07	12.1	0.005
	Co-O	2.02	1.86	8.8	
	Co-Cl	1.98	2.5	13.7	

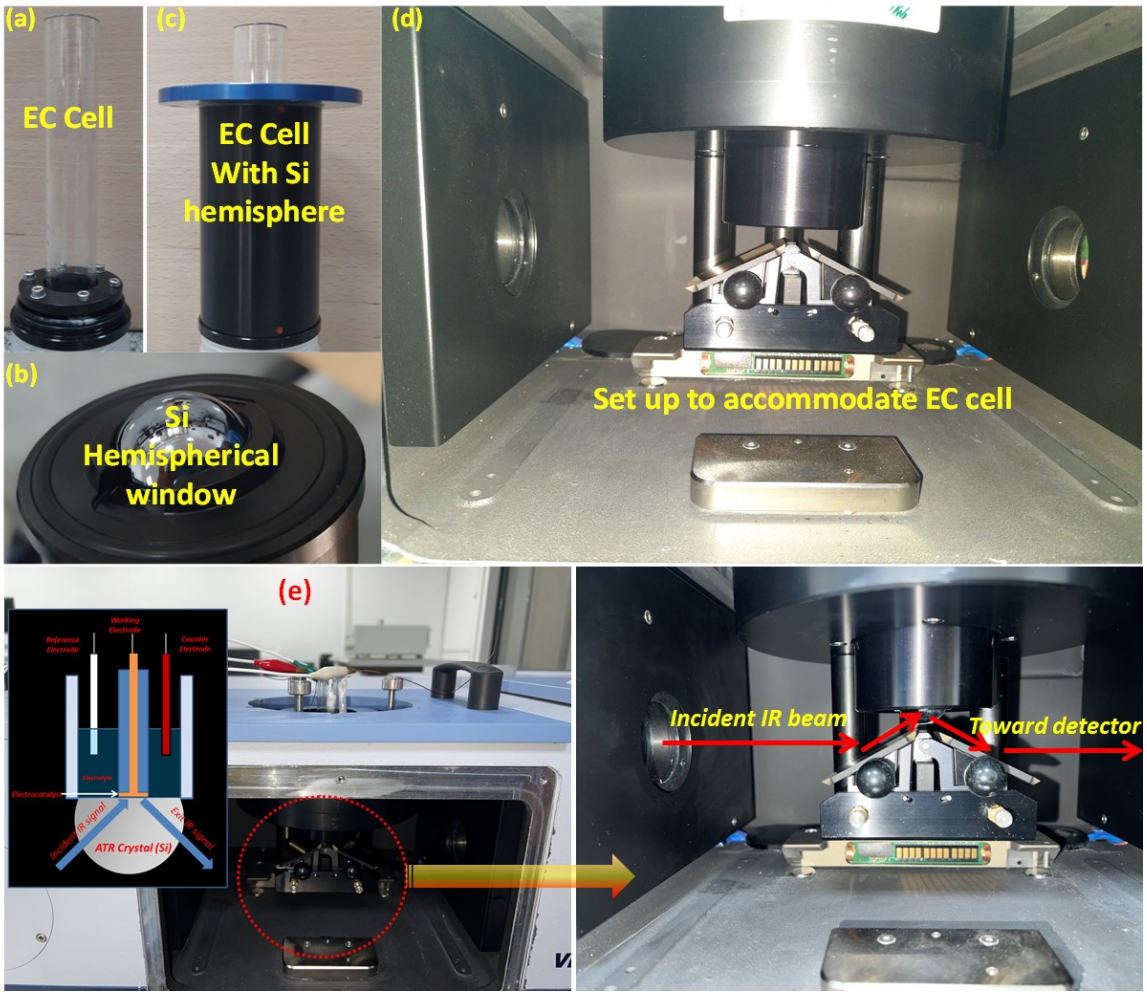


Fig. S32. (a) Electrochemical cell (EC) used for *in-situ* IR measurement (b) Picture of Si-hemisphere used during *in-situ* measurement (c) Photograph of EC cell connected with Si hemisphere (d) Attachments used during *in-situ* measurement. (e) Photograph of the overall set up including the schematic of the measurement process.

<u>Computational details for mechanistic study:</u>

The electrocatalytic mechanisms were investigated based on Nørskov's computational hydrogen electrode (CHE) model. This model offers an effective method for examining proton-electron transport in electrocatalysis without explicitly treating solvated protons and is commonly used in theoretical studies of electrocatalysis. In CHE model, the energy of an [e^- + H^+] pair is considered to be equal to half of the gaseous hydrogen (1/2 H_2) at an equilibrium potential. Thus, the total Gibbs free energy of a proton-electron pair is calculated as:

$$G(e^- + H^+) = 1/2\ G(H_2) - neU$$

where n is the number of electrons involved in the reaction (n = 1), e is the electronic charge, and U is the external potential. For CO_2RR, the corrections of zero-point energy (E_{ZPE}), heat capacity (C_p), temperature (T) and entropy (S) are introduced into the DFT-calculated total energy (E_{total}) to determine the Gibbs free energy (G) of each intermediate species at 298.15 K:

$$G = E_{total} + E_{ZPE} + \int C_p dT - TS$$

The Gibbs free energies (G) for all the intermediate species were calculated by using E_{total} along with the aforementioned corrections and listed in Table S34. Hence, the Gibbs free reaction energy for each elementary step at 298.15 K should be:

$$\Delta G = \Delta E_{total} + \Delta E_{ZPE} + \int C_p dT - T\Delta S$$

where ΔE_{total} is the difference of total electronic energy derived from DFT, ΔE_{ZPE} is the difference of zero-point energy correction (ZPE), $\int C_p dT$ is the enthalpy correction and $T\Delta S$ is the entropy change, as shown in Table S34. The Gibbs free energy change (ΔG) for each elementary step was calculated as:

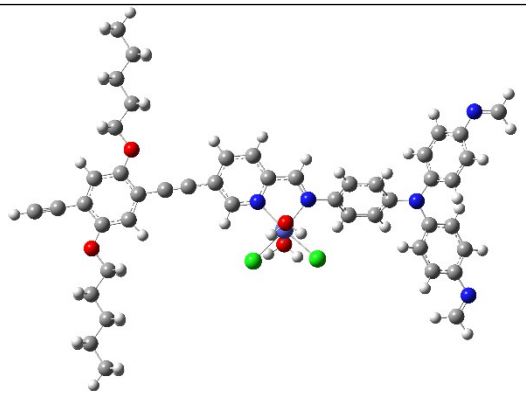
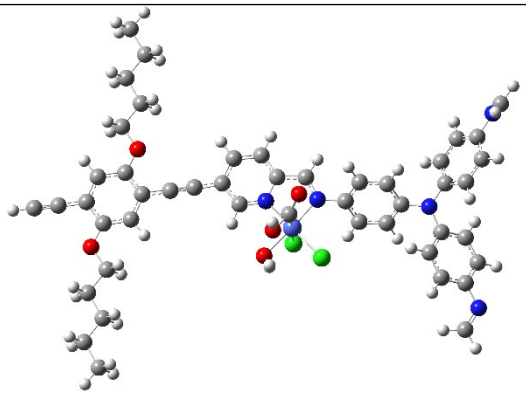
$$\Delta G = \sum G(\text{Product}) - \sum G(\text{Reactant})$$

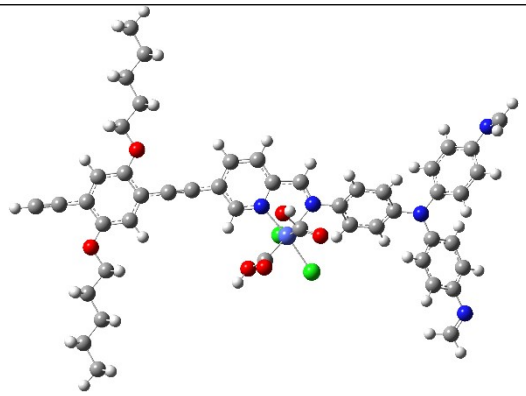
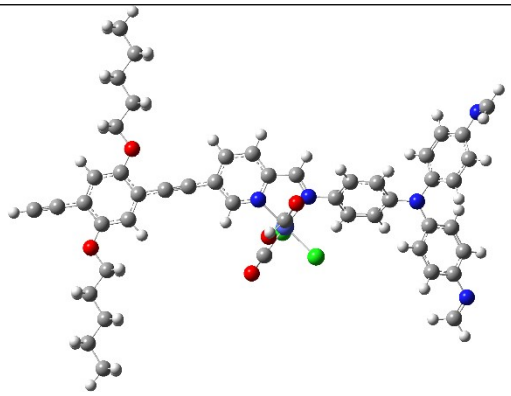
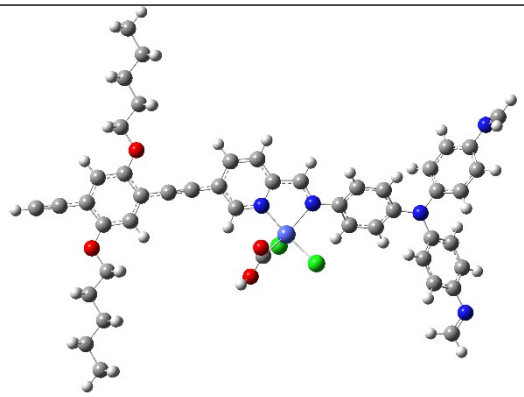
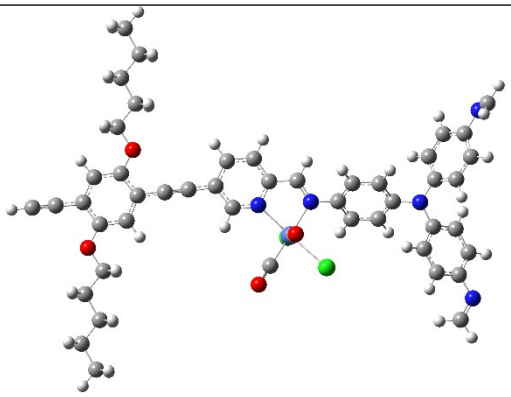
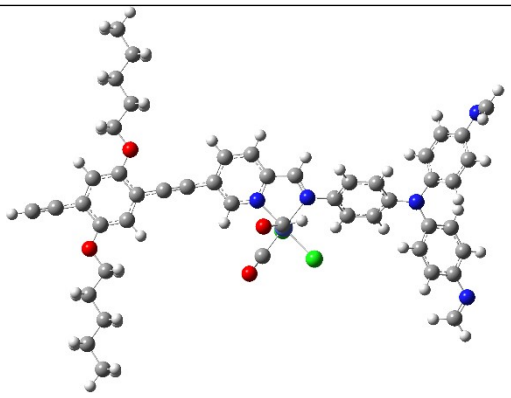
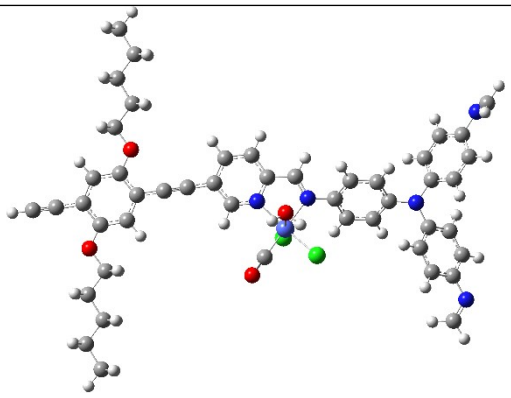
For the elementary steps involving proton-coupled reduction:

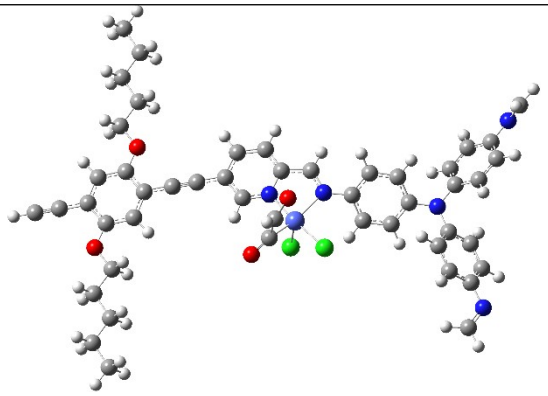
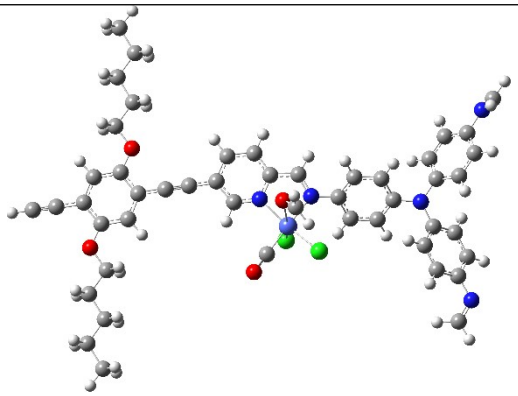
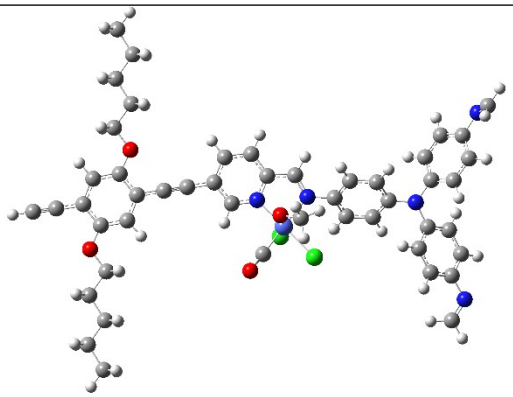
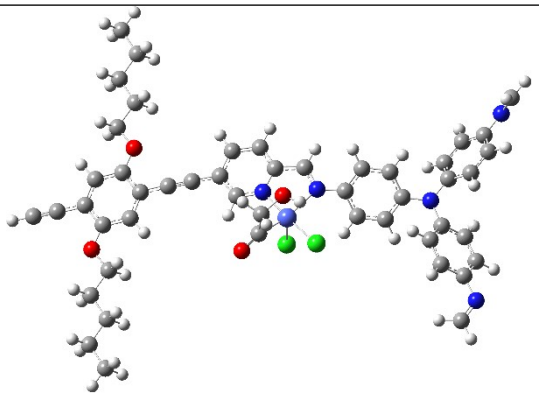
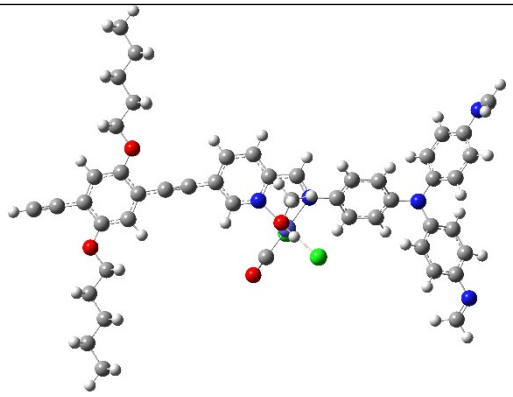
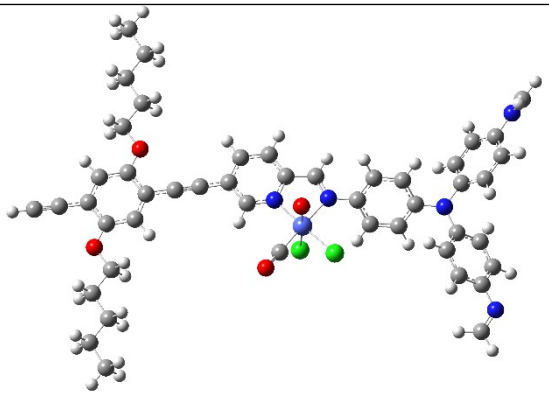
$$\Delta G\,(U) = \sum G\,(U = 0) + neU$$

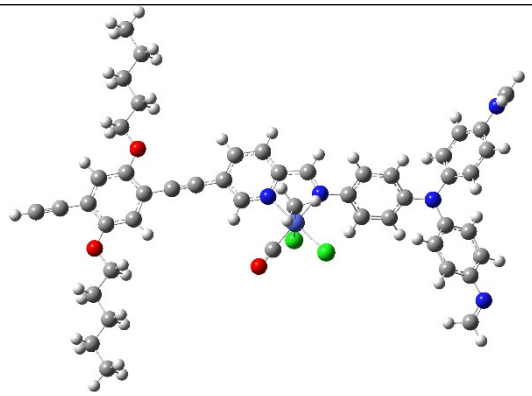
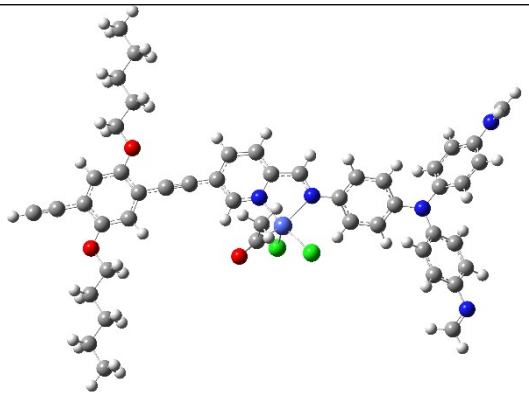
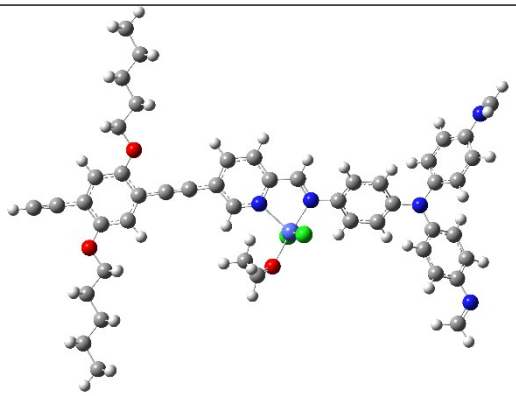
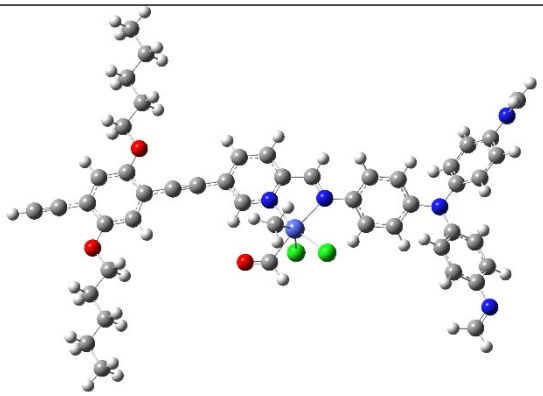
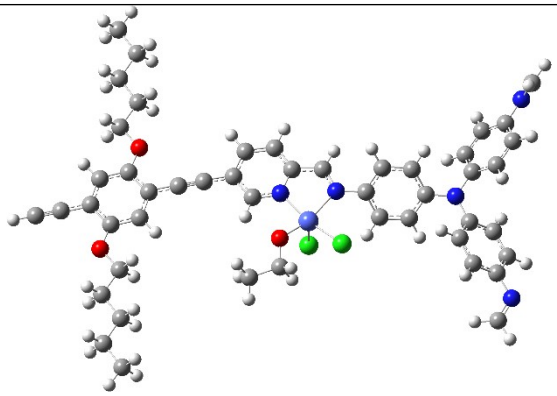
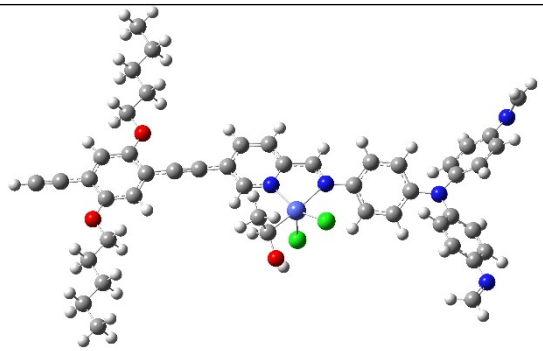
where n is the number of electrons involved in the reaction, e is the electronic charge and U is the applied external potential.

In Fig. S29, all the possible pathways for CO_2 electroreduction to ethanol on Co^{2+} metalated covalent organic framework based single atom catalyst were summarized.

	
(1) [Co^{II}(η^2-COF-N,N′)(H_2O)$_2Cl_2$] **(H_2O*OH_2)**	**(2)** [Co^{II}(η^2-COF-N,N′)(COOH)(H_2O)Cl_2] **(H_2O*COOH)**

 **(3)** [$Co^{II}(\eta^2$-COF-N,N′)$(COOH)_2Cl_2$] **(HOOC*COOH)**	 **(4)** [$Co^{II}(\eta^2$-COF-N,N′)(COOH)(CO)Cl_2] **(OC*COOH)**
 **(4a)** [$Co^{II}(\eta^2$-COF-N,N′)(COOH)Cl_2] **(*COOH)**	 **(5)** [$Co^{II}(\eta^2$-COF-N,N′)$(CO)_2Cl_2$] **(OC*CO)**
 **(6)** [$Co^{II}(\eta^2$-COF-N,N′)(CHO)(CO)Cl_2] **(OC*CHO)**	 **(6a)** [$Co^{II}(\eta^2$-COF-N,N′)(H_2O)(CO)Cl_2] **(OC*OH_2)**

	
(6b) [$Co^{II}(\eta^2$-COF-N,N′)(COCHO)Cl_2] **(*COCHO)**	**(7)** [$Co^{II}(\eta^2$-COF-N,N′)(OCH_2)(CO)Cl_2] **(OC*OCH_2)**
	
(8) [$Co^{II}(\eta^2$-COF-N,N′)(OCH_3)(CO)Cl_2] **(OC*OCH_3)**	**(8a)** [$Co^{II}(\eta^2$-COF-N,N′)($COCH_2OH$)Cl_2] **(*$COCH_2OH$)**
	
(9) [$Co^{II}(\eta^2$-COF-N,N′)($HOCH_3$)(CO)Cl_2] **(OC*$HOCH_3$)**	**(9a)** [$Co^{II}(\eta^2$-COF-N,N′)(O)(CO)Cl_2] **(OC*O)**

 **(10)** [$Co^{II}(\eta^2$-COF-N,N′)$(CH_3)(CO)Cl_2$] **(OC*CH_3)**	 **(10a)** [$Co^{II}(\eta^2$-COF-N,N′)$(COCH_3)Cl_2$] **(*$COCH_3$)**
 **(11)** [$Co^{II}(\eta^2$-COF-N,N′)$(OCHCH_3)Cl_2$] **(*$OCHCH_3$)**	 **(11a)** [$Co^{II}(\eta^2$-COF-N,N′)$(CH_3)(CHO)Cl_2$] **(OHC*CH_3)**
 **(12)** [$Co^{II}(\eta^2$-COF-N,N′)$(OCH_2CH_3)Cl_2$] **(*OCH_2CH_3)**	 **(12a)** [$Co^{II}(\eta^2$-COF-N,N′)$(CH(OH)CH_3)Cl_2$] **(*$CH(OH)CH_3$)**

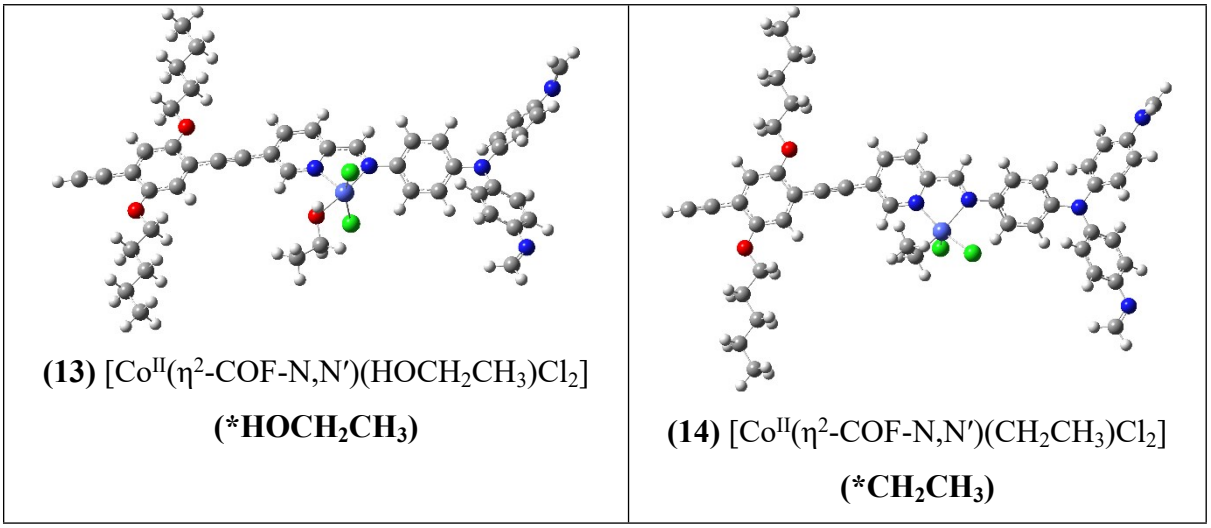


Fig. S33. Optimized geometries of all possible intermediates.

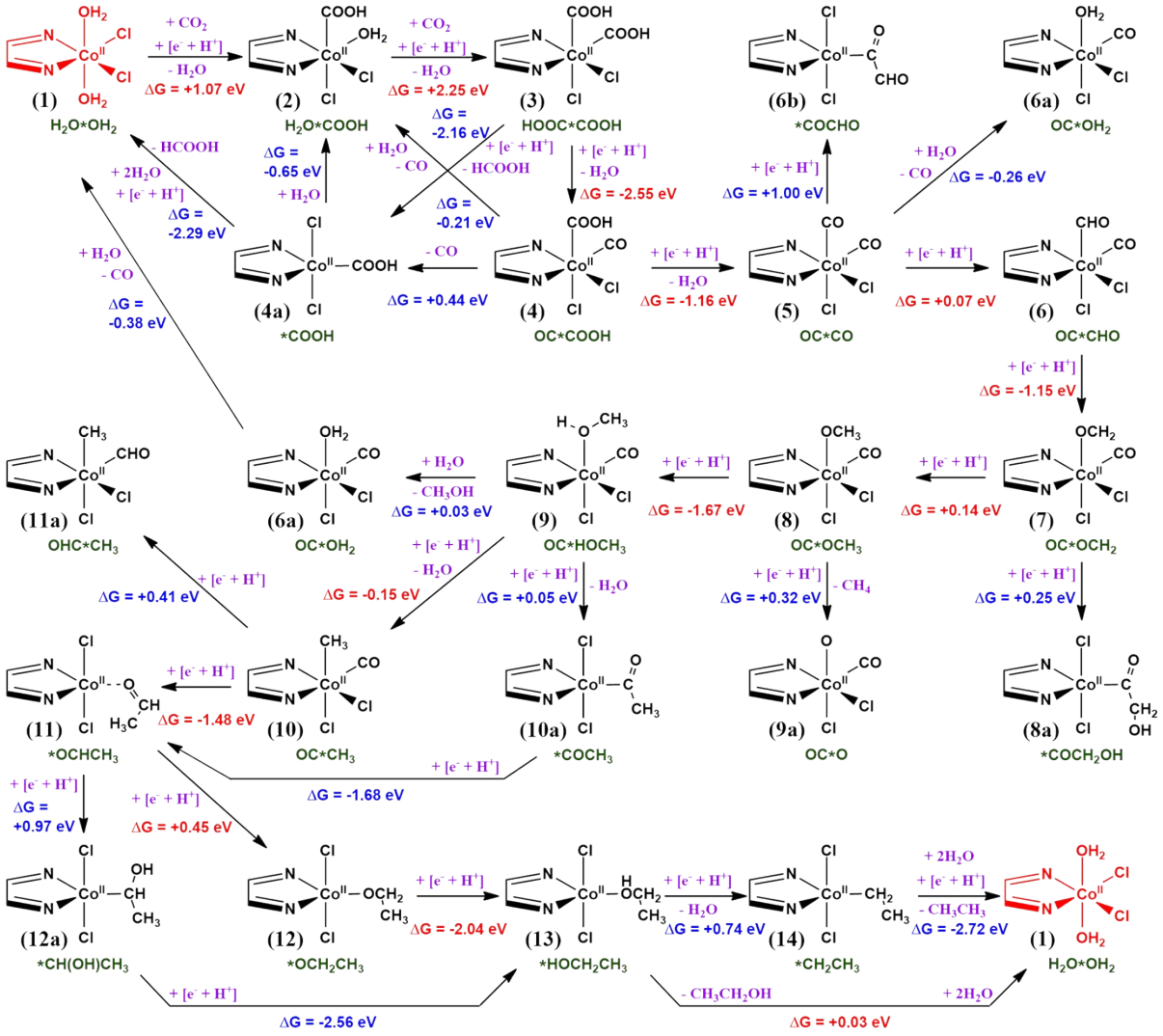


Fig. S34. Complete mechanism for electrocatalytic reduction of CO_2 to CH_3CH_2OH with respective relative Gibbs free energy values computed by DFT, at an applied potential of -0.67 V vs. RHE.

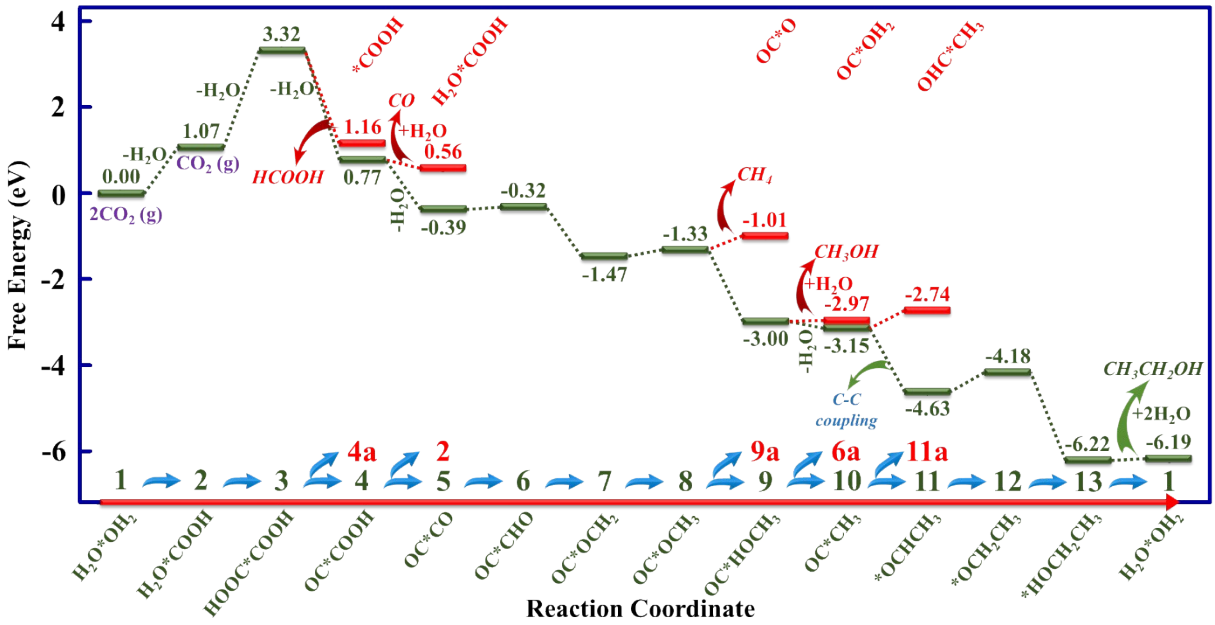


Fig. S35. Relative Gibbs free energy (ΔG) diagram computed by DFT, at an applied potential of -0.67 V vs. RHE for CO_2 to CH_3CH_2OH reduction process occurring on Co-TAPA-OPE COF. Asterisk (*) denotes Co-catalytic center adsorbed with intermediate species. The CH_3CH_2OH synthesis main pathway is drawn in green, whereas the other side products formation pathways are shown in red.

Cartesian coordinates of the computed structures

Coordinates are given in standard XYZ format

DFT-optimized geometry of **(1) $[Co^{II}(\eta^2\text{-COF-N,N'})(H_2O)_2Cl_2]$** (doublet) **$(H_2O^*OH_2)$**, computed at the UB3LYP-D3/ LANL2DZ (Co)/ 6-31+G* (HCNOCl) level in absence of any solvent.

Atom	x	y	z
C	-5.41513200	0.85701600	-0.07343500
C	-4.20941100	1.02914200	-0.07378200
C	-2.80937100	1.22777200	-0.07072900

C	-2.23449900	2.51390800	-0.11109400
C	-1.93880300	0.11308600	-0.01893000
C	-0.85069400	2.63497100	-0.10779100
H	-2.87476600	3.38968400	-0.14472000
N	-0.61384800	0.23564600	-0.01468700
H	-2.31867800	-0.90080300	0.03537400
C	-0.06324700	1.47973800	-0.06374000
H	-0.37454200	3.61047200	-0.14023800
C	1.38238900	1.49487900	-0.10165300
N	2.01121600	0.36378600	-0.10667100
H	1.91429900	2.44531400	-0.16539200
C	3.42646500	0.36925800	-0.12309700
C	4.15882700	1.16229900	0.77228400
C	4.10605900	-0.44355300	-1.04151000
C	5.55019300	1.13552500	0.75943800
H	3.63565100	1.74621700	1.52506600
C	5.49222200	-0.43851800	-1.08311800
H	3.53471000	-1.05634000	-1.72752300
C	6.23663200	0.33433600	-0.17040700
H	6.11026600	1.71744500	1.48424800
H	6.01240100	-1.05616100	-1.80782400
N	7.64818900	0.27810200	-0.17400300
C	8.41261800	1.43524700	0.12903600
C	8.30757000	-0.96364600	-0.38752900
C	8.07697100	2.67926500	-0.43294700
C	9.50754400	1.35977200	1.00544800
C	7.81614200	-2.14409800	0.19402600
C	9.47614500	-1.02243100	-1.16552100
C	8.81079000	3.81769000	-0.11630400
H	7.22855900	2.74674800	-1.10732400
C	10.26425200	2.49326100	1.29125900
H	9.75767800	0.40813200	1.46471500
C	8.45910300	-3.35933700	-0.02579000
H	6.92722000	-2.10689800	0.81659700
C	10.13857200	-2.23170000	-1.35127200
H	9.86770300	-0.11227500	-1.60981900
C	9.93383000	3.73815500	0.72463700
H	8.54260800	4.78191200	-0.53827000
H	11.08866500	2.42213700	1.99573600
C	9.62388300	-3.42298700	-0.81254500
H	8.07876600	-4.25759900	0.45285200
H	11.05037500	-2.27627300	-1.93970400
Co	0.77199400	-1.21015800	0.17465900
Cl	-0.84285700	-2.83905600	0.57347500
Cl	2.49513900	-2.72133000	0.50664600
O	0.76533600	-1.96902000	-2.02498600
O	0.84844100	-0.85450000	2.46818600
H	1.45804000	-2.62021900	-1.79902900
H	-0.06094300	-2.47757000	-1.93054600
H	1.64851500	-1.40610900	2.56158100
H	0.11674900	-1.47723300	2.63743900
C	-6.81262900	0.62921100	-0.06960200
C	-7.71922800	1.71639400	-0.14169800
C	-7.30868800	-0.68879500	0.00786900
C	-9.09022700	1.45921300	-0.13502700
O	-7.16520800	2.95671800	-0.21342600
C	-8.67891200	-0.94420800	0.01505100
H	-6.59027400	-1.49700600	0.06306600
C	-9.58550600	0.14413500	-0.05770500
H	-9.80893500	2.26723100	-0.18910200

C	-8.02084500	4.10098200	-0.28575500
O	-9.23194900	-2.18237300	0.08815200
C	-10.99164900	-0.08414800	-0.05271000
H	-8.65924700	4.03039900	-1.17889000
H	-8.67093500	4.13413300	0.60108100
C	-7.13389200	5.33552200	-0.35182100
C	-8.37430700	-3.32630500	0.16724700
C	-12.19149000	-0.25650500	-0.04981700
H	-6.47448800	5.24823300	-1.22551600
H	-6.48703300	5.35138900	0.53536700
C	-7.94952500	6.63232100	-0.43355900
H	-7.72381100	-3.36252500	-0.71923900
H	-7.73621000	-3.24901800	1.06000900
C	-9.25798200	-4.56238600	0.23988500
H	-13.24590400	-0.42139900	-0.04623100
H	-8.61624800	6.70470200	0.43900500
H	-8.60312400	6.60219800	-1.31844700
C	-7.07033500	7.88846100	-0.50022600
H	-9.91733900	-4.47269300	1.11309800
H	-9.90600000	-4.58432800	-0.64607700
C	-8.43613400	-5.85507200	0.32728900
H	-6.40427700	7.81658100	-1.37225600
H	-6.41744200	7.91897300	0.38409500
C	-7.88641900	9.18379000	-0.58186100
H	-7.78086000	-5.81769100	1.21059400
H	-7.77015600	-5.92951500	-0.54567200
C	-9.31003400	-7.11441200	0.40207700
H	-8.53842800	9.29527200	0.29411700
H	-7.23563300	10.06501200	-0.62846000
H	-8.52532300	9.19206300	-1.47439900
H	-9.97492700	-7.04072900	1.27480900
H	-9.96472300	-7.15217600	-0.48062700
C	-8.48796000	-8.40566400	0.48892800
H	-7.84688000	-8.40628200	1.37989600
H	-9.13486800	-9.28953700	0.54154300
H	-7.83691400	-8.51883100	-0.38754200
N	10.63918400	4.92935900	0.99803200
N	10.33873500	-4.61692400	-1.04772000
C	9.71188300	-5.70951200	-1.24352800
H	10.28542400	-6.62643900	-1.38179300
H	8.61647700	-5.78608900	-1.29444100
C	11.90875600	4.91147800	1.11071300
H	12.42701300	5.83680900	1.36352200
H	12.52429300	4.01385500	0.95523800

Total electronic Energy (E_{total}) = -3422.662896 (Hartree/Particle).

DFT-optimized geometry of **(2) [$Co^{II}(\eta^2$-COF-N,N′)(COOH)(H_2O)Cl_2]** (singlet) **(H_2O*COOH)**, computed at the B3LYP-D3/ LANL2DZ (Co)/ 6-31+G* (HCNOCl) level in absence of any solvent.

Atom	x	y	z
C	5.42209700	0.77769800	0.07301600
C	4.21758800	0.95762700	0.08428000

C	2.82396000	1.19588900	0.10056500
C	2.29354800	2.49868900	0.21933000
C	1.91324700	0.12072500	-0.00545500
C	0.91646300	2.67924100	0.23515400
H	2.96901800	3.34427200	0.29998500
N	0.60003100	0.31181300	0.00823100
H	2.24763600	-0.90468800	-0.10409100
C	0.08372200	1.56158600	0.12949900
H	0.48178100	3.66932100	0.33193500
C	-1.36058400	1.58589500	0.17980900
N	-1.97889100	0.45269800	0.11877800
H	-1.90240400	2.52098000	0.31178800
C	-3.39094200	0.40165400	0.14623900
C	-4.14295200	1.19875800	-0.72760900
C	-4.03205600	-0.46022600	1.04800200
C	-5.53217300	1.13362900	-0.70428800
H	-3.63326600	1.80220100	-1.47314500
C	-5.41738600	-0.49354800	1.09340100
H	-3.42864200	-1.07179400	1.70923500
C	-6.18844100	0.28737700	0.20850000
H	-6.11366700	1.71608200	-1.41144900
H	-5.91560900	-1.14398500	1.80463100
N	-7.59765600	0.19746700	0.22113500
C	-8.39048300	1.34370900	-0.05235600
C	-8.22866100	-1.05865600	0.43636800
C	-8.08759900	2.57771400	0.54944300
C	-9.50278800	1.25890000	-0.90433200
C	-7.72622300	-2.22327400	-0.16701700
C	-9.37937000	-1.14791300	1.23765600
C	-8.87105900	3.69817700	0.29440700
H	-7.24116500	2.64515300	1.22627900
C	-10.28310400	2.38396700	-1.16338800
H	-9.76071400	0.30391000	-1.35202700
C	-8.33946900	-3.45325700	0.05518400
H	-6.85137500	-2.16133000	-0.80729700
C	-10.01343600	-2.37193500	1.42568500
H	-9.77967400	-0.25003300	1.69884000
C	-9.96506800	3.62558300	-0.58460500
H	-8.65024800	4.64718400	0.77456700
H	-11.15728200	2.29203400	-1.80209200
C	-9.48577100	-3.54753300	0.86561900
H	-7.95131200	-4.33979200	-0.43885600
H	-10.91136900	-2.44013300	2.03285600
Co	-0.78536500	-1.05495400	-0.12633700
C	6.82186600	0.56474200	0.06074000
C	7.71155800	1.66566200	0.14027900
C	7.33868100	-0.74437200	-0.02969900
C	9.08654900	1.43049300	0.12594500
O	7.13822100	2.89558700	0.22609100
C	8.71271800	-0.97749400	-0.04278400
H	6.63366800	-1.56410600	-0.08721400
C	9.60226800	0.12441900	0.03534600
H	9.79229600	2.24951800	0.18461800
C	7.97485500	4.05305300	0.31833400
O	9.28621100	-2.20608000	-0.12630800
C	11.01176500	-0.08171700	0.02340000
H	8.61558300	3.97644500	1.20915400
H	8.62250100	4.11330700	-0.56878700
C	7.06686300	5.27058200	0.40862500
C	8.44888900	-3.36416100	-0.20019500

C	12.21410700	-0.23496300	0.01459500
H	6.41166800	5.15622200	1.28234200
H	6.41746500	5.29119100	-0.47663900
C	7.86009800	6.57971800	0.51164800
H	7.80368400	-3.41155100	0.68977800
H	7.80489800	-3.29886300	-1.09004400
C	9.35377900	-4.58469100	-0.27693400
H	13.27115400	-0.38217000	0.00665500
H	8.52287300	6.67946500	-0.36121900
H	8.51660100	6.54501900	1.39417300
C	6.95916300	7.81877600	0.60336300
H	10.00821800	-4.48291300	-1.15245700
H	10.00523400	-4.59543500	0.60658500
C	8.55497900	-5.89182200	-0.36183900
H	6.29705000	7.71941000	1.47565800
H	6.30332200	7.85384400	-0.27860900
C	7.75271300	9.12648700	0.70647400
H	7.89710200	-5.86640600	-1.24389900
H	7.89291400	-5.97799400	0.51313300
C	9.45074600	-7.13561600	-0.43869000
H	8.40015700	9.26532900	-0.16898000
H	7.08666600	9.99505700	0.77076100
H	8.39381100	9.12980500	1.59744100
H	10.11244200	-7.05004100	-1.31268500
H	10.10761200	-7.16178500	0.44266600
C	8.65156600	-8.44121500	-0.52393200
H	8.00923100	-8.45355200	-1.41402800
H	9.31391900	-9.31340000	-0.57765500
H	8.00447000	-8.56606400	0.35390800
N	-10.72112600	4.80008500	-0.79127400
N	-10.16945000	-4.75877200	1.10544800
C	-9.51398300	-5.83721000	1.28527000
H	-10.06346200	-6.76810900	1.42817900
H	-8.41639300	-5.88774100	1.31856000
C	-11.20372900	5.05919100	-1.94201500
H	-11.81659300	5.95247500	-2.06578200
H	-11.03038100	4.43840700	-2.83278400
Cl	-2.35545700	-2.65555800	-0.52218200
Cl	-0.66389900	-1.38792500	2.22712600
C	-0.77944400	-0.76516000	-2.03644200
O	-1.28781700	0.14623300	-2.65290800
O	-0.04402800	-1.72601300	-2.67789500
H	-0.10030800	-1.54809100	-3.63855000
O	0.57472900	-2.53310100	-0.20946800
H	0.22591400	-3.14627700	-0.88562700
H	0.36559100	-2.92457100	0.66733900

Total electronic Energy (E_{total}) = -3535.376832 (Hartree/Particle).

DFT-optimized geometry of **(3) [$Co^{II}(\eta^2$-COF-N,N′)$(COOH)_2Cl_2$]** (doublet) **(HOOC*COOH)**, computed at the UB3LYP-D3/ LANL2DZ (Co)/ 6-31+G* (HCNOCl) level in absence of any solvent.

Atom	x	y	z

C	5.43091200	0.87030600	0.07311800
C	4.22527200	1.04207800	0.05230300
C	2.83012000	1.26968000	0.03055300
C	2.28410900	2.56672300	0.11412700
C	1.93226300	0.18383300	-0.07611100
C	0.90516500	2.72098700	0.11150400
H	2.94519400	3.42369500	0.19395000
N	0.61486800	0.34515100	-0.10450500
H	2.29877400	-0.83306700	-0.12205500
C	0.08529600	1.59175000	0.00832600
H	0.45281200	3.70418000	0.20069800
C	-1.35899100	1.65741900	0.08034300
N	-2.02856100	0.55511400	0.04121200
H	-1.84685600	2.62153800	0.23367900
C	-3.43039800	0.51879800	0.10766400
C	-4.22593900	1.41928300	-0.62068000
C	-4.04014000	-0.46158400	0.90708800
C	-5.61055000	1.33849500	-0.55782700
H	-3.75646900	2.13401900	-1.29181000
C	-5.42266100	-0.51894100	0.99376000
H	-3.41445800	-1.14376600	1.47008200
C	-6.23124900	0.36561100	0.25186500
H	-6.22026300	2.00538500	-1.15852000
H	-5.88876200	-1.26530400	1.62826800
N	-7.63526500	0.25754500	0.29580100
C	-8.45144100	1.41511400	0.18355400
C	-8.24883600	-1.02341900	0.39587600
C	-8.14484800	2.57589500	0.91494000
C	-9.59279400	1.40798600	-0.63323700
C	-7.77913900	-2.10058000	-0.37232800
C	-9.34926400	-1.21837700	1.24648300
C	-8.95363300	3.70339800	0.81961500
H	-7.27672200	2.57963400	1.56725500
C	-10.39865800	2.54046800	-0.73195000
H	-9.85324600	0.50613100	-1.17895200
C	-8.37389100	-3.35483400	-0.26424400
H	-6.94410400	-1.95243400	-1.05060200
C	-9.96710300	-2.46270300	1.32314400
H	-9.72384500	-0.38574300	1.83436300
C	-10.07776500	3.71231100	-0.02362400
H	-8.73026800	4.59383000	1.40021700
H	-11.29472400	2.50661000	-1.34548600
C	-9.46923700	-3.55667800	0.59547000
H	-8.01292500	-4.17234600	-0.88224000
H	-10.82721800	-2.61271100	1.96903900
Co	-0.75515000	-1.12011200	-0.17396300
C	6.83157500	0.66523000	0.10127100
C	7.71460300	1.77340400	0.14667700
C	7.35611500	-0.64383800	0.08639600
C	9.09054200	1.54522800	0.17391100
O	7.13430300	3.00315400	0.15991000
C	8.73103700	-0.87005700	0.11541000
H	6.65617200	-1.46922200	0.05400000
C	9.61388400	0.23911500	0.15887300
H	9.79131500	2.36989600	0.20792000
C	7.96421000	4.16783300	0.21114500
O	9.31133200	-2.09819200	0.10564400
C	11.02414500	0.04026100	0.18832800
H	8.58680800	4.13921600	1.11753100
H	8.62978900	4.18688800	-0.66449400

C	7.04981700	5.38388500	0.22179200
C	8.48056900	-3.26287700	0.07274300
C	12.22700700	-0.10685500	0.21392700
H	6.37806200	5.31085700	1.08733400
H	6.41781700	5.35620200	-0.67579300
C	7.83570800	6.70046200	0.27331000
H	7.81581000	-3.26783000	0.94949700
H	7.85658500	-3.24650700	-0.83349500
C	9.39155200	-4.48123900	0.07899800
H	13.28456100	-0.24872800	0.23679200
H	8.51491800	6.75898000	-0.59061000
H	8.47509800	6.71388300	1.16887500
C	6.92833800	7.93815500	0.28455000
H	10.06482300	-4.42164600	-0.78605500
H	10.02322800	-4.44319900	0.97601400
C	8.59959000	-5.79483300	0.04436500
H	6.24994700	7.88010200	1.14803700
H	6.28945000	7.92501700	-0.61039700
C	7.71458200	9.25332400	0.33585100
H	7.96155900	-5.81831000	-0.85223000
H	7.91857300	-5.83877800	0.90787500
C	9.50128100	-7.03670200	0.05191800
H	8.37828800	9.35048200	-0.53301300
H	7.04404100	10.12079900	0.34295000
H	8.33833300	9.30522200	1.23755100
H	10.18178500	-6.99345600	-0.81067400
H	10.13857200	-7.01391000	0.94763000
C	8.70881100	-8.34869200	0.01728600
H	8.08646300	-8.41041800	-0.88485300
H	9.37532100	-9.21933100	0.02365400
H	8.04289000	-8.43079500	0.88602700
N	-10.85910200	4.88755800	-0.06465600
N	-10.13265100	-4.79542900	0.72636900
C	-9.46079000	-5.87838400	0.75071100
H	-9.99536900	-6.82675900	0.81118800
H	-8.36255700	-5.91729100	0.72672000
C	-11.38590300	5.27074400	-1.15999100
H	-12.01712700	6.15976700	-1.15673200
H	-11.23409600	4.76274700	-2.12322100
Cl	-2.09426300	-2.92474100	-0.17140800
Cl	-0.53749800	-1.17916000	2.10975600
C	-1.28413300	-0.66113400	-2.07271800
C	0.40186400	-2.38736900	-1.19475800
O	-2.31144600	-0.96085700	-2.60703700
O	-0.33236800	0.11989900	-2.64833200
O	0.50053100	-2.70377600	-2.34762900
O	1.18570400	-2.87832100	-0.20189800
H	-0.61232900	0.27804600	-3.57305600
H	1.71783900	-3.60914500	-0.58093900

Total electronic Energy (E_{total}) = -3648.031980 (Hartree/Particle).

DFT-optimized geometry of **(4) $[Co^{II}(\eta^2\text{-COF-N,N}')(COOH)(CO)Cl_2]$** (singlet) **(OC*COOH)**, computed at the B3LYP-D3/ LANL2DZ (Co)/ 6-31+G* (HCNOCl) level in absence of any solvent.

Atom	x	y	z
C	-5.41999200	0.83038800	-0.07279600
C	-4.21541600	1.01049700	-0.08180100
C	-2.82093500	1.24049900	-0.09407600
C	-2.27613900	2.53690500	-0.21387800
C	-1.91962400	0.15946200	0.01789800
C	-0.89774500	2.69808200	-0.22788400
H	-2.94112100	3.39032300	-0.29797800
N	-0.60065900	0.32577300	0.00799700
H	-2.28925600	-0.85364600	0.11527900
C	-0.07385900	1.57323400	-0.11882300
H	-0.45031700	3.68220700	-0.32715600
C	1.37027900	1.60536300	-0.17332600
N	1.99682600	0.47860300	-0.11498800
H	1.89905100	2.54854500	-0.30663200
C	3.40590200	0.43529600	-0.14460500
C	4.16166900	1.25022800	0.71094200
C	4.04746300	-0.44496300	-1.02952300
C	5.55024300	1.18586500	0.68520600
H	3.65458900	1.86751000	1.44684600
C	5.43264900	-0.47774500	-1.07882500
H	3.44403100	-1.06717000	-1.68044100
C	6.20575100	0.32184900	-0.21245500
H	6.13296200	1.78224600	1.37960700
H	5.92904100	-1.14108300	-1.77930700
N	7.61409000	0.23369500	-0.22740900
C	8.40778300	1.38327300	0.03012300
C	8.24694900	-1.02360100	-0.43320400
C	8.10394700	2.60999000	-0.58581400
C	9.52279800	1.30753300	0.87929100
C	7.75592800	-2.18105800	0.19247300
C	9.38812700	-1.11962700	-1.24693800
C	8.88916800	3.73278000	-0.34688200
H	7.25568300	2.66983300	-1.26107700
C	10.30486700	2.43496000	1.12224300
H	9.78139800	0.35767200	1.33740000
C	8.37071500	-3.41204500	-0.01998600
H	6.88900100	-2.11252800	0.84281300
C	10.02417300	-2.34401300	-1.42589300
H	9.77953700	-0.22661100	-1.72492900
C	9.98587200	3.66974300	0.52951300
H	8.66783100	4.67603500	-0.83798700
H	11.18114400	2.35008400	1.75902000
C	9.50725700	-3.51340000	-0.84320700
H	7.99203000	-4.29316800	0.49076800
H	10.91499400	-2.41768400	-2.04278900
Co	0.78523700	-1.06061800	0.14270500
C	-6.81905800	0.61434900	-0.06414000
C	-7.71125700	1.71342400	-0.13981600
C	-7.33189100	-0.69703200	0.01839500
C	-9.08563500	1.47410300	-0.12930400
O	-7.14109100	2.94512700	-0.21832000
C	-8.70516600	-0.93423300	0.02748800
H	-6.62484100	-1.51522700	0.07260900
C	-9.59751300	0.16612000	-0.04649100
H	-9.79368200	2.29132800	-0.18506300
C	-7.98085600	4.10088600	-0.30803300
O	-9.27530100	-2.16425800	0.10309400

C	-11.00635000	-0.04417100	-0.03833200
H	-8.61940600	4.02556900	-1.20045700
H	-8.63037700	4.15584100	0.57799900
C	-7.07618000	5.32128200	-0.39200000
C	-8.43481300	-3.32110900	0.17154800
C	-12.20818200	-0.20122000	-0.03268000
H	-6.41902300	5.21216300	-1.26492400
H	-6.42858100	5.34055600	0.49462600
C	-7.87311700	6.62845800	-0.49167500
H	-7.78805500	-3.36110700	-0.71755800
H	-7.79280500	-3.25914200	1.06298700
C	-9.33641600	-4.54447900	0.23931100
H	-13.26476000	-0.35207600	-0.02758600
H	-8.53781900	6.72298100	0.38029100
H	-8.52782000	6.59507300	-1.37556600
C	-6.97566400	7.87049300	-0.57708800
H	-9.99280200	-4.44979600	1.11418500
H	-9.98608900	-4.55188400	-0.64556200
C	-8.53372800	-5.84967700	0.31801400
H	-6.31161700	7.77631500	-1.44849500
H	-6.32162600	7.90425200	0.30628200
C	-7.77291500	9.17620200	-0.67690200
H	-7.87772100	-5.82762100	1.20148900
H	-7.86956700	-5.92861500	-0.55597000
C	-9.42604600	-7.09649300	0.38553400
H	-8.42242700	9.30989900	0.19780800
H	-7.10931900	10.04695000	-0.73670600
H	-8.41229300	9.18091400	-1.56908300
H	-10.08985900	-7.01808200	1.25863200
H	-10.08095500	-7.11932700	-0.49740100
C	-8.62306300	-8.40014200	0.46468700
H	-7.98255500	-8.41585800	1.35599700
H	-9.28296700	-9.27457300	0.51174500
H	-7.97364700	-8.51773600	-0.41238700
N	10.74390900	4.84573900	0.71940200
N	10.19201600	-4.72571500	-1.07402500
C	9.53739400	-5.80747900	-1.23582000
H	10.08761600	-6.73893300	-1.37193700
H	8.43969300	-5.86044900	-1.25971700
C	11.22890300	5.11906900	1.86581900
H	11.84330400	6.01295400	1.97689000
H	11.05616000	4.51013900	2.76484500
Cl	2.38784600	-2.62816500	0.55512000
Cl	0.65319700	-1.35789400	-2.20032500
C	0.77323500	-0.73517800	2.05956600
O	1.36706100	0.13900600	2.65009100
O	-0.06732600	-1.58877000	2.71597000
H	-0.01177400	-1.38347000	3.67268800
C	-0.28955300	-2.55540200	0.20600200
O	-0.94548600	-3.48537700	0.18583800

Total electronic Energy (E_{total}) = -3572.259619 (Hartree/Particle).

DFT-optimized geometry of **(4a) [$Co^{II}(\eta^2$-COF-N,N′)(COOH)Cl_2]** (singlet) **(*COOH)**, computed at the B3LYP-D3/ LANL2DZ (Co)/ 6-31+G* (HCNOCl) level in absence of any solvent.

Atom	x	y	z
C	5.35523200	0.85696400	-0.02060700
C	4.15348600	1.03299600	-0.11079100
C	2.76178300	1.26014400	-0.21147300
C	2.21343500	2.55984300	-0.21775800
C	1.86531900	0.17316100	-0.30785600
C	0.83592300	2.71829700	-0.28503500
H	2.87314500	3.41929900	-0.15387300
N	0.54889900	0.33597700	-0.40367300
H	2.22885600	-0.84660500	-0.29168800
C	0.01469800	1.58694600	-0.36324900
H	0.38640600	3.70652300	-0.26387500
C	-1.43469100	1.64415100	-0.31358800
N	-2.08879700	0.52994000	-0.28657600
H	-1.92278900	2.61660900	-0.21605200
C	-3.48541700	0.49206900	-0.16901800
C	-4.32929000	1.42542500	-0.79757000
C	-4.04978000	-0.53523200	0.60795400
C	-5.70731600	1.33307100	-0.65551700
H	-3.90922600	2.18122700	-1.45639500
C	-5.42337000	-0.60236900	0.78185800
H	-3.38910600	-1.24905600	1.08653500
C	-6.27718200	0.31870900	0.14190300
H	-6.35391800	2.02731900	-1.18216300
H	-5.84796600	-1.38473400	1.40188400
N	-7.67541400	0.20925300	0.27085300
C	-8.49287100	1.37187400	0.26518600
C	-8.28806300	-1.07268900	0.36221600
C	-8.13792700	2.49579200	1.03123700
C	-9.68208400	1.40413100	-0.47929100
C	-7.87779900	-2.12053000	-0.47728000
C	-9.33051900	-1.29722200	1.27629100
C	-8.94738100	3.62683600	1.04012800
H	-7.23122600	2.46777000	1.62812200
C	-10.48877400	2.54031600	-0.47399600
H	-9.97819500	0.52947500	-1.05055200
C	-8.47210700	-3.37577700	-0.37922400
H	-7.08907000	-1.94845500	-1.20357900
C	-9.94966200	-2.54133400	1.34536200
H	-9.65999000	-0.48718600	1.92006000
C	-10.12099800	3.67654400	0.26879800
H	-8.68591600	4.48826600	1.64792000
H	-11.42083300	2.53669900	-1.03233300
C	-9.50877200	-3.60750400	0.54347900
H	-8.15889300	-4.16950400	-1.05185900
H	-10.76573400	-2.71349500	2.04096000
C	6.75067900	0.64214900	0.08652100
C	7.64020500	1.74362300	0.15749100
C	7.26283700	-0.67132200	0.12472700
C	9.01052700	1.50469700	0.26243500
O	7.07134500	2.97829000	0.11628100
C	8.63220900	-0.90828600	0.23093700
H	6.55782200	-1.49128900	0.07099600
C	9.52176100	0.19419200	0.30025300
H	9.71617100	2.32405100	0.31775200
C	7.90825200	4.13662000	0.18962800
O	9.20061100	-2.14112400	0.27489300
C	10.92660900	-0.01561900	0.40825300

H	8.48168900	4.12025200	1.12821600
H	8.61948300	4.13332200	-0.64955800
C	7.00616000	5.36038900	0.12898100
C	8.36213400	-3.29934500	0.21281600
C	12.12502800	-0.17219600	0.50046300
H	6.28775100	5.30859900	0.95784400
H	6.42356600	5.32194100	-0.80103000
C	7.80042900	6.67099200	0.20033700
H	7.65059000	-3.28641900	1.05185100
H	7.78858100	-3.29049200	-0.72618400
C	9.26050200	-4.52490700	0.28514800
H	13.17851100	-0.32244800	0.58199100
H	8.52543300	6.70879000	-0.62671900
H	8.39105300	6.69457300	1.12860500
C	6.90538400	7.91631600	0.14200100
H	9.98124200	-4.48201700	-0.54184100
H	9.84181700	-4.48041500	1.21533200
C	8.46004000	-5.83231800	0.22288700
H	6.18111200	7.87881000	0.96859200
H	6.31536300	7.89321800	-0.78567700
C	7.69999600	9.22549600	0.21363000
H	7.87247500	-5.86196900	-0.70735800
H	7.73168900	-5.85967900	1.04748600
C	9.34900700	-7.08122300	0.29563800
H	8.41025800	9.30212600	-0.61974600
H	7.03819700	10.09861300	0.17013400
H	8.27492900	9.28757100	1.14660800
H	10.07708400	-7.05413400	-0.52792000
H	9.93540600	-7.05261200	1.22532300
C	8.54824600	-8.38710300	0.23217000
H	7.97696000	-8.45488100	-0.70272400
H	9.20566700	-9.26300400	0.28637400
H	7.83379900	-8.45293800	1.06288500
N	-10.89996200	4.85228800	0.33215500
N	-10.17025800	-4.84772400	0.66925700
C	-9.50586300	-5.93368000	0.60572200
H	-10.04180500	-6.88139700	0.66418900
H	-8.41192400	-5.97634400	0.50705200
C	-11.48774200	5.28993000	-0.71044900
H	-12.11525400	6.17759300	-0.62636400
H	-11.39269500	4.83090700	-1.70501600
Co	-0.76533500	-1.10639600	-0.62734800
Cl	-2.34138400	-2.54068400	-1.24581600
Cl	-0.48772200	-1.73096800	1.47313000
C	0.42336300	-2.23281600	-1.48216700
O	0.59071800	-1.80336100	-2.61244900
O	1.01908800	-3.32222400	-0.98811300
H	1.51911900	-3.74566300	-1.71663700

Total electronic Energy (E_{total}) = -3458.901227 (Hartree/Particle).

DFT-optimized geometry of **(5) [$Co^{II}(\eta^2$-COF-N,N′)$(CO)_2Cl_2$]** (doublet) **(OC*CO)**, computed at the UB3LYP-D3/ LANL2DZ (Co)/ 6-31+G* (HCNOCl) level in absence of any solvent.

Atom	x	y	z
C	-5.51201200	0.83225200	0.00935600
C	-4.30200600	0.97410700	0.00485300
C	-2.90062600	1.15845400	-0.00626900
C	-2.31504600	2.43802500	-0.11168500
C	-2.02284400	0.05095700	0.08992000
C	-0.93115200	2.55635800	-0.12532100
H	-2.95248400	3.31327800	-0.18769300
N	-0.70414100	0.17180500	0.08643000
H	-2.42128700	-0.95720600	0.16669300
C	-0.14541200	1.39880500	-0.02672700
H	-0.45692100	3.52934500	-0.21840400
C	1.30675100	1.43454000	-0.08690700
N	1.99715300	0.34107900	-0.06574500
H	1.80034000	2.40002300	-0.20837600
C	3.40738300	0.37597100	-0.10549500
C	4.13848700	1.29232100	0.66950500
C	4.08838400	-0.54477000	-0.91819600
C	5.52744200	1.28124700	0.64541800
H	3.61893900	1.96442400	1.34810300
C	5.47278900	-0.52610800	-0.97252800
H	3.51727400	-1.24546300	-1.51378900
C	6.21711700	0.36675400	-0.17620600
H	6.08559600	1.95575400	1.28628700
H	5.99052900	-1.23058700	-1.61442000
N	7.62476900	0.31641000	-0.17295100
C	8.38675300	1.49911300	0.02504000
C	8.29342700	-0.93559800	-0.29127400
C	8.06756000	2.67556000	-0.67513200
C	9.48589600	1.50445700	0.89778700
C	7.82357700	-2.06411700	0.39962000
C	9.44710200	-1.05025300	-1.08410300
C	8.82202800	3.83006300	-0.49502100
H	7.23300400	2.67048800	-1.36992100
C	10.23705100	2.66364800	1.08153200
H	9.75707200	0.59207500	1.42025100
C	8.47275400	-3.28889900	0.27074100
H	6.94293400	-1.98286000	1.02966000
C	10.11719000	-2.26599600	-1.17914600
H	9.82111200	-0.17845600	-1.61258500
C	9.90189400	3.84970800	0.40405100
H	8.58993500	4.73387600	-1.05101600
H	11.10250000	2.64093300	1.73803900
C	9.62245200	-3.41020900	-0.53104900
H	8.10696500	-4.14707800	0.82759800
H	11.01761900	-2.35395300	-1.77999600
Co	0.93088000	-1.38551600	0.06794400
C	-6.91803800	0.66532600	0.01320700
C	-7.77108300	1.79611500	-0.04798000
C	-7.47802800	-0.62772100	0.07612400
C	-9.15306800	1.60575300	-0.04303200
O	-7.15785200	3.00826000	-0.10780800
C	-8.85896300	-0.81609700	0.07962400
H	-6.80078700	-1.47136600	0.11970400
C	-9.71164200	0.31583100	0.02005200
H	-9.83145600	2.44839600	-0.08813700
C	-7.95642300	4.19359400	-0.18203500
O	-9.47261400	-2.02640100	0.13655000
C	-11.12712100	0.15583800	0.02282700

H	-8.59564200	4.15371100	-1.07632300
H	-8.60545400	4.25875800	0.70372800
C	-7.00953000	5.38276700	-0.24710500
C	-8.67422200	-3.21303500	0.18892700
C	-12.33383900	0.04181700	0.02411900
H	-6.35488900	5.26327900	-1.12055300
H	-6.36326800	5.36650300	0.64055400
C	-7.76006400	6.71831800	-0.32891900
H	-8.02748000	-3.26310100	-0.69976800
H	-8.03202000	-3.18747400	1.08209300
C	-9.61901000	-4.40439900	0.23712900
H	-13.39514200	-0.07108300	0.02533600
H	-8.42273300	6.82345800	0.54338900
H	-8.41388300	6.72064600	-1.21409700
C	-6.81964600	7.92935100	-0.39507800
H	-10.27313200	-4.29946400	1.11251800
H	-10.26701300	-4.37516100	-0.64850800
C	-8.86378000	-5.73856900	0.29699400
H	-6.15763600	7.82461700	-1.26683300
H	-6.16647300	7.92745100	0.48959000
C	-7.57059800	9.26345200	-0.47701800
H	-8.20893400	-5.75341000	1.18152100
H	-8.20140100	-5.82808000	-0.57737000
C	-9.80018300	-6.95357500	0.34456600
H	-8.21683400	9.40701400	0.39856000
H	-6.87691400	10.11129700	-0.52311400
H	-8.20763400	9.30346500	-1.36998700
H	-10.46218600	-6.86468900	1.21801600
H	-10.45404700	-6.93954500	-0.53931800
C	-9.04451200	-8.28619400	0.40473300
H	-8.40657600	-8.33849300	1.29650000
H	-9.73535200	-9.13704900	0.43760000
H	-8.39821000	-8.41362800	-0.47328300
N	10.62959300	5.05297700	0.53072400
N	10.33989900	-4.61668100	-0.67894900
C	9.71258700	-5.72109700	-0.78758100
H	10.28618100	-6.64558000	-0.86001800
H	8.61706300	-5.80105800	-0.82586500
C	11.08548600	5.41155800	1.66549400
H	11.67766500	6.32485100	1.72908700
H	10.90857500	4.85840200	2.59911200
Cl	2.81596600	-3.03451500	0.61955600
Cl	0.81126400	-1.46861200	-2.20321600
C	1.11029000	-1.37605500	1.90892100
C	-0.08703800	-2.94323700	-0.00889700
O	-0.68155100	-3.91089000	-0.10157400
O	1.22124600	-1.31860700	3.04402900

Total electronic Energy (E_{total}) = -3496.426386 (Hartree/Particle).

DFT-optimized geometry of **(6) [$Co^{II}(\eta^2$-COF-N,N′)(CHO)(CO)Cl_2]** (singlet) **(OC*CHO)**, computed at the B3LYP-D3/ LANL2DZ (Co)/ 6-31+G* (HCNOCl) level in absence of any solvent.

Atom	x	y	z

C	-5.39710400	0.82871900	-0.03163200
C	-4.19279400	1.01126400	-0.04123300
C	-2.79852200	1.23823900	-0.05758700
C	-2.25146200	2.53445600	-0.16240700
C	-1.90016600	0.15125200	0.03358500
C	-0.87243600	2.69177600	-0.16758700
H	-2.91398500	3.39068200	-0.23603600
N	-0.58154700	0.31136300	0.02098300
H	-2.27614000	-0.86011800	0.11965100
C	-0.05364300	1.56194600	-0.07126800
H	-0.42156800	3.67630600	-0.24670300
C	1.38979800	1.59181900	-0.08843200
N	2.01454000	0.46027700	-0.01296700
H	1.92419200	2.53236700	-0.21915600
C	3.42651900	0.41982600	-0.03405300
C	4.18431400	1.25002100	0.80596200
C	4.07299300	-0.46352400	-0.91352800
C	5.57347300	1.18971400	0.78265900
H	3.68280400	1.89821700	1.52044100
C	5.45797300	-0.49232900	-0.96256400
H	3.47202400	-1.08391600	-1.56814200
C	6.23201600	0.31639100	-0.10458900
H	6.15341500	1.80132500	1.46584800
H	5.95398600	-1.15773800	-1.66118800
N	7.63850600	0.23376200	-0.12146400
C	8.43063600	1.38269600	0.14925300
C	8.27966300	-1.01636100	-0.35108300
C	8.13419500	2.61217700	-0.46418000
C	9.53812300	1.30009900	1.00698100
C	7.80791600	-2.18535100	0.26702500
C	9.41141000	-1.09070700	-1.17963600
C	8.91949400	3.73246800	-0.21355100
H	7.29261700	2.67615300	-1.14748800
C	10.32060500	2.42481400	1.26158200
H	9.79131900	0.34700100	1.46149000
C	8.43186700	-3.40778400	0.03227600
H	6.94828800	-2.13319700	0.92850600
C	10.05727400	-2.30644500	-1.38114800
H	9.78796900	-0.18801200	-1.65134700
C	10.00864100	3.66279700	0.67180200
H	8.70491200	4.67816200	-0.70290000
H	11.19193800	2.33547700	1.90445300
C	9.55894300	-3.48759700	-0.80604600
H	8.06818100	-4.29905100	0.53621400
H	10.94121500	-2.36388700	-2.00949200
Co	0.78873000	-1.09329900	0.10868000
C	-6.79480000	0.60637500	-0.01773500
C	-7.69342200	1.69961100	-0.10300700
C	-7.30001200	-0.70693400	0.08087400
C	-9.06636100	1.45261700	-0.08689800
O	-7.13058800	2.93364500	-0.19578400
C	-8.67179300	-0.95176100	0.09664400
H	-6.58802200	-1.52018600	0.14364400
C	-9.57051300	0.14271300	0.01182300
H	-9.77924800	2.26506700	-0.15016500
C	-7.97731500	4.08362800	-0.29218800
O	-9.23469800	-2.18387400	0.18874100
C	-10.97807900	-0.07542200	0.02564800
H	-8.61742600	3.99792700	-1.18258000

H	-8.62517900	4.14143500	0.59487700
C	-7.08009400	5.30871700	-0.38724000
C	-8.38706100	-3.33457800	0.27443900
C	-12.17898600	-0.23926000	0.03583000
H	-6.42341000	5.19647700	-1.26011800
H	-6.43150300	5.33898000	0.49834800
C	-7.88507700	6.61018100	-0.49638900
H	-7.74143600	-3.38484500	-0.61495600
H	-7.74424300	-3.25441700	1.16373500
C	-9.28119300	-4.56206700	0.36305600
H	-13.23462800	-0.39625500	0.04536900
H	-8.54951900	6.70753800	0.37546700
H	-8.54041000	6.56583900	-1.37933400
C	-6.99537300	7.85698900	-0.59248700
H	-9.93639700	-4.45766300	1.23771200
H	-9.93252500	-4.58730100	-0.52029300
C	-8.47035900	-5.86095500	0.46061600
H	-6.33153200	7.75998500	-1.46374400
H	-6.34077900	7.90174700	0.28999500
C	-7.80071700	9.15696500	-0.70185600
H	-7.81240300	-5.82075600	1.34194600
H	-7.80781800	-5.94980100	-0.41364500
C	-9.35488500	-7.11191200	0.55025000
H	-8.45025800	9.29356700	0.17238700
H	-7.14257900	10.03131800	-0.76920700
H	-8.44094600	9.15066000	-1.59341900
H	-10.01691200	-7.02366500	1.42376800
H	-10.01191400	-7.15279600	-0.33048300
C	-8.54373400	-8.40923700	0.64802900
H	-7.90078700	-8.40674600	1.53769900
H	-9.19814000	-9.28682800	0.71084400
H	-7.89589000	-8.53684700	-0.22881600
N	10.76850300	4.83565000	0.87259400
N	10.25244600	-4.69043300	-1.05853400
C	9.60526800	-5.77431700	-1.23479900
H	10.16177100	-6.69936100	-1.38777100
H	8.50789900	-5.83480200	-1.25523800
C	11.24036900	5.10535000	2.02524100
H	11.85686800	5.99658200	2.14530100
H	11.05423900	4.49548500	2.92097600
Cl	2.36714900	-2.71139400	0.50385900
Cl	0.73339800	-1.23700000	-2.28205400
C	-0.30723500	-2.55976200	0.07377800
O	-0.98435700	-3.47414500	0.02144000
C	0.73446400	-0.94427100	2.03973800
H	1.73457100	-0.74551100	2.48652200
O	-0.25681400	-1.03880600	2.71483800

Total electronic Energy (E_{total}) = -3497.008852 (Hartree/Particle).

DFT-optimized geometry of **(6a) [Co^{II}(η^2-COF-N,N′)(H_2O)(CO)Cl_2]** (doublet) **(OC*OH_2)**, computed at the UB3LYP-D3/ LANL2DZ (Co)/ 6-31+G* (HCNOCl) level in absence of any solvent.

Atom	x	y	z

C	-5.43055300	0.80849100	0.01354500
C	-4.22552100	0.98255000	0.04995700
C	-2.82948200	1.20357100	0.08899800
C	-2.27370600	2.49855900	0.02371000
C	-1.93406700	0.11444400	0.19469100
C	-0.89348500	2.64861400	0.04714700
H	-2.92984300	3.35934600	-0.05639100
N	-0.61567600	0.26579300	0.23816300
H	-2.31313800	-0.90074400	0.23436900
C	-0.08178500	1.51268600	0.15175100
H	-0.43834100	3.63204800	-0.02301100
C	1.36387200	1.54922300	0.10065800
N	2.01084000	0.42877200	0.14197500
H	1.87768000	2.49989000	-0.04312300
C	3.41803200	0.39818500	0.05573900
C	4.21701200	1.32618500	0.74253500
C	4.02345000	-0.59791400	-0.72789200
C	5.60221300	1.26212700	0.64872800
H	3.75546400	2.05283100	1.40618200
C	5.40346400	-0.63622000	-0.84965900
H	3.39107600	-1.30471100	-1.25365900
C	6.21676800	0.28065700	-0.15339000
H	6.21631900	1.95316400	1.21690500
H	5.86478000	-1.39331400	-1.47490000
N	7.62198900	0.19643300	-0.23446400
C	8.41592300	1.37357900	-0.18450800
C	8.25795100	-1.07419800	-0.31184100
C	8.06416900	2.50187600	-0.94586200
C	9.57828500	1.41923500	0.60089500
C	7.82080800	-2.14105600	0.48970800
C	9.34919900	-1.27070800	-1.17433900
C	8.84987100	3.64898500	-0.91074800
H	7.17894900	2.46462400	-1.57365800
C	10.36098100	2.57146000	0.63947900
H	9.87323100	0.54240900	1.16941000
C	8.43787800	-3.38616100	0.40371000
H	6.99269200	-1.99234000	1.17620300
C	9.98964100	-2.50460500	-1.22925300
H	9.69875500	-0.44695800	-1.78942800
C	9.99539600	3.71110200	-0.09910300
H	8.59130400	4.51395500	-1.51476900
H	11.27342800	2.57798800	1.22935000
C	9.52419700	-3.58925600	-0.46702200
H	8.10151400	-4.19460700	1.04705600
H	10.84243200	-2.65453100	-1.88483000
Co	0.84281800	-1.14286400	0.39779200
C	-6.83021400	0.59854500	-0.03353200
C	-7.71700000	1.70326000	-0.08686100
C	-7.34952800	-0.71274300	-0.03063600
C	-9.09152000	1.46959100	-0.13304500
O	-7.14153600	2.93544300	-0.08835900
C	-8.72308400	-0.94449000	-0.07910600
H	-6.64685300	-1.53564200	0.00680700
C	-9.60975600	0.16133400	-0.12981000
H	-9.79510300	2.29159000	-0.17329300
C	-7.97498700	4.09660600	-0.15834400
O	-9.29822500	-2.17492600	-0.08222300
C	-11.01871800	-0.04297500	-0.17856300
H	-8.58265000	4.06126800	-1.07456900

H	-8.65486500	4.11711300	0.70623600
C	-7.06536900	5.31627600	-0.15993900
C	-8.46295000	-3.33664700	-0.04677900
C	-12.22055400	-0.19480200	-0.22036700
H	-6.37877000	5.24129700	-1.01356600
H	-6.44847600	5.29606900	0.74829900
C	-7.85552600	6.62933200	-0.23203400
H	-7.78781300	-3.33336000	-0.91544600
H	-7.84976200	-3.32343000	0.86682100
C	-9.36884500	-4.55854200	-0.07119700
H	-13.27709600	-0.34103600	-0.25785600
H	-8.54934100	6.69002200	0.62006700
H	-8.47989400	6.63503300	-1.13821900
C	-6.95303200	7.87063400	-0.23534900
H	-10.05323000	-4.50636900	0.78562900
H	-9.98938100	-4.51804000	-0.97585900
C	-8.57202700	-5.86913900	-0.03376800
H	-6.25988400	7.81019400	-1.08685200
H	-6.32933600	7.86547300	0.67032600
C	-7.74355500	9.18222800	-0.30796100
H	-7.94495500	-5.89490400	0.87042200
H	-7.88002500	-5.90573200	-0.88872200
C	-9.46871200	-7.11438600	-0.05910400
H	-8.42235400	9.28188300	0.54888800
H	-7.07646200	10.05238300	-0.30893700
H	-8.35206000	9.22615100	-1.22044000
H	-10.16042100	-7.07821500	0.79491800
H	-10.09461500	-7.08953000	-0.96277300
C	-8.67156300	-8.42345700	-0.02099900
H	-8.06047500	-8.48730100	0.88865400
H	-9.33450800	-9.29665300	-0.04036500
H	-7.99413700	-8.49838700	-0.88140100
N	10.75090600	4.90367900	-0.11893300
N	10.20932500	-4.81815600	-0.57741100
C	9.55869300	-5.91419700	-0.56238700
H	10.11079000	-6.85334200	-0.60789600
H	8.46195900	-5.97370000	-0.51882900
C	11.29851100	5.33516600	0.94786700
H	11.90910600	6.23708400	0.89736800
H	11.18437200	4.85706600	1.93140600
Cl	2.48481200	-2.52806900	1.35651400
Cl	0.74671600	-1.61480100	-1.96861400
C	-0.21861000	-2.62157800	0.55343800
O	-0.87204700	-3.55605200	0.60950000
O	0.86826300	-0.33398200	2.77622900
H	1.63197400	-0.94562300	2.84492700
H	0.16960700	-0.75235000	3.30245300

Total electronic Energy (E_{total}) = -3459.541642 (Hartree/Particle).

DFT-optimized geometry of **(6b) [Co^{II}(η^2-COF-N,N′)(COCHO)Cl_2]** (singlet) **(*COCHO)**, computed at the B3LYP-D3/ LANL2DZ (Co)/ 6-31+G* (HCNOCl) level in absence of any solvent.

Atom	x	y	z

C	-5.37432000	0.88310100	-0.01655600
C	-4.17841900	1.09374300	0.07730600
C	-2.78954200	1.33354300	0.18484400
C	-2.24649600	2.63569300	0.20269000
C	-1.88877800	0.24977300	0.28218100
C	-0.86995200	2.80041900	0.27765500
H	-2.90929200	3.49281700	0.13876300
N	-0.57464600	0.42205700	0.39302100
H	-2.24284800	-0.77432700	0.25826100
C	-0.04163800	1.67360500	0.35519300
H	-0.42572000	3.79113400	0.25887100
C	1.40864900	1.74082100	0.29953800
N	2.06902300	0.63341900	0.22468700
H	1.88692500	2.72139100	0.23734500
C	3.46192600	0.58539300	0.10801300
C	4.32023100	1.51697000	0.72178800
C	4.01238300	-0.46233400	-0.65261800
C	5.69597400	1.40379400	0.57847100
H	3.91256600	2.28877700	1.36961200
C	5.38446700	-0.55207200	-0.82660300
H	3.34028900	-1.17524100	-1.11696000
C	6.25145900	0.36854900	-0.20364600
H	6.35307800	2.09754300	1.09265400
H	5.79718900	-1.35108100	-1.43320100
N	7.64741000	0.23930500	-0.33216800
C	8.48085500	1.39083300	-0.33954400
C	8.24376900	-1.05103100	-0.41661300
C	8.14209400	2.51042800	-1.11899400
C	9.67017200	1.41461600	0.40493800
C	7.82504400	-2.08701500	0.43318300
C	9.27876600	-1.29534200	-1.33398100
C	8.96768400	3.62959700	-1.14091200
H	7.23534700	2.48821700	-1.71605600
C	10.49302900	2.53902000	0.38670700
H	9.95359000	0.54235900	0.98624600
C	8.40295800	-3.35039100	0.34167900
H	7.04190300	-1.89951700	1.16170000
C	9.88211800	-2.54754000	-1.39656600
H	9.61487300	-0.49441900	-1.98566400
C	10.14164700	3.67150100	-0.36964500
H	8.71879100	4.48738800	-1.75902100
H	11.42490400	2.52872300	0.94526600
C	9.43192600	-3.60195500	-0.58440500
H	8.08308000	-4.13535900	1.02141900
H	10.69241100	-2.73514500	-2.09490500
C	-6.75953000	0.61191400	-0.12792400
C	-7.69689900	1.67287600	-0.19555200
C	-7.21193900	-0.72320500	-0.17358900
C	-9.05492400	1.37325200	-0.30435700
O	-7.18376800	2.93177300	-0.14724500
C	-8.56910400	-1.02098700	-0.28392100
H	-6.47067300	-1.51078700	-0.12256200
C	-9.50685600	0.04122800	-0.34948100
H	-9.79655800	2.16034400	-0.35733500
C	-8.07135700	4.05133400	-0.22411800
O	-9.08087900	-2.27761200	-0.33523600
C	-10.90074300	-0.23050400	-0.46132300
H	-8.63961400	4.00934400	-1.16507300
H	-8.78541200	4.01610400	0.61199600

C	-7.22575100	5.31461600	-0.15972500
C	-8.18930000	-3.39717700	-0.28404100
C	-12.09083500	-0.43996200	-0.55664200
H	-6.50248900	5.29571800	-0.98572400
H	-6.64552800	5.30229600	0.77249100
C	-8.07838600	6.58787300	-0.23385300
H	-7.48013600	-3.34342900	-1.12322900
H	-7.61574900	-3.37018400	0.65438500
C	-9.03014400	-4.66210700	-0.36704500
H	-13.13622900	-0.63752500	-0.64114600
H	-8.80774700	6.59229100	0.59024900
H	-8.66573600	6.58508900	-1.16448700
C	-7.24115900	7.87257900	-0.17147100
H	-9.75003400	-4.66137100	0.46188000
H	-9.61529200	-4.63526700	-1.29555900
C	-8.16915400	-5.93122400	-0.32000400
H	-6.51264100	7.86852400	-0.99515000
H	-6.65434600	7.87581900	0.75853600
C	-8.09419900	9.14431900	-0.24577100
H	-7.57761200	-5.94259400	0.60794200
H	-7.44279700	-5.91609400	-1.14650900
C	-8.99921000	-7.21936700	-0.40321400
H	-8.81050900	9.18812600	0.58481100
H	-7.47299400	10.04664000	-0.19940300
H	-8.66770900	9.18064100	-1.18097900
H	-9.72487300	-7.23501600	0.42286900
H	-9.58972200	-7.20860900	-1.33075300
C	-8.13798400	-8.48694000	-0.35604600
H	-7.56027200	-8.53719600	0.57593700
H	-8.75394300	-9.39211300	-0.41714600
H	-7.42434200	-8.51050800	-1.18965900
N	10.93763000	4.83493500	-0.44656000
N	10.07675300	-4.85150700	-0.70382700
C	9.39775300	-5.92792600	-0.63308600
H	9.92062800	-6.88318000	-0.68696700
H	8.30346900	-5.95498500	-0.53283400
C	11.53001600	5.27717400	0.59145400
H	12.17046700	6.15452200	0.49731100
H	11.42666100	4.83215500	1.59155400
Co	0.74370000	-1.00529300	0.61553400
Cl	2.28539400	-2.57273800	1.14134000
Cl	0.45910600	-1.61429500	-1.49491700
C	-0.42506000	-2.22166700	1.44875600
O	-1.28975800	-3.01642100	1.18646000
C	-0.10294400	-1.73924900	2.86858500
H	-0.41712900	-2.27613200	3.78335100
O	0.49470500	-0.66702500	2.89999200

Total electronic Energy (E_{total}) = -3496.976633 (Hartree/Particle).

DFT-optimized geometry of **(7) $[Co^{II}(\eta^2\text{-COF-N,N}')(OCH_2)(CO)Cl_2]$** (doublet) **$(OC^*OCH_2)$**, computed at the UB3LYP-D3/ LANL2DZ (Co)/ 6-31+G* (HCNOCl) level in absence of any solvent.

Atom	x	y	z

C	-5.43747800	0.81651800	-0.03052400
C	-4.23295100	0.99414500	0.00240700
C	-2.83675300	1.21570400	0.03739900
C	-2.28242700	2.51104100	-0.02415100
C	-1.94191100	0.12552000	0.13466700
C	-0.90229300	2.66109900	0.00032000
H	-2.93911900	3.37183000	-0.09940900
N	-0.62363100	0.27651800	0.17474900
H	-2.32199100	-0.88881900	0.17327000
C	-0.09134800	1.52466500	0.09867400
H	-0.44677400	3.64477800	-0.06397400
C	1.35451400	1.56090300	0.05943900
N	1.99852200	0.43845100	0.10289200
H	1.87077000	2.51127000	-0.07882300
C	3.40643200	0.40611300	0.01868400
C	4.20708600	1.32491400	0.71520900
C	4.01017600	-0.57891200	-0.77998400
C	5.59280100	1.25944800	0.62171800
H	3.74667100	2.04945500	1.38236300
C	5.39048100	-0.61699400	-0.90256300
H	3.37606300	-1.27472500	-1.31815700
C	6.20540200	0.28791400	-0.19325400
H	6.20811900	1.94428500	1.19617600
H	5.85043400	-1.36496100	-1.53975400
N	7.61136600	0.20341500	-0.27649200
C	8.40500900	1.38020900	-0.21947300
C	8.24614500	-1.06649800	-0.36846600
C	8.04991200	2.51526500	-0.96923800
C	9.57046500	1.41974600	0.56190100
C	7.80508800	-2.14382000	0.41692200
C	9.33953500	-1.25364200	-1.23053800
C	8.83526600	3.66239200	-0.92688500
H	7.16237600	2.48328500	-1.59403400
C	10.35286200	2.57190600	0.60765900
H	9.86837900	0.53788800	1.12103400
C	8.42031400	-3.38869900	0.31584200
H	6.97460600	-2.00344200	1.10228200
C	9.97837100	-2.48763000	-1.29997100
H	9.69210000	-0.42264300	-1.83401100
C	9.98397800	3.71798100	-0.11928800
H	8.57401100	4.53250000	-1.52232300
H	11.26779000	2.57331600	1.19373000
C	9.50904100	-3.58187700	-0.55407300
H	8.08020800	-4.20553500	0.94653300
H	10.83267000	-2.62997000	-1.95528500
Co	0.81719500	-1.13604400	0.31313200
C	-6.83647100	0.60063900	-0.07318000
C	-7.72886500	1.70082400	-0.12566900
C	-7.34952200	-0.71298700	-0.06652100
C	-9.10231400	1.46049700	-0.16756300
O	-7.15941500	2.93599500	-0.13073700
C	-8.72212600	-0.95152900	-0.11049700
H	-6.64264600	-1.53228600	-0.02938700
C	-9.61432200	0.14970200	-0.16058600
H	-9.80998500	2.27902100	-0.20721400
C	-7.99875400	4.09258800	-0.20064900
O	-9.29103900	-2.18500500	-0.10960400
C	-11.02246400	-0.06139900	-0.20499300
H	-8.60848500	4.05282100	-1.11536800

H	-8.67679900	4.11131500	0.66546300
C	-7.09527700	5.31684800	-0.20640900
C	-8.44947300	-3.34218000	-0.07454900
C	-12.22371400	-0.21888800	-0.24325600
H	-6.40991000	5.24352200	-1.06115500
H	-6.47652400	5.30147500	0.70065300
C	-7.89207600	6.62579900	-0.27965200
H	-7.77701300	-3.33699800	-0.94526200
H	-7.83353100	-3.32405700	0.83707900
C	-9.34897800	-4.56888700	-0.09394600
H	-13.27959600	-0.37038300	-0.27758200
H	-8.58474000	6.68471300	0.57352800
H	-8.51803800	6.62664500	-1.18476000
C	-6.99582200	7.87159000	-0.28694600
H	-10.03092300	-4.51883800	0.76496600
H	-9.97260000	-4.53329000	-0.99670600
C	-8.54511300	-5.87517800	-0.05675300
H	-6.30381000	7.81291300	-1.13948900
H	-6.37055700	7.87130800	0.61767000
C	-7.79295900	9.17911600	-0.36079400
H	-7.91499800	-5.89598000	0.84542900
H	-7.85564400	-5.90959700	-0.91382500
C	-9.43525100	-7.12519400	-0.07704200
H	-8.47082900	9.27707800	0.49699900
H	-7.13023200	10.05261600	-0.36464700
H	-8.40323500	9.21818100	-1.27231600
H	-10.12442400	-7.09120000	0.77913400
H	-10.06417900	-7.10526600	-0.97874300
C	-8.63106400	-8.42997400	-0.03921100
H	-8.01668200	-8.48890500	0.86855500
H	-9.28940700	-9.30674300	-0.05490500
H	-7.95599300	-8.50278900	-0.90164100
N	10.73867200	4.91118800	-0.13178700
N	10.19229500	-4.81041200	-0.67919900
C	9.53949500	-5.90528600	-0.68201500
H	10.08993100	-6.84478900	-0.73886700
H	8.44249200	-5.96320000	-0.64345000
C	11.29354600	5.33221500	0.93544500
H	11.90315700	6.23505600	0.88979900
H	11.18675600	4.84414000	1.91493100
Cl	2.41825500	-2.55466900	1.19619400
Cl	0.72216500	-1.52043000	-2.07644900
C	-0.25950500	-2.60396700	0.46237300
O	-0.92273400	-3.53166500	0.51237000
C	1.21197000	-0.64313700	3.69271200
H	1.13876900	-0.21672100	4.71246800
O	0.57047400	-0.16690700	2.77574900
H	1.88118100	-1.50362700	3.52905100

Total electronic Energy (E_{total}) = -3497.623144 (Hartree/Particle).

DFT-optimized geometry of **(8) [$Co^{II}(\eta^2$-COF-N,N′)(OCH_3)(CO)Cl_2]** (singlet) **(OC*OCH_3)**, computed at the B3LYP-D3/ LANL2DZ (Co)/ 6-31+G* (HCNOCl) level in absence of any solvent.

Atom	x	y	z
C	-5.43255100	0.82078000	-0.06294100
C	-4.22936900	1.00873200	-0.03816400
C	-2.83587100	1.24317200	-0.00774200
C	-2.29227500	2.54226200	-0.07885000
C	-1.93240700	0.16011300	0.09524300
C	-0.91323800	2.70654000	-0.06037200
H	-2.95709500	3.39655000	-0.15577200
N	-0.61937900	0.33305300	0.12543500
H	-2.29970300	-0.85751900	0.14441500
C	-0.09162500	1.57978600	0.04204400
H	-0.46686700	3.69392000	-0.12908200
C	1.35371500	1.61613500	-0.00642800
N	1.99071500	0.49385600	0.04374500
H	1.87300900	2.56337500	-0.15399800
C	3.39657400	0.44647800	-0.03511200
C	4.19692500	1.32494200	0.71262800
C	3.99900100	-0.50580900	-0.87291700
C	5.58215500	1.25047600	0.63135800
H	3.73202000	2.01754900	1.40936700
C	5.38068700	-0.55378000	-0.97905200
H	3.36699100	-1.17342300	-1.44670800
C	6.19567100	0.30870500	-0.21819600
H	6.19646200	1.90158800	1.24454500
H	5.84170900	-1.27695400	-1.64345600
N	7.60018300	0.21076500	-0.28674500
C	8.40954100	1.37101900	-0.15157300
C	8.22108300	-1.06126000	-0.43583800
C	8.08609300	2.54914100	-0.84694800
C	9.55965900	1.35026300	0.65242200
C	7.76489100	-2.16834600	0.29745300
C	9.31673100	-1.21919800	-1.30049200
C	8.88727100	3.67995000	-0.72913900
H	7.21044900	2.56414600	-1.48898900
C	10.35803300	2.48590700	0.77392000
H	9.83283000	0.43566400	1.17003600
C	8.36783100	-3.41369700	0.14201400
H	6.93393400	-2.04993100	0.98646000
C	9.94291600	-2.45548000	-1.42429300
H	9.68146900	-0.36421400	-1.86183400
C	10.02049200	3.67429400	0.10188300
H	8.65068100	4.58444500	-1.28210500
H	11.26092700	2.44234800	1.37673400
C	9.45855800	-3.57778400	-0.73148600
H	8.01744400	-4.25465800	0.73414500
H	10.79949900	-2.57653700	-2.08087900
Co	0.76987400	-1.03169400	0.41335400
C	-6.82963800	0.59357100	-0.09559000
C	-7.73025200	1.68644200	-0.16042000
C	-7.33234300	-0.72386300	-0.06490800
C	-9.10210100	1.43509000	-0.19147200
O	-7.17012800	2.92520000	-0.18765900
C	-8.70318500	-0.97321300	-0.09737900
H	-6.61917800	-1.53710100	-0.01668300
C	-9.60379400	0.12079900	-0.16088400
H	-9.81619000	2.24749800	-0.24034000
C	-8.01892300	4.07542300	-0.25537600
O	-9.26314000	-2.21019700	-0.07273000
C	-11.01041800	-0.10168900	-0.19448600

H	-8.63671700	4.02651500	-1.16418900
H	-8.68876600	4.09289600	0.61700400
C	-7.12480600	5.30633000	-0.27522600
C	-8.41327900	-3.36071300	-0.01653600
C	-12.21053700	-0.26911700	-0.22394500
H	-6.44706300	5.23452700	-1.13620900
H	-6.49750300	5.29966300	0.62601800
C	-7.93227200	6.60886500	-0.34652100
H	-7.74398900	-3.36879600	-0.88972200
H	-7.79446700	-3.31916200	0.89228100
C	-9.30419900	-4.59374200	-0.00741700
H	-13.26542300	-0.42922200	-0.24961900
H	-8.61721400	6.66607500	0.51294100
H	-8.56673700	6.60113300	-1.24566400
C	-7.04561900	7.86136300	-0.36733600
H	-9.98260900	-4.53130700	0.85344100
H	-9.93203400	-4.58056300	-0.90787700
C	-8.49089200	-5.89335700	0.05219700
H	-6.36140700	7.80457000	-1.22631400
H	-6.41176400	7.86941700	0.53121400
C	-7.85342000	9.16246700	-0.43854700
H	-7.85657300	-5.89167800	0.95160800
H	-7.80515000	-5.94012200	-0.80733600
C	-9.37227100	-7.14970600	0.06100400
H	-8.52358200	9.25867800	0.42544900
H	-7.19743100	10.04092300	-0.45220300
H	-8.47282100	9.19330000	-1.34421700
H	-10.05734200	-7.10363200	0.91986700
H	-10.00582000	-7.15195500	-0.83769500
C	-8.55865800	-8.44781000	0.12049000
H	-7.93932200	-8.48443600	1.02602400
H	-9.21085700	-9.32926900	0.12559000
H	-7.88748300	-8.53303500	-0.74387300
N	10.79352900	4.85391200	0.16725600
N	10.13060100	-4.80592900	-0.90937300
C	9.46783100	-5.89338100	-0.96371900
H	10.00983200	-6.83449400	-1.06049000
H	8.37019000	-5.94277700	-0.93148200
C	11.32682500	5.21198100	1.26791400
H	11.95141600	6.10554600	1.28298500
H	11.18679400	4.67759700	2.21856400
Cl	2.35523500	-2.62450800	0.81420500
Cl	0.59058300	-1.55126500	-1.84188900
C	-0.30132100	-2.46380800	0.86813000
O	-0.96901600	-3.32875500	1.18534300
O	0.59156200	-0.45102200	2.21005700
C	1.65301500	-0.60862300	3.11289300
H	2.60895700	-0.22713600	2.71873600
H	1.39214500	-0.02345400	4.01043300
H	1.81371300	-1.65398000	3.41290000

Total electronic Energy (E_{total}) = -3498.210586 (Hartree/Particle).

DFT-optimized geometry of **(8a) [$Co^{II}(\eta^2$-COF-N,N′)($COCH_2OH$)Cl_2]** (singlet) **(*$COCH_2OH$)**, computed at the B3LYP-D3/ LANL2DZ (Co)/ 6-31+G* (HCNOCl) level in absence of any solvent.

Atom	x	y	z
C	-5.37851100	0.89322100	-0.02166000
C	-4.18327800	1.10264600	0.08173400
C	-2.79443000	1.33711200	0.20488200
C	-2.24455400	2.63587600	0.21687200
C	-1.90220200	0.24876600	0.32599000
C	-0.86766900	2.79074700	0.30361400
H	-2.90060600	3.49680800	0.13634800
N	-0.58758400	0.41142700	0.45216400
H	-2.26454900	-0.77243300	0.30785800
C	-0.04735300	1.65941100	0.40115100
H	-0.41559000	3.77773900	0.27471500
C	1.40338000	1.72648800	0.33845800
N	2.06623300	0.62235300	0.26823700
H	1.87651200	2.70925600	0.26006400
C	3.45808100	0.58113900	0.13467600
C	4.32132100	1.51403500	0.73922700
C	4.00206400	-0.46463300	-0.63342400
C	5.69634600	1.40438100	0.57967800
H	3.91859300	2.28780700	1.38819800
C	5.37229700	-0.54879600	-0.82568100
H	3.32496000	-1.17886800	-1.08884500
C	6.24442300	0.37330200	-0.21222400
H	6.35789600	2.10076500	1.08467400
H	5.77984200	-1.34504600	-1.43945200
N	7.63989000	0.25081400	-0.36167200
C	8.46577000	1.40743700	-0.38539100
C	8.24173300	-1.03585400	-0.45599200
C	8.10714200	2.52342400	-1.16119000
C	9.66701100	1.44063300	0.33945100
C	7.83671100	-2.07721500	0.39402800
C	9.26882100	-1.27261000	-1.38439200
C	8.92515700	3.64773700	-1.19889400
H	7.19079300	2.49436400	-1.74309100
C	10.48236100	2.57014600	0.30545000
H	9.96576900	0.57122700	0.91737400
C	8.41957100	-3.33753300	0.29239200
H	7.05943500	-1.89639000	1.13042000
C	9.87771200	-2.52155400	-1.45701000
H	9.59451100	-0.46828900	-2.03713800
C	10.11142900	3.69882300	-0.44725200
H	8.66064100	4.50262000	-1.81455200
H	11.42346100	2.56670000	0.84843200
C	9.44077700	-3.58107200	-0.64430000
H	8.10968900	-4.12659600	0.97205900
H	10.68181100	-2.70274000	-2.16416100
C	-6.76186000	0.61794500	-0.14759500
C	-7.70310300	1.67492300	-0.22073100
C	-7.20794000	-0.71884400	-0.20289900
C	-9.05863500	1.36988100	-0.34409400
O	-7.19592600	2.93609300	-0.16267700
C	-8.56263200	-1.02219500	-0.32841700
H	-6.46360300	-1.50324600	-0.14773300
C	-9.50435500	0.03604600	-0.39897100
H	-9.80316100	2.15393800	-0.40146400
C	-8.08747400	4.05170900	-0.24676000
O	-9.06792300	-2.28101900	-0.39043400
C	-10.89590400	-0.24124900	-0.52582800

H	-8.64570400	4.00919900	-1.19370500
H	-8.81025700	4.01186100	0.58167300
C	-7.24824900	5.31864600	-0.17106200
C	-8.17103400	-3.39643100	-0.33876700
C	-12.08409400	-0.45542100	-0.63383200
H	-6.51669000	5.30488500	-0.98980800
H	-6.67723100	5.30670000	0.76683200
C	-8.10580100	6.58824700	-0.25069800
H	-7.45438000	-3.33314800	-1.17084200
H	-7.60632600	-3.37321100	0.60508000
C	-9.00453100	-4.66499600	-0.43855700
H	-13.12767700	-0.65723800	-0.72967700
H	-8.84333400	6.58745900	0.56612900
H	-8.68390200	6.58503500	-1.18710700
C	-7.27508700	7.87657000	-0.17705800
H	-9.73205600	-4.67401100	0.38365200
H	-9.58123100	-4.63444000	-1.37224100
C	-8.13734800	-5.92994300	-0.39274800
H	-6.53849900	7.87779200	-0.99352800
H	-6.69742400	7.88021000	0.75867100
C	-8.13309100	9.14464900	-0.25671000
H	-7.55448000	-5.94513000	0.54059600
H	-7.40328600	-5.90482300	-1.21213300
C	-8.95977800	-7.22171300	-0.49340600
H	-8.85772800	9.18321700	0.56689200
H	-7.51648000	10.04967300	-0.20212800
H	-8.69757500	9.18062900	-1.19740800
H	-9.69313200	-7.24738900	0.32563300
H	-9.54158000	-7.20707800	-1.42639400
C	-8.09234200	-8.48510700	-0.44759800
H	-7.52310700	-8.53930900	0.48936500
H	-8.70288800	-9.39303000	-0.52129000
H	-7.37075200	-8.49860000	-1.27455300
N	10.89838500	4.86728800	-0.53976800
N	10.09021300	-4.82715800	-0.77459600
C	9.41694300	-5.90702400	-0.70130000
H	9.94369500	-6.85961900	-0.76385500
H	8.32380800	-5.93959300	-0.59063500
C	11.50717400	5.31448100	0.48657300
H	12.14011700	6.19580500	0.37962900
H	11.42548900	4.86991400	1.48890000
Co	0.71929900	-1.02940000	0.69942500
Cl	2.32679500	-2.57146300	1.22549900
Cl	0.44428500	-1.64208100	-1.42348700
C	-0.51255300	-2.17427400	1.54346600
O	-1.36486200	-2.95869700	1.22818200
C	-0.22479600	-1.68408600	2.96182000
H	-1.10756300	-1.21927900	3.41031800
H	0.15774400	-2.48036300	3.60617900
O	0.77302100	-0.63095400	2.76114400
H	1.65640900	-1.02339400	2.92298700

Total electronic Energy (E_{total}) = -3498.210055 (Hartree/Particle).

DFT-optimized geometry of **(9) [$Co^{II}(\eta^2$-COF-N,N′)($HOCH_3$)(CO)Cl_2]** (doublet) **(OC*$HOCH_3$)**, computed at the UB3LYP-D3/ LANL2DZ (Co)/ 6-31+G* (HCNOCl) level in absence of any solvent.

Atom	x	y	z
C	-5.45263500	0.81295600	-0.03846800
C	-4.24675600	0.98521800	-0.03812300
C	-2.84946500	1.19889400	-0.04251400
C	-2.28958900	2.49049000	-0.13444800
C	-1.95695900	0.10482900	0.04467400
C	-0.90844200	2.63442300	-0.14084200
H	-2.94348900	3.35376900	-0.20557200
N	-0.63791100	0.24903800	0.04675400
H	-2.34021700	-0.90721800	0.11019200
C	-0.10122100	1.49387400	-0.04814400
H	-0.45006000	3.61557700	-0.22272200
C	1.34505700	1.52566100	-0.08720900
N	1.99209300	0.40495800	-0.02174600
H	1.86317400	2.47444200	-0.22822500
C	3.40235700	0.38484300	-0.07058200
C	4.17353200	1.31024600	0.65094000
C	4.04030600	-0.59297200	-0.85140900
C	5.56170900	1.25591100	0.60392500
H	3.68689300	2.03242400	1.30196500
C	5.42373600	-0.62022400	-0.92806800
H	3.43111100	-1.29090800	-1.41408600
C	6.20867900	0.28844800	-0.18968500
H	6.15168100	1.94449700	1.19990900
H	5.90969500	-1.36324200	-1.55145900
N	7.61573100	0.21084400	-0.22303500
C	8.40292500	1.38933900	-0.12039600
C	8.25986200	-1.05582800	-0.30380900
C	8.07709100	2.53039500	-0.87412100
C	9.53374700	1.42347600	0.71025000
C	7.79958800	-2.14072000	0.45954700
C	9.38181500	-1.22989600	-1.13088200
C	8.85683100	3.67886800	-0.78742100
H	7.21731000	2.50203900	-1.53680500
C	10.31046600	2.57690100	0.80030500
H	9.80960700	0.53682700	1.27310400
C	8.42509400	-3.38136800	0.36979000
H	6.94649400	-2.01008200	1.11857800
C	10.02973900	-2.45978400	-1.18832000
H	9.74899800	-0.39217000	-1.71610400
C	9.96977900	3.72900900	0.06916500
H	8.61920100	4.55402600	-1.38532700
H	11.19955700	2.57493300	1.42484800
C	9.54257600	-3.56186300	-0.46570400
H	8.06950000	-4.20460000	0.98332700
H	10.90594600	-2.59262900	-1.81610000
Co	0.82586300	-1.18453100	0.12706700
C	-6.85289600	0.60318000	-0.04258000
C	-7.74142900	1.70689200	-0.08779700
C	-7.37110500	-0.70804300	-0.00457900
C	-9.11654500	1.47230200	-0.09207800
O	-7.16702500	2.93905700	-0.12397500

C	-8.74528100	-0.94076200	-0.01086600
H	-6.66703300	-1.52997200	0.02701900
C	-9.63363000	0.16412500	-0.05416400
H	-9.82154400	2.29339000	-0.12542300
C	-8.00301900	4.09882500	-0.18513500
O	-9.31951900	-2.17105900	0.02145100
C	-11.04326100	-0.04112700	-0.06062100
H	-8.63598500	4.05182800	-1.08353900
H	-8.65852800	4.12984300	0.69775200
C	-7.09480300	5.31882700	-0.22717900
C	-8.48262100	-3.33199400	0.05163900
C	-12.24570700	-0.19377400	-0.06683200
H	-6.43197800	5.23353100	-1.09844400
H	-6.45306200	5.31021100	0.66387400
C	-7.88773500	6.63050000	-0.29372500
H	-7.83188700	-3.34170500	-0.83539900
H	-7.84442800	-3.30448900	0.94753800
C	-9.38796600	-4.55436000	0.07079900
H	-13.30275700	-0.34100000	-0.07264400
H	-8.55822800	6.70116400	0.57609200
H	-8.53646200	6.62488200	-1.18262500
C	-6.98675300	7.87216400	-0.33653300
H	-10.04782100	-4.48995700	0.94583900
H	-10.03390600	-4.52730600	-0.81643500
C	-8.58934000	-5.86396700	0.10470100
H	-6.31692400	7.80183200	-1.20575900
H	-6.33870100	7.87825400	0.55189200
C	-7.78007200	9.18237900	-0.40341400
H	-7.93704300	-5.87644200	0.99110200
H	-7.92165100	-5.91256700	-0.76879300
C	-9.48541500	-7.10977900	0.12241500
H	-8.43542200	9.29199800	0.47030800
H	-7.11401700	10.05283600	-0.43304200
H	-8.41320100	9.21494700	-1.29946100
H	-10.15266000	-7.06178800	0.99511800
H	-10.13671300	-7.09798600	-0.76341800
C	-8.68645800	-8.41786500	0.15644400
H	-8.04970800	-8.46849400	1.04915000
H	-9.34899100	-9.29152100	0.16831600
H	-8.03367500	-8.50472400	-0.72170800
N	10.72158800	4.92365100	0.10031500
N	10.23675300	-4.78558900	-0.57678500
C	9.59046000	-5.88375700	-0.61087100
H	10.14768700	-6.81987900	-0.65589200
H	8.49312700	-5.94761600	-0.61065700
C	11.22635100	5.33690700	1.19507500
H	11.83561700	6.24105900	1.18455100
H	11.07610900	4.84050400	2.16461200
Cl	2.45397700	-2.66286200	1.00361400
Cl	0.80036700	-1.43911600	-2.27009600
C	-0.24809600	-2.66723900	0.13598800
O	-0.91050800	-3.59509500	0.10190600
O	0.54117100	-0.89496800	2.54380300
C	1.06238600	0.27733100	3.16834300
H	1.06189500	0.17745400	4.26179700
H	2.08154100	0.49376400	2.82221600
H	0.40565700	1.10633300	2.88952900
H	1.20108400	-1.61523600	2.62150300

Total electronic Energy (E_{total}) = -3498.847366 (Hartree/Particle).

DFT-optimized geometry of **(9a) [$Co^{II}(\eta^2$-COF-N,N′)(O)(CO)Cl_2]** (doublet) **(OC*O)**, computed at the UB3LYP-D3/ LANL2DZ (Co)/ 6-31+G* (HCNOCl) level in absence of any solvent.

Atom	x	y	z
C	5.40290800	0.80825500	0.01060200
C	4.19888200	0.99219800	-0.00397000
C	2.80534300	1.22552200	-0.01992700
C	2.26089700	2.52495900	0.05989700
C	1.90192200	0.14394800	-0.11974500
C	0.88273400	2.68966300	0.05087800
H	2.92627500	3.37907100	0.13349000
N	0.58544800	0.31581600	-0.13739100
H	2.26914300	-0.87301400	-0.17898800
C	0.05713200	1.56430800	-0.04630900
H	0.43723100	3.67711700	0.12269900
C	-1.38777000	1.60321600	0.00123500
N	-2.02263400	0.47975400	-0.04058100
H	-1.90714600	2.55310600	0.12848400
C	-3.42737900	0.42947400	0.00830400
C	-4.21191000	1.29860800	-0.76708000
C	-4.04731600	-0.51487200	0.84324700
C	-5.59810700	1.22535300	-0.71214400
H	-3.73223300	1.97779900	-1.46660900
C	-5.43021100	-0.56088400	0.92310900
H	-3.42732500	-1.17749200	1.43577900
C	-6.22927600	0.29438100	0.13666300
H	-6.19972700	1.86665700	-1.34778700
H	-5.90499600	-1.27634300	1.58612100
N	-7.63421700	0.19801900	0.17858800
C	-8.44089800	1.35522500	0.00510100
C	-8.25929500	-1.07125400	0.33536800
C	-8.13456200	2.54487300	0.68839400
C	-9.57191300	1.31957300	-0.82488600
C	-7.79255600	-2.18887200	-0.37486700
C	-9.36977200	-1.21501200	1.18329800
C	-8.93372300	3.67259700	0.53341100
H	-7.27401800	2.57134400	1.35017400
C	-10.36806600	2.45214700	-0.98379200
H	-9.83181300	0.39630900	-1.33386000
C	-8.40050000	-3.43091000	-0.21247300
H	-6.95036000	-2.08093700	-1.05187500
C	-10.00006300	-2.44850100	1.31388500
H	-9.74245200	-0.35143300	1.72598700
C	-10.04718300	3.65178000	-0.32370300
H	-8.71084600	4.58639500	1.07668600
H	-11.25645800	2.39780800	-1.60691900

C	-9.50602100	-3.58100200	0.64486200
H	-8.04224600	-4.28040100	-0.78745200
H	-10.86794900	-2.55913900	1.95732600
Co	-0.79569200	-1.05795000	-0.36435300
C	6.80109900	0.58793600	0.02893000
C	7.69566000	1.68540100	0.10075300
C	7.31084100	-0.72623300	-0.02374700
C	9.06919200	1.44164700	0.11705800
O	7.12852900	2.92005900	0.14881400
C	8.68324100	-0.96781300	-0.00638800
H	6.60209100	-1.54300100	-0.07706200
C	9.57793300	0.13088900	0.06452100
H	9.77900200	2.25746500	0.17088200
C	7.97103600	4.07487400	0.22349400
O	9.25043300	-2.20056400	-0.05282100
C	10.98597000	-0.08388900	0.08323000
H	8.59635100	4.01867100	1.12665400
H	8.63347000	4.10667000	-0.65404600
C	7.06967400	5.29988400	0.26523800
C	8.40738800	-3.35566000	-0.12074700
C	12.18716600	-0.24491600	0.10025400
H	6.39943300	5.21381300	1.13078600
H	6.43521600	5.30013200	-0.63102700
C	7.86987300	6.60640400	0.34547700
H	7.74494900	-3.38166400	0.75730000
H	7.78149000	-3.30360600	-1.02414100
C	9.30593100	-4.58263400	-0.15606600
H	13.24314000	-0.39932900	0.11485900
H	8.54760100	6.67778800	-0.51860900
H	8.51144400	6.59201000	1.23946300
C	6.97587700	7.85313100	0.38789600
H	9.97737900	-4.50221700	-1.02086200
H	9.94042600	-4.57973900	0.73979400
C	8.50028600	-5.88627800	-0.23033000
H	6.29886800	7.78219500	1.25152100
H	6.33491600	7.86779200	-0.50551700
C	7.77643100	9.15818500	0.46793500
H	7.85924200	-5.87435200	-1.12487600
H	7.82137000	-5.95108200	0.63345000
C	9.38942900	-7.13668400	-0.26572600
H	8.43908000	9.26853400	-0.40014100
H	7.11529100	10.03237000	0.49701700
H	8.40279200	9.18226200	1.36899900
H	10.06770700	-7.07255400	-1.12879800
H	10.02969400	-7.14920900	0.62810900
C	8.58348800	-8.43879900	-0.33995700
H	7.95763800	-8.46493500	-1.24135600
H	9.24114700	-9.31585700	-0.36401300
H	7.91939900	-8.54212600	0.52789700
N	-10.81956600	4.82910700	-0.42682800
N	-10.18341100	-4.80539800	0.82815700
C	-9.52390200	-5.89322500	0.90823200
H	-10.06938300	-6.83194900	1.00857700
H	-8.42598000	-5.94508000	0.89489500
C	-11.32485200	5.16921200	-1.54623500
H	-11.94992300	6.06143800	-1.59121000
H	-11.15980300	4.62029400	-2.48448600
Cl	-2.38779000	-2.60527300	-0.87470900
Cl	-0.66971100	-1.52927500	1.90582700
C	0.27094300	-2.53299500	-0.70444800

O	0.93404700	-3.42668100	-0.93869500
O	-0.74966600	-0.65030600	-2.14039700

Total electronic Energy (E_{total}) = -3458.230496 (Hartree/Particle).

DFT-optimized geometry of **(10) [$Co^{II}(\eta^2$-COF-N,N′)$(CH_3)(CO)Cl_2$]** (singlet) **(OC*CH_3)**, computed at the B3LYP-D3/ LANL2DZ (Co)/ 6-31+G* (HCNOCl) level in absence of any solvent.

Atom	x	y	z
C	-5.39692300	0.81652800	0.01063100
C	-4.19363100	1.00379800	0.03496400
C	-2.79973800	1.23772000	0.05778600
C	-2.25570900	2.53437300	-0.06576200
C	-1.89958700	0.16020000	0.20737300
C	-0.87806100	2.69628200	-0.04910400
H	-2.91975800	3.38482000	-0.18128400
N	-0.58075200	0.32599800	0.23837900
H	-2.27242900	-0.85269500	0.29484600
C	-0.05600300	1.57317300	0.10072700
H	-0.42860700	3.67840100	-0.16043300
C	1.38734000	1.60569100	0.05568300
N	2.01281700	0.47630200	0.13524300
H	1.91515400	2.54435800	-0.11207500
C	3.42121900	0.42889400	0.06169600
C	4.21747600	1.28567100	0.83665400
C	4.02515300	-0.49583900	-0.80518300
C	5.60409200	1.21171300	0.76033700
H	3.74911900	1.96356400	1.54581500
C	5.40704200	-0.53865500	-0.90890600
H	3.39325000	-1.14086600	-1.40468600
C	6.21946900	0.29756700	-0.11629200
H	6.21635700	1.84415900	1.39475700
H	5.87050900	-1.23803900	-1.59669500
N	7.62494700	0.20070000	-0.18395300
C	8.43409000	1.35578200	-0.01170200
C	8.24489900	-1.06698200	-0.36810400
C	8.11243700	2.55495500	-0.67117300
C	9.58260500	1.31047700	0.79379400
C	7.78094300	-2.19622000	0.32561500
C	9.34668800	-1.19986200	-1.22932200
C	8.91345700	3.68146600	-0.51685600
H	7.23820200	2.58985600	-1.31434400
C	10.38074500	2.44173400	0.95197100
H	9.85469500	0.38035100	1.28354800
C	8.38216000	-3.43737100	0.13422900
H	6.94454700	-2.09871800	1.01125700
C	9.97108200	-2.43300000	-1.38831400
H	9.71722900	-0.32835500	-1.76065200
C	10.04485800	3.65033400	0.31609400
H	8.67819500	4.60253000	-1.04239200
H	11.28233300	2.37929600	1.55510300
C	9.47902100	-3.57597000	-0.73593000
H	8.02484700	-4.29623600	0.69572700

H	10.83203500	-2.53488900	-2.04245200
Co	0.79658600	-1.06255800	0.42127900
C	-6.79414100	0.58988700	-0.02045300
C	-7.69352300	1.68219000	-0.10768500
C	-7.29796600	-0.72643400	0.03294000
C	-9.06553900	1.43146400	-0.13702800
O	-7.13219300	2.91973800	-0.15630400
C	-8.66893600	-0.97520200	0.00143300
H	-6.58561400	-1.53935600	0.09627200
C	-9.56840000	0.11838100	-0.08366500
H	-9.77881800	2.24342300	-0.20234100
C	-7.97952300	4.06885400	-0.25588300
O	-9.23005100	-2.21095100	0.04612200
C	-10.97512200	-0.10350700	-0.11646300
H	-8.59288400	3.99845600	-1.16623600
H	-8.65356600	4.10800200	0.61255300
C	-7.08408600	5.29811400	-0.30109900
C	-8.38133400	-3.36148900	0.11957500
C	-12.17529300	-0.27051600	-0.14555300
H	-6.40262800	5.20517900	-1.15709400
H	-6.46078500	5.31244500	0.60286800
C	-7.88990400	6.59932400	-0.40700300
H	-7.71061200	-3.38216300	-0.75223600
H	-7.76404500	-3.30790700	1.02883600
C	-9.27343300	-4.59343000	0.14419600
H	-13.23024800	-0.43025600	-0.17113400
H	-8.57883800	6.67750800	0.44761100
H	-8.52011400	6.57082100	-1.30869100
C	-7.00189800	7.85018100	-0.45334300
H	-9.95377900	-4.51822700	1.00251600
H	-9.89915800	-4.59240000	-0.75780800
C	-8.46145400	-5.89280400	0.22399400
H	-6.31366900	7.77237600	-1.30743500
H	-6.37232100	7.87904300	0.44781000
C	-7.80804500	9.14993700	-0.55933500
H	-7.82956200	-5.87923500	1.12503500
H	-7.77342600	-5.95208000	-0.63289200
C	-9.34404500	-7.14810900	0.24783200
H	-8.48225000	9.26728500	0.29888800
H	-7.15110700	10.02721600	-0.59075600
H	-8.42304300	9.15976900	-1.46845200
H	-10.03161000	-7.08941800	1.10394700
H	-9.97493400	-7.16234300	-0.65261100
C	-8.53180700	-8.44596900	0.32779800
H	-7.91518100	-8.47055400	1.23559600
H	-9.18485300	-9.32667400	0.34322700
H	-7.85815700	-8.54381600	-0.53327000
N	10.81726800	4.82770600	0.41946200
N	10.14907700	-4.79963100	-0.94918100
C	9.48362000	-5.88276200	-1.04330500
H	10.02367700	-6.82184400	-1.16709700
H	8.38567900	-5.92992000	-1.01996500
C	11.35183000	5.14994600	1.53056300
H	11.97580400	6.04302600	1.57402400
H	11.21360900	4.58467900	2.46346400
Cl	2.37781800	-2.68421000	0.76180800
Cl	0.59145400	-1.39629900	-1.92385800
C	-0.28452500	-2.49545600	0.67655600
O	-0.97339200	-3.39227000	0.83079300
C	0.88694100	-0.70431000	2.39964200

H	0.58663700	-1.58216800	2.97523300
H	1.93804700	-0.48681900	2.59704700
H	0.24694500	0.15196600	2.63509000

Total electronic Energy (E_{total}) = -3422.988417 (Hartree/Particle).

DFT-optimized geometry of **(10a) [$Co^{II}(\eta^2$-COF-N,N′)$(COCH_3)Cl_2$]** (singlet) **(*$COCH_3$)**, computed at the B3LYP-D3/ LANL2DZ (Co)/ 6-31+G* (HCNOCl) level in absence of any solvent.

Atom	x	y	z
C	5.35407300	0.89092800	-0.01638700
C	4.15880100	1.09892900	-0.12315100
C	2.76950900	1.32817000	-0.24573100
C	2.21507700	2.62504500	-0.27022200
C	1.88024000	0.23568500	-0.35106300
C	0.83772300	2.77506300	-0.35997600
H	2.86831100	3.48896200	-0.19927300
N	0.56354300	0.39126200	-0.47920400
H	2.24448500	-0.78442800	-0.32002500
C	0.02044300	1.64052400	-0.44658300
H	0.38303800	3.76114800	-0.34378100
C	-1.43062800	1.70318600	-0.39811300
N	-2.09150000	0.59521600	-0.33698600
H	-1.90725400	2.68435000	-0.32073600
C	-3.48367700	0.55639600	-0.20535800
C	-4.34545900	1.49616300	-0.80182200
C	-4.03074000	-0.48907500	0.56110300
C	-5.71999700	1.39160700	-0.63922700
H	-3.94247000	2.27061400	-1.44980000
C	-5.40061600	-0.56850900	0.75751700
H	-3.35745900	-1.20849300	1.01345700
C	-6.27080800	0.35894600	0.14948900
H	-6.37982400	2.09204000	-1.14075100
H	-5.80926600	-1.36502900	1.37010700
N	-7.66560500	0.24010300	0.30023800
C	-8.49003800	1.39787100	0.32262200
C	-8.27036500	-1.04558100	0.39595100
C	-8.13017200	2.51417000	1.09736100
C	-9.69155300	1.43113500	-0.40168600
C	-7.87390300	-2.08563800	-0.45947400
C	-9.29156900	-1.28116200	1.33089900
C	-8.94717200	3.63924700	1.13424200
H	-7.21381900	2.48471100	1.67924900
C	-10.50588200	2.56139100	-0.36848700
H	-9.99116400	0.56142600	-0.97869000
C	-8.45957300	-3.34458300	-0.35670800
H	-7.10143100	-1.90499500	-1.20098600
C	-9.90320700	-2.52869800	1.40512700
H	-9.61052600	-0.47714500	1.98737200
C	-10.13365700	3.69049800	0.38295000
H	-8.68184200	4.49445600	1.74908900
H	-11.44719300	2.55827200	-0.91108300
C	-9.47468400	-3.58736900	0.58681100

H	-8.15682600	-4.13286800	-1.04044200
H	-10.70294100	-2.70942800	2.11731100
C	6.73723500	0.61590800	0.10901100
C	7.67813100	1.67285900	0.18793300
C	7.18343400	-0.72124600	0.15723100
C	9.03364700	1.36735500	0.31053700
O	7.17080500	2.93411200	0.13588800
C	8.53807900	-1.02499500	0.28124900
H	6.43928000	-1.50543800	0.09700300
C	9.47946500	0.03332300	0.35832200
H	9.77804800	2.15116200	0.37254700
C	8.06236400	4.04952100	0.22484600
O	9.04378100	-2.28373200	0.33586500
C	10.87094700	-0.24437600	0.48440200
H	8.61986400	4.00329000	1.17202000
H	8.78565300	4.01274100	-0.60324200
C	7.22324900	5.31675300	0.15335800
C	8.14746700	-3.39939900	0.27420000
C	12.05908300	-0.45900800	0.59191600
H	6.49063100	5.29960800	0.97110300
H	6.65350500	5.30878600	-0.78536200
C	8.08074300	6.58598400	0.23945400
H	7.43015400	-3.34322700	1.10620300
H	7.58366300	-3.36857100	-0.66991100
C	8.98160500	-4.66822700	0.36427600
H	13.10259700	-0.66151600	0.68720500
H	8.81950400	6.58848500	-0.57624400
H	8.65740200	6.57891700	1.17672000
C	7.25018300	7.87463200	0.16979000
H	9.70953100	-4.67023900	-0.45761800
H	9.55778400	-4.64493900	1.29849700
C	8.11502900	-5.93317700	0.30774400
H	6.51230100	7.87252900	0.98509800
H	6.67403300	7.88214800	-0.76685400
C	8.10811000	9.14233000	0.25602000
H	7.53230400	-5.94084700	-0.62575000
H	7.38086400	-5.91528600	1.12722700
C	8.93815400	-7.22529800	0.39770200
H	8.83406000	9.18424800	-0.56625200
H	7.49161800	10.04758900	0.20415900
H	8.67107500	9.17442900	1.19776100
H	9.67147600	-7.24378700	-0.42155400
H	9.51997800	-7.21810500	1.33077500
C	8.07134900	-8.48869900	0.34138800
H	7.50209200	-8.53536400	-0.59594800
H	8.68238400	-9.39687700	0.40746500
H	7.34981300	-8.50947500	1.16823900
N	-10.91977200	4.85955500	0.47464000
N	-10.12660800	-4.83198200	0.71850000
C	-9.45639900	-5.91332600	0.63945300
H	-9.98513000	-6.86473800	0.70315900
H	-8.36400700	-5.94830700	0.52253800
C	-11.52764900	5.30671000	-0.55225500
H	-12.16002300	6.18852700	-0.44606800
H	-11.44564900	4.86161900	-1.55431000
Co	-0.71472900	-1.09029900	-0.67751800
Cl	-2.28949600	-2.57987400	-1.22279100
Cl	-0.29919700	-1.75193500	1.38939500
C	0.47859200	-2.12069900	-1.63395700
O	1.35254500	-2.90037600	-1.39117400

C	0.15416400	-1.58449800	-3.04585000
H	-0.29386300	-2.41071300	-3.60513100
H	-0.56974100	-0.75806400	-3.05850200
H	1.08811200	-1.25303200	-3.51132100

Total electronic Energy (E_{total}) = -3422.979772 (Hartree/Particle).

DFT-optimized geometry of **(11) [$Co^{II}(\eta^2$-COF-N,N′)($OCHCH_3$)Cl_2]** (doublet) **(*$OCHCH_3$)**, computed at the UB3LYP-D3/ LANL2DZ (Co)/ 6-31+G* (HCNOCl) level in absence of any solvent.

Atom	x	y	z
C	-5.39003600	0.81723500	-0.02094400
C	-4.18166000	0.96849900	0.00135600
C	-2.78132000	1.17262600	0.02594900
C	-2.21403500	2.46207900	-0.04544000
C	-1.89173100	0.07766600	0.12524200
C	-0.83194700	2.59713200	-0.04023500
H	-2.86220700	3.32977600	-0.11758600
N	-0.57346600	0.21154800	0.15641400
H	-2.27828600	-0.93550200	0.17170100
C	-0.03183700	1.44938600	0.05080000
H	-0.36840500	3.57646900	-0.11845100
C	1.41888000	1.50037000	-0.02199400
N	2.09230900	0.39873700	-0.05375100
H	1.91188800	2.47001800	-0.09770400
C	3.49988200	0.37547900	-0.09180100
C	4.28219500	1.32690000	0.58375200
C	4.13224700	-0.66050200	-0.79824000
C	5.66832700	1.25165600	0.54376500
H	3.80571200	2.08039200	1.20429500
C	5.51718200	-0.72034700	-0.85848200
H	3.52024300	-1.37935200	-1.33455900
C	6.30870600	0.22965800	-0.18407900
H	6.26539800	1.96618100	1.10115600
H	5.99718700	-1.50968600	-1.42762500
N	7.71653800	0.14393900	-0.21439100
C	8.50681100	1.32470300	-0.22316700
C	8.35536900	-1.12659900	-0.19569400
C	8.16967100	2.40128800	-1.06202400
C	9.65163900	1.42376400	0.58278300
C	7.90465600	-2.13862600	0.66719500
C	9.46389500	-1.37751000	-1.02140100
C	8.95272900	3.55061000	-1.08296100
H	7.29796800	2.32255800	-1.70470700
C	10.43156500	2.57835900	0.56474400
H	9.93506500	0.58620400	1.21303700
C	8.52584500	-3.38468900	0.67795000
H	7.06610600	-1.94314900	1.32902300
C	10.10751600	-2.61028300	-0.98047400
H	9.82447000	-0.59538100	-1.68271500
C	10.08037000	3.66756300	-0.25264900
H	8.70539800	4.37483400	-1.74578900
H	11.33069000	2.62534200	1.17295200

C	9.62960400	-3.64261800	-0.15586000
H	8.18148700	-4.14776900	1.37072100
H	10.97375300	-2.80116700	-1.60713900
C	-6.79614900	0.64556000	-0.05184800
C	-7.65269800	1.77523500	-0.04951200
C	-7.35368500	-0.64906600	-0.08753300
C	-9.03387700	1.58213500	-0.08007900
O	-7.04272100	2.99043400	-0.01602800
C	-8.73412200	-0.84030400	-0.12049600
H	-6.67455900	-1.49231700	-0.09283800
C	-9.58993600	0.28981400	-0.11543500
H	-9.71396000	2.42465400	-0.07802300
C	-7.84389600	4.17569800	-0.01905000
O	-9.34412900	-2.05458800	-0.15857800
C	-11.00493900	0.12711000	-0.14699600
H	-8.47023400	4.19734600	-0.92315600
H	-8.50606900	4.17759400	0.85949600
C	-6.89998800	5.36865900	0.01295100
C	-8.54218600	-3.23826000	-0.17848000
C	-12.21126000	0.01118300	-0.17336600
H	-6.23360800	5.31279100	-0.85797400
H	-6.26516600	5.29061900	0.90550900
C	-7.65340600	6.70504100	0.01623500
H	-7.88020400	-3.22298300	-1.05733700
H	-7.91468100	-3.27583200	0.72498300
C	-9.48248200	-4.43317500	-0.23183300
H	-13.27211900	-0.10268600	-0.19764100
H	-8.32704400	6.74693200	0.88550900
H	-8.29640600	6.76855100	-0.87463500
C	-6.71591300	7.91972200	0.04740500
H	-10.15250300	-4.39257600	0.63683800
H	-10.11485500	-4.34297500	-1.12457700
C	-8.72316000	-5.76609100	-0.25332200
H	-6.04314400	7.87836100	-0.82139700
H	-6.07334800	7.85657800	0.93753000
C	-7.46975200	9.25471600	0.05094400
H	-8.08463200	-5.84208800	0.64016600
H	-8.04455700	-5.79112000	-1.11951800
C	-9.65486000	-6.98431500	-0.30964900
H	-8.12677500	9.33461500	0.92665000
H	-6.77807700	10.10519000	0.07330200
H	-8.09631400	9.35646800	-0.84457400
H	-10.33345900	-6.95963400	0.55515000
H	-10.29210600	-6.90956100	-1.20249100
C	-8.89484100	-8.31566400	-0.32993500
H	-8.27361300	-8.42942400	0.56800500
H	-9.58242300	-9.16880300	-0.37067000
H	-8.23175900	-8.37851500	-1.20247700
N	10.83444700	4.85862900	-0.33172900
N	10.32086500	-4.87290300	-0.16888700
C	9.67583300	-5.96900800	-0.08451500
H	10.23312300	-6.90571100	-0.05514900
H	8.57877500	-6.03202700	-0.05172700
C	11.35548500	5.35968400	0.71781600
H	11.96580800	6.25830900	0.62387200
H	11.21817400	4.94571900	1.72713400
Co	1.04236800	-1.24661000	0.11460200
Cl	1.73089200	-1.37081900	2.30827800
Cl	0.90435400	-1.45599800	-2.17282300
O	0.10999900	-3.01560800	0.28878900

C	-0.67514900	-3.47247600	1.11073900
H	-0.93199100	-4.54162700	1.00988200
C	-1.32038000	-2.72726100	2.23162100
H	-1.05400700	-1.67123000	2.21923300
H	-2.40819300	-2.87737300	2.19009700
H	-0.96868100	-3.16063300	3.17762500

Total electronic Energy (E_{total}) = -3423.622222 (Hartree/Particle).

DFT-optimized geometry of **(11a) [$Co^{II}(\eta^2$-COF-N,N′)(CH_3)(CHO)Cl_2]** (doublet) **(OHC*CH_3)**, computed at the UB3LYP-D3/ LANL2DZ (Co)/ 6-31+G* (HCNOCl) level in absence of any solvent.

Atom	x	y	z
C	5.38132600	0.89036400	-0.05278600
C	4.17720900	1.06073900	-0.11800300
C	2.77890900	1.25664100	-0.19091500
C	2.19370400	2.53730000	-0.14088700
C	1.91573900	0.14470400	-0.32101700
C	0.81149600	2.64916500	-0.19805400
H	2.82480100	3.41538200	-0.04741700
N	0.59283400	0.26022400	-0.39286300
H	2.31279800	-0.86266900	-0.35647900
C	0.02509600	1.49583800	-0.31395500
H	0.32869800	3.62029200	-0.14167100
C	-1.42503400	1.54207200	-0.27779700
N	-2.09024800	0.43739400	-0.28738600
H	-1.91108800	2.51454100	-0.16184800
C	-3.49108500	0.42644300	-0.18894100
C	-4.30390500	1.36162900	-0.85327200
C	-4.08866100	-0.56618800	0.60698400
C	-5.68680400	1.30318200	-0.73080800
H	-3.85553200	2.09312300	-1.52107800
C	-5.46621800	-0.59674400	0.76206500
H	-3.45104500	-1.27913100	1.11671300
C	-6.28962000	0.32501700	0.08495900
H	-6.30996900	1.99926400	-1.28289500
H	-5.91788500	-1.35077500	1.39810100
N	-7.69336200	0.25236200	0.20013100
C	-8.47838900	1.43624900	0.17405300
C	-8.33800400	-1.01227100	0.29847900
C	-8.09593200	2.56120200	0.92547300
C	-9.66255000	1.49178200	-0.57748300
C	-7.93566500	-2.08349900	-0.51533000
C	-9.40353300	-1.19881100	1.19474000
C	-8.87335100	3.71445600	0.91374800
H	-7.19318200	2.51677700	1.52729200
C	-10.43703500	2.65005700	-0.59270800
H	-9.98059200	0.61780200	-1.13789000
C	-8.56079300	-3.32304300	-0.40950600
H	-7.12877500	-1.94154500	-1.22803200
C	-10.05282500	-2.42698900	1.27053000
H	-9.72677500	-0.37157700	1.81947300
C	-10.04138400	3.78621500	0.13571300

H	-8.59062100	4.57692500	1.51048100
H	-11.36602400	2.66418800	-1.15601500
C	-9.62118500	-3.51612100	0.49491400
H	-8.25263400	-4.13449200	-1.06314400
H	-10.88626300	-2.56895800	1.95224400
Co	-0.72178200	-1.27240800	-0.59849100
C	6.77704200	0.66521800	0.02607000
C	7.67881100	1.75621300	0.09985400
C	7.27578100	-0.65398500	0.03384600
C	9.04815200	1.50157900	0.17682700
O	7.12216000	2.99736000	0.08897700
C	8.64420000	-0.90681900	0.11268700
H	6.56072800	-1.46524100	-0.02039200
C	9.54623300	0.18533500	0.18425800
H	9.76330700	2.31257200	0.23334800
C	7.97210600	4.14501900	0.17480100
O	9.19957600	-2.14611100	0.12735100
C	10.95051900	-0.04031800	0.26445400
H	8.55935700	4.10226500	1.10400500
H	8.67090300	4.15297400	-0.67482400
C	7.08246300	5.37921100	0.15443100
C	8.34592500	-3.29405600	0.06899300
C	12.14871300	-0.21034100	0.33324700
H	6.37594400	5.31680400	0.99268200
H	6.48552500	5.36723300	-0.76717000
C	7.89189000	6.67950100	0.24216200
H	7.65115700	-3.28194000	0.92179700
H	7.75411600	-3.26793900	-0.85812100
C	9.23094900	-4.53064600	0.11020700
H	13.20171800	-0.37306300	0.39412100
H	8.60526200	6.72754700	-0.59446200
H	8.49615100	6.67674700	1.16191000
C	7.00978100	7.93523100	0.22380500
H	9.93522400	-4.48769500	-0.73091300
H	9.83162400	-4.50285600	1.02870900
C	8.41355200	-5.82771700	0.05101400
H	6.29708500	7.88745500	1.05985200
H	6.40620900	7.93854300	-0.69541400
C	7.81955700	9.23407300	0.31204800
H	7.80628500	-5.84042000	-0.86677100
H	7.70208400	-5.85497100	0.89012700
C	9.28878400	-7.08767500	0.09239300
H	8.51863700	9.32125800	-0.52972700
H	7.16679000	10.11493000	0.29708700
H	8.40846500	9.26974100	1.23766400
H	9.99969600	-7.06084400	-0.74609400
H	9.89499100	-7.07568500	1.00969900
C	8.47115000	-8.38327300	0.03279700
H	7.87919300	-8.43433900	-0.89020700
H	9.11890000	-9.26752000	0.06406700
H	7.77370000	-8.44906300	0.87782500
N	-10.78666100	4.98459600	0.17819900
N	-10.31402700	-4.73845800	0.62716200
C	-9.67529200	-5.84093200	0.59021200
H	-10.23493700	-6.77456000	0.65328700
H	-8.58119600	-5.91140500	0.51058600
C	-11.36148900	5.42131600	-0.87202400
H	-11.96330600	6.32790400	-0.80326300
H	-11.27953300	4.94326900	-1.85878800
Cl	-2.40684700	-2.67626200	-1.16242100

Cl	-0.61855500	-1.66927000	1.77419200
C	0.48575200	-2.86281500	-0.17671000
H	-0.19731600	-3.71614600	-0.06707100
O	1.67633300	-2.87093900	-0.14639200
C	0.08515200	-1.68797700	-2.37742200
H	-0.08704000	-2.70729600	-2.71970000
H	-0.54549400	-0.99041900	-2.94458600
H	1.13807200	-1.40643000	-2.40300400

Total electronic Energy (E_{total}) = -3423.550377 (Hartree/Particle).

DFT-optimized geometry of **(12) $[Co^{II}(\eta^2\text{-COF-N,N}')(OCH_2CH_3)Cl_2]$** (singlet) **(*$OCH_2CH_3$)**, computed at the B3LYP-D3/ LANL2DZ (Co)/ 6-31+G* (HCNOCl) level in absence of any solvent.

Atom	x	y	z
C	5.34339700	0.96930800	-0.02771400
C	4.14240800	1.17101000	-0.04875600
C	2.74547100	1.38580700	-0.07691000
C	2.17788200	2.67660100	-0.02476300
C	1.86431100	0.28260600	-0.15905700
C	0.79544300	2.81963000	-0.05150000
H	2.82669600	3.54429600	0.04097700
N	0.54875800	0.43821600	-0.19253100
H	2.20474300	-0.74618200	-0.21016700
C	-0.00557800	1.67510900	-0.13207400
H	0.33358200	3.80123700	-0.00395700
C	-1.45321700	1.67712300	-0.10723300
N	-2.06896400	0.53789400	-0.12844200
H	-1.99231100	2.62032900	-0.00981400
C	-3.47858200	0.49529100	-0.07736300
C	-4.26724300	1.36542700	-0.84756400
C	-4.10082800	-0.44144800	0.76417700
C	-5.65418200	1.29899100	-0.78499700
H	-3.79379100	2.04742800	-1.54935600
C	-5.48382900	-0.47988300	0.85472100
H	-3.48331600	-1.10538000	1.35665500
C	-6.28449600	0.37573900	0.07162700
H	-6.25652200	1.94309700	-1.41726900
H	-5.95712600	-1.19074500	1.52383500
N	-7.69090400	0.28907200	0.12513000
C	-8.48846800	1.45455700	-0.03127800
C	-8.32339400	-0.97591000	0.28212400
C	-8.16058700	2.63817300	0.65273300
C	-9.63131200	1.43475800	-0.84579200
C	-7.86403200	-2.09670000	-0.42823100
C	-9.43341500	-1.11409000	1.13192700
C	-8.95026700	3.77465700	0.51397100
H	-7.29073800	2.65302000	1.30257700
C	-10.41798800	2.57606700	-0.98833300
H	-9.90813000	0.51658000	-1.35505200
C	-8.47870900	-3.33525700	-0.26496000
H	-7.02167500	-1.99409400	-1.10580100
C	-10.07046300	-2.34399600	1.26325800

H	-9.80052400	-0.24887800	1.67575700
C	-10.07580000	3.76940800	-0.32745000
H	-8.71047300	4.68355500	1.05828700
H	-11.31560200	2.53337400	-1.59905200
C	-9.58400500	-3.47940100	0.59366300
H	-8.12555300	-4.18677300	-0.84013300
H	-10.93786200	-2.44964500	1.90821500
C	6.73259800	0.69718900	-0.00243700
C	7.67506900	1.75315900	0.07064200
C	7.18381400	-0.63831700	-0.04957500
C	9.03620000	1.44809100	0.09411300
O	7.16375200	3.01276100	0.11294800
C	8.54380700	-0.94165000	-0.02541500
H	6.43856000	-1.42181800	-0.10428000
C	9.48655700	0.11553700	0.04713100
H	9.78163400	2.23142200	0.14946700
C	8.05742100	4.12723300	0.19387000
O	9.05342200	-2.19999200	-0.06663900
C	10.88362900	-0.16161200	0.07305000
H	8.67403200	4.04221200	1.10088800
H	8.72660700	4.12950800	-0.67927500
C	7.21334400	5.39260700	0.23100900
C	8.15572600	-3.31310000	-0.13656400
C	12.07648600	-0.37573300	0.09620800
H	6.53399300	5.33680200	1.09185900
H	6.58529600	5.42276400	-0.66923000
C	8.07254000	6.66063500	0.31788300
H	7.48867900	-3.30551300	0.73825400
H	7.53683400	-3.23247500	-1.04259700
C	8.99292300	-4.58280600	-0.16591600
H	13.12434700	-0.57722100	0.11633300
H	8.75843800	6.70147700	-0.54178500
H	8.70712300	6.61576000	1.21587600
C	7.23711600	7.94745000	0.35631000
H	9.67145900	-4.53751300	-1.02775600
H	9.62276700	-4.61008800	0.73283500
C	8.12333800	-5.84467400	-0.24197000
H	6.55204200	7.90708200	1.21551400
H	6.60310800	7.99269800	-0.54104000
C	8.09671500	9.21397500	0.44305500
H	7.48765500	-5.80207200	-1.13934000
H	7.43775500	-5.87359500	0.61841700
C	8.94851800	-7.13829400	-0.27115800
H	8.76930400	9.29435400	-0.42069100
H	7.47668800	10.11792300	0.46918100
H	8.71787900	9.20804900	1.34803300
H	9.63319700	-7.11011100	-1.13112000
H	9.58323700	-7.18151200	0.62569000
C	8.07828200	-8.39828800	-0.34705800
H	7.45595200	-8.39432200	-1.25127200
H	8.69086700	-9.30756000	-0.36660900
H	7.40576100	-8.46617700	0.51779400
N	-10.83709600	4.95527000	-0.41409900
N	-10.26807500	-4.69989600	0.77823600
C	-9.61510100	-5.79194300	0.85488100
H	-10.16610500	-6.72732100	0.95634900
H	-8.51757600	-5.85075000	0.83759100
C	-11.35873300	5.30412600	-1.52329200
H	-11.97468400	6.20325600	-1.55454300
H	-11.21673300	4.75628100	-2.46595900

Co	-0.76174500	-1.04705000	-0.28950700
Cl	-2.33618800	-2.49450500	-0.89014600
Cl	-0.73207000	-1.33635100	1.90481600
O	0.59463100	-2.10620600	-0.76621700
C	0.59731300	-3.51140500	-0.63222900
H	0.04571700	-3.79457900	0.27433900
H	0.07190200	-3.96809700	-1.48341100
C	2.04430200	-3.99652700	-0.55510500
H	2.07974600	-5.09168600	-0.48505800
H	2.60181300	-3.68945400	-1.44866600
H	2.54204100	-3.57585600	0.32709000

Total electronic Energy (E_{total}) = -3424.193311 (Hartree/Particle).

DFT-optimized geometry of **(12a) $[Co^{II}(\eta^2\text{-COF-N,N'})(CH(OH)CH_3)Cl_2]$** (singlet) **(*$CH(OH)CH_3$)**, computed at the B3LYP-D3/ LANL2DZ (Co)/ 6-31+G* (HCNOCl) level in absence of any solvent.

Atom	x	y	z
C	5.39936900	0.90073600	-0.01765100
C	4.19182900	1.05785500	-0.03975500
C	2.79114300	1.25220000	-0.06940500
C	2.20749500	2.53485300	-0.07705600
C	1.92116800	0.14128700	-0.09275800
C	0.82537000	2.64164400	-0.10183500
H	2.84050100	3.41633100	-0.05909500
N	0.59297000	0.24098400	-0.12716700
H	2.33596500	-0.85766300	-0.08034600
C	0.03194400	1.48600500	-0.12356900
H	0.34328200	3.61470200	-0.09944400
C	-1.41749600	1.55876300	-0.10573000
N	-2.09644900	0.46440000	-0.10010800
H	-1.88201200	2.54667300	-0.04010800
C	-3.49596900	0.46065600	-0.05733200
C	-4.28519700	1.43415200	-0.69818900
C	-4.12943400	-0.57894800	0.64755600
C	-5.67079100	1.37089200	-0.63635800
H	-3.81460500	2.20194700	-1.30699200
C	-5.51156900	-0.61862100	0.74351900
H	-3.51421000	-1.32366500	1.13823200
C	-6.30733800	0.34514100	0.09236500
H	-6.27118900	2.09860600	-1.17268100
H	-5.98795900	-1.41169300	1.31015800
N	-7.71349300	0.26697400	0.14173100
C	-8.50047900	1.45000000	0.14520100
C	-8.35973700	-1.00120700	0.14580600
C	-8.15518100	2.53294200	0.97244700
C	-9.65121200	1.54408800	-0.65288900
C	-7.92674500	-2.02482700	-0.71212800
C	-9.45670300	-1.23651600	0.99095400
C	-8.93594800	3.68386900	0.98945900
H	-7.27923800	2.45728300	1.60970800
C	-10.42879800	2.70026100	-0.63904600
H	-9.94113400	0.70119000	-1.27296800

C	-8.55409600	-3.26767800	-0.69935000
H	-7.09448400	-1.84351000	-1.38566600
C	-10.10689700	-2.46648900	0.97394300
H	-9.80313600	-0.44520300	1.64893600
C	-10.06942100	3.79580800	0.16636300
H	-8.68272500	4.51310100	1.64376500
H	-11.33261000	2.74359000	-1.24051900
C	-9.64615900	-3.51035200	0.15407200
H	-8.22157800	-4.04129500	-1.38604300
H	-10.96434600	-2.64601900	1.61585300
C	6.80176400	0.70514300	0.01112400
C	7.67966600	1.81787200	0.02462600
C	7.33205100	-0.60158100	0.02724600
C	9.05668100	1.59647900	0.05321500
O	7.09364400	3.04520800	0.00791800
C	8.70819400	-0.82113600	0.05645300
H	6.63588700	-1.43077400	0.01766300
C	9.58605400	0.29273200	0.06934300
H	9.75382800	2.42484800	0.06398300
C	7.91871800	4.21417400	0.02861600
O	9.29346200	-2.04658100	0.07407700
C	10.99734600	0.10112600	0.09866400
H	8.54271800	4.21080500	0.93451300
H	8.58311900	4.21411900	-0.84813500
C	6.99954700	5.42653000	0.01008000
C	8.46726500	-3.21545000	0.06581000
C	12.20096900	-0.03988000	0.12356500
H	6.32782300	5.37148500	0.87698200
H	6.36784400	5.37508600	-0.88666800
C	7.78028300	6.74702400	0.03047900
H	7.80529700	-3.20655900	0.94457100
H	7.84032300	-3.21860100	-0.83840200
C	9.38320800	-4.42975200	0.09184600
H	13.25917800	-0.17683200	0.14598000
H	8.45945100	6.78776300	-0.83449400
H	8.41944900	6.78405500	0.92554800
C	6.86816700	7.98114100	0.01243000
H	10.05336400	-4.38358100	-0.77647300
H	10.01777700	-4.37254300	0.98583700
C	8.59622000	-5.74681000	0.08423000
H	6.18966500	7.94072700	0.87683800
H	6.22966100	7.94460700	-0.88213700
C	7.64933400	9.30017100	0.03312900
H	7.95447400	-5.78894500	-0.80890900
H	7.91873300	-5.77779600	0.95098100
C	9.50298800	-6.98471100	0.11041900
H	8.31298500	9.37950900	-0.83758300
H	6.97546000	10.16498500	0.01971000
H	8.27255700	9.37557900	0.93354000
H	10.17986700	-6.95428900	-0.75561500
H	10.14386800	-6.94337000	1.00295800
C	8.71559900	-8.30020600	0.10251300
H	8.08966600	-8.38035700	-0.79563200
H	9.38564000	-9.16798200	0.12165500
H	8.05342100	-8.36927200	0.97520100
N	-10.82085100	4.98871500	0.24124300
N	-10.34187400	-4.73762700	0.19180700
C	-9.70049900	-5.83665700	0.11706800
H	-10.26072100	-6.77200700	0.10680600
H	-8.60412700	-5.90320200	0.07430500

C	-11.34995200	5.48156000	-0.80816200
H	-11.95814700	6.38187700	-0.71681400
H	-11.22186000	5.05867200	-1.81498700
Co	-0.73834300	-1.26535900	-0.23805000
Cl	-2.28834900	-2.47048600	-1.25947800
Cl	-0.78603900	-1.56870500	1.97772100
C	0.59676300	-2.71458500	-0.39663900
H	1.37811900	-2.36653900	0.29339300
C	1.04585900	-2.77599100	-1.84198500
H	1.90389100	-3.45765300	-1.94345900
H	0.23036500	-3.14711600	-2.46723100
H	1.35218800	-1.78957900	-2.21133200
O	0.13604200	-3.96142900	0.00630400
H	-0.22196600	-3.86448600	0.90669000

Total electronic Energy (E_{total}) = -3424.172416 (Hartree/Particle).

DFT-optimized geometry of **(13) $[Co^{II}(\eta^2\text{-COF-N,N}')(HOCH_2CH_3)Cl_2]$** (doublet) **(*$HOCH_2CH_3$)**, computed at the UB3LYP-D3/ LANL2DZ (Co)/ 6-31+G* (HCNOCl) level in absence of any solvent.

Atom	x	y	z
C	5.38464700	0.90794800	-0.03055100
C	4.17888800	1.07820400	-0.00555100
C	2.78093200	1.29499100	0.02329100
C	2.22937200	2.59261200	0.08073100
C	1.87971400	0.20406600	-0.00446000
C	0.84882000	2.74941000	0.11244000
H	2.89012600	3.45351100	0.10423600
N	0.56548000	0.36467800	0.01790400
H	2.23402400	-0.82157200	-0.04137700
C	0.03508100	1.60936900	0.08208200
H	0.40131300	3.73784200	0.16525600
C	-1.41656300	1.65501200	0.13501700
N	-2.08076200	0.54465800	0.16873600
H	-1.92043200	2.62126400	0.16957700
C	-3.48773100	0.50440800	0.14259500
C	-4.25079300	1.44259000	-0.57366600
C	-4.14148400	-0.53678500	0.82192000
C	-5.63610900	1.35000300	-0.59878600
H	-3.75701200	2.20187000	-1.17337800
C	-5.52666600	-0.61482100	0.81667500
H	-3.54741300	-1.24451800	1.39152400
C	-6.29788700	0.32250400	0.10199600
H	-6.21485500	2.05550300	-1.18616400
H	-6.02297000	-1.40814500	1.36595100
N	-7.70379100	0.21966600	0.06681100
C	-8.50794000	1.39099800	0.02964800
C	-8.32658500	-1.05846200	0.02720200
C	-8.22559100	2.47563300	0.87814100
C	-9.61243400	1.47153600	-0.83243600
C	-7.82641200	-2.06973900	-0.80886900
C	-9.46876500	-1.31713000	0.80305400
C	-9.02246500	3.61537000	0.85391600

H	-7.38582800	2.41079700	1.56351400
C	-10.40622100	2.61652900	-0.85941200
H	-9.85418700	0.62732100	-1.47113200
C	-8.43363500	-3.32232800	-0.84159400
H	-6.96121900	-1.86817300	-1.43356400
C	-10.09695600	-2.55687900	0.73941800
H	-9.86747600	-0.53548800	1.44269400
C	-10.10898200	3.71400000	-0.03178000
H	-8.81821900	4.44591200	1.52347300
H	-11.27470200	2.64957600	-1.51146500
C	-9.57156200	-3.58789800	-0.05753100
H	-8.05084600	-4.08462300	-1.51479600
H	-10.98903400	-2.75386700	1.32668500
C	6.78579100	0.70067900	-0.05733700
C	7.67365300	1.80579800	-0.05414400
C	7.30671300	-0.60928900	-0.08640000
C	9.04890400	1.57384400	-0.08048700
O	7.09793700	3.03786300	-0.02506700
C	8.68126300	-0.83956300	-0.11201600
H	6.60366800	-1.43269100	-0.08727300
C	9.56846500	0.26613000	-0.10947900
H	9.75251900	2.39683100	-0.07902900
C	7.93245800	4.19956400	-0.01675100
O	9.25646400	-2.07094900	-0.13973800
C	10.97843600	0.06366700	-0.13556100
H	8.59080900	4.17677700	0.86436000
H	8.56306400	4.20952700	-0.91819000
C	7.02293200	5.41885200	0.01981700
C	8.42021000	-3.23115500	-0.13798000
C	12.18114300	-0.08612300	-0.15745900
H	6.38473200	5.35448300	0.91102100
H	6.35652900	5.38633200	-0.85230000
C	7.81420800	6.73311100	0.03089600
H	7.79087200	-3.23289100	0.76469500
H	7.75994500	-3.21342300	-1.01815800
C	9.32509300	-4.45387700	-0.16702000
H	13.23840900	-0.23017000	-0.17667900
H	8.46001600	6.78277900	-0.85885900
H	8.48757500	6.75131800	0.90118300
C	6.91181000	7.97394200	0.06720700
H	9.96280300	-4.39854300	-1.05888400
H	9.99315200	-4.41766900	0.70333400
C	8.52641700	-5.76380500	-0.16741600
H	6.26666300	7.92473000	0.95632000
H	6.23912600	7.95615300	-0.80249500
C	7.70346600	9.28683000	0.07829500
H	7.85170500	-5.78507500	-1.03681700
H	7.88129600	-5.80356800	0.72350700
C	9.42156000	-7.01007000	-0.19550800
H	8.33382100	9.37512800	-0.81601500
H	7.03638800	10.15665300	0.10428200
H	8.36144000	9.34346500	0.95509000
H	10.06603200	-6.97115400	-1.08551300
H	10.09550400	-6.98953200	0.67300700
C	8.62209500	-8.31829700	-0.19574000
H	7.96257300	-8.37774400	-1.07127800
H	9.28396600	-9.19229400	-0.21596600
H	7.99232900	-8.39621100	0.70001200
N	-10.88091800	4.89562300	0.00323400
N	-10.25094700	-4.82469400	-0.07053600

C	-9.59302300	-5.91509800	-0.12205700
H	-10.13993200	-6.85696000	-0.17285700
H	-8.49502200	-5.96817900	-0.10589000
C	-11.35197900	5.38675700	-1.07420600
H	-11.97761700	6.27782800	-1.01604100
H	-11.15626000	4.97133100	-2.07323300
Co	-0.97094100	-1.07570700	0.12349500
Cl	-1.56026800	-1.48888300	-2.08035800
Cl	-1.00967700	-1.27428400	2.42168100
O	0.28541200	-2.64973000	-0.13039400
C	0.10097800	-3.88196200	0.61723800
H	0.17993900	-3.58413900	1.66203900
H	-0.91736300	-4.24949000	0.44071800
C	1.15193700	-4.90581900	0.21883300
H	1.02542700	-5.81952200	0.81224900
H	1.06660600	-5.17768500	-0.84091800
H	2.15931000	-4.51342000	0.39703700
H	0.09003600	-2.81079000	-1.07910000

Total electronic Energy (E_{total}) = -3424.845277 (Hartree/Particle).

DFT-optimized geometry of **(14) [$Co^{II}(\eta^2$-COF-N,N′)(CH_2CH_3)Cl_2]** (singlet) **(*CH_2CH_3)**, computed at the B3LYP-D3/ LANL2DZ (Co)/ 6-31+G* (HCNOCl) level in absence of any solvent.

Atom	x	y	z
C	5.38709300	0.81830900	-0.02672700
C	4.18204700	0.98186800	-0.09279900
C	2.78468000	1.18689800	-0.17019300
C	2.21362100	2.47545600	-0.18527800
C	1.90702900	0.08319300	-0.23791700
C	0.83326000	2.59903800	-0.24454100
H	2.85514300	3.34978000	-0.13991700
N	0.58378400	0.20314800	-0.31819100
H	2.30188300	-0.92309800	-0.22520100
C	0.03219500	1.45062400	-0.29933600
H	0.36121700	3.57698600	-0.23720800
C	-1.41735800	1.51794800	-0.26763300
N	-2.08694400	0.41650700	-0.24296300
H	-1.88987200	2.50070800	-0.18859800
C	-3.48525600	0.40317600	-0.15093300
C	-4.30340200	1.35878600	-0.78095000
C	-4.08232000	-0.62487900	0.60060300
C	-5.68536400	1.28845500	-0.66446900
H	-3.86040300	2.11680300	-1.42199400
C	-5.45965800	-0.66988200	0.75089800
H	-3.44224200	-1.35596600	1.08077500
C	-6.28601100	0.27480900	0.11004500
H	-6.31095500	2.00112700	-1.19209800
H	-5.90866800	-1.45307000	1.35255800
N	-7.68902500	0.18989200	0.21546000
C	-8.48213800	1.36872200	0.22602700
C	-8.32687900	-1.08125000	0.26901900
C	-8.11190700	2.46928600	1.01851200

C	-9.66266500	1.44179500	-0.52965700
C	-7.91829300	-2.12063800	-0.58196800
C	-9.39184000	-1.30459800	1.15734300
C	-8.89778200	3.61660200	1.04279300
H	-7.21213600	2.41019000	1.62351200
C	-10.44551200	2.59431400	-0.50880900
H	-9.97110100	0.58561100	-1.12198400
C	-8.53703300	-3.36633600	-0.52055000
H	-7.11140900	-1.94942000	-1.28821900
C	-10.03464200	-2.53813700	1.18933500
H	-9.71973100	-0.50150000	1.81051400
C	-10.06207900	3.70708300	0.26112400
H	-8.62463300	4.45965900	1.67089900
H	-11.37154900	2.62158000	-1.07647600
C	-9.59673500	-3.59676700	0.37594100
H	-8.22408100	-4.15263600	-1.20201700
H	-10.86765600	-2.70856900	1.86501600
C	6.78672600	0.61665900	0.05209500
C	7.66813500	1.72577900	0.09871300
C	7.31097700	-0.69211000	0.08570400
C	9.04235000	1.49894400	0.17604700
O	7.08802500	2.95560000	0.06300700
C	8.68434100	-0.91711400	0.16400700
H	6.61217800	-1.51839700	0.05058800
C	9.56567300	0.19305100	0.20941500
H	9.74192900	2.32452700	0.21266800
C	7.91630200	4.12102800	0.11793700
O	9.26379700	-2.14504500	0.20147600
C	10.97426900	-0.00423700	0.28885400
H	8.50736000	4.11180400	1.04563900
H	8.61182600	4.12174500	-0.73436400
C	7.00307000	5.33713600	0.07130200
C	8.43373200	-3.31043000	0.16457500
C	12.17568800	-0.15007500	0.35652300
H	6.30044600	5.28127700	0.91329900
H	6.40376500	5.29174100	-0.84773400
C	7.78757700	6.65443700	0.12517500
H	7.74118400	-3.29849100	1.01938900
H	7.83903800	-3.31168500	-0.76119500
C	9.34350100	-4.52827500	0.22334900
H	13.23187400	-0.29115900	0.41657400
H	8.49726800	6.69614800	-0.71489300
H	8.39460600	6.68520000	1.04257800
C	6.88137500	7.89221500	0.08007600
H	10.04435400	-4.48484400	-0.62054300
H	9.94603500	-4.47326700	1.13936500
C	8.55240300	-5.84238300	0.18784100
H	6.17237600	7.85078300	0.91960000
H	6.27499200	7.86200900	-0.83680100
C	7.66629500	9.20806000	0.13439800
H	7.94272000	-5.88224700	-0.72762600
H	7.84441300	-5.87065200	1.02995700
C	9.45299500	-7.08368200	0.24629400
H	8.36087200	9.28848400	-0.71175300
H	6.99662900	10.07559800	0.10079000
H	8.25731300	9.27715100	1.05676600
H	10.16047200	-7.05588600	-0.59501600
H	10.06173900	-7.04468700	1.16113700
C	8.66151900	-8.39625500	0.21024700
H	8.06784500	-8.47418100	-0.70976700

H	9.32716600	-9.26655300	0.25332800
H	7.96833200	-8.46272900	1.05873300
N	-10.81655700	4.89774800	0.34118300
N	-10.28288300	-4.82683000	0.46443600
C	-9.63754700	-5.92358600	0.39028900
H	-10.19179800	-6.86208500	0.41990400
H	-8.54296700	-5.98483600	0.31009400
C	-11.38788100	5.36723100	-0.69674100
H	-11.99697700	6.26637100	-0.59994700
H	-11.29594300	4.92505800	-1.69922200
Co	-0.74131500	-1.28363600	-0.48076600
Cl	-2.35178600	-2.55909000	-1.32584000
Cl	-0.63938600	-1.73185100	1.68295400
C	0.56003200	-2.66570000	-0.91018800
H	1.39835100	-2.58235700	-0.21136300
H	0.06987000	-3.62602400	-0.74640800
C	0.94017600	-2.43842500	-2.36754300
H	1.69520000	-3.17180200	-2.69432200
H	0.06813200	-2.55242200	-3.02004300
H	1.36928300	-1.44216500	-2.54407900

Total electronic Energy (E_{total}) = -3348.950471 (Hartree/Particle).

DFT-optimized geometry of **H_2** (singlet), computed at the B3LYP-D3/ 6-31+G* (H) level in absence of any solvent.

Atom	x	y	z
H	0.00000000	0.00000000	0.37139400
H	0.00000000	0.00000000	-0.37139400

Total electronic Energy (E_{total}) = -1.175482 (Hartree/Particle).

DFT-optimized geometry of **CO_2** (singlet), computed at the B3LYP-D3/ 6-31+G* (CO) level in absence of any solvent.

Atom	x	y	z
C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.16949100
O	0.00000000	0.00000000	-1.16949100

Total electronic Energy (E_{total}) = -188.590582 (Hartree/Particle).

DFT-optimized geometry of **CO** (singlet), computed at the B3LYP-D3/ 6-31+G* (CO) level in absence of any solvent.

Atom	x	y	z
C	0.00000000	0.00000000	-0.64984200
O	0.00000000	0.00000000	0.48738200

Total electronic Energy (E_{total}) = -113.317323 (Hartree/Particle).

DFT-optimized geometry of **H_2O** (singlet), computed at the B3LYP-D3/ 6-31+G* (HO) level in absence of any solvent.

Atom	x	y	z
O	0.00000000	0.00000000	0.11732100
H	0.00000000	0.77131200	-0.46928400
H	0.00000000	-0.77131200	-0.46928400

Total electronic Energy (E_{total}) = -76.422582 (Hartree/Particle).

DFT-optimized geometry of **CH_3OH** (singlet), computed at the B3LYP-D3/ 6-31+G* (HCO) level in absence of any solvent.

Atom	x	y	z
C	0.04669600	0.66814000	0.00000000
H	1.09545200	0.97610200	0.00000000
H	-0.43988700	1.08085100	0.89629700
H	-0.43988700	1.08085100	-0.89629700
O	0.04669600	-0.75899400	0.00000000
H	-0.86942000	-1.07469300	0.00000000

Total electronic Energy (E_{total}) = -115.726317 (Hartree/Particle).

DFT-optimized geometry of **CH_4** (singlet), computed at the B3LYP-D3/ 6-31+G* (HC) level in absence of any solvent.

Atom	x	y	z
C	0.00000000	0.00000000	0.00000000
H	0.63189600	0.63189600	0.63189600
H	-0.63189600	-0.63189600	0.63189600
H	-0.63189600	0.63189600	-0.63189600
H	0.63189600	-0.63189600	-0.63189600

Total electronic Energy (E_{total}) = -40.520768 (Hartree/Particle).

DFT-optimized geometry of **CH_3CH_2OH** (singlet), computed at the B3LYP-D3/ 6-31+G* (HCO) level in absence of any solvent.

Atom	x	y	z
C	-1.17761200	-0.40071500	0.00000000
H	-2.12438900	0.15289700	0.00000000
H	-1.14693400	-1.04194100	0.88789900
H	-1.14693400	-1.04194100	-0.88789900
C	0.00000000	0.55947900	0.00000000
H	-0.03628200	1.20685900	0.89071500
H	-0.03628200	1.20685900	-0.89071500
O	1.19868000	-0.22512900	0.00000000
H	1.96704900	0.36571400	0.00000000

Total electronic Energy (E_{total}) = -155.048833 (Hartree/Particle).

DFT-optimized geometry of **CH_3CH_3** (singlet), computed at the B3LYP-D3/ 6-31+G* (HC) level in absence of any solvent.

Atom	x	y	z
C	0.00000000	0.00000000	0.76664200
H	0.00000000	1.02209500	1.16513900
H	-0.88516000	-0.51104700	1.16513900
H	0.88516000	-0.51104700	1.16513900
C	0.00000000	0.00000000	-0.76664200
H	0.00000000	-1.02209500	-1.16513900
H	-0.88516000	0.51104700	-1.16513900
H	0.88516000	0.51104700	-1.16513900

Total electronic Energy (E_{total}) = -79.835396 (Hartree/Particle).

Calculated total electronic energy (**E_{total}**), correction of zero-point energy (**E_{ZPE}**), entropy effect (**TS**), and enthalpy effect (**$\int C_P dT$**), and Gibbs free energy (**G**) of species in the reaction.

No.	Species	E_{total} (eV)	E_{ZPE} (eV)	TS (eV)	$\int C_P dT$ (eV)	G (eV)
1	H_2O*OH_2	-93135.449128	23.4041	4.719898	25.1087	-93091.6562
2	$H_2O*COOH$	-96202.553126	23.4406	4.660773	25.1369	-96158.6364
3	HOOC*COOH	-99268.057421	23.3402	4.811217	25.0903	-99224.4381
4	OC*COOH	-97206.185396	22.9473	4.710809	24.6540	-97163.2949
4a	*COOH	-94121.544848	22.7047	4.598066	24.3539	-94079.0843
5	OC*CO	-95142.656960	22.4685	4.736642	24.1660	-95100.7591
6	OC*CHO	-95158.506675	22.7960	4.661433	24.4793	-95115.8928
6a	$OC*OH_2$	-94138.971437	22.9272	4.737650	24.6339	-94096.1480
6b	*COCHO	-95157.629951	22.8158	4.638974	24.4892	-95114.9639
7	$OC*OCH_2$	-95175.222421	23.0431	4.847859	24.7816	-95132.2456
8	$OC*OCH_3$	-95191.207540	23.4384	4.674026	25.1353	-95147.3079
8a	$*COCH_2OH$	-95191.193091	23.4819	4.642194	25.1588	-95147.1946
9	$OC*HOCH_3$	-95208.535215	23.7200	4.830650	25.4630	-95164.1829
9a	OC*O	-94103.293319	22.3511	4.593102	23.9984	-94061.5369
10	$OC*CH_3$	-93144.307010	23.3046	4.611461	24.9716	-93100.6423
10a	$*COCH_3$	-93144.071768	23.3075	4.656248	24.9798	-93100.4407
11	$*OCHCH_3$	-93161.553732	23.6234	4.701862	25.3111	-93117.3211
11a	$OHC*CH_3$	-93159.598729	23.5712	4.658498	25.2512	-93115.4348
12	$*OCH_2CH_3$	-93177.093863	23.9882	4.624339	25.6552	-93132.0748
12a	$*CH(OH)CH_3$	-93176.525281	23.9671	4.642957	25.6432	-93131.5579
13	$*HOCH_2CH_3$	-93194.834771	24.2880	4.757393	25.9900	-93149.3142
14	$*CH_2CH_3$	-91129.630847	23.8406	4.570644	25.4857	-91084.8752
	H_2 (g)	-31.986511	0.2761	0.402512	0.3660	-31.7469
	CO_2 (g)	-5131.813763	0.3146	0.661122	0.4120	-5131.7483
	CO (g)	-3083.523003	0.1366	0.610685	0.2265	-3083.7706
	H_2O (g)	-2079.565448	0.5738	0.583431	0.6766	-2078.8985
	CH_3OH (g)	-3149.075102	1.3946	0.734780	1.5104	-3146.9049
	CH_4 (g)	-1102.626826	1.2236	0.575143	1.3272	-1100.6512
	CH_3CH_2OH (g)	-4219.095814	2.1782	0.832163	2.3200	-4215.4298

	CH_3CH_3 (g)	-2172.432895	2.0398	0.702754	2.1598	-2168.9360

XYZ Coordinates:

Staggard Conformation (AB stacking) of TAPA-OPE:

Fractional atomic coordinates for the unit cell of **TAPA-OPE COF** with AB stacking.

Space group: *P*1

Lattice parameters: a = 55.8364 Å, b = 55.822884 Å, c = 9.352275 Å and α = 90.21455˚, β = 90.08816˚, γ = 119.76684˚

Atom		x	y	z
C1	C	0.30290	0.65050	0.25248
C2	C	0.28961	0.62584	0.33058
C3	C	0.28678	0.65875	0.17378
C4	C	0.26085	0.60943	0.32782
H5	H	0.30158	0.61927	0.39337
C6	C	0.25804	0.64266	0.17332
H7	H	0.29629	0.67755	0.11193
C8	C	0.24475	0.61777	0.24841
H9	H	0.25160	0.59052	0.38871
H10	H	0.24588	0.64937	0.11284
N11	N	0.39742	0.61339	0.24310
C12	C	0.19921	0.57736	0.28786
H13	H	0.20769	0.56547	0.33401
C14	C	0.39597	0.83114	0.27697
C15	C	0.38726	0.84905	0.33100
N16	N	0.42143	0.84181	0.21586
C17	C	0.40483	0.87747	0.32181
H18	H	0.36719	0.84107	0.38091
C19	C	0.43885	0.86939	0.20544
C20	C	0.43091	0.88792	0.25899
H21	H	0.39814	0.89129	0.36463
H22	H	0.45894	0.87692	0.15629
C23	C	0.44933	0.91713	0.25216
C24	C	0.46457	0.94185	0.24884
C25	C	0.48229	0.97131	0.24794
C26	C	0.47115	0.98877	0.27086
C27	C	0.51064	0.98240	0.22745
H28	H	0.51843	0.96829	0.21058
O29	O	0.55733	0.02364	0.21049
C30	C	0.43060	0.99339	0.31917
H31	H	0.43933	0.00520	0.42019
H32	H	0.43465	0.00786	0.22917
C33	C	0.39961	0.97478	0.33534

H34	H	0.39123	0.96285	0.23444
H35	H	0.39585	0.95989	0.42276
C36	C	0.38483	0.99107	0.36936
H37	H	0.38864	0.00617	0.28295
H38	H	0.39296	0.00268	0.47142
C39	C	0.35377	0.97121	0.38279
H40	H	0.34562	0.96005	0.27977
H41	H	0.35003	0.95567	0.46654
C42	C	0.33809	0.98620	0.42145
H43	H	0.34070	0.00125	0.33704
H44	H	0.31579	0.97086	0.43084
H45	H	0.34560	0.00266	0.52503
C46	C	0.34937	0.65356	0.25203
C47	C	0.37411	0.66473	0.33094
C48	C	0.34109	0.62923	0.17275
C49	C	0.39048	0.65215	0.32841
H50	H	0.38079	0.68322	0.39436
C51	C	0.35710	0.61634	0.17271
H52	H	0.32225	0.62011	0.11046
C53	C	0.38195	0.62778	0.24847
H54	H	0.40935	0.66156	0.39015
H55	H	0.35021	0.59744	0.11223
N56	N	0.38676	0.78480	0.24238
C57	C	0.42237	0.62233	0.28782
H58	H	0.43457	0.64279	0.33336
C59	C	0.16919	0.56519	0.27648
C60	C	0.15177	0.53851	0.32962
N61	N	0.15800	0.57955	0.21602
C62	C	0.12327	0.52736	0.32044
H63	H	0.16022	0.52672	0.37856
C64	C	0.13026	0.56912	0.20583
C65	C	0.11223	0.54263	0.25867
H66	H	0.10986	0.50679	0.36194
H67	H	0.12231	0.58138	0.15696
C68	C	0.08293	0.53155	0.25185
C69	C	0.05810	0.52201	0.24854
C70	C	0.02872	0.51064	0.24779
C71	C	0.01099	0.48223	0.27109
C72	C	0.01774	0.52816	0.22765
H73	H	0.03207	0.54991	0.21097
O74	O	0.97683	0.53444	0.21030
C75	C	0.00583	0.43690	0.31962
H76	H	0.99422	0.43419	0.42050
H77	H	0.99120	0.42674	0.22934
C78	C	0.02401	0.42385	0.33547
H79	H	0.03558	0.42691	0.23417
H80	H	0.03921	0.43478	0.42259
C81	C	0.00741	0.39296	0.36969
H82	H	0.99200	0.38179	0.28374
H83	H	0.99612	0.38987	0.47208
C84	C	0.02702	0.38128	0.38259
H85	H	0.03794	0.38392	0.27954
H86	H	0.04279	0.39294	0.46618
C87	C	0.01189	0.35078	0.42166
H88	H	0.99645	0.33840	0.33815
H89	H	0.02709	0.34350	0.42996
H90	H	1.00124	0.34759	0.52604
C91	C	0.34610	0.69687	0.25106
C92	C	0.33513	0.71082	0.32895
C93	C	0.37044	0.71261	0.17240

C94	C	0.34785	0.73961	0.32642
H95	H	0.31665	0.69929	0.39215
C96	C	0.38346	0.74135	0.17223
H97	H	0.37937	0.70255	0.11111
C98	C	0.37226	0.75519	0.24733
H99	H	0.33865	0.74936	0.38804
H100	H	0.40241	0.75305	0.11266
N101	N	0.21525	0.60249	0.24274
C102	C	0.37806	0.80114	0.28817
H103	H	0.35775	0.79309	0.33427
C104	C	0.43473	0.60440	0.27661
C105	C	0.46126	0.61331	0.33091
N106	N	0.42015	0.57893	0.21513
C107	C	0.47234	0.59576	0.32181
H108	H	0.47320	0.63345	0.38080
C109	C	0.43054	0.56145	0.20485
C110	C	0.45692	0.56960	0.25887
H111	H	0.49284	0.60264	0.36436
H112	H	0.41816	0.54135	0.15508
C113	C	0.46802	0.55121	0.25193
C114	C	0.47759	0.53600	0.24861
C115	C	0.48920	0.51798	0.24775
C116	C	0.51767	0.52882	0.27114
C117	C	0.47180	0.48963	0.22732
H118	H	0.45001	0.48212	0.21046
O119	O	0.46590	0.44257	0.21005
C120	C	0.56294	0.56907	0.31969
H121	H	0.56598	0.56041	0.42067
H122	H	0.57313	0.56459	0.22968
C123	C	0.57569	0.60022	0.33546
H124	H	0.57233	0.60857	0.23428
H125	H	0.56477	0.60450	0.42249
C126	C	0.60664	0.61460	0.36978
H127	H	0.61777	0.61037	0.28365
H128	H	0.60998	0.60650	0.47197
C129	C	0.61815	0.64579	0.38320
H130	H	0.61525	0.65395	0.28032
H131	H	0.60656	0.64993	0.46700
C132	C	0.64873	0.66117	0.42202
H133	H	0.66101	0.65803	0.33830
H134	H	0.65590	0.68359	0.43027
H135	H	0.65223	0.65387	0.52627
C136	C	0.69717	0.34945	0.24261
C137	C	0.71052	0.37420	0.16541
C138	C	0.71320	0.34101	0.32058
C139	C	0.73932	0.39057	0.16856
H140	H	0.69865	0.38094	0.10310
C141	C	0.74197	0.35706	0.32142
H142	H	0.70366	0.32215	0.38181
C143	C	0.75532	0.38205	0.24743
H144	H	0.74863	0.40955	0.10827
H145	H	0.75407	0.35023	0.38154
N146	N	0.60282	0.38697	0.25324
C147	C	0.80089	0.42254	0.21022
H148	H	0.79245	0.43455	0.16509
C149	C	0.60369	0.16878	0.22137
C150	C	0.61247	0.15085	0.16885
N151	N	0.57816	0.15817	0.28153
C152	C	0.59491	0.12243	0.17861
H153	H	0.63260	0.15878	0.11973

C154	C	0.56073	0.13059	0.29247
C155	C	0.56876	0.11203	0.24046
H156	H	0.60167	0.10858	0.13702
H157	H	0.54059	0.12310	0.34084
C158	C	0.55035	0.08281	0.24781
C159	C	0.53514	0.05810	0.25145
C160	C	0.51743	0.02863	0.25260
C161	C	0.52858	0.01118	0.22971
C162	C	0.48907	0.01754	0.27313
H163	H	0.48127	0.03164	0.28997
O164	O	0.44240	0.97628	0.29003
C165	C	0.56906	0.00646	0.18158
H166	H	0.56031	0.99463	0.08065
H167	H	0.56497	0.99201	0.27172
C168	C	0.60008	0.02495	0.16533
H169	H	0.60851	0.03690	0.26614
H170	H	0.60391	0.03984	0.07778
C171	C	0.61469	0.00850	0.13149
H172	H	0.61080	0.99339	0.21803
H173	H	0.60651	0.99688	0.02951
C174	C	0.64578	0.02819	0.11798
H175	H	0.65399	0.03936	0.22092
H176	H	0.64962	0.04373	0.03411
C177	C	0.66128	0.01300	0.07951
H178	H	0.65857	0.99794	0.16403
H179	H	0.68361	0.02823	0.07009
H180	H	0.65372	1.00185	-0.02402
C181	C	0.65073	0.34659	0.24306
C182	C	0.62583	0.33541	0.16521
C183	C	0.65918	0.37108	0.32141
C184	C	0.60955	0.34807	0.16806
H185	H	0.61900	0.31681	0.10235
C186	C	0.64325	0.38404	0.32176
H187	H	0.67812	0.38023	0.38301
C188	C	0.61826	0.37255	0.24725
H189	H	0.59058	0.33863	0.10704
H190	H	0.65027	0.40302	0.38175
N191	N	0.61287	0.21515	0.25393
C192	C	0.57778	0.37795	0.21022
H193	H	0.56546	0.35740	0.16591
C194	C	0.83091	0.43470	0.22218
C195	C	0.84834	0.46150	0.17063
N196	N	0.84206	0.42023	0.28173
C197	C	0.87684	0.47266	0.18046
H198	H	0.83992	0.47337	0.12244
C199	C	0.86979	0.43068	0.29253
C200	C	0.88785	0.45729	0.24129
H201	H	0.89026	0.49332	0.14019
H202	H	0.87772	0.41833	0.34062
C203	C	0.91714	0.46842	0.24868
C204	C	0.94198	0.47800	0.25232
C205	C	0.97136	0.48940	0.25336
C206	C	0.98909	0.51782	0.23010
C207	C	0.98234	0.47189	0.27356
H208	H	0.96803	0.45013	0.29020
O209	O	0.02327	0.46563	0.29081
C210	C	0.99434	0.56317	0.18150
H211	H	0.00595	0.56585	0.08068
H212	H	0.00897	0.57330	0.27184
C213	C	0.97628	0.57636	0.16547

H214	H	0.96473	0.57338	0.26674
H215	H	0.96108	0.56547	0.07834
C216	C	0.99305	0.60724	0.13108
H217	H	0.00847	0.61837	0.21703
H218	H	0.00432	0.61025	0.02872
C219	C	0.97360	0.61911	0.11791
H220	H	0.96270	0.61656	0.22092
H221	H	0.95781	0.60749	0.03435
C222	C	0.98891	0.64960	0.07859
H223	H	0.00439	0.66193	0.16205
H224	H	0.97382	0.65702	0.07017
H225	H	0.00046	0.65270	-0.02579
C226	C	0.65377	0.30313	0.24406
C227	C	0.66473	0.28904	0.16710
C228	C	0.62930	0.28743	0.32198
C229	C	0.65192	0.26025	0.16988
H230	H	0.68330	0.30050	0.10440
C231	C	0.61619	0.25868	0.32241
H232	H	0.62035	0.29754	0.38267
C233	C	0.62740	0.24475	0.24838
H234	H	0.66111	0.25042	0.10889
H235	H	0.59717	0.24704	0.38163
N236	N	0.78484	0.39731	0.25375
C237	C	0.62162	0.19877	0.20966
H238	H	0.64201	0.20677	0.16462
C239	C	0.56542	0.39589	0.22198
C240	C	0.53877	0.38687	0.16939
N241	N	0.58013	0.42144	0.28235
C242	C	0.52767	0.40441	0.17908
H243	H	0.52673	0.36666	0.12038
C244	C	0.56972	0.43891	0.29319
C245	C	0.54322	0.43064	0.24090
H246	H	0.50708	0.39745	0.13784
H247	H	0.58221	0.45908	0.34205
C248	C	0.53207	0.44901	0.24834
C249	C	0.52248	0.46417	0.25198
C250	C	0.51084	0.48218	0.25311
C251	C	0.48236	0.47133	0.22977
C252	C	0.52824	0.51053	0.27359
H253	H	0.55004	0.51807	0.29041
O254	O	0.53411	0.55759	0.29080
C255	C	0.43706	0.43114	0.18129
H256	H	0.43404	0.43984	0.08039
H257	H	0.42692	0.43566	0.27141
C258	C	0.42418	0.39998	0.16541
H259	H	0.42748	0.39158	0.26653
H260	H	0.43504	0.39563	0.07831
C261	C	0.39323	0.38577	0.13111
H262	H	0.38217	0.39008	0.21730
H263	H	0.38996	0.39393	0.02897
C264	C	0.38153	0.35455	0.11754
H265	H	0.38436	0.34633	0.22038
H266	H	0.39305	0.35033	0.03371
C267	C	0.35095	0.33937	0.07868
H268	H	0.33874	0.34260	0.16243
H269	H	0.34363	0.31692	0.07038
H270	H	0.34752	0.34673	-0.02555
N271	N	0.33285	0.66707	0.25216
N272	N	0.66712	0.33294	0.24287
C273	C	0.97284	0.98057	0.75737

C274	C	0.95948	0.95579	0.83459
C275	C	0.95679	0.98898	0.67942
C276	C	0.93068	0.93943	0.83144
H277	H	0.97135	0.94906	0.89690
C278	C	0.92803	0.97294	0.67857
H279	H	0.96634	0.00786	0.61820
C280	C	0.91469	0.94795	0.75256
H281	H	0.92137	0.92045	0.89173
H282	H	0.91593	0.97977	0.61846
N283	N	0.06716	0.94304	0.74676
C284	C	0.86912	0.90747	0.78980
H285	H	0.87755	0.89545	0.83491
C286	C	0.06631	0.16120	0.77867
C287	C	0.05753	0.17917	0.83110
N288	N	0.09185	0.17185	0.71846
C289	C	0.07508	0.20756	0.82135
H290	H	0.03739	0.17122	0.88027
C291	C	0.10926	0.19940	0.70751
C292	C	0.10125	0.21799	0.75948
H293	H	0.06834	0.22142	0.86301
H294	H	0.12941	0.20690	0.65917
C295	C	0.11963	0.24717	0.75220
C296	C	0.13487	0.27191	0.74858
C297	C	0.15256	0.30136	0.74742
C298	C	0.14143	0.31883	0.77029
C299	C	0.18093	0.31247	0.72686
H300	H	0.18873	0.29836	0.71004
O301	O	0.22760	0.35372	0.70998
C302	C	0.10094	0.32354	0.81843
H303	H	0.10969	0.33537	0.91937
H304	H	0.10503	0.33800	0.72829
C305	C	0.06992	0.30505	0.83466
H306	H	0.06149	0.29310	0.73385
H307	H	0.06609	0.29017	0.92223
C308	C	0.05531	0.32150	0.86849
H309	H	0.05920	0.33661	0.78198
H310	H	0.06349	0.33312	0.97048
C311	C	0.02422	0.30181	0.88202
H312	H	0.01601	0.29064	0.77908
H313	H	0.02038	0.28627	0.96589
C314	C	0.00872	0.31700	0.92049
H315	H	0.01143	0.33206	0.83596
H316	H	0.01361	0.30177	0.92991
H317	H	0.01628	0.32815	1.02402
C318	C	0.01926	0.98344	0.75695
C319	C	0.04418	0.99458	0.83478
C320	C	0.01083	0.95891	0.67857
C321	C	0.06044	0.98194	0.83193
H322	H	0.05100	0.01319	0.89766
C323	C	0.02674	0.94597	0.67823
H324	H	0.99188	0.94977	0.61699
C325	C	0.05175	0.95743	0.75274
H326	H	0.07942	0.99137	0.89296
H327	H	0.01973	0.92698	0.61826
N328	N	0.05714	0.11485	0.74611
C329	C	0.09224	0.95204	0.78980
H330	H	0.10454	0.97260	0.83409
C331	C	0.83908	0.89529	0.77781
C332	C	0.82166	0.86851	0.82936
N333	N	0.82795	0.90977	0.71828

C334	C	0.79316	0.85733	0.81953
H335	H	0.83008	0.85663	0.87757
C336	C	0.80020	0.89932	0.70747
C337	C	0.78216	0.87271	0.75870
H338	H	0.77974	0.83668	0.85982
H339	H	0.79228	0.91167	0.65939
C340	C	0.75285	0.86158	0.75133
C341	C	0.72803	0.85200	0.74769
C342	C	0.69864	0.84060	0.74663
C343	C	0.68091	0.81218	0.76990
C344	C	0.68766	0.85811	0.72643
H345	H	0.70197	0.87987	0.70980
O346	O	0.64672	0.86437	0.70919
C347	C	0.67566	0.76683	0.81850
H348	H	0.66404	0.76415	0.91932
H349	H	0.66103	0.75670	0.72816
C350	C	0.69372	0.75364	0.83453
H351	H	0.70527	0.75662	0.73327
H352	H	0.70892	0.76453	0.92166
C353	C	0.67695	0.72276	0.86892
H354	H	0.66153	0.71163	0.78297
H355	H	0.66568	0.71975	0.97128
C356	C	0.69640	0.71089	0.88209
H357	H	0.70730	0.71344	0.77908
H358	H	0.71219	0.72251	0.96565
C359	C	0.68109	0.68040	0.92141
H360	H	0.66561	0.66807	0.83794
H361	H	0.69618	0.67299	0.92983
H362	H	0.67046	0.67730	1.02579
C363	C	0.01624	0.02692	0.75593
C364	C	0.00526	0.04094	0.83288
C365	C	0.04069	0.04255	0.67800
C366	C	0.01809	0.06977	0.83009
H367	H	0.98671	0.02951	0.89563
C368	C	0.05381	0.07133	0.67756
H369	H	0.04965	0.03246	0.61736
C370	C	0.04259	0.08524	0.75160
H371	H	0.00889	0.07958	0.89112
H372	H	0.07283	0.08296	0.61838
N373	N	0.88515	0.93268	0.74625
C374	C	0.04837	0.13124	0.79034
H375	H	0.02799	0.12323	0.83539
C376	C	0.10458	0.93411	0.77801
C377	C	0.13123	0.94313	0.83061
N378	N	0.08987	0.90856	0.71765
C379	C	0.14233	0.92559	0.82092
H380	H	0.14327	0.96334	0.87962
C381	C	0.10028	0.89109	0.70680
C382	C	0.12679	0.89936	0.75910
H383	H	0.16292	0.93255	0.86216
H384	H	0.08779	0.87092	0.65796
C385	C	0.13793	0.88099	0.75167
C386	C	0.14752	0.86583	0.74803
C387	C	0.15916	0.84782	0.74689
C388	C	0.18764	0.85867	0.77023
C389	C	0.14176	0.81947	0.72640
H390	H	0.11996	0.81193	0.70959
O391	O	0.13589	0.77241	0.70920
C392	C	0.23294	0.89886	0.81871
H393	H	0.23596	0.89016	0.91961

H394	H	0.24308	0.89434	0.72859
C395	C	0.24582	0.93002	0.83459
H396	H	0.24252	0.93842	0.73346
H397	H	0.23496	0.93437	0.92169
C398	C	0.27677	0.94423	0.86889
H399	H	0.28783	0.93992	0.78270
H400	H	0.28004	0.93607	0.97103
C401	C	0.28847	0.97545	0.88246
H402	H	0.28564	0.98367	0.77962
H403	H	0.27695	0.97967	0.96629
C404	C	0.31905	0.99063	0.92132
H405	H	0.33126	0.98740	0.83757
H406	H	0.32637	1.01308	0.92962
H407	H	0.32248	0.98327	1.02555
C408	C	0.36711	0.67951	0.74749
C409	C	0.38039	0.70415	0.66941
C410	C	0.38322	0.67124	0.82622
C411	C	0.40914	0.72057	0.67218
H412	H	0.36842	0.71073	0.60664
C413	C	0.41196	0.68734	0.82667
H414	H	0.37371	0.65245	0.88807
C415	C	0.42525	0.71223	0.75159
H416	H	0.41840	0.73948	0.61130
H417	H	0.42412	0.68063	0.88716
N418	N	0.27256	0.71661	0.75690
C419	C	0.47080	0.75265	0.71216
H420	H	0.46231	0.76453	0.66599
C421	C	0.27403	0.49885	0.72307
C422	C	0.28273	0.48096	0.66896
N423	N	0.24857	0.48820	0.78414
C424	C	0.26517	0.45253	0.67814
H425	H	0.30281	0.48893	0.61908
C426	C	0.23114	0.46060	0.79455
C427	C	0.23909	0.44210	0.74095
H428	H	0.27187	0.43872	0.63539
H429	H	0.21106	0.45308	0.84373
C430	C	0.22066	0.41285	0.74785
C431	C	0.20544	0.38817	0.75120
C432	C	0.18771	0.35868	0.75208
C433	C	0.19885	0.34124	0.72913
C434	C	0.15936	0.34760	0.77255
H435	H	0.15157	0.36171	0.78943
O436	O	0.11267	0.30636	0.78952
C437	C	0.23940	0.33661	0.68085
H438	H	0.23067	0.32480	0.57982
H439	H	0.23534	0.32214	0.77084
C440	C	0.27040	0.35522	0.66467
H441	H	0.27878	0.36715	0.76556
H442	H	0.27415	0.37011	0.57725
C443	C	0.28517	0.33893	0.63063
H444	H	0.28137	0.32383	0.71704
H445	H	0.27703	0.32732	0.52858
C446	C	0.31623	0.35879	0.61720
H447	H	0.32438	0.36995	0.72023
H448	H	0.31997	0.37433	0.53347
C449	C	0.33191	0.34380	0.57854
H450	H	0.32930	0.32875	0.66297
H451	H	0.35421	0.35914	0.56917
H452	H	0.32441	0.33266	0.47496
C453	C	0.32061	0.67646	0.74796

C454	C	0.29589	0.66526	0.66905
C455	C	0.32891	0.70076	0.82723
C456	C	0.27952	0.67786	0.67158
H457	H	0.28921	0.64678	0.60564
C458	C	0.31289	0.71366	0.82728
H459	H	0.34775	0.70989	0.88954
C460	C	0.28806	0.70221	0.75152
H461	H	0.26065	0.66843	0.60984
H462	H	0.31978	0.73256	0.88777
N463	N	0.28325	0.54520	0.75766
C464	C	0.24764	0.70767	0.71220
H465	H	0.23543	0.68721	0.66664
C466	C	0.50081	0.76480	0.72351
C467	C	0.51823	0.79149	0.67038
N468	N	0.51201	0.75045	0.78399
C469	C	0.54673	0.80263	0.67955
H470	H	0.50978	0.80328	0.62144
C471	C	0.53974	0.76088	0.79417
C472	C	0.55778	0.78737	0.74133
H473	H	0.56013	0.82321	0.63807
H474	H	0.54770	0.74862	0.84305
C475	C	0.58706	0.79845	0.74816
C476	C	0.61190	0.80799	0.75146
C477	C	0.64127	0.81936	0.75221
C478	C	0.65901	0.84777	0.72890
C479	C	0.65225	0.80184	0.77235
H480	H	0.63793	0.78009	0.78903
O481	O	0.69317	0.79556	0.78970
C482	C	0.66417	0.89310	0.68038
H483	H	0.67577	0.89581	0.57950
H484	H	0.67880	0.90326	0.77066
C485	C	0.64599	0.90615	0.66453
H486	H	0.63442	0.90309	0.76583
H487	H	0.63079	0.89522	0.57741
C488	C	0.66259	0.93704	0.63031
H489	H	0.67800	0.94822	0.71626
H490	H	0.67388	0.94013	0.52792
C491	C	0.64297	0.94872	0.61741
H492	H	0.63206	0.94608	0.72045
H493	H	0.62721	0.93706	0.53382
C494	C	0.65811	0.97922	0.57834
H495	H	0.67355	0.99160	0.66185
H496	H	0.64291	0.98650	0.57004
H497	H	0.66876	0.98241	0.47396
C498	C	0.32391	0.63317	0.74893
C499	C	0.33487	0.61916	0.67103
C500	C	0.29954	0.61737	0.82758
C501	C	0.32216	0.59040	0.67355
H502	H	0.35336	0.63071	0.60788
C503	C	0.28654	0.58866	0.82775
H504	H	0.29063	0.62745	0.88892
C505	C	0.29773	0.57480	0.75265
H506	H	0.33135	0.58064	0.61198
H507	H	0.26759	0.57694	0.88736
N508	N	0.45474	0.72750	0.75726
C509	C	0.29194	0.52887	0.71185
H510	H	0.31226	0.53690	0.66575
C511	C	0.23527	0.72561	0.72339
C512	C	0.20874	0.71669	0.66909
N513	N	0.24985	0.75107	0.78487

C514	C	0.19766	0.73425	0.67818
H515	H	0.19680	0.69655	0.61920
C516	C	0.23946	0.76855	0.79514
C517	C	0.21308	0.76040	0.74113
H518	H	0.17716	0.72736	0.63565
H519	H	0.25184	0.78865	0.84493
C520	C	0.20198	0.77879	0.74807
C521	C	0.19241	0.79400	0.75140
C522	C	0.18080	0.81202	0.75225
C523	C	0.15233	0.80118	0.72886
C524	C	0.19820	0.84037	0.77268
H525	H	0.21999	0.84789	0.78954
O526	O	0.20410	0.88743	0.78995
C527	C	0.10706	0.76093	0.68031
H528	H	0.10402	0.76959	0.57933
H529	H	0.09687	0.76541	0.77032
C530	C	0.09431	0.72978	0.66454
H531	H	0.09767	0.72143	0.76571
H532	H	0.10523	0.72550	0.57751
C533	C	0.06336	0.71540	0.63022
H534	H	0.05223	0.71963	0.71635
H535	H	0.06002	0.72350	0.52803
C536	C	0.05185	0.68421	0.61680
H537	H	0.05475	0.67605	0.71968
H538	H	0.06344	0.68007	0.53300
C539	C	0.02127	0.66883	0.57798
H540	H	0.00899	0.67196	0.66170
H541	H	0.01410	0.64641	0.56973
H542	H	0.01777	0.67613	0.47373
N543	N	0.00287	0.99700	0.75715
N544	N	0.33714	0.66288	0.74784

<u>Eclipsed Conformation (AA stacking) of TAPA-OPE</u>:

Space group: $P\bar{3}$

Lattice parameters: a = b = 55.932229 Å, c = 4.128009 Å and α = β = 90˚, γ = 120˚

Atom		x	y	z
C2	C	0.30319	-0.34952	3.12770
C3	C	0.28906	-0.37524	3.28573
C4	C	0.28724	-0.33997	2.97030
C5	C	0.26024	-0.39076	3.28715
H6	H	0.30022	-0.38370	3.40494
C7	C	0.25844	-0.35537	2.97200
H8	H	0.29692	-0.32034	2.84958
C9	C	0.24461	-0.38082	3.13037
H10	H	0.25066	-0.41038	3.41088
H11	H	0.24679	-0.34739	2.84884
N32	N	0.39568	-0.38940	3.12258
C35	C	0.19847	-0.41891	3.26562
H36	H	0.20630	-0.42947	3.41255
C41	C	0.40017	-0.16844	3.22929
C42	C	0.39240	-0.15056	3.37062
N43	N	0.42411	-0.15782	3.05691

C44	C	0.40930	-0.12209	3.33159
H45	H	0.37352	-0.15853	3.50982
C46	C	0.44091	-0.13018	3.01678
C47	C	0.43376	-0.11173	3.15360
H48	H	0.40338	-0.10820	3.44091
H49	H	0.45969	-0.12265	2.87685
C68	C	0.45129	-0.08248	3.11127
C69	C	0.46585	-0.05792	3.07718
C74	C	0.48305	-0.02851	3.03922
C75	C	0.47480	-0.01068	3.17250
C76	C	0.50785	-0.01805	2.86737
H79	H	0.51329	-0.03252	2.76552
O98	O	0.55062	0.02261	2.66039
C104	C	0.43861	-0.00527	3.43410
H105	H	0.45197	0.00954	3.62326
H106	H	0.43758	0.00625	3.22035
C107	C	0.40953	-0.02326	3.56901
H108	H	0.39700	-0.03956	3.38910
H109	H	0.41069	-0.03355	3.79396
C110	C	0.39566	-0.00613	3.64057
H111	H	0.39519	0.00459	3.41628
H112	H	0.40787	0.00981	3.82524
C113	C	0.36608	-0.02450	3.76319
H114	H	0.35375	-0.04042	3.57863
H115	H	0.36633	-0.03521	3.98842
C116	C	0.35211	-0.00758	3.83287
H117	H	0.35018	0.00206	3.60664
H118	H	0.33114	-0.02125	3.93247
H119	H	0.36422	0.00887	4.01258
N1	N	0.33333	-0.33333	3.12719

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