

Supporting Information

Enhanced photoelectrochemical water splitting with a donor-acceptor polyimide

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Scheme R1 Schematic diagram of the photoelectrode production process.

Fig. S1. TG curves of PI-PM, PI-BP, PI-NT and PI-PT with a heating rate of 10 °C/min in the air atmosphere.

Fig. S2. XPS spectra of (a) XPS survey, (b) C 1s, (c) N 1s, (d) O 1s of PI-PM before and after the PEC test.

Fig. S3. XPS spectra of (a) XPS survey, (b) C 1s, (c) N 1s, (d) O 1s of PI-BP before and after the PEC test.

Fig. S4. XPS spectra of (a) XPS survey, (b) C 1s, (c) N 1s, (d) O 1s of PI-PT before and after the PEC test.

Fig. S5. DFT calculated ESP distribution of optimized PI-PM, PI-BP and PI-PT models.

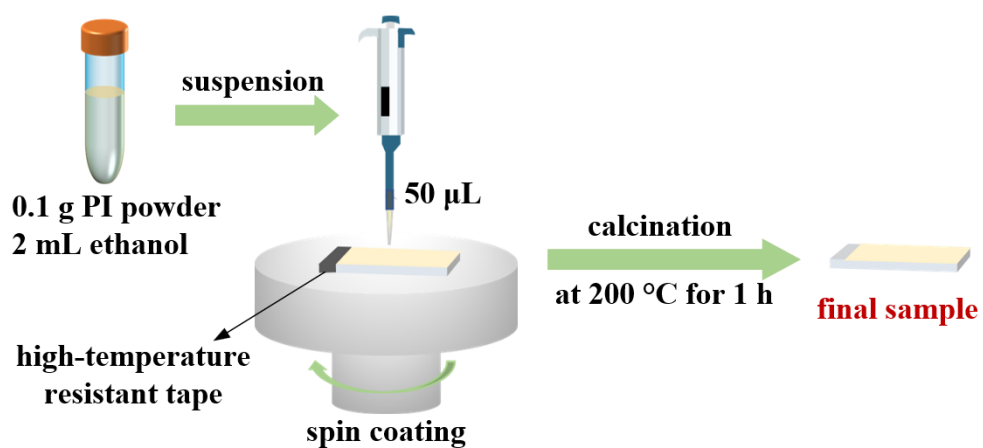
Fig. S6. DFT calculated HOMO and LUMO of optimized PI-PM, PI-BP and PI-PT models.

Text S1. The calculated coordinates of optimized PI-PM model.

Text S2. The calculated coordinates of optimized PI-BP model.

Text S3. The calculated coordinates of optimized PI-NT model.

Text S4. The calculated coordinates of optimized PI-PT model.



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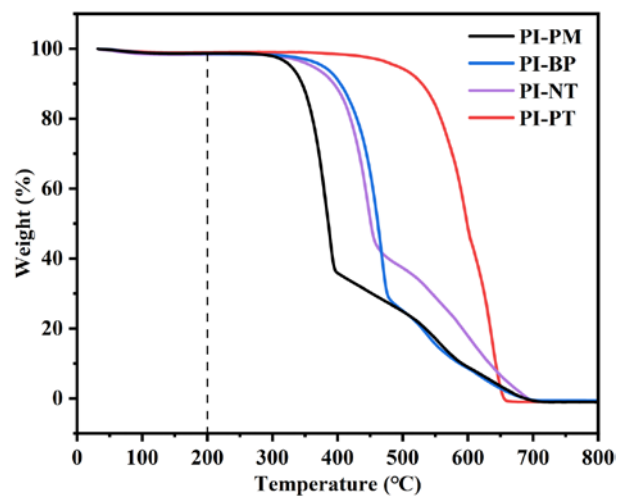


Fig. S1. TG curves of PI-PM, PI-BP, PI-NT and PI-PT with a heating rate of 10 °C/min in the air atmosphere.

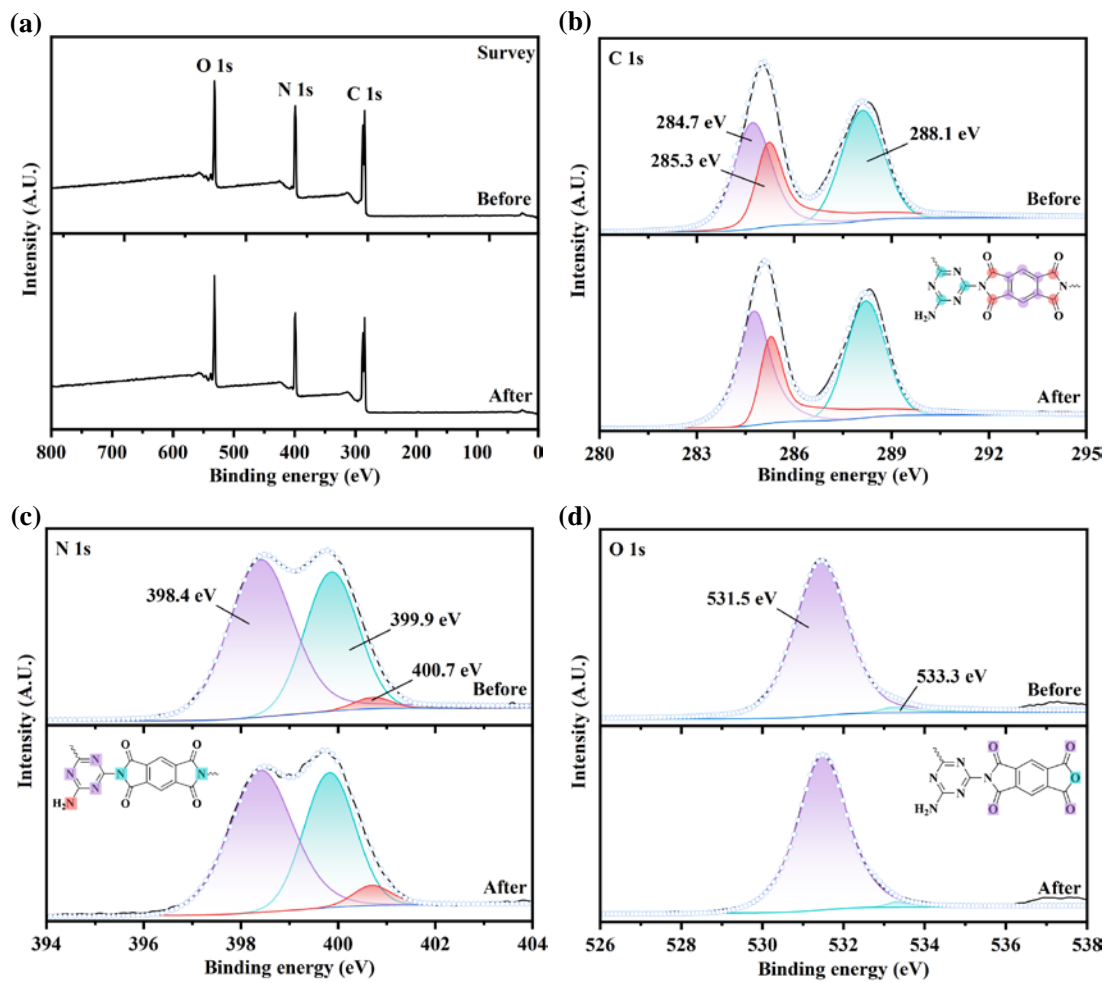


Fig. S2. XPS spectra of (a) XPS survey, (b) C 1s, (c) N 1s, (d) O 1s of PI-PM before and after the PEC test.

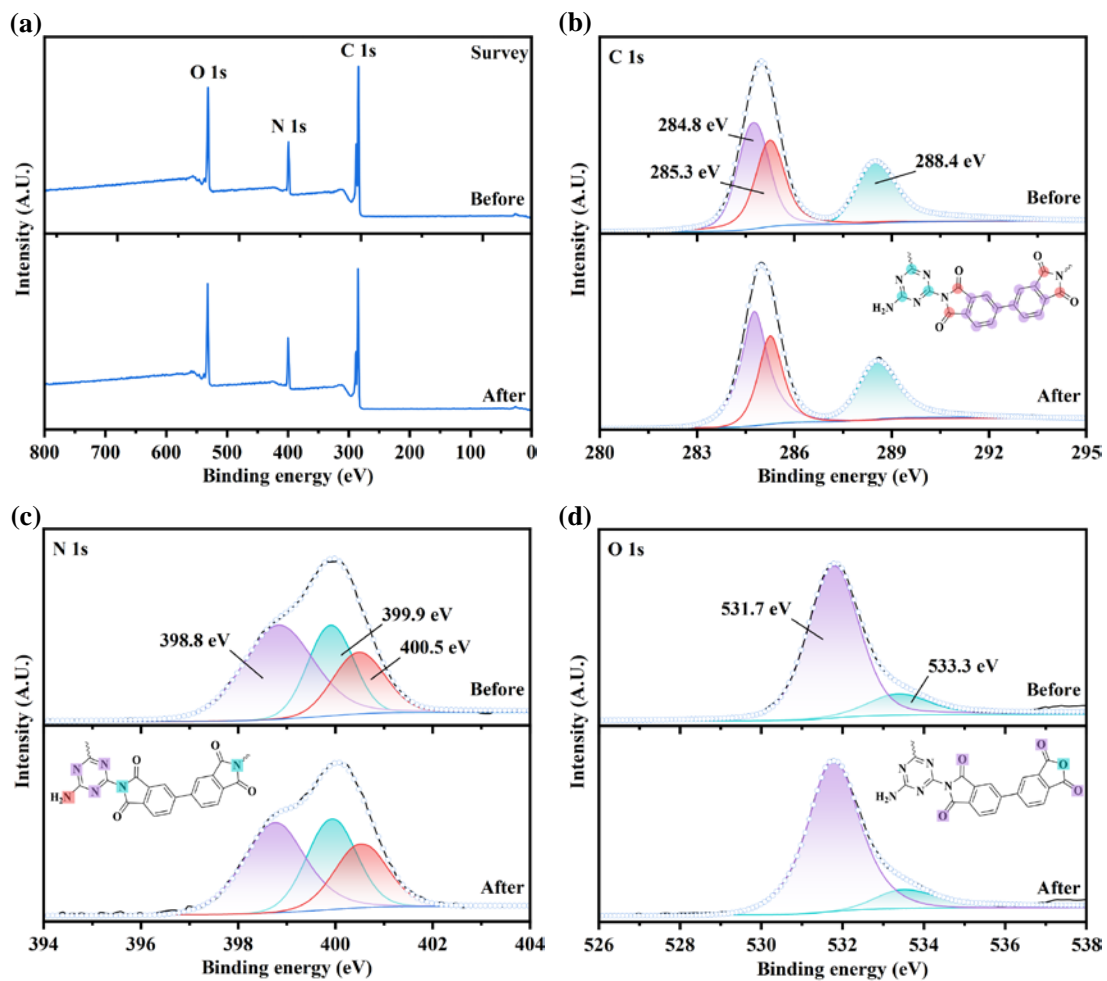


Fig. S3. XPS spectra of (a) XPS survey, (b) C 1s, (c) N 1s, (d) O 1s of PI-BP before and after the PEC test.

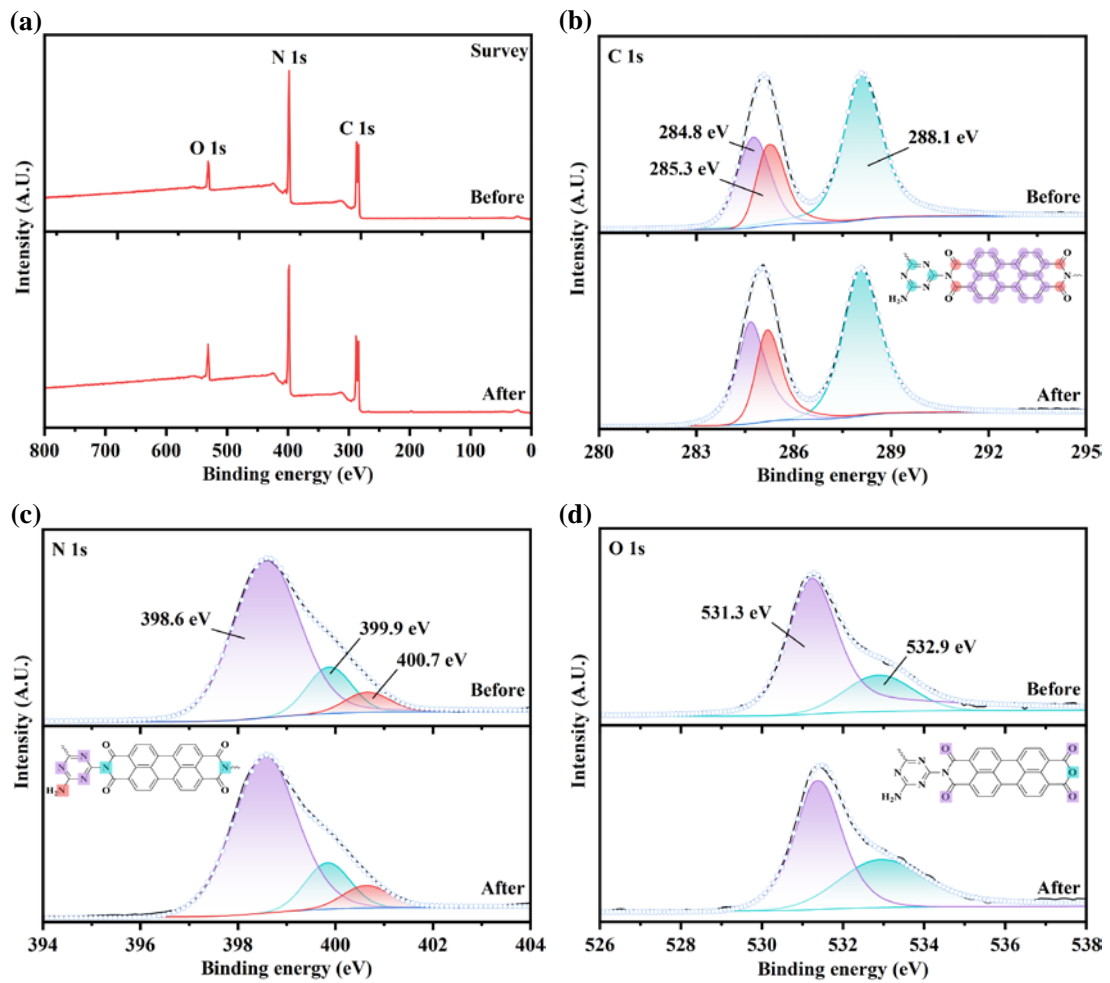


Fig. S4. XPS spectra of (a) XPS survey, (b) C 1s, (c) N 1s, (d) O 1s of PI-PT before and after the PEC test.

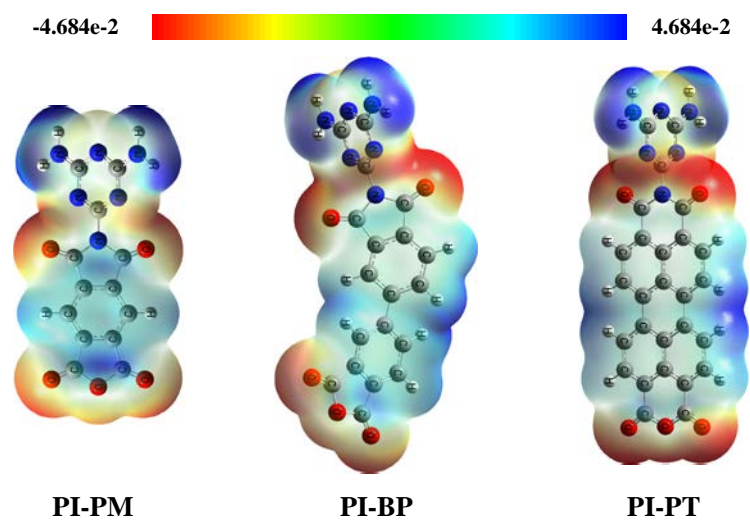


Fig. S5. DFT calculated ESP distribution of optimized PI-PM, PI-BP and PI-PT models.

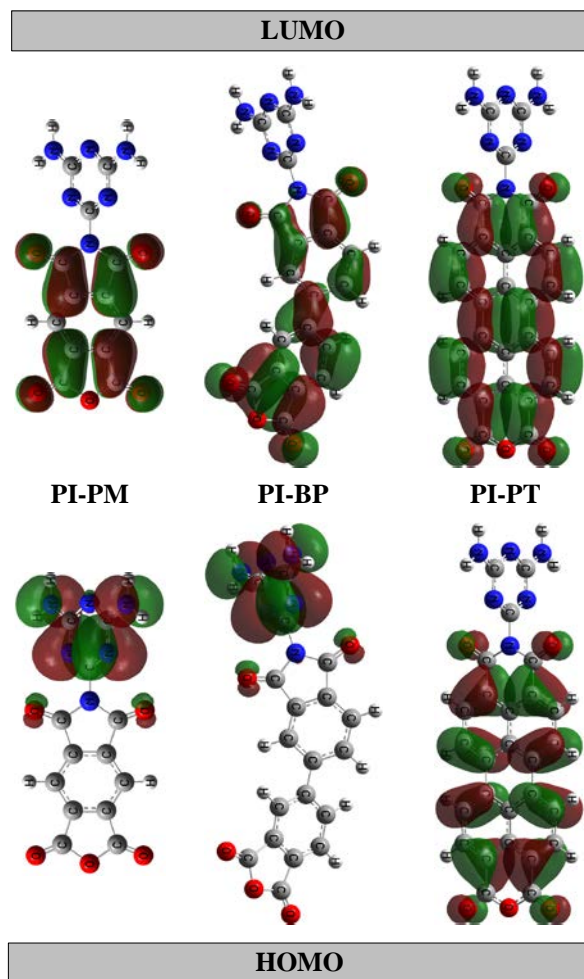


Fig. S6. DFT calculated HOMO and LUMO of optimized PI-PM, PI-BP and PI-PT models.

Text S1. The calculated coordinates of optimized PI-PM model.

Cartesian coordinates (Angstroms):	X	Y	Z
N	-5.24544000	-0.00003900	0.00005600
C	-4.52066200	0.88532900	0.69332300
N	-3.16951300	0.92079900	0.75244800
C	-2.59633400	0.00007600	-0.00013700
N	-3.16954400	-0.92055100	-0.75280700
C	-4.52068700	-0.88536100	-0.69329200
C	1.03849000	-0.67126200	0.19193200
C	1.03852500	0.67133100	-0.19191100
C	2.20772800	1.38971800	-0.40117300
C	3.37988000	0.66956500	-0.19297800
C	3.37984800	-0.66958400	0.19308700
C	2.20766200	-1.38965300	0.40137400
C	-0.38065200	-1.12724600	0.33325800
C	-0.38059600	1.12735000	-0.33333200
C	4.79573400	-1.10361500	0.31777700
C	4.79578600	1.10351600	-0.31771200
O	-0.77634200	-2.20423000	0.68661800
O	-0.77622200	2.20436600	-0.68666100
O	5.25505600	-2.15814800	0.62117500
O	5.25516100	2.15799600	-0.62121500
O	5.59207900	-0.00007800	0.00000200
N	-1.16681300	0.00003600	-0.00015000
N	-5.18099000	-1.81238800	-1.41527100
N	-5.18094100	1.81218400	1.41552500
H	2.20480700	2.43098900	-0.70145900
H	2.20468900	-2.43095700	0.70154300
H	-6.18283500	-1.86301400	-1.35864000
H	-4.65867500	-2.53105700	-1.88480600
H	-4.65865300	2.53105200	1.88478200
H	-6.18282800	1.86247100	1.35934100

Text S2. The calculated coordinates of optimized PI-BP model.

Cartesian coordinates (Angstroms):	X	Y	Z
N	-6.85478200	0.98840700	0.05137700
C	-6.34327900	0.23516900	-0.92918500
N	-5.06285800	-0.18927700	-1.00910800
C	-4.33040000	0.17182300	0.03012800
N	-4.69698100	0.88780500	1.07890000
C	-5.98442500	1.29398400	1.02055400
N	-6.42650900	2.05037000	2.04741900
N	-7.16049900	-0.11557800	-1.94403900
N	-2.97415300	-0.26547000	0.01814900
C	-1.86263400	0.60264900	0.16104400
O	-1.89531200	1.79832100	0.27550100
C	-1.08930100	-1.59666700	-0.09522600
C	-0.17928700	-2.63661000	-0.19346000
C	1.17620700	-2.32119000	-0.10313100
C	1.62088900	-0.99763100	0.08157100
C	0.67589100	0.03934400	0.17635600
C	-0.66485300	-0.28724300	0.08987800
C	-2.58065900	-1.61969300	-0.13862500
O	-3.30886600	-2.56983800	-0.24363500
C	3.07241400	-0.69904500	0.17356800
C	3.93077800	-1.54822000	0.90330500
C	5.29777900	-1.30365000	1.01249700
C	5.79849000	-0.18016000	0.37109400
C	4.96615300	0.66628100	-0.34774400
C	3.60630400	0.43420200	-0.46307900
C	5.80325700	1.75566200	-0.91058900
O	5.50891100	2.68834800	-1.58926200
C	7.17743900	0.35557300	0.28726000
O	8.19757300	-0.04518800	0.75246700
O	7.11632600	1.51615500	-0.49413500
H	-7.34746500	2.44973900	2.00211900
H	-5.76377700	2.37927700	2.72764500
H	-6.82301200	-0.75490900	-2.64204100
H	-8.13771300	0.11186800	-1.89126100
H	-0.51243200	-3.65714800	-0.34498600
H	1.90964400	-3.11350900	-0.20637700
H	0.97903100	1.06731400	0.34111000
H	3.50661500	-2.40415000	1.41635800
H	5.94490800	-1.96007600	1.58291300
H	2.98105000	1.09794500	-1.04916100

Text S3. The calculated coordinates of optimized PI-NT model.

Cartesian coordinates (Angstroms):	X	Y	Z
C	-0.55849400	1.23341500	-0.00029900
C	-1.25937800	2.42510000	-0.00024200
C	-2.66478600	2.42553800	-0.00026100
C	-3.36426600	1.23213300	-0.00013900
C	-2.67058000	-0.00000200	-0.00021400
C	-1.25068200	-0.00000100	-0.00047900
C	-0.55849600	-1.23341300	-0.00052900
C	-1.25938300	-2.42510100	-0.00000900
C	-2.66479000	-2.42554000	0.00023800
C	-3.36426800	-1.23213500	0.00001900
C	-4.84509700	-1.23853100	0.00025900
C	-4.84509000	1.23854100	0.00003100
C	0.93097800	-1.25439900	-0.00018400
C	0.93098700	1.25437900	-0.00016600
O	-5.52803400	-2.21986800	0.00046400
O	-5.52802400	2.21988300	0.00004300
O	-5.47448100	0.00000600	0.00019400
O	1.57362200	-2.28073100	0.00001500
O	1.57363900	2.28070400	-0.00012400
N	1.55997300	-0.00000700	-0.00011600
N	5.65676500	-0.00005600	0.00020500
C	4.93293800	-0.00025400	-1.12440100
N	3.58055700	-0.00025900	-1.18800700
C	3.01351200	-0.00001200	-0.00000300
N	3.58037200	0.00030900	1.18808900
C	4.93276000	0.00022800	1.12470600
N	5.59332500	0.00050900	2.29910500
N	5.59368100	-0.00059700	-2.29868800
H	-0.70379900	3.35515000	-0.00026700
H	-3.21763700	3.35734500	-0.00035300
H	-0.70381100	-3.35515500	0.00034800
H	-3.21764200	-3.35734800	0.00056400
H	5.07239900	0.00040300	3.15801400
H	6.59778500	0.00034400	2.30632200
H	5.07288200	0.00024300	-3.15766900
H	6.59814100	0.00009800	-2.30575700

Text S4. The calculated coordinates of optimized PI-PT model.

Cartesian coordinates (Angstroms):	X	Y	Z
N	-7.83969500	0.00075900	-0.00039700
C	-7.11463200	0.00046100	-1.12435200
N	-5.76317000	-0.00013100	-1.18786400
C	-5.19412400	-0.00052200	0.00006200
N	-5.76356300	-0.00035600	1.18775000
C	-7.11504600	0.00026200	1.12376100
N	-7.77635000	0.00072200	2.29857600
N	-7.77563400	0.00065200	-2.29931700
N	-3.74279000	-0.00063200	0.00013700
C	-3.10837400	-1.25054400	0.00025400
C	2.67986300	-1.24870200	0.00016600
C	3.37536700	0.00004100	0.00016100
C	4.80302900	0.00016500	0.00002000
C	5.51340000	-1.22225800	-0.00010300
C	4.82129100	-2.41848900	-0.00018700
C	3.42536500	-2.42721200	0.00000600
C	5.51318100	1.22271400	-0.00006600
C	4.82085900	2.41882400	0.00019900
C	3.42493100	2.42729700	0.00035000
C	2.67964100	1.24865700	0.00032000
C	-1.62376300	1.22345900	0.00020800
C	-0.93103600	2.41748600	0.00022800
C	0.46589500	2.42596000	0.00016100
C	1.21013200	1.24801600	0.00034400
C	0.51427000	-0.00023500	0.00022800
C	-0.91415200	-0.00036200	0.00024100
C	-1.62352400	-1.22430000	0.00032200
C	-0.93059900	-2.41820800	0.00021300
C	0.46632600	-2.42643000	0.00012800
C	1.21036100	-1.24834200	0.00024000
C	-3.10856000	1.24946800	-0.00002400
O	-3.75037300	-2.27987200	0.00033600
O	-3.75090000	2.27851000	-0.00012100
C	6.98936300	-1.23310900	-0.00030700
O	7.67003600	-2.21876600	-0.00049800
C	6.98914100	1.23382800	-0.00016100
O	7.66962700	2.21959500	-0.00013900
O	7.62520600	0.00041900	-0.00030700
H	-8.78072100	0.00119900	2.30556000
H	-7.25502000	0.00043500	3.15715600
H	-7.25411900	0.00233000	-3.15778100
H	-8.77999700	0.00303700	-2.30651200

H	5.37920900	-3.34738800	-0.00034500
H	2.92829400	-3.38805200	0.00006500
H	5.37860900	3.34782400	0.00016600
H	2.92770500	3.38805700	0.00046500
H	-1.49151200	3.34474900	0.00001200
H	0.96294600	3.38705200	0.00012400
H	-1.49093000	-3.34555700	0.00020000
H	0.96354600	-3.38743400	0.00007100