

## **Supporting Information**

### **One-Dimensional Multichannel g-C<sub>3</sub>N<sub>4.7</sub> Nanostructure Realizing an Efficient Photocatalytic Hydrogen Evolution Reaction and Theoretical Investigations**

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**Materials.** Tetraethyl orthosilicate (TEOS), triethanolamine (TEOA), dicyandiamide (C<sub>2</sub>H<sub>4</sub>N<sub>4</sub>), and triblock copolymer poly(ethylene glycol)-block-poly(propylene glycol)-block-poly(ethylene glycol) (pluronic P123, molecular weight = 5800, EO<sub>20</sub>PO<sub>70</sub>EO<sub>20</sub>) were obtained from Sigma Aldrich. Hydrochloric acid (HCl, GR grade) was obtained from Molychem.

**Synthesis of SBA-15 Template.** SBA-15 was prepared by using the same method as reported by Vinu et al.<sup>1</sup> Initially, 4g of the amphiphilic triblock copolymer (P123) was dissolved in 30 ml of DI water and 120 ml of 2M HCl. Afterwards the solution was stirred continuously for 5 h till complete dissolution of the triblock copolymer. Later, 9.6 ml of tetraethylorthosilicate (TEOS) was added drop-wise under constant stirring giving rise to a gel-like suspension. The mixture at this stage was transferred to the hydrothermal vessel and kept for aging at 40 °C for 24 h and then finally heated at 150 °C for 24 h. The product obtained was filtered hot and washed with

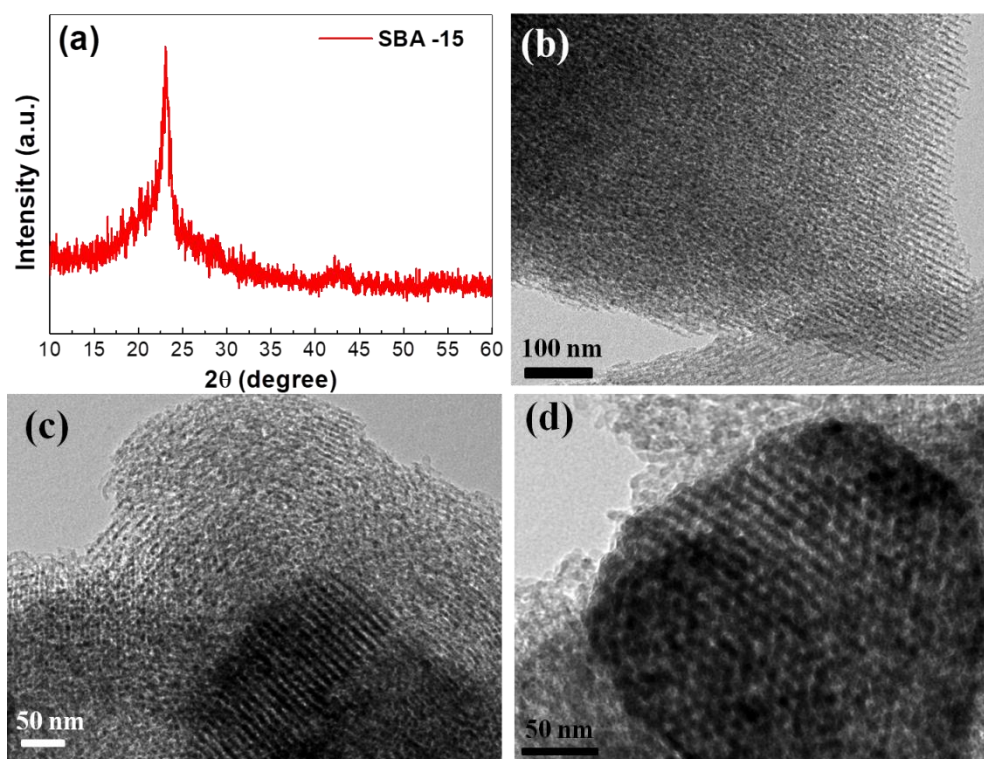
ethanol carefully. Further, it was dried overnight in oven at 60 °C. The white product obtained was finally calcined in air at 550°C for 6 hours in order to decompose the triblock polymer.

### **Characterization of the Samples/Instrumental techniques.**

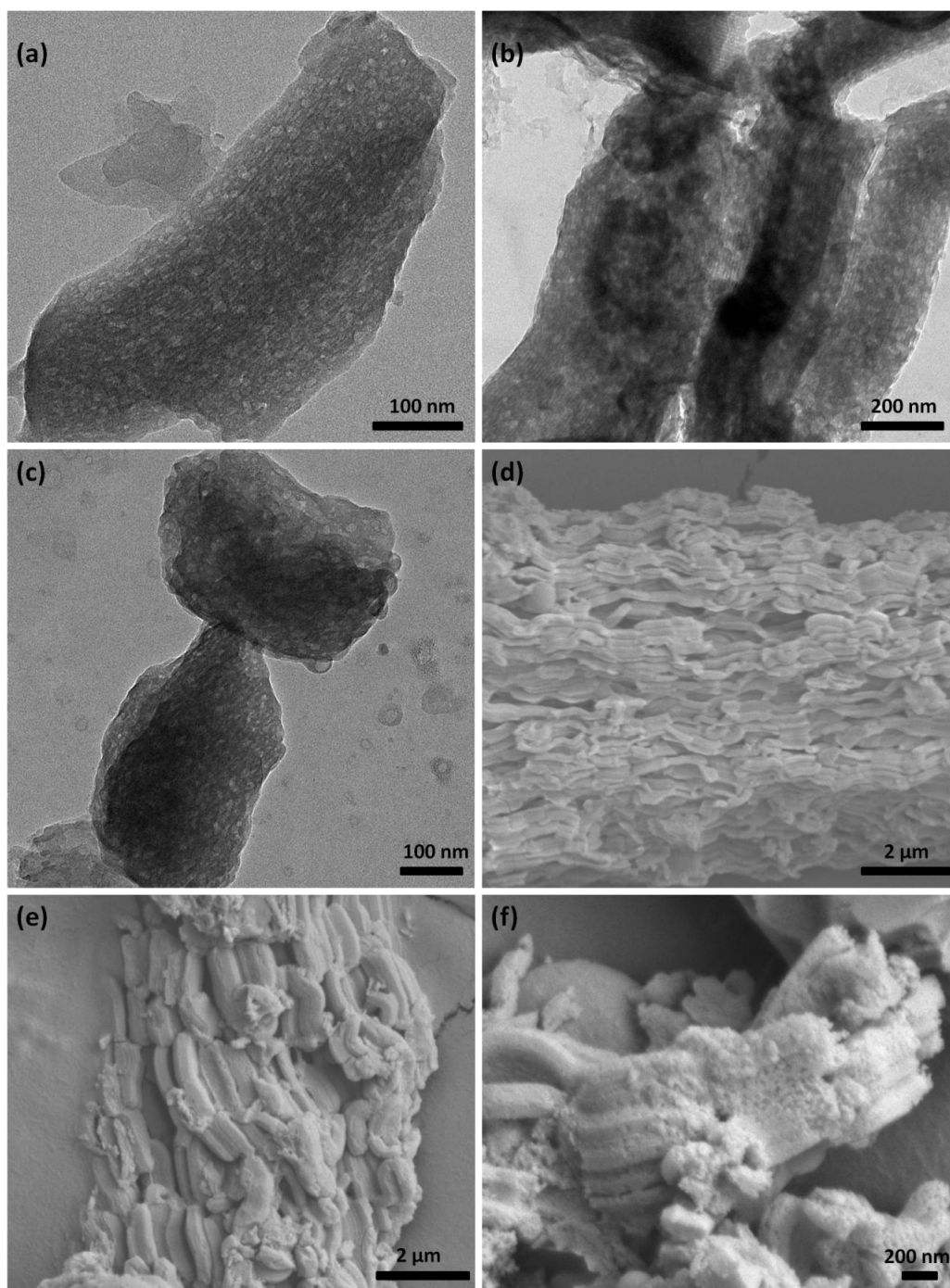
The crystalline structures were determined using X-ray diffraction (XRD) technique through a Bruker D8 Advance Diffractometer using monochromatic Cu K $\alpha$  ( $\lambda = 1.54 \text{ \AA}$ ) radiation source. The small angle X-ray scattering (SAXS) measurements were conducted through Xuess SAXS/WAXS system (Model C HP100 fm) equipped with a micro focused sealed tube having Cu anode as X-ray source. The surface area measurements were performed using a Quantachrome (Model ASI-CI-11) BET surface area analyzer, where the sample was degassed for 6h at 150 °C before the adsorption analysis. The Brunauer –Emmett-Teller (BET) method and Barrett-Joyner-Halenda (BJH) method were used to evaluate the specific surface area and pore size values, respectively. The FT-IR spectra were performed in the wavelength range of 400-4000  $\text{cm}^{-1}$  employing KBr method using RXI-Mid IR (Perkin Elmer) FT-IR spectrometer. Thermogravimetric measurements were performed under nitrogen atmosphere at a heating rate of 5°/ min to investigate the thermal stability using Mettler Toledo TGA 1 instrument. The morphological characteristics for the as-synthesized samples were studied by Transmission Electron Microscopy (TEM) using Thermo-Scientific Talos Cryo-Transmission Electron Microscope (Cryo-TEM). Similarly, the three dimensional morphological properties and the corresponding elemental composition were investigated by Field Emission Scanning Electron Microscopy (FESEM) using a JEOL JSM 6610 working at 20 kV equipped with Energy Dispersive X-ray spectrometer (EDX). The paramagnetic nature of the material was observed by Electron Paramagnetic Resonance (EPR) measurements using Bruker Model EMX MicroX spectrometer. In order to examine the surface states of the samples and the valence band-edge position, X-ray Photoelectron Spectroscopy (XPS) measurements and XPS valence band measurements were performed using Prevac MX650 XPS system employed with Scienta monochromator (Al K $\alpha$  anode, 1486.6 eV) and Scienta R3000HP differentially pumped analyzer. C1s peak at 284.4 eV was taken as a reference for all the other binding energies. The stoichiometry of the as-prepared samples were determined by CHN analysis using Elementar Analysensysteme (Model Vario Micro cube, Germany) CHNS analyzer. UV-Vis absorption spectra of the samples taking isopropanol as the reference were recorded using Perkin Elmer LAMDA 35 spectrophotometer. The room temperature photoluminescence (PL) study was

conducted on Cary Eclipse Fluorescence spectrophotometer. To examine the lifetime decay of the samples, Time-Resolved Photoluminescence (TRPL) on Horiba Yvon spectrophotometer at an excitation wavelength of 370 nm. Mott Schottky measurements were performed to investigate the absolute conduction band-edge positions relative to normal hydrogen electrode. Prior to deposition of sample ink over glassy carbon electrode (GCE), the sample ink was prepared. The ink was prepared as follows: 10 mg of the MDY sample was dispersed in 1 mL IPA followed by addition of 10  $\mu$ L of Nafion binder into it, and the resultant mixture was ultrasonicated for 30 mins to obtain a well dispersed sample ink. Flat band edge potential was determined using Dynamic impedance method.

**Photoelectrochemical Measurements:** The transient photocurrent response (TPC) plots and electrochemical impedance spectroscopy (EIS) measurements were conducted on CHI660E, USA at room temperature using a standard three-electrode system where a Pt wire and Ag/AgCl (saturated KCl) were used as counter and reference electrodes respectively. FTO electrode coated with carbon nitride sample was employed as the working electrode. The preparation of the working electrodes were done as follows: 10 mg of the samples (MDY, BDY) were dispersed in 0.5 ml DMF and 20  $\mu$ L of Nafion binder through sonication for 30 min. About, 100 $\mu$ L of this ink were spread onto FTO-coated glass slides (1 x 1 cm<sup>2</sup>). The films were dried at 60°C for 1 hour and then annealed at 200°C for 2 hours for better adhesion. The electrodes were immersed in an aqueous solution containing 0.5 M Na<sub>2</sub>SO<sub>4</sub> (inert electrolyte). Transient photocurrent responses were obtained under on/off illumination cycles at constant bias voltage of -0.2 V vs Ag/AgCl. Before the irradiation (dark), current equilibrium was achieved at applied bias voltage. The interval of light-on and light-off was 30 s.

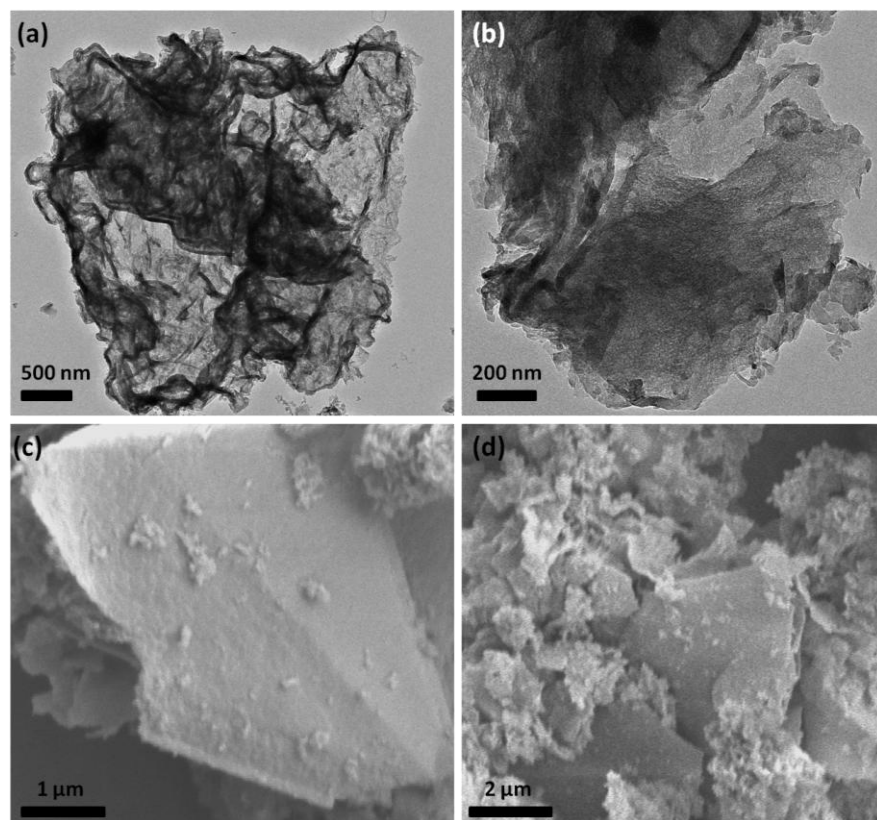


**Figure S1.** (a) Powder XRD pattern of SBA-15 template in the  $2\theta$  range from  $0^\circ$  to  $5^\circ$ . (Inset: Corresponding wide-angle XRD pattern). (b) Low-resolution transmission electron microscopy (TEM) image of SBA-15 template showing the mesoporous structure. (c) High-resolution TEM image illustrating the regular arrangement of pores. (d) High-resolution TEM image of the SBA-15 template.

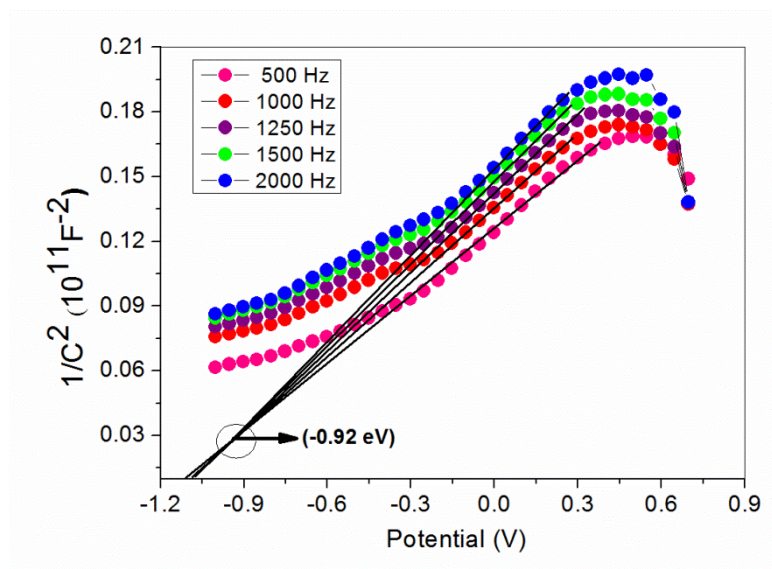


**Figure S2.** (a-c) TEM images of MDY sample exhibiting hexagonally ordered rope-like mesoporous structure. (d-f) FESEM images of MDY sample showing rope-like structure of MDY sample.

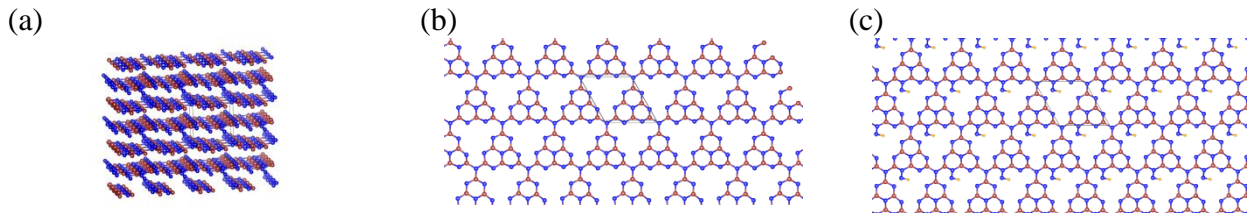




**Figure S3.** (a-b) TEM images of BDY sample showing sheet-kind of morphology with no observable porosity. (c-d) FESEM images of the BDY sample.



**Figure S4.** Mott-Schottky measurements of BDY sample.



**Figure S5.** Optimized geometric structure of (a) bulk g-C<sub>3</sub>N<sub>4</sub>, (b) mono layer of g-C<sub>3</sub>N<sub>4</sub> and (c) mono-layer of g-C<sub>3</sub>N<sub>4.7</sub>.

**Table S1.** Depiction of structural parameters of Mesoporous carbon nitride (MDY) and SBA-15 obtained using nanocasting technique.

Sample	S <sub>BET</sub> (m <sup>2</sup> g <sup>-1</sup> )	Pore volume <sup>a</sup> (cm <sup>3</sup> g <sup>-1</sup> )	Pore size <sup>b</sup> (nm)	Pore size from TEM (nm)	d <sub>100</sub> <sup>c</sup> (nm)	a <sub>o</sub> <sup>d</sup> (nm)	wall thickness <sup>e</sup> (nm)
SBA-15	305	0.31	6.9	7.0	5.9	20.43	2.47
MDY	220	0.72	6.2	6.2	5.5	19.02	1.05
BDY	23.5	0.079	0.13				

<sup>a</sup>Evaluated at  $P/P_o = 0.99$ , where  $P$  is the equilibrium pressure and  $P_o$  is the saturation pressure of nitrogen at 77K. <sup>b</sup>Determined using BJH method from the centre of the pore size distribution curve obtained from the adsorption branch. <sup>c</sup> $d(100)$  spacing of the characteristic reflection.

$$^d \text{Calculated using the equation}^2 a_o = 2d_{100}\sqrt{3}. \quad \text{S1}$$

$$^e \text{Determined using the following equations: } w_d = c d \left( \frac{\rho V_p}{1 + \rho V_p} \right)^{1/2} \quad \text{S2}$$

where:

$w_d$  is the primary mesopore diameter.

$d$  is the XRD (100) reflection plane spacing.

$c$  is a constant characteristic of the pore geometry and equals to 1.213 for circular as well as hexagonal pores.

$\rho$  is pore wall density and assumed to be 2.2 cm<sup>3</sup> g<sup>-1</sup>

The pore wall thickness  $b_d$  is determined further using the equation:

$$b_d = \left( \frac{2}{\sqrt{3}} \right) d_{100} - \frac{w_d}{1.050} \quad S3$$

**Table S2.** Analyzation of Structural parameters of Mesoporous carbon nitride (MDY) obtained with earlier reports.

SI. No.	Mesoporous carbon nitride materials	Measured Surface Area ( $\text{m}^2 \text{g}^{-1}$ )	Pore Volume ( $\text{cm}^3 \text{g}^{-1}$ )	Mesopores size (nm)	References
1.	MDY	220	0.72	6.2	This work
2.	Mesoporous g- $\text{C}_3\text{N}_4$ nanorods	100-200	-	3.9	3
3.	Uniformly graphitic carbon nitride	52	-	-	4
4.	Tubular g- $\text{C}_3\text{N}_4$	130		macroporous	5
5.	Nanoporous g- $\text{C}_3\text{N}_4$	135.1	1.39	60	6
6.	Porous-g $\text{C}_3\text{N}_4$	239.17	0.59	4.89	7
7.	N-rich mesoporous carbon nitride	298	0.66	5.8	8

**Table S3.** Corresponding CHN analysis of MDY sample to analyze the elemental composition.

Sample code	C [%]	N [%]	H [%]	C/N ratio	Stoichiometry
MDY	30.18	55.01	2.129	0.64	$\text{C}_3\text{N}_{4.7}$



**Table S4.** CHN analysis of conventional bulk carbon nitride samples prepared following literature methods and comparison with present as-synthesized samples (MDY and BDY).

Sl. No.	Sample code	C [%]	N [%]	H [%]	C/N ratio	Stoichiometry	References followed for synthesis
1	MDY	30.18	55.01	2.129	0.64	C <sub>3</sub> N <sub>4.7</sub>	This work
2	BDY	34.96	55.70	2.041	0.73	C <sub>3</sub> N <sub>4.0</sub>	This work
3	GC-1	35.77	58.23	2.113	0.72	C <sub>3</sub> N <sub>4.1</sub>	9
4	GC-2	35.36	56.82	2.097	0.73	C <sub>3</sub> N <sub>4.0</sub>	10
5	GC-3	36.28	58.11	1.733	0.73	C <sub>3</sub> N <sub>4.0</sub>	11
6	GC-4	35.07	56.77	2.052	0.72	C <sub>3</sub> N <sub>4.1</sub>	12
7	GC-5	35.16	55.76	1.932	0.73	C <sub>3</sub> N <sub>4.0</sub>	13

**Calculations of average lifetime:**

The average lifetime ( $\tau_a$ ) can be determined using the following equation:

$$\tau_a = \frac{A_1\tau_1^2 + A_2\tau_2^2 + A_3\tau_3^2}{A_1\tau_1 + A_2\tau_2 + A_3\tau_3} \quad S4$$

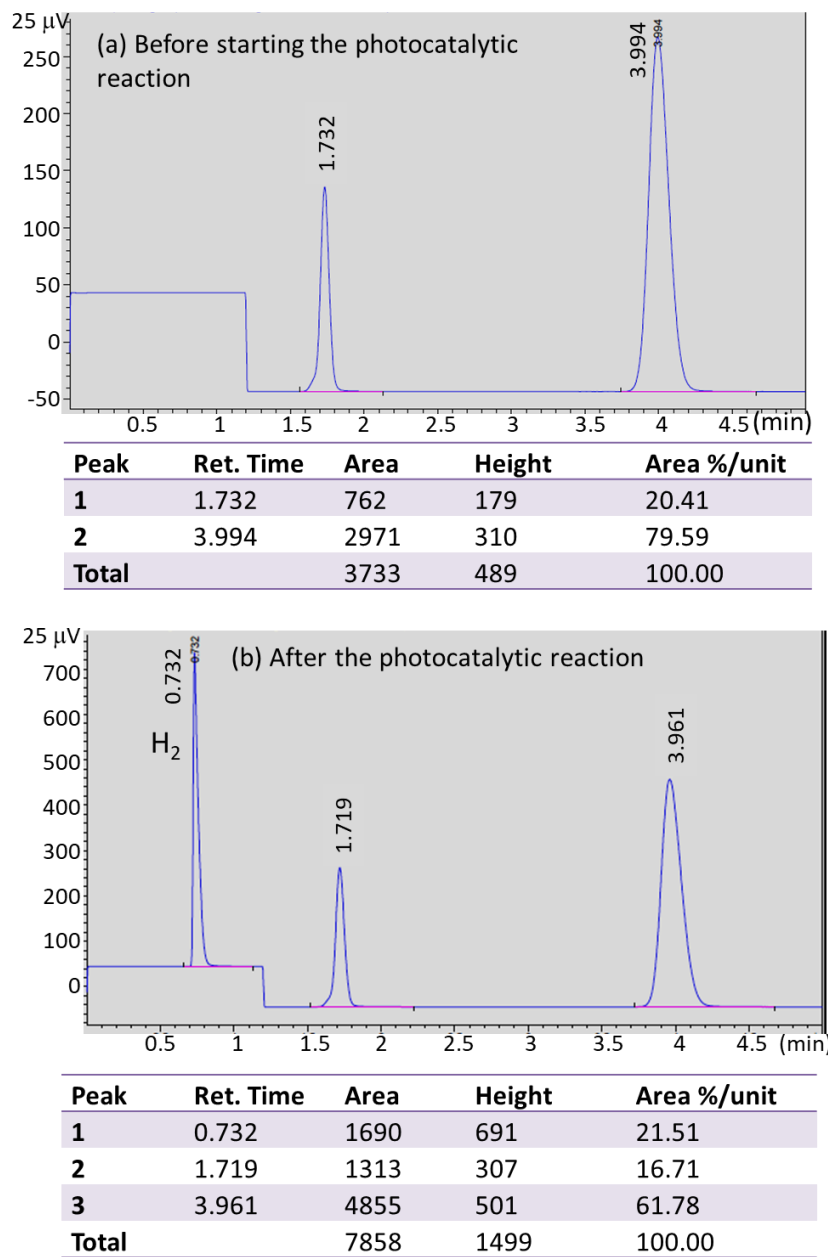
where  $\tau_1$ ,  $\tau_2$  and  $\tau_3$  are lifetime components and  $A_1$ ,  $A_2$  and  $A_3$  are the amplitudes of the components, respectively.

**Table S5.** The decay lifetimes and the average lifetime of photoexcited charge carriers in BDY and MDY photocatalysts are listed below:

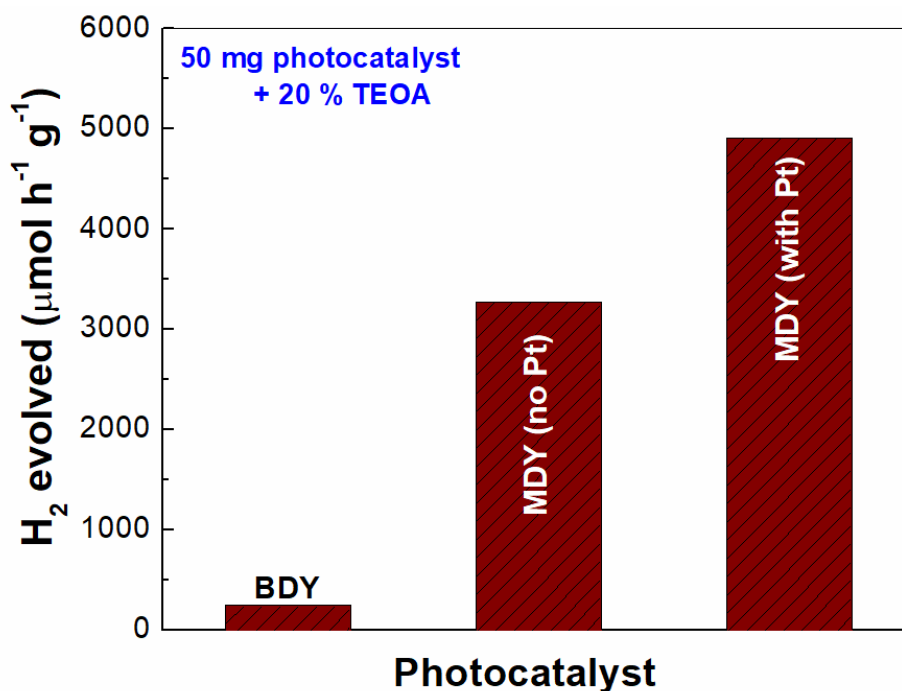
Sample	Decay life time (ns)			Avg. life time (ns)
	$\tau_1$	$\tau_2$	$\tau_3$	
BDY	0.23	1.61	11.6	<b>7.16</b>
MDY	3.42	0.61	18.4	<b>11.74</b>

**Table S6.** The corresponding measured pH values of different SRs used in the photocatalytic reaction.

Sl. No.	Sacrificial Agent (SRs)	Measured pH
1.	Water	7
2.	10 % MeOH	9.07
3.	10 % Lactic Acid	1.87
4.	10 % TEOA	10.6
5.	20 % TEOA	10.9



**Figure S6.** GC data (a) sample collected before starting the photocatalytic reaction and (b) sample collected after 3 hour of the photocatalytic reaction.



**Figure S7.** Amount of H<sub>2</sub> evolved per hour per gram of the studied MDY sample in absence and presence of Pt cocatalyst.

### Calculations:

**Determination of Donor Concentration ( $N_A$ ) of MDY sample using slope from Mott-Schottky plot.**

$$\text{slope} = 2/(\epsilon_o \epsilon_r q N_A) \quad \text{S5}$$

$\epsilon_o$  = permittivity of vacuum

$\epsilon_r$  = permittivity of vacuum

$q$  = electron charge

$N_A$  = donor concentration of MDY sample

$$\begin{aligned} \text{Therefore, } N_A &= 2 / (8.85 \times 10^{-10} * 9.58 * 1.602 \times 10^{-19} * 3.45 \times 10^9) \\ &= 4.26 \times 10^{17} \text{ cm}^{-3} \end{aligned}$$

### **Photocatalytic Reaction**

#### **1. Number of H<sub>2</sub> molecule produced from MDY using 3 wt% Pt**

Volume of gas liberated in reaction = 6.0 ml = 0.006 L

Form std. gas equation **PV= nRT**

$$n = 0.006 \text{ L} \times 1 \text{ atm} / 0.082 \text{ L.atm mol}^{-1} \text{ K}^{-1} \times 298 \text{ K}$$

$$\text{The corresponding amount of hydrogen in moles} = 0.000245 \text{ moles h}^{-1}$$

$$1 \text{ mole gas} = 6.023 \times 10^{23} \text{ molecules}$$

$$0.000245 \text{ moles will have} = 6.023 \times 10^{23} \times 0.000245$$

$$\begin{aligned} \text{H}_2 \text{ molecule (per cm}^2 \text{ per s)} &= (6.023 \times 10^{23} \times 0.000245) / (31.4 \times 60 \text{ min} \times 60 \text{ s}) \\ &= \mathbf{1.307 \times 10^{15}} \end{aligned}$$

$$\begin{aligned} \text{H}_2 \text{ molecule (per s)} &= (6.023 \times 10^{23} \times 0.000245) / (60 \text{ min} \times 60 \text{ s}) \\ &= \mathbf{4.09 \times 10^{16}} \end{aligned}$$

## **2. Number of H<sub>2</sub> molecule produced from MDY (no Pt)**

$$\text{Volume of gas liberated in reaction} = 4 \text{ ml} = 0.004 \text{ L}$$

$$\text{Form std. gas equation } \mathbf{PV = nRT}$$

$$n = 0.004 \text{ L} \times 1 \text{ atm} / 0.082 \text{ L.atm mol}^{-1} \text{ K}^{-1} \times 298 \text{ K}$$

$$\text{The corresponding amount of hydrogen in moles} = 0.0001635 \text{ moles h}^{-1}$$

$$1 \text{ mole gas} = 6.023 \times 10^{23} \text{ molecules}$$

$$0.0001635 \text{ moles will have} = 6.023 \times 10^{23} \times 0.0001635$$

$$\begin{aligned} \text{H}_2 \text{ molecule (per cm}^2 \text{ per s)} &= (6.023 \times 10^{23} \times 0.0001635) / (31.4 \times 60 \text{ min} \times 60 \text{ s}) \\ &= \mathbf{8.71 \times 10^{14}} \end{aligned}$$

$$\begin{aligned} \text{H}_2 \text{ molecule (per s)} &= (6.023 \times 10^{23} \times 0.0001635) / (60 \text{ min} \times 60 \text{ s}) \\ &= \mathbf{2.73 \times 10^{16}} \end{aligned}$$

## **3. For Bulk sample (BDY)**

$$\text{Volume of gas liberated in reaction} = 0.3 \text{ ml} = 0.0003 \text{ L}$$

$$\text{Form std. gas equation } \mathbf{PV = nRT}$$

$$n = 0.0003 \text{ L} \times 1 \text{ atm} / 0.082 \text{ L.atm mol}^{-1} \text{ K}^{-1} \times 298 \text{ K}$$

$$\text{The corresponding amount of hydrogen in moles} = 0.0000163 \text{ moles h}^{-1}$$

$$1 \text{ mole gas} = 6.023 \times 10^{23} \text{ molecules}$$

$$0.0000163 \text{ moles will have} = 6.023 \times 10^{23} \times 0.0000163$$

$$\text{H}_2 \text{ molecule (per cm}^2 \text{ per s)} = (6.023 \times 10^{23} \times 0.0000163) / (31.4 \times 60 \text{ min} \times 60 \text{ s})$$

$$= 8.7 \times 10^{13}$$

$$\text{H}_2 \text{ molecule ( per s)} = 2.72 \times 10^{15}$$

**Apparent quantum Yield (AQY):**

$$AQY = \frac{2.nH_2}{\text{number of incident photons}} \times 100 (\%)$$

$$AQY = \frac{2.nH_2}{(IA\lambda)/(hc)} \times 100 (\%) \quad S6$$

Where  $nH_2$  is the number of  $H_2$  molecule produced per second,  $I$  is the incident solar irradiance ( $W/cm^2$ ) over the irradiated area  $A$  ( $cm^2$ ),  $\lambda$  is the wavelength of the present study (nm),  $h$  Planck's constant and  $c$  is the speed of light.

$$I = 52500 \text{ lux} = 0.00768 \text{ W/cm}^2$$

$$A = 31.41 \text{ cm}^2$$

$$1 \text{ photon} = \frac{hc}{\lambda} = 6.626 \times 10^{-34} \times 3 \times 10^8 / (\lambda \times 10^{-9})$$

$$AQY = \frac{2 \times nH_2}{(0.00768 \times 31.41 \times \lambda \times 10^{-9}) / (6.626 \times 10^{-34} \times 3 \times 10^8)} \left( \frac{s^{-1}}{(\frac{W}{cm^2} \cdot cm^2 \cdot m) / (J \cdot s \cdot m \cdot s^{-1})} \right) \times 100\%$$

**Table S7.** The apparent quantum yield of BDY and MDY samples calculated at all wavelengths (5/10 nm intervals) till 420 nm from band gap absorption:

SI. N.	Wavelength ( $\lambda$ value in above equation S5)	AQY (%) (bulk BDY)	AQY (%) of MDY
1.	420	1.06	16.04
2.	425		15.86
3.	430	1.04	15.67
4.	435		15.49
5.	440	1.01	15.31
6.	445		15.14
7.	450	0.99	14.97
8.	455		14.81
9.	460	0.97	14.65
10.	465		14.49

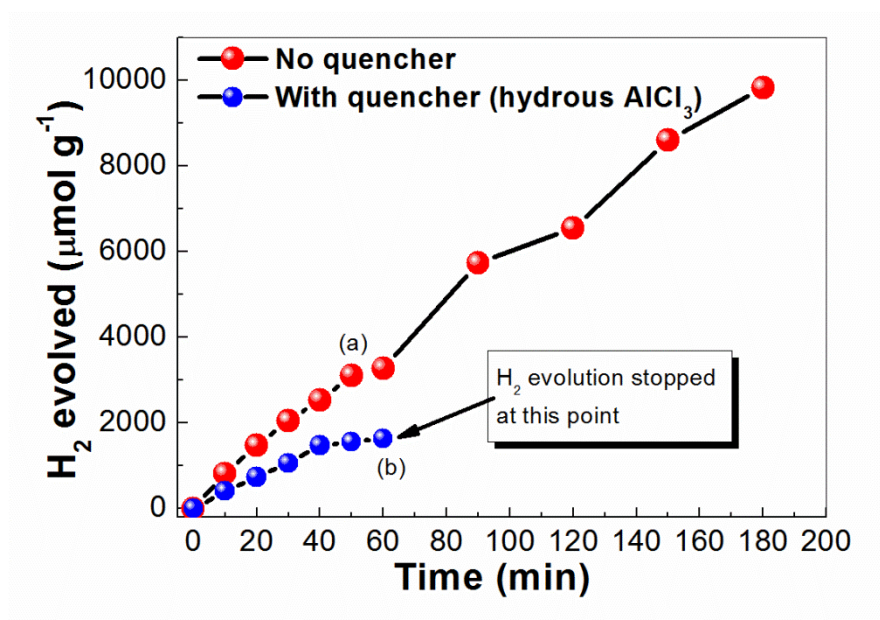


11.	470	0.95	14.34
12.	475		14.19
13.	479	0.93	14.07

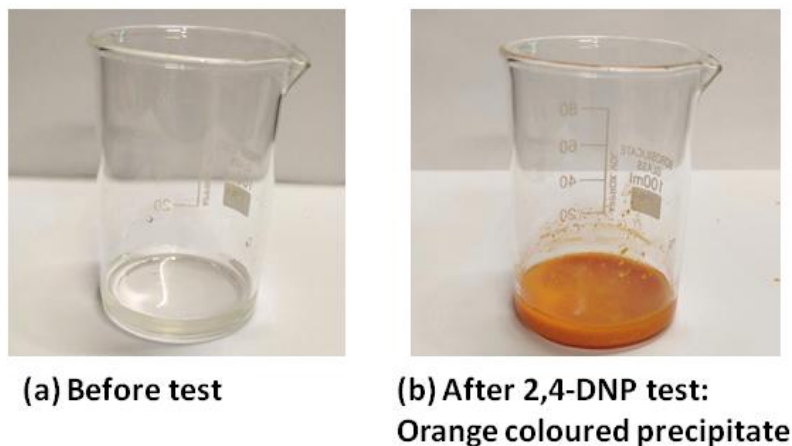
**Table S8.** Comparison of photocatalytic activity of present vermicular rope like mesoporous sample with other nanostructured mesoporous g-C<sub>3</sub>N<sub>4</sub> samples and other related photocatalysts.

Sl. No.	Photocatalyst	Amount of photocatalyst and Pt	Sacrificial agent	Photocatalytic Activity (mmol h <sup>-1</sup> g <sup>-1</sup> )	Apparent Quantum Efficiency (%)	Reference No.
1.	Mesoporous g-C <sub>3</sub> N <sub>4.7</sub>	50 mg + 3 wt % Pt	20 % vol TEOA	4.19	16.04 % at 420 nm	This work
		50 mg + without Pt		3.13	10.71 % at 420 nm	
2.	Mesoporous carbon nitride	100 mg + 3 wt % Pt	10% vol TEOA	0.3	0.21 % at 405 nm	14
3.	Mesoporous carbon nitride	30 mg + 3wt % Pt	10% vol TEOA	1.16	7.7% at 420 nm	15
4.	Rh <sub>x</sub> P/g-C <sub>3</sub> N <sub>4</sub>	50 mg	20% vol TEOA	3.055	18.4 % at 420 nm	16
5.	Holey graphitic carbon nitride nanotubes	20 mg + 0.5 wt% Pt	20% Lactic acid	1.07	-	17
6.	Pt@Au NRs/C <sub>3</sub> N <sub>4</sub> nanotubes	20 mg catalyst + 3wt % Pt	10 % TEOA	10.35	9.1 % at 420 nm	18
7.	2D FeS-FeS <sub>2</sub>	30 mg	0.35 M Na <sub>2</sub> SO <sub>3</sub> +0.15 Na <sub>2</sub> S	2.07	-	19
8.	P-doped g-C <sub>3</sub> N <sub>4</sub> nanosheets	50 mg + 1 wt% Pt	10% TEOA	2.61	7.7% at 420 nm	20
9.	Ni <sub>2</sub> P/ g-C <sub>3</sub> N <sub>4</sub>	50 mg + Ni <sub>2</sub> P	10% TEOA	2.84	18.8% at 420 nm	21
10.	1T PtS <sub>2</sub> /MCN	50 mg + 1 wt% PtS <sub>2</sub>	10% TEOA	0.29	1.16% at 405 nm	22
11.	MCN-8	100 mg + 3wt % Pt	10% vol TEOA	2.6	–	23

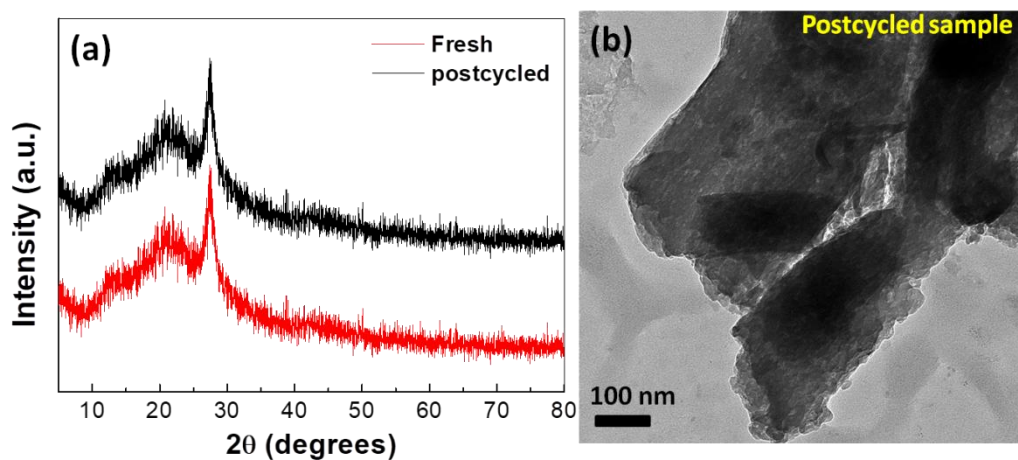
12.	CoNi-ZnIn <sub>2</sub> S <sub>4</sub>	30 mg	0.1 M ascorbic acid	3.336	-	24
13.	COP-TF@CNi <sub>2</sub> P	9 mg	Na <sub>2</sub> S + Na <sub>2</sub> SO <sub>3</sub>	2.5	1.4 % at 500 nm	25
14.	g-C <sub>3</sub> N <sub>4</sub> /Co@NC	10 mg + 1 wt% Pt	15% TEOA	1.56	6.85 at 420 nm	26
15.	Ni-single atom/CN	25 mg + 0.2 at% Ni	10 % TEOA	0.35	-	27
16.	PtSn-CN <sub>x</sub>	100 mg + PtSn	20% TEOA	2.96	8.42% at 435 nm	28
17.	Nitrogen vacancies into crystalline g-CN	50 mg + 2 wt% Pd	10 % MeOH	0.55	-	29



**Figure S8.** Prolonged 3 h continuous study of photocatalytic hydrogen evolution study using MDY (a) without radical scavenger, and (b) with scavenger (hydrous AlCl<sub>3</sub>).



**Figure S9.** 2,4-dinitrophenylhydrazine (2,4-DNP) test to detect the formation of aldehyde. (a) Solution left out after photocatalytic  $H_2$  evolution reaction and before the addition of 2,4-DNP reagent, (b) Same solution after the addition of 2,4-DNP reagent.



**Figure S10.** (a) Comparison of powder XRD patterns of fresh MDY sample and post catalytic MDY sample. (b) HRTEM images of the post-catalytic MDY sample.

**Table S9.** Comparison of efficacy of the present material in this work with the recent g-C<sub>3</sub>N<sub>4</sub> and similar co-catalyst with a similar reactor configuration (50 ml).

SI. No.	Photocatalyst	Amount of photocatalyst and Pt in 50 ml reactor	Sacrificial Agent	Photocatalytic activity (mmolh <sup>-1</sup> g <sup>-1</sup> )	Apparent Quantum Efficiency (%) at 420 nm	Reference No.
1.	Mesoporous g-C <sub>3</sub> N <sub>4.7</sub>	50 mg + 3 wt % Pt	20 % vol TEOA	4.19	16.04 % at 420 nm	This work
2.	Fish-scale structured g-C <sub>3</sub> N <sub>4</sub>	50 mg +3 wt% Pt	10 vol% TEOA	1.316	-	30
3.	g-C <sub>3</sub> N <sub>4</sub>	50 mg +3 wt% Pt	10 vol% TEOA	0.162	1.4	31
4.	g-C <sub>3</sub> N <sub>4</sub> nanostructure	50 mg +3 wt% Pt	10 vol% TEOA	3.135	21.03	32
5.	Holey graphitic carbon nitride	50 mg +3 wt% Pt in 40 ml reactor	10.7 vol% TEOA	8.290	-	33
6.	3D Ordered close-packed g-C <sub>3</sub> N <sub>4</sub> nanosphere arrays	50 mg +3 wt% Pt	10 vol% TEOA	3.138	5.07	34
7.	g-C <sub>3</sub> N <sub>4</sub>	50 mg +1 wt% Pt	10 vol% TEOA	2.7	-	35
8.	g-C <sub>3</sub> N <sub>4</sub>	50 mg +3 wt% Ni	10 vol% TEOA	0.11	2.6	36
9.	Porous oxygen doped g-C <sub>3</sub> N <sub>4</sub>	50 mg +3 wt% Pt	20 vol% TEOA	0.395	0.79	37
10.	Carbon-rich g-C <sub>3</sub> N <sub>4</sub> nanosheets	50 mg +3 wt% Pt	12 vol% TEOA	0.792	4.52	38
11.	Nanoporous g-C <sub>3</sub> N <sub>4</sub>	25 mg + 0.5 wt% Pt	10 vol% TEOA	0.008	-	39

**POSCAR for g-C<sub>3</sub>N<sub>4</sub>**g-C<sub>3</sub>N<sub>4</sub>\_heptazine\_Phase\_1

1.0000000000000000

6.8685919899354158	0.0062264310321799	0.0000000000000000
-3.4070984882571040	5.9639982045349234	0.0000000000000000
0.0000000000000000	0.0000000000000000	10.0000000000000000

C N  
6 8

Direct

0.9061677315109549	0.4158392555043307	0.2558324363580269
0.5841608585378850	0.0938324169186089	0.3544354636419698
0.2578923492893139	0.0945748645039401	0.3302903630821206
0.9054249980273639	0.7421076104179605	0.2799775369178832
0.9034806221731628	0.0965193691825377	0.3051340000000025
0.5703011148300945	0.4296989971626743	0.3051340000000025
0.3615030873623795	0.9801336808943262	0.3674864253266819
0.0198663928244898	0.6384969911753444	0.2427814746733148
0.9914881088844112	0.2812090883151868	0.2295154296835022
0.7187908965370866	0.0085119032234644	0.3807524703164944
0.6836034041766226	0.6497174564631223	0.2897546079783169
0.3502825971908337	0.3163967104806531	0.3205132920216798
0.0254067521785544	0.9745932353746269	0.3051340000000025
0.6875985365856536	0.3124015722939077	0.3051340000000025

**POSCAR for g-C<sub>3</sub>N<sub>4.7</sub>**

super cell

1.0000000000000000

9.5800000000000001	0.0000000000000000	0.0000000000000000
-4.7900000000000000	8.2965239999999998	0.0000000000000000
0.0000000000000000	0.0000000000000000	12.0000000000000000

C N H  
12 19 3

Direct

0.0923756571197032	0.3398857599075598	0.4279012586418034
0.6151942879454211	0.2855129802149463	0.3236202433205690
0.1490556245946664	0.7891275868695331	0.3778813118019642
0.6414617062374290	0.7931459392776503	0.3812416725399572
0.3845387774080322	0.3197370462956570	0.2953037364850459
0.8226226714451030	0.2789341572088304	0.3787278164043499
0.3608888234324610	0.7681510044017017	0.3564809386145953
0.8894043361646098	0.8178068817934872	0.3981138380239813
0.3879089933644195	0.5321486538029845	0.3431933722322853

0.9102418924251765	0.5688622428630339	0.4386265859063556
0.3442591579581133	0.0847534435989559	0.3764262578912394
0.8660991233074142	0.0425410107333803	0.3879602993380260
0.9297878898075780	0.2170347633508243	0.3902738164467934
0.4480135602783974	0.2161909042853765	0.3021073535185863
0.9842953078063630	0.7359732307491740	0.3970178799065849
0.4616986250360497	0.6981519851276872	0.3688342631319728
0.2237305030833454	0.4000170750762990	0.3470374896722035
0.7274224813341448	0.4368086401517601	0.3070458134872069
0.2698304883594176	0.9280516100622265	0.3244241262037306
0.7060817421518877	0.9520646325622550	0.3748364810349827
0.2287245567699472	0.2650665705039970	0.3081797483024431
0.6669972897034953	0.1868652686735999	0.3662232887417076
0.2052899059877120	0.6892458060178370	0.3982303096633544
0.7274202389790076	0.7188305082171595	0.3990350332525239
0.4803790181174890	0.4810343318465513	0.3017210617879300
0.8697376111478974	0.4446739019526191	0.3515661757891664
0.4026586566561647	0.9041100787676797	0.3046989809413745
0.9663075560343870	0.9807010257343833	0.3969690546080500
0.1020739829004498	0.3876156556340717	0.5272655872399241
0.8898169721979770	0.5487042429571645	0.5424098213304021
0.3304336834705168	0.1151656473778999	0.4770028562394941
0.2159949507008960	0.4795401107684683	0.5474484586536761
0.8397632349928728	0.4298033295742556	0.5663346594604022
0.2516969988519193	0.0144780883135809	0.5218287427206576

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