

Electronic Supplementary Information *for*

Rational Design of Reversibly Photochromic Molecules with Aggregation-Induced Emission by Introducing Photoactive Thienyl and Benzothienyl Groups

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Table of Contents

1. Experimental Section

2. Computational Details

3. Supplementary Schemes and Figures

3.1 Scheme S1. Synthesis routes of 2-TPVT, 3-TPVT, 2-TPVBT and 3-TPVBT.

3.2 Figure S1. Time-resolved PL decay curve of 2-TPVT solid.

3.3 Figure S2. PL spectra and images of solid forms of 2-TPVT (a), 3-TPVT (b), 2-TPVBT (c) and 3-TPVBT (d) before and after UV irradiation.

3.4 Figure S3. Images of solid form of 2-TPVT irradiated by UV light with different wavelengths ranging from 280 nm to 450 nm for 2 min.

3.5 Figure S4. Photochromic recycles of 3-TPVT (a), 2-TPVBT (b), and 3-TPVBT (c) in acetonitrile as a function of exposure to UV-light (365 nm) and visible-light respectively.

3.6 Figure S5. Time-dependent UV-vis absorption spectra of 2-TPVT in sucrose octaacetate film after different periods of UV-light irradiation from 0 to 270 s.

3.7 Figure S6. Time-dependent decoloration processes of the colored films of 3-TPVT (a), 2-TPVBT (b) and 3-TPVBT (c) under continuous white light irradiation.

3.8 Figure S7. Time-resolved PL spectra of 3-TPVT (a), 2-TPVBT (b), and 3-TPVBT (c) in film under continuous UV light irradiation.

3.9 Figure S8. Optimized structures of reactants, *E*-products and *Z*-products of cyclization reactions of TPE, 2-TPVT, 2-TPVBT and 3-TPVBT.

3.10 Figure S9. HOMOs and LUMOs of 3-TPVT, 2-TPVBT and 3-TPVBT calculated with B3LYP/6-311+G(d,p) level.

3.11 Figure S10. HOMOs and LUMOs of *E*-products of 3-TPVT, 2-TPVBT and 3-

TPVBT calculated with B3LYP/6-311+G(d,p) level.

4. Supplementary Tables

4.1 Table S1. Optical properties of the four compounds in solution, film and solid

4.2 Table S2. Compositions of HOMOs and LUMOs of 3-TPVT, 3-TPVBT and 2-TPVBT Calculated at B3LYP/6-311+G(d,p) Level

4.3 Table S3. Compositions of HOMOs and LUMOs of *E*-products of 3-TPVT, 2-TPVBT and 3-TPVBT Calculated at B3LYP/6-311+G(d,p) Level

4.4 Table S4. Experimental and calculated absorption maxima of 3-TPVT, 2-TPVBT and 3-TPVBT and their products in acetonitrile

5. Spectra of Compounds

5.1 ¹H NMR spectrum of 2-(1,2,2-triphenylvinyl)thiophene (2-TPVT) in CDCl₃

5.2 ¹³C NMR spectrum of 2-(1,2,2-triphenylvinyl)thiophene (2-TPVT) in CDCl₃

5.3 ¹H NMR spectrum of 3-(1,2,2-triphenylvinyl)thiophene (3-TPVT) in CDCl₃

5.4 ¹³C NMR spectrum of 3-(1,2,2-triphenylvinyl)thiophene (3-TPVT) in CDCl₃

5.5 ¹H NMR spectrum of 2-(1,2,2-triphenylvinyl)benzo[*b*]thiophene (2-TPVBT) in CDCl₃

5.6 ¹³C NMR spectrum of 2-(1,2,2-triphenylvinyl)benzo[*b*]thiophene (2-TPVBT) in CDCl₃

5.7 ¹H NMR spectrum of 3-(1,2,2-triphenylvinyl)benzo[*b*]thiophene (3-TPVBT) in CDCl₃

5.8 ¹³C NMR spectrum of 3-(1,2,2-triphenylvinyl)benzo[*b*]thiophene (3-TPVBT) in CDCl₃

5.9 Mass spectrum of 2-(1,2,2-triphenylvinyl)thiophene (2-TPVT)

5.10 Mass spectrum of 3-(1,2,2-triphenylvinyl)thiophene (3-TPVT)

5.11 Mass spectrum of 2-(1,2,2-triphenylvinyl)benzo[*b*]thiophene (2-TPVBT)

5.12 Mass spectrum of 3-(1,2,2-triphenylvinyl)benzo[*b*]thiophene (3-TPVBT)

6. Cartesian Coordinates

7. References

1. Experimental Section

Synthesis of 2-(1,2,2-TriPhenylVinyl)Thiophene (2-TPVT). 2-Thienylboronic acid (1.02 g, 9.0 mmol), 1-bromo-1,2,2-triphenylethylene (2.01 g, 6.0 mmol), and potassium carbonate (1.24 g, 9.0 mmol) were dissolved in a mixed solution of toluene (100 mL) and tetrahydrofuran (50 mL). The reaction solution was stirred at room temperature under nitrogen for 30 min, and then Pd (PPh₃)₄ (50 mg, 0.043 mmol) was added. The resulting solution was heated at 80 °C for 16 h. After the reaction was completed, the mixture was poured into water and extracted 3 times with dichloromethane. The organic layer was dried over anhydrous sodium sulfate. After removing the solvent under reduced pressure, the crude product was purified by column chromatography on silica gel (petroleum ether) to obtain a white solid (1.47 g, 72.3%). Molecular formula: C₂₄H₁₈S. ¹H NMR (600 MHz, CDCl₃): δ (ppm) 7.36 (t, J = 7 Hz, 4H), 7.30 (d, J = 8 Hz, 4H), 7.16 (m, J = 7 Hz, 4H), 7.05 (m, J = 7 Hz, 4H), 6.94 (m, J = 7 Hz, 2H). ¹³C NMR (150 MHz, CDCl₃): δ (ppm) 143.78, 143.56, 141.08, 141.05, 131.28, 130.98, 130.87, 130.34, 130.31, 129.52, 128.21, 128.00, 127.95, 127.87, 127.70, 127.58, 127.00, 122.17. MS (EI) m/z: [M⁺], 338.1 (calcd. for C₂₄H₁₈S, 338.1).

Synthesis of 3-(1,2,2-TriPhenylVinyl)Thiophene (3-TPVT). 3-Thienylboronic acid (1.02 g, 9.0 mmol), 1-bromo-1,2,2-triphenylethylene (2.01 g, 6.0 mmol), and potassium carbonate (1.24 g, 9.0 mmol) were dissolved in a mixed solution of toluene (60 mL) and tetrahydrofuran (30 mL). The reaction solution was stirred at room temperature under nitrogen for 30 min, and then Pd (PPh₃)₄ (50 mg, 0.043 mmol) was added. The resulting solution was heated at 80 °C for 18 h. After the reaction was completed, the mixture was poured into water and extracted 3 times with dichloromethane. The organic layer was dried over anhydrous sodium sulfate. After removing the solvent under reduced pressure, the crude product was purified by column chromatography on silica gel (petroleum ether) to obtain a white solid powder (1.43 g, 70.5%). ¹H NMR (600 MHz, CDCl₃): δ (ppm) 7.18 (m, J = 7 Hz, 3H), 7.11 (m, J = 7 Hz, 5H), 7.08-7.05 (m, J = 7 Hz, 5H), 6.99 (m, J = 7 Hz, 3H), 6.73 (d, J = 7 Hz, 1H), 6.56 (d, J = 7 Hz, 1H). ¹³C NMR (150 MHz, CDCl₃): δ (ppm) 144.12, 144.02, 143.43, 143.42, 140.66, 135.47, 131.21, 131.15, 130.83, 130.06, 127.94, 127.65, 127.58, 126.73, 126.57, 126.32, 125.98, 123.65. MS (EI) m/z: [M⁺], 338.1 (calcd.

for C₂₄H₁₈S, 338.1).

Synthesis of 2-(1,2,2-TriphenylVinyl)Benzo[*b*]Thiophene (2-TPVBT). 2-Benzothierylboronic acid (1.02 g, 6.0 mmol), 1-bromo-1,2,2-triphenylethylene (1.34 g, 4.0 mmol), and potassium carbonate (0.83 g, 6.0 mmol) were dissolved in a mixed solution of toluene (60 mL) and tetrahydrofuran (30 mL). The reaction solution was stirred at room temperature under nitrogen for 30 min, and then Pd (PPh₃)₄ (50 mg, 0.043 mmol) was added and the solution heated at 80 °C for 18 h. After the reaction was completed, the mixture was poured into water and extracted 3 times with dichloromethane. The organic layer was dried over anhydrous sodium sulfate. After removing the solvent under reduced pressure, the crude product was purified by column chromatography on silica gel (petroleum ether) to obtain a white solid (0.87 g, 56.1%). Molecular formula: C₂₈H₂₀S. ¹H NMR (600 MHz, CDCl₃): δ (ppm) 7.52 (d, J = 8 Hz, 1H), 7.43 (d, J = 7 Hz, 1H), 7.19 (m, J = 7 Hz, 2H), 7.16 (m, J = 7 Hz, 4H), 7.12 (m, J = 7 Hz, 3H), 7.08 (m, J = 7 Hz, 3H), 7.00 (m, J = 7 Hz, 3H), 6.92 (m, J = 7 Hz, 2H), 6.75 (s, 1H). ¹³C NMR (150 MHz, CDCl₃): δ (ppm) 146.69, 143.07, 143.02, 143.00, 142.91, 140.73, 139.25, 134.09, 131.33, 131.05, 130.98, 128.26, 127.79, 127.62, 127.47, 127.07, 126.65, 126.41, 124.11, 123.93, 123.45, 121.92. MS (EI) m/z: [M⁺], 388.2 (calcd. for C₂₈H₂₀S, 388.1).

Synthesis of 3-(1,2,2-TriPhenylVinyl)Benzo[*b*]Thiophene (3-TPVBT). 1-Bromo-1,2,2-triphenylethylene (1.34g, 4.0 mmol), 2-benzothierylboronic acid (1.02 g, 6.0 mmol), and potassium carbonate (0.83 g, 6.0 mmol) were dissolved in a mixed solution of toluene (60 mL) and tetrahydrofuran (30 mL). The reaction solution was stirred at room temperature under nitrogen for 30 min, then Pd (PPh₃)₄ (50 mg, 0.043 mmol) was added and the solution heated at 80 °C for 18 h. After the reaction was completed, the mixture was poured into water and extracted 3 times with dichloromethane. The organic layer was dried over anhydrous sodium sulfate. After removing the solvent under reduced pressure, the crude product was purified by column chromatography on silica gel (petroleum ether) to obtain a white solid powder (0.91 g, 58.5%). Molecular formula: C₂₈H₂₀S. ¹H NMR (600 MHz, CDCl₃): δ (ppm) 7.69 (t, J = 7 Hz, 1H), 7.30 (m, J = 7 Hz, 1H), 7.15 (t, J = 7 Hz, 1H), 7.09-7.07 (m, J = 7 Hz, 5H), 7.04 (m, J = 7 Hz, 2H), 7.02 (m, J = 7 Hz, 4H), 6.95 (m, J = 7 Hz, 6H). ¹³C NMR (150 MHz, CDCl₃): δ (ppm) 143.86, 143.54, 142.99, 141.99, 139.92, 138.92, 138.73, 134.56, 131.49, 131.46, 130.58, 130.56, 130.14, 130.11, 127.80,

127.63, 127.09, 126.75, 126.65, 123.86, 123.50, 122.51. MS (EI) m/z: [M⁺], 388.1 (calcd. for C₂₈H₂₀S, 388.1).

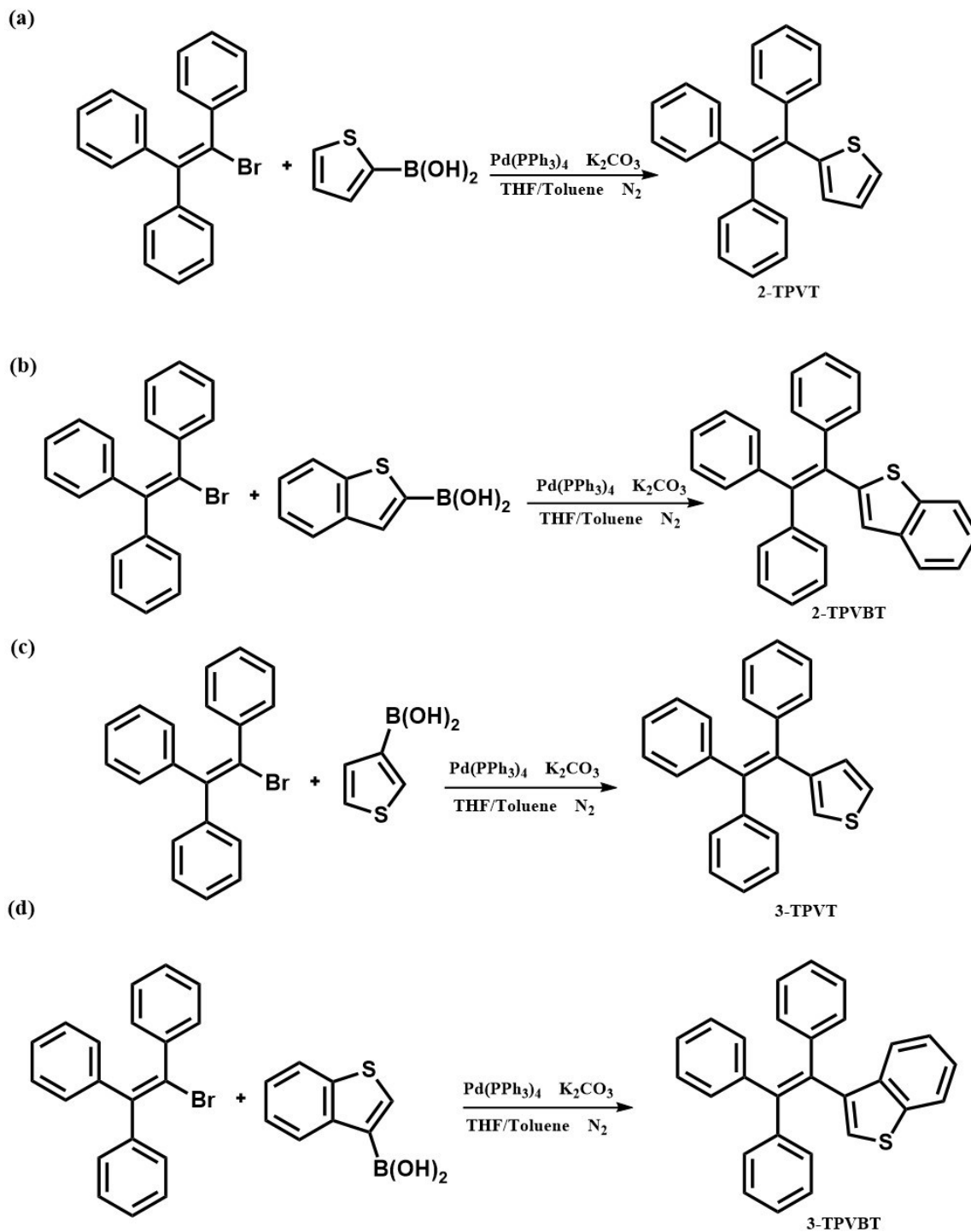
Characterization of UV-Visible and Fluorescence Properties of All Samples.

UV-vis absorption spectra were recorded using an Agilent Cary 5000 UV-Vis-NIR spectrophotometer. Steady PL spectra of all samples were performed on an Edinburgh Instruments model FLS980 fluorescence spectrophotometer equipped with a xenon arc lamp using a front face sample holder. Time-resolved fluorescence measurements were conducted with EPL-series lasers. The absolute PL quantum yields of all samples were determined using an integrating sphere equipped in FLS980 spectrophotometer for at least three times.

2. Computational Details

All the calculations were performed with density functional theory (DFT) and time-dependent density functional theory (TDDFT) implemented in Gaussian 09 program package.¹ The ground state equilibrium geometries and the normal modes of vibration of the single-molecules of TPE, 3-TPVT, 2-TPVT, 3-TPVBT and 2-TPVBT were computed using density functional theory (DFT) with the hybrid B3LYP functional at 6-311+G(d,p) level.² NBO analysis of all the four compounds and their photocyclized products were performed with the same basis set to the optimization. Excitation energies and absorption maxima of all the four molecules and their *E*-products were calculated using PBE0 functional with 6-311+G(d,p) level based on the optimized structure in acetonitrile with SCRF.³

3. Supplementary Schemes and Figures



Scheme S1. Synthesis routes of 2-TPVT, 3-TPVT, 2-TPVBT and 3-TPVBT.

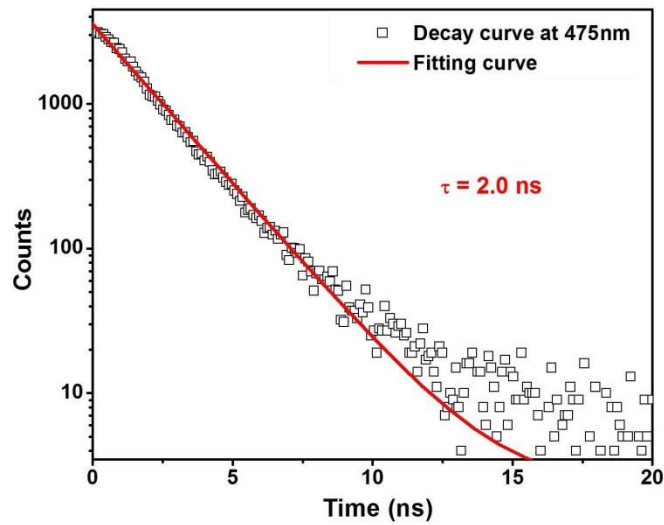


Figure S1. Time-resolved PL decay curve of 2-TPVT solid.

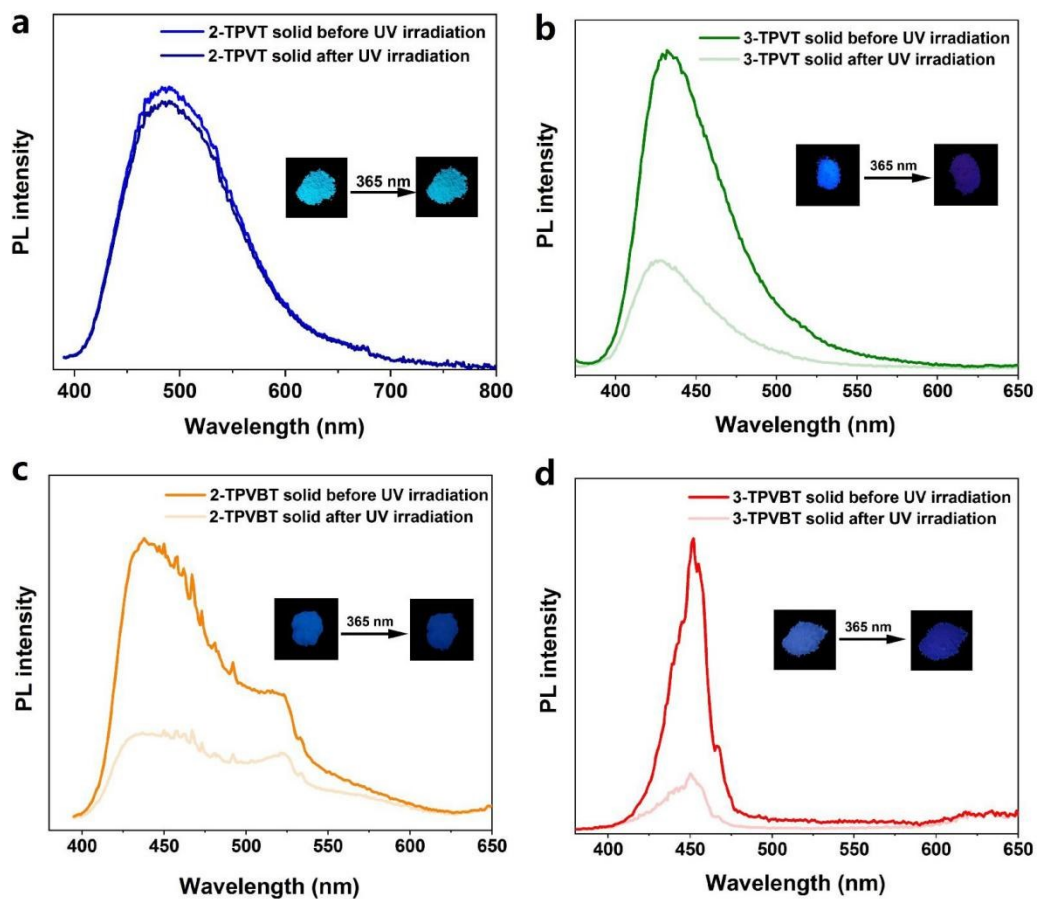


Figure S2. PL spectra and images of solid forms of 2-TPVT (a), 3-TPVT (b), 2-TPVBT (c) and 3-TPVBT (d) before and after UV irradiation.

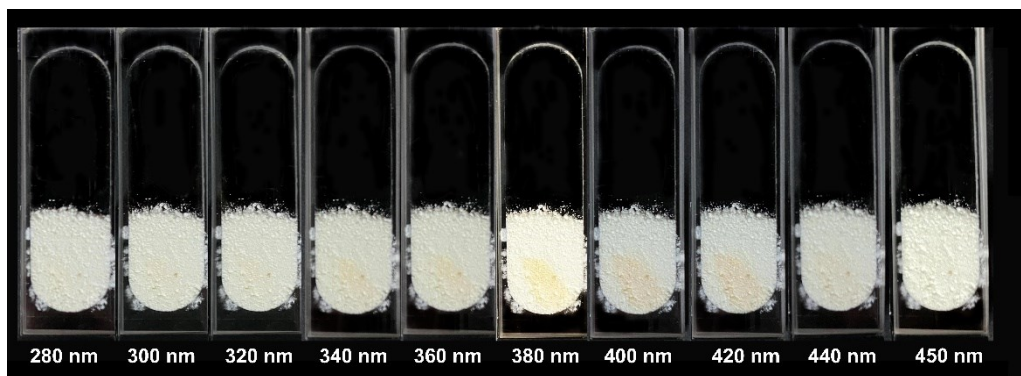


Figure S3. Images of solid form of 2-TPVT irradiated by UV light with different wavelengths ranging from 280 nm to 450 nm for 2 min.

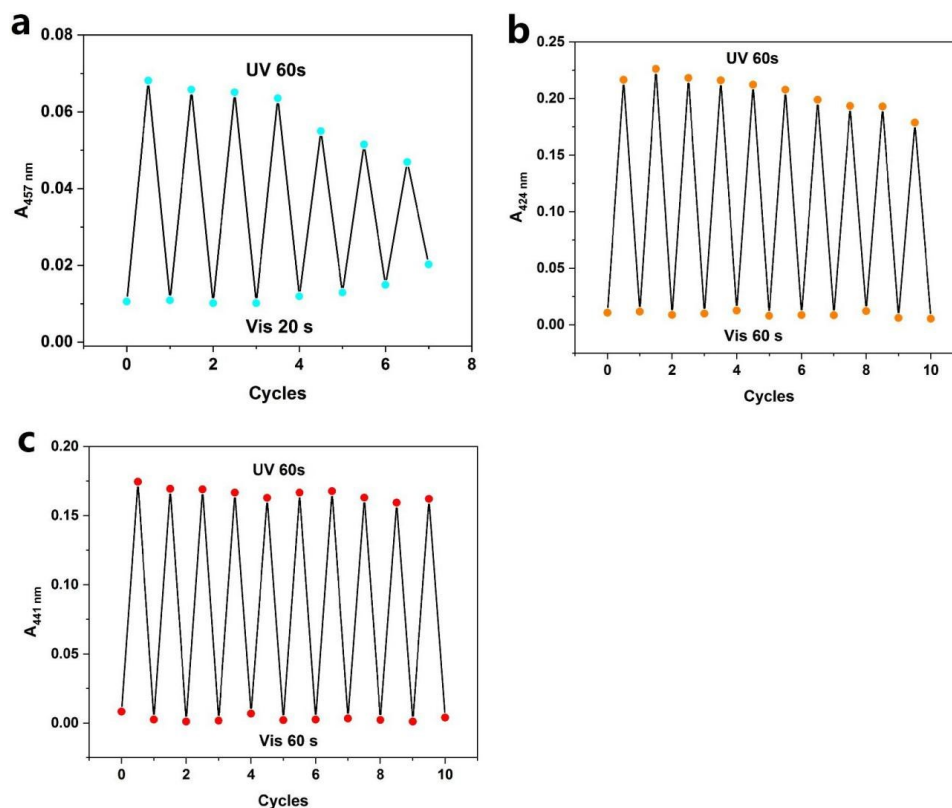


Figure S4. Photochromic cycles of 3-TPVT (a), 2-TPVBT (b), and 3-TPVBT (c) in acetonitrile as a function of exposure to UV-light (365 nm) and visible-light respectively.

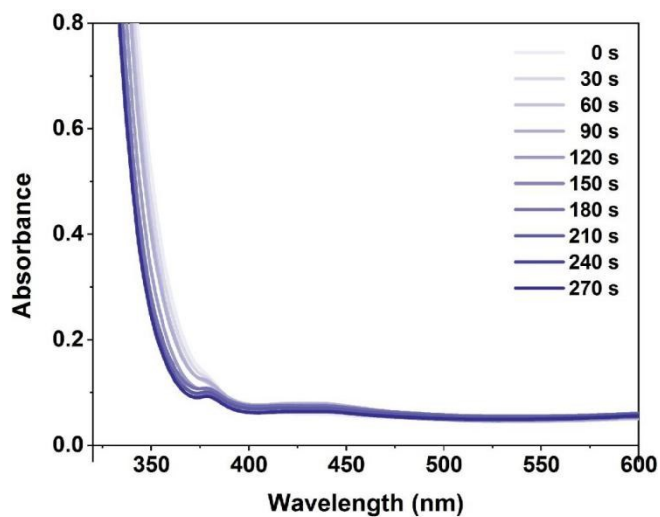


Figure S5. Time-dependent UV-vis absorption spectra of 2-TPVT in sucrose octaacetate film after different periods of UV-light irradiation from 0 to 270 s.

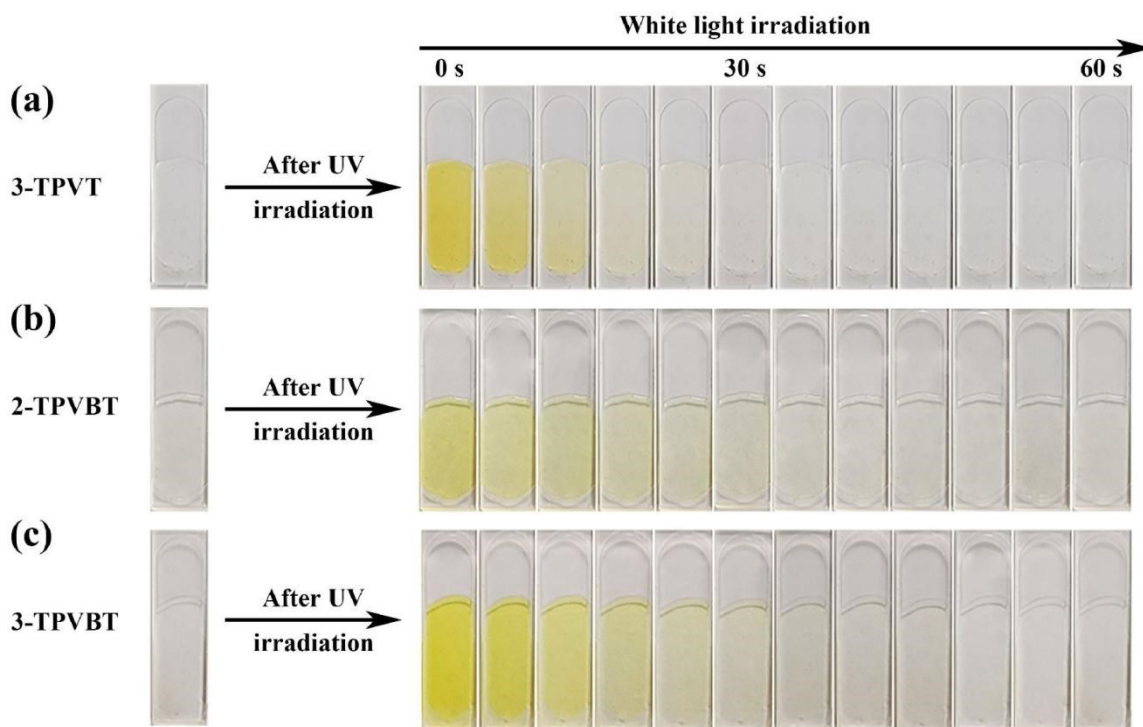


Figure S6. Time-dependent decoloration processes of the colored films of 3-TPVT (a), 2-TPVBT (b) and 3-TPVBT (c) under continuous white light irradiation.

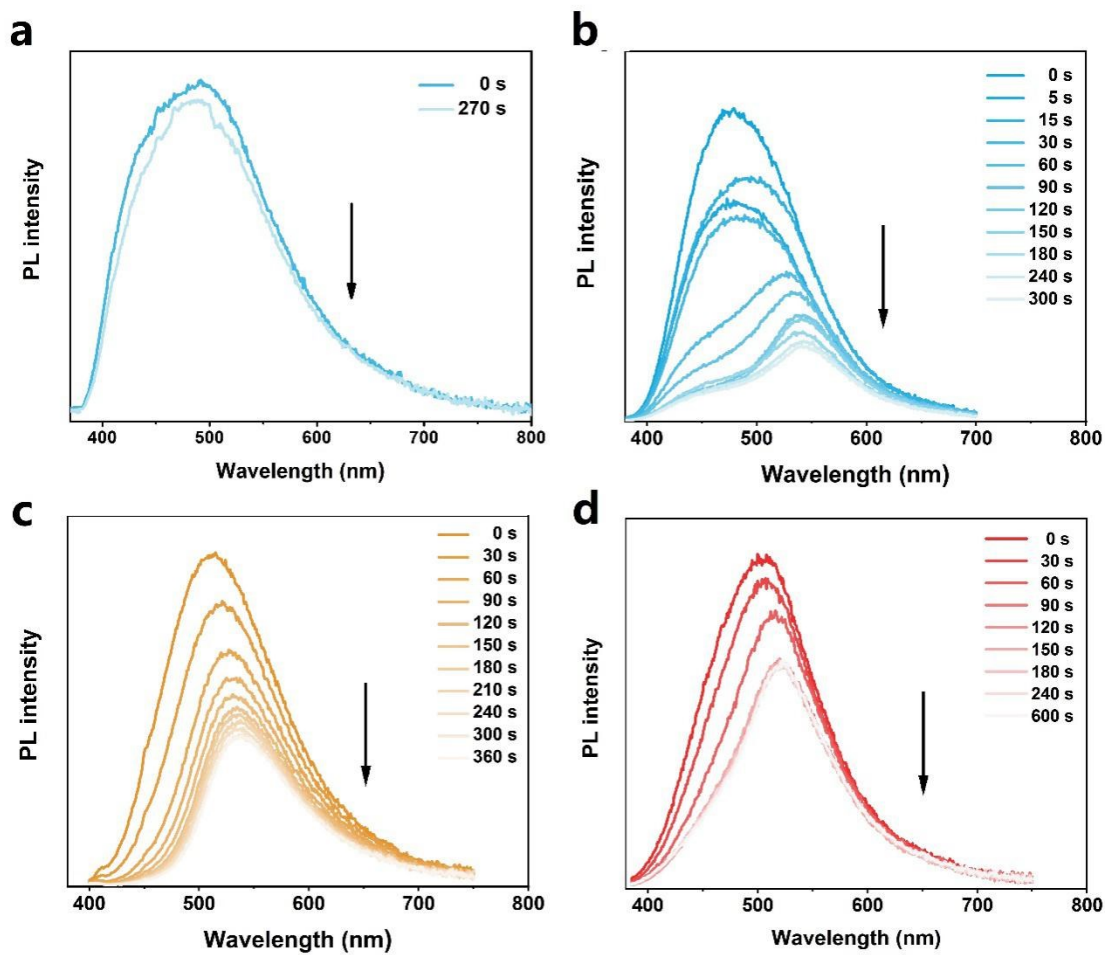


Figure S7. Time-resolved PL spectra of 3-TPVT (a), 2-TPVBT (b), and 3-TPVBT (c) in film under continuous UV light irradiation.

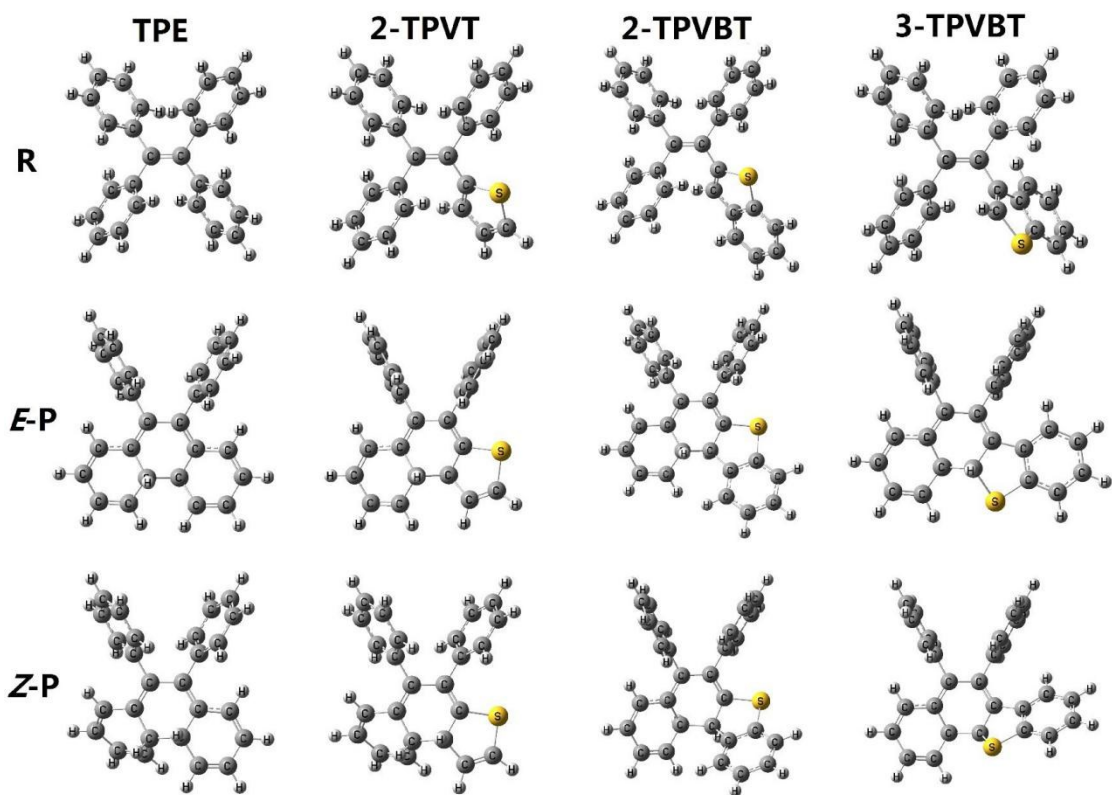


Figure S8. Optimized structures of reactants, *E*-products and *Z*-products of cyclization reactions of TPE, 2-TPVT, 2-TPVBT and 3-TPVBT.

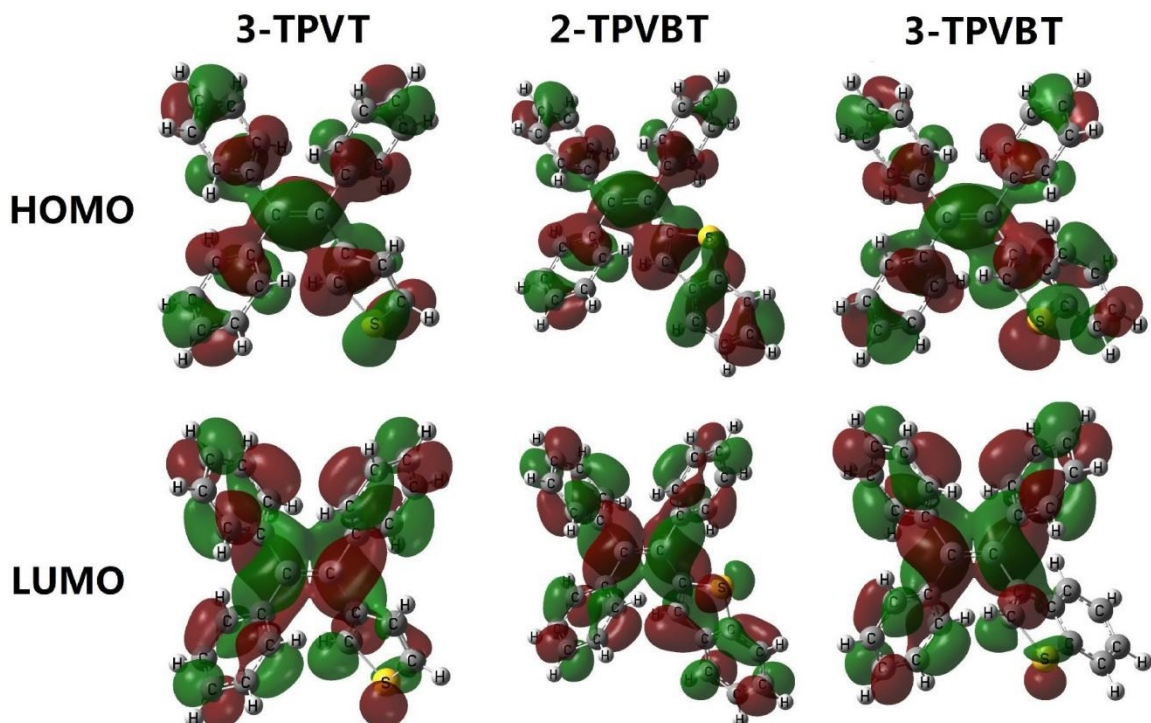


Figure S9. HOMOs and LUMOs of 3-TPVT, 2-TPVBT and 3-TPVBT calculated with B3LYP/6-311+G(d,p) level.

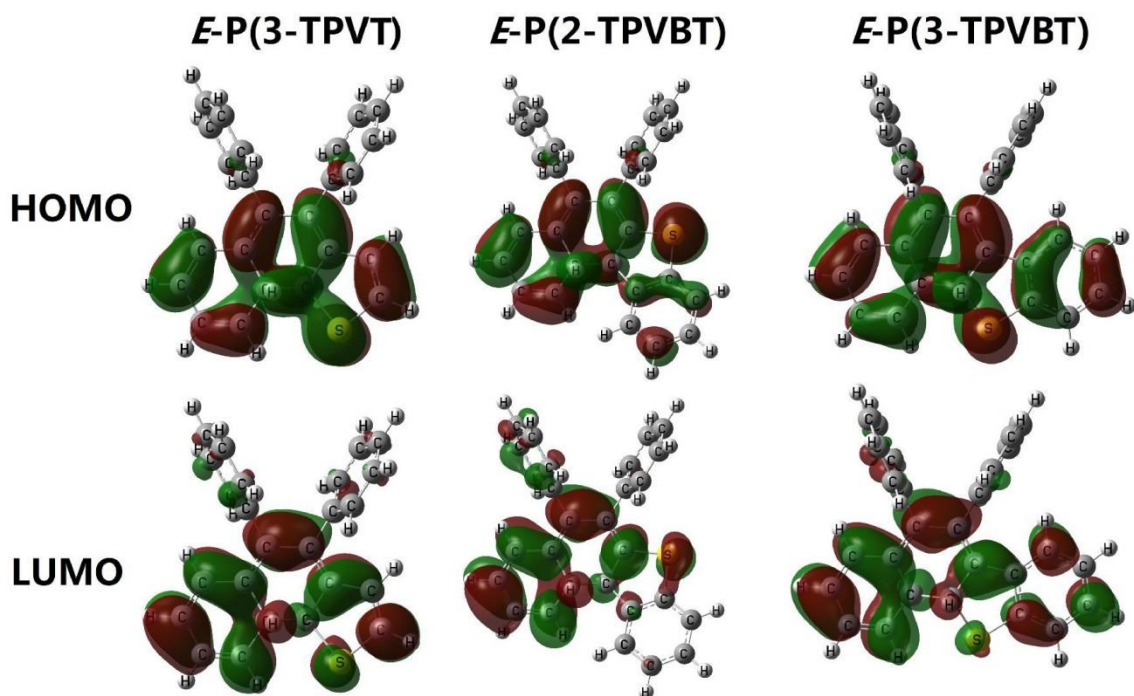


Figure S10. HOMOs and LUMOs of *E*-products of 3-TPVT, 2-TPVBT and 3-TPVBT calculated with B3LYP/6-311+G(d,p) level.

4. Supplementary Tables

Table S1. Optical properties of the four compounds in solution, film and solid.

	Solution		Film				Solid		
	λ_{ab}^a (nm)	λ_{ab}^b (nm)	λ_{ab}^a (nm)	λ_{ab}^b (nm)	λ_{fl}^a (nm)	λ_{fl}^b (nm)	λ_{ab}^a (nm)	λ_{ab}^b (nm)	λ_{fl}^a (nm)
2-TPVT	282	-	342	-	495	495	352	475	485
3-TPVT	302	456	385	460	480	540	385	508	432
2-TPVBT	322	424	383	430	510	535	383	458	435
3-TPVBT	311	440	372	442	510	525	372	503	450

λ_{ab} and λ_{fl} represents absorption maximum and fluorescence maximum respectively.

^a The open form. ^b The closed form.

Table S2. Compositions of HOMOs and LUMOs of 3-TPVT, 3-TPVBT and 2-TPVBT Calculated at B3LYP/6-311+G(d,p) Level

Group	Contribution to HOMO (%)	Contribution to LUMO (%)
3-TPVT		
Vinyl group	27.3	33.1
Phenyl groups	48.9	50.4
Thienyl group	23.0	12.0
2-TPVBT		
Vinyl group	21.3	31.3
Phenyl groups	38.1	37.6
Benzothienyl group	39.8	27.5
3-TPVBT		
Vinyl group	21.1	33.2
Phenyl groups	40.5	52.6
Benzothienyl group	37.6	9.7

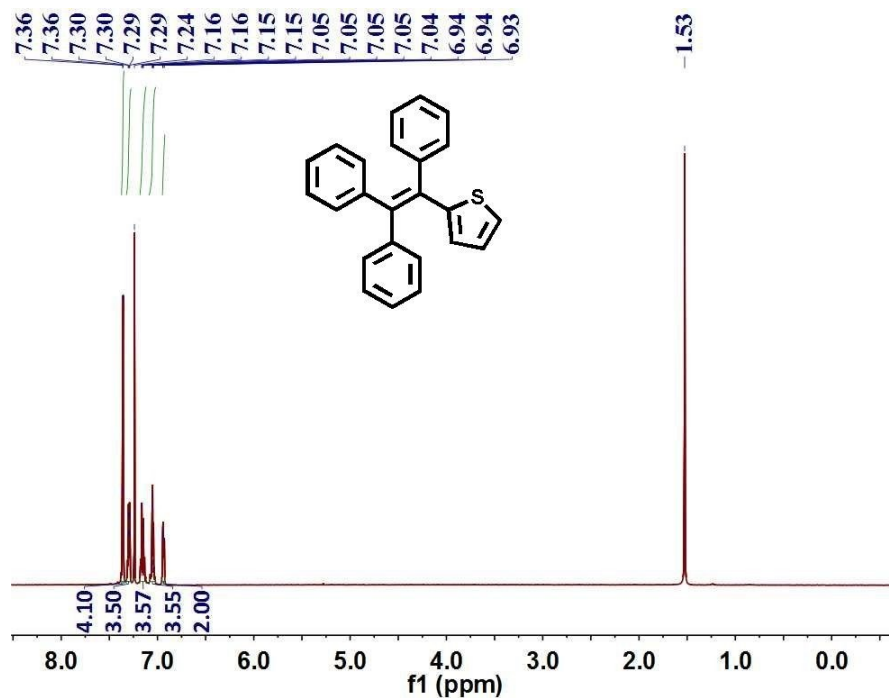
Table S3. Compositions of HOMOs and LUMOs of *E*-products of 3-TPVT, 2-TPVBT and 3-TPVBT Calculated at B3LYP/6-311+G(d,p) Level

Group	Contribution to HOMO (%)	Contribution to LUMO (%)
<i>E</i>-Product of 3-TPVT		
Phenyl groups	3.6	4.0
Dihydronaphththienyl group	94.9	92.6
<i>E</i>-Product of 2-TPVBT		
Phenyl groups	2.1	5.4
Dihydronaphthbenzothienyl group	96.3	90.9
<i>E</i>-Product of 3-TPVBT		
Phenyl groups	1.4	3.4
Dihydronaphthbenzothienyl group	97.1	93.7

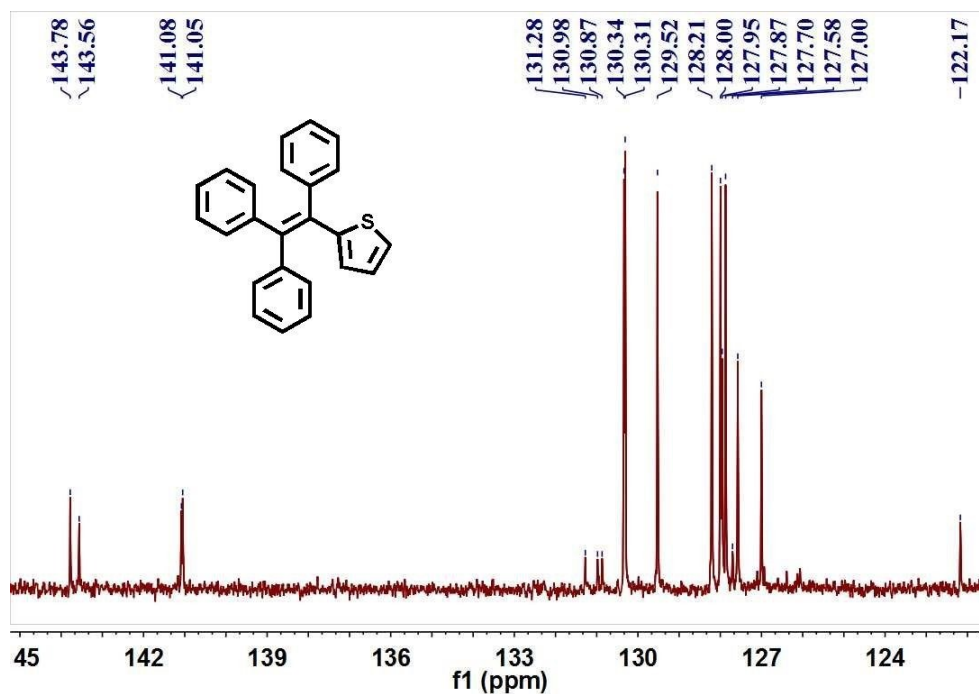
Table S4. Experimental and calculated absorption maxima of 3-TPVT, 2-TPVBT and 3-TPVBT and their products in acetonitrile.

	λ_{ab}^{exp} (nm)	λ_{ab}^{cal} (nm)	f_{cal}
3-TPVT	302	336	0.2637
2-TPVBT	322	381	0.1946
3-TPVBT	311	386	0.1043
<i>E</i> -P of 3-TPVT	456	500	0.1238
<i>E</i> -P of 2-TPVBT	424	442	0.1633
<i>E</i> -P of 3-TPVBT	440	485	0.1784

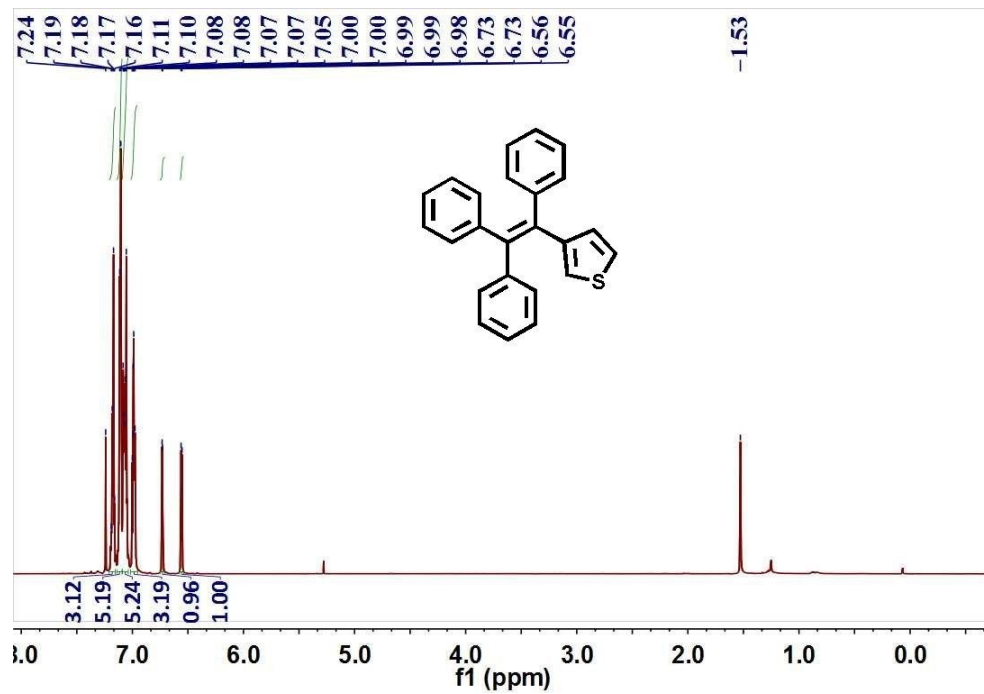
5. NMR and MS Spectra of Compounds



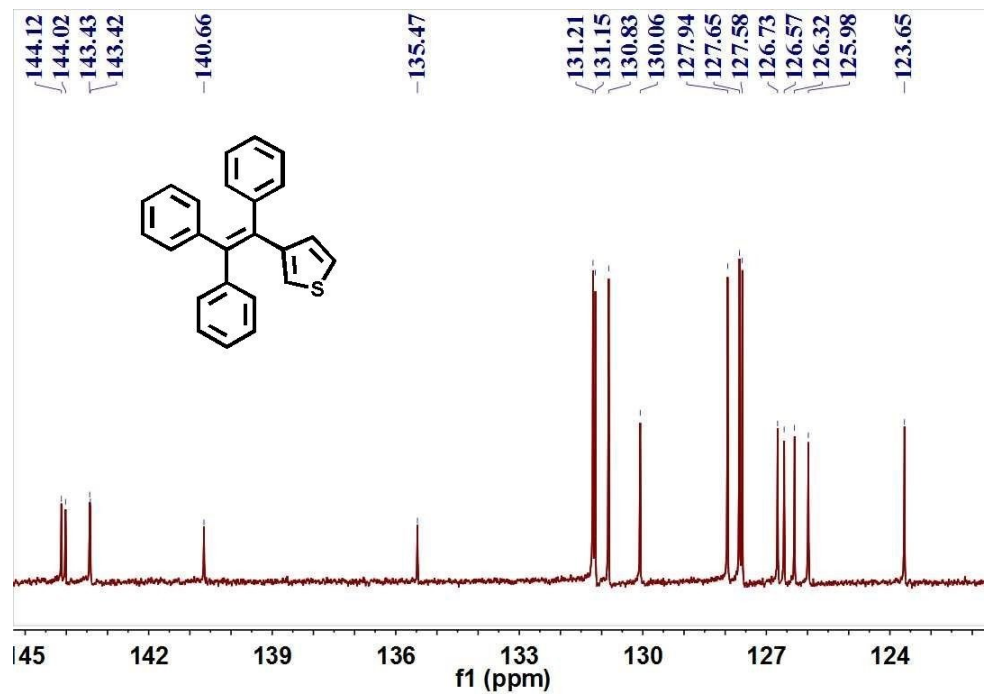
¹H NMR spectrum of 2-(1,2,2-triphenylvinyl)thiophene (2-TPVT) in CDCl₃



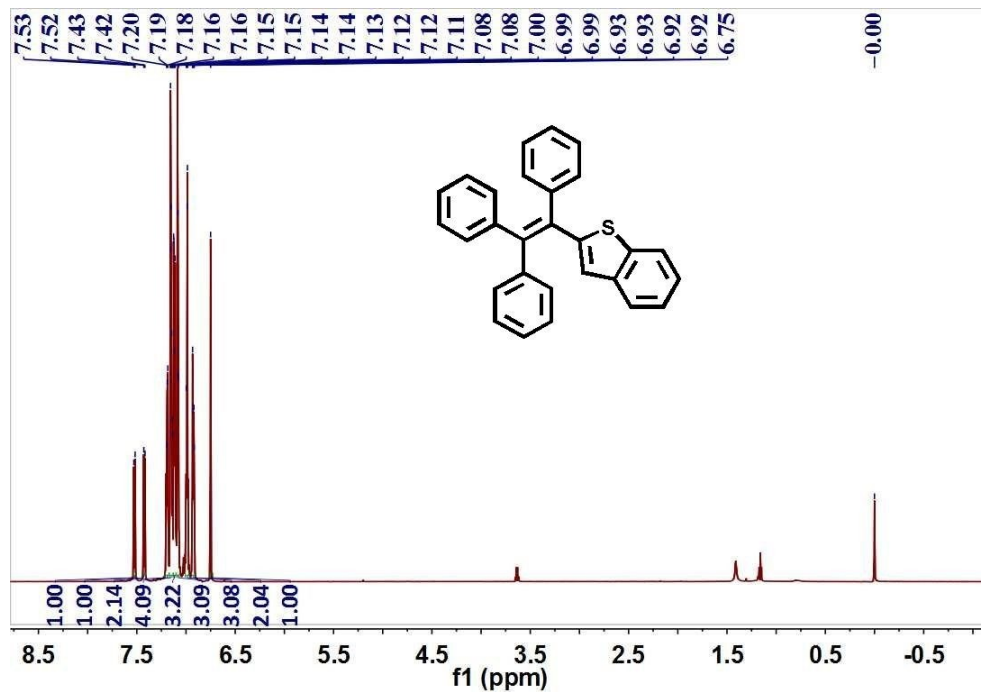
¹³C NMR spectrum of 2-(1,2,2-triphenylvinyl)thiophene (2-TPVT) in CDCl₃



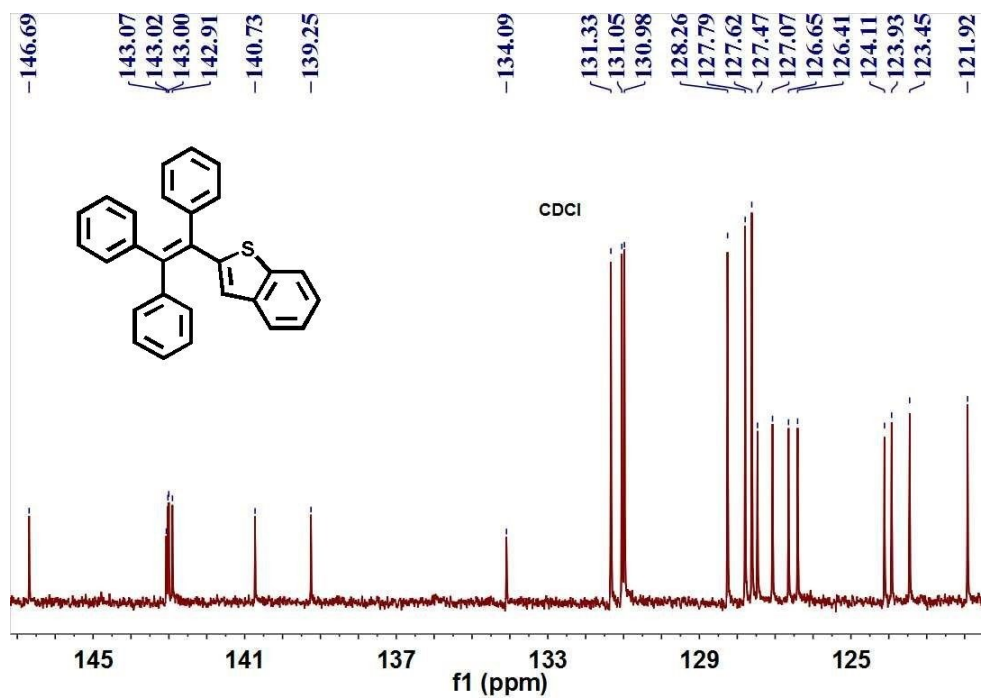
^1H NMR spectrum of 3-(1,2,2-triphenylvinyl)thiophene (3-TPVT) in CDCl_3



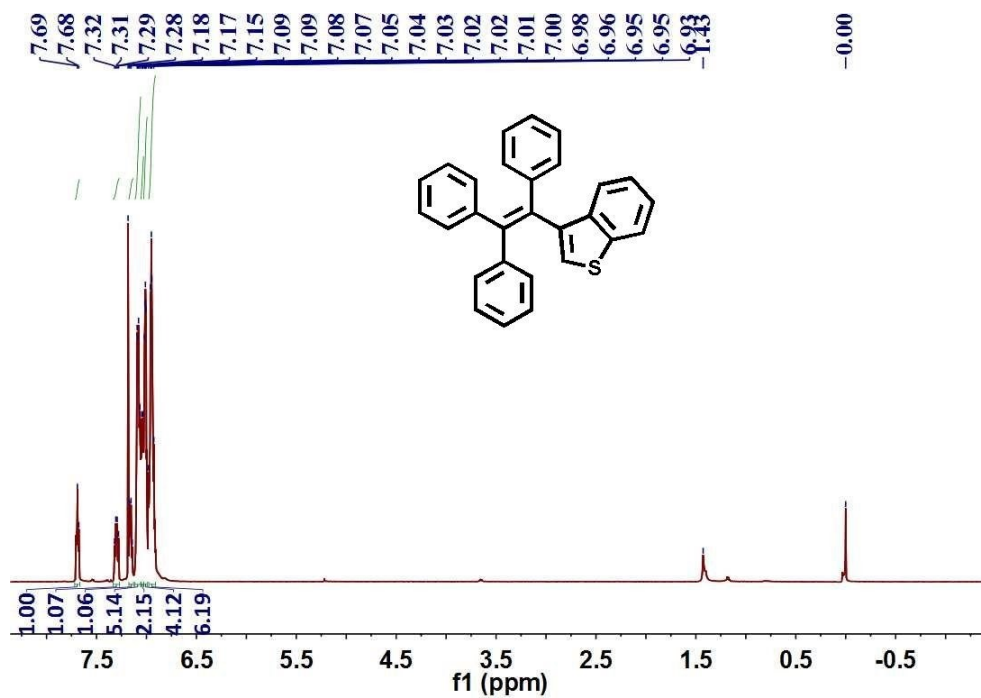
^{13}C NMR spectrum of 3-(1,2,2-triphenylvinyl)thiophene (3-TPVT) in CDCl_3



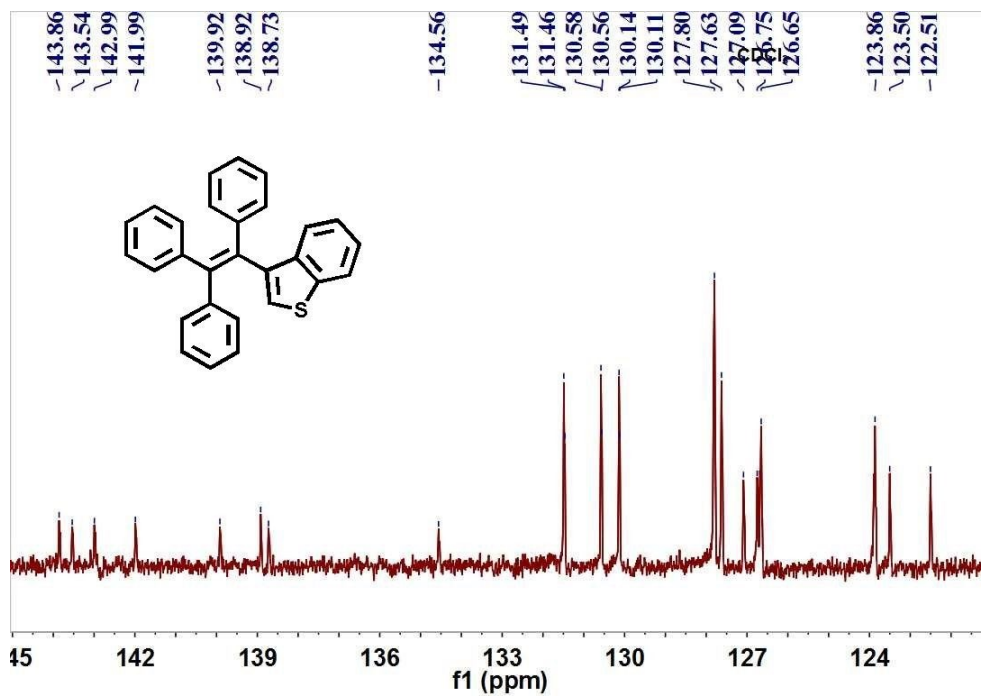
^1H NMR spectrum of 2-(1,2,2-triphenylvinyl)benzo[*b*]thiophene (2-TPVBT) in CDCl_3



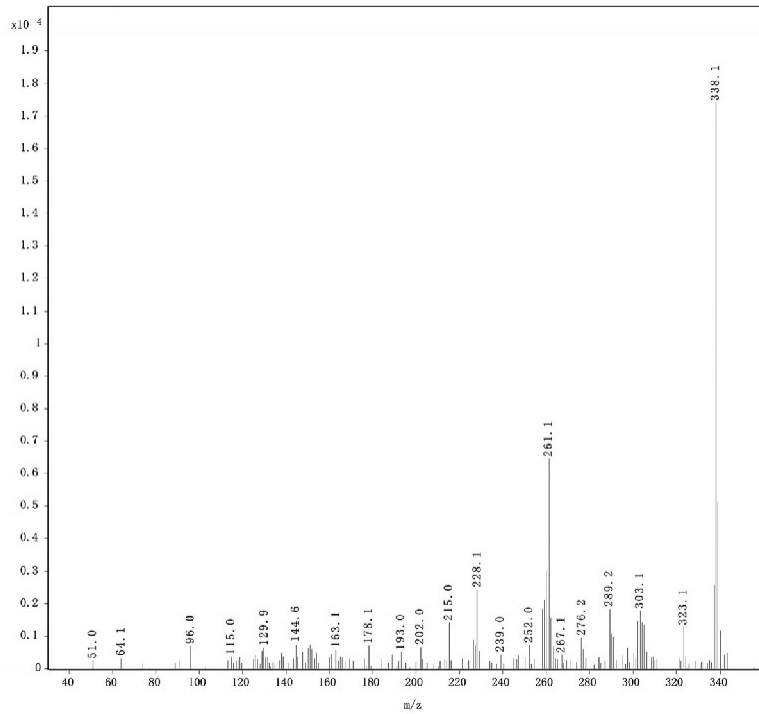
^{13}C NMR spectrum of 2-(1,2,2-triphenylvinyl)benzo[*b*]thiophene (2-TPVBT) in CDCl_3



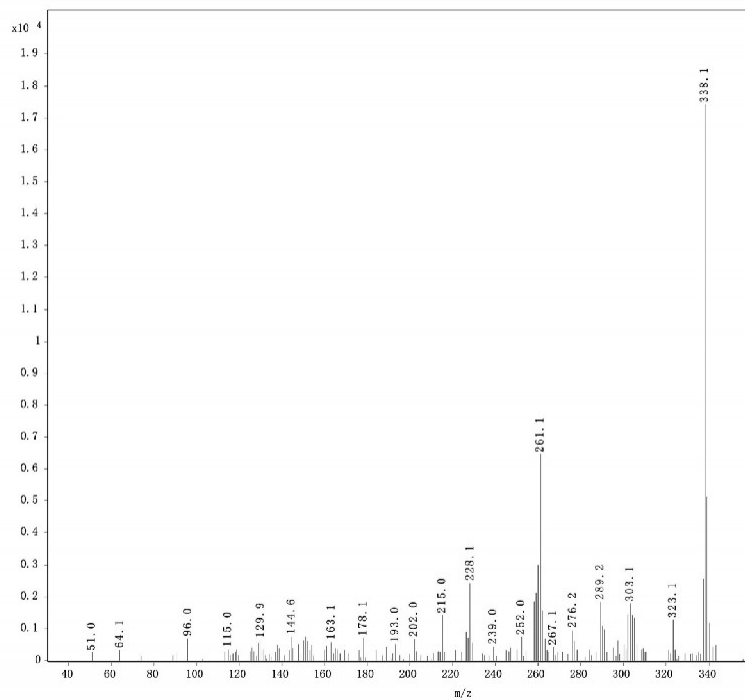
^1H NMR spectrum of 3-(1,2,2-triphenylvinyl)benzo[*b*]thiophene (3-TPVBT) in CDCl_3



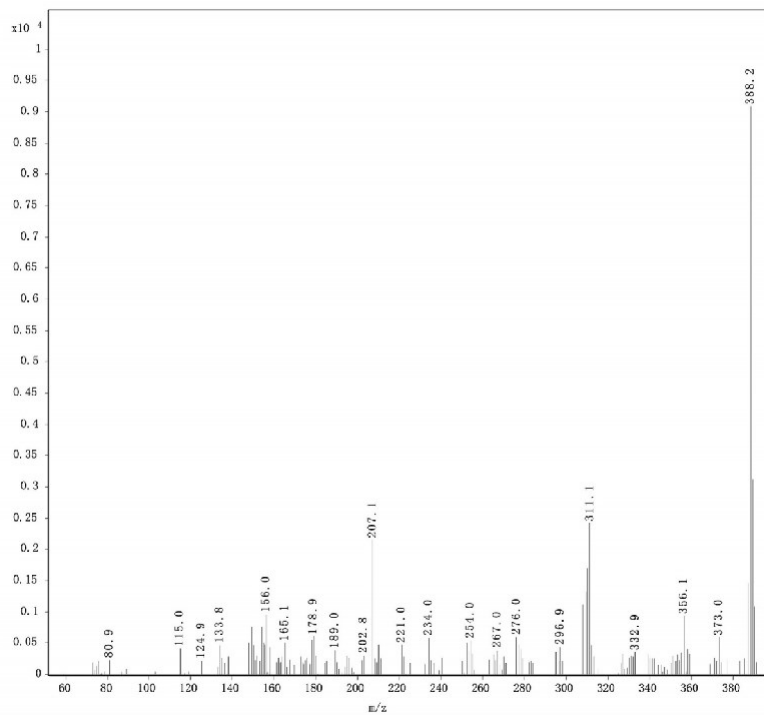
^{13}C NMR spectrum of 3-(1,2,2-triphenylvinyl)benzo[*b*]thiophene (3-TPVBT) in CDCl_3



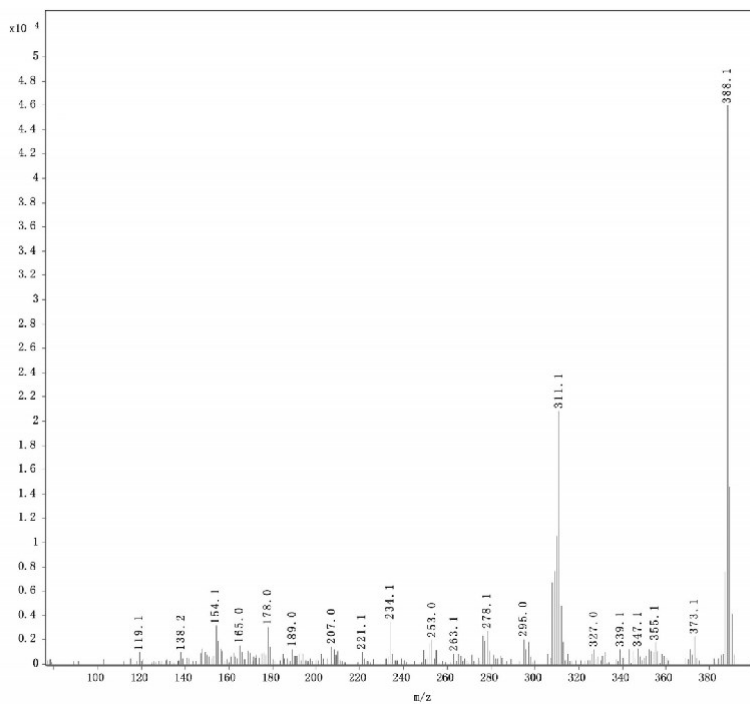
Mass spectrum of 2-(1,2,2-triphenylvinyl)thiophene (2-TPVT)



Mass spectrum of 3-(1,2,2-triphenylvinyl)thiophene (3-TPVT)



Mass spectrum of 2-(1,2,2-triphenylvinyl)benzo[*b*]thiophene (2-TPVBT)



Mass spectrum of 3-(1,2,2-triphenylvinyl)benzo[*b*]thiophene (3-TPVBT)

6. Cartesian Coordinates

TPE

C	5.61270700	12.34645900	14.33039300
C	6.63421900	12.24237000	13.24377800
C	4.90547500	13.00813700	16.64278500
C	6.26934700	12.43748900	11.90289700
H	5.24143400	12.68444600	11.66186400
C	3.24796000	12.87719900	18.91458400
C	5.80817200	13.08954100	15.45404400
C	3.57851200	14.11174300	18.35645500
H	3.19381600	15.02651400	18.79399000
C	7.20882300	12.32424400	10.88195200
H	6.90816200	12.49289000	9.85366400
C	4.36040000	11.56842700	14.08286600
C	4.57285800	11.77483800	17.22122600
H	4.96104900	10.86239300	16.78491400
C	3.75506700	11.70970600	18.34624300
H	3.51522000	10.74515700	18.78003800
C	4.40859700	14.17634300	17.24087300
H	4.67217700	15.14135600	16.82262200
C	4.42570300	10.22713200	13.67534200
H	5.39393300	9.75307300	13.55929300
C	3.09672800	12.16552500	14.19688600
H	3.02587700	13.20495000	14.49405700
C	3.26657900	9.49813400	13.42499700
H	3.33964500	8.45861400	13.12454600
C	8.52933800	11.98695800	11.17767700
C	2.01634200	10.10282400	13.55150900
C	1.93717200	11.44159900	13.93174700
H	0.97058500	11.92520200	14.02077100
C	8.90047200	11.76657600	12.50311600
H	9.92149600	11.49095900	12.74323500
H	9.25966000	11.88968000	10.38221600
H	1.11334400	9.53810000	13.34828600
H	2.60796300	12.82645800	19.78833500
C	7.96331400	11.89531400	13.52499300
H	8.26070800	11.72253800	14.55228700
C	6.94205100	14.05324300	15.59742900
C	7.74617200	14.04078800	16.74739100
C	7.19870800	15.02567100	14.62026200

C	8.79235200	14.94658100	16.89891100
H	7.55008700	13.31142700	17.52542000
C	8.23545100	15.94187000	14.77764900
H	6.57804700	15.06390500	13.73314700
C	9.04129900	15.90235300	15.91430700
H	9.41014100	14.91012900	17.78955300
H	8.41222500	16.68874700	14.01146000
H	9.85080800	16.61342400	16.03552300

***E*-Product of Photocyclization of TPE in gas**

C	5.58583800	12.43510200	14.27884300
C	6.48650300	12.49284100	13.24409700
C	4.98710400	12.75272900	16.73961700
C	6.24428000	11.87562500	11.95978300
H	5.37400400	11.24176100	11.84560400
C	3.29044800	12.28517500	18.93293600
C	5.90576200	13.00538100	15.58273100
C	2.90222200	13.15820800	17.91753200
H	1.94360400	13.66240400	17.97131200
C	7.04675900	12.11731300	10.89264300
H	6.83196700	11.65311900	9.93655400
C	4.27184100	11.74132300	14.08363100
C	5.36751900	11.88135000	17.76761900
H	6.33032500	11.38515300	17.71151500
C	4.52664200	11.64710900	18.85463300
H	4.83877800	10.96704700	19.63971300
C	3.74222200	13.38754000	16.83025600
H	3.43181900	14.06745000	16.04522300
C	4.03758900	10.47006400	14.62192100
H	4.81585900	9.98315900	15.19834100
C	3.25303900	12.34918100	13.34009700
H	3.42290200	13.33223600	12.91449700
C	2.81926400	9.82498100	14.42201600
H	2.65769100	8.83889800	14.84348300
C	8.13941300	13.06602100	10.98737100
C	1.81053600	10.44251000	13.68366800
C	2.03118500	11.70734800	13.14253900
H	1.25390400	12.19560000	12.56489100
C	8.50303200	13.56841100	12.17797900
H	9.30484000	14.29518500	12.24024600
H	8.63986600	13.38441800	10.07895900

H	0.86146700	9.94097200	13.53072700
H	2.63518800	12.10489900	19.77777100
C	7.01497600	13.79658400	15.75232900
C	9.29742200	14.53109600	14.97142300
C	9.56653100	14.99775000	16.20103500
H	10.08357300	14.46995400	14.22765800
H	10.57098600	15.31318100	16.46294500
C	7.89063700	14.15694200	14.56036300
H	7.43762800	15.07430900	14.12218200
C	7.87163700	13.08479200	13.46447500
H	8.50267700	12.24253500	13.82666900
C	8.52616800	15.05200600	17.20998600
H	8.73999600	15.52040100	18.16423800
C	7.32838300	14.44870900	17.00354100
H	6.59982800	14.41204800	17.80349400

Z-Product of Photocyclization of TPE in gas

C	5.74357900	12.08284500	14.29559200
C	6.54491300	12.28906600	13.20301500
C	5.03692700	12.79443400	16.64615400
C	6.11902800	12.15021400	11.81858200
H	5.35828000	11.42636100	11.55231900
C	3.06345900	13.05310500	18.63632700
C	6.09809000	12.66178800	15.60047600
C	2.93563000	13.73403100	17.42636300
H	2.07535600	14.37021000	17.24940300
C	6.58146500	13.03823100	10.89985600
H	6.22589100	12.99383400	9.87629200
C	4.43229100	11.37625700	14.14806400
C	5.15421200	12.11877200	17.86817200
H	6.01852000	11.48718000	18.04249100
C	4.17701300	12.24431100	18.85398600
H	4.28591900	11.70873000	19.79079700
C	3.91121800	13.60313900	16.44117000
H	3.80436200	14.13964900	15.50559900
C	4.22571700	10.15380200	14.80144900
H	5.01708300	9.74000900	15.41657700
C	3.39388600	11.89516100	13.36464700
H	3.52914100	12.84726500	12.86474400
C	3.02375100	9.46466300	14.66550500
H	2.88661000	8.51716100	15.17486700

C	7.44275500	14.14157300	11.30260300
C	1.99900600	9.99037700	13.87921800
C	2.18734000	11.20933300	13.23177900
H	1.39413900	11.63063100	12.62382900
C	8.05901900	14.12282900	12.49937100
H	8.69458500	14.93594600	12.83004100
H	7.56436100	14.98275700	10.62830800
H	1.06125400	9.45601100	13.77598900
H	2.30223800	13.15248900	19.40201700
C	7.35368600	13.17266300	15.81499400
C	9.73318000	13.57497700	14.99059800
C	9.96380900	14.35280800	16.06039900
H	10.50186500	13.42536100	14.23816300
H	10.92134100	14.84797200	16.18333700
C	8.43725400	12.83750000	14.80307700
H	8.65754700	11.77056300	14.97743100
C	7.93773500	12.86247500	13.33194100
H	8.59554600	12.13970600	12.82009600
C	8.93736600	14.55563500	17.06533700
H	9.15521600	15.19715000	17.91188200
C	7.70635400	13.99507500	16.94332600
H	6.94655000	14.20528800	17.68559900

1-TPVT in gas

C	5.59173800	12.36674300	14.33439400
C	6.58665800	12.31321900	13.22081700
C	4.95491000	12.91072500	16.70192900
C	6.19549700	12.58226700	11.90110100
H	5.16566300	12.85231400	11.69560300
C	3.37660100	12.63750600	19.01313200
C	5.81285400	13.06345600	15.48634400
C	3.64679600	13.90325200	18.49356200
H	3.24509700	14.78660800	18.97769200
C	7.11259200	12.51311400	10.85531600
H	6.79250900	12.73907400	9.84405000
C	4.33292000	11.60214700	14.08709400
C	4.68288900	11.64535600	17.23985800
H	5.08813500	10.76471000	16.75617000
C	3.90376100	11.50992800	18.38567700
H	3.71005300	10.52234600	18.78946600
C	4.43793000	14.03851300	17.35651400

H	4.65489200	15.02598300	16.96445000
C	4.38458400	10.28963500	13.59207800
H	5.34816900	9.82827200	13.40753700
C	3.07320700	12.18493400	14.28938100
H	3.01154600	13.20353500	14.65259200
C	3.21778600	9.57295200	13.34273600
H	3.28078900	8.55477100	12.97466600
C	8.43466200	12.14757700	11.10481800
C	1.97235800	10.16253000	13.55781900
C	1.90566200	11.47386300	14.02574900
H	0.94249500	11.94647800	14.18370700
C	8.83080800	11.85296400	12.40908200
H	9.85333000	11.55423300	12.61226000
H	9.14734100	12.08497300	10.29011900
H	1.06316400	9.60757200	13.35538300
H	2.76688900	12.53189500	19.90346900
C	6.91666100	14.03434600	15.60878100
C	8.40936500	15.78991900	15.18369000
C	8.88116400	15.37602800	16.39789900
H	8.83693400	16.61436000	14.62815900
H	9.70681700	15.77373300	16.96818100
C	7.29404800	15.02799200	14.73814800
H	6.78233400	15.20231100	13.80139400
C	7.91734300	11.93792600	13.45574900
H	8.23379800	11.70963300	14.46662600
S	7.95779300	14.05267600	17.02380600

***E*-Product of Photocyclization of 2-TPVT in gas**

C	5.57295000	12.43826700	14.24896000
C	6.51121500	12.44433900	13.25003900
C	5.04225900	12.71553600	16.76585800
C	6.29217500	11.82146900	11.96289300
H	5.37687300	11.26239300	11.81271600
C	3.49667900	12.15518300	19.04223800
C	5.88445800	13.01743700	15.56654400
C	3.04451200	13.07345300	18.09596300
H	2.09358100	13.57534700	18.23654700
C	7.17699300	11.95043300	10.94516700
H	6.97807500	11.47647400	9.99058000
C	4.23058100	11.81046300	14.03686600
C	5.48839900	11.79733300	17.72405500

H	6.44309700	11.30301200	17.58133900
C	4.72196500	11.51850300	18.85403700
H	5.08249800	10.80462500	19.58650900
C	3.81164500	13.35166400	16.96689800
H	3.45432000	14.06564300	16.23372700
C	3.93087100	10.54547400	14.55727100
H	4.68318200	10.01014900	15.12507800
C	3.24338400	12.48317300	13.30635300
H	3.46367200	13.46280300	12.89631700
C	2.67972700	9.96838500	14.35102500
H	2.46721300	8.98622300	14.75872000
C	8.36887800	12.76921500	11.08833900
C	1.70392400	10.64894100	13.62426600
C	1.98963500	11.90860600	13.10166400
H	1.23807500	12.44532300	12.53303000
C	8.69625300	13.30692400	12.27289300
H	9.58843200	13.91597000	12.37041800
H	8.98567200	12.95214600	10.21460700
H	0.72966400	10.20025700	13.46565600
H	2.89903200	11.93913200	19.92078000
C	6.95030100	13.84418600	15.66260400
C	9.06653900	14.82228000	15.00713900
C	9.02604400	15.11712100	16.30703600
H	9.90808600	15.07810200	14.37600100
H	9.79222700	15.61434800	16.88633900
C	7.79413500	14.22200800	14.46032000
H	7.25590700	15.01757300	13.90557900
C	7.90690900	13.01570400	13.52659300
H	8.46299500	12.23226800	14.08344700
S	7.52846000	14.64169000	17.13790700

Z-Product of Photocyclization of 2-TPVT in gas

C	5.74382300	12.06594700	14.27414600
C	6.54809900	12.29573200	13.19471300
C	5.05879800	12.78470000	16.65954100
C	6.13904300	12.16190000	11.80034400
H	5.40697100	11.41579800	11.51520900
C	3.13213700	13.16818700	18.67194700
C	6.10371200	12.60310000	15.60990400
C	2.97367100	13.76869100	17.42332300
H	2.10717700	14.39008600	17.22568200

C	6.58587000	13.07384000	10.89983700
H	6.24827700	13.03196900	9.87012400
C	4.43478200	11.36120500	14.12415500
C	5.20799400	12.19037700	17.91941300
H	6.07590400	11.57014100	18.11433700
C	4.25311900	12.37835900	18.91699100
H	4.38520300	11.90533600	19.88390200
C	3.92623300	13.57697900	16.42668500
H	3.79615300	14.05140600	15.46121200
C	4.20640200	10.16807400	14.82441200
H	4.98138200	9.77711300	15.47428400
C	3.41504300	11.85321000	13.29919700
H	3.56362000	12.78608900	12.76830700
C	3.00491500	9.47885400	14.68966300
H	2.85170300	8.55394600	15.23465600
C	7.41414000	14.19493500	11.32924000
C	2.00018400	9.97615100	13.85981200
C	2.20830400	11.16723800	13.16839100
H	1.42970700	11.56783500	12.52843000
C	8.03046200	14.16617200	12.52503100
H	8.64285200	14.98849100	12.87704200
H	7.51171500	15.05442800	10.67442600
H	1.06206200	9.44215000	13.75823800
H	2.38809900	13.31575700	19.44670400
C	7.36016900	13.06021800	15.80264100
C	9.60709700	13.72768200	15.15746400
C	9.46879000	14.35087300	16.32813000
H	10.49920800	13.80252100	14.54732100
H	10.18838400	14.99687900	16.81249400
C	8.45665600	12.83062500	14.78677300
H	8.78465500	11.78843700	14.93310600
C	7.94232100	12.88269800	13.32530500
H	8.59536800	12.18033600	12.78118900
S	7.93133900	14.04714900	17.16362100

2-TPVT in gas

C	5.57388300	12.41354000	14.31854700
C	6.55058200	12.41294600	13.18645200
C	4.95206200	12.91891400	16.69811600
C	6.12576500	12.69132300	11.87907600

H	5.08286900	12.92607000	11.69699000
C	3.42565100	12.59785100	19.04079900
C	5.79026000	13.10124300	15.47371000
C	3.68240600	13.87339000	18.53941400
H	3.29018500	14.74676100	19.04888500
C	7.02503200	12.67501300	10.81574000
H	6.67794200	12.90705200	9.81479600
C	4.34040400	11.60489400	14.07901000
C	4.69501000	11.64298500	17.22003500
H	5.09141400	10.77211900	16.71205300
C	3.94147100	11.48392800	18.37976800
H	3.75858500	10.48815800	18.76841300
C	4.44788900	14.03211700	17.38728400
H	4.65397700	15.02781100	17.01072800
C	4.43316000	10.29758700	13.57677500
H	5.41060600	9.87185300	13.37946500
C	3.06318900	12.14156800	14.29747800
H	2.96990100	13.15530800	14.66780200
C	3.28991300	9.54096700	13.33600000
H	3.38498900	8.52747300	12.96185900
C	8.36426700	12.35483900	11.03443100
C	2.02670900	10.08492000	13.56717000
C	1.91863600	11.39086100	14.04245100
H	0.94103800	11.82811700	14.21321900
C	8.79501700	12.05152000	12.32553700
H	9.83155900	11.78781100	12.50479000
H	9.06355300	12.33420400	10.20611800
H	1.13562200	9.49902700	13.37144400
H	2.83567800	12.47368600	19.94196600
C	6.88235400	14.09743800	15.62453800
C	8.67647000	15.15833000	16.68812400
H	9.45348400	15.41184500	17.39278500
C	7.14808000	15.11078500	14.73743000
H	6.64741700	15.32141500	13.80557300
C	7.89808300	12.08228600	13.38967800
H	8.24101200	11.84708900	14.39036100
C	7.76515200	14.14785700	16.75787000
H	7.71469400	13.44764100	17.58119100
S	8.47015700	16.10099400	15.24611600

***E*-Product of Photocyclization of 3-TPVT in gas**

C	5.56561700	12.44994400	14.21632600
C	6.47041700	12.48091500	13.18231300
C	5.08026800	12.70183600	16.73553600
C	6.21082900	11.88878700	11.88927200
H	5.29551400	11.32556600	11.75681300
C	3.55708800	12.16905300	19.03807800
C	5.91365500	12.99852700	15.52888400
C	3.06090600	13.01542900	18.04733600
H	2.08463300	13.47323400	18.16284600
C	7.05674500	12.05298700	10.84296800
H	6.82541600	11.60226000	9.88446200
C	4.22866700	11.80191800	14.02759100
C	5.56911900	11.85550500	17.73869800
H	6.54699800	11.40191000	17.61871500
C	4.81446400	11.58978800	18.88056100
H	5.20932500	10.92968100	19.64514500
C	3.81513000	13.27818800	16.90627000
H	3.42114900	13.93654600	16.14084300
C	3.96460100	10.52724000	14.54353800
H	4.73862800	10.00295300	15.09229800
C	3.21463200	12.45982900	13.32101900
H	3.40710400	13.44661500	12.91396700
C	2.72160600	9.92662100	14.35677300
H	2.53679800	8.93719100	14.76038000
C	8.24574200	12.87919300	10.96200100
C	1.71832100	10.59296900	13.65452900
C	1.96866300	11.86190400	13.13628000
H	1.19568600	12.38761500	12.58641500
C	8.61485800	13.38182600	12.14928100
H	9.50433100	13.99744200	12.23839900
H	8.82488100	13.09570200	10.07059500
H	0.75040600	10.12583900	13.51115100
H	2.96834100	11.96367200	19.92510100
C	7.00933000	13.80458700	15.64542500
C	8.75936800	15.00325700	16.63785700
H	9.34631000	15.51788900	17.38640700
C	7.79243900	14.18724600	14.40567500
H	7.29831300	15.04700700	13.92636800
C	7.87773100	13.03730200	13.42044900
H	8.45725500	12.23169300	13.91997200
C	7.54561700	14.44055100	16.82339300

H	7.03973300	14.43373000	17.77946200
S	9.42801000	14.83416000	15.01913300

Z-Product of Photocyclization of 3-TPVT in gas

C	5.75107600	12.07430100	14.25279700
C	6.55144400	12.26939100	13.15996800
C	5.10306500	12.78396400	16.64301200
C	6.13004400	12.11232200	11.77363000
H	5.38455400	11.37134200	11.51102600
C	3.21131500	13.11878700	18.70087300
C	6.12835900	12.62296400	15.57033300
C	3.01454200	13.72169400	17.45894100
H	2.13197600	14.32678900	17.28287600
C	6.58112600	12.99978600	10.85003500
H	6.23325500	12.94063500	9.82465200
C	4.42976800	11.38805900	14.11350000
C	5.28941500	12.18632600	17.89710000
H	6.17312900	11.58140500	18.06840000
C	4.35319900	12.35008600	18.91653100
H	4.51521200	11.87358700	19.87728200
C	3.94901300	13.55377100	16.44065400
H	3.78750600	14.03095400	15.48135500
C	4.19036200	10.19596500	14.81122200
H	4.96526200	9.79076800	15.45237100
C	3.41078800	11.89789700	13.29881300
H	3.56998400	12.82884900	12.76740700
C	2.97692500	9.52587200	14.68570300
H	2.81470800	8.60136400	15.22874200
C	7.41947400	14.12256700	11.25112300
C	1.97215100	10.04159900	13.86735500
C	2.19218900	11.23145300	13.17740900
H	1.41435300	11.64555900	12.54519100
C	8.03985500	14.11840100	12.44524400
H	8.65525200	14.94307000	12.78194800
H	7.51741000	14.96846600	10.57899800
H	1.02509500	9.52229500	13.77272600
H	2.48120700	13.24693200	19.49210700
C	7.39265300	13.09771800	15.75962500
C	9.17377400	14.35178200	16.62870200
H	9.73176400	15.00510200	17.28551200
C	8.44922300	12.79059700	14.72093900

H	8.77086300	11.75931500	14.89712400
C	7.95439700	12.84578600	13.26459000
H	8.59572600	12.13163200	12.72246000
C	7.91295200	13.90947400	16.82955900
H	7.32521000	14.19188500	17.69234900
S	9.93297900	13.83273200	15.13083100

2-TPVBT in gas

C	3.54108700	15.20332800	13.60250000
C	4.54458400	15.15149500	12.49680000
C	2.93259900	15.50969000	16.02213500
C	4.22977500	15.65931300	11.22781700
H	3.25685500	16.10755000	11.06001500
C	1.27703100	15.18618100	18.27132600
C	3.83634300	15.68486800	14.84342800
C	1.76872700	16.44782800	17.93784700
H	1.51161400	17.30928600	18.54430800
C	5.15177200	15.60074000	10.18593400
H	4.89379100	16.01191500	9.21613500
C	2.18486600	14.69149600	13.24292600
C	2.43958300	14.24580400	16.37410600
H	2.70357400	13.38568200	15.77062400
C	1.62116200	14.08509900	17.48875400
H	1.25409800	13.09807200	17.74735500
C	2.59771700	16.60546800	16.83106700
H	2.98780900	17.58689500	16.58492900
C	2.04383500	13.46406500	12.57717400
H	2.92759200	12.88131500	12.34328400
C	1.02875200	15.43949500	13.50877300
H	1.11850700	16.39772300	14.00603800
C	0.78666900	12.98468500	12.22097200
C	6.39849800	15.00931700	10.38517600
C	-0.35510300	13.73571200	12.49880200
C	-0.22772900	14.96812100	13.13772500
H	-1.10810500	15.56581300	13.34664400
C	6.71479000	14.47827800	11.63517200
H	7.67710500	14.00547300	11.79740700
H	7.11391800	14.95592200	9.57225900
H	-1.33395200	13.36707000	12.21332600
H	0.63774400	15.06146800	19.13811100
H	0.69866100	12.02690900	11.72000500

C	7.24144600	17.26631000	16.11485500
C	6.83795700	17.98205300	14.96194600
C	7.64432200	19.04013500	14.50522000
C	8.80987800	19.35636700	15.18495000
C	9.19388600	18.63332500	16.32746900
C	8.41497200	17.58555900	16.80156800
C	5.08231000	16.42930800	15.11147500
H	7.35197300	19.59861600	13.62263400
H	9.43470300	20.16941300	14.83327300
H	10.10872900	18.89576000	16.84640200
H	8.71283000	17.03056200	17.68358900
C	5.79833400	14.55040600	12.68032800
H	6.05284800	14.13597800	13.64869400
C	5.60658800	17.48201700	14.42239300
H	5.13123000	17.89347900	13.54170800
S	6.09084200	16.00367100	16.50839800

***E*-Product of Photocyclization of 2-TPVBT in gas**

C	3.54544600	15.35810300	13.60976400
C	4.51935300	15.45439700	12.65354900
C	2.78802000	15.57733400	16.06820300
C	4.35519100	14.91699300	11.31898800
H	3.49968000	14.28352400	11.12077200
C	0.95921600	15.07598900	18.13923700
C	3.77568700	15.85030600	14.97659300
C	0.67339700	16.03378400	17.16772300
H	-0.25710400	16.58907900	17.20880300
C	5.20836000	15.23130900	10.31339400
H	5.05379700	14.82385700	9.32070300
C	2.22991100	14.71845600	13.29091100
C	3.06689700	14.62025800	17.05125600
H	4.00200500	14.07272600	17.00870100
C	2.15976300	14.37074800	18.07907700
H	2.39161100	13.62555300	18.83207900
C	1.58104200	16.28237800	16.14050600
H	1.35201600	17.02776100	15.38745100
C	1.91028300	13.44132600	13.76816300
H	2.62614800	12.90595700	14.38112900
C	1.29043000	15.38999500	12.49897000
H	1.52653000	16.37890600	12.12165300
C	0.68688200	12.85098800	13.45961200

C	6.26753900	16.19910700	10.52639200
C	-0.24212300	13.53093900	12.67312900
C	0.06339100	14.80294900	12.19359300
H	-0.65198500	15.33974500	11.58016700
C	6.57124100	16.61619600	11.76548000
H	7.32525900	17.37865000	11.91391900
H	6.78581800	16.61009200	9.66627600
H	-1.19568100	13.07259900	12.43598600
H	0.25224200	14.88184400	18.93807300
H	0.45920700	11.85920800	13.83441600
C	6.98888500	17.51214500	16.28123700
C	7.19208400	17.24270700	14.91838900
C	8.49348200	17.29068400	14.42326700
C	9.55651000	17.62770800	15.26596100
C	9.32647200	17.92727700	16.60675700
C	8.03447100	17.86538100	17.12815200
C	4.88291600	16.58277800	15.22802500
H	8.70051500	17.05955500	13.38690900
H	10.56494200	17.65443200	14.86978800
H	10.15381500	18.19304500	17.25489900
H	7.85280500	18.06973800	18.17696200
C	5.90792000	16.00860800	12.98693600
H	6.51340000	15.12992400	13.28770600
C	5.88866000	16.98472000	14.17112900
H	5.54645500	17.96494600	13.78336700
S	5.29963300	17.29109700	16.79774800

Z-Product of Photocyclization of 2-TPVBT in gas

C	3.51894900	15.66908800	13.56243500
C	4.42837300	15.94025500	12.57298000
C	2.53502100	16.16012100	15.90370500
C	4.53033800	15.18255000	11.34796800
H	3.84069100	14.36344100	11.19040500
C	0.68460300	15.74422400	17.97633400
C	3.53917200	16.42506900	14.82864600
C	0.75348000	16.98023900	17.33884700
H	0.09284300	17.78614000	17.63882500
C	5.47907400	15.44503300	10.41466600
H	5.53234300	14.84017100	9.51644700
C	2.51497700	14.57212000	13.40138000
C	2.45740900	14.92171500	16.55389800

H	3.12234200	14.11895200	16.26002600
C	1.54299900	14.71758100	17.58281300
H	1.50242100	13.75525000	18.08095800
C	1.67577800	17.18659400	16.31363300
H	1.72829300	18.15035100	15.81907500
C	2.90703900	13.22730900	13.39618700
H	3.95485500	12.98036600	13.52827300
C	1.15535100	14.87008000	13.24287900
H	0.83268000	15.90506900	13.24950300
C	1.96869000	12.20950300	13.23174800
C	6.45181700	16.50453400	10.60307000
C	0.61982800	12.52010000	13.07115100
C	0.21680200	13.85487700	13.07658800
H	-0.83051600	14.10692500	12.95195700
C	6.38428000	17.31346900	11.67205400
H	7.09569100	18.12263300	11.80183800
H	7.23366400	16.63703600	9.86267400
H	-0.11125000	11.72951600	12.94450500
H	-0.02932700	15.58121100	18.77593800
H	2.29244600	11.17439000	13.23290000
C	6.78831800	17.30401700	16.24002000
C	6.93796600	17.16194400	14.84813800
C	8.17222600	16.76509600	14.34382400
C	9.24020100	16.52868000	15.21593500
C	9.08218900	16.70423200	16.58860400
C	7.84791000	17.09236600	17.11385400
C	4.56729900	17.26887300	15.09075000
H	8.30948500	16.63274900	13.27843200
H	10.19571200	16.20738400	14.81752400
H	9.91491900	16.52347500	17.25897600
H	7.71526600	17.20396300	18.18385300
C	5.26981000	17.20602400	12.67749700
H	4.55728900	18.00801000	12.40584600
C	5.66939500	17.60448200	14.12053300
H	5.74985700	18.70185600	14.09251300
S	5.11500500	17.71790900	16.73888200

3-TPVBT in gas

C	3.72397700	15.94074000	14.01296600
C	4.55401000	16.41140200	12.86219600
C	3.02923500	16.06113800	16.42876500

C	5.07549000	15.49211600	11.93972200
H	4.88262300	14.43380600	12.07601500
C	1.30576800	15.58984300	18.60567700
C	3.96125900	16.33775200	15.29376900
C	0.79775600	16.05984300	17.39485100
H	-0.26468100	16.24950800	17.28833100
C	5.84129200	15.91967300	10.85830200
H	6.24673700	15.19059500	10.16529700
C	2.63165400	14.98888400	13.64656100
C	4.79400100	17.77611000	12.64638800
H	6.69570800	15.59736000	14.99972400
C	3.52864400	15.61090200	17.66008700
H	4.59430200	15.44731300	17.77330700
C	2.67569000	15.36686900	18.73337500
H	3.08319400	15.00867700	19.67236500
C	1.64926200	16.29195400	16.31905900
H	1.24376300	16.65893800	15.38405200
C	2.48718500	13.75878000	14.30383600
H	3.16400800	13.50550600	15.11105400
C	1.75722700	15.28389100	12.58961100
H	1.86774600	16.21985700	12.05355800
C	1.48963700	12.86195400	13.93018500
C	6.08081900	17.27913800	10.66220800
C	0.61208000	13.17880600	12.89444900
C	0.74956400	14.39501700	12.22591000
H	0.07558000	14.64889300	11.41510400
C	5.54795200	18.20554900	11.55758500
H	5.71682200	19.26617800	11.40737900
H	6.67046000	17.61367300	9.81609200
H	-0.16661200	12.48176800	12.60579100
H	0.64168700	15.40785500	19.44316700
H	1.39930600	11.91359900	14.44835800
C	6.59573800	18.75940800	16.58676400
C	5.26734300	18.34733100	16.33090600
C	4.21756900	19.20864500	16.69694600
C	4.50300500	20.42381500	17.30003400
C	5.83015200	20.81062300	17.54980100
C	6.88620400	19.98331200	17.19402200
C	6.45446100	16.53920100	15.46905100
C	5.21003000	17.05537000	15.66989700
H	3.19053100	18.91652900	16.51500300

H	3.69208300	21.08438200	17.58504500
H	6.03334900	21.76442900	18.02313300
H	7.91135800	20.28171800	17.38057500
H	4.38212900	18.50411300	13.33520700
S	7.75090800	17.55899500	16.03369200

***E*-Product of Photocyclization of 3-TPVBT in gas**

C	3.81841300	15.88095200	13.92612400
C	4.58209400	16.30442000	12.87104600
C	2.86913000	16.29140800	16.25510500
C	4.45027200	15.77503700	11.53181400
H	3.65710900	15.06424100	11.33633200
C	0.79874700	15.94282300	18.12103000
C	3.96485400	16.49530300	15.25524800
C	0.89761000	17.13011900	17.39756900
H	0.17624700	17.92452300	17.55453900
C	5.30984200	16.11755800	10.54234700
H	5.18996200	15.69464500	9.55123500
C	2.79849700	14.80017600	13.73140000
C	5.54647500	17.46978700	13.07806700
H	6.82526100	16.50854800	14.52005300
C	2.75737700	15.10111500	16.98291500
H	3.47964200	14.30861400	16.82462700
C	1.73216800	14.92869600	17.91075100
H	1.66210000	14.00123700	18.46828300
C	1.92452100	17.30157400	16.47114800
H	2.00328400	18.22931800	15.91511700
C	3.19102700	13.45631100	13.72019100
H	4.23810400	13.20909500	13.85847900
C	1.44422900	15.10222000	13.54520400
H	1.12341000	16.13763100	13.54935700
C	2.25542500	12.44015800	13.53078900
C	6.43370300	17.00308600	10.79598800
C	0.91004000	12.75359800	13.34798700
C	0.50790000	14.08839600	13.35389000
H	-0.53648500	14.34193500	13.20908500
C	6.57827300	17.60617300	11.98499000
H	7.41719200	18.26951100	12.16924100
H	7.16405400	17.16021000	10.00945600
H	0.18100000	11.96473600	13.20032000
H	-0.00008300	15.80789100	18.84162200

H	2.57886000	11.40497800	13.52469500
C	6.57731700	18.77200300	16.60220100
C	5.48484900	17.89420500	16.78561500
C	4.95657100	17.76632000	18.08087000
C	5.49340200	18.49700400	19.13612100
C	6.56613500	19.36657000	18.92630600
C	7.11929700	19.50334800	17.65562300
C	6.14682900	17.37396800	14.47053200
C	5.07856300	17.22899200	15.54436300
H	4.13303000	17.09329500	18.26759300
H	5.07652200	18.38293600	20.13004200
H	6.97871600	19.93141500	19.75468700
H	7.96047000	20.16596700	17.48863300
H	4.93716000	18.39677600	13.06219500
S	7.15797700	18.85678600	14.93269000

Z-Product of Photocyclization of 3-TPVBT in gas

C	3.65970700	16.12053700	13.83350100
C	4.50795900	16.45197200	12.80941700
C	2.73765500	16.44748500	16.19470700
C	4.63721800	15.68712300	11.59445900
H	3.97875100	14.84101800	11.44444200
C	0.94257700	15.73538400	18.23324600
C	3.69068700	16.84799500	15.11026100
C	0.68177000	16.84084300	17.42585800
H	-0.21530100	17.42994600	17.58203900
C	5.59428800	15.96686500	10.67259000
H	5.68046500	15.35289500	9.78314700
C	2.75241500	14.93487800	13.70743200
C	5.27602300	17.76115200	12.88391000
H	5.67491400	19.30006100	14.30585100
C	2.98836800	15.33833800	17.00951600
H	3.88794700	14.75413100	16.85430900
C	2.09934100	14.98647300	18.02248700
H	2.31118900	14.12659900	18.64826100
C	1.57515300	17.19424100	16.41540200
H	1.37259000	18.05873200	15.79205400
C	3.25688900	13.63401200	13.82546300
H	4.31362200	13.49104200	14.02328300
C	1.38586000	15.10021500	13.45253300
H	0.97825700	16.10027600	13.35615100

C	2.41936000	12.52794600	13.69002400
C	6.54684900	17.04037200	10.87535800
C	1.06129000	12.70565600	13.43382000
C	0.54740000	13.99608400	13.31457400
H	-0.50765100	14.14436000	13.11223900
C	6.42866700	17.87330400	11.92210000
H	7.13076800	18.68621300	12.07481400
H	7.36183100	17.15913300	10.16948500
H	0.40859400	11.84646300	13.32750900
H	0.24989400	15.45916800	19.02030500
H	2.82911200	11.52826500	13.78464200
C	6.64728900	18.12571500	16.63642300
C	5.23231000	18.13738700	16.68015900
C	4.59812300	18.41989500	17.89166000
C	5.35804900	18.67476200	19.03403200
C	6.75082200	18.63746900	18.97969500
C	7.40524900	18.36268700	17.77736100
C	5.62667200	18.20836100	14.30701600
C	4.67163200	17.76093900	15.36757400
H	3.51793100	18.44702900	17.94496900
H	4.85883000	18.90385100	19.96843200
H	7.33403400	18.83329400	19.87255900
H	8.48800200	18.34308600	17.73236800
H	4.53837600	18.52272500	12.56397600
S	7.31559500	17.74408100	15.02409600

7. References

(1) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Borthers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Rahavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, G.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc. Wallingford CT, 2009.

(2) Becke, A. D. Density-functional thermochemistry. III. The role of exact exchange. *J. Chem. Phys.* **1993**, *98*, 5648–5652.

(3) Adamo, C.; Jacquemin, D. The calculations of excited-state properties with time-dependent density functional theory. *Chem. Soc. Rev.* **2013**, *42*, 845–856.