Supporting Information for

Substituent Effect of Conjugated Microporous Polymers on the Photocatalytic Hydrogen Evolution Activity

Xiaomin Gao,[a] Chang Shu,[a] Chong Zhang,[a,*] Wenyan Ma,[a] Shi-Bin Ren,[b,*] Feng Wang,[c] Yu Chen,[a] Jing Hui Zeng,[a] and Jia-Xing Jiang[a,*]

[a] *Key Laboratory for Macromolecular Science of Shaanxi Province, Shaanxi Engineering Laboratory for Advanced Energy Technology, School of Materials Science and Engineering, Shaanxi Normal University, Xi'an, Shaanxi 710062, P. R. China.*

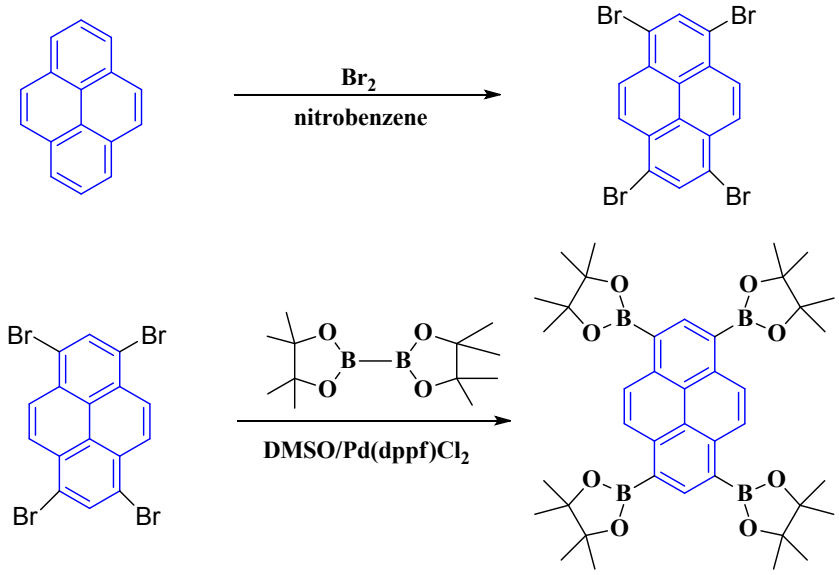
[b] *School of Pharmaceutical and Materials Engineering, Taizhou University, Taizhou 318000, P. R. China.*

[c] *Key Laboratory for Green Chemical Process of Ministry of Education, School of Chemical Engineering and Pharmacy, Wuhan Institute of Technology, Wuhan 430073, P. R. China.*

** E-mail: chongzhangabc@snnu.edu.cn; renshibin@126.com; jiaxing@snnu.edu.cn*

Experimental Section

Synthesis of 1,3,6,8-tetrakis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pyrene

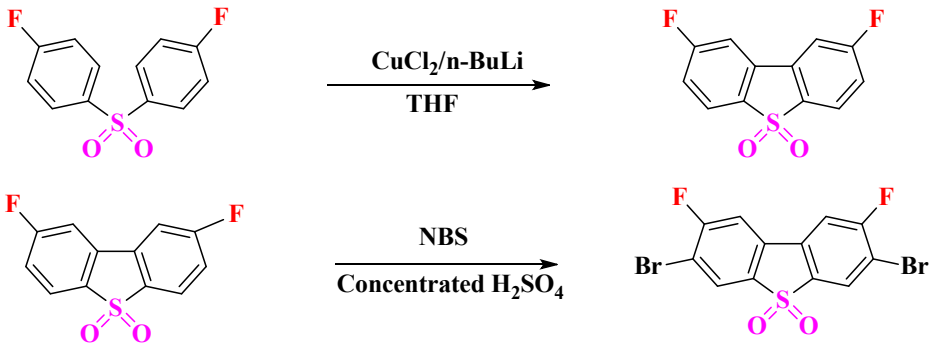


Liquid bromine (6.6 mL) was added into the solution of pyrene (6.0 g) in 100 mL nitrobenzene at room temperature with strong stirring. The reaction solution was

heated to 160 ºC and stirred for 6 h and then cooled to room temperature. The mixture was poured into acetone and filtered. The obtained product was washed with acetone for several times to give 1,3,6,8-tetrabromopyrene as a white solid.

Bis(pinacolato)diboron (35.2 g, 138.8 mmol) was added into the solution of 1,3,6,8-tetrabromopyrene (12.0 g, 23 mmol), Pd(dppf)Cl_2 (1.28 g, 2 mmol) and potassium acetate (14 g, 142.8 mmol) in DMSO (240 mL, anhydrous) with stirring at under nitrogen atmosphere. The reaction solution was heated to 80 ºC and stirred for 48 h. The reaction mixture was cooled to room temperature, and poured into 1 L of water and filtered. The product was purifed by column chromatography on silica gel using dichloromethane and petroleum ether as the eluent. The product was obtained as pale white solid (8.6 g, 52%). ^{1}H NMR (ppm, 400 MHz; $CDCl_3$): δ 9.20 (s, 4H), 9.06 (s, 2H), 1.48 (s, 48H); ^{13}C NMR (ppm, 300 MHz; $CDCl_3$): δ 143.3, 136.0, 133.1, 128.0, 122.0, 86.6, 20.0.

Synthesis of 2,8-difluoro-3,7-dibromo-benzothiophene-S,S-dioxide

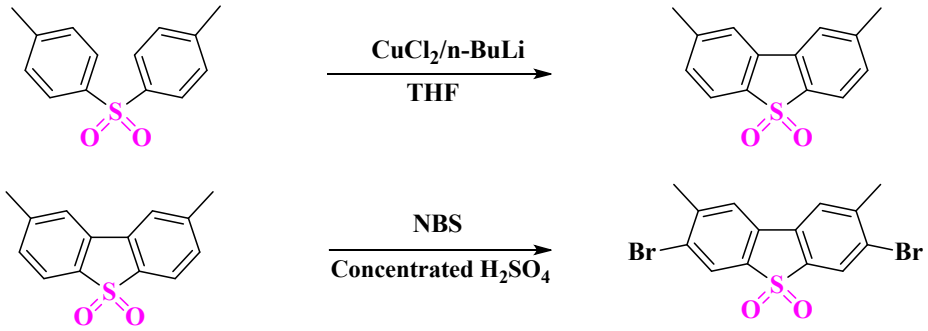


A 500 mL single neck round-bottom flask was charged with dry THF (250 mL) and bis-(4-fluorophenyl) sulfone (10.0 g, 39.4 mmol). The reaction symtem was purged with nitrogen and cooled to -78 ºC in a dry-ice/acetone bath. n-Butyl lithium in cyclohexane (2.0 M, 40.3 mL, 80.6 mmol) was slowly added into the solution via syringe. The reaction solution was stirred for an hour at -78 ºC and removed from the

cold bath. Anhydrous copper (II) chloride (10.6 g, 77.8 mmol) was added to the mixture. Then, the reaction solution was refluxed for 20 h and 3% hydrochloric acid (660 mL) was added. After work-up, the resulting yellow solid was recrystallized from THF to give the product of 2,8-difluoro-dibenzothiophene-S,S-dioxide as white solid (yield, 25%). ^{1}H NMR (ppm, 400 MHz; $CDCl_3$): δ 7.75 (d, 2H), 7.68 (s, 2H), 7.34 (d, 2H). ^{13}C NMR (ppm, 300 MHz; $CDCl_3$): δ 167.70, 134.60, 133.8, 125.4, 119.6, 103.7.

2,8-Difluoro-dibenzothiophene-S,S-dioxide (4.8 g, 18.9 mmol) was dissolved in concentrated H_2SO_4 (150 mL). NBS (5 g, 28.1 mmol) was added into the solution in three times and the resulting mixture was stirred at ice-water for 7 h. The mixture was carefully poured into ice/water. The off-white solid was filtered off, washed with 20% aqueous sodium hydrogen carbonate, water and dried to afford white solid. The product was further recrystallized from trichloromethane to give 2,8-difluoro-3,7-dibromo-benzothiophene-S,S-dioxide as white crystal in 60 % yield. ^{1}H NMR (ppm, 400 MHz; $CDCl_3$): δ 8.02 (s, 2H), 7.44 (d, 2H). ^{13}C NMR (ppm, 300 MHz; $CDCl_3$): δ 164.98, 135.45, 133.86, 127.68, 119.69, 107.34.

Synthesis of 2,8-dimethyl -3,7-dibromo-benzothiophene-S,S-dioxide



A 500mL single neck round-bottom flask was charged with dry THF (250 mL) and bis-(4-methylphenyl) sulfone (9.7 g, 39.4 mmol). The reaction symtem was

purged with nitrogen and cooled to -78℃ in a dry-ice/acetone bath. n-Butyl lithium in cyclohexane (2.0 M, 40.3 mL, 80.6 mmol) was slowly added into the solution via syringe. The reaction solution was stirred for an hour at -78 ℃ and removed from the cold bath. Anhydrous copper (II) chloride (10.6 g, 77.8 mmol) was added into the mixture. Then, the reaction solution was refluxed for 20 h and 3% hydrochloric acid (660 mL) was added. After work-up, the resulting crude product was recrystallized from THF to give 2,8-dimethyl-dibenzothiophene-S,S-dioxide as white solid (yield, 34%). ^{1}H NMR (ppm, 400 MHz; $CDCl_3$): δ 7.83 (d, 2H), 7.42 (s, 2H), 7.25 (d, 2H), 1.57 (s, 6H). ^{13}C NMR (ppm, 300 MHz; $CDCl_3$): δ 134.40, 124.73, 118.34, 109.65, 30.13.

2,8-Dimethyl-dibenzothiophene-S,S-dioxide (4.6 g, 18.7mmol) was dissolved in concentrated H_2SO_4 (150 mL). NBS (5 g, 28.1 mmol) was added into the solution in three portions and the resulting mixture was stirred at ice/water for 7 h. The mixture was carefully poured into ice/water. The white solid was filtered off, washed with 20% aqueous $NaHCO_3$, water and dried to afford white solid. The product was further recrystallized from trichloromethane to give 2,8-dimethyl -3,7-dibromo-benzothiophene-S,S-dioxide as white crystal in 60 % yield. ^{1}H NMR (ppm, 400 MHz; $CDCl_3$): δ 7.93 (s, 2H), 7.61 (d, 2H), 2.49 (s, 6H). ^{13}C NMR (ppm, 300 MHz; $CDCl_3$): δ 144.84, 136.58, 130.15, 126.22, 123.38, 23.93.

Characterization

Elemental composition was measured by EURO EA3000 Elemental Analyzer. Thermogravimetric analysis (TGA) measurement was performed by using a differential thermal analysis instrument (Q1000DSC + LNCS + FACS Q600SDT) over the temperature range from 30 to 800 °C under a nitrogen atmosphere with a heating rate of 10 °C min^{-1}. Fourier-transform infrared (FT-IR) spectra were collected

on a Tensor 27 FT-IR spectrometer (Bruker) using KBr disks. Solid-state ^{13}C NMR spectra were obtained on a JEOL RESONRNCE ECZ 400R NMR spectrometer at a MAS rate of 12 kHz. Powder X-ray diffraction measurement (PXRD) was performed by X-ray diffractometer (D/Max-3c). The morphology analysis was performed by using a field emission scanning electron microscope (SEM) (JSM-6700F). The UV-Vis adsorption spectra of the polymers were carried out by a Scan UV-Vis spectrophotometer (UV-Lambda 950, PerkinElmer, US) using $BaSO_4$ as a reference sample. The fluorescence properties of the polymers were measured with a Shimadzu F-7000 PC fluorescence spectrometer by using excitation wavelength of 365 nm at room temperature. N_2 adsorption isotherms at −196 °C were obtained using an ASAP 2420-4 (Micromeritics) volumetric adsorption analyzer. Samples were degassed at 120 °C for 15 h under vacuum (10^{-5} bar) before analysis. The surface areas were calculated from nitrogen adsorption data by Brunauere-Emmette-Teller (BET) analysis. Pore size distributions were calculated by DFT methods via the adsorption branch. Pd content was obtained by inductively coupled plasma mass spectrometry (ICP-MS) and energy dispersive X-ray spectroscopy (EDX). Cyclic voltammetry (CV) measurements were carried out on CHI660E (Chenhua, Shanghai) electrochemical workstation in a three-electrode-cell system. A platinum plate and a saturated calomel electrode were employed as the counter electrode and reference electrode, respectively. The photocurrent was measured on CHI660E electrochemical workstation with a bias voltage of 0.02 V under UV-Vis light irradiation with 25 s light on-off cycles. The prepared electrode from the polymer catalyst and 5 wt % Nafion (mass ratio of 1:30) was immersed in 1 M Na_2SO_4 aqueous solution.

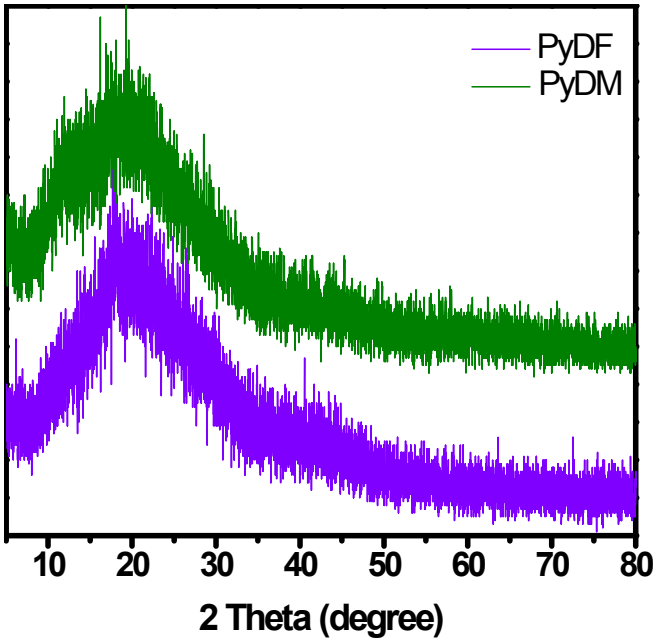


Figure S1. Powder XRD patterns of the PyDF and PyDM polymers.

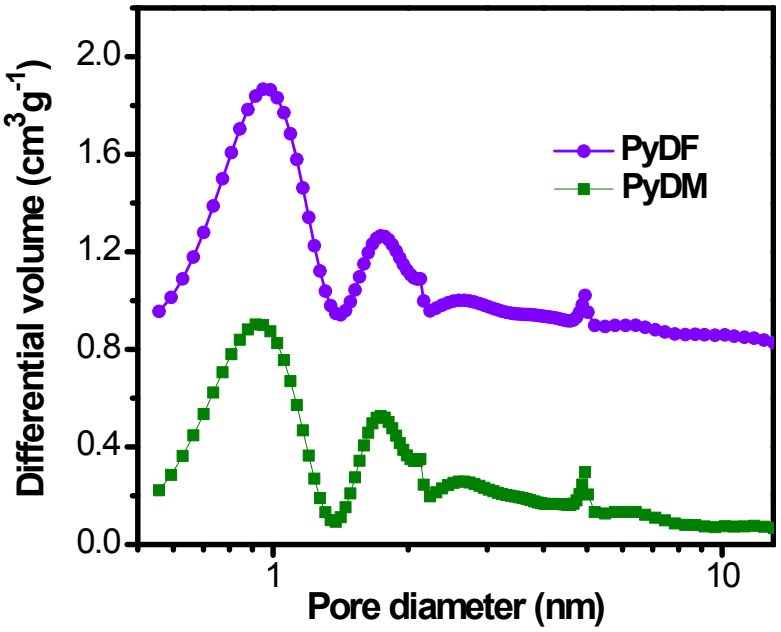


Figure S2. Pore size distribution curves for PyDF and PyDM.

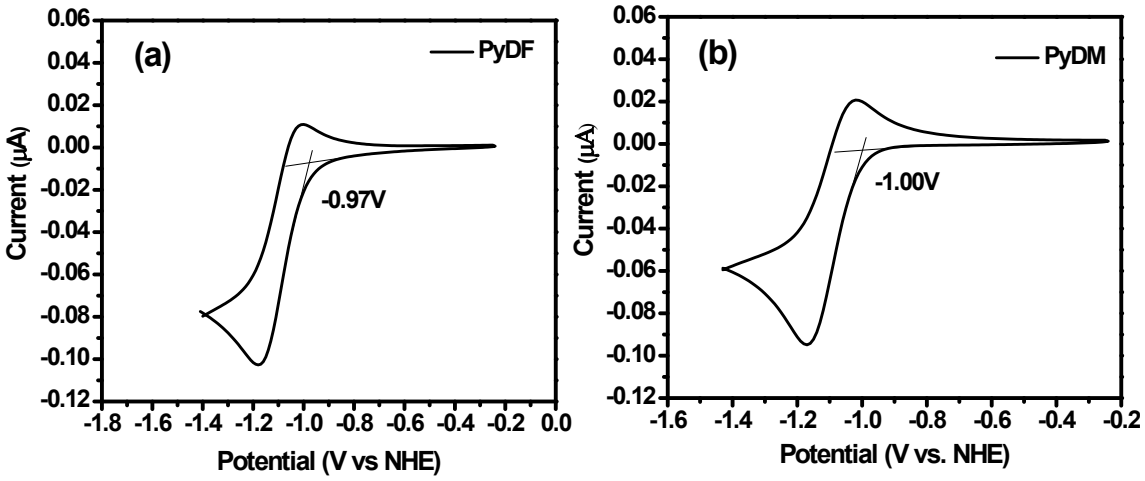


Figure S3. Cyclic voltammetry curves for PyDF and PyDM.

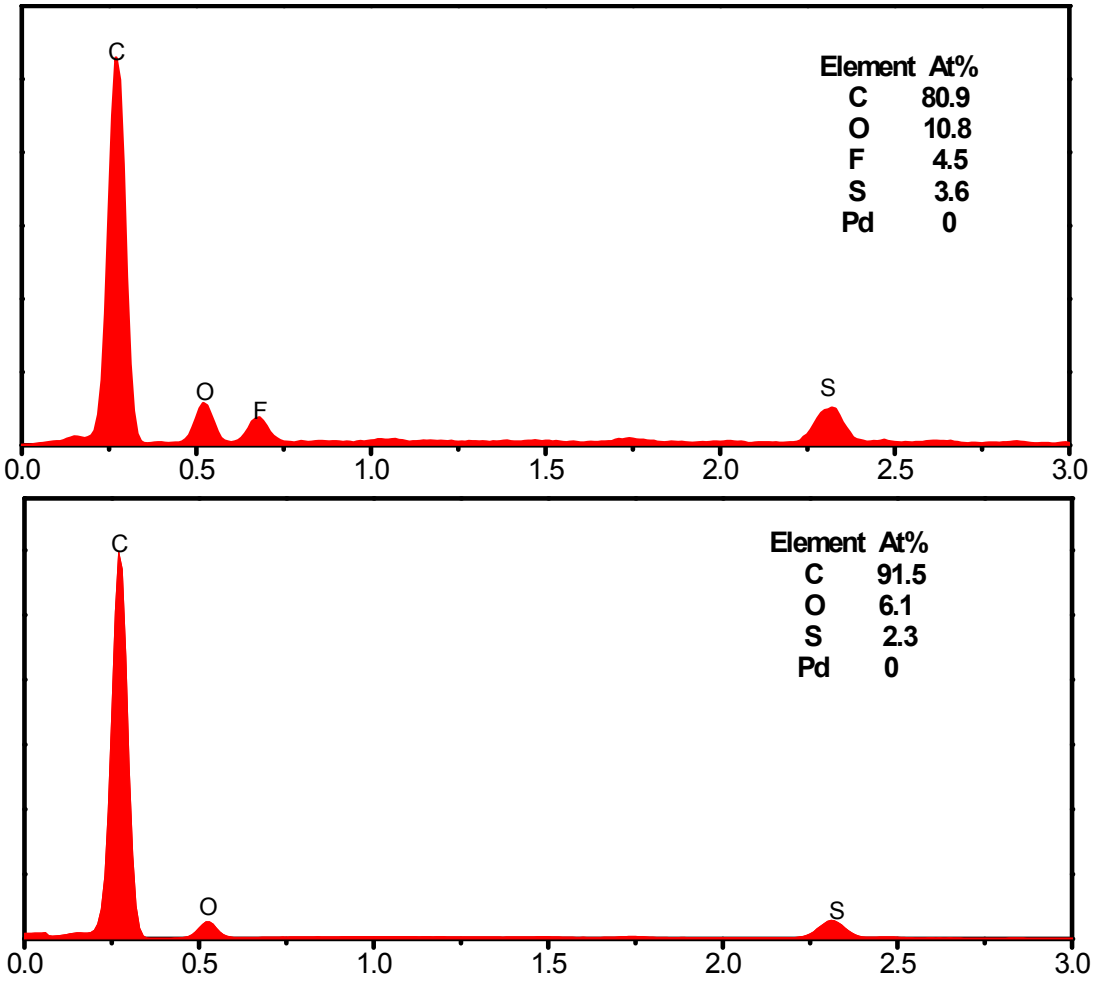


Figure S4. Energy dispersive X-ray spectroscopy (EDX) spectra of (top) PyDF and (bottom) PyDM.

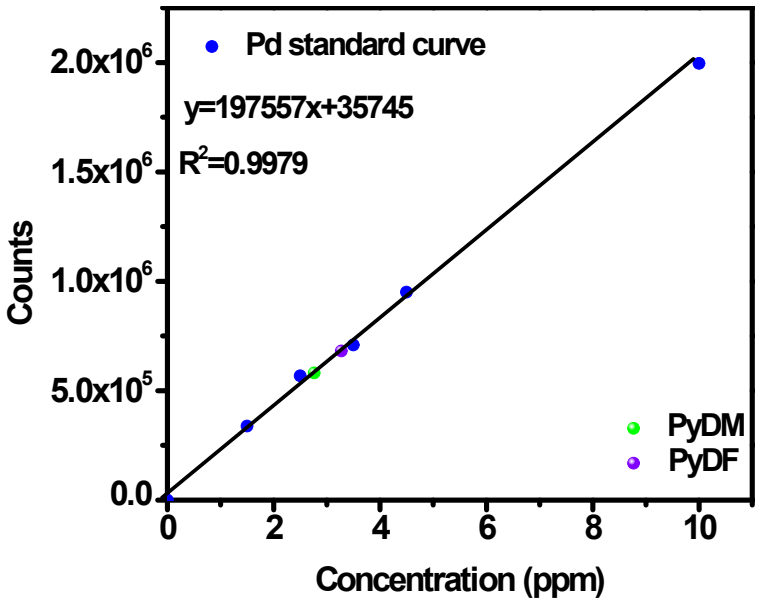


Figure S5. The residual Pd contents in PyDF and PyDM measured by ICP-MS.

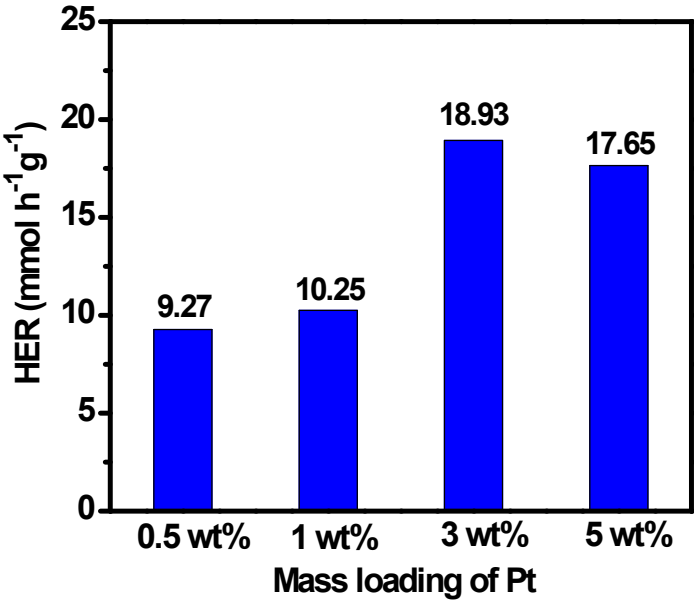


Figure S6. H_2 production of PyDF loaded with different amounts of Pt co-catalyst under UV-visible light.

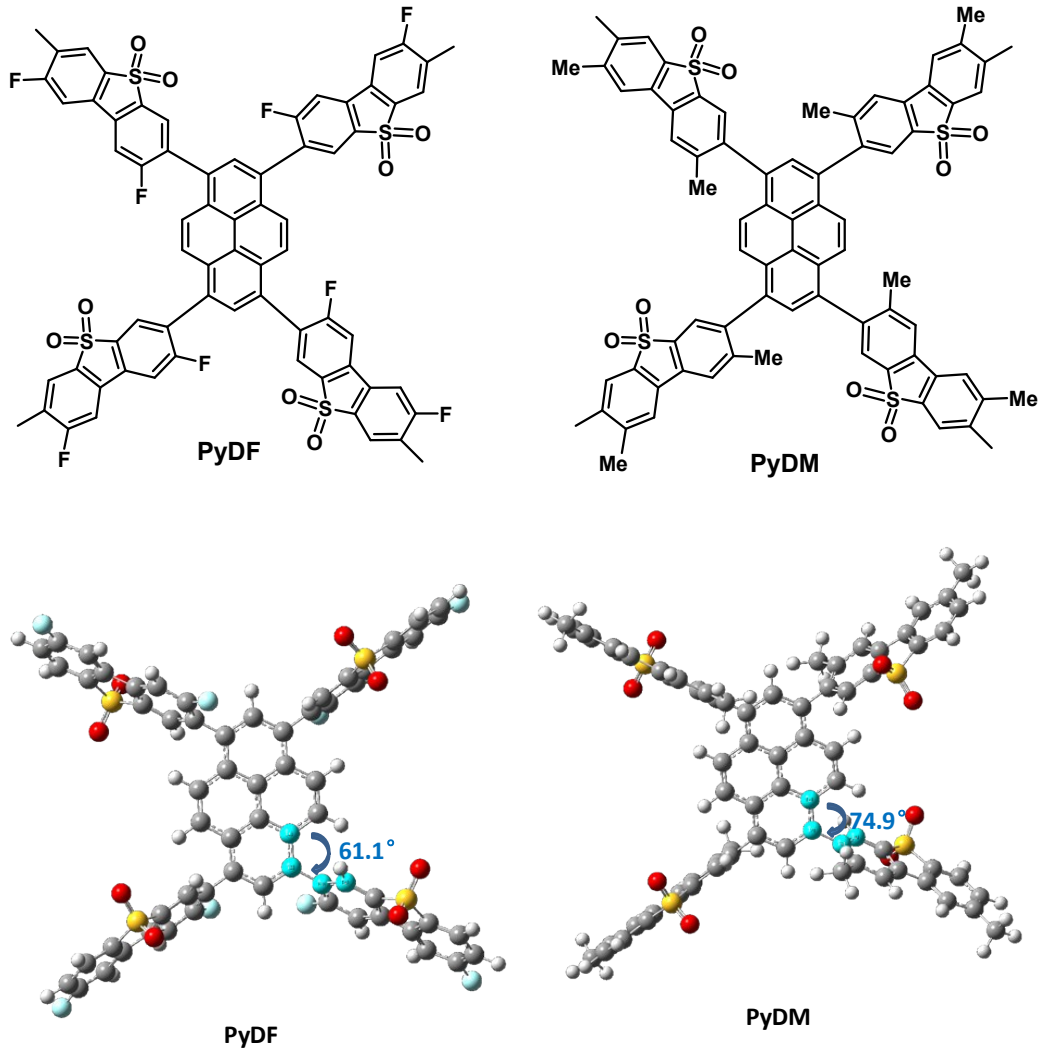


Figure S7. The molecular fragments of PyDF and PyDM were used for DFT simulation (top), the DFT geometry optimizations and the dihedral angles of the polymers (bottom).

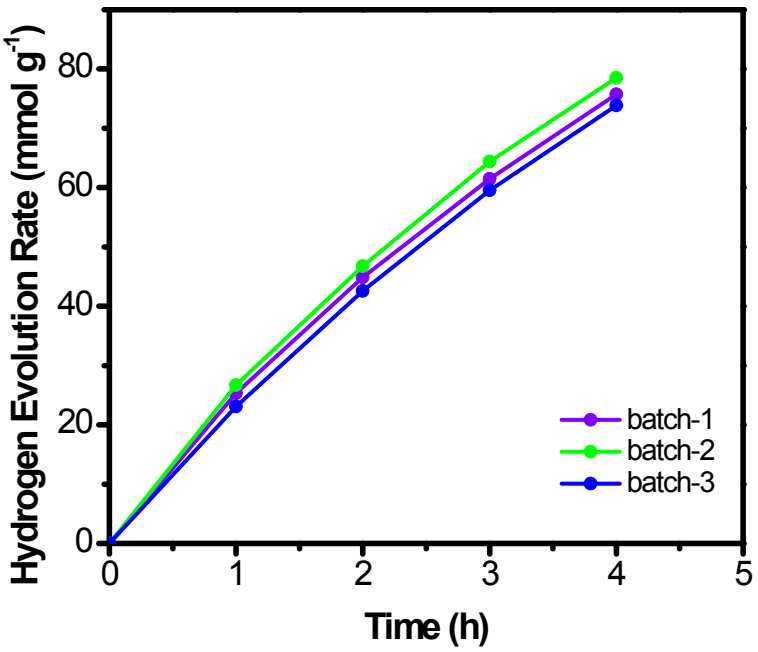


Figure S8. Hydrogen generation of PyDF produced from different batches with 3 wt% Pt under UV−Vis light irradiation (λ > 300 nm).

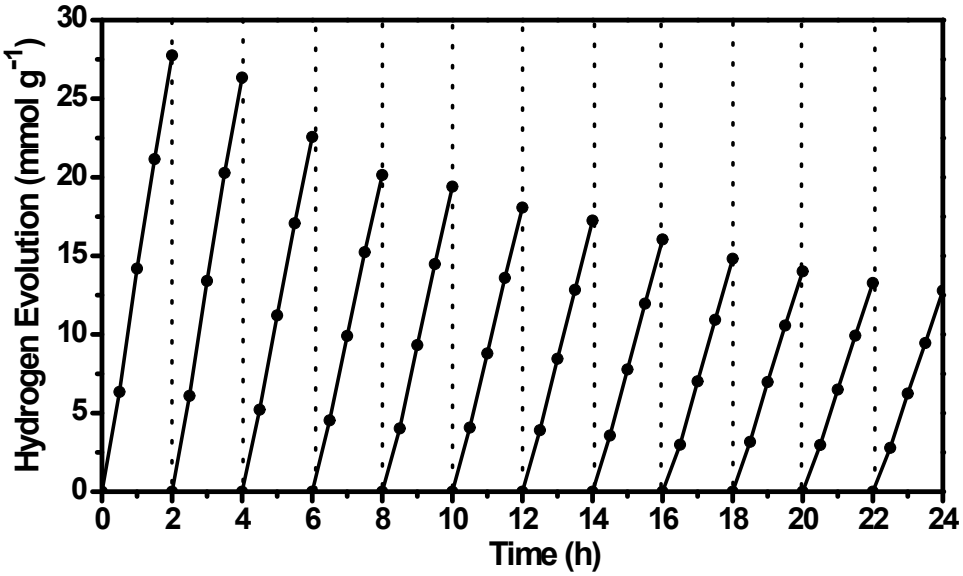


Figure S9. Stability test of PyDF with 3 wt% Pt from water containing 20 vol% triethanolamine and irradiated by visible light (λ > 420 nm) for 24 h.

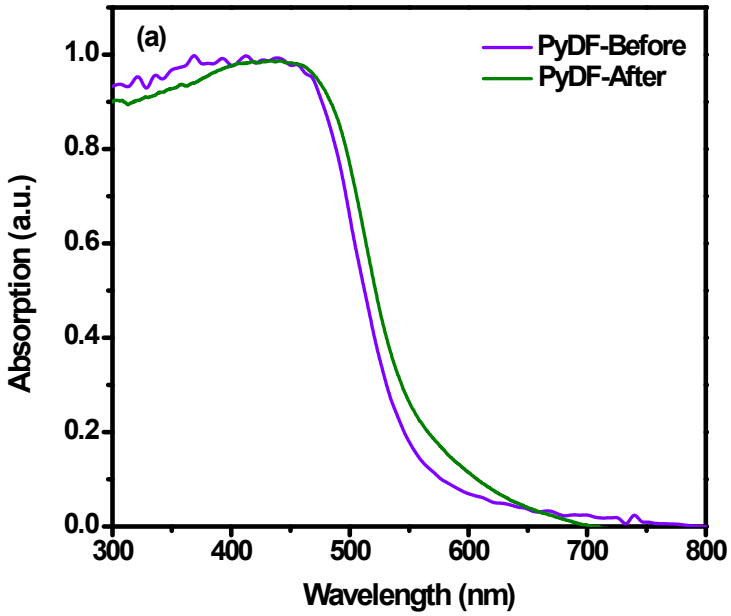


Figure S10. UV-Vis absorption spectra for the polymer PyDF before and after photocatalytic reaction under visible light (λ > 420 nm) for 24 h in a triethanolamine/water mixture.

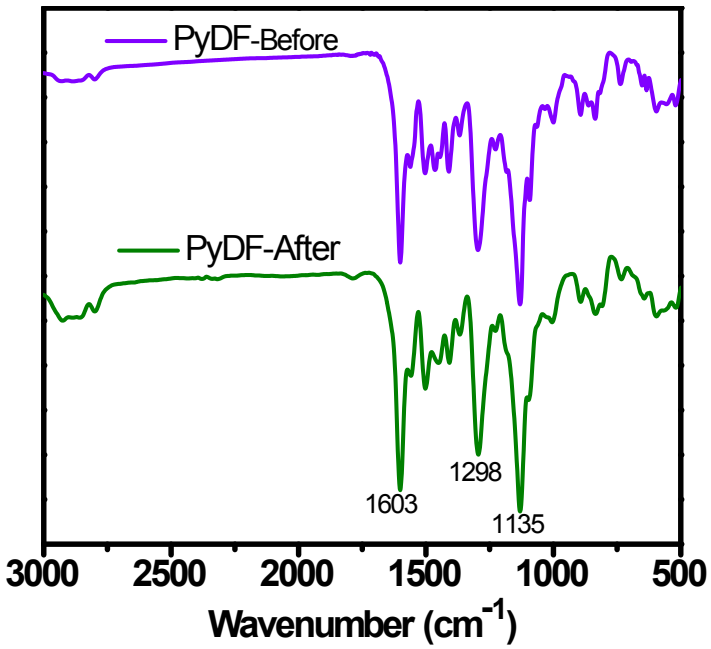


Figure S11. FT-IR spectra for the polymer PyDF before and after photocatalytic reaction under visible light (λ > 420 nm) for 24 h in a triethanolamine/water mixture.

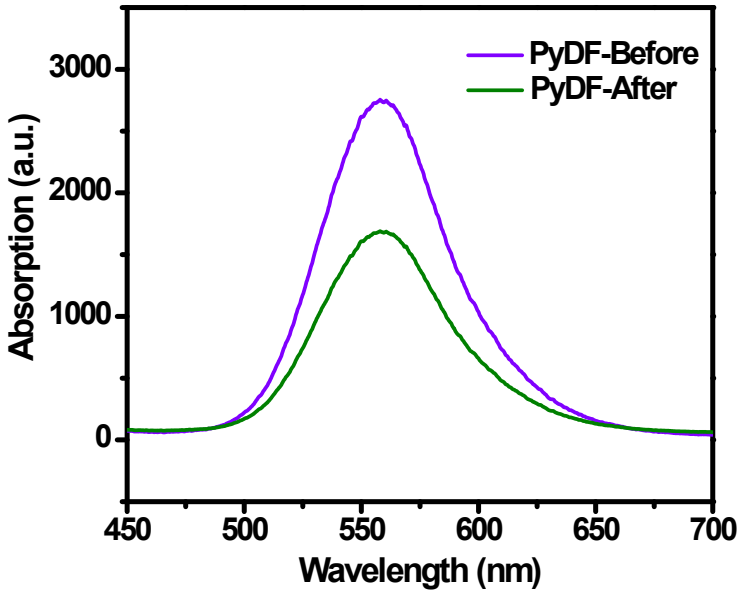


Figure S12. Photoluminescence spectra of the polymer PyDF before and after photocatalytic reaction under visible light (λ > 420 nm) for 24 h in a mixture of triethanolamine/water ($\lambda_{excitation}$ = 365 nm).

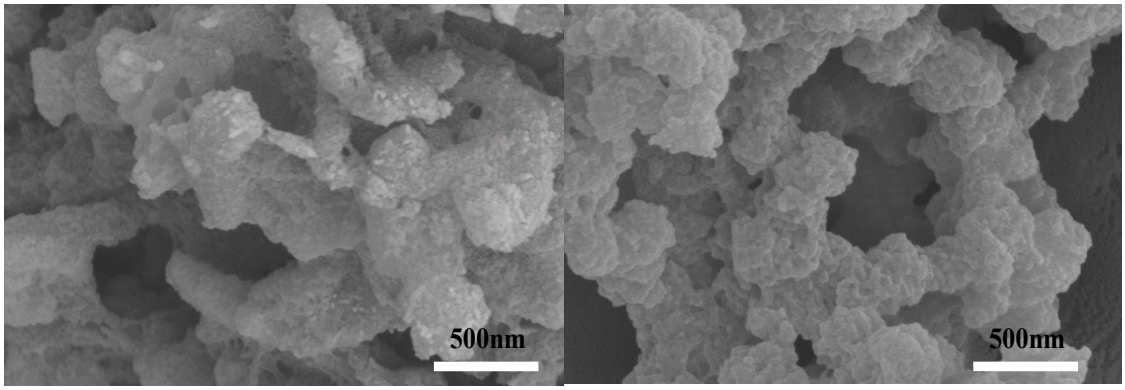


Figure S13. Scanning electron microscope (SEM) images of PyDF before (a) and after (b) photocatalytic reaction under visible light (λ >420 nm) for 24 h in a triethanolamine/water mixture.

Table S1. Summary of Pore Properties for the Polymer Networks

Polymer	S_{BET}[a] ($m^2 g^{-1}$)	S_{Micro}[b] ($m^2 g^{-1}$)	V_{Micro}[c] ($cm^3 g^{-1}$)	V_{Total}[d] ($cm^3 g^{-1}$)	S_{Micro}/ S_{BET} (%)	V_{Micro}/ V_{Total} (%)
PyDF	825	701	0.33	0.59	0.85	0.56
PyDM	827	679	0.33	0.65	0.82	0.51

[a] Surface area calculated from N_2 adsorption isotherm in the relative pressure (P/P_0) range from 0.05 to 0.20; [b] Micropore surface area calculated from the N_2 adsorption isotherm using *t*-plot method based on the Harkins Jura Equation; [c] The micropore volume devised from the *t*-plot method; [d] Total pore volume at P/P_0 =0.90.

Table S2. Fitted decay time of the polymers

Polymer	τ_1 (ns)	τ_2 (ns)
PyDF	0.6701	0.3899
PyDM	1.1007	0.6743

Table S3. The summary of the photocatalytic performances of polymeric photocatalysts for hydrogen evolution from water splitting.

Photocatalysts	cocatalyst	HER ($mmol\ h^{-1} g^{-1}$)	EQE (%)	λ >nm	References
PyDF	3 wt% Pt	18.93	---	300	This work
PyDF	3 wt% Pt	13.47	4.5	420	This work
PyDOBT-1	3 wt% Pt	8.52	6.1	420	1
PDBTSO	3 wt% Pt	44.2	8.4	420	2
P16PySO	3 wt% Pt	11.2	3.5	420	3
TFPT-OCH3	3 wt% Pt	0.442	1.03	420	4

Ta-CMO-CN	3 wt% Pt	0.698	0.15	420	5
DBTD-CMP1	3 wt% Pt	4.6	3.3	420	6
4-CzPN	3 wt% Pt	2.1	6.4	420	7
PyBT-2	3 wt% Pt	0.296	0.22	420	8
ter-CTF-0.7	3 wt% Pt	19.3	22.8	420	9
CTF-15	3 wt% Pt	2.946	15.9	420	10
CTF-BT/Th-1	3 wt% Pt	6.6	7.3	420	11
TFPT-COF/Pt	2.2 wt% Pt	1.97	3.9	420	12
Flu-SO	3 wt% Pt	6.06	2.13	420	13
F0.5CMP	--	0.66	5.8	420	14
PCP10	--	8.63	1.05	300	15
P-FSO	--	8	8.5	420	16
P1	3 wt% Pt	1	3.58	420	17
COP-TP3:1	3 wt% Pt	4.2	1.5	400	18
P64	--	6.04	20.7	300	19

Table S4. Cartesian coordinates of the DFT-optimized structure of PyDF depicted in Figure 5.

	X	Y	Z
C	-2.69960000	1.38180000	-0.87440000
C	-1.35060000	1.36130000	-0.77000000
C	-0.65900000	0.20220000	-0.68490000
C	-1.35300000	-0.95780000	-0.62740000
C	-2.70630000	-0.97780000	-0.57240000
C	-3.33300000	0.20380000	-0.72240000
C	-0.64670000	2.50170000	-0.67130000
C	0.68480000	2.50150000	-0.56460000
C	1.39110000	1.35950000	-0.51580000
C	0.70110000	0.20490000	-0.65650000
C	1.40010000	-0.94730000	-0.76690000
C	0.69540000	-2.09080000	-0.74060000
C	-0.63940000	-2.09540000	-0.68780000
C	2.73950000	1.37610000	-0.39880000
C	3.37860000	0.20870000	-0.60200000
C	2.75210000	-0.96090000	-0.82950000
C	-5.54060000	-5.45200000	0.59970000
C	-4.82950000	-6.08240000	1.54730000
C	-5.25830000	-7.24640000	2.05830000
C	-6.40770000	-7.77820000	1.61340000
C	-7.12620000	-7.15230000	0.66690000
C	-6.69150000	-5.98630000	0.16000000
C	-4.95550000	-4.31000000	0.21130000
C	-3.80240000	-4.08320000	0.85180000
S	-3.30890000	-5.29010000	2.09280000
C	-5.37130000	-3.41880000	-0.69850000
C	-4.64380000	-2.31970000	-0.96540000

C	-3.46280000	-2.08370000	-0.34780000
C	-3.07890000	-2.98770000	0.57960000
O	-3.45860000	-4.72860000	3.42830000
O	-2.13580000	-6.02190000	1.63480000
C	5.07170000	-4.23330000	-1.64530000
C	5.42870000	-3.35700000	-0.69820000
C	4.66800000	-2.28210000	-0.44270000
C	3.51230000	-2.05240000	-1.10340000
C	3.18500000	-2.93430000	-2.07590000
C	3.95000000	-4.00720000	-2.34220000
C	5.94600000	-5.24250000	-1.76700000
C	6.96340000	-5.13140000	-0.89910000
S	6.94780000	-3.70790000	0.20150000
C	5.90130000	-6.28250000	-2.61540000
C	6.87480000	-7.20850000	-2.59330000
C	7.88960000	-7.08990000	-1.72150000
C	7.93860000	-6.05220000	-0.87160000
O	7.98580000	-2.75480000	-0.16600000
O	6.64520000	-4.10840000	1.56870000
C	-5.00770000	4.67860000	-1.62450000
C	-5.38950000	3.76320000	-0.72540000
C	-4.63010000	2.68330000	-0.48850000
C	-3.45320000	2.48450000	-1.12110000
C	-3.09910000	3.40770000	-2.04470000
C	-3.86160000	4.48710000	-2.29170000
C	-5.88580000	5.68550000	-1.73610000
C	-6.93160000	5.53230000	-0.90920000
S	-6.93960000	4.06840000	0.13720000
C	-5.82110000	6.75860000	-2.54090000
C	-6.80310000	7.67540000	-2.51660000

C	-7.84660000	7.51450000	-1.68640000
C	-7.91550000	6.44380000	-0.87990000
O	-7.95990000	3.12410000	-0.29690000
O	-6.68550000	4.42260000	1.52690000
C	5.88640000	5.65830000	0.68110000
C	6.93620000	5.55390000	-0.14830000
C	7.91080000	6.47560000	-0.13250000
C	7.82860000	7.50740000	0.72190000
C	6.78100000	7.61960000	1.55500000
C	5.80820000	6.69280000	1.53380000
C	5.01890000	4.64890000	0.52010000
C	5.41310000	3.77860000	-0.41770000
S	6.96220000	4.13950000	-1.26050000
C	3.87180000	4.41730000	1.17270000
C	3.11950000	3.34460000	0.87180000
C	3.48580000	2.46830000	-0.09170000
C	4.66490000	2.70360000	-0.70730000
O	6.70570000	4.55180000	-2.63360000
O	7.98970000	3.18600000	-0.86560000
F	-2.01860000	3.25600000	-2.79960000
F	-6.74240000	8.73470000	-3.30850000
F	-8.25940000	-7.68320000	0.23450000
F	-5.11090000	-1.51950000	-1.91410000
F	2.12950000	-2.74500000	-2.85720000
F	6.83370000	-8.23510000	-3.42830000
F	2.03530000	3.14940000	1.61120000
F	6.70700000	8.64090000	2.39430000
H	-4.43240000	0.20900000	-0.71640000
H	-1.12370000	3.49430000	-0.64010000
H	1.15970000	3.49550000	-0.54730000

H	1.17420000	-3.08310000	-0.73200000
H	-1.10390000	-3.09310000	-0.72980000
H	4.47930000	0.21060000	-0.57970000
H	-4.67720000	-7.76550000	2.83810000
H	-6.76550000	-8.73470000	2.02930000
H	-7.29610000	-5.49100000	-0.61560000
H	-6.31010000	-3.57560000	-1.25290000
H	-2.18060000	-2.82310000	1.19870000
H	5.00230000	-1.62540000	0.37740000
H	3.64210000	-4.68460000	-3.15430000
H	5.07870000	-6.40050000	-3.33770000
H	8.68800000	-7.85040000	-1.70380000
H	8.77540000	-5.96290000	-0.15960000
H	-4.98760000	1.99290000	0.29340000
H	-3.53220000	5.19820000	-3.06560000
H	-4.97500000	6.91130000	-3.22870000
H	-8.65190000	8.26750000	-1.66680000
H	-8.77540000	6.32030000	-0.20130000
H	8.77390000	6.39210000	-0.81330000
H	8.62620000	8.26860000	0.73970000
H	4.95850000	6.80550000	2.22480000
H	3.53210000	5.08960000	1.97620000
H	5.03080000	2.05160000	-1.51780000

Table S5. Cartesian coordinates of the DFT-optimized structure of PyDM depicted in Figure 5.

	X	Y	Z
C	1.79250000	-2.88590000	-0.11830000
C	1.24400000	-1.65290000	-0.05430000
C	1.99430000	-0.55690000	0.19730000
C	3.31980000	-0.71470000	0.41670000
C	3.90330000	-1.93560000	0.40020000
C	3.10660000	-2.99000000	0.15100000
C	-0.08460000	-1.48690000	-0.16280000
C	-0.64730000	-0.27680000	-0.09900000
C	0.08160000	0.82400000	0.14910000
C	1.42080000	0.67350000	0.25070000
C	2.17550000	1.78100000	0.42050000
C	3.46120000	1.59610000	0.76200000
C	4.01250000	0.37940000	0.77880000
C	-0.50350000	2.03940000	0.24520000
C	0.30640000	3.11260000	0.30690000
C	1.64780000	3.02460000	0.36980000
C	9.26980000	-2.62090000	0.31160000
C	9.73040000	-1.64150000	-0.48110000
C	11.04440000	-1.52390000	-0.72020000
C	11.89710000	-2.39530000	-0.15920000
C	11.45210000	-3.38550000	0.63560000
C	10.13010000	-3.48990000	0.86580000
C	7.93550000	-2.57940000	0.43630000
C	7.39370000	-1.56620000	-0.24790000
S	8.51390000	-0.52910000	-1.20120000
C	7.12710000	-3.38800000	1.13480000
C	5.79140000	-3.20350000	1.16070000

C	5.23800000	-2.16840000	0.47990000
C	6.06850000	-1.37340000	-0.22880000
O	8.58150000	0.79960000	-0.60820000
O	8.33930000	-0.78100000	-2.62500000
C	3.78390000	6.49650000	0.59920000
C	2.66390000	6.31860000	1.30850000
C	1.96930000	5.17780000	1.19880000
C	2.37610000	4.16900000	0.39800000
C	3.49150000	4.37040000	-0.34830000
C	4.17910000	5.52430000	-0.23340000
C	4.35110000	7.68950000	0.82880000
C	3.66040000	8.40790000	1.72650000
S	2.17740000	7.65450000	2.41180000
C	5.46840000	8.19810000	0.28540000
C	5.90180000	9.42420000	0.63280000
C	5.19620000	10.13160000	1.53400000
C	4.07870000	9.63080000	2.08310000
O	0.97880000	8.31720000	1.91660000
O	2.38260000	7.26530000	3.80020000
C	-0.09390000	-6.37750000	-1.06000000
C	0.72960000	-6.28430000	-0.01010000
C	1.34660000	-5.12690000	0.26260000
C	1.14930000	-4.02120000	-0.48770000
C	0.34660000	-4.13110000	-1.57530000
C	-0.26690000	-5.30210000	-1.84040000
C	-0.62150000	-7.60370000	-1.18600000
C	-0.19820000	-8.43350000	-0.22070000
S	0.94440000	-7.76140000	0.99540000
C	-1.47470000	-8.04990000	-2.12160000
C	-1.91050000	-9.32320000	-2.09930000

C	-1.47510000	-10.14200000	-1.12450000
C	-0.62200000	-9.70500000	-0.18520000
O	2.28830000	-8.29390000	0.81720000
O	0.29800000	-7.58650000	2.28880000
C	-5.79540000	3.11840000	-0.00230000
C	-5.91420000	4.07530000	-0.93460000
C	-7.12020000	4.56820000	-1.25110000
C	-8.21010000	4.09530000	-0.62680000
C	-8.10950000	3.13390000	0.30910000
C	-6.89140000	2.65070000	0.61610000
C	-4.51840000	2.75190000	0.17940000
C	-3.67550000	3.43720000	-0.60150000
S	-4.40000000	4.64510000	-1.72170000
C	-4.01780000	1.84320000	1.02730000
C	-2.69540000	1.58900000	1.08770000
C	-1.84200000	2.25380000	0.26970000
C	-2.35820000	3.19800000	-0.54610000
O	-4.31820000	4.17240000	-3.09700000
O	-4.07160000	5.99980000	-1.30010000
C	0.19140000	-3.04590000	-2.62880000
C	-2.87000000	-9.81010000	-3.16010000
C	12.40780000	-4.36920000	1.26970000
C	5.00470000	-4.12590000	2.07770000
C	3.97060000	3.42070000	-1.43540000
C	7.16120000	9.98180000	0.01170000
C	-2.24640000	0.64550000	2.19210000
C	-9.33360000	2.60010000	1.01590000
H	3.58560000	-3.97090000	-0.00650000
H	-0.77460000	-2.33560000	-0.29150000
H	-1.73630000	-0.23930000	-0.26020000

H	4.10470000	2.43080000	1.08570000
H	5.05690000	0.33540000	1.12790000
H	-0.15530000	4.11410000	0.31970000
H	11.42610000	-0.72140000	-1.37260000
H	12.97590000	-2.29170000	-0.36140000
H	9.77500000	-4.30250000	1.51820000
H	7.55740000	-4.21670000	1.71850000
H	5.67910000	-0.57070000	-0.87830000
H	1.08390000	5.07530000	1.84880000
H	5.07200000	5.67020000	-0.86140000
H	6.05280000	7.62640000	-0.45200000
H	5.53330000	11.13780000	1.83310000
H	3.51350000	10.22380000	2.82090000
H	1.98150000	-5.10060000	1.16490000
H	-0.89910000	-5.37310000	-2.73940000
H	-1.83650000	-7.38680000	-2.92250000
H	-1.81890000	-11.18890000	-1.08770000
H	-0.27600000	-10.38970000	0.60660000
H	-7.22150000	5.35450000	-2.01710000
H	-9.19810000	4.50560000	-0.89320000
H	-6.81840000	1.86430000	1.38310000
H	-4.68900000	1.30300000	1.71320000
H	-1.71770000	3.76250000	-1.24510000
H	0.95990000	-2.24560000	-2.56560000
H	0.32610000	-3.47860000	-3.64650000
H	-0.82360000	-2.58950000	-2.60550000
H	-3.08430000	-10.89910000	-3.07830000
H	-3.84000000	-9.26880000	-3.07710000
H	-2.45120000	-9.63060000	-4.17650000
H	13.47450000	-4.11160000	1.08480000

H	12.26170000	-4.39910000	2.37350000
H	12.23170000	-5.39080000	0.86230000
H	4.06510000	-3.66770000	2.45750000
H	4.77500000	-5.09230000	1.57430000
H	5.58470000	-4.36890000	2.99680000
H	3.20340000	2.68450000	-1.75850000
H	4.21440000	3.98770000	-2.36290000
H	4.89820000	2.88370000	-1.13460000
H	7.39780000	11.00930000	0.36760000
H	8.03250000	9.33330000	0.25860000
H	7.05830000	10.02840000	-1.09650000
H	-1.16350000	0.71680000	2.43160000
H	-2.76060000	0.90090000	3.14680000
H	-2.50380000	-0.41220000	1.95940000
H	-10.25120000	3.18610000	0.78550000
H	-9.51980000	1.54480000	0.71180000
H	-9.19340000	2.62980000	2.12050000

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