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# **†Electronic Supporting Information**

### for

# AIEE compounds based on 9, 10-dithienylanthracene-substituted

# triphenylamine: design, synthesis, and applications in cell imaging

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Figure S1. NMR spectra data for TPA-DTA-C in DMSO-d<sub>6</sub>: (A) <sup>1</sup>H-NMR spectra; (B) <sup>13</sup>C-NMR

spectra.



(B)

Figure S2. NMR spectra data for TPA-DTA-PAM in DMSO-d<sub>6</sub>: (A) <sup>1</sup>H-NMR spectra; (B) <sup>13</sup>C-

NMR spectra.



Figure S3. NMR spectra data for TPA-DTA-PA in DMSO-d<sub>6</sub>: (A) <sup>1</sup>H-NMR spectra; (B) <sup>13</sup>C-

NMR spectra.



(B)

Figure S4. NMR spectra data for TPA-DTA-PATF in DMSO-d<sub>6</sub>: (A) <sup>1</sup>H-NMR spectra; (B) <sup>13</sup>C-

NMR spectra.



Figure S5. HRMS-ESI spectra of TPA-DTA-C.



Figure S6. HRMS-ESI spectra of TPA-DTA-PAM.



Figure S7. HRMS-ESI spectra of TPA-DTA-PA.



Figure S8. HRMS-ESI spectra of TPA-DTA-PATF.



**Figure S9.** The changes of absorption, fluorescence spectra and photos in THF/H<sub>2</sub>O with different fraction for **TPA-DTA-C** (A), **TPA-DTA-PA** (B), and **TPA-DTA-PATF** ( $\lambda_{ex}$  = 400 nm, *C* =2.0 × 10<sup>-5</sup> mol/L).



Figure S10. Size distribution curve of TPA-DTA-C (A), TPA-DTA-PA (B) TPA-DTA-PATF

(C) in THF-H<sub>2</sub>O ( $f_w$ =90%) mixture.





(B)





# Figure S11. SEM images of TPA-DTA-C (A), TPA-DTA-PA (B) and TPA-DTA-PATF (C) in

THF/H<sub>2</sub>O ( $f_w = 90\%$ )..



Figure S12. Photographic images of TPA-DTA-C in various states under 365 nm UV irradiation.

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Figure S13. (A) Solid state PL spectra of TPA-DTA-PA before and after the grinding, and after treatment with DCM vapor. (B) XRD curves of TPA-DTA-PA in pristine, ground, and fumed form, (C-E) Photographic images of TPA-DTA-PA in various states under 365 nm UV irradiation.



**Figure S14.** (A) Solid state PL spectra of **TPA-DTA-PATF** before and after the grinding, and after treatment with DCM vapor, (B) XRD curves of **TPA-DTA-PATF** in pristine, ground, and fumed form, (C-E) Photographic images of **TPA-DTA-PATF** in various states under 365 nm UV

irradiation.



Figure S15. % cell viability of HeLa cells treated with different concentrations (10 $\rightarrow$ 50  $\mu$ M) of

TPA-DTAs for 24 h determined by MTT assay.

Symbolic Z Mai			
	-0.883	0.47461	0
	-1.917	1.29261	-0.227
	-3.171	1.11361	0.252
	-3.327	0.13361	1.186
	-2.302	-0.74239	1.313
	-1.098	-0.60639	0.746
	-4.211	1.91261	-0.117
	-5.391	1.70861	0.526
	-5.497	0.84761	1.563
	-4.487	-0.00039	1.89
	-6.548	2.25961	0.084
	-7.698	2.24061	0.768
	-7.703	1.64561	1.961
	-6.61	0.96461	2.326
	-4.152	2.92261	-1.031
	-4.727	-0.94539	2.844
	-4.765	4.11061	-0.866
	-4.519	4.96261	-1.864
	-3.675	4.40961	-2.745
	-3.289	3.09561	-2.212
	-3.93485	-2.02155	3.04078
	-4.30998	-2.76524	4.08608
	-5.36259	-2.1788	4.66504
	-5.67493	-0.92448	3.97597
	-3.233	4.95261	-3.901
	-2.364	4.34161	-4.729
	-1.96	4.88961	-5.887
	-2.369	6.09461	-6.343
	-3.229	6.69761	-5.49
	-3.643	6.16061	-4.331
	-1.985	6.61461	-7.468
	-1.975	7.90361	-7.618
	-1.617	5.84461	-8.446
	-2.125	8.51261	-8.82
	-2.122	9.84461	-8.991
	-1.959	10.65961	-7.943
	-1.804	10.10861	-6.733
	-1.816	8.77361	-6.591
	-0.742	6.22861	-9.406
	-0.351	5.44361	-10 423
	-0.832	4,19961	-10 539
	-1.701	3.77161	-9 616
	-2 071	4 57761	-8 608
	2.071		0.000

 Table S1. Symbolic Z-Matrix of TPA-DTA-C.

С	-5.97542	-2.68939	5.77015
0	-6.9384	-2.23526	6.353
Н	0.112	0.65861	-0.442
Н	-1.605	2.13761	-0.849
Н	-2.351	-1.67339	1.887
Н	-0.293	-1.34239	0.909
Н	-6.634	2.77061	-0.888
Н	-8.603	2.74161	0.386
Н	-8.602	1.67461	2.6
Н	-6.702	0.50661	3.324
Н	-5.402	4.41561	-0.021
Н	-4.975	5.96061	-1.905
Н	-3.04018	-2.29748	2.46301
Н	-3.81362	-3.69085	4.40782
Н	-1.929	3.35761	-4.48
Н	-1.195	4.30261	-6.426
Н	-3.718	7.65261	-5.747
Н	-4.376	6.75361	-3.76
Н	-2.342	7.94261	-9.739
Н	-2.277	10.27661	-9.995
Н	-1.954	11.75461	-8.071
Н	-1.646	10.76061	-5.857
Н	-1.606	8.42861	-5.564
Н	-0.228	7.20461	-9.37
Н	0.384	5.81061	-11.159
Н	-0.521	3.54661	-11.37
Н	-2.129	2.75761	-9.704
Н	-2.848	4.14861	-7.952
Н	-5.5101	-3.63219	6.14763

 Table S2. Total energies of TPA-DTA-C.

Zero-point correction	0.558239 (Hartree/Particle)
Thermal correction to Energy	0.594417
Thermal correction to Enthalpy	0.595361
Thermal correction to Gibbs Free Energy	0.482156
Sum of electronic and zero-point Energies	-2504.619982
Sum of electronic and thermal Energies	-2504.583804
Sum of electronic and thermal Enthalpies	-2504.582860
Sum of electronic and thermal Free Energies	-2504.696065

С	-1.22212	-5.53657	0.45127
С	-1.92683	-4.38169	0.23902
С	-1.26613	-3.12876	0.02401
С	0.17894	-3.10685	0.07737
С	0.87362	-4.34056	0.29279
С	0.19914	-5.5188	0.46727
С	-1.97891	-1.92698	-0.21327
С	0.87311	-1.88484	-0.07044
С	0.16051	-0.68191	-0.27967
С	-1.28141	-0.70298	-0.36703
С	-1.95755	0.52915	-0.6432
Н	-3.03674	0.52537	-0.73125
С	-1.26992	1.70452	-0.78928
С	0.14598	1.72942	-0.66756
С	0.83588	0.57237	-0.42417
Н	-1.75142	-6.47109	0.61702
Н	-3.01003	-4.40196	0.24266
Н	1.95716	-4.32221	0.32534
Н	0.74899	-6.44171	0.63074
Н	-1.80872	2.62439	-0.99987
Н	0.68046	2.6695	-0.77439
Н	1.91623	0.58944	-0.33415
С	-3.44835	-1.95513	-0.32105
С	-4.30797	-2.13989	-1.37061
С	-5.63709	-2.03296	-0.84935
Н	-4.01995	-2.31521	-2.39778
С	-5.49868	-1.7914	0.48274
Н	-6.5654	-2.12208	-1.39634
С	2.35656	-1.86519	-0.01148
С	3.16925	-1.74081	1.087
С	4.56394	-1.76376	0.77637
Н	2.77415	-1.63469	2.09187
С	4.80487	-1.90735	-0.56127
Н	5.3489	-1.67683	1.52011
S	3.32839	-2.01604	-1.46593
S	-4.18103	-1.73819	0.82497
С	6.16231	-1.97626	-1.2853
Н	6.19419	-2.09154	-2.34859
С	7.31662	-1.89139	-0.58036
C	8.66971	-1.9612	-1.31238
N	9 67715	-2.01318	-1 85741
C	7.27988	-1.72538	0.95023
			0.0000000000000000000000000000000000000

 Table S3. Symbolic Z-Matrix of TPA-DTA-PAM.

С	7.25291	-0.44902	1.51296
С	7.27345	-2.85098	1.77396
С	7.22021	-0.29839	2.89912
Н	7.25877	0.43819	0.86329
С	7.23974	-2.70048	3.16055
Н	7.29452	-3.85702	1.3306
С	7.21326	-1.42446	3.72322
Н	7.19959	0.70762	3.34276
Н	7.23427	-3.58816	3.80976
С	-6.49583	-1.58076	1.63726
С	-6.94889	-2.67423	2.37586
С	-6.94596	-0.29684	1.94463
С	-7.8524	-2.48381	3.42115
Н	-6.59442	-3.68641	2.13279
С	-7.84899	-0.10608	2.99085
Н	-6.58884	0.56511	1.36272
С	-8.30235	-1.19929	3.72901
Н	-8.21004	-3.34571	4.00297
Н	-8.20341	0.9064	3.23323
Ν	-9.25457	-0.9989	4.83084
С	-10.70054	-1.04627	4.57041
С	-11.38662	0.11999	4.23038
С	-11.38668	-2.25712	4.66312
С	-12.75863	0.07543	3.9838
Н	-10.84553	1.07459	4.15812
С	-12.75893	-2.30205	4.41553
Н	-10.84607	-3.17644	4.93093
С	-13.44499	-1.13602	4.07604
Н	-13.29958	0.99476	3.71639
Н	-13.29958	-3.25697	4.4883
Н	-14.52677	-1.17092	3.88151
С	-8.76082	-0.75115	6.19309
С	-8.52712	-1.82234	7.05589
С	-8.52585	0.55477	6.6231
С	-8.05919	-1.58752	8.34861
Н	-8.71319	-2.85174	6.71683
С	-8.05685	0.78977	7.91585
Н	-8.70983	1.39913	5.94315
С	-7.82363	-0.28108	8.77866
Н	-7.87556	-2.43175	9.02894
Н	-7.87129	1.81951	8.25448
Н	-7.45463	-0.09618	9.79795
0	7.179	-1.27024	5.14447
С	7.19454	0.12115	5.47415

Н	6.3418	0.60007	5.04014
Н	7.16539	0.23607	6.53756
Н	8.08806	0.56841	5.09143

 Table S4. Total energies of TPA-DTA-PAM.

Zero-point correction	0.693761 (Hartree/Particle)
Thermal correction to Energy	0.739369
Thermal correction to Enthalpy	0.740313
Thermal correction to Gibbs Free Energy	0.603621
Sum of electronic and zero-point Energies	-2906.177911
Sum of electronic and thermal Energies	-2906.132303
Sum of electronic and thermal Enthalpies	-2906.131359
Sum of electronic and thermal Free Energies	-2906.268051

С	-1.22212	-5.53657	0.45127
С	-1.92683	-4.38169	0.23902
С	-1.26613	-3.12876	0.02401
С	0.17894	-3.10685	0.07737
С	0.87362	-4.34056	0.29279
С	0.19914	-5.5188	0.46727
С	-1.97891	-1.92698	-0.21327
С	0.87311	-1.88484	-0.07044
С	0.16051	-0.68191	-0.27967
С	-1.28141	-0.70298	-0.36703
С	-1.95755	0.52915	-0.6432
Н	-3.03674	0.52537	-0.73125
С	-1.26992	1.70452	-0.78928
С	0.14598	1.72942	-0.66756
С	0.83588	0.57237	-0.42417
Н	-1.75142	-6.47109	0.61702
Н	-3.01003	-4.40196	0.24266
Н	1.95716	-4.32221	0.32534
Н	0.74899	-6.44171	0.63074
Н	-1.80872	2.62439	-0.99987
Н	0.68046	2.6695	-0.77439
Н	1.91623	0.58944	-0.33415
С	-3.44835	-1.95513	-0.32105
С	-4.30797	-2.13989	-1.37061
С	-5.63709	-2.03296	-0.84935
Н	-4.01995	-2.31521	-2.39778
С	-5.49868	-1.7914	0.48274
Н	-6.5654	-2.12208	-1.39634
С	2.35656	-1.86519	-0.01148
С	3.16925	-1.74081	1.087
С	4.56394	-1.76376	0.77637
Н	2.77415	-1.63469	2.09187
С	4.80487	-1.90735	-0.56127
Н	5.3489	-1.67683	1.52011
S	3.32839	-2.01604	-1.46593
S	-4.18103	-1.73819	0.82497
С	6.16231	-1.97626	-1.2853
Н	6.19419	-2.09154	-2.34859
С	7.31662	-1.89139	-0.58036
С	8.66971	-1.9612	-1.31238
Ν	9.67715	-2.01318	-1.85741
С	7.27988	-1.72538	0.95023

 Table S5. Symbolic Z-Matrix of TPA-DTA-PA.

C         7.27345         -2.85098         1.77396           C         7.22021         -0.29839         2.89912           H         7.25877         0.43819         0.86229           C         7.23974         -2.70048         3.16055           H         7.29452         -3.85702         1.3306           C         7.21326         -1.42446         3.72322           H         7.19959         0.70762         3.34276           II         7.23427         -3.58816         3.80976           C         -6.94889         -2.67423         2.37586           C         -6.94889         -2.67423         2.37586           C         -7.8524         -2.48381         3.42115           H         -6.59442         -3.68641         2.13279           C         -7.84899         -0.10608         2.99085           H         -6.58844         0.56511         1.36272           C         -8.30235         -1.1929         3.72901           H         -8.20341         0.9064         3.23323           N         -9.25457         -0.9989         4.8084           C         -10.7005         -1.0462         4.57041		С	7.25291	-0.44902	1.51296
C         7.22021         -0.29839         2.89912           H         7.23877         0.43819         0.86329           C         7.23974         -2.70048         3.16055           H         7.29452         -3.85702         1.3306           C         7.21326         -1.42446         3.72322           H         7.19959         0.70762         3.34276           II         7.23427         -3.58816         3.80976           C         -6.49583         -1.58076         1.63726           C         -6.94889         -2.67423         2.3786           C         -6.94894         2.468381         3.42115           H         -6.59424         -3.68641         2.13279           C         -7.8524         -2.48381         3.42115           H         -6.58844         0.56511         1.36272           C         -8.30235         -1.19929         3.72901           H         -8.20041         0.9064         3.23323           N         -9.25457         -0.9989         4.83084           C         -10.7005         -1.0462         4.57041           C         -11.3866         0.1199         4.23038		С	7.27345	-2.85098	1.77396
H         7.25877         0.43819         0.86329           C         7.23974         -2.70048         3.16055           H         7.29452         -3.85702         1.3306           C         7.21326         -1.42446         3.72322           H         7.19959         0.70762         3.34276           II         7.23427         -3.58816         3.80976           C         -6.49583         -1.58076         1.63726           C         -6.94889         -2.67423         2.37586           C         -6.94894         -2.67423         2.37586           C         -7.8524         -2.48381         3.42115           H         -6.594842         -3.66641         2.13279           C         -7.8524         -2.48381         3.42115           H         -6.58884         0.56511         1.36272           C         -8.30235         -1.19929         3.72901           H         -8.20341         0.9064         3.2323           N         -9.25457         -0.9989         4.8304           C         -10.7005         -1.0462         4.57041           C         -11.3866         0.21571         4.66312		С	7.22021	-0.29839	2.89912
C         7,23974         -2,70048         3,16055           H         7,29452         -3,85702         1,3306           C         7,21326         -1,42446         3,72322           H         7,19959         0,70762         3,34276           H         7,23427         -3,58816         3,80976           C         -6,49583         -1,58076         1,63726           C         -6,94889         -2,67423         2,37586           C         -6,94869         -0,20684         1,44415           H         -6,59442         -3,68641         2,13279           C         -7,84899         -0,10608         2.99085           H         -6,5884         0,56511         1,36272           C         -8,30235         -1,19929         3,72901           H         -8,20341         0,9064         3,23323           N         -9,25457         -0,9899         4,83084           C         -10,7005         -1,0462         4,57041           C         -11,3866         -2,2571         4,66312           C         -11,3866         -2,2571         4,66312           C         -12,7586         0,0754         3,9838		Н	7.25877	0.43819	0.86329
H         7.29452         -3.85702         1.3306           C         7.21326         -1.42446         3.72322           H         7.19959         0.70762         3.34276           C         -6.49583         -1.58076         1.63726           C         -6.94596         -0.29684         1.94463           C         -7.8524         -2.48381         3.4215           H         -6.59442         -3.68641         2.1327           C         -7.84899         -0.10608         2.99085           C         -7.84899         -0.10608         2.99085           H         -6.5884         0.56511         1.36272           C         -8.30235         -1.19929         3.72901           H         -8.21004         -3.34571         4.00297           H         -8.20341         0.9064         2.3323           N         -9.25457         -0.9989         4.83084           C         -10.7005         -1.0462         4.57041           C         -11.3866         0.1199         4.23038           C         -12.7589         -2.302         4.41553           H         -10.8455         1.0745         4.15812     <		С	7.23974	-2.70048	3.16055
C         7.21326         -1.42446         3.72322           H         7.19959         0.70762         3.34276           H         7.23427         -3.58816         3.80976           C         -6.49583         -1.58076         1.63726           C         -6.94889         -2.67423         2.37586           C         -6.94889         -2.67423         2.37586           C         -7.8524         -2.48381         3.42115           H         -6.59442         -3.68641         2.13279           C         -7.84899         -0.10608         2.99085           H         -6.5884         0.56511         1.36272           C         -8.30235         -1.19929         3.72901           H         -8.21004         -3.34571         4.00297           H         -8.20341         0.9064         3.23323           N         -9.25457         -0.9989         4.83084           C         -10.7005         -1.0462         4.57041           C         -11.3866         0.1199         4.23038           C         -11.3866         0.2571         4.66312           C         -12.7589         -2.302         4.41552		Н	7.29452	-3.85702	1.3306
H         7.19959         0.70762         3.34276           H         7.23427         -3.58816         3.80976           C         -6.49583         -1.58076         1.63726           C         -6.94889         -2.67423         2.37586           C         -6.94896         -0.29684         1.94463           C         -7.8524         -2.48381         3.42115           H         -6.59442         -3.68641         2.13279           C         -7.84899         -0.10608         2.99085           H         -6.58884         0.56511         1.36272           C         -8.30235         -1.19929         3.72901           H         -8.21004         -3.34571         4.00297           H         -8.20341         0.9064         3.23323           N         -9.25457         -0.9989         4.83084           C         -10.7005         -1.0462         4.57041           C         -11.3866         0.1199         4.23038           H         -10.8455         1.0745         4.15812           C         -12.7586         0.0754         3.9838           H         -10.846         -3.1764         4.93093		С	7.21326	-1.42446	3.72322
H         7.23427         -3.58816         3.80976           C         -6.49583         -1.58076         1.63726           C         -6.94889         -2.67423         2.37586           C         -6.94596         -0.29684         1.94463           C         -7.8524         -2.48381         3.42115           H         -6.59442         -3.68641         2.13279           C         -7.84899         -0.10608         2.99085           H         -6.58884         0.56511         1.36272           C         -8.30235         -1.19929         3.72901           H         -8.21004         -3.34571         4.00297           H         -8.20341         0.9064         3.23323           N         -9.25457         -0.9989         4.83084           C         -10.7005         -1.0462         4.57041           C         -11.3866         0.1199         4.23038           C         -11.3866         0.0754         3.9838           H         -10.8455         1.0745         4.15812           C         -12.7589         -2.302         4.41553           H         -10.846         -3.1764         4.93093		Н	7.19959	0.70762	3.34276
C         -6.49583         -1.58076         1.63726           C         -6.94889         -2.67423         2.37586           C         -6.94596         -0.29684         1.94463           C         -7.8524         -2.48381         3.42115           H         -6.59442         -3.66641         2.13279           C         -7.84899         -0.16608         2.99085           H         -6.58844         0.56511         1.36272           C         -8.30235         -1.19929         3.72901           H         -8.21004         -3.34571         4.00297           H         -8.20341         0.9064         3.23323           N         -9.25457         -0.9989         4.83084           C         -10.7005         -1.0462         4.57041           C         -11.3866         0.1199         4.23038           C         -11.3866         -2.2571         4.66312           C         -12.7586         0.0754         3.9838           H         -10.8455         1.0745         4.15812           C         -12.7589         -2.302         4.41553           G         -13.4449         -1.136         4.07604		Н	7.23427	-3.58816	3.80976
C         -6.94889         -2.67423         2.37586           C         -6.94596         -0.29684         1.94463           C         -7.8524         -2.48381         3.42115           H         -6.59442         -3.68641         2.13279           C         -7.84899         -0.10608         2.99085           H         -6.58884         0.56511         1.36272           C         -8.30235         -1.19929         3.72901           H         -8.21004         -3.34571         4.00297           H         -8.20341         0.9064         3.23323           N         -9.25457         -0.9989         4.83084           C         -10.7005         -1.0462         4.57041           C         -11.3866         0.1199         4.23038           C         -11.3866         -2.2571         4.66312           C         -12.7586         0.0754         3.9838           H         -10.846         -3.1764         4.93093           C         -13.4449         -1.136         4.07604           H         -13.2995         -3.2569         4.44853           H         -13.2995         -3.2569         4.4883		С	-6.49583	-1.58076	1.63726
C         -6.94596         -0.29684         1.94463           C         -7.8524         -2.48381         3.42115           H         -6.59442         -3.68641         2.13279           C         -7.84899         -0.10608         2.99085           H         -6.58884         0.56511         1.36272           C         -8.30235         -1.19929         3.72901           H         -8.21004         -3.34571         4.00297           H         -8.20341         0.9064         3.23323           N         -9.25457         -0.9989         4.83084           C         -10.7005         -1.0462         4.57041           C         -11.3866         0.1199         4.23038           C         -11.3866         0.1199         4.23038           C         -11.3866         0.1795         4.1581           C         -12.7589         -2.302         4.41553           H         -10.8455         1.0745         4.1581           C         -13.4449         -1.136         4.07604           H         -13.2995         0.9947         3.71639           H         -13.2995         0.52477         6.6231 <td></td> <td>С</td> <td>-6.94889</td> <td>-2.67423</td> <td>2.37586</td>		С	-6.94889	-2.67423	2.37586
C         -7.8524         -2.48381         3.42115           H         -6.59442         -3.68641         2.13279           C         -7.84899         -0.10608         2.99085           H         -6.58884         0.56511         1.36272           C         -8.30235         -1.19929         3.72901           H         -8.21004         -3.34571         4.00297           H         -8.20341         0.9064         3.23323           N         -9.25457         -0.9989         4.83084           C         -10.7005         -1.0462         4.57041           C         -11.3866         0.1199         4.23038           C         -11.3866         -2.2571         4.66312           C         -12.7586         0.0754         3.9838           H         -10.8455         1.0745         4.15812           C         -12.7589         -2.302         4.41553           H         -10.846         -3.1764         4.93093           C         -13.4449         -1.136         4.07604           H         -13.2995         -3.2569         4.4883           H         -14.5267         -1.1709         3.88151 <td></td> <td>С</td> <td>-6.94596</td> <td>-0.29684</td> <td>1.94463</td>		С	-6.94596	-0.29684	1.94463
H         -6.59442         -3.68641         2.13279           C         -7.84899         -0.10608         2.99085           H         -6.58884         0.56511         1.36272           C         -8.30235         -1.19929         3.72901           H         -8.21004         -3.34571         4.00297           H         -8.20341         0.9064         3.23323           N         -9.25457         -0.9989         4.83084           C         -10.7005         -1.0462         4.57041           C         -11.3866         0.1199         4.23038           C         -11.3866         0.1199         4.23038           C         -11.3866         -2.2571         4.66312           C         -12.7586         0.0754         3.9838           H         -10.8455         1.0745         4.15812           C         -12.7589         -2.302         4.41553           H         -10.8455         1.0745         4.15812           C         -13.4449         -1.136         4.07604           H         -13.2995         0.9947         3.71639           H         -13.2995         -3.2569         4.4883		С	-7.8524	-2.48381	3.42115
C         -7.84899         -0.10608         2.99085           H         -6.58884         0.56511         1.36272           C         -8.30235         -1.19929         3.72901           H         -8.21004         -3.34571         4.00297           H         -8.20341         0.9064         3.23323           N         -9.25457         -0.9989         4.83084           C         -10.7005         -1.0462         4.57041           C         -11.3866         0.1199         4.23038           C         -11.3866         0.12971         4.66312           C         -12.7586         0.0754         3.9838           H         -10.8455         1.0745         4.15812           C         -12.7589         -2.302         4.41553           H         -10.846         -3.1764         4.93093           C         -13.4449         -1.136         4.07604           H         -13.2995         0.9947         3.71639           H         -13.2995         -3.2569         4.4883           H         -14.5267         -1.1709         3.88151           C         -8.52585         0.55477         6.6231		Н	-6.59442	-3.68641	2.13279
H         -6.58884         0.56511         1.36272           C         -8.30235         -1.19929         3.72901           H         -8.21004         -3.34571         4.00297           H         -8.20341         0.9064         3.23323           N         -9.25457         -0.9989         4.83084           C         -10.7005         -1.0462         4.57041           C         -11.3866         0.1199         4.23038           C         -11.3866         -2.2571         4.66312           C         -11.3866         -2.2571         4.66312           C         -12.7586         0.0754         3.9838           H         -10.8455         1.0745         4.15812           C         -12.7589         -2.302         4.41553           H         -10.846         -3.1764         4.93093           C         -13.4449         -1.136         4.07604           H         -13.2995         0.9947         3.71639           H         -13.2995         -3.2569         4.4883           H         -14.5267         -1.1709         3.88151           C         -8.52712         -1.82234         7.05589		С	-7.84899	-0.10608	2.99085
C         -8.30235         -1.19929         3.72901           H         -8.21004         -3.34571         4.00297           H         -8.20341         0.9064         3.23323           N         -9.25457         -0.9989         4.83084           C         -10.7005         -1.0462         4.57041           C         -11.3866         0.1199         4.23038           C         -11.3866         -2.2571         4.66312           C         -12.7586         0.0754         3.9838           H         -10.8455         1.0745         4.15812           C         -12.7589         -2.302         4.41553           H         -10.846         -3.1764         4.93093           C         -13.4449         -1.136         4.07604           H         -13.2995         0.9947         3.71639           H         -13.2995         0.9947         3.71639           H         -13.2995         0.9947         3.71639           H         -13.2995         0.55477         6.6231           C         -8.76082         -0.75115         6.19309           C         -8.52585         0.55477         6.6231		Н	-6.58884	0.56511	1.36272
H         -8.21004         -3.34571         4.00297           H         -8.20341         0.9064         3.23323           N         -9.25457         -0.9989         4.83084           C         -10.7005         -1.0462         4.57041           C         -11.3866         0.1199         4.23038           C         -11.3866         -2.2571         4.66312           C         -12.7586         0.0754         3.9838           H         -10.8455         1.0745         4.15812           C         -12.7589         -2.302         4.41553           H         -10.846         -3.1764         4.93093           C         -13.4449         -1.136         4.07604           H         -13.2995         0.9947         3.71639           H         -13.2995         0.9947         3.71639           H         -13.2995         0.55477         6.6231           C         -8.76082         -0.75115         6.19309           C         -8.52712         -1.82234         7.05589           C         -8.52585         0.55477         6.6231           C         -8.52585         0.55477         6.6231		С	-8.30235	-1.19929	3.72901
H-8.203410.90643.23323N-9.25457-0.99894.83084C-10.7005-1.04624.57041C-11.38660.11994.23038C-11.3866-2.25714.66312C-12.75860.07543.9838H-10.84551.07454.15812C-12.7589-2.3024.41553H-10.846-3.17644.93093C-13.4449-1.1364.07604H-13.29950.99473.71639H-13.2995-3.25694.4883H-14.5267-1.17093.88151C-8.76082-0.751156.19309C-8.525850.554776.6231C-8.525850.554776.6231C-8.05919-1.587528.34861H-8.71319-2.851746.71683C-8.056850.789777.91585H-8.709831.399135.94315C-7.82363-0.281088.77866H-7.87556-2.431759.02894H-7.87566-2.431759.02894H-7.87566-2.431759.02894H-7.87663-0.096189.79795H7.18762-1.309074.78667		Н	-8.21004	-3.34571	4.00297
N         -9.25457         -0.9989         4.83084           C         -10.7005         -1.0462         4.57041           C         -11.3866         0.1199         4.23038           C         -11.3866         -2.2571         4.66312           C         -12.7586         0.0754         3.9838           H         -10.8455         1.0745         4.15812           C         -12.7589         -2.302         4.41553           H         -10.846         -3.1764         4.93093           C         -13.4449         -1.136         4.07604           H         -13.2995         0.9947         3.71639           H         -13.2995         -3.2569         4.4883           H         -14.5267         -1.1709         3.88151           C         -8.76082         -0.75115         6.19309           C         -8.52712         -1.82234         7.05589           C         -8.52712         -1.82234         7.05589           C         -8.52585         0.55477         6.6231           C         -8.05685         0.78977         7.91585           H         -8.70983         1.39913         5.94315		Н	-8.20341	0.9064	3.23323
C-10.7005-1.04624.57041C-11.38660.11994.23038C-11.3866-2.25714.66312C-12.75860.07543.9838H-10.84551.07454.15812C-12.7589-2.3024.41553H-10.846-3.17644.93093C-13.4449-1.1364.07604H-13.29950.99473.71639H-13.2995-3.25694.4883H-14.5267-1.17093.88151C-8.76082-0.751156.19309C-8.52712-1.822347.05589C-8.525850.554776.6231C-8.05919-1.587528.34861H-8.71319-2.851746.71683C-8.056850.789777.91585H-8.709831.399135.94315C-7.82363-0.281088.77866H-7.871291.819518.25448H-7.45463-0.096189.79795H7.18762-1.309074.78667		Ν	-9.25457	-0.9989	4.83084
C-11.38660.11994.23038C-11.3866-2.25714.66312C-12.75860.07543.9838H-10.84551.07454.15812C-12.7589-2.3024.41553H-10.846-3.17644.93093C-13.4449-1.1364.07604H-13.29950.99473.71639H-13.2995-3.25694.4883H-14.5267-1.17093.88151C-8.76082-0.751156.19309C-8.52712-1.822347.05589C-8.525850.554776.6231C-8.05919-1.587528.34861H-8.71319-2.851746.71683C-8.056850.789777.91585H-8.709831.399135.94315C-7.82363-0.281088.77866H-7.87556-2.431759.02894H-7.871291.819518.25448H-7.18762-1.309074.78667		С	-10.7005	-1.0462	4.57041
C-11.3866-2.25714.66312C-12.75860.07543.9838H-10.84551.07454.15812C-12.7589-2.3024.41553H-10.846-3.17644.93093C-13.4449-1.1364.07604H-13.29950.99473.71639H-13.2995-3.25694.4883H-14.5267-1.17093.88151C-8.76082-0.751156.19309C-8.525850.554776.6231C-8.525850.554776.6231C-8.056850.789777.91585H-8.709831.399135.94315C-7.82363-0.281088.77866H-7.87556-2.431759.02894H-7.871291.819518.25448H-7.45463-0.096189.79795H7.18762-1.309074.78667		С	-11.3866	0.1199	4.23038
C-12.75860.07543.9838H-10.84551.07454.15812C-12.7589-2.3024.41553H-10.846-3.17644.93093C-13.4449-1.1364.07604H-13.29950.99473.71639H-13.2995-3.25694.4883H-14.5267-1.17093.88151C-8.76082-0.751156.19309C-8.52712-1.822347.05589C-8.525850.554776.6231C-8.05919-1.587528.34861H-8.71319-2.851746.71683C-8.056850.789777.91585H-8.709831.399135.94315C-7.82363-0.281088.77866H-7.87556-2.431759.02894H-7.871291.819518.25448H-7.45463-0.096189.79795H7.18762-1.309074.78667		С	-11.3866	-2.2571	4.66312
H-10.84551.07454.15812C-12.7589-2.3024.41553H-10.846-3.17644.93093C-13.4449-1.1364.07604H-13.29950.99473.71639H-13.2995-3.25694.4883H-14.5267-1.17093.88151C-8.76082-0.751156.19309C-8.52712-1.822347.05589C-8.525850.554776.6231C-8.05919-1.587528.34861H-8.71319-2.851746.71683C-8.056850.789777.91585H-8.709831.399135.94315C-7.82363-0.281088.77866H-7.87556-2.431759.02894H-7.871291.819518.25448H-7.45463-0.096189.79795H7.18762-1.309074.78667		С	-12.7586	0.0754	3.9838
C-12.7589-2.3024.41553H-10.846-3.17644.93093C-13.4449-1.1364.07604H-13.29950.99473.71639H-13.2995-3.25694.4883H-14.5267-1.17093.88151C-8.76082-0.751156.19309C-8.52712-1.822347.05589C-8.525850.554776.6231C-8.05919-1.587528.34861H-8.71319-2.851746.71683C-8.056850.789777.91585H-8.709831.399135.94315C-7.82363-0.281088.77866H-7.87556-2.431759.02894H-7.871291.819518.25448H-7.45463-0.096189.79795H7.18762-1.309074.78667		Н	-10.8455	1.0745	4.15812
H-10.846-3.17644.93093C-13.4449-1.1364.07604H-13.29950.99473.71639H-13.2995-3.25694.483H-14.5267-1.17093.88151C-8.76082-0.751156.19309C-8.52712-1.822347.05589C-8.525850.554776.6231C-8.05919-1.587528.34861H-8.71319-2.851746.71683C-8.056850.789777.91585H-8.709831.399135.94315C-7.82363-0.281088.77866H-7.87556-2.431759.02894H-7.45463-0.096189.79795H7.18762-1.309074.78667		С	-12.7589	-2.302	4.41553
C-13.4449-1.1364.07604H-13.29950.99473.71639H-13.2995-3.25694.4883H-14.5267-1.17093.88151C-8.76082-0.751156.19309C-8.52712-1.822347.05589C-8.525850.554776.6231C-8.05919-1.587528.34861H-8.71319-2.851746.71683C-8.056850.789777.91585H-8.709831.399135.94315C-7.82363-0.281088.77866H-7.871291.819518.25448H-7.45463-0.096189.79795H7.18762-1.309074.78667		Н	-10.846	-3.1764	4.93093
H-13.29950.99473.71639H-13.2995-3.25694.4883H-14.5267-1.17093.88151C-8.76082-0.751156.19309C-8.52712-1.822347.05589C-8.525850.554776.6231C-8.05919-1.587528.34861H-8.71319-2.851746.71683C-8.056850.789777.91585H-8.709831.399135.94315C-7.82363-0.281088.77866H-7.87556-2.431759.02894H-7.45463-0.096189.79795H7.18762-1.309074.78667		C	-13.4449	-1.136	4.07604
H-13.2995-3.25694.4883H-14.5267-1.17093.88151C-8.76082-0.751156.19309C-8.52712-1.822347.05589C-8.525850.554776.6231C-8.05919-1.587528.34861H-8.71319-2.851746.71683C-8.056850.789777.91585H-8.709831.399135.94315C-7.82363-0.281088.77866H-7.87556-2.431759.02894H-7.871291.819518.25448H-7.45463-0.096189.79795H7.18762-1.309074.78667		Н	-13.2995	0.9947	3.71639
H-14.5267-1.17093.88151C-8.76082-0.751156.19309C-8.52712-1.822347.05589C-8.525850.554776.6231C-8.05919-1.587528.34861H-8.71319-2.851746.71683C-8.056850.789777.91585H-8.709831.399135.94315C-7.82363-0.281088.77866H-7.87556-2.431759.02894H-7.45463-0.096189.79795H7.18762-1.309074.78667		Н	-13.2995	-3.2569	4.4883
C-8.76082-0.751156.19309C-8.52712-1.822347.05589C-8.525850.554776.6231C-8.05919-1.587528.34861H-8.71319-2.851746.71683C-8.056850.789777.91585H-8.709831.399135.94315C-7.82363-0.281088.77866H-7.87556-2.431759.02894H-7.45463-0.096189.79795H7.18762-1.309074.78667		Н	-14.5267	-1.1709	3.88151
C-8.52712-1.822347.05589C-8.525850.554776.6231C-8.05919-1.587528.34861H-8.71319-2.851746.71683C-8.056850.789777.91585H-8.709831.399135.94315C-7.82363-0.281088.77866H-7.87556-2.431759.02894H-7.871291.819518.25448H-7.45463-0.096189.79795H7.18762-1.309074.78667		C	-8.76082	-0.75115	6.19309
C-8.525850.554776.6231C-8.05919-1.587528.34861H-8.71319-2.851746.71683C-8.056850.789777.91585H-8.709831.399135.94315C-7.82363-0.281088.77866H-7.87556-2.431759.02894H-7.45463-0.096189.79795H7.18762-1.309074.78667		С	-8.52712	-1.82234	7.05589
C-8.05919-1.587528.34861H-8.71319-2.851746.71683C-8.056850.789777.91585H-8.709831.399135.94315C-7.82363-0.281088.77866H-7.87556-2.431759.02894H-7.871291.819518.25448H-7.45463-0.096189.79795H7.18762-1.309074.78667		С	-8.52585	0.55477	6.6231
H-8.71319-2.851746.71683C-8.056850.789777.91585H-8.709831.399135.94315C-7.82363-0.281088.77866H-7.87556-2.431759.02894H-7.871291.819518.25448H-7.45463-0.096189.79795H7.18762-1.309074.78667		С	-8.05919	-1.58752	8.34861
C-8.056850.789777.91585H-8.709831.399135.94315C-7.82363-0.281088.77866H-7.87556-2.431759.02894H-7.871291.819518.25448H-7.45463-0.096189.79795H7.18762-1.309074.78667		Н	-8.71319	-2.85174	6.71683
H-8.709831.399135.94315C-7.82363-0.281088.77866H-7.87556-2.431759.02894H-7.871291.819518.25448H-7.45463-0.096189.79795H7.18762-1.309074.78667		C	-8.05685	0.78977	7.91585
C-7.82363-0.281088.77866H-7.87556-2.431759.02894H-7.871291.819518.25448H-7.45463-0.096189.79795H7.18762-1.309074.78667		Н	-8.70983	1.39913	5.94315
H-7.87556-2.431759.02894H-7.871291.819518.25448H-7.45463-0.096189.79795H7.18762-1.309074.78667		C	-7.82363	-0.28108	8.77866
H-7.871291.819518.25448H-7.45463-0.096189.79795H7.18762-1.309074.78667		Н	-7.87556	-2.43175	9.02894
H-7.45463-0.096189.79795H7.18762-1.309074.78667		Н	-7.87129	1.81951	8.25448
Н 7.18762 -1.30907 4.78667		Н	-7.45463	-0.09618	9.79795
	_	Н	7.18762	-1.30907	4.78667

Table S6. Total energies of TPA-DTA-PA

Zero-point correction	0.660927 (Hartree/Particle)
Thermal correction to Energy	0.703963
Thermal correction to Enthalpy	0.704907
Thermal correction to Gibbs Free Energy	0.573940
Sum of electronic and zero-point Energies	-2791.686982
Sum of electronic and thermal Energies	-2791.643946
Sum of electronic and thermal Enthalpies	-2791.643001
Sum of electronic and thermal Free Energies	-2791.773968

С	-1.22212	-5.53657	0.45127
С	-1.92683	-4.38169	0.23902
С	-1.26613	-3.12876	0.02401
С	0.17894	-3.10685	0.07737
С	0.87362	-4.34056	0.29279
С	0.19914	-5.5188	0.46727
С	-1.97891	-1.92698	-0.21327
С	0.87311	-1.88484	-0.07044
С	0.16051	-0.68191	-0.27967
С	-1.28141	-0.70298	-0.36703
С	-1.95755	0.52915	-0.6432
Н	-3.03674	0.52537	-0.73125
С	-1.26992	1.70452	-0.78928
С	0.14598	1.72942	-0.66756
С	0.83588	0.57237	-0.42417
Н	-1.75142	-6.47109	0.61702
Н	-3.01003	-4.40196	0.24266
Н	1.95716	-4.32221	0.32534
Н	0.74899	-6.44171	0.63074
Н	-1.80872	2.62439	-0.99987
Н	0.68046	2.6695	-0.77439
Н	1.91623	0.58944	-0.33415
С	-3.44835	-1.95513	-0.32105
С	-4.30797	-2.13989	-1.37061
С	-5.63709	-2.03296	-0.84935
Н	-4.01995	-2.31521	-2.39778
С	-5.49868	-1.7914	0.48274
Н	-6.5654	-2.12208	-1.39634
С	2.35656	-1.86519	-0.01148
С	3.16925	-1.74081	1.087
С	4.56394	-1.76376	0.77637
Н	2.77415	-1.63469	2.09187
С	4.80487	-1.90735	-0.56127
Н	5.3489	-1.67683	1.52011
S	3.32839	-2.01604	-1.46593
S	-4.18103	-1.73819	0.82497
С	6.16231	-1.97626	-1.2853
Н	6.19419	-2.09154	-2.34859
С	7.31662	-1.89139	-0.58036
С	8.66971	-1.9612	-1.31238
Ν	9.67715	-2.01318	-1.85741
С	7.27988	-1.72538	0.95023

Table S7. Symbolic Z-Matrix of TPA-DTA-PATF.

С	7.25291	-0.44902	1.51296
С	7.27345	-2.85098	1.77396
С	7.22021	-0.29839	2.89912
Н	7.25877	0.43819	0.86329
С	7.23974	-2.70048	3.16055
Н	7.29452	-3.85702	1.3306
С	7.21326	-1.42446	3.72322
Н	7.19959	0.70762	3.34276
Н	7.23427	-3.58816	3.80976
С	7.17707	-1.25779	5.25375
F	6.51368	-0.12465	5.56745
F	8.43879	-1.18671	5.72863
F	6.54701	-2.3159	5.80686
С	-6.49583	-1.58076	1.63726
С	-6.94889	-2.67423	2.37586
С	-6.94596	-0.29684	1.94463
С	-7.8524	-2.48381	3.42115
Н	-6.59442	-3.68641	2.13279
С	-7.84899	-0.10608	2.99085
Н	-6.58884	0.56511	1.36272
С	-8.30235	-1.19929	3.72901
Н	-8.21004	-3.34571	4.00297
Н	-8.20341	0.9064	3.23323
Ν	-9.25457	-0.9989	4.83084
С	-10.7005	-1.0462	4.57041
С	-11.3866	0.1199	4.23038
С	-11.3866	-2.2571	4.66312
С	-12.7586	0.0754	3.9838
Н	-10.8455	1.0745	4.15812
С	-12.7589	-2.302	4.41553
Н	-10.846	-3.1764	4.93093
С	-13.4449	-1.136	4.07604
Н	-13.2995	0.9947	3.71639
Н	-13.2995	-3.2569	4.4883
Н	-14.5267	-1.1709	3.88151
С	-8.76082	-0.75115	6.19309
С	-8.52712	-1.82234	7.05589
С	-8.52585	0.55477	6.6231
С	-8.05919	-1.58752	8.34861
Н	-8.71319	-2.85174	6.71683
С	-8.05685	0.78977	7.91585
Н	-8.70983	1.39913	5.94315
С	-7.82363	-0.28108	8.77866
Н	-7.87556	-2.43175	9.02894

Н	-7.87129	1.81951	8.25448
Н	-7.45463	-0.09618	9.79795

Table S8. Total energies of TPA-DTA-PATF.

Zero-point correction	0.665673 (Hartree/Particle)
Thermal correction to Energy	0.712348
Thermal correction to Enthalpy	0.713292
Thermal correction to Gibbs Free Energy	0.573009
Sum of electronic and zero-point Energies	-3128.718801
Sum of electronic and thermal Energies	-3128.672126
Sum of electronic and thermal Enthalpies	-3128.671182
Sum of electronic and thermal Free Energies	-3128.811466