Supporting Information

Green, Sustainable synthesis of TPD-based donor-acceptor-type conjugated polymer photocatalysts for hydrogen production under visible light

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Experimental section

Materials

5-(2-octyl-1-dodecyl)-4H-thieno[3,4-c]pyrrole-4,6(5H)-dione, 3,3'-dioctyl-2,2'-bithiophene, 4,4-dioctyl-cyclopenta[2,1-b:3,4-b]dithiophene, 8-bis(octyloxy)benzo[1,2-b:4,5-b]dithiophene, silver carbonate (Ag_2CO_3), and potassium acetate (KOAc) were purchased from Beijing J&K Scientific Co., LTD. Ascorbic acid (AA) and chloroplatinic acid (H_2PtCl_6) were obtained from Tianjin Heowns Biochem Technologies LLC. Trans-bis(acetato)bis[2-[bis(2-methylphenyl)phosphino]benzyl]-dipalladium(II) (Herrmann's catalyst), dichloro[1,1'-bis(diphenylphosphino)ferrocene] palladium(II) ($Pd(dppf)Cl_2$), bis(tertbutyldicylcohexylphosphine)dichloropalladium(II) [$Pd(tbdchp)_2Cl_2$], tetrakis(triphenylphosphine)palladium(0) ($Pd(PPh_3)_4$), di-t-butylmethylphosphonium tetrafluoroborate [$P(t\text{-}Bu)_2MeHBF_4$], tricyclohexyl phosphine[PCy_3], tricyclohexylphosphonium tetrafluoroborate[PCy_3HBF_4], and tris(2-methoxyphenyl)phosphine [$P(2\text{-}MeOC_6H_4)_3$ were bought from Sigma-Aldrich (Shanghai) Trading Co., LTD. Anhydrous *N*, *N*-dimethylacetamide (DMAc) and xylene were purchased from Beijing J&K Scientific Co., LTD. Tetrahydrofuran (THF), trichloromethane ($CHCl_3$), anhydrous methanol, and n-hexane were provided by Tianjin Hengshan Chemical Co. All other solvents and reagents (analytical and spectroscopic grades) were obtained commercially and used directly, unless otherwise stated.

Instruments

^1H, ^{13}C, HSQC and HMBC NMR spectra were obtained on a Bruker AV400 at 25°C using tetramethylsilane (TMS) as an internal standard. Number-average (M_n) and polydispersity index (PDI) were determined by size exclusion chromatography (SEC) in tetrahydrofuran at 25 °C using Waters 1525 with Waters Styragel HT gel columns. Monodisperse polystyrene standards (Shodex) was used to establish the calibration curve. UV-Vis absorption spectra were recorded using a Shimadzu UV-2550 and dropcast films on glass plates were used for the solid-state measurements. Optical bandgap was determined from the onset of the absorption band. Fluorescence spectra were collected on a Hitachi F-4600 fluorescence spectrophotometer equipped with a xenon lamp excitation source. Thermogravimetric analysis (TGA) was used to determine the decomposition temperature, which was ramped up from 25 °C to 1000 °C at a rate of 10 °C/min. Particle size measurements were performed using a Morven ZetaSizerNanoZS90. Transmission electron microscopy (TEM) images of the synthesized nanoparticles were obtained using a FEIT ecnai G2 Spirit TWIN transmission electron microscope while energy-dispersive spectroscopy (EDS) data were obtained. Water contact angles were measured using KRUSS DSA100 measurement instrument (Shanghai Fang Rui Instrument Co. Ltd.). Pd content was determined by inductively coupled plasma optical emission spectrometer (Agilent ICP-OES 725). Time-resolved PL was acquired on an Edinburgh FLS980 spectrophotometer.

Electrochemical measurements

Cyclic voltammetry (CV) was performed on an LK2005A electrochemical apparatus in a three-neck flask consisting of a three-electrode structure under a nitrogen atmosphere. A glassy carbon electrode, a saturated heat electrode and a platinum electrode were used as the working, reference and counter electrodes, respectively. Bu_4NPF_6 (0.1 mol/L) in anhydrous acetonitrile was used as the supporting electrode. The electrodes were polished with aluminum powder and cleaned with distilled water and acetonitrile. The polymer drop-cast film prepared with chloroform solution on the working electrode was scanned at least three times at a rate of 100 mV^{-1}.

Electrochemical impedance spectra (EIS) were recorded on a CIMPS-2 electrochemical workstation (Zahner Electrochemie, Germany) with a standard three-electrode system. A platinum plate as counter electrode, glassy carbon electrode as working electrode, saturated calomel electrode (SCE) as reference electrode, and 0.2 M Na_2SO_4 solution as electrolyte were applied in the measurements (pH = 6.8), respectively. Time-current curves were obtained on an LK2005A electrochemical apparatus (Lanlike, China) in a three-neck flask consisting of a three-electrode structure under a nitrogen atmosphere. A fluorine doped tin oxide (FTO) coated glass, a platinum electrode and a saturated calomel electrode were used as the working, counter and reference electrodes, respectively. An electrolyte solution of 0.2 M was prepared with ultrapure water and Na_2SO_4, and irradiated every 30 s using a CEL-HXF300E light source.

Apparent quantum yields measurements

The apparent quantum yield at different wavelengths was measured by inserting 400 nm, 450 nm, 500 nm, 550 nm, and 600 nm band-pass filters, and the irradiation was continued for 2 h for each wavelength region. The light intensity in the photocatalytic reaction was measured using a calibrated power meter (Model 843R, Newport). The apparent quantum yields (AQY) was calculated according to the following equation:

$$AQY = \frac{number\ of\ evolved\ H_2\ molecules \times 2}{number\ of\ incident\ photons} \times 100\%$$

$$AQY = \frac{2M \times N_A \times h \times c}{S \times P \times t \times \lambda} \times 100\%$$

where M is the amount of H_2 molecules (mol); NA is the Avogadro constant (6.022×10^{23} mol^{-1}); h is the Planck constant (6.626×10^{-34} J•s); c is vacuum light velocity (2.997×10^{8} $m•s^{-1}$); the irradiation area (S) is 25.5 cm^2 in our experiment; P is the intensity of the irradiating light ($W•cm^{-2}$); t is the photoreaction time (s); and λ is the wavelength of the monochromatic light (m).

DFT calculations

All calculations were performed based on the density functional theory in Gaussian 09 programs [1]. The geometry optimizations and the spin density surfaces of the polymers were performed at the B3LYP/6-31G [2-6]. Four repeating units were used and the side chains were replaced with methyl groups to reduce the computation time according to the literatures [7]. All optimized structures were not imaginary frequency.

The reaction Gibbs free energy (ΔG_{H*}) for hydrogen adsorption is determined by:

$\Delta G_{H*} = \Delta E_{H*} + \Delta E_{ZPE} - T\Delta S_H$

the ΔE_{H*} is the integral adsorption energy of H absorbates calculated by the formula of $\Delta E_{H*} = E_{oligomer+H} - E_{oligomer} - 1/2\ E_{H_2}$, where $E_{oligomer+H}$, $E_{oligomer}$ and E_{H_2} represent the total energies of oligomer with one absorbed H atoms, total energies of oligomer and H_2 gas, respectively. ΔE_{ZPE} and ΔS_H are the changes in the zero-point energy and entropy between H atoms adsorption state and the gas-phase state of H_2. The ΔE_{ZPE} is calculated by the formula of $\Delta E_{ZPE} = E_{ZPE\ (oligomer\ +\ H)} - E_{ZPE\ (oligomer)} - 1/2\ E_{ZPE\ (H_2)}$. The ΔS_H is calculated by the formula of $\Delta S_H \approx 1/2\ S_{H_2}$, where S_{H_2} is entropy of the gas-phase state of H_2 at standard condition.

Table S1. The screening of the reaction conditions for the polymerization of TPD2T by C-H/C-H cross-coupling polycondensation [a]

Entry	Catalyst	Additive	Solvent (v/v)	T (°C)	Yield [b] (%)	M_n [c] (kDa)	PDI
1	Heremann's cat.	-	DMAc	100	58.7	3.8	1.84
2	Heremann's cat.	PCy_3	DMAc	100	56.7	5.0	1.47
3	Heremann's cat.	$P(2\text{-}MeOC_6H_4)_3$	DMAc	100	53.7	4.0	1.71
4	Heremann's cat.	PCy_3HBF_4	DMAc	100	58.5	4.7	1.46
5	Heremann's cat.	$P(t\text{-}Bu)_2MeHBF_4$	DMAc	100	70.4	10.7	2.11
6	$Pd(dppf)Cl_2$	$P(t\text{-}Bu)_2MeHBF_4$	DMAc	80	52.7	3.7	1.87
7	$Pd(tbdchp)_2Cl_2$	$P(t\text{-}Bu)_2MeHBF_4$	DMAc	80	32.1	4.6	1.34
8	$Pd(PPh_3)_4$	$P(t\text{-}Bu)_2MeHBF_4$	DMAc	80	63.4	12.5	1.21
9	$Pd(PPh_3)_4$	$P(t\text{-}Bu)_2MeHBF_4$	DMAc/xylene (20:1)	80	55.3	9.1	1.67
10	$Pd(PPh_3)_4$	$P(t\text{-}Bu)_2MeHBF_4$	DMAc/xylene (10:1)	80	48.2	9.3	1.53
11	$Pd(PPh_3)_4$	$P(t\text{-}Bu)_2MeHBF_4$	DMAc/xylene (7:3)	80	46.7	10.3	1.54
12	$Pd(PPh_3)_4$	$P(t\text{-}Bu)_2MeHBF_4$	DMAc/xylene (1:1)	80	57.5	18.1	1.26

[a] Reaction conditions: TPD (0.1 mmol), 2T (0.1 mmol), catalyst (10 mol%), additive (20 mol%), Ag_2CO_3 (0.4 mmol), KOAc (0.4 mmol) in 1 mL of solvent for 48 h. [b] Isolated yield after purification. [c] Estimated by GPC measurements (eluent: THF, standard: polystyrene).

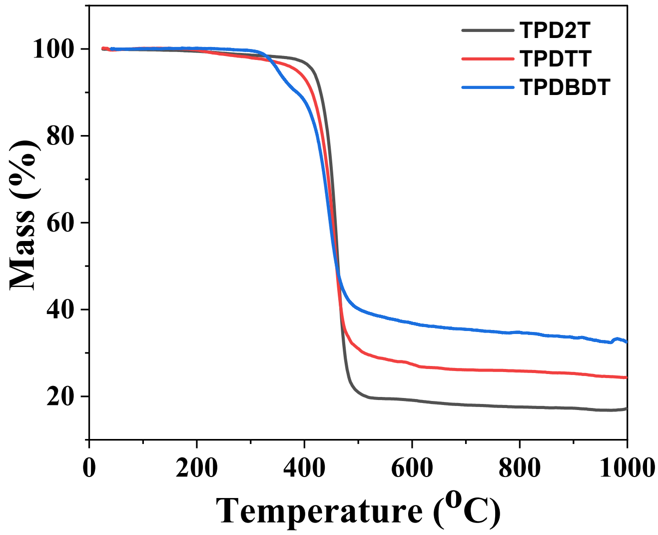

Fig. S1. TGA curves of polymers TPD2T, TPDTT, and TPDBDT.

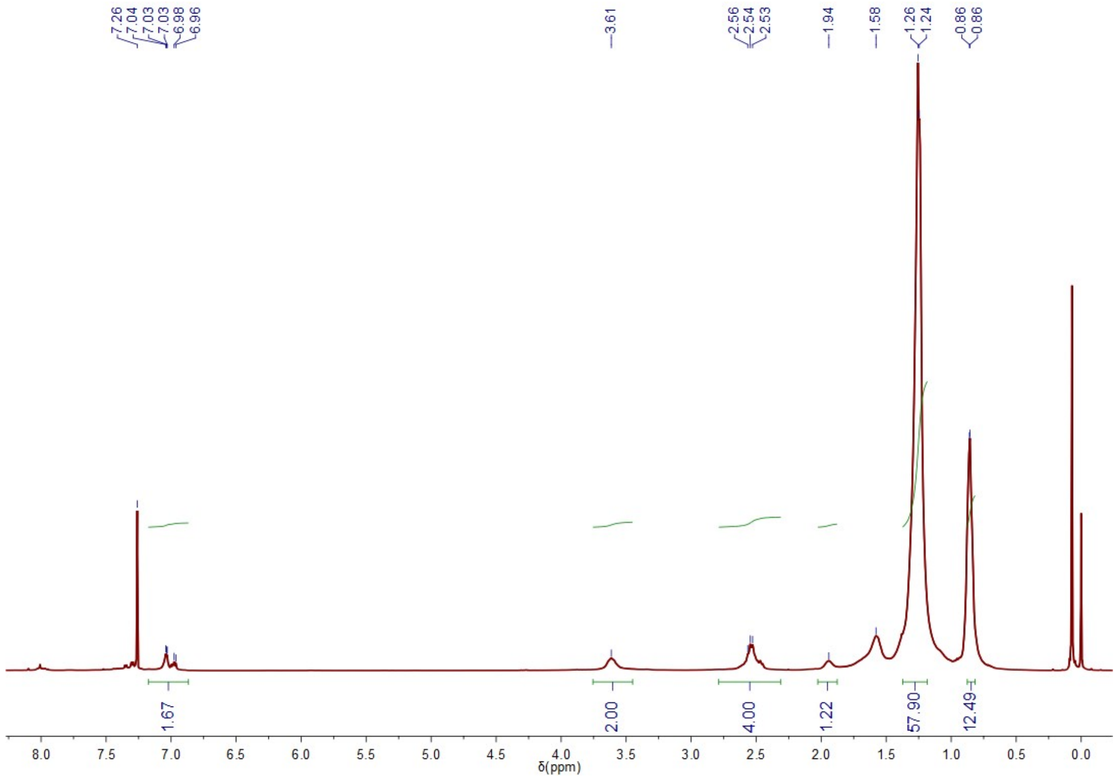

Fig. S2. ^{1}H NMR spectrum in $CDCl_3$ of TPD2T (entry 12, Table S1).

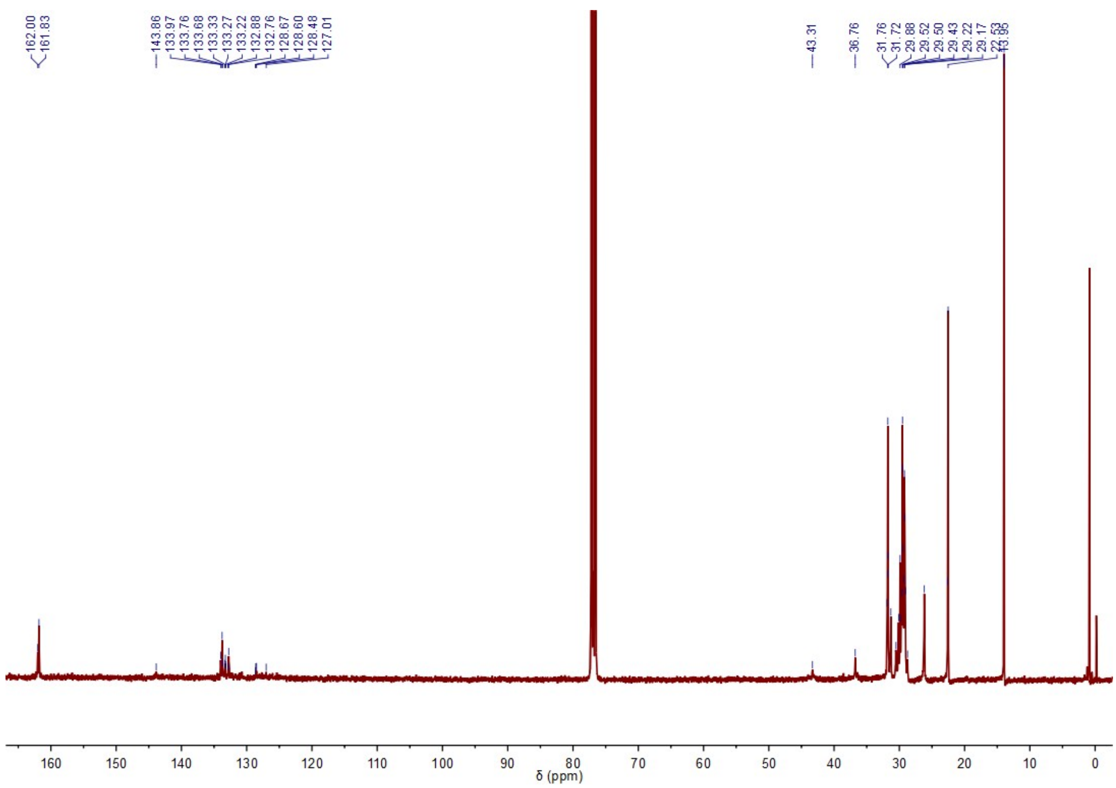

Fig. S3. ^{13}C NMR spectrum in $CDCl_3$ of TPD2T (entry 12, Table S1).

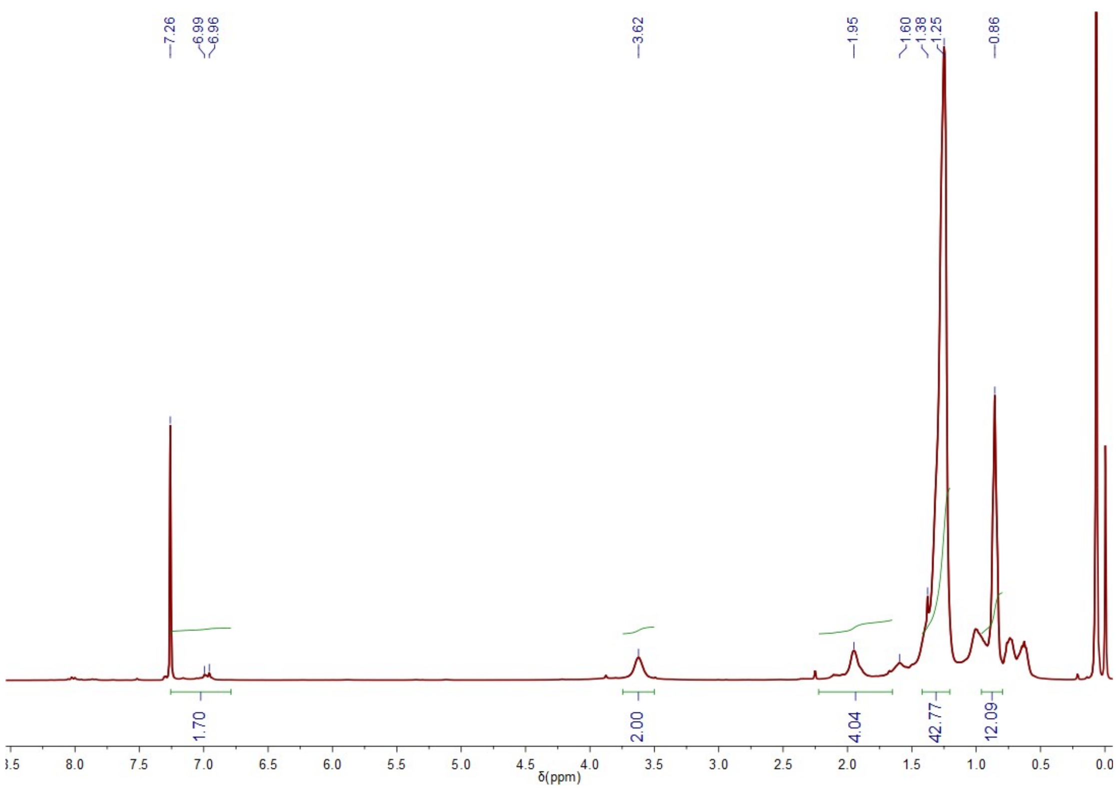

Fig. S4. ^{1}H NMR spectrum in $CDCl_3$ of TPDTT

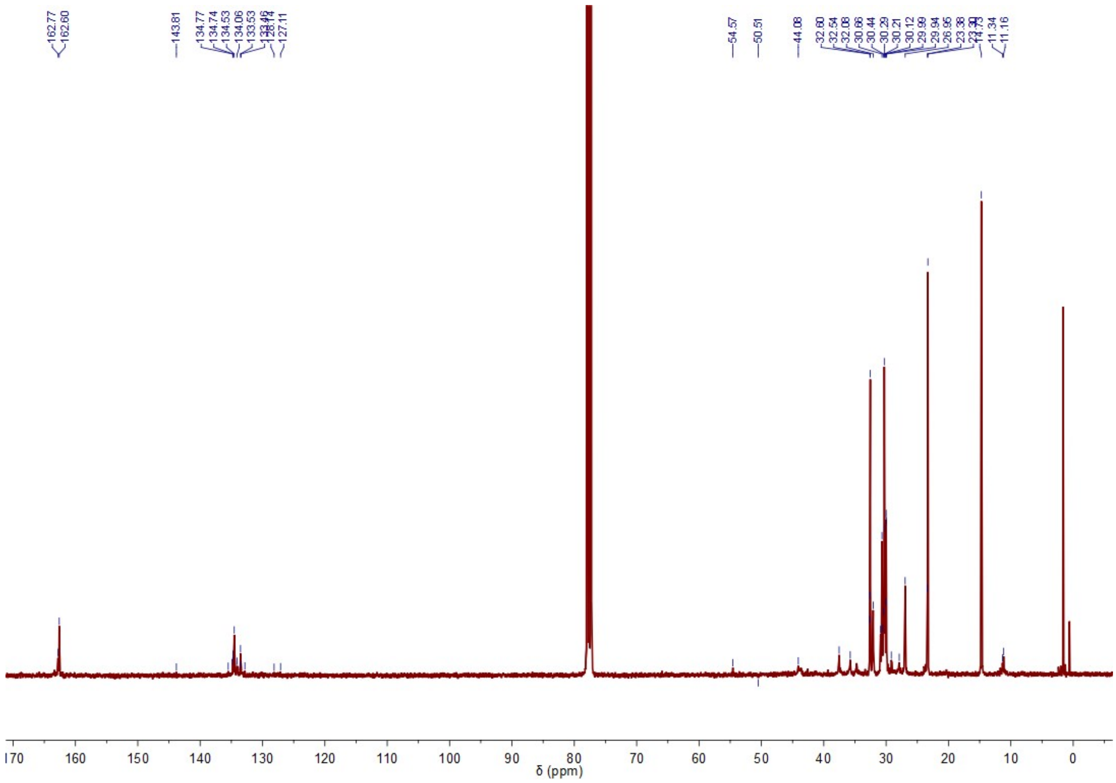

Fig. S5. ^{13}C NMR spectrum in $CDCl_3$ of TPDTT

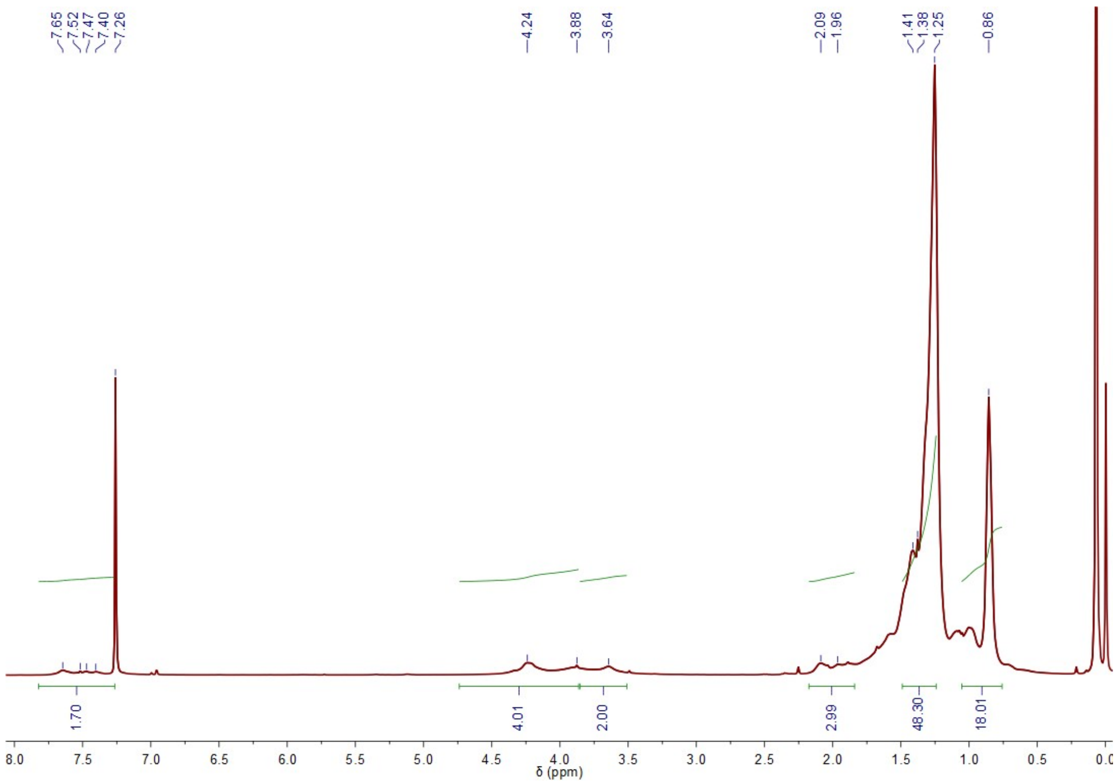

Fig. S6. ^{1}H NMR spectrum in $CDCl_3$ of TPDBDT

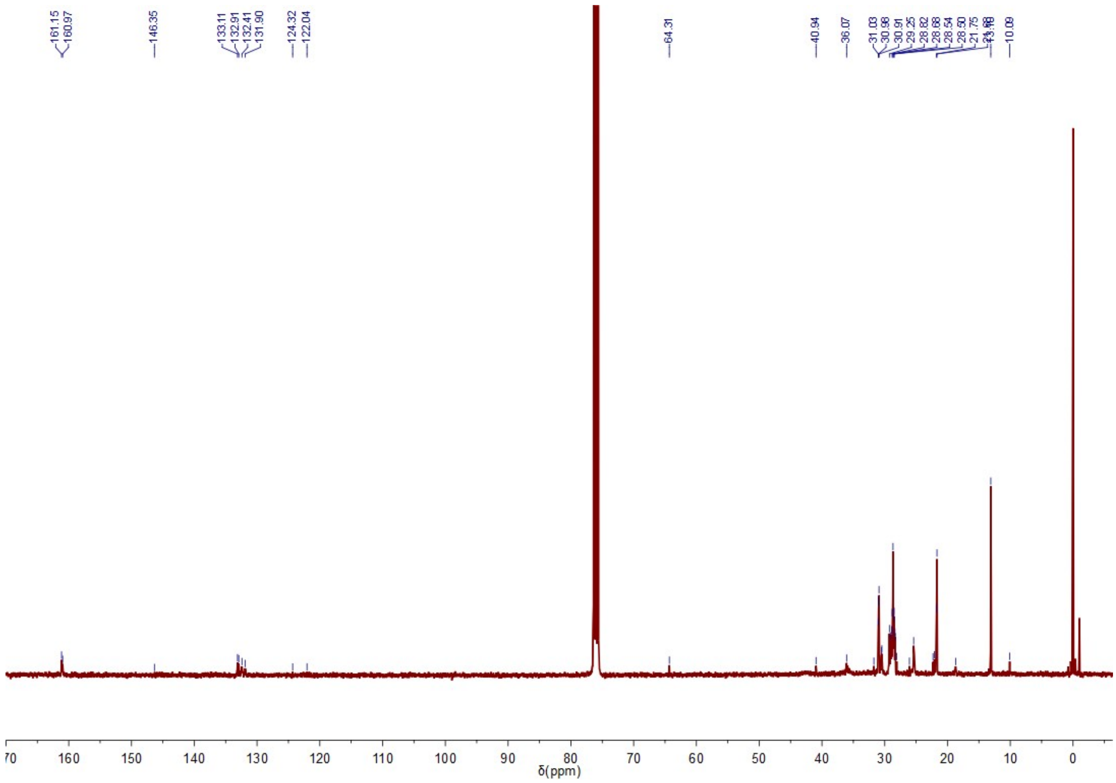

Fig. S7. ^{13}C NMR spectrum in $CDCl_3$ of TPDBDT

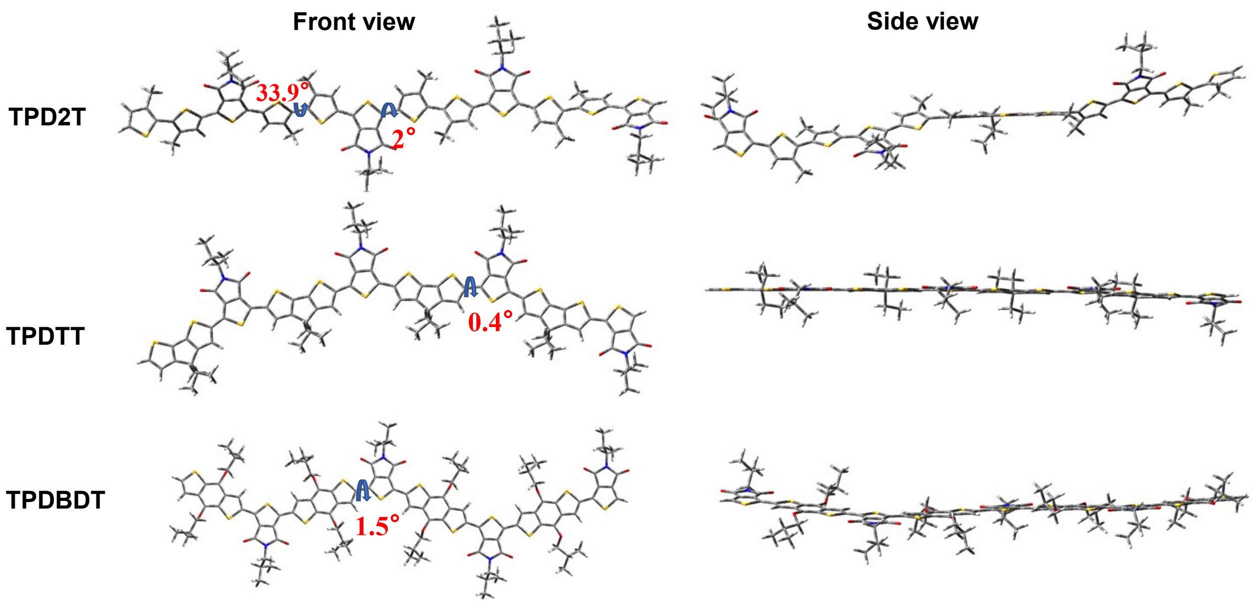

Fig. S8. Optimized molecular geometries of TPD2T, TPDTT, and TPDBDT.

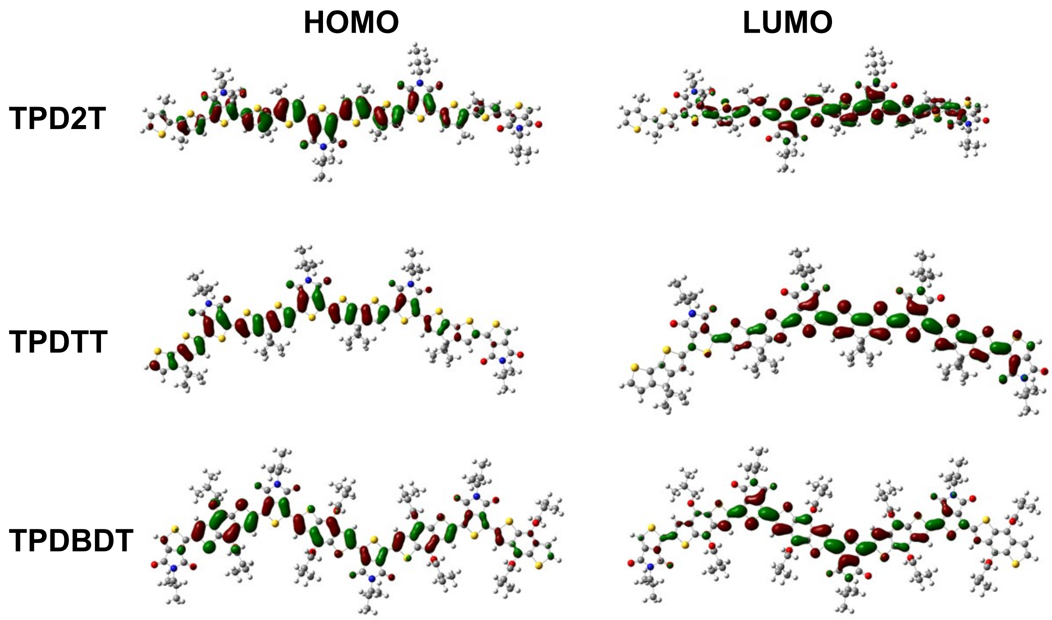

Fig. S9. The HOMO and LUMO of TPD2T, TPDTT, TPDBDT.

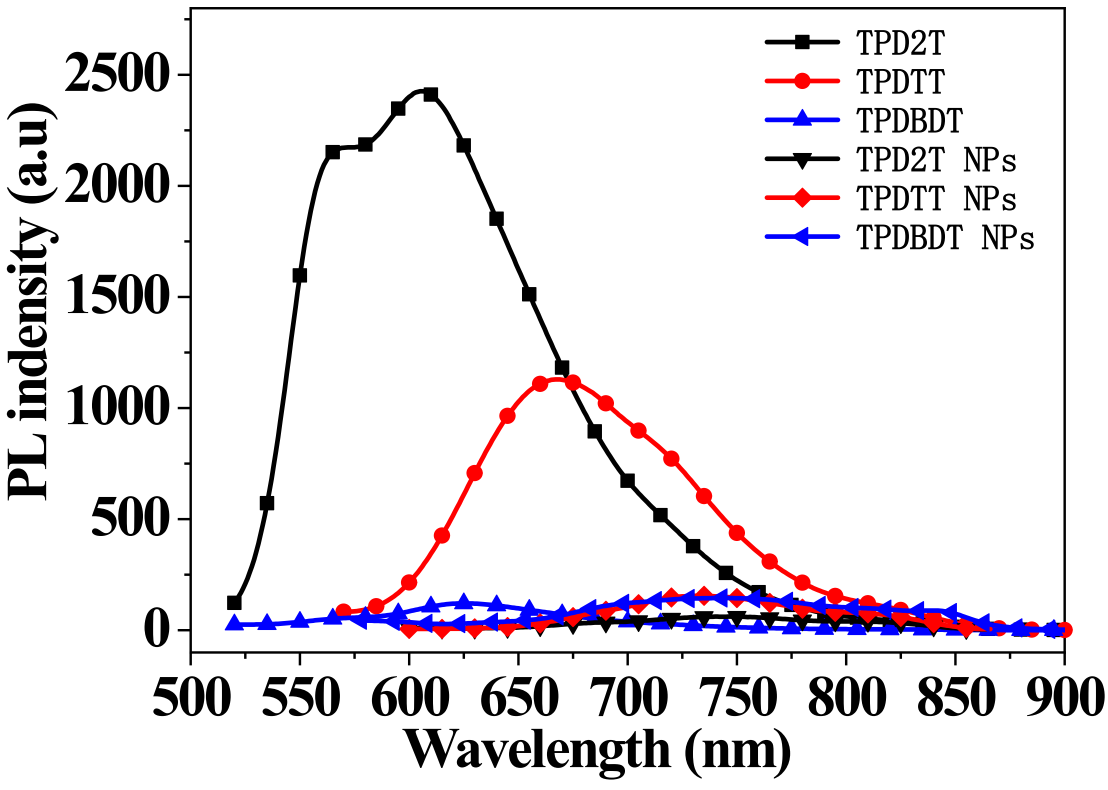

Fig. S10. PL spectra of TPD2T, TPDTT, TPDBDT, and TPD2T NPs, TPDTT NPs, TPDBDT NPs.

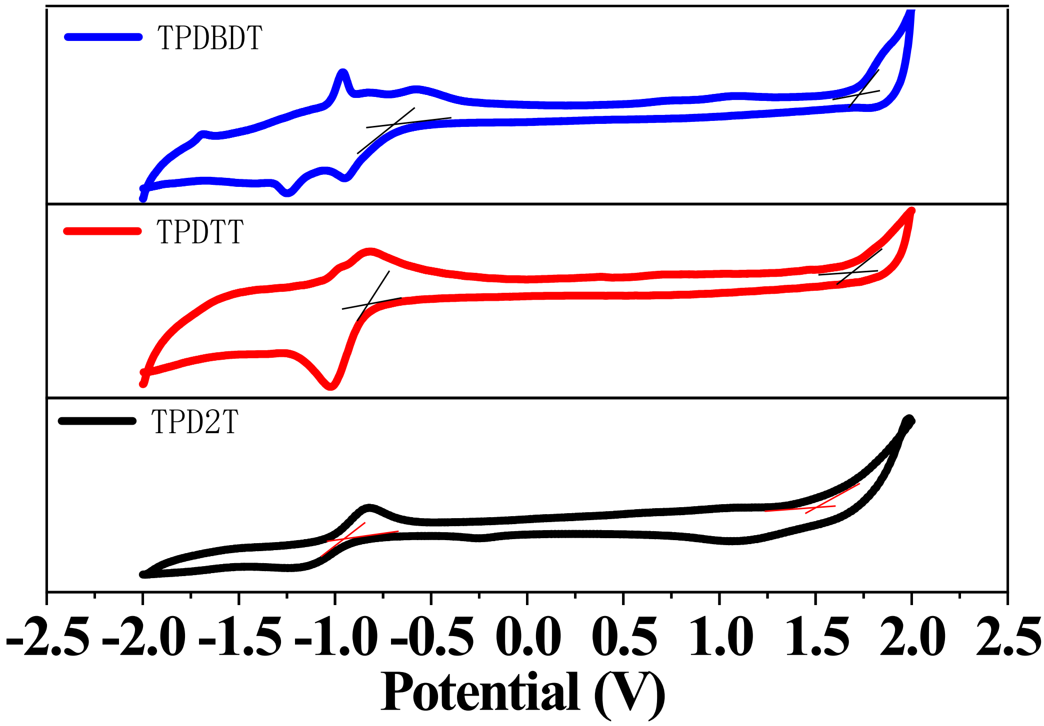

Fig. S11. The CV curves of polymers TPD2T, TPDTT, and TPDBDT.

Table S2. Fitted decay time of TPD2T, TPDTT, and TPDBDT

paramters	TPD2T	TPDTT	TPDBDT
λ	520	540	520
τ_1(ns)	0.487	0.685	0.622
B_1	21.15%	62.33%	78.77%
τ_2(ns)	2.452	2.249	2.158
B_2	78.85%	37.67%	21.23%
τ_{Av}(ns)	2.04	1.27	0.95
x^2	1.117	1.196	1.177

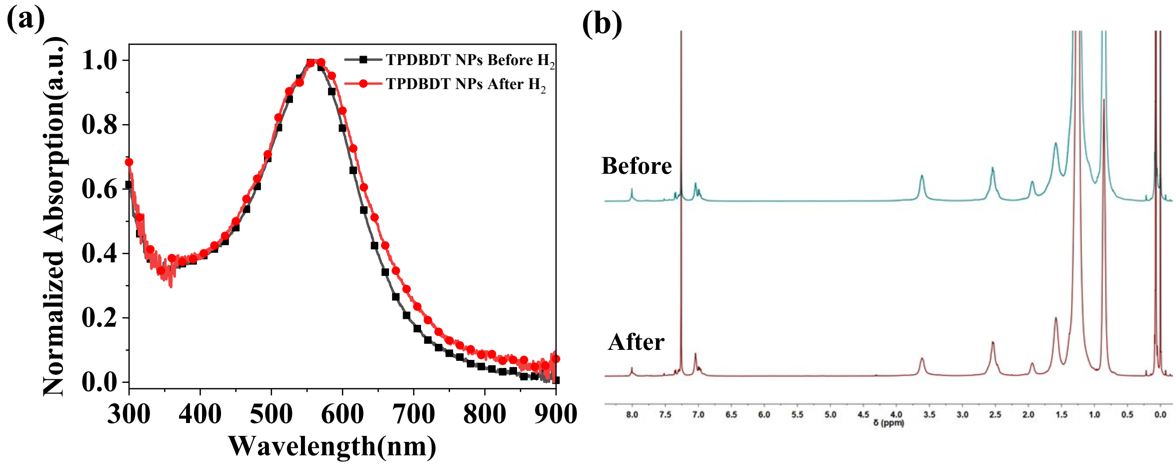

Fig. S12. (a) UV−vis spectra and (b) [1]H NMR of TPDBDT NPs after H_2 production

Table S3. Summary of the photocatalytic hydrogen production performances of organic photocatalysts.

Polymer catalyst	Metal co-Catalyst	λ (nm)	Other conditions	HER (mmol $h^{-1} \cdot g^{-1}$)	AQY	Ref.
PFODTBT[a]	0.1 wt% Pd residue	＞550	AA/H_2O	50	0.6%@550 nm	8
PBDT-B3T[a]	4 wt% Pt	＞420	AA/H_2O	14.1	0.5%@420 nm	9
PFBT[a]	--	＞420	AA/H_2O	8.3	0.5%@420 nm	10
PG6[a]	4 wt % Pt	＞420	AA/H_2O	5.84	0.7%@420 nm	11
PFTBTA[a]	Pd residue	＞420	DEA/H_2O	0.44	0.56%@420 nm	12
PFTBTA[a]	Pd residue	＞420	TEA/H_2O	1.05	--	13
PFTBDD[a]	Pd residue	＞420	AA/H_2O	0.02	0.56%@420 nm	14
LE-CP-dots[a]	--	＞420	AA/H_2O	0.77	--	15
PyPm[a]	3 wt% Pt	＞300	TEOA/H_2O	0.37	1.1%@420 nm	16
PFTFQ-PtPy15[b]	--	＞420	DEA/H_2O	12.7	0.4%@515 nm	17
PFTBTA-PtPy[b]	2.3 wt% Pt + Pd residue	＞420	TEA/H_2O	7.34	0.27%@420 nm	13
PFTBDD-Ir-TPy[b]	-	＞420	AA/H_2O	0.44	--	14
FP-R[c]	--	＞420	TEA/MeOH/H_2O	2.9	10.0%@420 nm	18
PBDTBT-7EO[c]	3wt.% Pt	＞420	AA/H_2O	12.8	0.25% @550 nm	19
PFN-Br[d]	3 wt% Pt	＞420	AA/TEOA/H_2O	0.08	0.12@550 nm	20
PFBT-CPE[d]	0.04 wt% Pd	＞420	TEA/MeOH/H_2O	5.12	0.3% @420 nm	21
PSO-FBBr[d]	0.15 wt% Pt	＞420	TEOA/H_2O	20.5	3.5% @420 nm	22
TPDBDT NPs[a]	--	＞300	AA/H_2O	7.42	0.55%@550 nm	This work
TPD2T NPs[a]	--	＞300	AA/H_2O	0.38	--	This work
TPDTT NPs[a]	--	＞300	AA/H_2O	0.81	--	This work

[a] organic nanoparticles (NPs). [b] metal complex-contained polymer nanoparticles(NPs). [c] OEG-functionalized conjugated polymers. [d] Conjugated Polyelectrolyte. AA: ascorbic acid, DEA: diethylamine, TEOA: triethanolamine, and TEA: trimethylamine.

The TPD2T optimized geometries of the stationary points

Stand orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	18.846772	0.558603	0.233428
2	6	0	19.440102	-0.666705	0.610893
3	6	0	20.829473	-0.583931	0.679659
4	6	0	21.313004	0.679091	0.374952
5	16	0	20.056803	1.658699	0.046291
6	6	0	19.047752	-2.015745	0.957189
7	7	0	20.281467	-2.672561	1.209515
8	6	0	21.416214	-1.845493	1.053005
9	8	0	22.579063	-2.18321	1.211275
10	8	0	17.965808	-2.576475	1.055288
11	6	0	20.360501	-4.081185	1.581178
12	6	0	20.176761	-5.038472	0.387152
13	6	0	21.255917	-4.828424	-0.686349
14	6	0	20.184998	-6.496296	0.873132
15	6	0	11.135785	0.716039	-0.117676
16	6	0	11.629187	-0.5847	0.112734
17	6	0	13.020333	-0.66235	0.118348
18	6	0	13.612776	0.60807	-0.103934
19	16	0	12.413971	1.696249	-0.359078
20	6	0	17.471711	0.922044	0.022944
21	6	0	16.982829	2.19643	-0.32855
22	6	0	15.594306	2.250429	-0.438824
23	6	0	15.000159	0.99418	-0.152379
24	16	0	16.199649	-0.090005	0.118029
25	6	0	14.953052	3.525727	-0.938165
26	6	0	13.672375	-2.022936	0.222361
27	6	0	7.247911	0.971608	-0.165384
28	6	0	7.733767	2.282154	-0.346258
29	6	0	9.131067	2.356985	-0.341064
30	6	0	9.754437	1.106903	-0.163157
31	16	0	8.556989	-0.001617	0.014243
32	6	0	7.177387	3.598907	-0.548715
33	7	0	8.320978	4.419593	-0.658953
34	6	0	9.545758	3.727738	-0.52349
35	8	0	10.638903	4.277725	-0.5589
36	8	0	6.03353	4.03089	-0.62428
37	6	0	8.233899	5.862265	-0.860592

38	6	0	7.918496	6.645236	0.429347
39	6	0	8.995463	6.443238	1.506571
40	6	0	7.759159	8.140547	0.112107
41	6	0	-0.403006	-0.092577	-0.335508
42	6	0	-0.045616	1.260007	-0.478038
43	6	0	1.326732	1.494514	-0.442707
44	6	0	2.046132	0.280653	-0.260675
45	16	0	0.976754	-0.950976	-0.159997
46	6	0	5.915453	0.434449	-0.12477
47	6	0	5.565169	-0.919862	0.036732
48	6	0	4.189899	-1.147291	0.008662
49	6	0	3.472528	0.066715	-0.171012
50	16	0	4.542092	1.299225	-0.272684
51	6	0	3.643956	-2.548416	0.161743
52	6	0	1.868895	2.897978	-0.590686
53	6	0	-4.235844	-0.813464	-0.401037
54	6	0	-3.596605	-2.063619	-0.262251
55	6	0	-2.201683	-1.970429	-0.242684
56	6	0	-1.724746	-0.648032	-0.35683
57	16	0	-3.04776	0.30844	-0.537721
58	6	0	-4.001323	-3.441536	-0.119387
59	7	0	-2.772241	-4.128208	-0.018213
60	6	0	-1.637219	-3.292375	-0.100357
61	8	0	-0.486789	-3.71149	-0.060425
62	8	0	-5.088194	-4.005868	-0.083111
63	6	0	-2.6928	-5.578589	0.120648
64	6	0	-2.908047	-6.334459	-1.205657
65	6	0	-1.857406	-5.958578	-2.262016
66	6	0	-2.892199	-7.850942	-0.95684
67	6	0	-11.947439	-0.625865	-0.144729
68	6	0	-11.447115	-1.93849	-0.049576
69	6	0	-10.056313	-2.011747	-0.118985
70	6	0	-9.481553	-0.720861	-0.273572
71	16	0	-10.683337	0.386697	-0.325324
72	6	0	-5.620545	-0.431397	-0.433256
73	6	0	-6.122713	0.876609	-0.571725
74	6	0	-7.515085	0.945664	-0.539004
75	6	0	-8.089104	-0.344358	-0.373326
76	16	0	-6.886167	-1.449208	-0.297191
77	6	0	-8.21572	2.279328	-0.665481
78	6	0	-9.356643	-3.348611	-0.026357
79	6	0	-15.835139	-0.374223	0.107458
80	6	0	-15.356916	0.943866	-0.045744
81	6	0	-13.96513	1.023411	-0.157743

82	6	0	-13.328884	-0.233673	-0.088658
83	16	0	-14.514753	-1.350996	0.095864
84	6	0	-15.91662	2.273312	-0.117634
85	7	0	-14.784858	3.100257	-0.279743
86	6	0	-13.55849	2.40008	-0.30813
87	8	0	-12.471173	2.950325	-0.432368
88	8	0	-17.060476	2.709331	-0.062491
89	6	0	-14.882283	4.552941	-0.375884
90	6	0	-15.066117	5.245476	0.989211
91	6	0	-13.892304	4.96815	1.941205
92	6	0	-15.243961	6.759351	0.792938
93	6	0	-23.444408	-1.334797	0.763735
94	6	0	-23.126171	0.010593	0.619311
95	6	0	-21.74036	0.204754	0.498022
96	6	0	-21.032544	-1.023568	0.555263
97	16	0	-22.110637	-2.246223	0.745579
98	6	0	-17.15558	-0.912643	0.254912
99	6	0	-17.512611	-2.263423	0.404007
100	6	0	-18.883162	-2.481169	0.525859
101	6	0	-19.605425	-1.256208	0.469432
102	16	0	-18.535672	-0.035693	0.279618
103	6	0	-19.417159	-3.885581	0.692453
104	6	0	-21.186846	1.60241	0.33132
105	1	0	22.357289	0.983864	0.362174
106	1	0	19.590359	-4.290055	2.345533
107	1	0	21.328594	-4.284783	2.070033
108	1	0	19.189005	-4.842437	-0.075463
109	1	0	21.125333	-5.537706	-1.522719
110	1	0	21.213715	-3.812337	-1.115007
111	1	0	22.267589	-4.978668	-0.269688
112	1	0	20.016231	-7.196778	0.036686
113	1	0	19.389941	-6.676156	1.619065
114	1	0	21.152139	-6.75586	1.340701
115	1	0	11.00478	-1.466541	0.26862
116	1	0	17.608645	3.073046	-0.506968
117	1	0	15.686749	4.127891	-1.503126
118	1	0	14.157022	3.320926	-1.669815
119	1	0	14.603759	4.175708	-0.118896
120	1	0	12.961861	-2.813678	-0.077353
121	1	0	14.505349	-2.129723	-0.488726
122	1	0	13.974783	-2.27154	1.253135
123	1	0	7.452928	6.066782	-1.614989
124	1	0	9.171665	6.239895	-1.30219
125	1	0	6.954056	6.280975	0.836126

126	1	0	8.764129	7.03244	2.411731
127	1	0	9.068078	5.387576	1.819709
128	1	0	9.98885	6.758868	1.142304
129	1	0	7.49214	8.714325	1.016706
130	1	0	6.961713	8.311165	-0.633483
131	1	0	8.696173	8.564889	-0.29212
132	1	0	-0.737137	2.086325	-0.628246
133	1	0	6.277959	-1.7371	0.161387
134	1	0	4.46117	-3.275692	0.307209
135	1	0	2.990972	-2.63963	1.045907
136	1	0	3.096265	-2.875488	-0.738195
137	1	0	1.049288	3.629061	-0.699297
138	1	0	2.443044	3.21239	0.297009
139	1	0	2.495445	3.002513	-1.492571
140	1	0	-3.449015	-5.904851	0.85722
141	1	0	-1.719928	-5.864911	0.554719
142	1	0	-3.906637	-6.068305	-1.605896
143	1	0	-2.013401	-6.528928	-3.194854
144	1	0	-1.908041	-4.88846	-2.526689
145	1	0	-0.83541	-6.171522	-1.902145
146	1	0	-3.085811	-8.410397	-1.888764
147	1	0	-3.667494	-8.147333	-0.227564
148	1	0	-1.913694	-8.180618	-0.562763
149	1	0	-12.062242	-2.831399	0.075464
150	1	0	-5.507285	1.771085	-0.683407
151	1	0	-7.485393	3.095945	-0.798843
152	1	0	-8.878007	2.313765	-1.546839
153	1	0	-8.792767	2.527885	0.241119
154	1	0	-10.087898	-4.168934	0.075481
155	1	0	-8.771914	-3.570178	-0.9351
156	1	0	-8.701447	-3.408807	0.858982
157	1	0	-15.731165	4.808281	-1.035391
158	1	0	-13.989149	4.960222	-0.879202
159	1	0	-15.989699	4.854822	1.461136
160	1	0	-14.030177	5.494399	2.902503
161	1	0	-13.798614	3.893448	2.17354
162	1	0	-12.93585	5.305976	1.504894
163	1	0	-15.418632	7.269006	1.756623
164	1	0	-16.107881	6.982009	0.14116
165	1	0	-14.34678	7.21001	0.331006
166	1	0	-24.450742	-1.738084	0.875366
167	1	0	-23.867601	0.809838	0.603202
168	1	0	-16.821628	-3.103419	0.429256
169	1	0	-18.597039	-4.623978	0.697684

170	1	0	-19.947042	-4.01071	1.652422
171	1	0	-20.081252	-4.172455	-0.140956
172	1	0	-22.002183	2.346434	0.325866
173	1	0	-20.520571	1.884328	1.164088
174	1	0	-20.654896	1.723867	-0.627403

The TPDTT optimized geometries of the stationary points

Stand orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	18.953037	-1.489818	-0.281879
2	6	0	19.729797	-2.626283	-0.129924
3	6	0	21.131683	-2.384574	-0.191407
4	6	0	21.475002	-1.084772	-0.389822
5	16	0	20.039164	-0.105499	-0.510947
6	6	0	19.531311	-4.074875	0.095385
7	7	0	20.826849	-4.624025	0.171298
8	6	0	21.8499	-3.671172	-0.007698
9	8	0	23.040764	-3.910563	-0.006761
10	8	0	18.509541	-4.737652	0.197372
11	6	0	21.075247	-6.04978	0.356479
12	6	0	20.914208	-6.536023	1.810217
13	6	0	21.09464	-8.060203	1.852243
14	6	0	21.884117	-5.832437	2.7681
15	6	0	15.203478	-0.442665	-0.313081
16	16	0	16.772207	0.272605	-0.40375
17	6	0	17.524143	-1.327915	-0.277755
18	6	0	16.564415	-2.331278	-0.173777
19	6	0	15.250844	-1.828223	-0.182038
20	6	0	13.838127	-2.417656	-0.129602
21	6	0	13.013828	-1.132147	-0.248505
22	6	0	13.83941	-0.014087	-0.352803
23	6	0	11.654887	-0.780915	-0.230562
24	6	0	11.437399	0.593611	-0.340789
25	16	0	12.973942	1.47538	-0.453759
26	6	0	13.637085	-3.36917	-1.34713
27	6	0	13.532871	-3.10147	1.237117
28	6	0	14.309797	-4.387659	1.538305
29	6	0	12.250597	-4.006527	-1.484874
30	6	0	7.602001	1.69475	-0.357833

31	6	0	8.392878	2.822518	-0.443904
32	6	0	9.793766	2.581622	-0.4499
33	6	0	10.163364	1.254799	-0.367375
34	16	0	8.678188	0.281706	-0.280016
35	6	0	8.175046	4.280969	-0.538959
36	7	0	9.462223	4.846148	-0.586036
37	6	0	10.487645	3.882932	-0.550854
38	8	0	11.679806	4.136227	-0.602816
39	8	0	7.138833	4.923815	-0.578692
40	6	0	9.69864	6.280371	-0.714506
41	6	0	9.523356	7.068614	0.598316
42	6	0	10.49622	6.602621	1.689012
43	6	0	9.684804	8.567743	0.308678
44	6	0	3.713306	1.728384	-0.291938
45	16	0	5.026498	2.844224	-0.382158
46	6	0	6.18101	1.496918	-0.32596
47	6	0	5.517252	0.271028	-0.245239
48	6	0	4.120249	0.397407	-0.213383
49	6	0	2.913842	-0.545791	-0.170719
50	6	0	1.779927	0.482099	-0.238116
51	6	0	2.283009	1.780163	-0.305441
52	6	0	0.377292	0.462254	-0.197332
53	6	0	-0.194711	1.73468	-0.254018
54	16	0	1.05489	2.9921	-0.343312
55	6	0	2.949025	-1.477903	-1.418569
56	6	0	2.815789	-1.32716	1.173621
57	6	0	3.914269	-2.362208	1.437476
58	6	0	1.776032	-2.45201	-1.569688
59	6	0	-4.18495	1.786616	-0.211054
60	6	0	-3.719498	3.08538	-0.248499
61	6	0	-2.304799	3.22226	-0.269866
62	6	0	-1.597947	2.037483	-0.248014
63	16	0	-2.773929	0.70469	-0.201025
64	6	0	-4.314448	4.437818	-0.276001
65	7	0	-3.222118	5.323317	-0.301063
66	6	0	-1.978933	4.663445	-0.313707
67	8	0	-0.896452	5.223652	-0.358667
68	8	0	-5.483794	4.78614	-0.283012
69	6	0	-3.372494	6.773327	-0.3657
70	6	0	-3.728673	7.431144	0.98186
71	6	0	-2.651457	7.190878	2.047285
72	6	0	-3.970208	8.931015	0.759553
73	6	0	-7.944597	0.792711	-0.133869
74	16	0	-6.972148	2.217615	-0.174748

75	6	0	-5.503264	1.220566	-0.184225
76	6	0	-5.820546	-0.139089	-0.159302
77	6	0	-7.201062	-0.386348	-0.118622
78	6	0	-8.116749	-1.614559	-0.118709
79	6	0	-9.48171	-0.919221	-0.135324
80	6	0	-9.338414	0.466871	-0.142288
81	6	0	-10.829324	-1.309642	-0.093737
82	6	0	-11.71637	-0.231714	-0.090058
83	16	0	-10.842766	1.313019	-0.121835
84	6	0	-7.855873	-2.446427	-1.409873
85	6	0	-7.987171	-2.454794	1.186811
86	6	0	-6.651864	-3.175632	1.398939
87	6	0	-8.734802	-3.68598	-1.606287
88	6	0	-15.579169	-1.236634	-0.040344
89	6	0	-15.473208	0.139277	-0.019685
90	6	0	-14.144021	0.645591	-0.036062
91	6	0	-13.15003	-0.309821	-0.0685
92	16	0	-13.932703	-1.906799	-0.080745
93	6	0	-16.403089	1.286106	0.014829
94	7	0	-15.582627	2.429008	0.029635
95	6	0	-14.209778	2.121818	-0.014166
96	8	0	-13.314011	2.949676	-0.03394
97	8	0	-17.623211	1.315777	0.024292
98	6	0	-16.110098	3.789144	0.031931
99	6	0	-16.607891	4.270369	1.409
100	6	0	-15.490847	4.274931	2.460385
101	6	0	-17.237675	5.662324	1.256728
102	6	0	-18.942625	-3.190343	-0.005737
103	16	0	-18.381377	-1.560562	0.011899
104	6	0	-16.700256	-2.132472	-0.037529
105	6	0	-16.64961	-3.526383	-0.068308
106	6	0	-17.917461	-4.130613	-0.037808
107	6	0	-18.481534	-5.554535	-0.089749
108	6	0	-19.982282	-5.244556	-0.079175
109	6	0	-20.204289	-3.876616	-0.02924
110	6	0	-21.192889	-5.988714	-0.054305
111	6	0	-22.299639	-5.17628	-0.005143
112	16	0	-21.888047	-3.479333	0.026049
113	6	0	-18.023654	-6.236937	-1.413242
114	6	0	-18.123953	-6.38306	1.180159
115	6	0	-16.644474	-6.736876	1.364181
116	6	0	-18.551073	-7.653786	-1.662467
117	1	0	22.455554	-0.636275	-0.472241
118	1	0	22.095428	-6.231066	0.003953

119	1	0	20.378341	-6.590202	-0.292291
120	1	0	19.885673	-6.303579	2.11686
121	1	0	20.942998	-8.442175	2.867868
122	1	0	20.381174	-8.569177	1.193192
123	1	0	22.10681	-8.346568	1.538102
124	1	0	21.743142	-6.193853	3.793287
125	1	0	21.732193	-4.747839	2.775828
126	1	0	22.926694	-6.019577	2.483426
127	1	0	16.852886	-3.373767	-0.098869
128	1	0	10.837458	-1.486818	-0.132784
129	1	0	14.393754	-4.160626	-1.285963
130	1	0	13.865841	-2.800718	-2.256624
131	1	0	13.726311	-2.366008	2.027362
132	1	0	12.456756	-3.312457	1.2779
133	1	0	14.026325	-4.769175	2.525685
134	1	0	14.099501	-5.178536	0.810159
135	1	0	15.391478	-4.221159	1.549835
136	1	0	12.225221	-4.655693	-2.367199
137	1	0	11.467935	-3.251439	-1.613837
138	1	0	11.989306	-4.623199	-0.617892
139	1	0	9.000262	6.659252	-1.467772
140	1	0	10.718956	6.391087	-1.094536
141	1	0	8.495965	6.894747	0.944706
142	1	0	10.343284	7.174652	2.61145
143	1	0	10.359048	5.543121	1.93024
144	1	0	11.538142	6.739416	1.374559
145	1	0	9.522772	9.158898	1.216779
146	1	0	8.968344	8.911799	-0.44668
147	1	0	10.69507	8.792626	-0.05757
148	1	0	6.051908	-0.672161	-0.218545
149	1	0	-0.224995	-0.436321	-0.120358
150	1	0	3.887218	-2.046198	-1.391885
151	1	0	3.007038	-0.840594	-2.308991
152	1	0	2.809015	-0.591491	1.986723
153	1	0	1.838093	-1.823929	1.207411
154	1	0	3.744162	-2.848301	2.404613
155	1	0	3.935571	-3.149027	0.675365
156	1	0	4.905828	-1.899242	1.476069
157	1	0	1.905982	-3.054591	-2.47555
158	1	0	0.821357	-1.924137	-1.664212
159	1	0	1.69965	-3.144775	-0.724333
160	1	0	-4.157127	6.986975	-1.098793
161	1	0	-2.42281	7.164335	-0.743789
162	1	0	-4.669281	6.978992	1.323326

163	1	0	-2.935174	7.66286	2.995061
164	1	0	-2.502533	6.12324	2.240988
165	1	0	-1.686625	7.609564	1.735949
166	1	0	-4.268167	9.419617	1.693835
167	1	0	-4.762861	9.106741	0.022588
168	1	0	-3.059751	9.42865	0.400743
169	1	0	-5.056538	-0.90862	-0.178007
170	1	0	-11.173001	-2.337607	-0.058367
171	1	0	-6.801283	-2.749299	-1.411913
172	1	0	-7.979255	-1.775806	-2.268608
173	1	0	-8.175112	-1.784606	2.034111
174	1	0	-8.799658	-3.192069	1.198706
175	1	0	-6.674283	-3.732551	2.342324
176	1	0	-6.435996	-3.893943	0.600289
177	1	0	-5.816147	-2.470479	1.457172
178	1	0	-8.463605	-4.191458	-2.539871
179	1	0	-9.795518	-3.423084	-1.674883
180	1	0	-8.61612	-4.412439	-0.794761
181	1	0	-16.933661	3.820578	-0.688867
182	1	0	-15.302307	4.433029	-0.329549
183	1	0	-17.391933	3.572117	1.730822
184	1	0	-15.875146	4.614156	3.42934
185	1	0	-15.064861	3.276315	2.604541
186	1	0	-14.673705	4.945085	2.166679
187	1	0	-17.640914	6.01373	2.212967
188	1	0	-18.05834	5.656128	0.529502
189	1	0	-16.494626	6.397102	0.920159
190	1	0	-15.710409	-4.066729	-0.117854
191	1	0	-21.263342	-7.07053	-0.06614
192	1	0	-23.340855	-5.469132	0.011824
193	1	0	-16.926559	-6.254357	-1.426065
194	1	0	-18.325268	-5.587463	-2.243676
195	1	0	-18.47241	-5.819497	2.053885
196	1	0	-18.714906	-7.307377	1.161195
197	1	0	-16.510584	-7.316485	2.284465
198	1	0	-16.256064	-7.341957	0.537451
199	1	0	-16.022015	-5.840117	1.450683
200	1	0	-18.16733	-8.032848	-2.616329
201	1	0	-19.644296	-7.673939	-1.719556
202	1	0	-18.238729	-8.356625	-0.882128

The TPDBDT optimized geometries of the stationary points

Stand orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-20.86846	-1.85924	-0.51446
2	6	0	-22.28966	-1.82569	-0.57767
3	6	0	-22.82679	-0.57639	-0.57757
4	16	0	-21.55842	0.61182	-0.49523
5	6	0	-20.2763	-0.6106	-0.46461
6	6	0	-20.44974	-3.28039	-0.52909
7	7	0	-21.64444	-4.022	-0.61518
8	6	0	-22.80217	-3.21834	-0.63305
9	6	0	-21.67372	-5.48097	-0.62211
10	6	0	-21.32398	-6.1133	-1.98348
11	6	0	-21.28303	-7.64059	-1.83138
12	6	0	-22.29963	-5.6883	-3.08839
13	8	0	-19.34079	-3.78774	-0.47246
14	8	0	-23.94344	-3.63122	-0.67916
15	6	0	-16.37383	-0.20008	-0.28946
16	6	0	-15.00212	-0.39395	-0.22416
17	6	0	-14.19034	0.75457	-0.1452
18	6	0	-14.76141	2.06566	-0.14492
19	6	0	-16.14725	2.25483	-0.2108
20	6	0	-16.9588	1.09859	-0.28287
21	6	0	-12.76834	0.78776	-0.07673
22	6	0	-12.2353	2.05399	-0.05146
23	16	0	-13.49796	3.29848	-0.10605
24	6	0	-18.38428	1.04998	-0.34983
25	6	0	-18.88669	-0.22698	-0.39628
26	16	0	-17.60021	-1.45461	-0.35097
27	8	0	-14.44136	-1.64855	-0.19841
28	8	0	-16.80236	3.44662	-0.25885
29	6	0	-16.34901	4.55667	0.53986
30	6	0	-17.49738	5.55496	0.68976
31	6	0	-18.68093	4.96789	1.4695
32	6	0	-16.968	6.83665	1.35169
33	6	0	-14.1912	-2.23428	-1.49525
34	6	0	-13.55186	-3.60669	-1.29731
35	6	0	-14.47344	-4.55328	-0.517
36	6	0	-13.15836	-4.19448	-2.66052
37	6	0	-8.73168	3.46507	0.1198
38	6	0	-10.1478	3.58009	0.05895
39	6	0	-10.83141	2.38289	0.0167

40	16	0	-9.64109	1.07147	0.06172
41	6	0	-8.25796	2.16731	0.12421
42	6	0	-8.15628	4.83006	0.13387
43	7	0	-9.26059	5.69685	0.09414
44	6	0	-10.49421	5.02133	0.03469
45	6	0	-9.13195	7.15063	0.06466
46	6	0	-8.82882	7.78582	1.43587
47	6	0	-8.60609	9.2937	1.251
48	6	0	-9.93402	7.50639	2.4624
49	8	0	-6.99531	5.20903	0.16658
50	8	0	-11.57881	5.57158	-0.02931
51	6	0	-4.41091	1.38689	0.2531
52	6	0	-3.02435	1.45517	0.28297
53	6	0	-2.31072	0.23874	0.25806
54	6	0	-3.01371	-1.00105	0.23898
55	6	0	-4.40343	-1.06817	0.23245
56	6	0	-5.11891	0.14733	0.22252
57	6	0	-0.90034	0.04055	0.24371
58	6	0	-0.52332	-1.28364	0.22168
59	16	0	-1.92472	-2.37665	0.21402
60	6	0	-6.53275	0.33366	0.16887
61	6	0	-6.91179	1.6543	0.16814
62	16	0	-5.51413	2.75378	0.22177
63	8	0	-2.36476	2.66029	0.28362
64	8	0	-5.04017	-2.2782	0.16723
65	6	0	-5.62564	-2.75328	1.40217
66	6	0	-6.38296	-4.04703	1.11541
67	6	0	-5.45476	-5.14097	0.57156
68	6	0	-7.11681	-4.503	2.38517
69	6	0	-2.05794	3.18808	1.59318
70	6	0	-1.31177	4.50967	1.42635
71	6	0	-2.16022	5.54872	0.68159
72	6	0	-0.8614	5.0253	2.80114
73	6	0	2.79914	-3.08804	0.18208
74	6	0	1.37879	-3.03837	0.22518
75	6	0	0.83527	-1.77148	0.18881
76	16	0	2.1675	-0.60822	0.07966
77	6	0	3.4175	-1.85449	0.10996
78	6	0	3.21812	-4.50718	0.25975
79	7	0	2.02146	-5.23838	0.36018
80	6	0	0.87247	-4.42818	0.32898
81	6	0	1.96241	-6.69569	0.42107
82	6	0	1.68159	-7.25673	1.82875
83	6	0	1.52639	-8.78162	1.73914

84	6	0	2.76836	-6.86439	2.83788
85	8	0	4.32961	-5.01259	0.24034
86	8	0	-0.26754	-4.85417	0.3757
87	6	0	7.32821	-1.51951	0.00452
88	6	0	8.69732	-1.74795	1.63E-04
89	6	0	9.54626	-0.62465	-0.08754
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91	6	0	7.61537	0.91288	-0.14367
92	6	0	6.76523	-0.20925	-0.05816
93	6	0	10.96943	-0.58931	-0.13993
94	6	0	11.49351	0.68112	-0.22764
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96	6	0	5.33905	-0.23221	-0.01105
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105	6	0	9.53807	-3.51324	1.3541
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107	6	0	11.3079	-5.02227	0.35266
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113	6	0	15.4737	0.79199	-0.3599
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115	7	0	14.46636	4.31445	-0.55598
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121	8	0	16.73127	3.82472	-0.62358
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151	1	0	-22.26723	-8.03558	-1.5476
152	1	0	-22.02242	-6.14721	-4.04443
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191	1	0	-4.68822	-5.40813	1.31078
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196	1	0	-1.4436	2.45922	2.13952
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210	1	0	2.53692	-7.26893	3.82992
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212	1	0	3.74829	-7.2531	2.53445
213	1	0	11.57599	-1.4878	-0.12904
214	1	0	4.71376	0.65192	-0.02615
215	1	0	5.80946	1.93366	-1.76115

216	1	0	7.38059	2.66695	-2.17264
217	1	0	5.218	3.93286	-0.42878
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221	1	0	4.80078	5.45463	-2.37732
222	1	0	4.47248	3.76557	-2.79716
223	1	0	5.9688	4.54752	-3.34742
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225	1	0	8.64499	-3.47221	1.99186
226	1	0	9.25434	-5.52769	0.74308
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228	1	0	11.121	-4.60743	-0.64205
229	1	0	12.13574	-4.46181	0.80792
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239	1	0	14.2908	6.79735	2.64259
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243	1	0	24.19629	-3.0648	-0.47724
244	1	0	16.47441	-1.84472	-0.26134
245	1	0	18.96686	-4.10931	1.7726
246	1	0	17.47331	-3.22089	1.38238
247	1	0	16.63641	-5.17558	0.11358
248	1	0	17.75175	-7.40149	0.31395
249	1	0	18.82521	-6.2343	-0.48167
250	1	0	19.08706	-6.66799	1.21813
251	1	0	16.09993	-6.59056	2.11435
252	1	0	15.96354	-4.86437	2.48643
253	1	0	17.3784	-5.78669	3.03517
254	1	0	22.33654	0.97494	-2.4542
255	1	0	20.74437	1.75791	-2.58349
256	1	0	21.63099	3.75435	-1.40599
257	1	0	24.07902	4.03432	-1.01999
258	1	0	23.45344	2.65659	-0.09342
259	1	0	24.37469	2.38317	-1.58657

260	1	0	23.02149	4.61565	-3.30342
261	1	0	21.63941	3.68687	-3.90638
262	1	0	23.25941	2.9658	-3.89492

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