Electronic Supplementary Material (ESI) for Nanoscale Horizons.

Supporting Information

A Highly Selective and Active Metal-free Catalyst for Ammonia Production

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EXPERIMENTAL PROCEDURES

1 Materials

Carbon fiber cloth was purchased from CeTech (Taiwan). Diisopropylamine (DIPA), ethynyltrimethylsilane, and triphenylphosphine (PPh_3) were purchased from Energy Chemical. Tetrahydrofuran (THF) is refluxed with sodium to remove the remaining water. All other reagents, unless otherwise specified, were analytical grade and used without further purification. Ultrapure water was produced from the Millipore Milli-Q water purification system. The high-purity N_2 (≥ 99.999%) gas used for NRR was first purified by alkaline aqueous solution to remove NO_x, followed by being dried by drying tower, before being bubbled into the electrolytes.

2 Synthesis of 3D fluorographdiyne networks

FGDY was synthesized according to the previous report.[1] Several pieces of copper foil and commercial carbon fiber cloth (CF) were kept at 50 °C for 2 hours in a three-necked flask containing 5 mL pyridine, 50 ml acetone and 1 mL TMEDA solution. Subsequently, 50ml acetone of the monomer 1,3,5-triethynyl-2,4,6-trifluorobenzene was added in a very slow speed into the above reactor. After a 12 h reaction at 50 °C in dark, the surface of CF turned black, suggesting the successful loading of cFGDY. Then the fresh-prepared FGDY was washed with hot acetone and DMF, KOH (4 M), HCl (6 M), KOH (4 M) and water sequentially, and followed by drying in 40 ℃ vacuum oven for 12 hours.

3 Electrochemical measurements

All electrochemical measurements were conducted by using an electrochemical workstation (CHI 660E). The H-type electrolyte cell separated by the pre-treated Nafion 117 membrane was used as the electrochemical reactor. For NRR, 30 mL N_2-saturated 0.1 M Na_2SO_4 was used as the electrolyte. During the NRR process, the N_2 was continuously bubbled into the electrolyte.

4 NH_3 determination

The calibrated standard curves were recorded to determine the concentration of NH_3. In 0.1 M Na_2SO_4 solution, a spectrophotometry method was employed to detect the resulted NH_3. Firstly, 4 mL of post-tested solution was removed from the cathodic chamber, secondly 50 μL oxidizing solution [a mixture of NaClO (ρCl=4~4.9) and 0.75 M NaOH], 500 μL coloring solution (a mixture of 0.4 M $C_7H_5O_3Na$ and 0.32 M NaOH) and 50 μL $Na_2[Fe(CN)_5NO]\cdot 2H_2O$ (1.0 wt.%) were added into above solution. A UV-Vis absorption measurements were conducted after 2 h. For each standard solution, the absorbance at the wavelength of 655 nm was plotted against NH_4Cl concentration. The calibration curve showed good linear relationship (y=0.145x-0.034).

The average NH_3 yield (y_{NH3}) can be calculated using the following equation:

$$y_{NH3} = \frac{0.318 \times C_{NH4^+} \times V}{t \times m_{cat}}$$

where C_{NH4Cl} is the mass concentration of NH_4Cl, V is volume of cathodic electrolyte, t is the time for NRR, $m_{cat.}$ is the mass loading of the sample.

Faradic efficiency (FE) can be calculated as following:

$$FE = \frac{3 \times F \times 0.318 \times C_{NH4^+} \times V}{Q}$$

where F is Faradic Constant and Q is the electric quantity.

5 Computational Details

5.1 NRR Calculations

Density functional theory (DFT) calculations based on the CASTEP code have been performed for NRR investigation of FGDY[2]. The generalized gradient approximation (GGA) in the parametrization of Perdew-Burke-Ernzerhof (PBE) for the exchange-correlation energy was used and the cutoff energy of the plane-wave basis set was set to be 380 eV [3,4]. The Hellmann-Feynman forces during all the geometry optimization will be converged to less than 0.001 eV/A, meanwhile, the total energy and inter-ionic displacement will be set as 5×10^{-5} eV/atom and

0.005 Å. The coarse k-point has been applied for the energy minimization based on the Broyden-Fletcher-Goldfarb-Shannon (BFGS) algorithm [5]. The band energy tolerance for the optical properties calculation has been set as 1×10^{-5} eV.

5.2 Geometry Optimizations and Energy Calculations

The Vienna ab initio package (VASP) was employed for the comprehensive structural analysis to resolve the intrinsic crystal structure of FGDY. All the geometry optimizations and energy calculations of related structures in this work were performed with plane-wave density functional theory (DFT) calculations by the Vienna ab initio package (VASP), under the generalized gradient approximation (GGA) with the Perdew-Burke-Ernzerhof (PBE) functional.

The Gibbs free energies difference of intermediates involved in NRR pathways can be calculated by utilizing the computational hydrogen electrode model [1, 2]:

$$\Delta G = \Delta E + \Delta ZPE - T\Delta S \qquad (1)$$

Where ΔE is the energy difference of adsorption. ΔZPE and TΔS are the zero-point energy correction term and the entropy correction term, respectively. The two terms are obtained by the frequency calculation at T=300K [3]. The Gibbs free energy of $(H^+ + e^-)$ is equivalent to the energy of $1/2G_{H2}$ in the study.

ZPE values of adsorbed species is derived after the frequency calculation by [1]:

$$ZPE = \frac{1}{2}\sum h\nu_i \qquad (2)$$

TS values of adsorbed species is also calculated using the vibrational frequencies by [4]:

$$TS_\nu = k_B T\left[\sum_K \ln\left(\frac{1}{1-e^{-h\nu_K/k_B T}}\right) + \sum_K \frac{h\nu_K}{k_B T}\frac{1}{(e^{h\nu_K/k_B T}-1)}\right] \qquad (3)$$

Where k_B is the Boltzmann constant, T is Temperature, K is vibrational mode, ν is vibrational frequency for the intermediates, which is obtained from DFT calculations.

References

[1]J. K. Norskov *et al.*, Origin of the overpotential for oxygen reduction at a fuel-cell cathode. *J. Phys. Chem. B* 2004, *108*, 17886.

[2]Y. Jiao, Y. Zheng, M. Jaroniec, S. Z. Qiao, Origin of the Electrocatalytic Oxygen

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[3]B. Delley, An all-electron numerical-method for solving the local density functional for polyatomic-molecules. *J. Chem. Phys.* 1990, *92*, 508.

L. I. Bendavid, E. A. Carter, CO_2 Adsorption on Cu_2O(111): A DFT+U and DFT-D Study. *J. Phys. Chem. C* 2013, *117*, 26048.

6 Structural Analysis of cFGDY

6.1 Symmetry Analysis

Herein, we decide to perform a comprehensive structural analysis to resolve the intrinsic crystal structure of cFGDY by using Vienna ab initio package (VASP). According to the symmetric nature of the monomer, a single layer of cFGDY should exhibit hexagonal pores with the D6h point group symmetry (Figure S6a, shown as red crosses) and a periodic structure of the P6/mmm space group where the unit cell contains two monomer units (Figure S5a, shown as the blue diamond). The selective area electron diffraction (SAED) pattern of cFGDY from the normal direction of its 2D plane (Figure S5b) was obtained from the transmission electron microscopy (TEM). Indeed, the SAED pattern clearly reflects a reciprocal lattice complying with the D6h point group and the P6/mmm space group of the expected cFGDY structure of a single layer.

6.2 Theory of Stacking Modes

Subsequently, we need to consider the stacking mode of the multi-layer cFGDY and resolve the actual stacking mode which has formed the SAED pattern. Firstly, we define the in-plane component of the minimum offset vector of a 2D layer with respect to its adjacent identical 2D layer as the stacking vector (***S***), which describes how much two adjacent 2D layers offsetting each other within the 2D plane. Taking account of the intrinsic 2D symmetries, ***S*** represents a group of crystallographic directions which are geometrically identical to each other. For example, the cFGDY single layer bears D_{6h} symmetry and its ***S*** with respect to a certain stacking mode should contain six identical vector elements. Therefore, by applying those identical vector

elements of $\boldsymbol{S}$ with respect to a specific stacking mode, the minimum number of layers needed (n) to exhaust all the possibilities of layer offsetting in 2D without overlapping, is used to identify this specific stacking mode as n-fold stacking. Therefore, each stacking mode must be characteristic of a unique $\boldsymbol{S}$ and a corresponding unique $|\boldsymbol{S}|$, namely $\mathbf{S}_n$ and $|\boldsymbol{S}_n|$ with respect to n-fold stacking. For example, AA stacking is a 1-fold stacking characteristic of $\boldsymbol{S}_1$ (vector size $|\boldsymbol{S}_1|$ equal to the lattice constant $|\boldsymbol{a}|$) and ABC stacking is a 3-fold stacking characteristic of $\boldsymbol{S}_3$ (vector size $|\boldsymbol{S}_3|$).

6.3 Stacking Mode Analysis

We listed possible stacking modes of cFGDY (i.e. the P6/mmm space group) from 1-fold stacking exhibiting the largest possible $|\boldsymbol{S}_n|$ (i.e. $|\boldsymbol{S}_1|$) to 12-fold stacking with a small $|\boldsymbol{S}_{12}|$, as shown in Figure S6. Because all the atoms contained in a single-layer 2D unit cell as a whole become the minimal repeat unit in the translation symmetry of the cFGDY topological structure, atoms in the 2D unit cell will only generate one first-order reflection in the reciprocal space. Therefore, we use a filled circle to represent all atoms in a 2D unit cell, namely the 2D real-space translational symmetry stacking diagram (Figure S6, a-e). Due to the P6/mmm symmetry and the ergodic theorem applying to symmetrically identical points, there can only be 1-fold stacking, 3-fold stacking, 4-fold stacking, 9-fold stacking and 12-fold stacking existent below and as high as 12-fold. For example, "2-fold" stacking will require a green-filled circle (any point within the unit cell is colored green) in the center of the 1-fold stacking diagram (Figure S6, a); however, that central position is symmetrically identical to the middle points of the edges of the unit cell, therefore requiring blue-filled circles (points shared by the edge couples of the unit cell are colored blue) to be produced at the middle of edges, which leads to 4-fold stacking (Figure S6, c) and causes absence of "2-fold stacking" for a P6/mmm unit cell. Indeed, each stacking mode has a unique |Sn| (Figure S6, f-j), which offsets adjacent layers by $|\boldsymbol{S}_n|$ in one of the Sn directions (Figure S6, k-o).

Apparently, each stacking mode higher than 1-fold can generate a higher translational symmetry and thereby producing a smaller $|\boldsymbol{S_n}|$ than the lattice constant $|\boldsymbol{a}|$ (Figure S6), which should result in its unique SAED pattern. To characterize stacking from the experimental SAED pattern of cFGDY, we need to calculate the diffraction natures of different stacking modes in the first place. Herein, we performed geometry optimization to derive lattice constants for cFGDY with different stacking modes using plane-wave density functional theory (DFT) calculations by the Vienna ab initio package (VASP), under the generalized gradient approximation (GGA) with the Perdew-Burke-Ernzerhof (PBE) functional. As shown in Table S1, the maximum plane distance (d) of 9-fold stacking cFGDY (corresponding to d of the highest-density {3 0 0} planes $d_{\{3\ 0\ 0\}}$) calculated from VASP ($d_{max,calc}$ = 0.472 nm) is highly consistent with that determined from experimental SAED pattern ($d_{max,SAED}$ = 0.467 nm, Figure S6, b) with a relative error δ as low as 1.1%. Therefore, the actual stacking mode of the synthesized cFGDY must be 9-fold stacking, uniquely determined from correlation between SAED and DFT calculations.

6.4 Analyzing Driving Force of 9-Fold Stacking Mode Formation

Acknowledging 9-fold stacking of the synthesized cFGDY, we were extremely curious about the driving force and the reason behind this preference for 9-fold stacking over other stacking modes. Firstly, we derived the total energies of the bilayer unit cells under different stacking modes (Figure S6, k-o). The stacking energy of a specific stacking mode is defined as the energy difference between the stacking mode of interest and the 1-fold stacking (Figure S8, a), with respect to the bilayer unit cell model of the respective stacking mode. Interestingly, 4-fold stacking has the lowest stacking energy of -2554 kcal/mol per cell, while 9-fold stacking is the second lowest (-2278 kcal/mol). We were thus driven to the question why 9-fold stacking wins over 4-fold despite a higher stacking energy. Obviously, the stacking energy derived from the bilayer unit cell model only reflects the driving force of two infinitely expanded 2D layers of cFGDY to be stacked together, where only C and F atoms exist. Therefore, the preference of 9-

fold stacking over 4-fold must happen during the nucleation and formation of a new cFGDY layer on the previous layer, where H atoms at the unreacted acetylenic groups must play a role. Indeed, in the corresponding models where a monomer, a dimer or a trimer respectively lies on an intact cFGDY layer, established for 9-fold stacking (Figure S7, c-e) and 4-fold stacking (Figure S7, f-h), we noticed equivalent F-F repulsion (denoted in red squared) for both stacking modes, but additional F-H hydrogen bonds in 9-fold stacking which should largely reduce the energy by electrostatic attraction. Indeed, energy calculations after restrictive geometry optimization by plane-wave DFT revealed that all of the monomer-, dimer- and trimer-cFGDY models with the 4-fold stacking mode exhibit substantially higher energy as compared to the respective models with the 9-fold stacking mode (Figure S7, c-h, denoted below models). Although the commonly available computational capacity cannot support further larger models, it is already clear that the unreacted acetylenic H atoms which are present during formation and nucleation have determined this preference of 9-fold stacking over 4-fold stacking by generating F-H hydrogen bonds. In this way, continued growth of the layer will be based on the relaxed fragment, keeping the 9-fold stacking mode all along.

Supplementary Figures and Tables

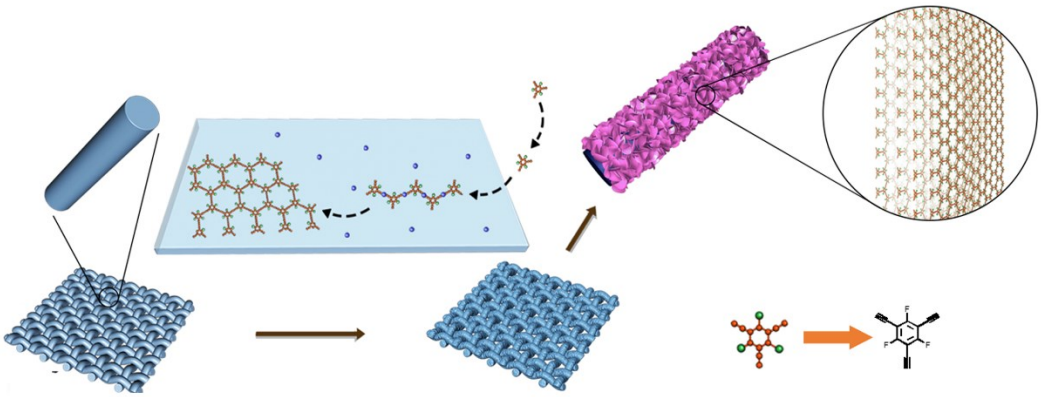

Figure S1. Schematic representation of the synthetic route for cFGDY.

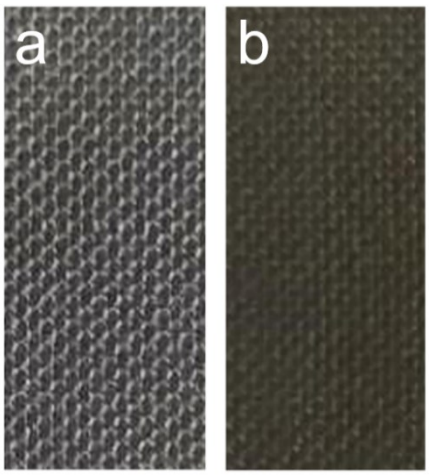

Figure S2. The photographs of (a) pure CF and (b) cFGDY samples.

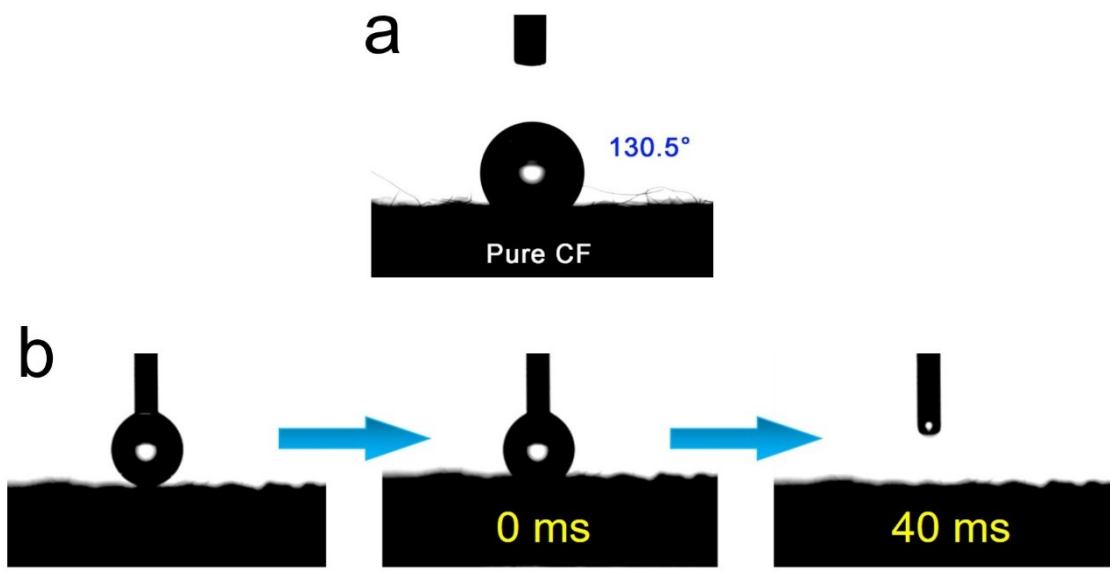

Figure S3. Contact angle measurements of (a) pure CF and (b) cFGDY.

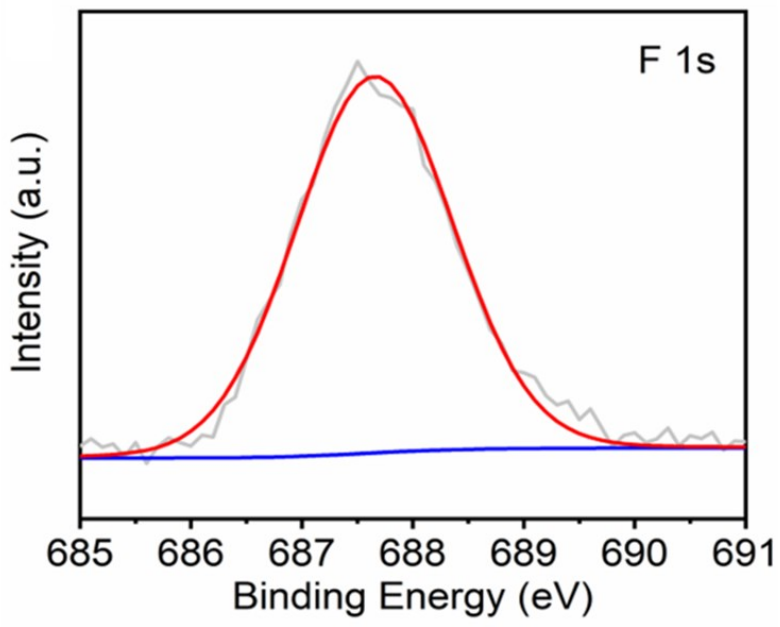

Figure S4. The high-resolution (a) C 1s and (b) F 1s XPS spectra of as-prepared cFGDY.

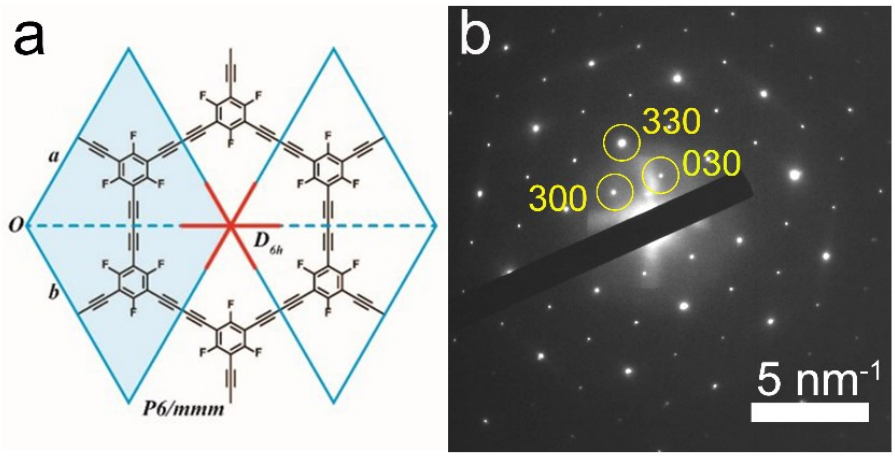

Figure S5. (a) Symmetry analysis of cFGDY, with the point group D6h of hexagonal pore and the space group P6/mmm of the periodic structure identified. (b) The experimental SAED pattern of cFGDY.

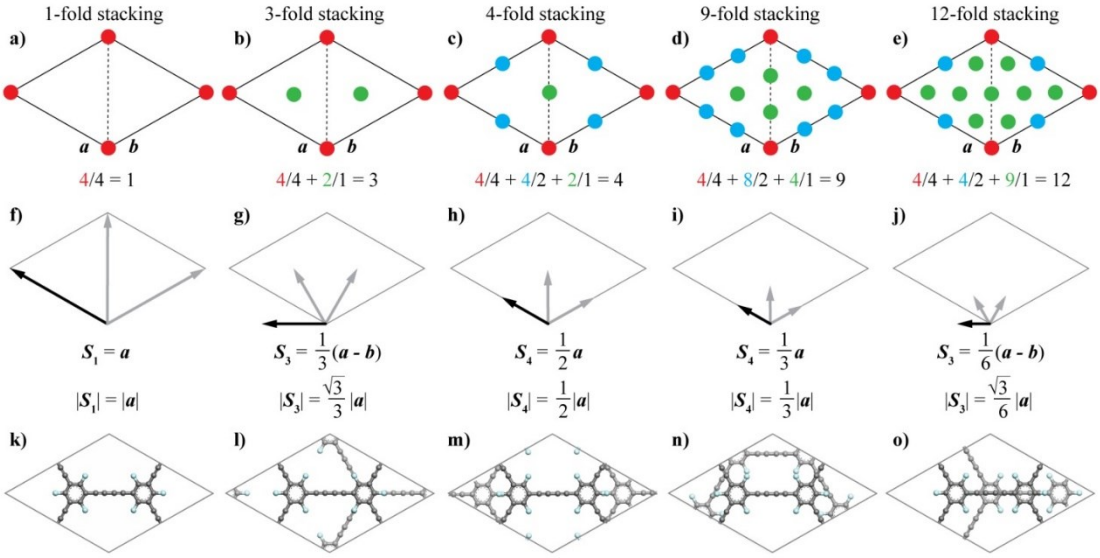

Figure S6. Stacking analysis of cFGDY. (a-e) 2D real-space translational symmetry stacking diagrams of (a) 1-fold stacking, (b) 3-fold stacking, (c) 4-fold stacking, (d) 9-fold stacking and (e) 12-fold stacking. (f-j) Stacking vectors of (f) 1-fold stacking, (g) 3-fold stacking, (h) 4-fold stacking, (i) 9-fold stacking and (j) 12-fold stacking. (k-o) The bilayer unit cell models with (a) 1-fold stacking, (b) 3-fold stacking, (c) 4-fold stacking, (d) 9-fold stacking and (e) 12-fold stacking modes respectively

Table S1. Characterization of the stacking mode of the synthesized cFGDY.

Stacking	$\|\boldsymbol{a}\|$ calculated[a]	Highest-density planes[b]	$d_{max,calc}$[c]	$d_{max,SAED}$[d]	δ[e]
1-fold	1.628 nm	{1 0 0}	1.410 nm	0.467 nm	-
3-fold	1.632 nm	{1 1 0}	0.816 nm		-
4-fold	1.648 nm	{2 0 0}	0.714 nm		-
9-fold	1.634 nm	{3 0 0}	0.472 nm		1.1%
12-fold	1.632 nm	{4 0 0}	0.353 nm		-

[a]Calculated lattice constant |a| from plane-wave DFT. [b]The plane family that exhibit the highest atom density and the largest plane spacing. [c]Calculated maximum plane spacing that corresponds to the highest-density planes, from plane-wave DFT. [d]Maximum plane spacing determined from the experimental SAED pattern by taking the reciprocal of the measured distance to the origin for the reflection closed to the origin (Figure S5, b). [e]The relative error of the experimentally determined $d_{max,SAED}$ with respect to $d_{max,calc}$ of the 9-fold stacking model, expressed as $\delta = |d_{max,SAED} - d_{max,calc}|/d_{max,calc} \times 100\%$; $d_{max,calc}$ is set to be the denominator because the plane-wave DFT method is believed to be of higher accuracy, compared with the SAED method where capturing, post-processing and measurement of the SAED image could generate non-negligible errors.

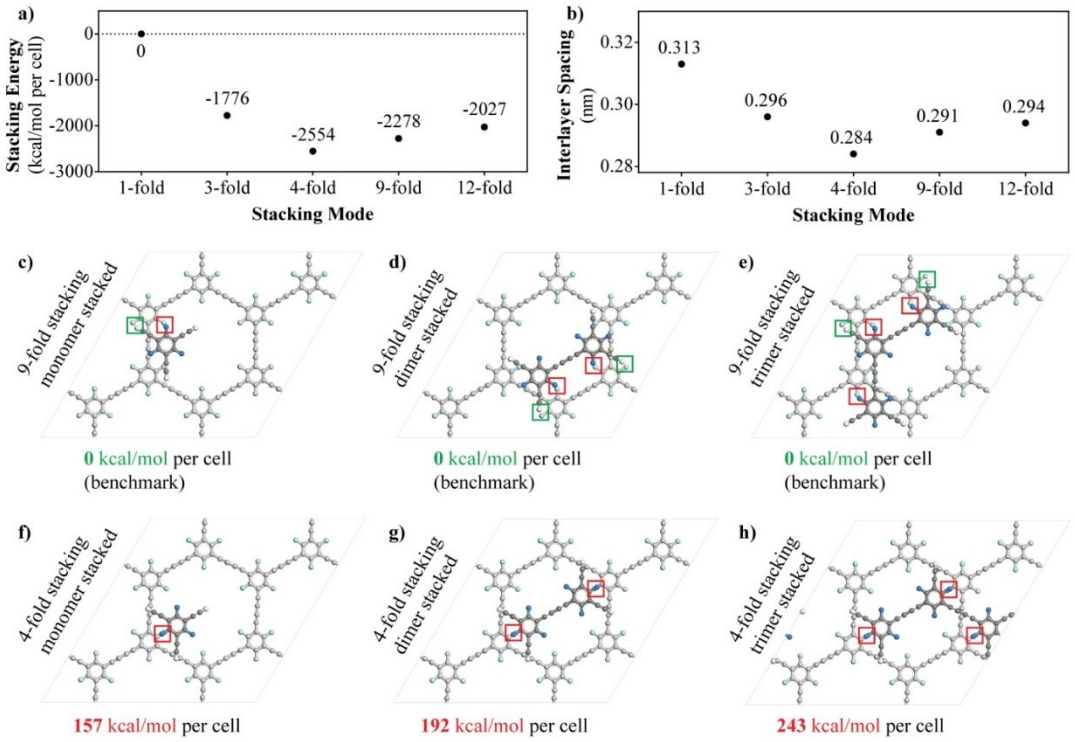

Figure S7. (a) Plot of stacking energies versus different stacking modes. (b) Plot of interlayer spacing versus different stacking modes. (c-h) Restrictively optimized cFGDY nucleation models where (c and f) the monomer, (d and g) the dimer and (e and h) the trimer were respectively stacked on a 2 × 2 supercell single layer cFGDY with (c-e) the 9-fold stacking mode or (f-g) the 4-fold stacking mode in comparison; F-H hydrogen bond interactions were denoted in green squares and F-F repulsions were denoted in red squares; the incremented energy of 4-fold stacking models compared with the corresponding 9-fold stacking models were denoted below the model cell; during restrictive optimization, the position of the monomer, dimer or trimer is horizontally restricted to guarantee the energy is calculated for the studied stacking mode without sliding to other modes, but is vertically relaxed to find their minimum energy geometries while stacking; sufficient vacuum space were made above the monomer, dimer or trimer to mimic the actual surface interaction.

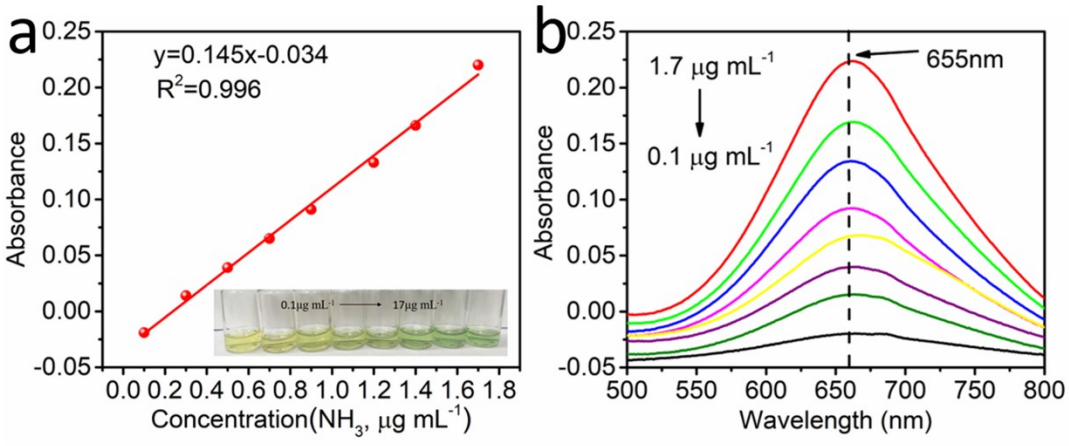

Figure S8. Determination of NH_3 in 0.1 M Na_2SO_4. (a) Corresponding calibration curve. (b) UV-Vis absorption spectra of indophenol assays for standard NH_3 solutions with different concentrations: 0.1 (–), 0.3(–), 0.5(–), 0.7(–), 0.9(–), 1.2(–), 1.4(–) and 1.7 (–) μg mL^{-1}, respectively.

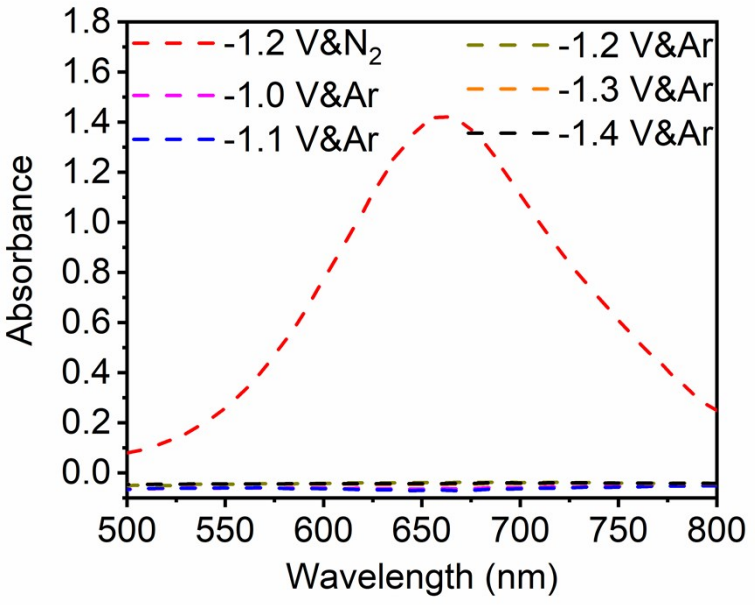

Figure S9. Detection of NH_3 after NRR in N_2- and Ar-saturated 0.1 M Na_2SO_4 at different applied potentials.

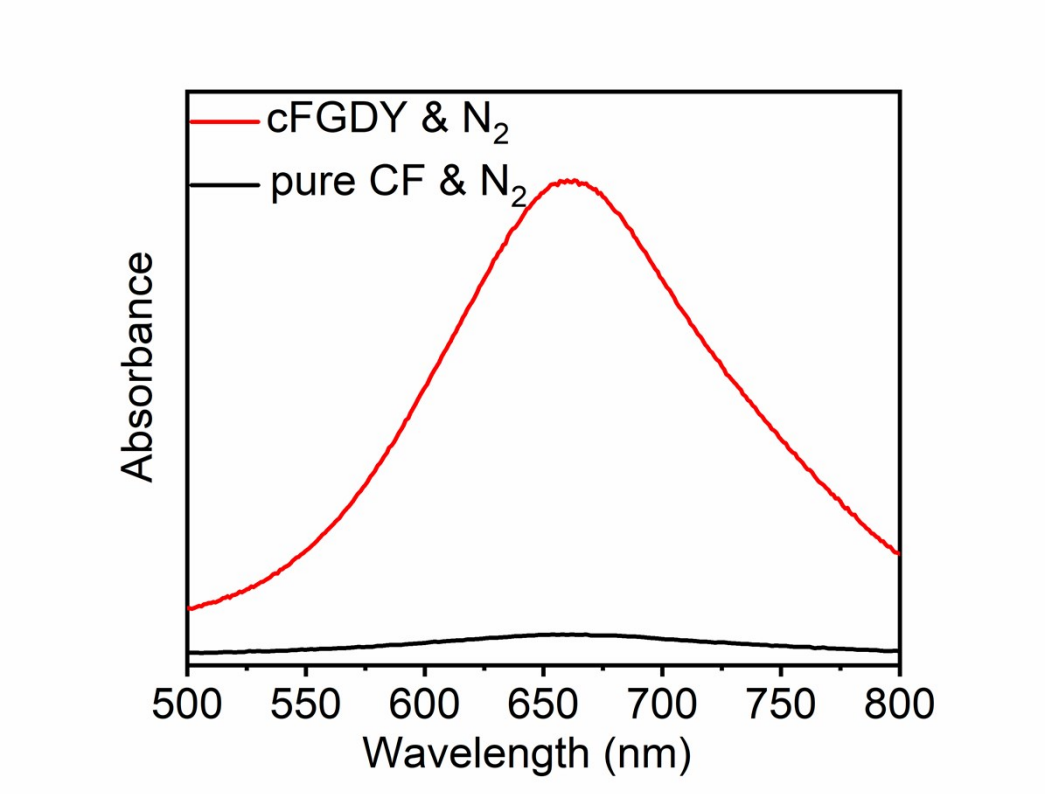

Figure S10. UV-vis absorption spectra of cFGDY (red line) and pure CF (black line) under N_2 saturated electrolytes.

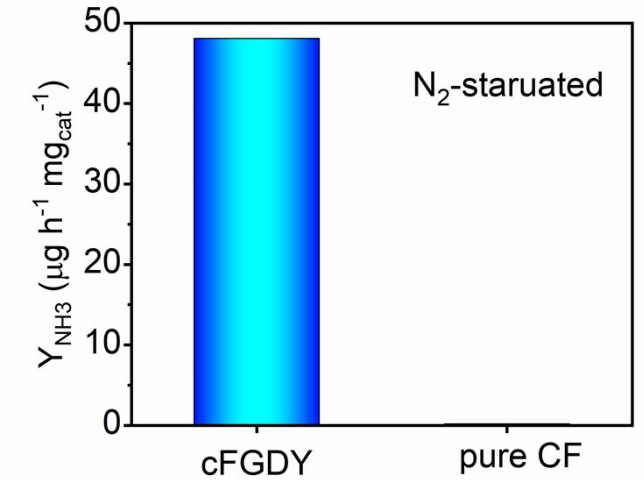

Figure S11. Amounts of NH_3 produced using pure CF and cFGDY electrodes after 2 h-electrolysis at −1.2 V vs SCE.

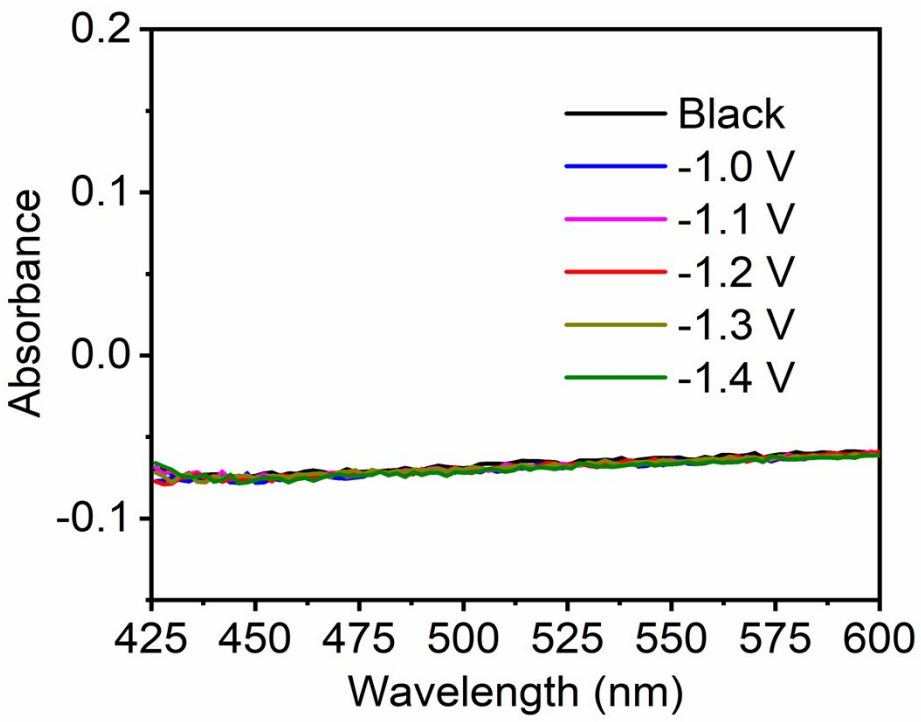

Figure S12. Detection of N_2H_4 after NRR tests in 0.1 M Na_2SO_4.

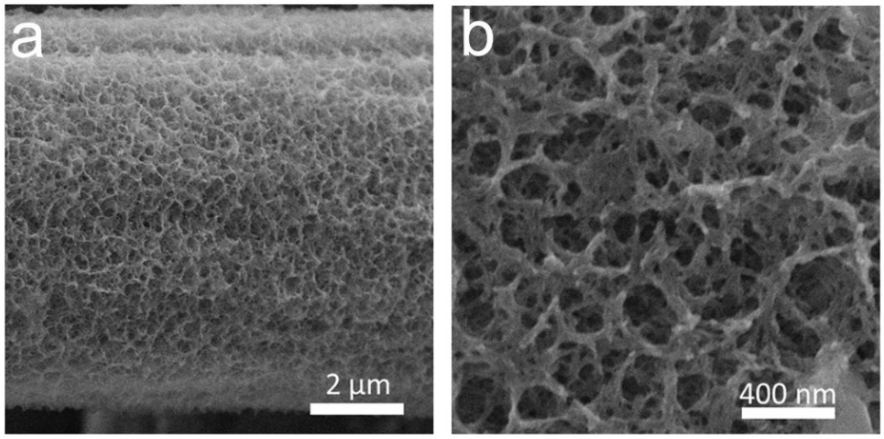

Figure S13. (a) Low- and (b) high-magnification SEM images of cFGDY obtained after the NRR test in 0.1 M Na_2SO_4.

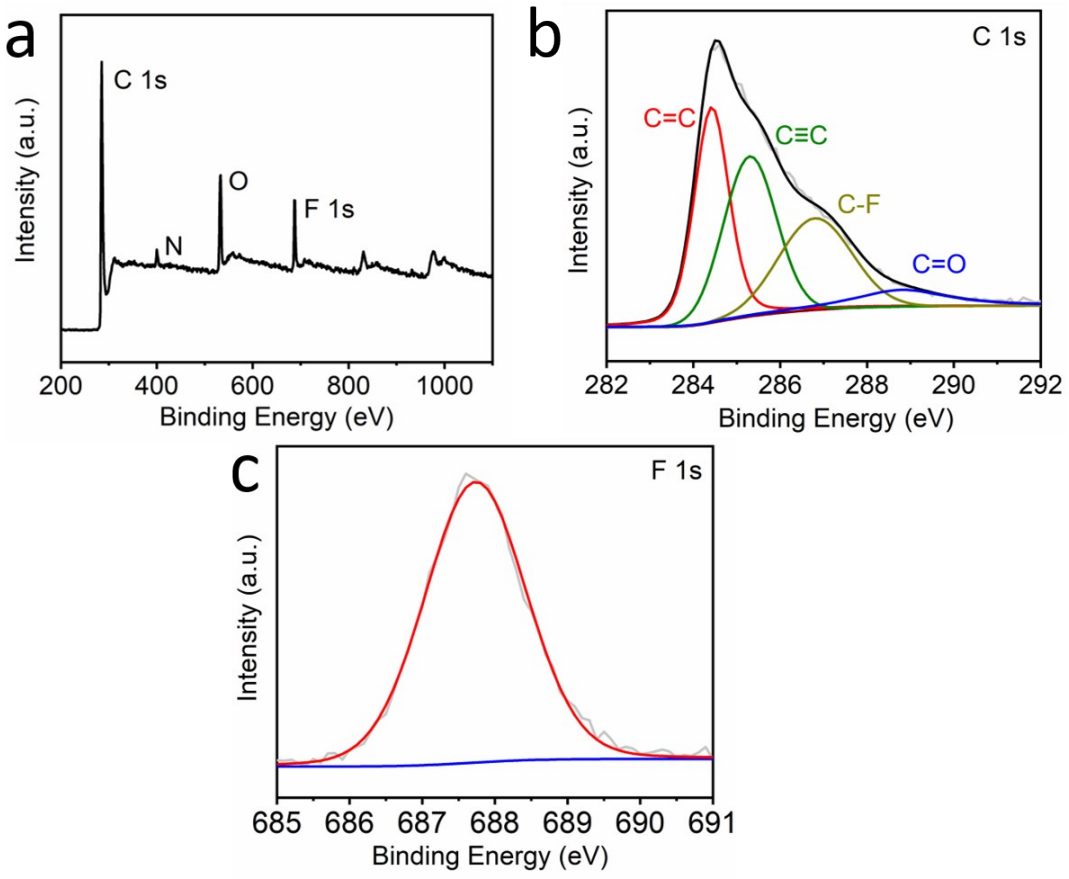

Figure S14. The (a) survey, (b) C 1s and (c) F 1s XPS spectra of the cFGDY obtained after NRR test in 0.1 M Na_2SO_4.

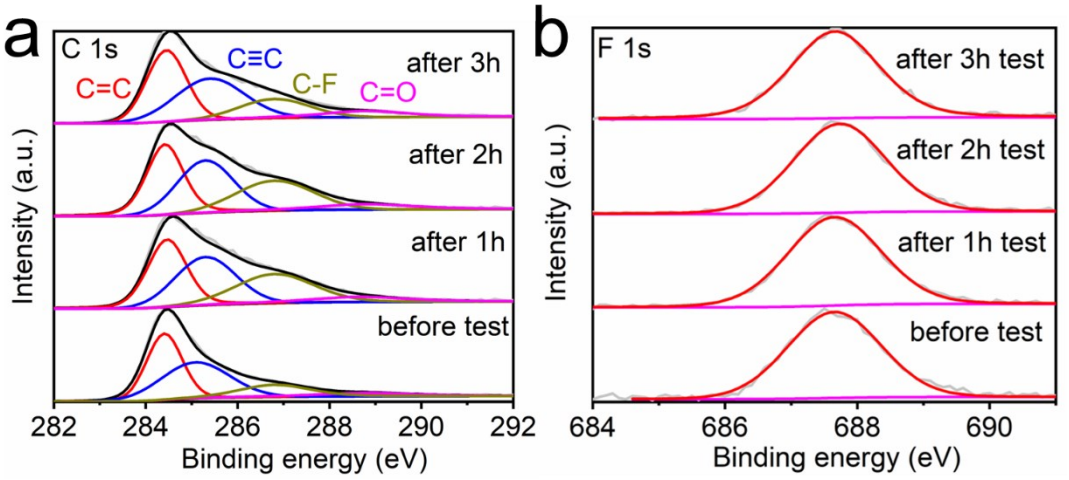

Figure S15. The (a) C 1s and (b) F 1s XPS spectra of the cFGDY obtained before and 1-, 2-, and 3-h NRR tests in 0.1 M Na_2SO_4.

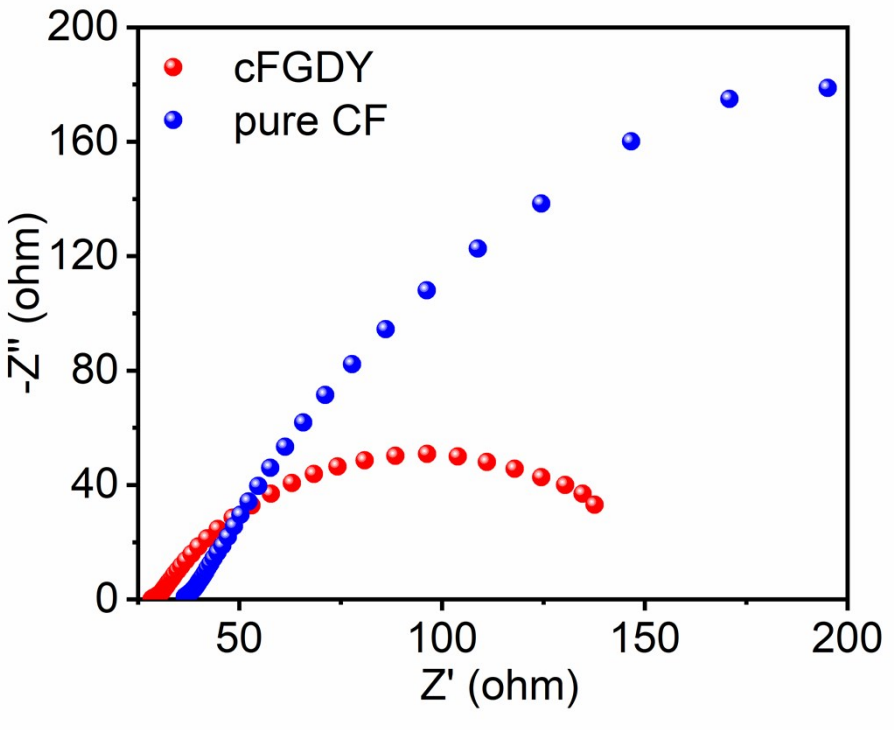

Figure S16. Nyquist plots of cFGDY (red dots) and pure CF (blue dots).

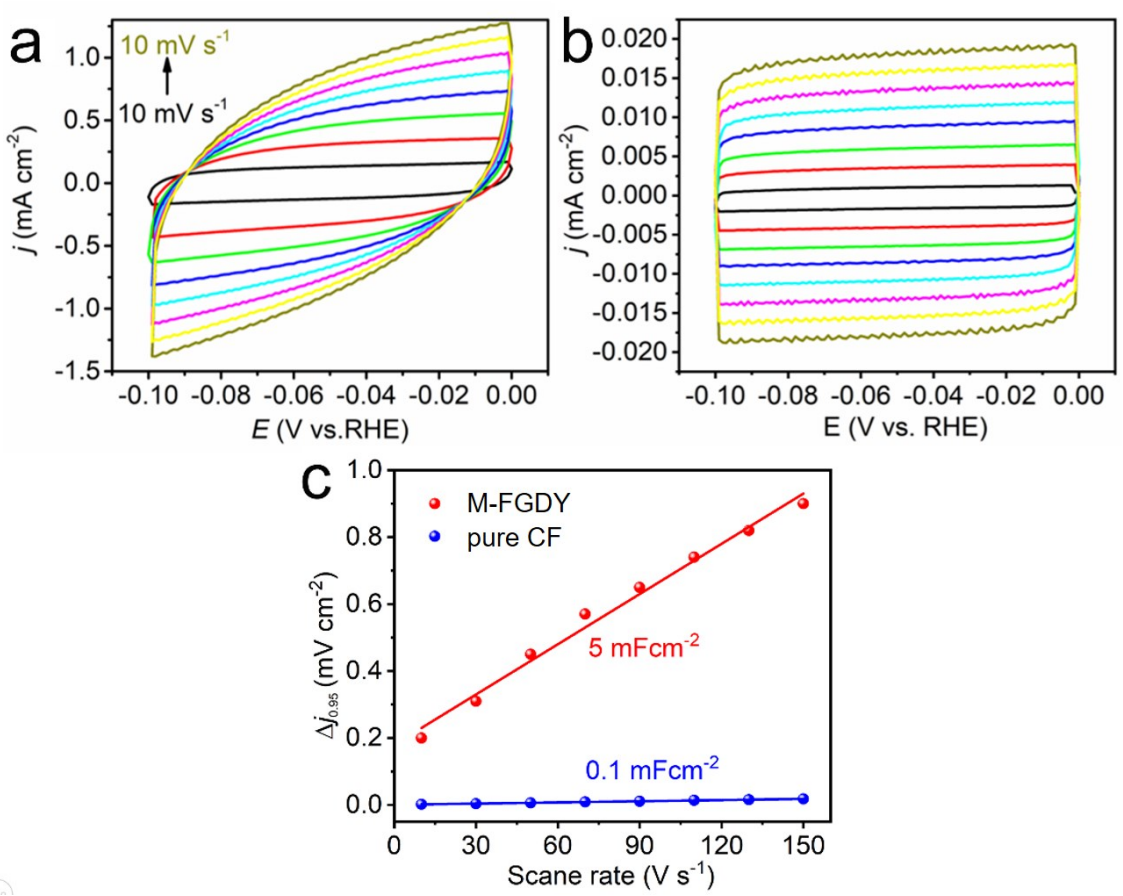

Figure S17. CV curves of (a) cFGDY (b) pure CF in the region of -0.1 V -0 V vs. RHE at various scan rates. (c) Corresponding capacitive current densities as a function of scan rates for cFGDY (read line) and pure CF (blue line).

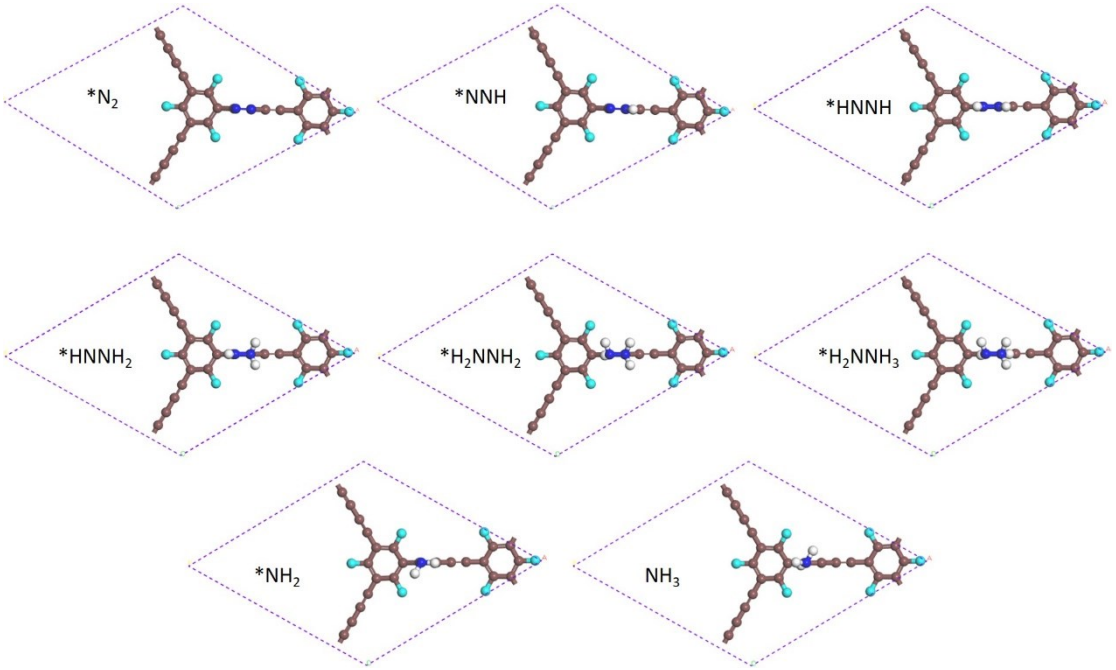

Figure S18. The structures of the intermediates.

Table S2. Comparison of electrochemical NRR performances of cFGDY with other reported metal-free catalysts under ambient temperature and ambient pressures.

Catalysts	Yield	FE (%)	Electrolytes	References
cFGDY	44.1 mg h^{-1} mg_{cat}^{-1}	25.95	0.1 M Na_2SO_4	This work
Cl-GDY	10.7 μg h^{-1} cm^{-2}	8.7	0.1 M HCl	*ACS Catal.* **2019**, *9*, 10649−10655
B_4C/GCE	14.70 mg h^{-1} mg_{cat}^{-1}	9.24	0.1 M Na_2SO_4	*Nat. Commun.* **2018**, *9*, 3485
BG	9.8 mg h^{-1} cm^{-2}	10.8	0.05 M H_2SO_4	*Joule* **2018**, *2*, 1610–1622
FL-BP NSs/CF	31.37 mg h^{-1} mg_{cat}^{-1}	5.07	0.01 M HCl	*Angew. Chem. Int. Ed.* **2019**, *58*, 2612 – 2616
PCN-NV4	8.09 mg h^{-1} mg_{cat}^{-1}	11.59	0.1 M HCl	*Angew. Chem. Int. Ed.* **2018**, *57*,10246–10250
NPC	1.40 mmol g^{-1} h^{-1}	1.42	0.05 M H_2SO_4	*ACS Catal.* **2018**, *8*, 1186−1191
BCN	7.75 mg h^{-1} mg_{cat}^{-1}	13.79	0.1 M HCl	*Small* **2019**, *15*, 1805029
NP-C-MOF-5	1.08 mg h^{-1} mg_{cat}^{-1}	0.0754	0.1 M HCl	*ACS Appl. Mater. Interfaces* **2019**, *11*, 12408−12414
SDG/CP	28.56 mg h^{-1} mg_{cat}^{-1}	7.07	0.5 M $LiClO_4$	*Chem. Commun.* **2019**, *55*, 3152-3155
oxidized carbon nanotube material (O-CNT)	32.33 mgh^{-1} mg_{cat}^{-1}	12.5	0.1 M $LiClO_4$	*Chem. Commun.* **2019**, *55*, 4997--5000
mesoporous boron nitride (MBN)	18.2 mg h^{-1} mg_{cat}^{-1}	5.5	0.1 M Na_2SO_4	*Nanoscale* **2019**, *11*, 4231–4235
defect-rich fluorographene nanosheet	9.3 mg h^{-1} mg_{cat}^{-1}	4.2	0.1 M Na_2SO_4	*Chem. Commun.*, **2019**, *55*, 4266-4269
NSG	7.7 mg h^{-1} mg_{cat}^{-1}	5.8	0.1 M HCl	*J. Mater Sci* **2019**, *54*, 9088–9097

Table S3. Comparison of electrochemical NRR performances of cFGDY with other reported metal-based catalysts under ambient temperature and ambient pressures.

Catalysts	**Yield ($\mu g \cdot h^{-1} \cdot mg^{-1}_{cat}$)**	**FE (%)**	**Electrolytes**	**References**
cFGDY	44.1	25.95	0.1M Na_2SO_4	This work
Mo^0/GDY	145.4	21	0.1M Na_2SO_4	*J. Am. Chem. Soc.* **2019,** *141*, 10677−10683
Pd/C	4.5	8.2	0.1M PBS	*Nat. Commun.* **2018**, *9*, 1795
MIL-125(Ti)	14.8	17.8	0.1 M $LiClO_4$	*Angew. Chem. Int. Ed.* **2019**, 58, 13101 – 13106
DR MoS_2 nanoflower	29.28	8.34	0.1 M Na_2SO_4	Adv. Energy Mater. **2018**, 8, 1801357
pAu/NF	9.42	13.36	0.1 M Na_2SO_4	*Small* **2019**, *15*, 1804769
Sn/SnS_2	23.8	3.4	0.1 m PBS	*Small* **2019**, 1902535
MoS_2–rGO	24.82	4.58	0.1 M $LiClO_4$	*J. Mater. Chem. A* **2019**, *7*, 2524–2528
SnO2/RGO	25.6	7.1	0.1 M Na_2SO_4	ACS Appl. Mater. Interfaces **2019**, 11, 31806-31815
SDG/CP	28.56	7.07	0.5 M $LiClO_4$	*Chem. Commun.* **2019**, *55*, 3152-3155
O-CNT	32.33	12.5	0.1 M $LiClO_4$	*Chem. Commun.* **2019**, *55*, 4997-5000
mesoporous boron nitride	18.2	5.5	0.1M Na_2SO_4	*Nanoscale* **2019**, *11*, 4231–4235
b-FeOOH nanorods	23.32	6.7	0.5 M $LiClO_4$	*Chem. Commun.* **2018**, *54*, 11332-11335
Fe_2O_3 nanorods.	15.9	0.94	0.1 M Na_2SO_4	*ChemCatChem* **2018**, *10*, 4530– 4535
b-FeO(OH,F) nanorod	42.38	9.02	0.5 M $LiClO_4$	*Chem. Commun.* **2019**, *55*, 3987-3990

Optimized Molecular Coordinates

The bilayer unit cell model with 1-fold stacking:

_cell_length_a	16.2780
_cell_length_b	16.2780
_cell_length_c	6.2621
_cell_angle_alpha	90.0000
_cell_angle_beta	90.0000
_cell_angle_gamma	120.0050

C1	C	0.38381	0.76759	0.24692	0.00000	Uiso	1.00
C2	C	0.43315	0.86628	0.24692	0.00000	Uiso	1.00
C3	C	0.47635	0.95270	0.24692	0.00000	Uiso	1.00
C4	C	0.23241	0.61619	0.24692	0.00000	Uiso	1.00
C5	C	0.13372	0.56685	0.24692	0.00000	Uiso	1.00
C6	C	0.04730	0.52365	0.24692	0.00000	Uiso	1.00
C7	C	0.38380	0.61620	0.24692	0.00000	Uiso	1.00
C8	C	0.43314	0.56686	0.24692	0.00000	Uiso	1.00
C9	C	0.47635	0.52365	0.24692	0.00000	Uiso	1.00
C10	C	0.61619	0.23241	0.24692	0.00000	Uiso	1.00
C11	C	0.56685	0.13372	0.24692	0.00000	Uiso	1.00
C12	C	0.52365	0.04730	0.24692	0.00000	Uiso	1.00
C13	C	0.76759	0.38381	0.24692	0.00000	Uiso	1.00
C14	C	0.86628	0.43315	0.24692	0.00000	Uiso	1.00
C15	C	0.95270	0.47635	0.24692	0.00000	Uiso	1.00
C16	C	0.61620	0.38380	0.24692	0.00000	Uiso	1.00

C17	C	0.56686	0.43314	0.24692	0.00000	Uiso	1.00
C18	C	0.52365	0.47635	0.24692	0.00000	Uiso	1.00
C19	C	0.28445	0.56891	0.24692	0.00000	Uiso	1.00
C20	C	0.43109	0.71555	0.24692	0.00000	Uiso	1.00
C21	C	0.28447	0.71553	0.24692	0.00000	Uiso	1.00
C22	C	0.71555	0.43109	0.24692	0.00000	Uiso	1.00
C23	C	0.56891	0.28445	0.24692	0.00000	Uiso	1.00
C24	C	0.71553	0.28447	0.24692	0.00000	Uiso	1.00
C25	C	0.38381	0.76759	0.74692	0.00000	Uiso	1.00
C26	C	0.43315	0.86628	0.74692	0.00000	Uiso	1.00
C27	C	0.47635	0.95270	0.74692	0.00000	Uiso	1.00
C28	C	0.23241	0.61619	0.74692	0.00000	Uiso	1.00
C29	C	0.13372	0.56685	0.74692	0.00000	Uiso	1.00
C30	C	0.04730	0.52365	0.74692	0.00000	Uiso	1.00
C31	C	0.38380	0.61620	0.74692	0.00000	Uiso	1.00
C32	C	0.43314	0.56686	0.74692	0.00000	Uiso	1.00
C33	C	0.47635	0.52365	0.74692	0.00000	Uiso	1.00
C34	C	0.61619	0.23241	0.74692	0.00000	Uiso	1.00
C35	C	0.56685	0.13372	0.74692	0.00000	Uiso	1.00
C36	C	0.52365	0.04730	0.74692	0.00000	Uiso	1.00
C37	C	0.76759	0.38381	0.74692	0.00000	Uiso	1.00
C38	C	0.86628	0.43315	0.74692	0.00000	Uiso	1.00
C39	C	0.95270	0.47635	0.74692	0.00000	Uiso	1.00
C40	C	0.61620	0.38380	0.74692	0.00000	Uiso	1.00
C41	C	0.56686	0.43314	0.74692	0.00000	Uiso	1.00
C42	C	0.52365	0.47635	0.74692	0.00000	Uiso	1.00

C43	C	0.28445	0.56891	0.74692	0.00000	Uiso	1.00
C44	C	0.43109	0.71555	0.74692	0.00000	Uiso	1.00
C45	C	0.28447	0.71553	0.74692	0.00000	Uiso	1.00
C46	C	0.71555	0.43109	0.74692	0.00000	Uiso	1.00
C47	C	0.56891	0.28445	0.74692	0.00000	Uiso	1.00
C48	C	0.71553	0.28447	0.74692	0.00000	Uiso	1.00
F49	F	0.23686	0.76314	0.24692	0.00000	Uiso	1.00
F50	F	0.23682	0.47369	0.24692	0.00000	Uiso	1.00
F51	F	0.52631	0.76318	0.24692	0.00000	Uiso	1.00
F52	F	0.76314	0.23686	0.24692	0.00000	Uiso	1.00
F53	F	0.76318	0.52631	0.24692	0.00000	Uiso	1.00
F54	F	0.47369	0.23682	0.24692	0.00000	Uiso	1.00
F55	F	0.23686	0.76314	0.74692	0.00000	Uiso	1.00
F56	F	0.23682	0.47369	0.74692	0.00000	Uiso	1.00
F57	F	0.52631	0.76318	0.74692	0.00000	Uiso	1.00
F58	F	0.76314	0.23686	0.74692	0.00000	Uiso	1.00
F59	F	0.76318	0.52631	0.74692	0.00000	Uiso	1.00
F60	F	0.47369	0.23682	0.74692	0.00000	Uiso	1.00

The bilayer unit cell model with 3-fold stacking:

_cell_length_a	16.3233
_cell_length_b	16.3233
_cell_length_c	5.9132
_cell_angle_alpha	90.0000
_cell_angle_beta	90.0000
_cell_angle_gamma	120.0070

C1	C	0.71718	0.43431	0.24692	0.00000	Uiso	1.00
C2	C	0.76650	0.53296	0.24692	0.00000	Uiso	1.00
C3	C	0.80970	0.61940	0.24692	0.00000	Uiso	1.00
C4	C	0.56569	0.28282	0.24692	0.00000	Uiso	1.00
C5	C	0.46704	0.23350	0.24692	0.00000	Uiso	1.00
C6	C	0.38060	0.19030	0.24692	0.00000	Uiso	1.00
C7	C	0.71717	0.28283	0.24692	0.00000	Uiso	1.00
C8	C	0.76648	0.23352	0.24692	0.00000	Uiso	1.00
C9	C	0.80970	0.19030	0.24692	0.00000	Uiso	1.00
C10	C	0.94954	0.89912	0.24692	0.00000	Uiso	1.00
C11	C	0.90020	0.80043	0.24692	0.00000	Uiso	1.00
C12	C	0.85699	0.71398	0.24692	0.00000	Uiso	1.00
C13	C	0.10088	0.05046	0.24692	0.00000	Uiso	1.00
C14	C	0.19957	0.09980	0.24692	0.00000	Uiso	1.00
C15	C	0.28602	0.14301	0.24692	0.00000	Uiso	1.00
C16	C	0.94955	0.05045	0.24692	0.00000	Uiso	1.00
C17	C	0.90021	0.09979	0.24692	0.00000	Uiso	1.00
C18	C	0.85699	0.14301	0.24692	0.00000	Uiso	1.00
C19	C	0.61802	0.23603	0.24692	0.00000	Uiso	1.00
C20	C	0.76397	0.38198	0.24692	0.00000	Uiso	1.00
C21	C	0.61804	0.38196	0.24692	0.00000	Uiso	1.00
C22	C	0.04881	0.09763	0.24692	0.00000	Uiso	1.00
C23	C	0.90237	0.95119	0.24692	0.00000	Uiso	1.00
C24	C	0.04879	0.95121	0.24692	0.00000	Uiso	1.00
C25	C	0.38379	0.76755	0.74692	0.00000	Uiso	1.00
C26	C	0.43314	0.86624	0.74692	0.00000	Uiso	1.00

C27	C	0.47635	0.95269	0.74692	0.00000	Uiso	1.00
C28	C	0.23245	0.61621	0.74692	0.00000	Uiso	1.00
C29	C	0.13376	0.56686	0.74692	0.00000	Uiso	1.00
C30	C	0.04731	0.52365	0.74692	0.00000	Uiso	1.00
C31	C	0.38378	0.61622	0.74692	0.00000	Uiso	1.00
C32	C	0.43313	0.56687	0.74692	0.00000	Uiso	1.00
C33	C	0.47635	0.52365	0.74692	0.00000	Uiso	1.00
C34	C	0.61616	0.23235	0.74692	0.00000	Uiso	1.00
C35	C	0.56684	0.13371	0.74692	0.00000	Uiso	1.00
C36	C	0.52363	0.04727	0.74692	0.00000	Uiso	1.00
C37	C	0.76765	0.38384	0.74692	0.00000	Uiso	1.00
C38	C	0.86629	0.43316	0.74692	0.00000	Uiso	1.00
C39	C	0.95273	0.47637	0.74692	0.00000	Uiso	1.00
C40	C	0.61617	0.38383	0.74692	0.00000	Uiso	1.00
C41	C	0.56685	0.43315	0.74692	0.00000	Uiso	1.00
C42	C	0.52363	0.47637	0.74692	0.00000	Uiso	1.00
C43	C	0.28452	0.56904	0.74692	0.00000	Uiso	1.00
C44	C	0.43096	0.71548	0.74692	0.00000	Uiso	1.00
C45	C	0.28454	0.71546	0.74692	0.00000	Uiso	1.00
C46	C	0.71532	0.43063	0.74692	0.00000	Uiso	1.00
C47	C	0.56937	0.28468	0.74692	0.00000	Uiso	1.00
C48	C	0.71530	0.28470	0.74692	0.00000	Uiso	1.00
F49	F	0.57068	0.42932	0.24692	0.00000	Uiso	1.00
F50	F	0.57063	0.14131	0.24692	0.00000	Uiso	1.00
F51	F	0.85869	0.42937	0.24692	0.00000	Uiso	1.00
F52	F	0.09628	0.90372	0.24692	0.00000	Uiso	1.00

F53	F	0.09634	0.19262	0.24692	0.00000	Uiso	1.00
F54	F	0.80738	0.90366	0.24692	0.00000	Uiso	1.00
F55	F	0.23706	0.76294	0.74692	0.00000	Uiso	1.00
F56	F	0.23700	0.47405	0.74692	0.00000	Uiso	1.00
F57	F	0.52595	0.76300	0.74692	0.00000	Uiso	1.00
F58	F	0.76265	0.23735	0.74692	0.00000	Uiso	1.00
F59	F	0.76271	0.52536	0.74692	0.00000	Uiso	1.00
F60	F	0.47464	0.23729	0.74692	0.00000	Uiso	1.00

The bilayer unit cell model with 4-fold stacking:

_cell_length_a	16.4752
_cell_length_b	16.4773
_cell_length_c	5.6777
_cell_angle_alpha	90.0000
_cell_angle_beta	90.0000
_cell_angle_gamma	120.9090

C1	C	0.88881	0.26564	0.24692	0.00000	Uiso	1.00
C2	C	0.93926	0.36536	0.24692	0.00000	Uiso	1.00
C3	C	0.97862	0.45231	0.24692	0.00000	Uiso	1.00
C4	C	0.73436	0.11119	0.24692	0.00000	Uiso	1.00
C5	C	0.63464	0.06074	0.24692	0.00000	Uiso	1.00
C6	C	0.54769	0.02138	0.24692	0.00000	Uiso	1.00
C7	C	0.88582	0.11418	0.24692	0.00000	Uiso	1.00
C8	C	0.93434	0.06566	0.24692	0.00000	Uiso	1.00
C9	C	0.97676	0.02324	0.24692	0.00000	Uiso	1.00
C10	C	0.11119	0.73436	0.24692	0.00000	Uiso	1.00

C11	C	0.06074	0.63464	0.24692	0.00000	Uiso	1.00
C12	C	0.02138	0.54769	0.24692	0.00000	Uiso	1.00
C13	C	0.26564	0.88881	0.24692	0.00000	Uiso	1.00
C14	C	0.36536	0.93926	0.24692	0.00000	Uiso	1.00
C15	C	0.45231	0.97862	0.24692	0.00000	Uiso	1.00
C16	C	0.11418	0.88582	0.24692	0.00000	Uiso	1.00
C17	C	0.06566	0.93434	0.24692	0.00000	Uiso	1.00
C18	C	0.02324	0.97676	0.24692	0.00000	Uiso	1.00
C19	C	0.78563	0.06498	0.24692	0.00000	Uiso	1.00
C20	C	0.93502	0.21437	0.24692	0.00000	Uiso	1.00
C21	C	0.78862	0.21138	0.24692	0.00000	Uiso	1.00
C22	C	0.21437	0.93502	0.24692	0.00000	Uiso	1.00
C23	C	0.06498	0.78563	0.24692	0.00000	Uiso	1.00
C24	C	0.21138	0.78862	0.24692	0.00000	Uiso	1.00
C25	C	0.38881	0.76564	0.74692	0.00000	Uiso	1.00
C26	C	0.43926	0.86536	0.74692	0.00000	Uiso	1.00
C27	C	0.47862	0.95231	0.74692	0.00000	Uiso	1.00
C28	C	0.23436	0.61119	0.74692	0.00000	Uiso	1.00
C29	C	0.13464	0.56074	0.74692	0.00000	Uiso	1.00
C30	C	0.04769	0.52138	0.74692	0.00000	Uiso	1.00
C31	C	0.38582	0.61418	0.74692	0.00000	Uiso	1.00
C32	C	0.43434	0.56566	0.74692	0.00000	Uiso	1.00
C33	C	0.47676	0.52324	0.74692	0.00000	Uiso	1.00
C34	C	0.61119	0.23436	0.74692	0.00000	Uiso	1.00
C35	C	0.56074	0.13464	0.74692	0.00000	Uiso	1.00
C36	C	0.52138	0.04769	0.74692	0.00000	Uiso	1.00

C37	C	0.76564	0.38881	0.74692	0.00000	Uiso	1.00
C38	C	0.86536	0.43926	0.74692	0.00000	Uiso	1.00
C39	C	0.95231	0.47862	0.74692	0.00000	Uiso	1.00
C40	C	0.61418	0.38582	0.74692	0.00000	Uiso	1.00
C41	C	0.56566	0.43434	0.74692	0.00000	Uiso	1.00
C42	C	0.52324	0.47676	0.74692	0.00000	Uiso	1.00
C43	C	0.28563	0.56498	0.74692	0.00000	Uiso	1.00
C44	C	0.43502	0.71437	0.74692	0.00000	Uiso	1.00
C45	C	0.28862	0.71138	0.74692	0.00000	Uiso	1.00
C46	C	0.71437	0.43502	0.74692	0.00000	Uiso	1.00
C47	C	0.56498	0.28563	0.74692	0.00000	Uiso	1.00
C48	C	0.71138	0.28862	0.74692	0.00000	Uiso	1.00
F49	F	0.74176	0.25824	0.24692	0.00000	Uiso	1.00
F50	F	0.73630	0.96910	0.24692	0.00000	Uiso	1.00
F51	F	0.03090	0.26370	0.24692	0.00000	Uiso	1.00
F52	F	0.25824	0.74176	0.24692	0.00000	Uiso	1.00
F53	F	0.26370	0.03090	0.24692	0.00000	Uiso	1.00
F54	F	0.96910	0.73630	0.24692	0.00000	Uiso	1.00
F55	F	0.24176	0.75824	0.74692	0.00000	Uiso	1.00
F56	F	0.23630	0.46910	0.74692	0.00000	Uiso	1.00
F57	F	0.53090	0.76370	0.74692	0.00000	Uiso	1.00
F58	F	0.75824	0.24176	0.74692	0.00000	Uiso	1.00
F59	F	0.76370	0.53090	0.74692	0.00000	Uiso	1.00
F60	F	0.46910	0.23630	0.74692	0.00000	Uiso	1.00

The bilayer unit cell model with 9-fold stacking:

_cell_length_a 16.3364

_cell_length_b 16.3364

_cell_length_c 5.8116

_cell_angle_alpha 90.0000

_cell_angle_beta 90.0000

_cell_angle_gamma 120.0560

_atom_site_fract_z

_atom_site_U_iso_or_equiv

_atom_site_adp_type

_atom_site_occupancy

C1	C	0.71726	0.10075	0.24692	0.00000	Uiso	1.00
C2	C	0.76684	0.19948	0.24692	0.00000	Uiso	1.00
C3	C	0.81031	0.28597	0.24692	0.00000	Uiso	1.00
C4	C	0.56582	0.94941	0.24692	0.00000	Uiso	1.00
C5	C	0.46704	0.89969	0.24692	0.00000	Uiso	1.00
C6	C	0.38056	0.85729	0.24692	0.00000	Uiso	1.00
C7	C	0.71716	0.94949	0.24692	0.00000	Uiso	1.00
C8	C	0.76649	0.90012	0.24692	0.00000	Uiso	1.00
C9	C	0.80967	0.85699	0.24692	0.00000	Uiso	1.00
C10	C	0.94941	0.56582	0.24692	0.00000	Uiso	1.00
C11	C	0.89969	0.46704	0.24692	0.00000	Uiso	1.00
C12	C	0.85729	0.38056	0.24692	0.00000	Uiso	1.00
C13	C	0.10075	0.71726	0.24692	0.00000	Uiso	1.00
C14	C	0.19948	0.76684	0.24692	0.00000	Uiso	1.00
C15	C	0.28597	0.81031	0.24692	0.00000	Uiso	1.00
C16	C	0.94949	0.71716	0.24692	0.00000	Uiso	1.00

C17	C	0.90012	0.76649	0.24692	0.00000	Uiso	1.00
C18	C	0.85699	0.80967	0.24692	0.00000	Uiso	1.00
C19	C	0.61798	0.90250	0.24692	0.00000	Uiso	1.00
C20	C	0.76434	0.04877	0.24692	0.00000	Uiso	1.00
C21	C	0.61803	0.04864	0.24692	0.00000	Uiso	1.00
C22	C	0.04877	0.76434	0.24692	0.00000	Uiso	1.00
C23	C	0.90250	0.61798	0.24692	0.00000	Uiso	1.00
C24	C	0.04864	0.61803	0.24692	0.00000	Uiso	1.00
C25	C	0.38393	0.76751	0.74692	0.00000	Uiso	1.00
C26	C	0.43365	0.86630	0.74692	0.00000	Uiso	1.00
C27	C	0.47604	0.95278	0.74692	0.00000	Uiso	1.00
C28	C	0.23259	0.61607	0.74692	0.00000	Uiso	1.00
C29	C	0.13385	0.56649	0.74692	0.00000	Uiso	1.00
C30	C	0.04736	0.52302	0.74692	0.00000	Uiso	1.00
C31	C	0.38384	0.61617	0.74692	0.00000	Uiso	1.00
C32	C	0.43321	0.56685	0.74692	0.00000	Uiso	1.00
C33	C	0.47634	0.52366	0.74692	0.00000	Uiso	1.00
C34	C	0.61607	0.23259	0.74692	0.00000	Uiso	1.00
C35	C	0.56649	0.13385	0.74692	0.00000	Uiso	1.00
C36	C	0.52302	0.04736	0.74692	0.00000	Uiso	1.00
C37	C	0.76751	0.38393	0.74692	0.00000	Uiso	1.00
C38	C	0.86630	0.43365	0.74692	0.00000	Uiso	1.00
C39	C	0.95278	0.47604	0.74692	0.00000	Uiso	1.00
C40	C	0.61617	0.38384	0.74692	0.00000	Uiso	1.00
C41	C	0.56685	0.43321	0.74692	0.00000	Uiso	1.00
C42	C	0.52366	0.47634	0.74692	0.00000	Uiso	1.00

C43	C	0.28457	0.56899	0.74692	0.00000	Uiso	1.00
C44	C	0.43083	0.71536	0.74692	0.00000	Uiso	1.00
C45	C	0.28469	0.71531	0.74692	0.00000	Uiso	1.00
C46	C	0.71536	0.43083	0.74692	0.00000	Uiso	1.00
C47	C	0.56899	0.28457	0.74692	0.00000	Uiso	1.00
C48	C	0.71531	0.28469	0.74692	0.00000	Uiso	1.00
F49	F	0.57103	0.09644	0.24692	0.00000	Uiso	1.00
F50	F	0.57025	0.80743	0.24692	0.00000	Uiso	1.00
F51	F	0.85928	0.09640	0.24692	0.00000	Uiso	1.00
F52	F	0.09644	0.57103	0.24692	0.00000	Uiso	1.00
F53	F	0.09640	0.85928	0.24692	0.00000	Uiso	1.00
F54	F	0.80743	0.57025	0.24692	0.00000	Uiso	1.00
F55	F	0.23690	0.76230	0.74692	0.00000	Uiso	1.00
F56	F	0.23694	0.47406	0.74692	0.00000	Uiso	1.00
F57	F	0.52590	0.76308	0.74692	0.00000	Uiso	1.00
F58	F	0.76230	0.23690	0.74692	0.00000	Uiso	1.00
F59	F	0.76308	0.52590	0.74692	0.00000	Uiso	1.00
F60	F	0.47406	0.23694	0.74692	0.00000	Uiso	1.00

The bilayer unit cell model with 12-fold stacking:

_cell_length_a	16.3167
_cell_length_b	16.3167
_cell_length_c	5.8811
_cell_angle_alpha	90.0000
_cell_angle_beta	90.0000
_cell_angle_gamma	119.9840

_atom_site_U_iso_or_equiv

_atom_site_adp_type

_atom_site_occupancy

C1	C	0.55092	0.60081	0.24692	0.00000	Uiso	1.00
C2	C	0.59977	0.69947	0.24692	0.00000	Uiso	1.00
C3	C	0.64302	0.78590	0.24692	0.00000	Uiso	1.00
C4	C	0.39919	0.44908	0.24692	0.00000	Uiso	1.00
C5	C	0.30053	0.40023	0.24692	0.00000	Uiso	1.00
C6	C	0.21410	0.35698	0.24692	0.00000	Uiso	1.00
C7	C	0.55032	0.44968	0.24692	0.00000	Uiso	1.00
C8	C	0.59970	0.40030	0.24692	0.00000	Uiso	1.00
C9	C	0.64297	0.35703	0.24692	0.00000	Uiso	1.00
C10	C	0.78293	0.06569	0.24692	0.00000	Uiso	1.00
C11	C	0.73355	0.96698	0.24692	0.00000	Uiso	1.00
C12	C	0.69031	0.88055	0.24692	0.00000	Uiso	1.00
C13	C	0.93431	0.21707	0.24692	0.00000	Uiso	1.00
C14	C	0.03303	0.26645	0.24692	0.00000	Uiso	1.00
C15	C	0.11945	0.30969	0.24692	0.00000	Uiso	1.00
C16	C	0.78306	0.21694	0.24692	0.00000	Uiso	1.00
C17	C	0.73370	0.26630	0.24692	0.00000	Uiso	1.00
C18	C	0.69042	0.30958	0.24692	0.00000	Uiso	1.00
C19	C	0.45122	0.40209	0.24692	0.00000	Uiso	1.00
C20	C	0.59791	0.54878	0.24692	0.00000	Uiso	1.00
C21	C	0.45195	0.54805	0.24692	0.00000	Uiso	1.00
C22	C	0.88228	0.26422	0.24692	0.00000	Uiso	1.00
C23	C	0.73578	0.11772	0.24692	0.00000	Uiso	1.00

C24	C	0.88218	0.11782	0.24692	0.00000	Uiso	1.00
C25	C	0.38374	0.76764	0.74692	0.00000	Uiso	1.00
C26	C	0.43311	0.86636	0.74692	0.00000	Uiso	1.00
C27	C	0.47636	0.95278	0.74692	0.00000	Uiso	1.00
C28	C	0.23236	0.61626	0.74692	0.00000	Uiso	1.00
C29	C	0.13364	0.56689	0.74692	0.00000	Uiso	1.00
C30	C	0.04722	0.52364	0.74692	0.00000	Uiso	1.00
C31	C	0.38361	0.61639	0.74692	0.00000	Uiso	1.00
C32	C	0.43296	0.56704	0.74692	0.00000	Uiso	1.00
C33	C	0.47624	0.52376	0.74692	0.00000	Uiso	1.00
C34	C	0.61575	0.23252	0.74692	0.00000	Uiso	1.00
C35	C	0.56689	0.13387	0.74692	0.00000	Uiso	1.00
C36	C	0.52365	0.04743	0.74692	0.00000	Uiso	1.00
C37	C	0.76748	0.38425	0.74692	0.00000	Uiso	1.00
C38	C	0.86613	0.43311	0.74692	0.00000	Uiso	1.00
C39	C	0.95257	0.47635	0.74692	0.00000	Uiso	1.00
C40	C	0.61635	0.38365	0.74692	0.00000	Uiso	1.00
C41	C	0.56696	0.43304	0.74692	0.00000	Uiso	1.00
C42	C	0.52369	0.47631	0.74692	0.00000	Uiso	1.00
C43	C	0.28439	0.56912	0.74692	0.00000	Uiso	1.00
C44	C	0.43088	0.71561	0.74692	0.00000	Uiso	1.00
C45	C	0.28449	0.71551	0.74692	0.00000	Uiso	1.00
C46	C	0.71545	0.43125	0.74692	0.00000	Uiso	1.00
C47	C	0.56875	0.28455	0.74692	0.00000	Uiso	1.00
C48	C	0.71472	0.28528	0.74692	0.00000	Uiso	1.00
F49	F	0.40430	0.59570	0.24692	0.00000	Uiso	1.00

F50	F	0.40400	0.30716	0.24692	0.00000	Uiso	1.00
F51	F	0.69284	0.59600	0.24692	0.00000	Uiso	1.00
F52	F	0.92966	0.07034	0.24692	0.00000	Uiso	1.00
F53	F	0.92957	0.35916	0.24692	0.00000	Uiso	1.00
F54	F	0.64084	0.07043	0.24692	0.00000	Uiso	1.00
F55	F	0.23700	0.76300	0.74692	0.00000	Uiso	1.00
F56	F	0.23710	0.47418	0.74692	0.00000	Uiso	1.00
F57	F	0.52582	0.76290	0.74692	0.00000	Uiso	1.00
F58	F	0.76237	0.23763	0.74692	0.00000	Uiso	1.00
F59	F	0.76266	0.52617	0.74692	0.00000	Uiso	1.00
F60	F	0.47383	0.23734	0.74692	0.00000	Uiso	1.00

2×2 unit cell model of 9-fold stacking with a monomer stacked:

_cell_length_a	32.6729
_cell_length_b	32.6729
_cell_length_c	11.6232
_cell_angle_alpha	90.0000
_cell_angle_beta	90.0000
_cell_angle_gamma	120.0560

C1	C	0.28291	0.47470	0.62346	0.00000	Uiso	1.00
C2	C	0.23352	0.44984	0.62346	0.00000	Uiso	1.00
C3	C	0.19028	0.42864	0.62346	0.00000	Uiso	1.00
C4	C	0.35858	0.47474	0.62346	0.00000	Uiso	1.00
C5	C	0.38324	0.45006	0.62346	0.00000	Uiso	1.00
C6	C	0.40484	0.42850	0.62346	0.00000	Uiso	1.00
C7	C	0.30899	0.45125	0.62346	0.00000	Uiso	1.00

C8	C	0.19196	0.38376	0.87346	0.00000	Uiso	1.00
C9	C	0.21682	0.43315	0.87346	0.00000	Uiso	1.00
C10	C	0.23802	0.47639	0.87346	0.00000	Uiso	1.00
C11	C	0.11629	0.30803	0.87346	0.00000	Uiso	1.00
C12	C	0.06693	0.28325	0.87346	0.00000	Uiso	1.00
C13	C	0.02368	0.26151	0.87346	0.00000	Uiso	1.00
C14	C	0.19192	0.30809	0.87346	0.00000	Uiso	1.00
C15	C	0.21661	0.28342	0.87346	0.00000	Uiso	1.00
C16	C	0.23817	0.26183	0.87346	0.00000	Uiso	1.00
C17	C	0.30803	0.11629	0.87346	0.00000	Uiso	1.00
C18	C	0.28325	0.06693	0.87346	0.00000	Uiso	1.00
C19	C	0.26151	0.02368	0.87346	0.00000	Uiso	1.00
C20	C	0.38376	0.19196	0.87346	0.00000	Uiso	1.00
C21	C	0.43315	0.21682	0.87346	0.00000	Uiso	1.00
C22	C	0.47639	0.23802	0.87346	0.00000	Uiso	1.00
C23	C	0.30809	0.19192	0.87346	0.00000	Uiso	1.00
C24	C	0.28342	0.21661	0.87346	0.00000	Uiso	1.00
C25	C	0.26183	0.23817	0.87346	0.00000	Uiso	1.00
C26	C	0.14228	0.28450	0.87346	0.00000	Uiso	1.00
C27	C	0.21542	0.35768	0.87346	0.00000	Uiso	1.00
C28	C	0.14235	0.35765	0.87346	0.00000	Uiso	1.00
C29	C	0.35768	0.21542	0.87346	0.00000	Uiso	1.00
C30	C	0.28450	0.14228	0.87346	0.00000	Uiso	1.00
C31	C	0.35765	0.14235	0.87346	0.00000	Uiso	1.00
F32	F	0.28513	0.40372	0.62346	0.00000	Uiso	1.00
F33	F	0.11845	0.38115	0.87346	0.00000	Uiso	1.00

F34	F	0.11847	0.23703	0.87346	0.00000	Uiso	1.00
F35	F	0.26295	0.38154	0.87346	0.00000	Uiso	1.00
F36	F	0.38115	0.11845	0.87346	0.00000	Uiso	1.00
F37	F	0.38154	0.26295	0.87346	0.00000	Uiso	1.00
F38	F	0.23703	0.11847	0.87346	0.00000	Uiso	1.00
C39	C	0.69196	0.38376	0.87346	0.00000	Uiso	1.00
C40	C	0.71682	0.43315	0.87346	0.00000	Uiso	1.00
C41	C	0.73802	0.47639	0.87346	0.00000	Uiso	1.00
C42	C	0.61629	0.30803	0.87346	0.00000	Uiso	1.00
C43	C	0.56693	0.28325	0.87346	0.00000	Uiso	1.00
C44	C	0.52368	0.26151	0.87346	0.00000	Uiso	1.00
C45	C	0.69192	0.30809	0.87346	0.00000	Uiso	1.00
C46	C	0.71661	0.28342	0.87346	0.00000	Uiso	1.00
C47	C	0.73817	0.26183	0.87346	0.00000	Uiso	1.00
C48	C	0.80803	0.11629	0.87346	0.00000	Uiso	1.00
C49	C	0.78325	0.06693	0.87346	0.00000	Uiso	1.00
C50	C	0.76151	0.02368	0.87346	0.00000	Uiso	1.00
C51	C	0.88376	0.19196	0.87346	0.00000	Uiso	1.00
C52	C	0.93315	0.21682	0.87346	0.00000	Uiso	1.00
C53	C	0.97639	0.23802	0.87346	0.00000	Uiso	1.00
C54	C	0.80809	0.19192	0.87346	0.00000	Uiso	1.00
C55	C	0.78342	0.21661	0.87346	0.00000	Uiso	1.00
C56	C	0.76183	0.23817	0.87346	0.00000	Uiso	1.00
C57	C	0.64228	0.28450	0.87346	0.00000	Uiso	1.00
C58	C	0.71542	0.35768	0.87346	0.00000	Uiso	1.00
C59	C	0.64235	0.35765	0.87346	0.00000	Uiso	1.00

C60	C	0.85768	0.21542	0.87346	0.00000	Uiso	1.00
C61	C	0.78450	0.14228	0.87346	0.00000	Uiso	1.00
C62	C	0.85765	0.14235	0.87346	0.00000	Uiso	1.00
F63	F	0.61845	0.38115	0.87346	0.00000	Uiso	1.00
F64	F	0.61847	0.23703	0.87346	0.00000	Uiso	1.00
F65	F	0.76295	0.38154	0.87346	0.00000	Uiso	1.00
F66	F	0.88115	0.11845	0.87346	0.00000	Uiso	1.00
F67	F	0.88154	0.26295	0.87346	0.00000	Uiso	1.00
F68	F	0.73703	0.11847	0.87346	0.00000	Uiso	1.00
C69	C	0.35863	0.55037	0.62346	0.00000	Uiso	1.00
C70	C	0.38342	0.59974	0.62346	0.00000	Uiso	1.00
C71	C	0.40516	0.64299	0.62346	0.00000	Uiso	1.00
C72	C	0.38217	0.52438	0.62346	0.00000	Uiso	1.00
C73	C	0.30901	0.52432	0.62346	0.00000	Uiso	1.00
C74	C	0.19196	0.88376	0.87346	0.00000	Uiso	1.00
C75	C	0.21682	0.93315	0.87346	0.00000	Uiso	1.00
C76	C	0.23802	0.97639	0.87346	0.00000	Uiso	1.00
C77	C	0.11629	0.80803	0.87346	0.00000	Uiso	1.00
C78	C	0.06693	0.78325	0.87346	0.00000	Uiso	1.00
C79	C	0.02368	0.76151	0.87346	0.00000	Uiso	1.00
C80	C	0.19192	0.80809	0.87346	0.00000	Uiso	1.00
C81	C	0.21661	0.78342	0.87346	0.00000	Uiso	1.00
C82	C	0.23817	0.76183	0.87346	0.00000	Uiso	1.00
C83	C	0.30803	0.61629	0.87346	0.00000	Uiso	1.00
C84	C	0.28325	0.56693	0.87346	0.00000	Uiso	1.00
C85	C	0.26151	0.52368	0.87346	0.00000	Uiso	1.00

C86	C	0.38376	0.69196	0.87346	0.00000	Uiso	1.00
C87	C	0.43315	0.71682	0.87346	0.00000	Uiso	1.00
C88	C	0.47639	0.73802	0.87346	0.00000	Uiso	1.00
C89	C	0.30809	0.69192	0.87346	0.00000	Uiso	1.00
C90	C	0.28342	0.71661	0.87346	0.00000	Uiso	1.00
C91	C	0.26183	0.73817	0.87346	0.00000	Uiso	1.00
C92	C	0.14228	0.78450	0.87346	0.00000	Uiso	1.00
C93	C	0.21542	0.85768	0.87346	0.00000	Uiso	1.00
C94	C	0.14235	0.85765	0.87346	0.00000	Uiso	1.00
C95	C	0.35768	0.71542	0.87346	0.00000	Uiso	1.00
C96	C	0.28450	0.64228	0.87346	0.00000	Uiso	1.00
C97	C	0.35765	0.64235	0.87346	0.00000	Uiso	1.00
F98	F	0.28552	0.54822	0.62346	0.00000	Uiso	1.00
F99	F	0.42964	0.54820	0.62346	0.00000	Uiso	1.00
F100	F	0.11845	0.88115	0.87346	0.00000	Uiso	1.00
F101	F	0.11847	0.73703	0.87346	0.00000	Uiso	1.00
F102	F	0.26295	0.88154	0.87346	0.00000	Uiso	1.00
F103	F	0.38115	0.61845	0.87346	0.00000	Uiso	1.00
F104	F	0.38154	0.76295	0.87346	0.00000	Uiso	1.00
F105	F	0.23703	0.61847	0.87346	0.00000	Uiso	1.00
C106	C	0.69196	0.88376	0.87346	0.00000	Uiso	1.00
C107	C	0.71682	0.93315	0.87346	0.00000	Uiso	1.00
C108	C	0.73802	0.97639	0.87346	0.00000	Uiso	1.00
C109	C	0.61629	0.80803	0.87346	0.00000	Uiso	1.00
C110	C	0.56693	0.78325	0.87346	0.00000	Uiso	1.00
C111	C	0.52368	0.76151	0.87346	0.00000	Uiso	1.00

C112	C	0.69192	0.80809	0.87346	0.00000	Uiso	1.00
C113	C	0.71661	0.78342	0.87346	0.00000	Uiso	1.00
C114	C	0.73817	0.76183	0.87346	0.00000	Uiso	1.00
C115	C	0.80803	0.61629	0.87346	0.00000	Uiso	1.00
C116	C	0.78325	0.56693	0.87346	0.00000	Uiso	1.00
C117	C	0.76151	0.52368	0.87346	0.00000	Uiso	1.00
C118	C	0.88376	0.69196	0.87346	0.00000	Uiso	1.00
C119	C	0.93315	0.71682	0.87346	0.00000	Uiso	1.00
C120	C	0.97639	0.73802	0.87346	0.00000	Uiso	1.00
C121	C	0.80809	0.69192	0.87346	0.00000	Uiso	1.00
C122	C	0.78342	0.71661	0.87346	0.00000	Uiso	1.00
C123	C	0.76183	0.73817	0.87346	0.00000	Uiso	1.00
C124	C	0.64228	0.78450	0.87346	0.00000	Uiso	1.00
C125	C	0.71542	0.85768	0.87346	0.00000	Uiso	1.00
C126	C	0.64235	0.85765	0.87346	0.00000	Uiso	1.00
C127	C	0.85768	0.71542	0.87346	0.00000	Uiso	1.00
C128	C	0.78450	0.64228	0.87346	0.00000	Uiso	1.00
C129	C	0.85765	0.64235	0.87346	0.00000	Uiso	1.00
F130	F	0.61845	0.88115	0.87346	0.00000	Uiso	1.00
F131	F	0.61847	0.73703	0.87346	0.00000	Uiso	1.00
F132	F	0.76295	0.88154	0.87346	0.00000	Uiso	1.00
F133	F	0.88115	0.61845	0.87346	0.00000	Uiso	1.00
F134	F	0.88154	0.76295	0.87346	0.00000	Uiso	1.00
F135	F	0.73703	0.61847	0.87346	0.00000	Uiso	1.00
H136	H	0.14997	0.40888	0.62346	0.00000	Uiso	1.00
H137	H	0.42542	0.68330	0.62346	0.00000	Uiso	1.00

H138	H	0.42499	0.40837	0.62346	0.00000	Uiso	1.00

2×2 unit cell model of 9-fold stacking with a dimer stacked:

_cell_length_a	32.6729
_cell_length_b	32.6729
_cell_length_c	11.6232
_cell_angle_alpha	90.0000
_cell_angle_beta	90.0000
_cell_angle_gamma	120.0560

C1	C	0.28291	0.47470	0.58556	0.01267	Uiso	1.00
C2	C	0.23352	0.44984	0.57247	0.01267	Uiso	1.00
C3	C	0.19028	0.42864	0.56550	0.01267	Uiso	1.00
C4	C	0.35858	0.47474	0.61291	0.01267	Uiso	1.00
C5	C	0.38324	0.45006	0.62560	0.01267	Uiso	1.00
C6	C	0.40484	0.42850	0.63279	0.01267	Uiso	1.00
C7	C	0.47470	0.28291	0.58556	0.01267	Uiso	1.00
C8	C	0.44984	0.23352	0.57247	0.01267	Uiso	1.00
C9	C	0.42864	0.19028	0.56550	0.01267	Uiso	1.00
C10	C	0.47474	0.35858	0.61291	0.01267	Uiso	1.00
C11	C	0.45006	0.38324	0.62560	0.01267	Uiso	1.00
C12	C	0.42850	0.40484	0.63279	0.01267	Uiso	1.00
C13	C	0.30899	0.45125	0.59946	0.01267	Uiso	1.00
C14	C	0.45125	0.30899	0.59946	0.01267	Uiso	1.00
C15	C	0.19196	0.38376	0.87346	0.01267	Uiso	1.00
C16	C	0.21682	0.43315	0.87346	0.01267	Uiso	1.00
C17	C	0.23802	0.47639	0.87346	0.01267	Uiso	1.00

C18	C	0.11629	0.30803	0.87346	0.01267	Uiso	1.00
C19	C	0.06693	0.28325	0.87346	0.01267	Uiso	1.00
C20	C	0.02368	0.26151	0.87346	0.01267	Uiso	1.00
C21	C	0.19192	0.30809	0.87346	0.01267	Uiso	1.00
C22	C	0.21661	0.28342	0.87346	0.01267	Uiso	1.00
C23	C	0.23817	0.26183	0.87346	0.01267	Uiso	1.00
C24	C	0.30803	0.11629	0.87346	0.01267	Uiso	1.00
C25	C	0.28325	0.06693	0.87346	0.01267	Uiso	1.00
C26	C	0.26151	0.02368	0.87346	0.01267	Uiso	1.00
C27	C	0.38376	0.19196	0.87346	0.01267	Uiso	1.00
C28	C	0.43315	0.21682	0.87346	0.01267	Uiso	1.00
C29	C	0.47639	0.23802	0.87346	0.01267	Uiso	1.00
C30	C	0.30809	0.19192	0.87346	0.01267	Uiso	1.00
C31	C	0.28342	0.21661	0.87346	0.01267	Uiso	1.00
C32	C	0.26183	0.23817	0.87346	0.01267	Uiso	1.00
C33	C	0.14228	0.28450	0.87346	0.01267	Uiso	1.00
C34	C	0.21542	0.35768	0.87346	0.01267	Uiso	1.00
C35	C	0.14235	0.35765	0.87346	0.01267	Uiso	1.00
C36	C	0.35768	0.21542	0.87346	0.01267	Uiso	1.00
C37	C	0.28450	0.14228	0.87346	0.01267	Uiso	1.00
C38	C	0.35765	0.14235	0.87346	0.01267	Uiso	1.00
C39	C	0.55037	0.35863	0.59699	0.01267	Uiso	1.00
C40	C	0.59974	0.38342	0.59340	0.01267	Uiso	1.00
C41	C	0.64299	0.40516	0.59093	0.01267	Uiso	1.00
C42	C	0.52438	0.38217	0.60960	0.01267	Uiso	1.00
C43	C	0.52432	0.30901	0.58581	0.01267	Uiso	1.00

C44	C	0.69196	0.38376	0.87346	0.01267	Uiso	1.00
C45	C	0.71682	0.43315	0.87346	0.01267	Uiso	1.00
C46	C	0.73802	0.47639	0.87346	0.01267	Uiso	1.00
C47	C	0.61629	0.30803	0.87346	0.01267	Uiso	1.00
C48	C	0.56693	0.28325	0.87346	0.01267	Uiso	1.00
C49	C	0.52368	0.26151	0.87346	0.01267	Uiso	1.00
C50	C	0.69192	0.30809	0.87346	0.01267	Uiso	1.00
C51	C	0.71661	0.28342	0.87346	0.01267	Uiso	1.00
C52	C	0.73817	0.26183	0.87346	0.01267	Uiso	1.00
C53	C	0.80803	0.11629	0.87346	0.01267	Uiso	1.00
C54	C	0.78325	0.06693	0.87346	0.01267	Uiso	1.00
C55	C	0.76151	0.02368	0.87346	0.01267	Uiso	1.00
C56	C	0.88376	0.19196	0.87346	0.01267	Uiso	1.00
C57	C	0.93315	0.21682	0.87346	0.01267	Uiso	1.00
C58	C	0.97639	0.23802	0.87346	0.01267	Uiso	1.00
C59	C	0.80809	0.19192	0.87346	0.01267	Uiso	1.00
C60	C	0.78342	0.21661	0.87346	0.01267	Uiso	1.00
C61	C	0.76183	0.23817	0.87346	0.01267	Uiso	1.00
C62	C	0.64228	0.28450	0.87346	0.01267	Uiso	1.00
C63	C	0.71542	0.35768	0.87346	0.01267	Uiso	1.00
C64	C	0.64235	0.35765	0.87346	0.01267	Uiso	1.00
C65	C	0.85768	0.21542	0.87346	0.01267	Uiso	1.00
C66	C	0.78450	0.14228	0.87346	0.01267	Uiso	1.00
C67	C	0.85765	0.14235	0.87346	0.01267	Uiso	1.00
C68	C	0.35863	0.55037	0.59699	0.01267	Uiso	1.00
C69	C	0.38342	0.59974	0.59340	0.01267	Uiso	1.00

C70	C	0.40516	0.64299	0.59093	0.01267	Uiso	1.00
C71	C	0.38217	0.52438	0.60960	0.01267	Uiso	1.00
C72	C	0.30901	0.52432	0.58581	0.01267	Uiso	1.00
C73	C	0.19196	0.88376	0.87346	0.01267	Uiso	1.00
C74	C	0.21682	0.93315	0.87346	0.01267	Uiso	1.00
C75	C	0.23802	0.97639	0.87346	0.01267	Uiso	1.00
C76	C	0.11629	0.80803	0.87346	0.01267	Uiso	1.00
C77	C	0.06693	0.78325	0.87346	0.01267	Uiso	1.00
C78	C	0.02368	0.76151	0.87346	0.01267	Uiso	1.00
C79	C	0.19192	0.80809	0.87346	0.01267	Uiso	1.00
C80	C	0.21661	0.78342	0.87346	0.01267	Uiso	1.00
C81	C	0.23817	0.76183	0.87346	0.01267	Uiso	1.00
C82	C	0.30803	0.61629	0.87346	0.01267	Uiso	1.00
C83	C	0.28325	0.56693	0.87346	0.01267	Uiso	1.00
C84	C	0.26151	0.52368	0.87346	0.01267	Uiso	1.00
C85	C	0.38376	0.69196	0.87346	0.01267	Uiso	1.00
C86	C	0.43315	0.71682	0.87346	0.01267	Uiso	1.00
C87	C	0.47639	0.73802	0.87346	0.01267	Uiso	1.00
C88	C	0.30809	0.69192	0.87346	0.01267	Uiso	1.00
C89	C	0.28342	0.71661	0.87346	0.01267	Uiso	1.00
C90	C	0.26183	0.73817	0.87346	0.01267	Uiso	1.00
C91	C	0.14228	0.78450	0.87346	0.01267	Uiso	1.00
C92	C	0.21542	0.85768	0.87346	0.01267	Uiso	1.00
C93	C	0.14235	0.85765	0.87346	0.01267	Uiso	1.00
C94	C	0.35768	0.71542	0.87346	0.01267	Uiso	1.00
C95	C	0.28450	0.64228	0.87346	0.01267	Uiso	1.00

C96	C	0.35765	0.64235	0.87346	0.01267	Uiso	1.00
C97	C	0.69196	0.88376	0.87346	0.01267	Uiso	1.00
C98	C	0.71682	0.93315	0.87346	0.01267	Uiso	1.00
C99	C	0.73802	0.97639	0.87346	0.01267	Uiso	1.00
C100	C	0.61629	0.80803	0.87346	0.01267	Uiso	1.00
C101	C	0.56693	0.78325	0.87346	0.01267	Uiso	1.00
C102	C	0.52368	0.76151	0.87346	0.01267	Uiso	1.00
C103	C	0.69192	0.80809	0.87346	0.01267	Uiso	1.00
C104	C	0.71661	0.78342	0.87346	0.01267	Uiso	1.00
C105	C	0.73817	0.76183	0.87346	0.01267	Uiso	1.00
C106	C	0.80803	0.61629	0.87346	0.01267	Uiso	1.00
C107	C	0.78325	0.56693	0.87346	0.01267	Uiso	1.00
C108	C	0.76151	0.52368	0.87346	0.01267	Uiso	1.00
C109	C	0.88376	0.69196	0.87346	0.01267	Uiso	1.00
C110	C	0.93315	0.71682	0.87346	0.01267	Uiso	1.00
C111	C	0.97639	0.73802	0.87346	0.01267	Uiso	1.00
C112	C	0.80809	0.69192	0.87346	0.01267	Uiso	1.00
C113	C	0.78342	0.71661	0.87346	0.01267	Uiso	1.00
C114	C	0.76183	0.73817	0.87346	0.01267	Uiso	1.00
C115	C	0.64228	0.78450	0.87346	0.01267	Uiso	1.00
C116	C	0.71542	0.85768	0.87346	0.01267	Uiso	1.00
C117	C	0.64235	0.85765	0.87346	0.01267	Uiso	1.00
C118	C	0.85768	0.71542	0.87346	0.01267	Uiso	1.00
C119	C	0.78450	0.64228	0.87346	0.01267	Uiso	1.00
C120	C	0.85765	0.64235	0.87346	0.01267	Uiso	1.00
F1	F	0.28513	0.40372	0.60087	0.01267	Uiso	1.00

F2	F	0.40372	0.28513	0.60087	0.01267	Uiso	1.00
F3	F	0.11845	0.38115	0.87346	0.01267	Uiso	1.00
F4	F	0.11847	0.23703	0.87346	0.01267	Uiso	1.00
F5	F	0.26295	0.38154	0.87346	0.01267	Uiso	1.00
F6	F	0.38115	0.11845	0.87346	0.01267	Uiso	1.00
F7	F	0.38154	0.26295	0.87346	0.01267	Uiso	1.00
F8	F	0.23703	0.11847	0.87346	0.01267	Uiso	1.00
F9	F	0.54822	0.28552	0.57474	0.01267	Uiso	1.00
F10	F	0.54820	0.42964	0.61834	0.01267	Uiso	1.00
F11	F	0.61845	0.38115	0.87346	0.01267	Uiso	1.00
F12	F	0.61847	0.23703	0.87346	0.01267	Uiso	1.00
F13	F	0.76295	0.38154	0.87346	0.01267	Uiso	1.00
F14	F	0.88115	0.11845	0.87346	0.01267	Uiso	1.00
F15	F	0.88154	0.26295	0.87346	0.01267	Uiso	1.00
F16	F	0.73703	0.11847	0.87346	0.01267	Uiso	1.00
F17	F	0.28552	0.54822	0.57474	0.01267	Uiso	1.00
F18	F	0.42964	0.54820	0.61834	0.01267	Uiso	1.00
F19	F	0.11845	0.88115	0.87346	0.01267	Uiso	1.00
F20	F	0.11847	0.73703	0.87346	0.01267	Uiso	1.00
F21	F	0.26295	0.88154	0.87346	0.01267	Uiso	1.00
F22	F	0.38115	0.61845	0.87346	0.01267	Uiso	1.00
F23	F	0.38154	0.76295	0.87346	0.01267	Uiso	1.00
F24	F	0.23703	0.61847	0.87346	0.01267	Uiso	1.00
F25	F	0.61845	0.88115	0.87346	0.01267	Uiso	1.00
F26	F	0.61847	0.73703	0.87346	0.01267	Uiso	1.00
F27	F	0.76295	0.88154	0.87346	0.01267	Uiso	1.00

F28	F	0.88115	0.61845	0.87346	0.01267	Uiso	1.00
F29	F	0.88154	0.76295	0.87346	0.01267	Uiso	1.00
F30	F	0.73703	0.61847	0.87346	0.01267	Uiso	1.00
H1	H	0.15257	0.41024	0.55694	0.01267	Uiso	1.00
H2	H	0.41023	0.15257	0.55694	0.01267	Uiso	1.00
H3	H	0.68088	0.42453	0.58923	0.01267	Uiso	1.00
H4	H	0.42454	0.68088	0.58923	0.01267	Uiso	1.00

2×2 unit cell model of 9-fold stacking with a trimer stacked:

_cell_length_a	32.6729
_cell_length_b	32.6729
_cell_length_c	11.6232
_cell_angle_alpha	90.0000
_cell_angle_beta	90.0000
_cell_angle_gamma	120.0560

C1	C	0.28291	0.47470	0.57415	0.01267	Uiso	1.00
C2	C	0.23352	0.44984	0.56107	0.01267	Uiso	1.00
C3	C	0.19028	0.42864	0.55388	0.01267	Uiso	1.00
C4	C	0.35858	0.47474	0.60024	0.01267	Uiso	1.00
C5	C	0.38324	0.45006	0.61195	0.01267	Uiso	1.00
C6	C	0.40484	0.42850	0.61790	0.01267	Uiso	1.00
C7	C	0.47470	0.28291	0.57664	0.01267	Uiso	1.00
C8	C	0.44984	0.23352	0.56261	0.01267	Uiso	1.00
C9	C	0.42864	0.19028	0.55460	0.01267	Uiso	1.00
C10	C	0.47474	0.35858	0.60268	0.01267	Uiso	1.00
C11	C	0.45006	0.38324	0.61369	0.01267	Uiso	1.00

C12	C	0.42850	0.40484	0.61865	0.01267	Uiso	1.00
C13	C	0.30899	0.45125	0.58868	0.01267	Uiso	1.00
C14	C	0.45125	0.30899	0.59081	0.01267	Uiso	1.00
C15	C	0.19196	0.38376	0.87346	0.01267	Uiso	1.00
C16	C	0.21682	0.43315	0.87346	0.01267	Uiso	1.00
C17	C	0.23802	0.47639	0.87346	0.01267	Uiso	1.00
C18	C	0.11629	0.30803	0.87346	0.01267	Uiso	1.00
C19	C	0.06693	0.28325	0.87346	0.01267	Uiso	1.00
C20	C	0.02368	0.26151	0.87346	0.01267	Uiso	1.00
C21	C	0.19192	0.30809	0.87346	0.01267	Uiso	1.00
C22	C	0.21661	0.28342	0.87346	0.01267	Uiso	1.00
C23	C	0.23817	0.26183	0.87346	0.01267	Uiso	1.00
C24	C	0.30803	0.11629	0.87346	0.01267	Uiso	1.00
C25	C	0.28325	0.06693	0.87346	0.01267	Uiso	1.00
C26	C	0.26151	0.02368	0.87346	0.01267	Uiso	1.00
C27	C	0.38376	0.19196	0.87346	0.01267	Uiso	1.00
C28	C	0.43315	0.21682	0.87346	0.01267	Uiso	1.00
C29	C	0.47639	0.23802	0.87346	0.01267	Uiso	1.00
C30	C	0.30809	0.19192	0.87346	0.01267	Uiso	1.00
C31	C	0.28342	0.21661	0.87346	0.01267	Uiso	1.00
C32	C	0.26183	0.23817	0.87346	0.01267	Uiso	1.00
C33	C	0.14228	0.28450	0.87346	0.01267	Uiso	1.00
C34	C	0.21542	0.35768	0.87346	0.01267	Uiso	1.00
C35	C	0.14235	0.35765	0.87346	0.01267	Uiso	1.00
C36	C	0.35768	0.21542	0.87346	0.01267	Uiso	1.00
C37	C	0.28450	0.14228	0.87346	0.01267	Uiso	1.00

C38	C	0.35765	0.14235	0.87346	0.01267	Uiso	1.00
C39	C	0.55037	0.35863	0.58608	0.01267	Uiso	1.00
C40	C	0.59974	0.38342	0.58175	0.01267	Uiso	1.00
C41	C	0.64299	0.40516	0.57858	0.01267	Uiso	1.00
C42	C	0.52438	0.38217	0.59937	0.01267	Uiso	1.00
C43	C	0.52432	0.30901	0.57565	0.01267	Uiso	1.00
C44	C	0.69196	0.38376	0.87346	0.01267	Uiso	1.00
C45	C	0.71682	0.43315	0.87346	0.01267	Uiso	1.00
C46	C	0.73802	0.47639	0.87346	0.01267	Uiso	1.00
C47	C	0.61629	0.30803	0.87346	0.01267	Uiso	1.00
C48	C	0.56693	0.28325	0.87346	0.01267	Uiso	1.00
C49	C	0.52368	0.26151	0.87346	0.01267	Uiso	1.00
C50	C	0.69192	0.30809	0.87346	0.01267	Uiso	1.00
C51	C	0.71661	0.28342	0.87346	0.01267	Uiso	1.00
C52	C	0.73817	0.26183	0.87346	0.01267	Uiso	1.00
C53	C	0.80803	0.11629	0.87346	0.01267	Uiso	1.00
C54	C	0.78325	0.06693	0.87346	0.01267	Uiso	1.00
C55	C	0.76151	0.02368	0.87346	0.01267	Uiso	1.00
C56	C	0.88376	0.19196	0.87346	0.01267	Uiso	1.00
C57	C	0.93315	0.21682	0.87346	0.01267	Uiso	1.00
C58	C	0.97639	0.23802	0.87346	0.01267	Uiso	1.00
C59	C	0.80809	0.19192	0.87346	0.01267	Uiso	1.00
C60	C	0.78342	0.21661	0.87346	0.01267	Uiso	1.00
C61	C	0.76183	0.23817	0.87346	0.01267	Uiso	1.00
C62	C	0.64228	0.28450	0.87346	0.01267	Uiso	1.00
C63	C	0.71542	0.35768	0.87346	0.01267	Uiso	1.00

C64	C	0.64235	0.35765	0.87346	0.01267	Uiso	1.00
C65	C	0.85768	0.21542	0.87346	0.01267	Uiso	1.00
C66	C	0.78450	0.14228	0.87346	0.01267	Uiso	1.00
C67	C	0.85765	0.14235	0.87346	0.01267	Uiso	1.00
C68	C	0.35863	0.55037	0.58228	0.01267	Uiso	1.00
C69	C	0.38342	0.59974	0.57617	0.01267	Uiso	1.00
C70	C	0.40516	0.64299	0.56998	0.01267	Uiso	1.00
C71	C	0.47470	0.78291	0.57763	0.01267	Uiso	1.00
C72	C	0.44984	0.73352	0.56983	0.01267	Uiso	1.00
C73	C	0.42864	0.69028	0.56736	0.01267	Uiso	1.00
C74	C	0.47474	0.85858	0.60246	0.01267	Uiso	1.00
C75	C	0.45006	0.88324	0.61799	0.01267	Uiso	1.00
C76	C	0.42850	0.90484	0.62608	0.01267	Uiso	1.00
C77	C	0.38217	0.52438	0.59620	0.01267	Uiso	1.00
C78	C	0.30901	0.52432	0.57253	0.01267	Uiso	1.00
C79	C	0.45125	0.80899	0.59311	0.01267	Uiso	1.00
C80	C	0.19196	0.88376	0.87346	0.01267	Uiso	1.00
C81	C	0.21682	0.93315	0.87346	0.01267	Uiso	1.00
C82	C	0.23802	0.97639	0.87346	0.01267	Uiso	1.00
C83	C	0.11629	0.80803	0.87346	0.01267	Uiso	1.00
C84	C	0.06693	0.78325	0.87346	0.01267	Uiso	1.00
C85	C	0.02368	0.76151	0.87346	0.01267	Uiso	1.00
C86	C	0.19192	0.80809	0.87346	0.01267	Uiso	1.00
C87	C	0.21661	0.78342	0.87346	0.01267	Uiso	1.00
C88	C	0.23817	0.76183	0.87346	0.01267	Uiso	1.00
C89	C	0.30803	0.61629	0.87346	0.01267	Uiso	1.00

C90	C	0.28325	0.56693	0.87346	0.01267	Uiso	1.00
C91	C	0.26151	0.52368	0.87346	0.01267	Uiso	1.00
C92	C	0.38376	0.69196	0.87346	0.01267	Uiso	1.00
C93	C	0.43315	0.71682	0.87346	0.01267	Uiso	1.00
C94	C	0.47639	0.73802	0.87346	0.01267	Uiso	1.00
C95	C	0.30809	0.69192	0.87346	0.01267	Uiso	1.00
C96	C	0.28342	0.71661	0.87346	0.01267	Uiso	1.00
C97	C	0.26183	0.73817	0.87346	0.01267	Uiso	1.00
C98	C	0.14228	0.78450	0.87346	0.01267	Uiso	1.00
C99	C	0.21542	0.85768	0.87346	0.01267	Uiso	1.00
C100	C	0.14235	0.85765	0.87346	0.01267	Uiso	1.00
C101	C	0.35768	0.71542	0.87346	0.01267	Uiso	1.00
C102	C	0.28450	0.64228	0.87346	0.01267	Uiso	1.00
C103	C	0.35765	0.64235	0.87346	0.01267	Uiso	1.00
C104	C	0.55037	0.85863	0.58161	0.01267	Uiso	1.00
C105	C	0.59974	0.88342	0.57659	0.01267	Uiso	1.00
C106	C	0.64299	0.90516	0.57420	0.01267	Uiso	1.00
C107	C	0.52438	0.88217	0.59583	0.01267	Uiso	1.00
C108	C	0.52432	0.80901	0.57309	0.01267	Uiso	1.00
C109	C	0.69196	0.88376	0.87346	0.01267	Uiso	1.00
C110	C	0.71682	0.93315	0.87346	0.01267	Uiso	1.00
C111	C	0.73802	0.97639	0.87346	0.01267	Uiso	1.00
C112	C	0.61629	0.80803	0.87346	0.01267	Uiso	1.00
C113	C	0.56693	0.78325	0.87346	0.01267	Uiso	1.00
C114	C	0.52368	0.76151	0.87346	0.01267	Uiso	1.00
C115	C	0.69192	0.80809	0.87346	0.01267	Uiso	1.00

C116	C	0.71661	0.78342	0.87346	0.01267	Uiso	1.00
C117	C	0.73817	0.76183	0.87346	0.01267	Uiso	1.00
C118	C	0.80803	0.61629	0.87346	0.01267	Uiso	1.00
C119	C	0.78325	0.56693	0.87346	0.01267	Uiso	1.00
C120	C	0.76151	0.52368	0.87346	0.01267	Uiso	1.00
C121	C	0.88376	0.69196	0.87346	0.01267	Uiso	1.00
C122	C	0.93315	0.71682	0.87346	0.01267	Uiso	1.00
C123	C	0.97639	0.73802	0.87346	0.01267	Uiso	1.00
C124	C	0.80809	0.69192	0.87346	0.01267	Uiso	1.00
C125	C	0.78342	0.71661	0.87346	0.01267	Uiso	1.00
C126	C	0.76183	0.73817	0.87346	0.01267	Uiso	1.00
C127	C	0.64228	0.78450	0.87346	0.01267	Uiso	1.00
C128	C	0.71542	0.85768	0.87346	0.01267	Uiso	1.00
C129	C	0.64235	0.85765	0.87346	0.01267	Uiso	1.00
C130	C	0.85768	0.71542	0.87346	0.01267	Uiso	1.00
C131	C	0.78450	0.64228	0.87346	0.01267	Uiso	1.00
C132	C	0.85765	0.64235	0.87346	0.01267	Uiso	1.00
F1	F	0.28513	0.40372	0.59080	0.01267	Uiso	1.00
F2	F	0.40372	0.28513	0.59313	0.01267	Uiso	1.00
F3	F	0.11845	0.38115	0.87346	0.01267	Uiso	1.00
F4	F	0.11847	0.23703	0.87346	0.01267	Uiso	1.00
F5	F	0.26295	0.38154	0.87346	0.01267	Uiso	1.00
F6	F	0.38115	0.11845	0.87346	0.01267	Uiso	1.00
F7	F	0.38154	0.26295	0.87346	0.01267	Uiso	1.00
F8	F	0.23703	0.11847	0.87346	0.01267	Uiso	1.00
F9	F	0.54822	0.28552	0.56320	0.01267	Uiso	1.00

F10	F	0.54820	0.42964	0.60885	0.01267	Uiso	1.00
F11	F	0.61845	0.38115	0.87346	0.01267	Uiso	1.00
F12	F	0.61847	0.23703	0.87346	0.01267	Uiso	1.00
F13	F	0.76295	0.38154	0.87346	0.01267	Uiso	1.00
F14	F	0.88115	0.11845	0.87346	0.01267	Uiso	1.00
F15	F	0.88154	0.26295	0.87346	0.01267	Uiso	1.00
F16	F	0.73703	0.11847	0.87346	0.01267	Uiso	1.00
F17	F	0.28552	0.54822	0.55987	0.01267	Uiso	1.00
F18	F	0.42964	0.54820	0.60530	0.01267	Uiso	1.00
F19	F	0.40372	0.78513	0.59898	0.01267	Uiso	1.00
F20	F	0.11845	0.88115	0.87346	0.01267	Uiso	1.00
F21	F	0.11847	0.73703	0.87346	0.01267	Uiso	1.00
F22	F	0.26295	0.88154	0.87346	0.01267	Uiso	1.00
F23	F	0.38115	0.61845	0.87346	0.01267	Uiso	1.00
F24	F	0.38154	0.76295	0.87346	0.01267	Uiso	1.00
F25	F	0.23703	0.61847	0.87346	0.01267	Uiso	1.00
F26	F	0.54822	0.78552	0.55971	0.01267	Uiso	1.00
F27	F	0.54820	0.92964	0.60334	0.01267	Uiso	1.00
F28	F	0.61845	0.88115	0.87346	0.01267	Uiso	1.00
F29	F	0.61847	0.73703	0.87346	0.01267	Uiso	1.00
F30	F	0.76295	0.88154	0.87346	0.01267	Uiso	1.00
F31	F	0.88115	0.61845	0.87346	0.01267	Uiso	1.00
F32	F	0.88154	0.76295	0.87346	0.01267	Uiso	1.00
F33	F	0.73703	0.61847	0.87346	0.01267	Uiso	1.00
H1	H	0.15262	0.41019	0.54487	0.01267	Uiso	1.00
H2	H	0.41018	0.15263	0.54434	0.01267	Uiso	1.00

H3	H	0.68081	0.42443	0.57498	0.01267	Uiso	1.00
H4	H	0.68086	0.92441	0.57234	0.01267	Uiso	1.00
H5	H	0.40970	0.92365	0.63656	0.01267	Uiso	1.00

2×2 unit cell model of 4-fold stacking with a monomer stacked:

_cell_length_a	32.9505
_cell_length_b	32.9546
_cell_length_c	11.3555
_cell_angle_alpha	90.0000
_cell_angle_beta	90.0000
_cell_angle_gamma	120.9090

C1	C	0.19441	0.38282	0.87346	0.00000	Uiso	1.00
C2	C	0.21963	0.43268	0.87346	0.00000	Uiso	1.00
C3	C	0.23931	0.47616	0.87346	0.00000	Uiso	1.00
C4	C	0.11718	0.30559	0.87346	0.00000	Uiso	1.00
C5	C	0.06732	0.28037	0.87346	0.00000	Uiso	1.00
C6	C	0.02384	0.26069	0.87346	0.00000	Uiso	1.00
C7	C	0.19291	0.30709	0.87346	0.00000	Uiso	1.00
C8	C	0.21717	0.28283	0.87346	0.00000	Uiso	1.00
C9	C	0.23838	0.26162	0.87346	0.00000	Uiso	1.00
C10	C	0.30559	0.11718	0.87346	0.00000	Uiso	1.00
C11	C	0.28037	0.06732	0.87346	0.00000	Uiso	1.00
C12	C	0.26069	0.02384	0.87346	0.00000	Uiso	1.00
C13	C	0.38282	0.19441	0.87346	0.00000	Uiso	1.00
C14	C	0.43268	0.21963	0.87346	0.00000	Uiso	1.00
C15	C	0.47616	0.23931	0.87346	0.00000	Uiso	1.00

C16	C	0.30709	0.19291	0.87346	0.00000	Uiso	1.00
C17	C	0.28283	0.21717	0.87346	0.00000	Uiso	1.00
C18	C	0.26162	0.23838	0.87346	0.00000	Uiso	1.00
C19	C	0.14281	0.28249	0.87346	0.00000	Uiso	1.00
C20	C	0.21751	0.35719	0.87346	0.00000	Uiso	1.00
C21	C	0.14431	0.35569	0.87346	0.00000	Uiso	1.00
C22	C	0.35719	0.21751	0.87346	0.00000	Uiso	1.00
C23	C	0.28249	0.14281	0.87346	0.00000	Uiso	1.00
C24	C	0.35569	0.14431	0.87346	0.00000	Uiso	1.00
F25	F	0.36815	0.48455	0.62346	0.00000	Uiso	1.00
F26	F	0.12088	0.37912	0.87346	0.00000	Uiso	1.00
F27	F	0.11815	0.23455	0.87346	0.00000	Uiso	1.00
F28	F	0.26545	0.38185	0.87346	0.00000	Uiso	1.00
F29	F	0.37912	0.12088	0.87346	0.00000	Uiso	1.00
F30	F	0.38185	0.26545	0.87346	0.00000	Uiso	1.00
F31	F	0.23455	0.11815	0.87346	0.00000	Uiso	1.00
C32	C	0.69441	0.38282	0.87346	0.00000	Uiso	1.00
C33	C	0.71963	0.43268	0.87346	0.00000	Uiso	1.00
C34	C	0.73931	0.47616	0.87346	0.00000	Uiso	1.00
C35	C	0.61718	0.30559	0.87346	0.00000	Uiso	1.00
C36	C	0.56732	0.28037	0.87346	0.00000	Uiso	1.00
C37	C	0.52384	0.26069	0.87346	0.00000	Uiso	1.00
C38	C	0.69291	0.30709	0.87346	0.00000	Uiso	1.00
C39	C	0.71717	0.28283	0.87346	0.00000	Uiso	1.00
C40	C	0.73838	0.26162	0.87346	0.00000	Uiso	1.00
C41	C	0.80559	0.11718	0.87346	0.00000	Uiso	1.00

C42	C	0.78037	0.06732	0.87346	0.00000	Uiso	1.00
C43	C	0.76069	0.02384	0.87346	0.00000	Uiso	1.00
C44	C	0.88282	0.19441	0.87346	0.00000	Uiso	1.00
C45	C	0.93268	0.21963	0.87346	0.00000	Uiso	1.00
C46	C	0.97616	0.23931	0.87346	0.00000	Uiso	1.00
C47	C	0.80709	0.19291	0.87346	0.00000	Uiso	1.00
C48	C	0.78283	0.21717	0.87346	0.00000	Uiso	1.00
C49	C	0.76162	0.23838	0.87346	0.00000	Uiso	1.00
C50	C	0.64281	0.28249	0.87346	0.00000	Uiso	1.00
C51	C	0.71751	0.35719	0.87346	0.00000	Uiso	1.00
C52	C	0.64431	0.35569	0.87346	0.00000	Uiso	1.00
C53	C	0.85719	0.21751	0.87346	0.00000	Uiso	1.00
C54	C	0.78249	0.14281	0.87346	0.00000	Uiso	1.00
C55	C	0.85569	0.14431	0.87346	0.00000	Uiso	1.00
F56	F	0.62088	0.37912	0.87346	0.00000	Uiso	1.00
F57	F	0.61815	0.23455	0.87346	0.00000	Uiso	1.00
F58	F	0.76545	0.38185	0.87346	0.00000	Uiso	1.00
F59	F	0.87912	0.12088	0.87346	0.00000	Uiso	1.00
F60	F	0.88185	0.26545	0.87346	0.00000	Uiso	1.00
F61	F	0.73455	0.11815	0.87346	0.00000	Uiso	1.00
C62	C	0.44441	0.63282	0.62346	0.00000	Uiso	1.00
C63	C	0.46963	0.68268	0.62346	0.00000	Uiso	1.00
C64	C	0.48931	0.72616	0.62346	0.00000	Uiso	1.00
C65	C	0.36718	0.55559	0.62346	0.00000	Uiso	1.00
C66	C	0.31732	0.53037	0.62346	0.00000	Uiso	1.00
C67	C	0.27384	0.51069	0.62346	0.00000	Uiso	1.00

C68	C	0.44291	0.55709	0.62346	0.00000	Uiso	1.00
C69	C	0.46717	0.53283	0.62346	0.00000	Uiso	1.00
C70	C	0.48838	0.51162	0.62346	0.00000	Uiso	1.00
C71	C	0.39281	0.53249	0.62346	0.00000	Uiso	1.00
C72	C	0.46751	0.60719	0.62346	0.00000	Uiso	1.00
C73	C	0.39431	0.60569	0.62346	0.00000	Uiso	1.00
C74	C	0.19441	0.88282	0.87346	0.00000	Uiso	1.00
C75	C	0.21963	0.93268	0.87346	0.00000	Uiso	1.00
C76	C	0.23931	0.97616	0.87346	0.00000	Uiso	1.00
C77	C	0.11718	0.80559	0.87346	0.00000	Uiso	1.00
C78	C	0.06732	0.78037	0.87346	0.00000	Uiso	1.00
C79	C	0.02384	0.76069	0.87346	0.00000	Uiso	1.00
C80	C	0.19291	0.80709	0.87346	0.00000	Uiso	1.00
C81	C	0.21717	0.78283	0.87346	0.00000	Uiso	1.00
C82	C	0.23838	0.76162	0.87346	0.00000	Uiso	1.00
C83	C	0.30559	0.61718	0.87346	0.00000	Uiso	1.00
C84	C	0.28037	0.56732	0.87346	0.00000	Uiso	1.00
C85	C	0.26069	0.52384	0.87346	0.00000	Uiso	1.00
C86	C	0.38282	0.69441	0.87346	0.00000	Uiso	1.00
C87	C	0.43268	0.71963	0.87346	0.00000	Uiso	1.00
C88	C	0.47616	0.73931	0.87346	0.00000	Uiso	1.00
C89	C	0.30709	0.69291	0.87346	0.00000	Uiso	1.00
C90	C	0.28283	0.71717	0.87346	0.00000	Uiso	1.00
C91	C	0.26162	0.73838	0.87346	0.00000	Uiso	1.00
C92	C	0.14281	0.78249	0.87346	0.00000	Uiso	1.00
C93	C	0.21751	0.85719	0.87346	0.00000	Uiso	1.00

C94	C	0.14431	0.85569	0.87346	0.00000	Uiso	1.00
C95	C	0.35719	0.71751	0.87346	0.00000	Uiso	1.00
C96	C	0.28249	0.64281	0.87346	0.00000	Uiso	1.00
C97	C	0.35569	0.64431	0.87346	0.00000	Uiso	1.00
F98	F	0.37088	0.62912	0.62346	0.00000	Uiso	1.00
F99	F	0.12088	0.87912	0.87346	0.00000	Uiso	1.00
F100	F	0.11815	0.73455	0.87346	0.00000	Uiso	1.00
F101	F	0.26545	0.88185	0.87346	0.00000	Uiso	1.00
F102	F	0.37912	0.62088	0.87346	0.00000	Uiso	1.00
F103	F	0.38185	0.76545	0.87346	0.00000	Uiso	1.00
F104	F	0.23455	0.61815	0.87346	0.00000	Uiso	1.00
C105	C	0.69441	0.88282	0.87346	0.00000	Uiso	1.00
C106	C	0.71963	0.93268	0.87346	0.00000	Uiso	1.00
C107	C	0.73931	0.97616	0.87346	0.00000	Uiso	1.00
C108	C	0.61718	0.80559	0.87346	0.00000	Uiso	1.00
C109	C	0.56732	0.78037	0.87346	0.00000	Uiso	1.00
C110	C	0.52384	0.76069	0.87346	0.00000	Uiso	1.00
C111	C	0.69291	0.80709	0.87346	0.00000	Uiso	1.00
C112	C	0.71717	0.78283	0.87346	0.00000	Uiso	1.00
C113	C	0.73838	0.76162	0.87346	0.00000	Uiso	1.00
C114	C	0.80559	0.61718	0.87346	0.00000	Uiso	1.00
C115	C	0.78037	0.56732	0.87346	0.00000	Uiso	1.00
C116	C	0.76069	0.52384	0.87346	0.00000	Uiso	1.00
C117	C	0.88282	0.69441	0.87346	0.00000	Uiso	1.00
C118	C	0.93268	0.71963	0.87346	0.00000	Uiso	1.00
C119	C	0.97616	0.73931	0.87346	0.00000	Uiso	1.00

C120	C	0.80709	0.69291	0.87346	0.00000	Uiso	1.00
C121	C	0.78283	0.71717	0.87346	0.00000	Uiso	1.00
C122	C	0.76162	0.73838	0.87346	0.00000	Uiso	1.00
C123	C	0.64281	0.78249	0.87346	0.00000	Uiso	1.00
C124	C	0.71751	0.85719	0.87346	0.00000	Uiso	1.00
C125	C	0.64431	0.85569	0.87346	0.00000	Uiso	1.00
C126	C	0.85719	0.71751	0.87346	0.00000	Uiso	1.00
C127	C	0.78249	0.64281	0.87346	0.00000	Uiso	1.00
C128	C	0.85569	0.64431	0.87346	0.00000	Uiso	1.00
F129	F	0.51545	0.63185	0.62346	0.00000	Uiso	1.00
F130	F	0.62088	0.87912	0.87346	0.00000	Uiso	1.00
F131	F	0.61815	0.73455	0.87346	0.00000	Uiso	1.00
F132	F	0.76545	0.88185	0.87346	0.00000	Uiso	1.00
F133	F	0.87912	0.62088	0.87346	0.00000	Uiso	1.00
F134	F	0.88185	0.76545	0.87346	0.00000	Uiso	1.00
F135	F	0.73455	0.61815	0.87346	0.00000	Uiso	1.00
H136	H	0.50751	0.76637	0.62346	0.00000	Uiso	1.00
H137	H	0.23362	0.49248	0.62346	0.00000	Uiso	1.00
H138	H	0.50826	0.49174	0.62346	0.00000	Uiso	1.00

2×2 unit cell model of 4-fold stacking with a dimer stacked:

_cell_length_a	32.9505
_cell_length_b	32.9546
_cell_length_c	11.3555
_cell_angle_alpha	90.0000
_cell_angle_beta	90.0000

_cell_angle_gamma 120.9090

C1	C	0.19441	0.38282	0.87346	0.01267	Uiso	1.00
C2	C	0.21963	0.43268	0.87346	0.01267	Uiso	1.00
C3	C	0.23931	0.47616	0.87346	0.01267	Uiso	1.00
C4	C	0.11718	0.30559	0.87346	0.01267	Uiso	1.00
C5	C	0.06732	0.28037	0.87346	0.01267	Uiso	1.00
C6	C	0.02384	0.26069	0.87346	0.01267	Uiso	1.00
C7	C	0.19291	0.30709	0.87346	0.01267	Uiso	1.00
C8	C	0.21717	0.28283	0.87346	0.01267	Uiso	1.00
C9	C	0.23838	0.26162	0.87346	0.01267	Uiso	1.00
C10	C	0.30559	0.11718	0.87346	0.01267	Uiso	1.00
C11	C	0.28037	0.06732	0.87346	0.01267	Uiso	1.00
C12	C	0.26069	0.02384	0.87346	0.01267	Uiso	1.00
C13	C	0.38282	0.19441	0.87346	0.01267	Uiso	1.00
C14	C	0.43268	0.21963	0.87346	0.01267	Uiso	1.00
C15	C	0.47616	0.23931	0.87346	0.01267	Uiso	1.00
C16	C	0.30709	0.19291	0.87346	0.01267	Uiso	1.00
C17	C	0.28283	0.21717	0.87346	0.01267	Uiso	1.00
C18	C	0.26162	0.23838	0.87346	0.01267	Uiso	1.00
C19	C	0.14281	0.28249	0.87346	0.01267	Uiso	1.00
C20	C	0.21751	0.35719	0.87346	0.01267	Uiso	1.00
C21	C	0.14431	0.35569	0.87346	0.01267	Uiso	1.00
C22	C	0.35719	0.21751	0.87346	0.01267	Uiso	1.00
C23	C	0.28249	0.14281	0.87346	0.01267	Uiso	1.00
C24	C	0.35569	0.14431	0.87346	0.01267	Uiso	1.00
C25	C	0.55559	0.36718	0.58626	0.01267	Uiso	1.00

C26	C	0.53037	0.31732	0.57787	0.01267	Uiso	1.00
C27	C	0.51069	0.27384	0.57369	0.01267	Uiso	1.00
C28	C	0.63282	0.44441	0.58626	0.01267	Uiso	1.00
C29	C	0.68268	0.46963	0.57763	0.01267	Uiso	1.00
C30	C	0.72616	0.48931	0.57364	0.01267	Uiso	1.00
C31	C	0.55709	0.44291	0.61136	0.01267	Uiso	1.00
C32	C	0.53283	0.46717	0.62720	0.01267	Uiso	1.00
C33	C	0.51162	0.48838	0.63772	0.01267	Uiso	1.00
C34	C	0.60719	0.46751	0.60197	0.01267	Uiso	1.00
C35	C	0.53249	0.39281	0.60192	0.01267	Uiso	1.00
C36	C	0.60569	0.39431	0.58056	0.01267	Uiso	1.00
C37	C	0.69441	0.38282	0.87346	0.01267	Uiso	1.00
C38	C	0.71963	0.43268	0.87346	0.01267	Uiso	1.00
C39	C	0.73931	0.47616	0.87346	0.01267	Uiso	1.00
C40	C	0.61718	0.30559	0.87346	0.01267	Uiso	1.00
C41	C	0.56732	0.28037	0.87346	0.01267	Uiso	1.00
C42	C	0.52384	0.26069	0.87346	0.01267	Uiso	1.00
C43	C	0.69291	0.30709	0.87346	0.01267	Uiso	1.00
C44	C	0.71717	0.28283	0.87346	0.01267	Uiso	1.00
C45	C	0.73838	0.26162	0.87346	0.01267	Uiso	1.00
C46	C	0.80559	0.11718	0.87346	0.01267	Uiso	1.00
C47	C	0.78037	0.06732	0.87346	0.01267	Uiso	1.00
C48	C	0.76069	0.02384	0.87346	0.01267	Uiso	1.00
C49	C	0.88282	0.19441	0.87346	0.01267	Uiso	1.00
C50	C	0.93268	0.21963	0.87346	0.01267	Uiso	1.00
C51	C	0.97616	0.23931	0.87346	0.01267	Uiso	1.00

C52	C	0.80709	0.19291	0.87346	0.01267	Uiso	1.00
C53	C	0.78283	0.21717	0.87346	0.01267	Uiso	1.00
C54	C	0.76162	0.23838	0.87346	0.01267	Uiso	1.00
C55	C	0.64281	0.28249	0.87346	0.01267	Uiso	1.00
C56	C	0.71751	0.35719	0.87346	0.01267	Uiso	1.00
C57	C	0.64431	0.35569	0.87346	0.01267	Uiso	1.00
C58	C	0.85719	0.21751	0.87346	0.01267	Uiso	1.00
C59	C	0.78249	0.14281	0.87346	0.01267	Uiso	1.00
C60	C	0.85569	0.14431	0.87346	0.01267	Uiso	1.00
C61	C	0.44441	0.63282	0.58626	0.01267	Uiso	1.00
C62	C	0.46963	0.68268	0.57787	0.01267	Uiso	1.00
C63	C	0.48931	0.72616	0.57369	0.01267	Uiso	1.00
C64	C	0.36718	0.55559	0.58626	0.01267	Uiso	1.00
C65	C	0.31732	0.53037	0.57763	0.01267	Uiso	1.00
C66	C	0.27384	0.51069	0.57364	0.01267	Uiso	1.00
C67	C	0.44291	0.55709	0.61136	0.01267	Uiso	1.00
C68	C	0.46717	0.53283	0.62720	0.01267	Uiso	1.00
C69	C	0.48838	0.51162	0.63772	0.01267	Uiso	1.00
C70	C	0.39281	0.53249	0.60197	0.01267	Uiso	1.00
C71	C	0.46751	0.60719	0.60192	0.01267	Uiso	1.00
C72	C	0.39431	0.60569	0.58056	0.01267	Uiso	1.00
C73	C	0.19441	0.88282	0.87346	0.01267	Uiso	1.00
C74	C	0.21963	0.93268	0.87346	0.01267	Uiso	1.00
C75	C	0.23931	0.97616	0.87346	0.01267	Uiso	1.00
C76	C	0.11718	0.80559	0.87346	0.01267	Uiso	1.00
C77	C	0.06732	0.78037	0.87346	0.01267	Uiso	1.00

C78	C	0.02384	0.76069	0.87346	0.01267	Uiso	1.00
C79	C	0.19291	0.80709	0.87346	0.01267	Uiso	1.00
C80	C	0.21717	0.78283	0.87346	0.01267	Uiso	1.00
C81	C	0.23838	0.76162	0.87346	0.01267	Uiso	1.00
C82	C	0.30559	0.61718	0.87346	0.01267	Uiso	1.00
C83	C	0.28037	0.56732	0.87346	0.01267	Uiso	1.00
C84	C	0.26069	0.52384	0.87346	0.01267	Uiso	1.00
C85	C	0.38282	0.69441	0.87346	0.01267	Uiso	1.00
C86	C	0.43268	0.71963	0.87346	0.01267	Uiso	1.00
C87	C	0.47616	0.73931	0.87346	0.01267	Uiso	1.00
C88	C	0.30709	0.69291	0.87346	0.01267	Uiso	1.00
C89	C	0.28283	0.71717	0.87346	0.01267	Uiso	1.00
C90	C	0.26162	0.73838	0.87346	0.01267	Uiso	1.00
C91	C	0.14281	0.78249	0.87346	0.01267	Uiso	1.00
C92	C	0.21751	0.85719	0.87346	0.01267	Uiso	1.00
C93	C	0.14431	0.85569	0.87346	0.01267	Uiso	1.00
C94	C	0.35719	0.71751	0.87346	0.01267	Uiso	1.00
C95	C	0.28249	0.64281	0.87346	0.01267	Uiso	1.00
C96	C	0.35569	0.64431	0.87346	0.01267	Uiso	1.00
C97	C	0.69441	0.88282	0.87346	0.01267	Uiso	1.00
C98	C	0.71963	0.93268	0.87346	0.01267	Uiso	1.00
C99	C	0.73931	0.97616	0.87346	0.01267	Uiso	1.00
C100	C	0.61718	0.80559	0.87346	0.01267	Uiso	1.00
C101	C	0.56732	0.78037	0.87346	0.01267	Uiso	1.00
C102	C	0.52384	0.76069	0.87346	0.01267	Uiso	1.00
C103	C	0.69291	0.80709	0.87346	0.01267	Uiso	1.00

C104	C	0.71717	0.78283	0.87346	0.01267	Uiso	1.00
C105	C	0.73838	0.76162	0.87346	0.01267	Uiso	1.00
C106	C	0.80559	0.61718	0.87346	0.01267	Uiso	1.00
C107	C	0.78037	0.56732	0.87346	0.01267	Uiso	1.00
C108	C	0.76069	0.52384	0.87346	0.01267	Uiso	1.00
C109	C	0.88282	0.69441	0.87346	0.01267	Uiso	1.00
C110	C	0.93268	0.71963	0.87346	0.01267	Uiso	1.00
C111	C	0.97616	0.73931	0.87346	0.01267	Uiso	1.00
C112	C	0.80709	0.69291	0.87346	0.01267	Uiso	1.00
C113	C	0.78283	0.71717	0.87346	0.01267	Uiso	1.00
C114	C	0.76162	0.73838	0.87346	0.01267	Uiso	1.00
C115	C	0.64281	0.78249	0.87346	0.01267	Uiso	1.00
C116	C	0.71751	0.85719	0.87346	0.01267	Uiso	1.00
C117	C	0.64431	0.85569	0.87346	0.01267	Uiso	1.00
C118	C	0.85719	0.71751	0.87346	0.01267	Uiso	1.00
C119	C	0.78249	0.64281	0.87346	0.01267	Uiso	1.00
C120	C	0.85569	0.64431	0.87346	0.01267	Uiso	1.00
F1	F	0.36815	0.48455	0.60819	0.01267	Uiso	1.00
F2	F	0.48455	0.36815	0.60834	0.01267	Uiso	1.00
F3	F	0.12088	0.37912	0.87346	0.01267	Uiso	1.00
F4	F	0.11815	0.23455	0.87346	0.01267	Uiso	1.00
F5	F	0.26545	0.38185	0.87346	0.01267	Uiso	1.00
F6	F	0.37912	0.12088	0.87346	0.01267	Uiso	1.00
F7	F	0.38185	0.26545	0.87346	0.01267	Uiso	1.00
F8	F	0.23455	0.11815	0.87346	0.01267	Uiso	1.00
F9	F	0.62912	0.37088	0.56990	0.01267	Uiso	1.00

F10	F	0.62088	0.37912	0.87346	0.01267	Uiso	1.00
F11	F	0.61815	0.23455	0.87346	0.01267	Uiso	1.00
F12	F	0.76545	0.38185	0.87346	0.01267	Uiso	1.00
F13	F	0.87912	0.12088	0.87346	0.01267	Uiso	1.00
F14	F	0.88185	0.26545	0.87346	0.01267	Uiso	1.00
F15	F	0.73455	0.11815	0.87346	0.01267	Uiso	1.00
F16	F	0.37088	0.62912	0.56990	0.01267	Uiso	1.00
F17	F	0.12088	0.87912	0.87346	0.01267	Uiso	1.00
F18	F	0.11815	0.73455	0.87346	0.01267	Uiso	1.00
F19	F	0.26545	0.88185	0.87346	0.01267	Uiso	1.00
F20	F	0.37912	0.62088	0.87346	0.01267	Uiso	1.00
F21	F	0.38185	0.76545	0.87346	0.01267	Uiso	1.00
F22	F	0.23455	0.61815	0.87346	0.01267	Uiso	1.00
F23	F	0.51545	0.63185	0.60834	0.01267	Uiso	1.00
F24	F	0.63185	0.51545	0.60819	0.01267	Uiso	1.00
F25	F	0.62088	0.87912	0.87346	0.01267	Uiso	1.00
F26	F	0.61815	0.73455	0.87346	0.01267	Uiso	1.00
F27	F	0.76545	0.88185	0.87346	0.01267	Uiso	1.00
F28	F	0.87912	0.62088	0.87346	0.01267	Uiso	1.00
F29	F	0.88185	0.76545	0.87346	0.01267	Uiso	1.00
F30	F	0.73455	0.61815	0.87346	0.01267	Uiso	1.00
H1	H	0.49221	0.23598	0.57041	0.01267	Uiso	1.00
H2	H	0.76404	0.50780	0.57029	0.01267	Uiso	1.00
H3	H	0.50779	0.76402	0.57041	0.01267	Uiso	1.00
H4	H	0.23596	0.49220	0.57029	0.01267	Uiso	1.00

2×2 unit cell model of 4-fold stacking with a trimer stacked:

_cell_length_a	32.9505
_cell_length_b	32.9546
_cell_length_c	11.3555
_cell_angle_alpha	90.0000
_cell_angle_beta	90.0000
_cell_angle_gamma	120.9090

C1	C	0.05559	0.36718	0.58363	0.01267	Uiso	1.00
C2	C	0.03037	0.31732	0.57605	0.01267	Uiso	1.00
C3	C	0.01069	0.27384	0.57334	0.01267	Uiso	1.00
C4	C	0.13282	0.44441	0.58530	0.01267	Uiso	1.00
C5	C	0.18268	0.46963	0.57892	0.01267	Uiso	1.00
C6	C	0.22616	0.48931	0.57589	0.01267	Uiso	1.00
C7	C	0.05709	0.44291	0.60784	0.01267	Uiso	1.00
C8	C	0.03283	0.46717	0.62460	0.01267	Uiso	1.00
C9	C	0.01162	0.48838	0.63397	0.01267	Uiso	1.00
C10	C	0.10719	0.46751	0.59956	0.01267	Uiso	1.00
C11	C	0.03249	0.39281	0.59852	0.01267	Uiso	1.00
C12	C	0.10569	0.39431	0.57921	0.01267	Uiso	1.00
C13	C	0.19441	0.38282	0.87346	0.01267	Uiso	1.00
C14	C	0.21963	0.43268	0.87346	0.01267	Uiso	1.00
C15	C	0.23931	0.47616	0.87346	0.01267	Uiso	1.00
C16	C	0.11718	0.30559	0.87346	0.01267	Uiso	1.00
C17	C	0.06732	0.28037	0.87346	0.01267	Uiso	1.00
C18	C	0.02384	0.26069	0.87346	0.01267	Uiso	1.00
C19	C	0.19291	0.30709	0.87346	0.01267	Uiso	1.00

C20	C	0.21717	0.28283	0.87346	0.01267	Uiso	1.00
C21	C	0.23838	0.26162	0.87346	0.01267	Uiso	1.00
C22	C	0.30559	0.11718	0.87346	0.01267	Uiso	1.00
C23	C	0.28037	0.06732	0.87346	0.01267	Uiso	1.00
C24	C	0.26069	0.02384	0.87346	0.01267	Uiso	1.00
C25	C	0.38282	0.19441	0.87346	0.01267	Uiso	1.00
C26	C	0.43268	0.21963	0.87346	0.01267	Uiso	1.00
C27	C	0.47616	0.23931	0.87346	0.01267	Uiso	1.00
C28	C	0.30709	0.19291	0.87346	0.01267	Uiso	1.00
C29	C	0.28283	0.21717	0.87346	0.01267	Uiso	1.00
C30	C	0.26162	0.23838	0.87346	0.01267	Uiso	1.00
C31	C	0.14281	0.28249	0.87346	0.01267	Uiso	1.00
C32	C	0.21751	0.35719	0.87346	0.01267	Uiso	1.00
C33	C	0.14431	0.35569	0.87346	0.01267	Uiso	1.00
C34	C	0.35719	0.21751	0.87346	0.01267	Uiso	1.00
C35	C	0.28249	0.14281	0.87346	0.01267	Uiso	1.00
C36	C	0.35569	0.14431	0.87346	0.01267	Uiso	1.00
C37	C	0.55559	0.36718	0.58652	0.01267	Uiso	1.00
C38	C	0.53037	0.31732	0.57743	0.01267	Uiso	1.00
C39	C	0.51069	0.27384	0.57316	0.01267	Uiso	1.00
C40	C	0.63282	0.44441	0.58654	0.01267	Uiso	1.00
C41	C	0.68268	0.46963	0.57745	0.01267	Uiso	1.00
C42	C	0.72616	0.48931	0.57313	0.01267	Uiso	1.00
C43	C	0.55709	0.44291	0.61257	0.01267	Uiso	1.00
C44	C	0.53283	0.46717	0.62889	0.01267	Uiso	1.00
C45	C	0.51162	0.48838	0.63929	0.01267	Uiso	1.00

C46	C	0.60719	0.46751	0.60247	0.01267	Uiso	1.00
C47	C	0.53249	0.39281	0.60243	0.01267	Uiso	1.00
C48	C	0.60569	0.39431	0.58094	0.01267	Uiso	1.00
C49	C	0.69441	0.38282	0.87346	0.01267	Uiso	1.00
C50	C	0.71963	0.43268	0.87346	0.01267	Uiso	1.00
C51	C	0.73931	0.47616	0.87346	0.01267	Uiso	1.00
C52	C	0.61718	0.30559	0.87346	0.01267	Uiso	1.00
C53	C	0.56732	0.28037	0.87346	0.01267	Uiso	1.00
C54	C	0.52384	0.26069	0.87346	0.01267	Uiso	1.00
C55	C	0.69291	0.30709	0.87346	0.01267	Uiso	1.00
C56	C	0.71717	0.28283	0.87346	0.01267	Uiso	1.00
C57	C	0.73838	0.26162	0.87346	0.01267	Uiso	1.00
C58	C	0.80559	0.11718	0.87346	0.01267	Uiso	1.00
C59	C	0.78037	0.06732	0.87346	0.01267	Uiso	1.00
C60	C	0.76069	0.02384	0.87346	0.01267	Uiso	1.00
C61	C	0.88282	0.19441	0.87346	0.01267	Uiso	1.00
C62	C	0.93268	0.21963	0.87346	0.01267	Uiso	1.00
C63	C	0.97616	0.23931	0.87346	0.01267	Uiso	1.00
C64	C	0.80709	0.19291	0.87346	0.01267	Uiso	1.00
C65	C	0.78283	0.21717	0.87346	0.01267	Uiso	1.00
C66	C	0.76162	0.23838	0.87346	0.01267	Uiso	1.00
C67	C	0.64281	0.28249	0.87346	0.01267	Uiso	1.00
C68	C	0.71751	0.35719	0.87346	0.01267	Uiso	1.00
C69	C	0.64431	0.35569	0.87346	0.01267	Uiso	1.00
C70	C	0.85719	0.21751	0.87346	0.01267	Uiso	1.00
C71	C	0.78249	0.14281	0.87346	0.01267	Uiso	1.00

C72	C	0.85569	0.14431	0.87346	0.01267	Uiso	1.00
C73	C	0.44441	0.63282	0.58454	0.01267	Uiso	1.00
C74	C	0.46963	0.68268	0.57650	0.01267	Uiso	1.00
C75	C	0.48931	0.72616	0.57320	0.01267	Uiso	1.00
C76	C	0.36718	0.55559	0.58646	0.01267	Uiso	1.00
C77	C	0.31732	0.53037	0.57978	0.01267	Uiso	1.00
C78	C	0.27384	0.51069	0.57639	0.01267	Uiso	1.00
C79	C	0.44291	0.55709	0.61081	0.01267	Uiso	1.00
C80	C	0.46717	0.53283	0.62770	0.01267	Uiso	1.00
C81	C	0.48838	0.51162	0.63851	0.01267	Uiso	1.00
C82	C	0.39281	0.53249	0.60174	0.01267	Uiso	1.00
C83	C	0.46751	0.60719	0.60047	0.01267	Uiso	1.00
C84	C	0.39431	0.60569	0.57960	0.01267	Uiso	1.00
C85	C	0.19441	0.88282	0.87346	0.01267	Uiso	1.00
C86	C	0.21963	0.93268	0.87346	0.01267	Uiso	1.00
C87	C	0.23931	0.97616	0.87346	0.01267	Uiso	1.00
C88	C	0.11718	0.80559	0.87346	0.01267	Uiso	1.00
C89	C	0.06732	0.78037	0.87346	0.01267	Uiso	1.00
C90	C	0.02384	0.76069	0.87346	0.01267	Uiso	1.00
C91	C	0.19291	0.80709	0.87346	0.01267	Uiso	1.00
C92	C	0.21717	0.78283	0.87346	0.01267	Uiso	1.00
C93	C	0.23838	0.76162	0.87346	0.01267	Uiso	1.00
C94	C	0.30559	0.61718	0.87346	0.01267	Uiso	1.00
C95	C	0.28037	0.56732	0.87346	0.01267	Uiso	1.00
C96	C	0.26069	0.52384	0.87346	0.01267	Uiso	1.00
C97	C	0.38282	0.69441	0.87346	0.01267	Uiso	1.00

C98	C	0.43268	0.71963	0.87346	0.01267	Uiso	1.00
C99	C	0.47616	0.73931	0.87346	0.01267	Uiso	1.00
C100	C	0.30709	0.69291	0.87346	0.01267	Uiso	1.00
C101	C	0.28283	0.71717	0.87346	0.01267	Uiso	1.00
C102	C	0.26162	0.73838	0.87346	0.01267	Uiso	1.00
C103	C	0.14281	0.78249	0.87346	0.01267	Uiso	1.00
C104	C	0.21751	0.85719	0.87346	0.01267	Uiso	1.00
C105	C	0.14431	0.85569	0.87346	0.01267	Uiso	1.00
C106	C	0.35719	0.71751	0.87346	0.01267	Uiso	1.00
C107	C	0.28249	0.64281	0.87346	0.01267	Uiso	1.00
C108	C	0.35569	0.64431	0.87346	0.01267	Uiso	1.00
C109	C	0.69441	0.88282	0.87346	0.01267	Uiso	1.00
C110	C	0.71963	0.93268	0.87346	0.01267	Uiso	1.00
C111	C	0.73931	0.97616	0.87346	0.01267	Uiso	1.00
C112	C	0.61718	0.80559	0.87346	0.01267	Uiso	1.00
C113	C	0.56732	0.78037	0.87346	0.01267	Uiso	1.00
C114	C	0.52384	0.76069	0.87346	0.01267	Uiso	1.00
C115	C	0.69291	0.80709	0.87346	0.01267	Uiso	1.00
C116	C	0.71717	0.78283	0.87346	0.01267	Uiso	1.00
C117	C	0.73838	0.76162	0.87346	0.01267	Uiso	1.00
C118	C	0.80559	0.61718	0.87346	0.01267	Uiso	1.00
C119	C	0.78037	0.56732	0.87346	0.01267	Uiso	1.00
C120	C	0.76069	0.52384	0.87346	0.01267	Uiso	1.00
C121	C	0.88282	0.69441	0.87346	0.01267	Uiso	1.00
C122	C	0.93268	0.71963	0.87346	0.01267	Uiso	1.00
C123	C	0.97616	0.73931	0.87346	0.01267	Uiso	1.00

C124	C	0.80709	0.69291	0.87346	0.01267	Uiso	1.00
C125	C	0.78283	0.71717	0.87346	0.01267	Uiso	1.00
C126	C	0.76162	0.73838	0.87346	0.01267	Uiso	1.00
C127	C	0.64281	0.78249	0.87346	0.01267	Uiso	1.00
C128	C	0.71751	0.85719	0.87346	0.01267	Uiso	1.00
C129	C	0.64431	0.85569	0.87346	0.01267	Uiso	1.00
C130	C	0.85719	0.71751	0.87346	0.01267	Uiso	1.00
C131	C	0.78249	0.64281	0.87346	0.01267	Uiso	1.00
C132	C	0.85569	0.64431	0.87346	0.01267	Uiso	1.00
F1	F	0.36815	0.48455	0.60792	0.01267	Uiso	1.00
F2	F	0.12912	0.37088	0.56861	0.01267	Uiso	1.00
F3	F	0.48455	0.36815	0.60806	0.01267	Uiso	1.00
F4	F	0.12088	0.37912	0.87346	0.01267	Uiso	1.00
F5	F	0.11815	0.23455	0.87346	0.01267	Uiso	1.00
F6	F	0.26545	0.38185	0.87346	0.01267	Uiso	1.00
F7	F	0.37912	0.12088	0.87346	0.01267	Uiso	1.00
F8	F	0.38185	0.26545	0.87346	0.01267	Uiso	1.00
F9	F	0.23455	0.11815	0.87346	0.01267	Uiso	1.00
F10	F	0.62912	0.37088	0.56909	0.01267	Uiso	1.00
F11	F	0.98455	0.36815	0.60471	0.01267	Uiso	1.00
F12	F	0.62088	0.37912	0.87346	0.01267	Uiso	1.00
F13	F	0.61815	0.23455	0.87346	0.01267	Uiso	1.00
F14	F	0.76545	0.38185	0.87346	0.01267	Uiso	1.00
F15	F	0.87912	0.12088	0.87346	0.01267	Uiso	1.00
F16	F	0.88185	0.26545	0.87346	0.01267	Uiso	1.00
F17	F	0.73455	0.11815	0.87346	0.01267	Uiso	1.00

F18	F	0.37088	0.62912	0.56783	0.01267	Uiso	1.00
F19	F	0.13185	0.51545	0.60480	0.01267	Uiso	1.00
F20	F	0.12088	0.87912	0.87346	0.01267	Uiso	1.00
F21	F	0.11815	0.73455	0.87346	0.01267	Uiso	1.00
F22	F	0.26545	0.88185	0.87346	0.01267	Uiso	1.00
F23	F	0.37912	0.62088	0.87346	0.01267	Uiso	1.00
F24	F	0.38185	0.76545	0.87346	0.01267	Uiso	1.00
F25	F	0.23455	0.61815	0.87346	0.01267	Uiso	1.00
F26	F	0.51545	0.63185	0.60731	0.01267	Uiso	1.00
F27	F	0.63185	0.51545	0.60817	0.01267	Uiso	1.00
F28	F	0.62088	0.87912	0.87346	0.01267	Uiso	1.00
F29	F	0.61815	0.73455	0.87346	0.01267	Uiso	1.00
F30	F	0.76545	0.88185	0.87346	0.01267	Uiso	1.00
F31	F	0.87912	0.62088	0.87346	0.01267	Uiso	1.00
F32	F	0.88185	0.76545	0.87346	0.01267	Uiso	1.00
F33	F	0.73455	0.61815	0.87346	0.01267	Uiso	1.00
H1	H	0.99267	0.23603	0.56936	0.01267	Uiso	1.00
H2	H	0.99308	0.50696	0.64538	0.01267	Uiso	1.00
H3	H	0.76396	0.50735	0.56897	0.01267	Uiso	1.00
H4	H	0.50733	0.76398	0.56902	0.01267	Uiso	1.00
H5	H	0.49267	0.23604	0.56899	0.01267	Uiso	1.00

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