Supporting Information

Enhanced photocatalytic hydrogen production through modification of B←N coordination units

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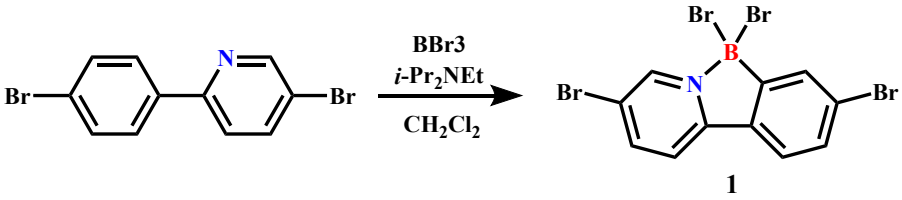
General Methods

All reactions and manipulations were carried out under an argon atmosphere by using standard Schlenk techniques or an inter-atmosphere glovebox. Prior to use CH_2Cl_2, Et_2O, THF and toluene were dried by refluxing and degassed by applying three freeze-pump-thaw cycles. $CDCl_3$ was dried by 4 Å molecular sieve (2-3 days). All chemicals (reagents and solvents) were obtained from commercial suppliers (Energy Chemical, Heowns) and directly used without further purification.

Synthetic Methods



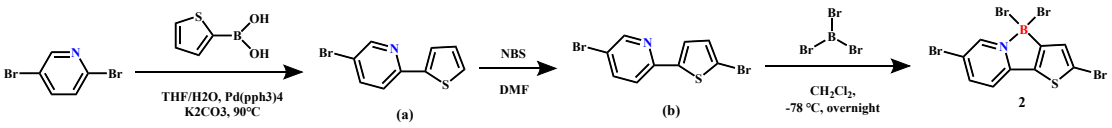
1

Compound 1: To a stirred solution of 5-bromo-2-(4-bromophenyl)pyridine (3.00 g, 9.58 mmol) and *i*-Pr_2NEt (1.6 mL, 9.20 mmol) in CH_2Cl_2 (50 mL) at -78 °C, BBr_3 (1.0 M in CH_2Cl_2, 20 mL, 20.00 mmol) was added dropwise. After being stirred at room temperature for 12 h, saturated K_2CO_3 aqueous solution was added to the reaction mixture. The formed precipitate was collected via filtration and washed with water and acetone to afford **Compound 1** as a pale-yellow solid (4.20 g, 8.70 mmol, 91%). ^{1}H NMR (400MHz, $CDCl_3$, ppm): δ 9.01 (d, J = 1.5 Hz, 1H), 8.27 (dd, J = 8.4, 2.1 Hz, 1H), 7.99 (s,1H), 7.80 (dd, J = 8.4, 0.6 Hz, 1H), 7.57-7.59 (m, 2H).

Monomer 1: To a stirred solution of **Compound 1** (2.41 g, 5.00 mmol) in toluene (50 mL) at room temperature was added $AlMe_3$ (1.1 M in hexane, 10 mL, 11.00 mmol). After being stirred at this temperature for 2 h, the reaction was quenched by adding water. The organic layer was separated and extracted with ethyl acetate (twice), washed with water (once), brine (once), and dried over $MgSO_4$ and concentrated. The residue was purified by preparative thin layer chromatography on silica gel to afford **Monomer 1** (1.44 g, 4.08 mmol, 82 % yield). ^{1}H NMR (400 MHz, CDCl3, ppm): δ 8.49 (s, 1H), 8.07 (d, J = 8.0 Hz, 1H), 7.79 (d, J = 8.0 Hz, 1H), 7.73

(s, 1H), 7.65 (d, J = 8.0 Hz, 1H), 7.41 (d, J = 8.0 Hz, 1H), 0.03 (s, 6H). $^{13}C\{^{1}H\}$ NMR (100 MHz, CDCl3, ppm): δ 155.03, 143.91, 142.49, 132.75, 132.42, 128.69, 128.59, 126.81, 123.16, 118.81, 117.03, 8.90.

Monomer 2: Diphenylzinc: Under argon atmosphere, 10 mL of dry tetrahydrofuran was added to a 100 mL flask containing ZnBr2 (7.46 g, 33.12 mmol), LiCl (1.40 g, 33.12 mmol). Phenylmagnesium bromide 66.24 mL (66.24 mmol, 1.0 M) was added dropwise and the reaction lasted for 3 h. A yellow solution was obtained, and the crude product was directly purified in the next step. Under argon atmosphere, added 40 mL of deoxidized dry dichloromethane to a 100 mL flask containing compound 1 (2.00 g, 4.14 mmol). System temperature was cooled down to 0 °C, the above diphenyl zinc solution was added, and the reaction lasted for 12 h. After the reaction was completed, the reaction was quenched by adding 100 mL of water and extracted with ethyl acetate (3 × 100 mL), with the organic phases combined. The product was dried over anhydrous magnesium sulfate and evaporated to obtain the crude product. The crude product was separated by silica gel chromatography (V_{PE}: V_{DCM} = 4:1) and dried in a vacuum oven at 60 °C to obtain 1.01 g of white solid product (51% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.55 (d, J = 1.5 Hz, 1H), 8.16 (dd, J = 8.6, 2.0 Hz, 1H), 7.90 (dd, J = 8.6, 0.4 Hz, 1H), 7.81 (d, J = 1.7 Hz, 1H), 7.70 (d, J = 8.2 Hz, 1H), 7.47 (dd, J = 8.2, 1.9 Hz, 1H), 7.25-7.16 (m, 10H), ^{13}C NMR (101 MHz, $CDCl_3$): δ 156.31, 145.36, 143.67, 133.86, 133.72, 133.03, 129.54, 127.69, 127.53, 126.23, 123.20, 118.99, 117.44.



Compound (a): Under argon atmosphere, added a deoxygenated solvent mixture (100 mL of tetrahydrofuran, 50 mL of distilled water) to a 250 mL flask containing 5-dibromopyridine (5.00 g, 21.11 mmol), 2-thiopheneboronic acid (2.70 g, 21.11 mmol), potassium carbonate (8.75 g, 63.33 mmol), and tetrakis(triphenylphosphine-palladium)

(0.62 g, 0.53 mmol). Heated to 90 °C and maintained for 24 h. After the reaction was completed, 100 mL of water was added to quench the reaction and extracted with ethyl acetate (3 × 100 mL), with the organic phases combined. Dried over anhydrous magnesium sulfate and evaporated to obtain the crude product. The crude product was separated by silica gel chromatography (V_{PE}: V_{DCM} = 1:1) and dried in a vacuum oven at 60 °C to obtain 3.29 g of white solid product (65% yield).

Compound (b): Under argon atmosphere, added 20 mL of dimethylformamide to a 100 mL flask containing compound (a) (3.00 g, 12.49 mmol). Reduce the system temperature to 0 °C, add N-bromosuccinimide (3.56 g, 20.01 mmol), and the reaction lasted for 12 h. After the reaction was completed, 100 mL of water was added to quench the reaction and extracted with ethyl acetate (3 × 100 mL), with the organic phases combined. Dried over anhydrous magnesium sulfate and evaporated to obtain the crude product. The crude product was separated by silica gel chromatography (V_{PE}: V_{DCM} = 1:1) and dried in a vacuum oven at 60 °C to obtain 3.59 g of white solid product (90% yield). 1H NMR (400 MHz, CDCl3): δ 8.56 (s, 1H), 7.76 (dd, J = 8.4, 2.4 Hz, 1H), 7.45 (d, J = 8.8 Hz, 1H), 7.28 (d, J = 3.6 Hz, 1H), 7.04 (d, J = 3.6 Hz, 1H).

Compound 2: Under argon atmosphere, added Compound (b) (2.01 g, 6.30 mmol), 1 mL diisopropylethylamine, and 40 mL of deoxygenated dry dichloromethane solvent to a 100 mL flask. After the reaction system was cooled down to 78 °C, 8 mL of boron tribromide (1.0 mol/L) was added, and the solution changed from white to yellow. After that, restored the system temperature to room

temperature gradually and reacted overnight. The next day, 50 mL of water was added to quench, the resulting precipitate was washed with 300 mL of acetone, and then dried in a vacuum oven at 60 °C to obtain a solid product of 2.71 g (88% yield).

Monomer 3: Under argon atmosphere, added 40 mL of deoxidized dry dichloromethane to a 100 mL flask containing compound 2 (2.00 g, 4.09 mmol). Reduce the temperature of the system to 0 °C, add the above diphenyl zinc solution, and the reaction lasted for 12 h. After the reaction was completed, 100 mL of water was added to quench the reaction and extracted with ethyl acetate (3 × 100 mL), with the organic phases combined. Dried over anhydrous magnesium sulfate and evaporated to obtain the crude product. The crude product was separated by silica gel chromatography (V_{PE}: V_{DCM} = 1:1) and dried in a vacuum oven at 60 °C to obtain 1.05 g of white solid product (53% yield).

Electrochemical impedance test method

Electrochemical impedance spectra were recorded using a CHI-760E electrochemical workstation in a standard three electrode configuration. The polymer (4.0 mg) was dispersed in ethanol (0.5 mL) containing 1 % nafion by ultrasound for 1 hour. The work electrodes were prepared via drop-casting the mixture 20 μL onto the surface of FTO glass substrate electrode with 1 cm^2 illuminated area and then being filmed at 80 ºC in vacuum oven. The Pt plate served as the counter electrode, and a saturated Ag/AgCl electrode as a reference electrode. A 0.5 M Na_2SO_4 solution was used as the electrolyte. A 300 W Xenon lamp equipped with a 420 nm cut-off filter (100 mW cm^{-1}) was used as the light source in the photocurrent response

measurement. The electrochemical impedance spectroscopy (EIS) measurements were performed over a frequency range from 0.01 to 100000 Hz with a 50 mV amplitude.

Characterization of polymers

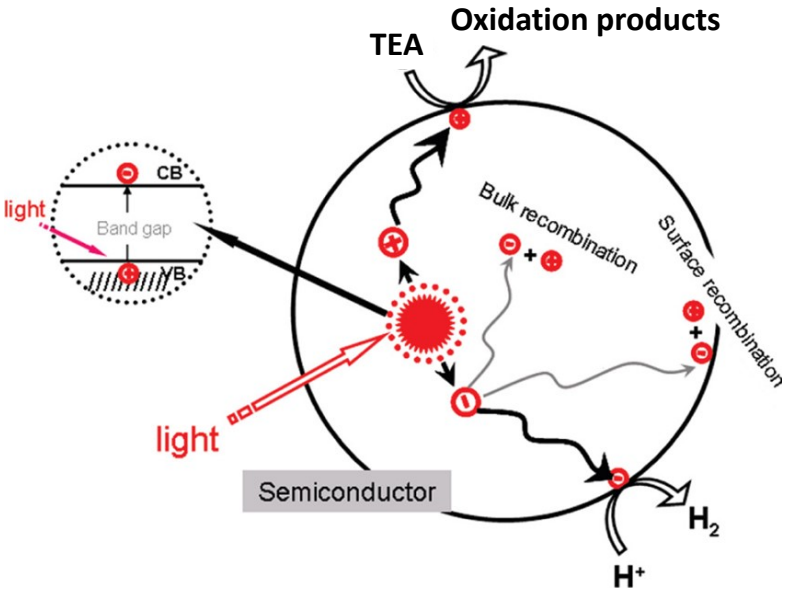


Figure S1. Processes in photocatalytic water splitting.

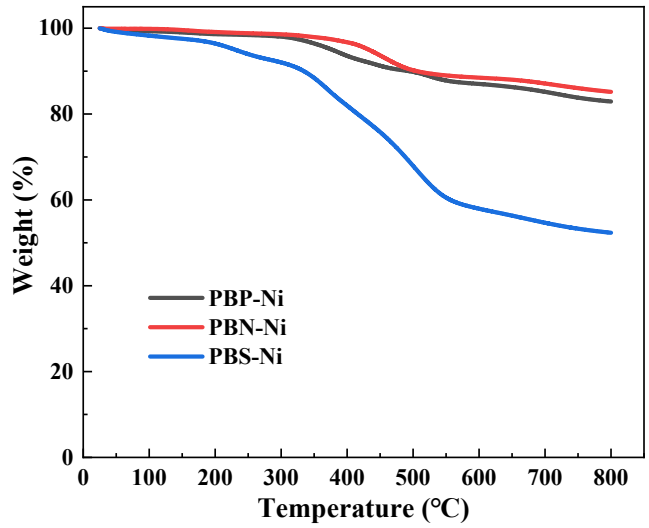


Figure S2. TGA analysis under nitrogen atmosphere.

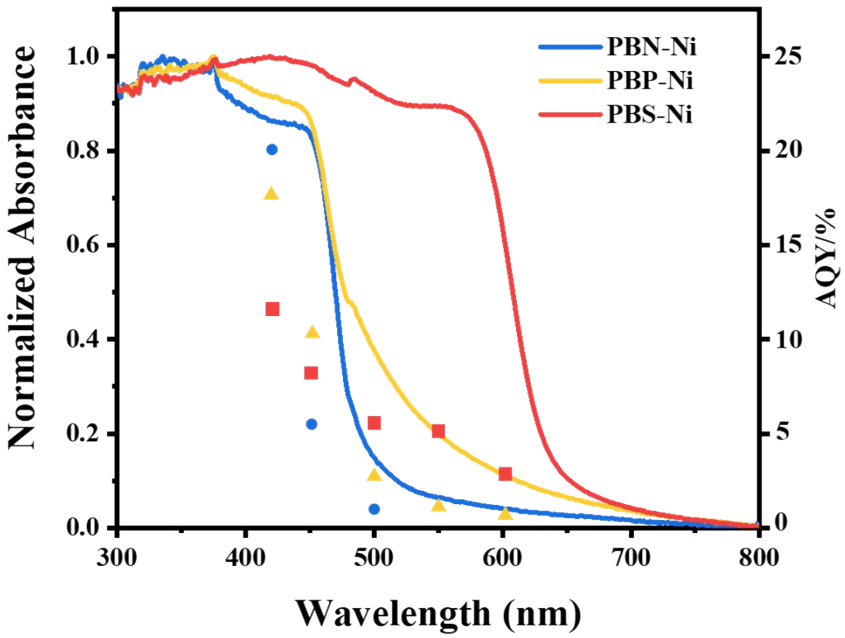


Figure S3. Wavelength-dependent AQYs of polymers superimposed on their absorption curves.

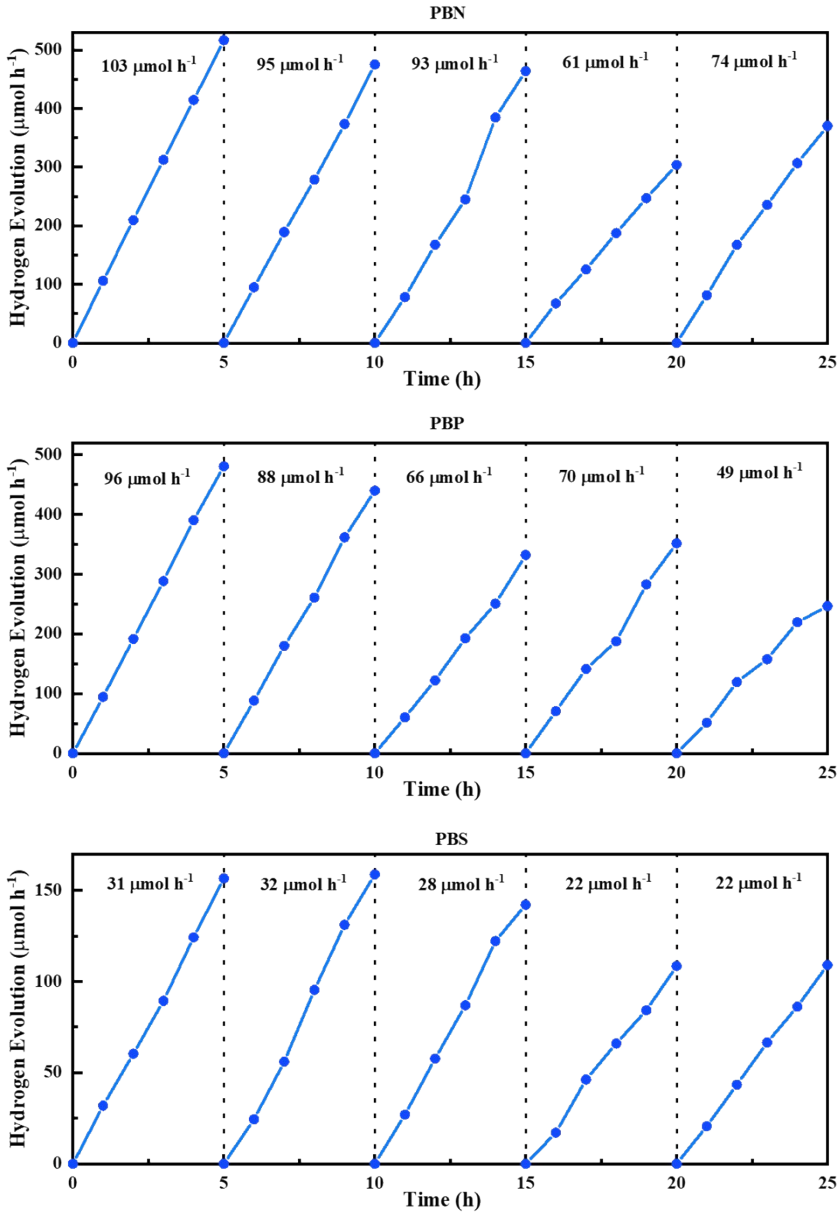


Figure S4. Photostability and reusability using polymers as a photocatalysts under visible-light illumination ($\lambda > 420$ nm).

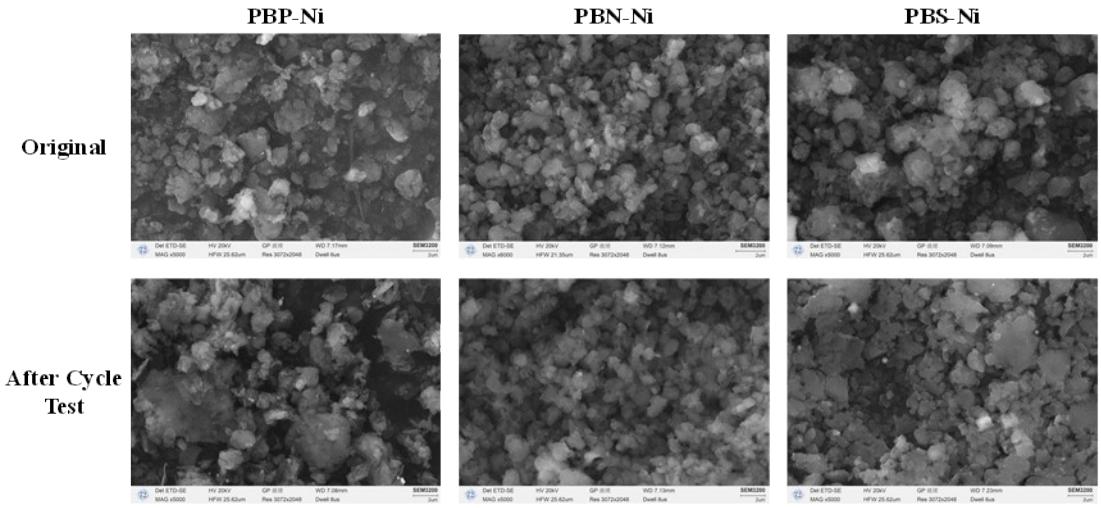
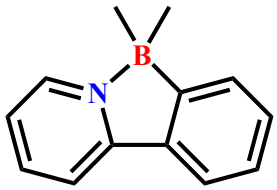


Figure S5. SEM images of polymers before and after cycle test.

Cartesian coordinates for the optimized geometries



MBN1-DFT

Coordinates from Gaussian 09-B3LYP/6-311G (d, p)

C	0.79095	-0.81191	0.00003
C	-0.66559	-0.87106	0.00003
N	-1.1929	0.3825	-0.00037
B	-0.0255	1.54732	0.00011
C	1.22509	0.53048	0.00014
C	2.603	0.76113	0.0002
C	3.50008	-0.30542	0.0001
C	3.04369	-1.62945	-0.00012
C	1.68051	-1.89261	-0.00024
C	-1.5135	-1.98398	0.00022
C	-2.88546	-1.789	0.0003
C	-3.40288	-0.49017	-0.00025
C	-2.51744	0.57337	-0.00053
C	-0.17658	2.42562	-1.36126
C	-0.17753	2.42522	1.36162
H	2.98423	1.77773	0.00038

H	4.56799	-0.11238	0.00019
H	3.75511	-2.44742	-0.00023
H	1.32465	-2.91795	-0.00046
H	-1.09217	-2.98064	0.00026
H	-3.55527	-2.64125	0.00043
H	-2.84829	1.60424	-0.00084
H	-1.10517	3.01099	-1.38226
H	0.64514	3.14776	-1.42991
H	-0.14582	1.82058	-2.27473
H	-1.10607	3.0107	1.38199
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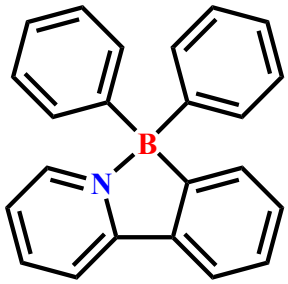

MBP1-DFT

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B	-0.2488	0.01618	-0.12375
C	0.95579	0.13785	-1.19632
C	0.9438	0.37667	-2.57155
C	2.13946	0.46845	-3.28213
C	3.37356	0.32941	-2.63559
C	3.41723	0.09477	-1.26776
C	2.99988	-0.4626	1.84907
C	2.58998	-0.68498	3.15419
C	1.22698	-0.68761	3.4641
C	0.31662	-0.46494	2.44623
H	0.0005	0.49514	-3.09451
H	2.11777	0.65331	-4.35105
H	4.29388	0.40701	-3.203
H	4.37241	-0.01035	-0.76369

H	4.04948	-0.46055	1.58642
H	3.32487	-0.85901	3.93175
H	-0.75275	-0.46076	2.61168
H	0.87693	-0.86204	4.47257
C	-1.20505	-1.29161	-0.27884
C	-2.44966	-1.37581	0.37005
C	-0.80353	-2.41855	-1.01558
C	-3.2456	-2.51855	0.29618
H	-2.81706	-0.5205	0.92885
C	-1.59326	-3.56435	-1.10117
H	0.14545	-2.39873	-1.5416
C	-2.81915	-3.62025	-0.44193
H	-4.20249	-2.54517	0.80776
H	-1.25239	-4.41315	-1.68545
H	-3.43772	-4.50894	-0.50818
C	-1.03357	1.4297	0.05362
C	-2.13909	1.71892	-0.76614
C	-0.61926	2.44769	0.9274
C	-2.79433	2.94756	-0.71528
H	-2.50139	0.96164	-1.45391
C	-1.27231	3.67857	0.99239
H	0.23873	2.29049	1.57422

C	-2.3652	3.93508	0.16935
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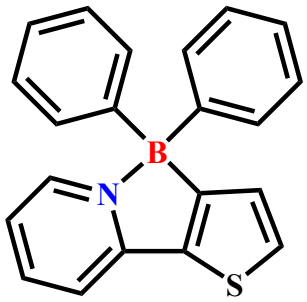

MBS1-DFT

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S	-3.46784	0.1852	-1.63305
C	-2.38284	0.39697	-2.97712
C	-1.97778	-0.18078	0.844
N	-0.65326	-0.19865	1.17944
C	-0.27005	-0.39634	2.44558
C	-1.19247	-0.57603	3.46223
C	-2.5537	-0.555	3.14156
C	-2.95476	-0.35856	1.83008
B	0.32563	0.01476	-0.14485
C	1.13509	1.41668	-0.00516
C	1.24787	-1.31734	-0.26986
C	0.75141	2.45958	0.85252
C	1.43067	3.67757	0.88465

C	2.51887	3.89436	0.04415
C	2.91708	2.88082	-0.82545
C	2.23579	1.66566	-0.84424
C	2.49562	-1.41218	0.37072
C	3.26324	-2.57542	0.3218
C	2.80368	-3.68655	-0.38151
C	1.57347	-3.61993	-1.0318
C	0.81207	-2.45372	-0.97174
H	-0.25809	0.46882	-3.32272
H	-2.79789	0.54732	-3.96289
H	0.79809	-0.40872	2.62019
H	-0.85342	-0.73165	4.47728
H	-3.29647	-0.69518	3.91848
H	-4.00211	-0.34319	1.55767
H	-0.10175	2.33218	1.51182
H	1.10614	4.45841	1.56506
H	3.04979	4.83993	0.06567
H	3.7632	3.035	-1.4874
H	2.57234	0.88768	-1.52205
H	2.887	-0.55071	0.90301
H	4.22362	-2.61122	0.82616
H	3.4001	-4.59147	-0.42774

H	1.20717	-4.47645	-1.5887
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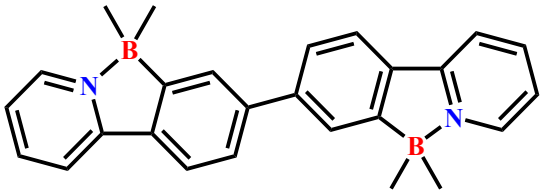

MBN2-DFT

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3(N) --> Charge: 7.000000 x,y,z(Bohr): -5.712662 0.870542 0.120856

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7(C) --> Charge: 6.000000 x,y,z(Bohr): -14.512496 -0.845149 0.144138

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46(H) --> Charge: 1.000000 x,y,z(Bohr):   5.298417   5.028832 -1.964387

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49(H) --> Charge: 1.000000 x,y,z(Bohr): 16.337596   0.860148   0.358458

50(H) --> Charge: 1.000000 x,y,z(Bohr): 13.361891 -2.696358   1.315170

51(H) --> Charge: 1.000000 x,y,z(Bohr):   7.939341 -1.950435   5.162740

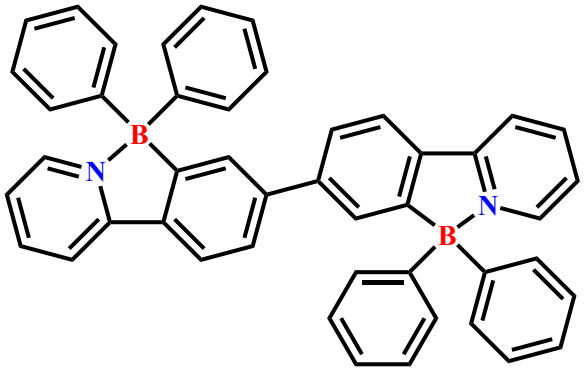
52(H) --> Charge: 1.000000 x,y,z(Bohr):   6.641232 -4.905419   4.355417

53(H) --> Charge: 1.000000 x,y,z(Bohr):   9.936545 -4.524609   4.408122

54(H) --> Charge: 1.000000 x,y,z(Bohr):   8.605179 -4.679096 -2.966352

55(H) --> Charge: 1.000000 x,y,z(Bohr):   7.048398 -6.615078 -0.751396

56(H) --> Charge: 1.000000 x,y,z(Bohr): 10.331797 -6.192462 -0.535364



MBP2-DFT

1(C) --> Charge: 6.000000 x,y,z(Bohr): 8.647089 4.472654 -0.219411

2(C) --> Charge: 6.000000 x,y,z(Bohr): 6.049071 3.628547 -0.571840

3(N) --> Charge: 7.000000 x,y,z(Bohr): 5.889068 1.075258 -0.357328

4(B) --> Charge: 5.000000 x,y,z(Bohr): 8.657808 -0.224310 0.246393

5(C) --> Charge: 6.000000 x,y,z(Bohr): 10.235398 2.393693 0.282726

6(C) --> Charge: 6.000000 x,y,z(Bohr): 12.799902 2.876501 0.663570

7(C) --> Charge: 6.000000 x,y,z(Bohr): 13.723749 5.341535 0.555858

8(C) --> Charge: 6.000000 x,y,z(Bohr): 12.110072 7.377238 0.055282

9(C) --> Charge: 6.000000 x,y,z(Bohr): 9.550466 6.954745 -0.340161

10(C) --> Charge: 6.000000 x,y,z(Bohr): 3.863363 5.029094 -1.056309

11(C) --> Charge: 6.000000 x,y,z(Bohr): 1.577038 3.789361 -1.322541

12(C) --> Charge: 6.000000 x,y,z(Bohr): 1.431468 1.143174 -1.101549

13(C) --> Charge: 6.000000 x,y,z(Bohr): 3.680995 -0.127820 -0.594361

14(C) --> Charge: 6.000000 x,y,z(Bohr): -5.507222 -2.839741 -1.975794

15(C) --> Charge: 6.000000 x,y,z(Bohr): -8.052859 -3.888117 -2.092719

16(N) --> Charge: 7.000000 x,y,z(Bohr): -9.732701 -2.291971 -0.983489

17(B) --> Charge: 5.000000 x,y,z(Bohr): -8.361041 0.273226 0.134046

18(C) --> Charge: 6.000000 x,y,z(Bohr): -5.525305 -0.498829 -0.709248

19(C) --> Charge: 6.000000 x,y,z(Bohr): -3.237717   0.770656 -0.436861

20(C) --> Charge: 6.000000 x,y,z(Bohr): -0.981180 -0.243484 -1.389688

21(C) --> Charge: 6.000000 x,y,z(Bohr): -1.035008 -2.591318 -2.644614

22(C) --> Charge: 6.000000 x,y,z(Bohr): -3.286714 -3.895940 -2.942291

23(C) --> Charge: 6.000000 x,y,z(Bohr): -8.884206 -6.174870 -3.119608

24(C) --> Charge: 6.000000 x,y,z(Bohr): -11.428844 -6.783068 -2.982819

25(C) --> Charge: 6.000000 x,y,z(Bohr): -13.117130 -5.115573 -1.823414

26(C) --> Charge: 6.000000 x,y,z(Bohr): -12.189632 -2.878374 -0.836377

27(H) --> Charge: 1.000000 x,y,z(Bohr): 14.091436   1.329517   1.042625

28(H) --> Charge: 1.000000 x,y,z(Bohr): 15.720800   5.694060   0.858593

29(H) --> Charge: 1.000000 x,y,z(Bohr): 12.860417   9.281549 -0.027015

30(H) --> Charge: 1.000000 x,y,z(Bohr):   8.296328   8.528391 -0.734771

31(H) --> Charge: 1.000000 x,y,z(Bohr):   3.976953   7.062861 -1.236492

32(H) --> Charge: 1.000000 x,y,z(Bohr): -0.118274   4.858605 -1.742112

33(H) --> Charge: 1.000000 x,y,z(Bohr):   3.740379 -2.154313 -0.327737

34(H) --> Charge: 1.000000 x,y,z(Bohr): -3.187347   2.558934   0.565014

35(H) --> Charge: 1.000000 x,y,z(Bohr):   0.689776 -3.358865 -3.438001

36(H) --> Charge: 1.000000 x,y,z(Bohr): -3.297061 -5.690216 -3.933711

37(H) --> Charge: 1.000000 x,y,z(Bohr): -7.542001 -7.442876 -3.997816

38(H) --> Charge: 1.000000 x,y,z(Bohr): -12.104584 -8.550346 -3.767063

39(H) --> Charge: 1.000000 x,y,z(Bohr): -15.110846 -5.542965 -1.680818

40(H) --> Charge: 1.000000 x,y,z(Bohr): -13.383996 -1.508763   0.101400

41(C) --> Charge: 6.000000 x,y,z(Bohr):   9.482549 -2.010912 -2.115483

42(C) --> Charge: 6.000000 x,y,z(Bohr): 11.464492 -3.755425 -1.812157

43(C) --> Charge: 6.000000 x,y,z(Bohr):   8.439854 -1.819311 -4.548142

44(C) --> Charge: 6.000000 x,y,z(Bohr): 12.348246 -5.225239 -3.810034

45(H) --> Charge: 1.000000 x,y,z(Bohr): 12.324738 -3.981625   0.035808

46(C) --> Charge: 6.000000 x,y,z(Bohr):   9.299233 -3.291862 -6.559206

47(H) --> Charge: 1.000000 x,y,z(Bohr):   6.927792 -0.480098 -4.911003

48(C) --> Charge: 6.000000 x,y,z(Bohr): 11.262040 -5.005734 -6.199084

49(H) --> Charge: 1.000000 x,y,z(Bohr): 13.882611 -6.550290 -3.498939

50(H) --> Charge: 1.000000 x,y,z(Bohr):   8.440113 -3.089645 -8.410923

51(H) --> Charge: 1.000000 x,y,z(Bohr): 11.938869 -6.152547 -7.757370

52(C) --> Charge: 6.000000 x,y,z(Bohr):   8.408540 -1.672317   2.948222

53(C) --> Charge: 6.000000 x,y,z(Bohr):   8.869803 -0.429122   5.248568

54(C) --> Charge: 6.000000 x,y,z(Bohr):   7.602822 -4.199430   3.105908

55(C) --> Charge: 6.000000 x,y,z(Bohr):   8.543990 -1.627737   7.571981

56(H) --> Charge: 1.000000 x,y,z(Bohr):   9.510969   1.518712   5.227565

57(C) --> Charge: 6.000000 x,y,z(Bohr):   7.259849 -5.414571   5.419121

58(H) --> Charge: 1.000000 x,y,z(Bohr):   7.271518 -5.258265   1.379874

59(C) --> Charge: 6.000000 x,y,z(Bohr):   7.730133 -4.129128   7.667511

60(H) --> Charge: 1.000000 x,y,z(Bohr):   8.929025 -0.608197   9.309565

61(H) --> Charge: 1.000000 x,y,z(Bohr):   6.639459 -7.369107   5.464912

62(H) --> Charge: 1.000000 x,y,z(Bohr):   7.476965 -5.069065   9.471664

63(C) --> Charge: 6.000000 x,y,z(Bohr): -8.892921   0.335172   3.159935

64(C) --> Charge: 6.000000 x,y,z(Bohr): -11.034095   1.540417   4.170943

65(C) --> Charge: 6.000000 x,y,z(Bohr): -7.307385 -0.914636   4.884605

66(C) --> Charge: 6.000000 x,y,z(Bohr): -11.572593   1.495031   6.750260

67(H) --> Charge: 1.000000 x,y,z(Bohr): -12.290430   2.572621   2.920109

68(C) --> Charge: 6.000000 x,y,z(Bohr): -7.821628 -0.964486   7.467851

69(H) --> Charge: 1.000000 x,y,z(Bohr): -5.622218 -1.862313   4.200483

70(C) --> Charge: 6.000000 x,y,z(Bohr): -9.963459   0.239480   8.412520

71(H) --> Charge: 1.000000 x,y,z(Bohr): -13.239853   2.453376   7.463132

72(H) --> Charge: 1.000000 x,y,z(Bohr): -6.545605 -1.938186   8.744189

73(H) --> Charge: 1.000000 x,y,z(Bohr): -10.367201   0.210104 10.421941

74(C) --> Charge: 6.000000 x,y,z(Bohr): -9.343958   2.733516 -1.424028

75(C) --> Charge: 6.000000 x,y,z(Bohr): -10.472063   2.608627 -3.822061

76(C) --> Charge: 6.000000 x,y,z(Bohr): -8.900161   5.165801 -0.447730

77(C) --> Charge: 6.000000 x,y,z(Bohr): -11.139150   4.774821 -5.168113

78(H) --> Charge: 1.000000 x,y,z(Bohr): -10.837530   0.784296 -4.688060

79(C) --> Charge: 6.000000 x,y,z(Bohr): -9.545791   7.342288 -1.781641

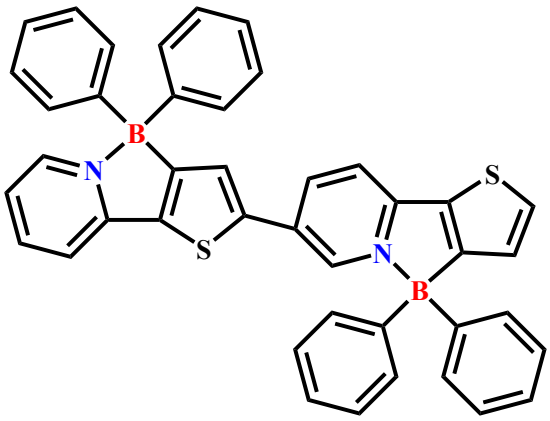
80(H) --> Charge: 1.000000 x,y,z(Bohr): -8.049978   5.361217   1.408475

81(C) --> Charge: 6.000000 x,y,z(Bohr): -10.676760   7.157068 -4.152772

82(H) --> Charge: 1.000000 x,y,z(Bohr): -12.015181   4.598716 -7.014188

83(H) --> Charge: 1.000000 x,y,z(Bohr): -9.178266   9.186326 -0.962456

84(H) --> Charge: 1.000000 x,y,z(Bohr): -11.192459   8.846563 -5.192190



PBS2-DFT

1(C) --> Charge: 6.000000 x,y,z(Bohr): -3.339810 1.729526 0.397831

2(C) --> Charge: 6.000000 x,y,z(Bohr): -5.481976 0.237277 -0.187196

3(C) --> Charge: 6.000000 x,y,z(Bohr): -4.794495 -1.888191 -1.532996

4(S) --> Charge: 16.000000 x,y,z(Bohr): -1.570566 -2.105793 -2.120664

5(C) --> Charge: 6.000000 x,y,z(Bohr): -1.087812 0.745895 -0.479199

6(C) --> Charge: 6.000000 x,y,z(Bohr): -6.893253 -3.475119 -2.198618

7(N) --> Charge: 7.000000 x,y,z(Bohr): -9.067942 -2.388880 -1.325622

8(C) --> Charge: 6.000000 x,y,z(Bohr): -11.302744 -3.519040 -1.665105

9(C) --> Charge: 6.000000 x,y,z(Bohr): -11.504165 -5.801071 -2.929926

10(C) --> Charge: 6.000000 x,y,z(Bohr): -9.302856 -6.936119 -3.852004

11(C) --> Charge: 6.000000 x,y,z(Bohr): -6.981136 -5.780647 -3.489443

12(B) --> Charge: 5.000000 x,y,z(Bohr): -8.518117 0.311917 0.173283

13(C) --> Charge: 6.000000 x,y,z(Bohr): -9.531502 -0.034729 3.049145

14(C) --> Charge: 6.000000 x,y,z(Bohr): -9.753505 2.640591 -1.401386

15(C) --> Charge: 6.000000 x,y,z(Bohr): -8.009867 -1.109909 4.940606

16(C) --> Charge: 6.000000 x,y,z(Bohr): -8.905779 -1.518954 7.383533

17(C) --> Charge: 6.000000 x,y,z(Bohr): -11.377770 -0.865236   8.010825

18(C) --> Charge: 6.000000 x,y,z(Bohr): -12.931345   0.206838   6.176296

19(C) --> Charge: 6.000000 x,y,z(Bohr): -12.012258   0.615971   3.740471

20(C) --> Charge: 6.000000 x,y,z(Bohr): -9.984780   5.019280 -0.238683

21(C) --> Charge: 6.000000 x,y,z(Bohr): -10.887459   7.123342 -1.538395

22(C) --> Charge: 6.000000 x,y,z(Bohr): -11.600949   6.914141 -4.064830

23(C) --> Charge: 6.000000 x,y,z(Bohr): -11.387860   4.584208 -5.266810

24(C) --> Charge: 6.000000 x,y,z(Bohr): -10.469905   2.492367 -3.950873

25(C) --> Charge: 6.000000 x,y,z(Bohr): 13.019075   2.694177   0.788470

26(C) --> Charge: 6.000000 x,y,z(Bohr): 10.410136   2.096977   0.552201

27(C) --> Charge: 6.000000 x,y,z(Bohr):   8.958165   4.265254   0.560170

28(S) --> Charge: 16.000000 x,y,z(Bohr): 10.712712   7.033071   0.856240

29(C) --> Charge: 6.000000 x,y,z(Bohr): 13.465508   5.238041   0.972722

30(C) --> Charge: 6.000000 x,y,z(Bohr):   6.302518   3.788348   0.308736

31(N) --> Charge: 7.000000 x,y,z(Bohr):   5.920541   1.245655   0.082870

32(C) --> Charge: 6.000000 x,y,z(Bohr):   3.600046   0.290573 -0.143941

33(C) --> Charge: 6.000000 x,y,z(Bohr):   1.445873   1.813111 -0.213031

34(C) --> Charge: 6.000000 x,y,z(Bohr):   1.827891   4.443372   0.000877

35(C) --> Charge: 6.000000 x,y,z(Bohr):   4.228031   5.429615   0.274781

36(B) --> Charge: 5.000000 x,y,z(Bohr):   8.623578 -0.358377   0.200195

37(C) --> Charge: 6.000000 x,y,z(Bohr):   9.121921 -1.734706 -2.498231

38(C) --> Charge: 6.000000 x,y,z(Bohr):   8.449203 -2.233651   2.624304

39(C) --> Charge: 6.000000 x,y,z(Bohr): 10.996248 -3.610956 -2.670867

40(C) --> Charge: 6.000000 x,y,z(Bohr): 11.612828 -4.758181 -4.958609

41(C) --> Charge: 6.000000 x,y,z(Bohr): 10.357616 -4.066402 -7.168196

42(C) --> Charge: 6.000000 x,y,z(Bohr):   8.496582 -2.210963 -7.056331

43(C) --> Charge: 6.000000 x,y,z(Bohr):   7.903721 -1.064753 -4.757297

44(C) --> Charge: 6.000000 x,y,z(Bohr):   7.464101 -4.691742   2.413346

45(C) --> Charge: 6.000000 x,y,z(Bohr):   7.200513 -6.270602   4.506693

46(C) --> Charge: 6.000000 x,y,z(Bohr):   7.933952 -5.433668   6.892213

47(C) --> Charge: 6.000000 x,y,z(Bohr):   8.928538 -3.010705   7.157343

48(C) --> Charge: 6.000000 x,y,z(Bohr):   9.172839 -1.444322   5.053588

49(H) --> Charge: 1.000000 x,y,z(Bohr): -3.420094   3.462148   1.482553

50(H) --> Charge: 1.000000 x,y,z(Bohr): -12.925063 -2.544482 -0.889054

51(H) --> Charge: 1.000000 x,y,z(Bohr): -13.337252 -6.669293 -3.179504

52(H) --> Charge: 1.000000 x,y,z(Bohr): -9.409257 -8.724326 -4.844973

53(H) --> Charge: 1.000000 x,y,z(Bohr): -5.251048 -6.629645 -4.174304

54(H) --> Charge: 1.000000 x,y,z(Bohr): -6.076374 -1.634009   4.499590

55(H) --> Charge: 1.000000 x,y,z(Bohr): -7.672535 -2.344167   8.799040

56(H) --> Charge: 1.000000 x,y,z(Bohr): -12.081220 -1.176865   9.910753

57(H) --> Charge: 1.000000 x,y,z(Bohr): -14.855825   0.738912   6.644812

58(H) --> Charge: 1.000000 x,y,z(Bohr): -13.242228   1.499014   2.356633

59(H) --> Charge: 1.000000 x,y,z(Bohr): -9.465210   5.225390   1.734895

60(H) --> Charge: 1.000000 x,y,z(Bohr): -11.043900   8.926782 -0.574367

61(H) --> Charge: 1.000000 x,y,z(Bohr): -12.313968   8.545046 -5.080891

62(H) --> Charge: 1.000000 x,y,z(Bohr): -11.931361   4.391618 -7.234988

63(H) --> Charge: 1.000000 x,y,z(Bohr): -10.307006   0.712989 -4.959384

64(H) --> Charge: 1.000000 x,y,z(Bohr): 14.525294   1.311021   0.818464

65(H) --> Charge: 1.000000 x,y,z(Bohr): 15.257337   6.195770   1.168366

66(H) --> Charge: 1.000000 x,y,z(Bohr):   3.486242 -1.750120 -0.242297

67(H) --> Charge: 1.000000 x,y,z(Bohr):   0.216531   5.702963 -0.084402

68(H) --> Charge: 1.000000 x,y,z(Bohr):   4.524462   7.446872   0.436742

69(H) --> Charge: 1.000000 x,y,z(Bohr): 11.983550 -4.199050 -0.972036

70(H) --> Charge: 1.000000 x,y,z(Bohr): 13.069774 -6.200545 -5.015144

71(H) --> Charge: 1.000000 x,y,z(Bohr): 10.825940 -4.960961 -8.951920

72(H) --> Charge: 1.000000 x,y,z(Bohr):   7.506542 -1.645864 -8.761326

73(H) --> Charge: 1.000000 x,y,z(Bohr):   6.461329   0.394138 -4.751059

74(H) --> Charge: 1.000000 x,y,z(Bohr):   6.928716 -5.405001   0.565756

75(H) --> Charge: 1.000000 x,y,z(Bohr):   6.436922 -8.159684   4.272455

76(H) --> Charge: 1.000000 x,y,z(Bohr):   7.743265 -6.659818   8.523872

77(H) --> Charge: 1.000000 x,y,z(Bohr):   9.518008 -2.340893   9.003969

78(H) --> Charge: 1.000000 x,y,z(Bohr):   9.954144   0.435059   5.307290