Electronic supplementary information for

Highly responsive ethylenediamine vapor sensor based on perylenediimide–camphorsulfonic acid complex *via* ionic self-assembly

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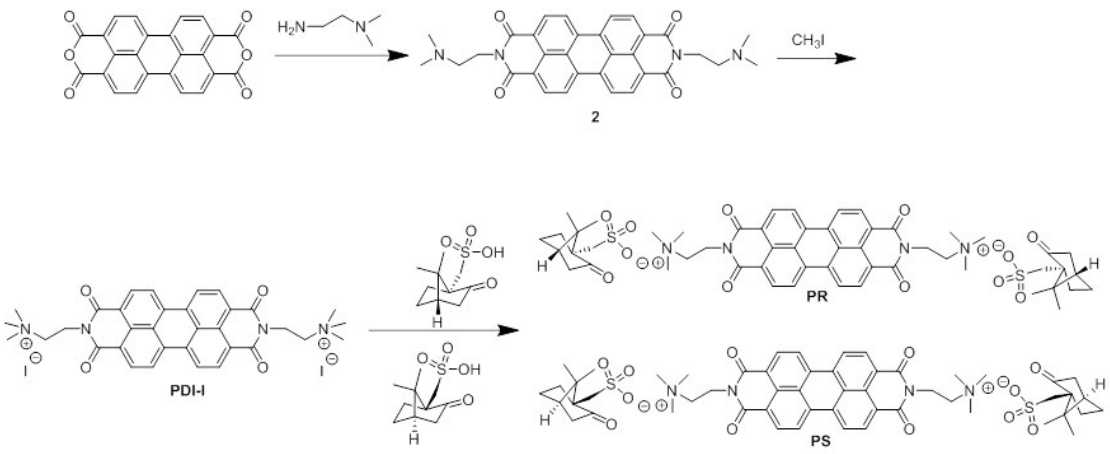
1. Synthesis of PR and PS



***N*,*N'*-Bis(2-(dimethylammoethyl)perylene-3,4,9,10-tetracarboxyldiimide (2)**

3,4:9,10-perylenedicarboximide (2.00 g, 5 mmol) and N, N'-dimethylethylenediamine (7.05 g, 80 mmol) was stirred in 20 mL 1-benzazine for 24 h at 160 ^{o}C under argon atmosphere. The mixture was cooled to room temperature, subsequently added 50 mL CH_3OH into the mixture, then stirred overnight and filtered, and dried in vacuum at 60 ^{o}C to give dark red **2** (2.40 g). This product was used in the next step without further purification.

***N*,*N'*-Bis(2-(trimethylammoniumiodide)ethylene)perylene-3,4,9,10-tetracarboxyldiimide iodide (PDI-I)**

2 (1.33 g, 2.5 mmol) and iodomethane (2.84 g, 20 mmol) was stirred in methylbenzene (80 mL) for 6 h at 100 ^{o}C. The mixture was cooled to room temperature, stirred overnight and filtered, washed with ether, and dried in vacuum at 60 ^{o}C to give dark red **PDI-I** (1.55 g, 76 %).^{1}H NMR (400 MHz, DMSO-d_6): δ 8.66 (d, 4 H, J = 8 Hz), 8.40 (d, 4 H, J = 8 Hz), 4.48-4.52 (m, 4 H), 3.67-3.70 (m, 4 H), 3.28-3.33 (m, 18 H).

***N*,*N'*-bis(2-(trimethylammoniumethylene)perylene-3,4,9,10-tetracarboxyldiimide-(*R*)-(-)-camphorsulfonic acid salt (PR)**

3 (0.05 g, 0.06 mmol) and (R)-(-)-camphorsulfonic acid (0.14 g, 0.60 mmol) was

stirred in CH_3OH (20 mL) for 24 h at 70 °C, then methylbenzene (150 mL) was added, the mixture was stirred overnight. The precipitate was recovered by filtration, dried in vacuum at 60 °C. This solid was further purified by recrystallization with ethanol to give the dark red solid (0.04 g, 65.03%).^{1}H NMR (400 MHz, DMSO-d_6): δ 9.02 (d, 4 H, J = 8 Hz), 8.65 (d, 4 H, J = 8 Hz), 4.51 (m, 4 H), 3.66 (m, 4 H), 3.24 (s, 18 H), 2.85 (d, 2 H J = 16 Hz), 2.70 (m, 4 H), 2.35 (d, 2 H J = 16 Hz), 2.25 (m, 1 H), 2.21 (m, 1 H), 1.93 (m, 2 H), 1.79 (m, 2 H), 1.25 (m, 4 H), 1.02 (s, 6 H), 0.74 (s, 6 H). Anal. Calcd for $C_{54}H_{64}N_4O_{12}S_2$: C, 63.26; H, 6.29; N, 5.46; S, 6.25. Found: C, 63.29; H, 6.24; N, 5.38; S, 6.21.

_N_,_N_′-bis(2-(trimethylammoniumethylene)perylene-3,4,9,10-tetracarboxyldiimide-(_S_)-(+)-camphorsulfonic acid salt (PS)

3 (0.05 g, 0.06 mmol) and (1S)-(+)-10-camphorsulfonic acid (0.14 g, 0.60 mmol)was stirred in CH_3OH (20 mL) for 24 h at 70 °C, then methylbenzene (150 mL) was added, the mixture was stirred overnight. The precipitate was recovered by filtration, dried in vacuum at 70 °C. This solid was further purified by recrystallization with ethanol to give the dark red solid (0.05 g, 83.33%).^{1}H NMR (400 MHz, DMSO-d_6): δ 8.86 (d, 4 H, J = 8 Hz), 8.54 (d, 4 H, J = 8 Hz), 4.51 (m, 4 H), 3.68 (m, 4 H), 3.26 (s, 18 H), 2.86 (d, 2 H J = 16 Hz), 2.68 (m, 4 H), 2.36 (d, 2 H J = 16 Hz), 2.25 (m, 1 H), 2.21 (m, 1 H), 1.93 (m, 2 H), 1.79 (m, 2 H), 1.25 (m, 4 H), 1.04 (s, 6 H), 0.73 (s, 6 H). Anal. Calcd for $C_{54}H_{64}N_4O_{12}S_2$: C, 63.26; H, 6.29; N, 5.46; S, 6.25. Found: C, 63.31; H, 6.27; N, 5.42; S, 6.20.

2. Supporting Figures and Table

Table S1 The dipole moment of the liquid analytes tested[1] and the corresponding increment of current measured at concentration of 100 ppm.

analytes	μ (D)	Current (PS/PR, μA)
ethylenediamine	1.99±0.10	0.176/0.016
hydrazine	1.75±0.09	0.05/0.004
ammonia	1.4718±0.0002	0.048/0.003
ethylamine	1.22±0.10	0.001/0.001
butylamine	1.0	-/-
triethylamine	0.66±0.05	-/-
diethylamine	0.92±0.05	-/-
aniline	1.13±0.02	-/-

Table S2. The average hydrogen-bonding distances (in Å) in PR and PS monomers and dimers (in bracket) at the different computational levels

	PR		PS	
	$H\text{-}bond_{avg}$		$H\text{-}bond_{avg}$	
	monomer	dimer	monomer	dimer
AM1	2.054	2.197	2.057	2.210
HF/6-31G(d, p)	2.296	2.365	2.128	2.336
BP86/def2-SVP	2.013	2.125	1.994	2.179
BP86-(D3BJ)/def2-SVP	2.001	2.072	1.961	2.144

Table S3. Dimerization energies ΔE(dimerization) (in kcal/mol) at the different computational levels.

Methods	PR dimer	PS dimer
AM1	-17.6	-27.0
HF/6-31G(d, p)	-24.1	-29.6
BP86/def2-SVP	-24.8	-27.9
RI-BP86-(D3BJ)/def2-SVP	-75.6	-107.6

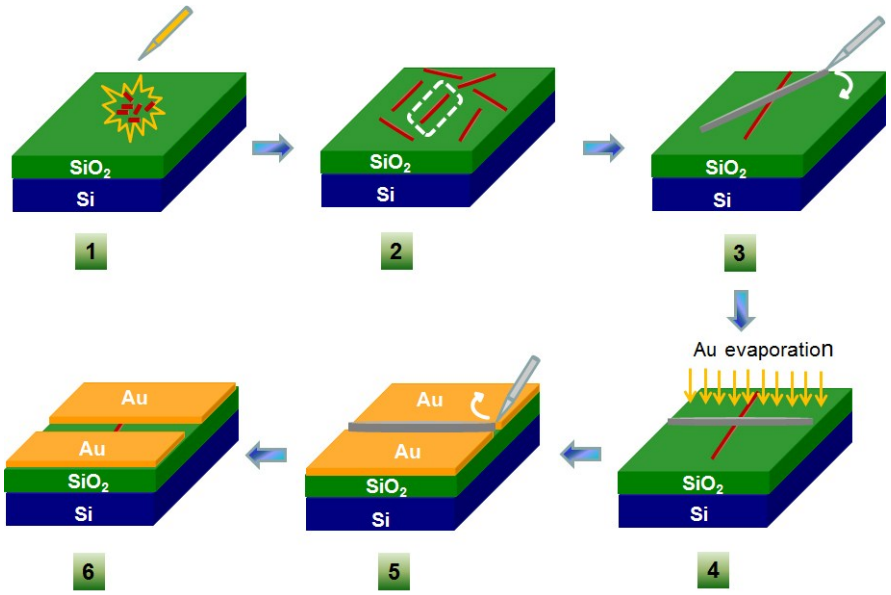


Fig. S1 Schematic diagram of device fabrication by using ‘‘organic ribbon mask’’ technique; the dashed line in Stage **2** shows the selected nanofiber using to prepare the sensing device in next stage.

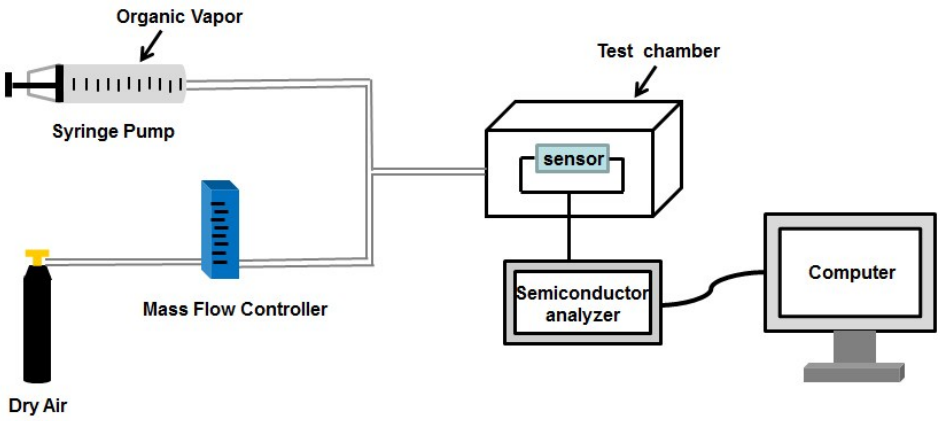


Fig. S2 Schematic diagram for the vapor sensing measurement system.

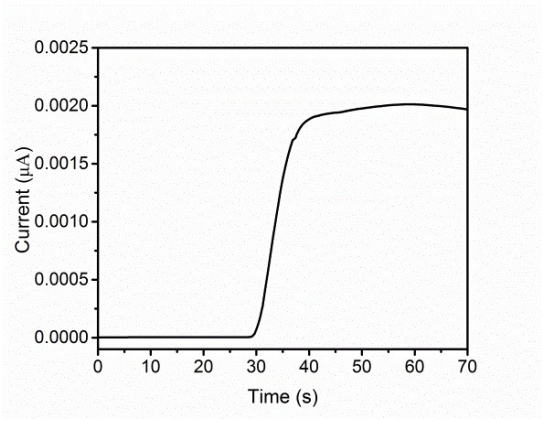


Fig. S3 Responses of PDI-I devices in ethylenediamine vapor (100 ppm).

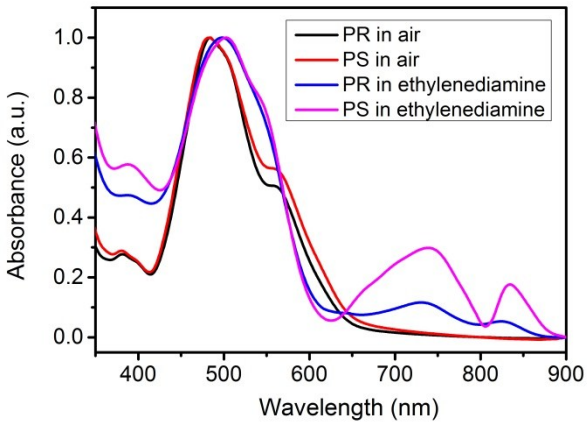


Fig. S4 The absorption spectra of PR and PS films in air and in ethylenediamine vapor (100 ppm).

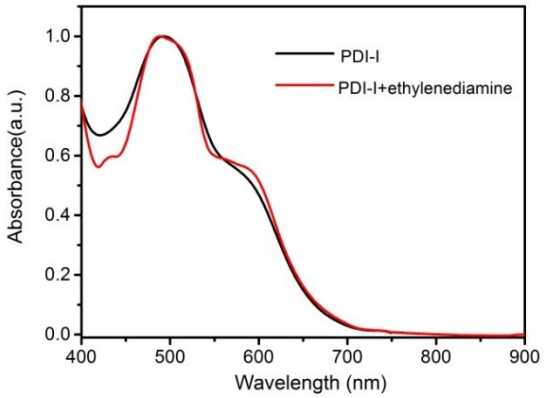
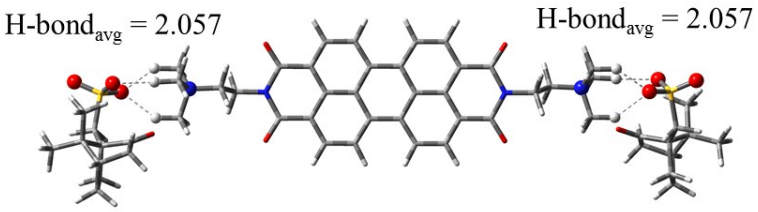


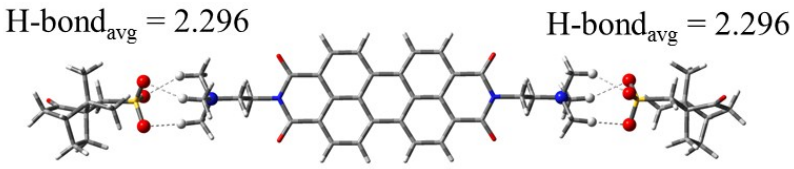
Fig. S5 UV-vis spectra of PDI-I in air and in ethylenediamine (100 ppm).

(a) PR monomer

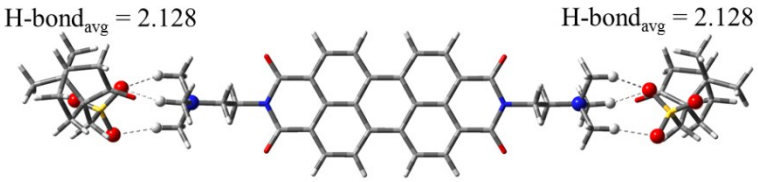


(b) PS monomer

Fig. S6 Optimized structures of (a) PR monomer, and (b) PS monomer at the AM1 level. The average hydrogen bond distances are in Å. The color code, N: blue, O: red, C: gray, H: white.

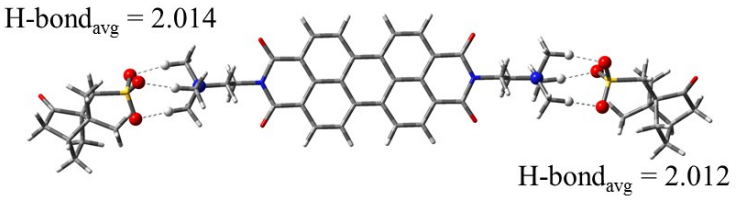


(a) PR monomer

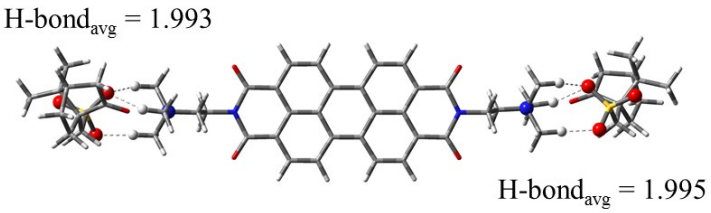


(b) PS monomer

Fig. S7 Optimized structures of (a) PR monomer, and (b) PS monomer at the HF/6-31G(d,p) level. The average hydrogen bond distances are in Å. The color code, N: blue, O: red, C: gray, H: white.

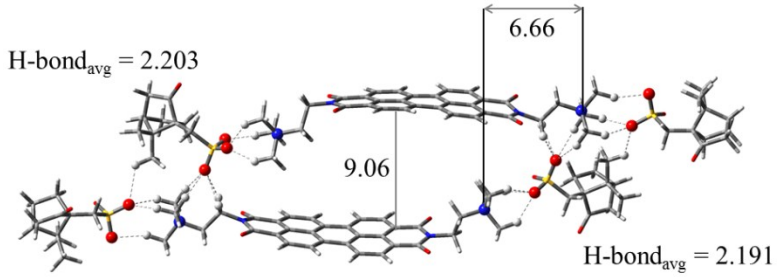


(a) PR monomer



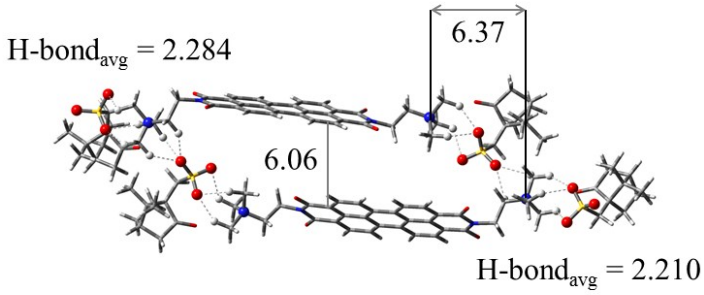
(b) PS monomer

Fig. S8 Optimized structures of (a) PR monomer, and (b) PS monomer at the bp86/def2-SVP level. The average hydrogen bond distances are in Å. The color code, N: blue, O: red, C: gray, H: white.



ΔE(dimerization) = -17.6

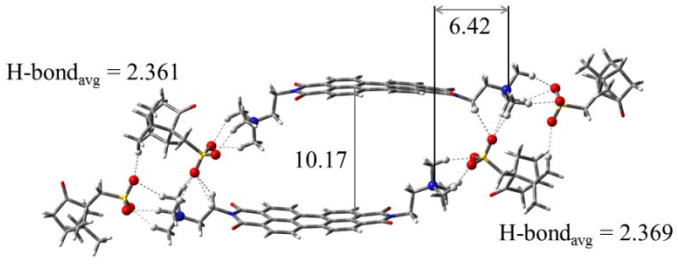
(a) PR dimer



ΔE(dimerization) = -27.0

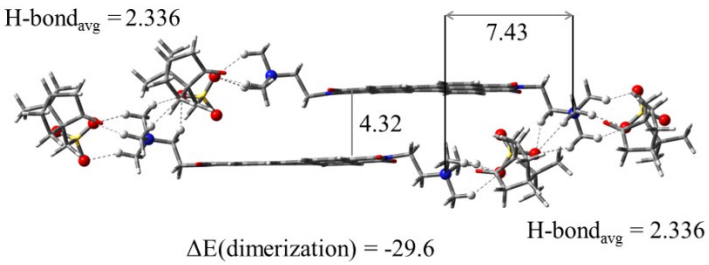
(b) PS dimer

Fig. S9 Optimized structures of (a) PR dimer, and (b) PS dimer at the AM1 level. The average hydrogen bond distances are in Å. Dimerization energies ΔE(dimerization) are in kcal/mol. The color code, N: blue, O: red, C: gray, H: white.



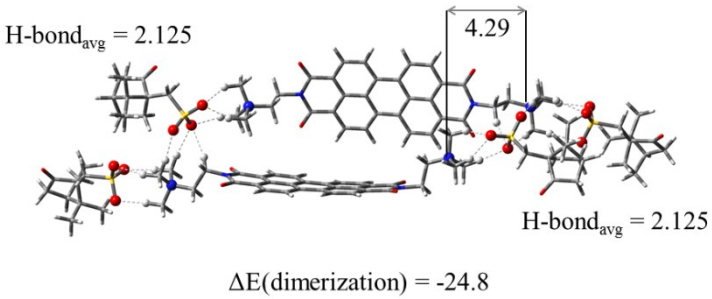
ΔE(dimerization) = -24.1

(a) PR dimer

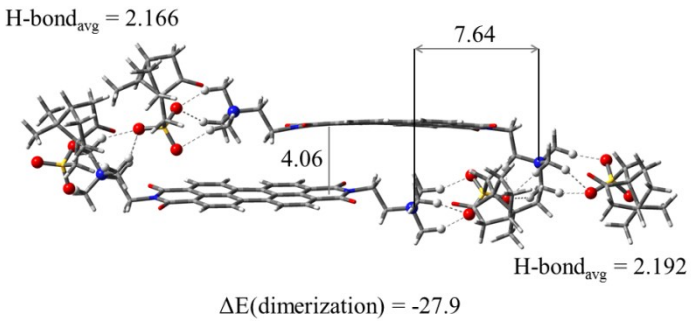


(b) PS dimer

Fig. S10 Optimized structures of (a) PR dimer, and (b) PS dimer at the AM1 level. The average hydrogen bond distances are in Å. Dimerization energies ΔE(dimerization) are in kcal/mol. The color code, N: blue, O: red, C: gray, H: white.



(a) PR dimer



(b) PS dimer

Fig. S11 Optimized structures of (a) PR dimer, and (b) PS dimer at the AM1 level. The average hydrogen bond distances are in Å. Dimerization energies ΔE(dimerization) are in kcal/mol. The color code, N: blue, O: red, C: gray, H: white.

SI x. Coordinates and energies (kcal/mol) of the calculated structures at the BP86-D3(BJ)/def2-SVP level

PR-monomer

Energy = -2517811.1

C	0.1071590	0.7258760	-0.4023853
C	0.2127962	1.4194523	0.8521726
C	0.1084635	0.7254421	2.1065324
C	0.4276712	2.8415111	0.8522983
C	0.5320069	3.5467820	2.0853645
C	0.4234824	2.8529171	3.2947180
C	0.2174456	1.4667837	3.3010831
C	0.2115756	1.4678305	-1.5969892
C	0.4158727	2.8541348	-1.5905131
C	0.5279722	3.5468915	-0.3809450
C	0.7442277	5.0101948	-0.4045687
N	0.8951152	5.6373332	0.8518723
C	0.7497602	5.0106553	2.1108526
O	0.8086401	5.6749615	3.1444923
O	0.7969356	5.6772954	-1.4383108
C	1.1458931	7.0778742	0.8426238
C	-0.1924205	7.8176530	0.7594393
N	-0.0881261	9.3138992	0.5753154
C	0.7230180	9.6451838	-0.6581022
C	-1.4866352	9.8575822	0.3990541
C	0.5362496	9.9635330	1.7864520
C	-0.4868802	15.3820068	-2.7107995
C	-1.7316820	15.9963619	-3.4186063
C	-2.5261624	16.6256182	-2.2466504
C	-1.7260347	17.8498010	-1.7742524
C	-0.5215824	17.1901130	-1.0866610
C	-0.7394996	15.6625449	-1.1916626
C	-2.3092238	15.5834930	-1.0932890
C	-2.8243763	16.0169822	0.2884553
C	-2.9436011	14.2245019	-1.4320682
C	0.1769306	14.9483863	-0.2147845
S	-0.0015158	13.1498774	-0.0047315
O	1.2742841	12.7179693	0.6778343
O	-1.2167881	12.9209868	0.8746598
O	-0.1580141	12.5352827	-1.3812631
O	0.4276712	17.7523588	-0.5734807
H	-3.5909144	16.8336115	-2.4725417
H	0.5053687	3.4217648	4.2319453
H	0.1400433	0.9584362	4.2706091
H	0.1315458	0.9599401	-2.5665076
H	0.4938226	3.4237878	-2.5275828
H	1.6824413	7.3204318	1.7767029
H	1.7718379	7.2944952	-0.0408008
H	-0.7663372	7.4367532	-0.1068364
H	-0.7750059	7.6447974	1.6847654
H	0.5322741	10.7048439	-0.9379094
H	1.7931812	9.5028526	-0.4319820
H	0.4085450	8.9629890	-1.4689623
H	-1.4507773	10.9689870	0.4398442
H	-2.1116047	9.4690759	1.2235906
H	-1.8755163	9.5083927	-0.5739031
H	-0.1387407	9.8142471	2.6478036
H	1.5124841	9.4862596	1.9802774
H	0.6910074	11.0439754	1.5653912
H	-0.4038041	14.2867613	-2.8457689
H	0.4712995	15.8302197	-3.0432504
H	-1.4594539	16.7587005	-4.1760186
H	-2.3257896	15.2208985	-3.9390601
H	-2.2662143	18.4756903	-1.0350351
H	-1.3898199	18.5260814	-2.5866235
H	-2.5694755	15.2326591	1.0291226
H	-2.3887158	16.9709308	0.6472492
H	-3.9281984	16.1307327	0.2781407
H	-2.8226277	13.5264730	-0.5844376
H	-4.0277657	14.3705389	-1.6265875
H	-2.4940889	13.7375486	-2.3154780
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H	0.0747222	15.3521360	0.8111584
C	-0.1071590	-0.7258760	-0.4023853
C	-0.2127962	-1.4194523	0.8521726
C	-0.1084635	-0.7254421	2.1065324
C	-0.4276712	-2.8415111	0.8522983
C	-0.5320069	-3.5467820	2.0853645
C	-0.4234824	-2.8529171	3.2947180
C	-0.2174456	-1.4667837	3.3010831
C	-0.2115756	-1.4678305	-1.5969892
C	-0.4158727	-2.8541348	-1.5905131
C	-0.5279722	-3.5468915	-0.3809450
C	-0.7442277	-5.0101948	-0.4045687
N	-0.8951152	-5.6373332	0.8518723
C	-0.7497602	-5.0106553	2.1108526
O	-0.8086401	-5.6749615	3.1444923

O	-0.7969356	-5.6772954	-1.4383108
C	-1.1458931	-7.0778742	0.8426238
C	0.1924205	-7.8176530	0.7594393
N	0.0881261	-9.3138992	0.5753154
C	-0.7230180	-9.6451838	-0.6581022
C	1.4866352	-9.8575822	0.3990541
C	-0.5362496	-9.9635330	1.7864520
C	0.4868802	-15.3820068	-2.7107995
C	1.7316820	-15.9963619	-3.4186063
C	2.5261624	-16.6256182	-2.2466504
C	1.7260347	-17.8498010	-1.7742524
C	0.5215824	-17.1901130	-1.0866610
C	0.7394996	-15.6625449	-1.1916626
C	2.3092238	-15.5834930	-1.0932890
C	2.8243763	-16.0169822	0.2884553
C	2.9436011	-14.2245019	-1.4320682
C	-0.1769306	-14.9483863	-0.2147845
S	0.0015158	-13.1498774	-0.0047315
O	-1.2742841	-12.7179693	0.6778343
O	1.2167881	-12.9209868	0.8746598
O	0.1580141	-12.5352827	-1.3812631
O	-0.4276712	-17.7523588	-0.5734807
H	3.5909144	-16.8336115	-2.4725417
H	-0.5053687	-3.4217648	4.2319453
H	-0.1400433	-0.9584362	4.2706091
H	-0.1315458	-0.9599401	-2.5665076
H	-0.4938226	-3.4237878	-2.5275828
H	-1.6824413	-7.3204318	1.7767029
H	-1.7718379	-7.2944952	-0.0408008
H	0.7663372	-7.4367532	-0.1068364
H	0.7750059	-7.6447974	1.6847654
H	-0.5322741	-10.7048439	-0.9379094
H	-1.7931812	-9.5028526	-0.4319820
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H	1.4507773	-10.9689870	0.4398442
H	2.1116047	-9.4690759	1.2235906
H	1.8755163	-9.5083927	-0.5739031
H	0.1387407	-9.8142471	2.6478036
H	-1.5124841	-9.4862596	1.9802774
H	-0.6910074	-11.0439754	1.5653912
H	0.4038041	-14.2867613	-2.8457689
H	-0.4712995	-15.8302197	-3.0432504
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H	2.3257896	-15.2208985	-3.9390601
H	2.2662143	-18.4756903	-1.0350351
H	1.3898199	-18.5260814	-2.5866235
H	2.5694755	-15.2326591	1.0291226
H	2.3887158	-16.9709308	0.6472492
H	3.9281984	-16.1307327	0.2781407
H	2.8226277	-13.5264730	-0.5844376
H	4.0277657	-14.3705389	-1.6265875
H	2.4940889	-13.7375486	-2.3154780
H	-1.2337668	-15.0894044	-0.5139898
H	-0.0747222	-15.3521360	0.8111584

PS-monomer

Energy = -2517808.4

C	-2.7732275	0.9611010	2.0597930
C	-3.4425526	0.9738383	0.8319234
C	-2.7507547	0.6027622	-0.3564124
C	-1.3661074	0.2193158	-0.2929883
C	-0.6954616	0.2192674	0.9783980
C	-1.4233409	0.5915240	2.1275395
C	-3.4332746	0.6049338	-1.6064643
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References

1 W. M. Haynes, CRC *Handbook of Chemistry and Physics*, 91st ed; CRC Press: Boulder, CO, USA, 2010-2011.