Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

Deep Blue Fluorophors Incorporated Sulfone-Locked Triphenylamine: the Key for Highly Efficient Fluorescence/Phosphorescence Hybrid White OLEDs with Simplified Structure

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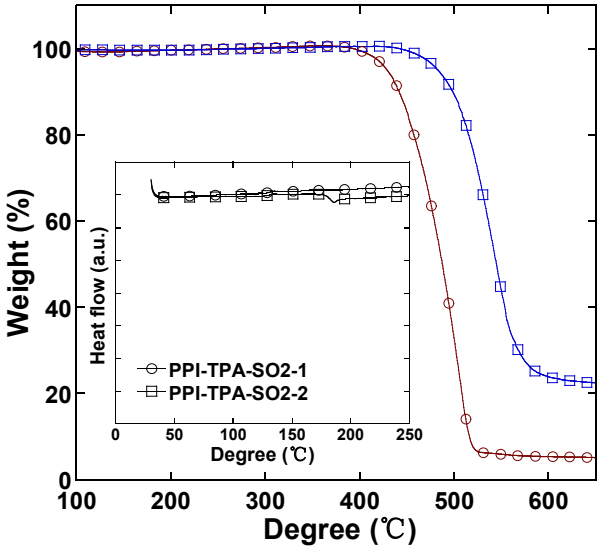


Figure S1. TGA and DSC (inset) curves of PPI-TPA-SO2-1 (○) and PPI-TPA-SO2-2 (□).

Lippert-Mataga calculation: To determine the change in dipole moment upon excitation, Δμ, Lippert-Mataga equation, Eq. (1), is used to express the Stokes shift as a function of the solvent polarity parameter Δf (ε, n).

$$hc(\nu_a - \nu_f) = hc(\nu_a^0 - \nu_f^0) - \frac{2(\mu_e - \mu_g)^2}{a^3} f(\varepsilon,n) \quad (1),$$

where f is the orientational polarizability of the solvent, ν_a-ν_f corresponds to the Stokes shift when f is zero, μ_e is the excited state dipole moment, μ_g is the ground-state dipole moment; a is the solvent cavity (Onsager) radius, derived from the Avogadro number (N), molecular weight (M), and density (d=1.0 g/cm^3); ε and n are the solvent dielectric and the solvent refractive index, respectively; f(ε,n) and a can be calculated respectively as follows:

$$f(\varepsilon,n) = \frac{\varepsilon - 1}{2\varepsilon + 1} - \frac{n^2 - 1}{2n^2 + 1} \quad (2),$$

$$a = (^{3M}/_{4\pi Nd})^{1/3} \quad (3).$$

Through the investigation of the fitted line in high-polarity solvents, the slope value of the fitted line was acquired.

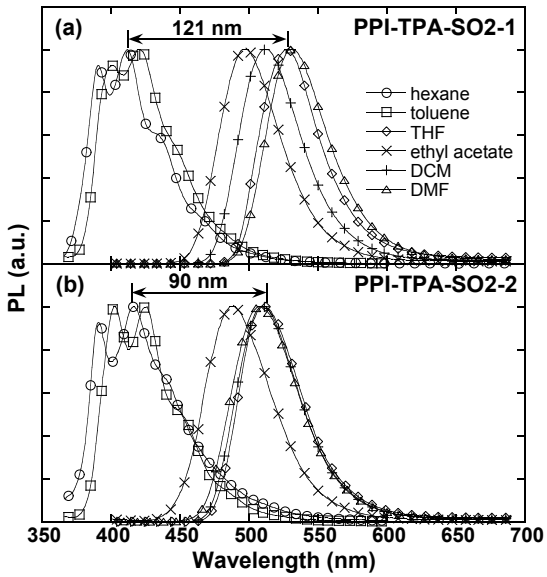


Figure S2. PL spectra of PPI-TPA-SO2-1 (a) and PPI-TPA-SO2-2 (b) in various solvents with different polarities: n-hexane (○), toluene (□), THF(◇), ethyl acetate (×), DCM (＋), and DMF (△).

Table S1. Detailed absorption and emission peak positions in different solvents

solvent	Δf (ε, n)	PPI-TPA-SO2-1			PPI-TPA-SO2-2		
		v_a	v_f	$\Delta v(v_a-v_f)$	v_a	v_f	$\Delta v(v_a-v_f)$
n-hexane	0.0012	365	412	3125.42	365	383	3416.45
toluene	0.014	365	417	3416.45	365	395	3293.08
ethyl acetate	0.20	365	499	7537.08	365	490	6989.10
THF	0.21	365	526	8385.85	365	509	7750.90
DCM	0.217	365	512	7866.01	365	512	7866.01
DMF	0.276	365	529	8493.67	365	510	7789.42

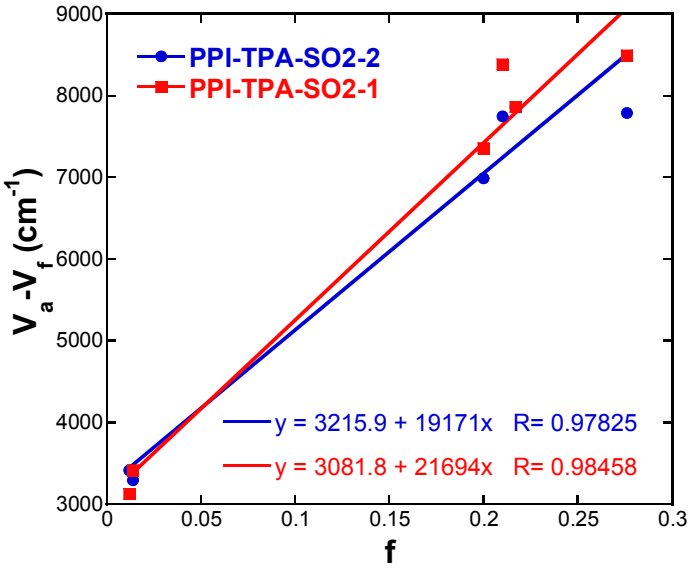


Figure S3. Linear correlation of the orientation polarization (*f*) of the solvent media with the Stokes shift (v_a-v_f) for PPI-TPA-SO2-1 and PPI-TPA-SO2-2.

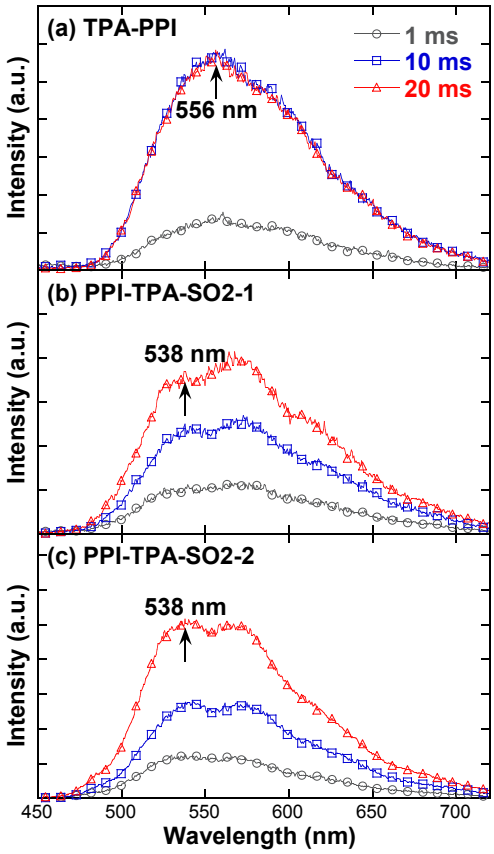


Figure S4. Phosphorescence spectra of TPA-PPI, PPI-TPA-SO2-1, and PPI-TPA-SO2-2 measured in a frozen 2-methyltetrahydrofuran matrix at 77 K at different delayed times.

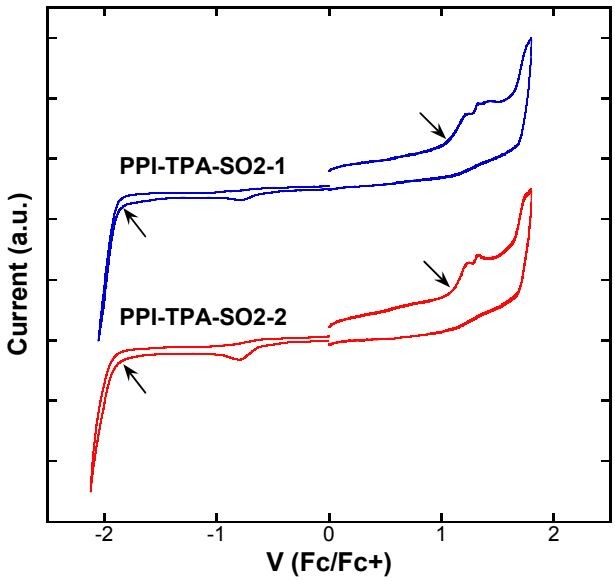


Figure S5. Cyclic voltammograms of PPI-TPA-SO2-1 and PPI-TPA-SO2-2 in CH_3CN/DCM (volume ratio: 1/4).

Figure S6. Calculated singlet and triplet excited energies of PPI-TPA-SO2-1 and PPI-TPA-SO2-2.

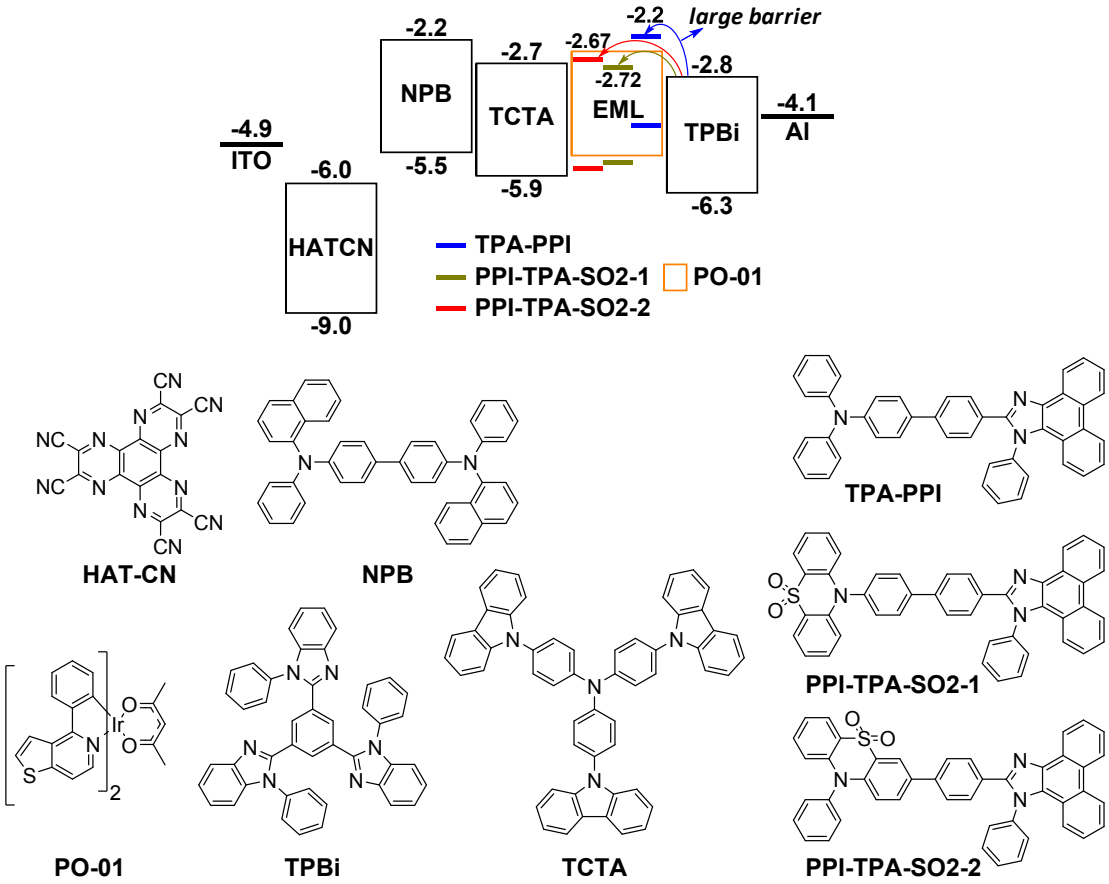


Figure S7. Energy level diagrams (eV) of the devices with TPA-PPI, PPI-TPA-SO2-1, and PPI-TPA-SO2-2 as the blue emitter as well as the host for a yellow phosphor PO-01. Also shown are the molecular structures of the materials used.

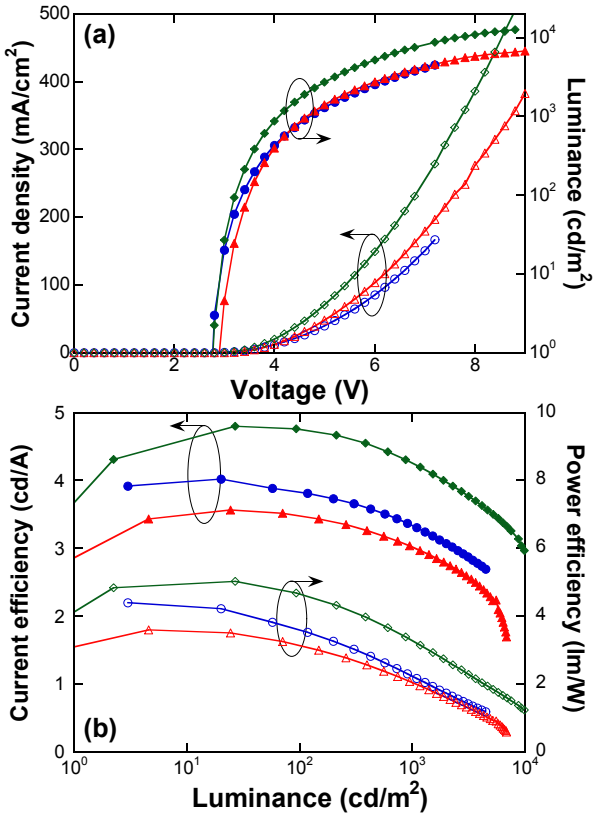


Figure S8. (a) Current density and luminance versus driving voltage (*J*-*V*-*L*) and (b) current and power efficiency versus luminance characteristics of the nondoped blue OLEDs based on TPA-PPI (●○), PPI-TPA-SO2-1 (▲△), and PPI-TPA-SO2-2 (◆◇) as the emitter.

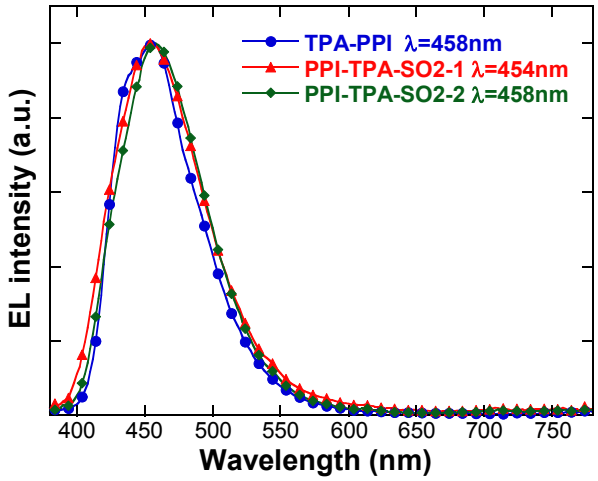


Figure S9. EL spectra of the nondoped blue OLEDs in a structure of ITO (95 nm)/ HATCN (5 nm)/ NPB (40 nm)/ TCTA (5 nm)/ EML (20 nm)/ TPBI (40 nm)/ LiF (1 nm)/ Al (>80 nm) at 10 mA cm^{-2}. EML: TPA-PPI (●), PPI-TPA-SO2-1 (▲), and PPI-TPA-SO2-2 (◆).

Table S2. Summary of the device performance of the nondoped blue OLEDs in a structure of ITO (95 nm)/ HATCN (5 nm)/ NPB (40 nm)/ TCTA (5 nm)/ EML (20 nm)/ TPBI (40 nm)/ LiF (1 nm)/ Al (80 nm)

EML	V_{on}[a] (V)	CE_{max} (cd A^{-1})	PE_{max} (lm W^{-1})	EQE_{max} (%)	at 100 cd m^{-2}					at 1000 cd m^{-2}				
					V (V)	CE (cd A^{-1})	PE (lm W^{-1})	CIE (x, y)	EQE (%)	V (V)	CE (cd A^{-1})	PE (lm W^{-1})	CIE (x, y)	EQE (%)
TPA-PPI	2.7	4.02	4.40	4.11	3.4	3.81	3.52	(0.148, 0.107)	3.89	4.7	3.33	2.25	(0.148, 0.106)	3.40
PPI-TPA-SO2-1	2.8	3.56	3.59	3.50	3.5	3.48	3.12	(0.152, 0.122)	3.42	4.6	3.00	2.05	(0.149, 0.116)	2.95
PPI-TPA-SO2-2	2.7	4.80	5.02	4.62	3.2	4.76	4.67	(0.145, 0.124)	4.58	4.1	4.25	3.21	(0.145, 0.121)	4.09

[a]at the luminance of 1 cd m^{-2}.

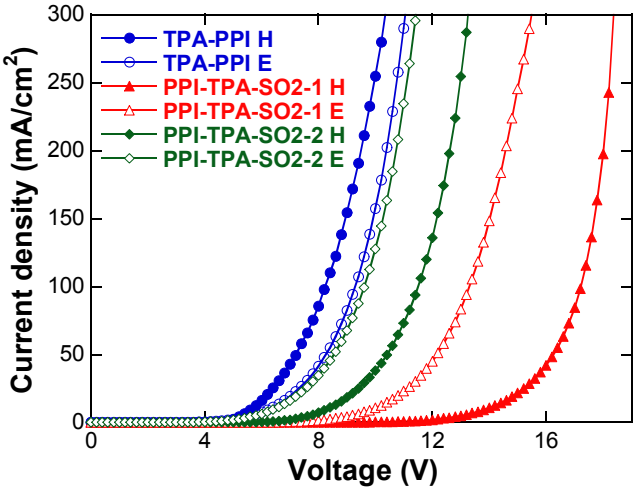


Figure S10. Current density versus driving voltage characteristics of the hole-only (solid symbol) and electron-only devices (open symbol) based on TPA-PPI (○●), PPI-TPA-SO2-1 (△▲), and PPI-TPA-SO2-2 (◇◆).

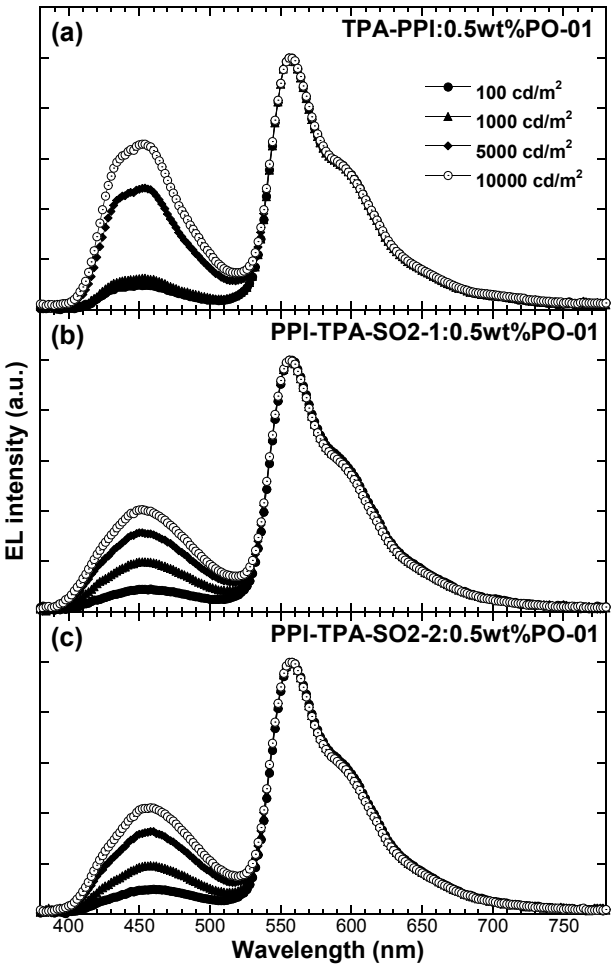


Figure S11. EL spectra of the F/P hybrid WOLEDs at different luminances with TPA-PPI, PPI-TPA-SO2-1, and PPI-TPA-SO2-2 as the blue emitter as well as the host of the phosphorescent emitter PO-01 at 0.5 wt% doping concentration.

Table S3. Summary of the performance of the F/P hybrid WOLEDs with simplified EMLs just containing the emitting component for white light emission.

Blue emitter	forward CE_{max} (cd A^{-1})	forward PE_{max} (lm W^{-1})	total[a] PE_{max} (lm W^{-1})	EQE_{max} (%)	Ref.
DADBT	--	--	67.2	15.6[b]	1a
DFBC	21.5	22.5	--	--	1b
TPA-o-OXD	4.7	7.9	--	5.2	1c
CPhBzIm	15.5	12.8	--	7	1d
CzS1	--	42.1	71.6	16.4[b]	1e
POTA	--	--	59.8	14.5[b]	1f
DAPSF	--	--	57.3	12.8[b]	1g
TPA-SO2	39.6	47.9	81.4	13.2	1h
PPI-TPA-SO2-1	44.2	49.5	84.2	14.4	this work
PPI-TPA-SO2-2	47.6	53.4	90.8	15.6	this work

[a]Total efficiency with 1.7 times enhancement as compared to the forward-viewing efficiency. [b]The external quantum efficiency was calculated by dividing the original total external quantum efficiency with a factor of 1.7.

Table S4. Summary of the performance of the typical fully phosphorescent WOLEDs without using any out-coupling technology.

Host	forward PE_{max} (lm W^{-1})	EQE_{max} (%)	Ref.
PVK/OXD-7	20.3	19.1	2a
DCzPPy/TCTA	55	26	2b
H2	50	26	2c
o-DBFPPO	35.7	12.7	2d
PVK/OXD-7	42.1	16.4	2e
CBP	34	26.2	2f
mCP	42.5	19.3	2g
PPI-TPA-SO2-1[a]	49.5	14.4	this work
PPI-TPA-SO2-2[a]	53.4	15.6	this work

[a]The current F/P hybrid WOLEDs with simplified EMLs with blue fluorescent emitter instead of blue phosphorescent emitter.

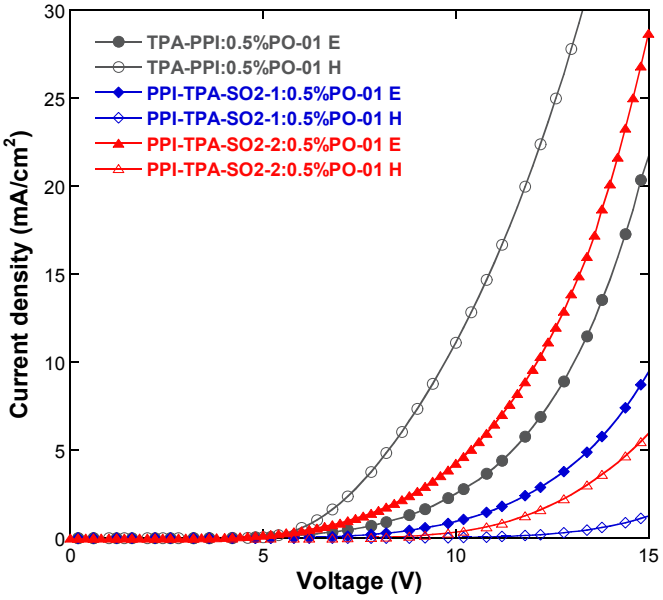
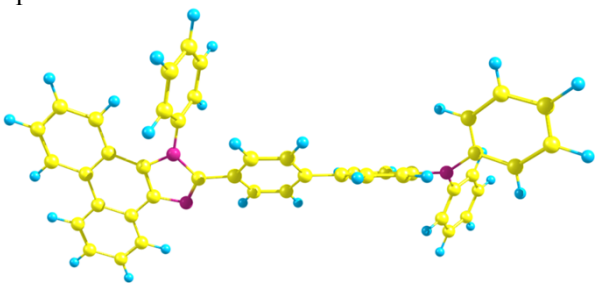


Figure S12. Current density versus driving voltage characteristics of the hole-only (*open symbol*) and electron-only devices (*solid symbol*) based on TPA-PPI (○●), PPI-TPA-SO2-1 (◇◆) and PPI-TPA-SO2-2 (△▲) doped with 0.5 wt% PO-01.

Molecular orbital quantum calculation:

Optimized molecular coordinates of **TPA-PPI**:



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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5	6	0	8.555761	-2.674798	-0.422232
6	6	0	8.306026	-4.015072	-0.662619
7	6	0	5.097669	-1.300350	-0.232434
8	6	0	7.738059	-0.317499	0.005634
9	6	0	6.644130	0.603598	0.144599
10	6	0	5.323454	0.054403	-0.016895
11	6	0	6.918624	1.958531	0.444574
12	1	0	6.101509	2.653993	0.575187
13	6	0	8.216121	2.415382	0.585537
14	6	0	9.290178	1.527555	0.433598
15	6	0	9.045864	0.194670	0.154227
16	1	0	6.795633	-5.540242	-0.946709
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18	1	0	9.587329	-2.349064	-0.357251
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24	6	0	3.721840	1.997425	0.282191
25	6	0	3.862288	2.944384	-0.737765
26	6	0	3.257631	2.379241	1.542705
27	6	0	3.539362	4.278197	-0.489833
28	1	0	4.225796	2.628314	-1.710226
29	6	0	2.930348	3.714441	1.781688
30	1	0	3.155337	1.630597	2.321118
31	6	0	3.071453	4.664346	0.768716
32	1	0	3.650279	5.014122	-1.280296
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34	1	0	2.817662	5.702781	0.958442
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37	6	0	0.954270	0.819790	-0.566223
38	6	0	-0.448978	-1.426403	0.283859
39	1	0	1.483874	-2.324980	0.577556
40	6	0	-0.437170	0.825288	-0.553337
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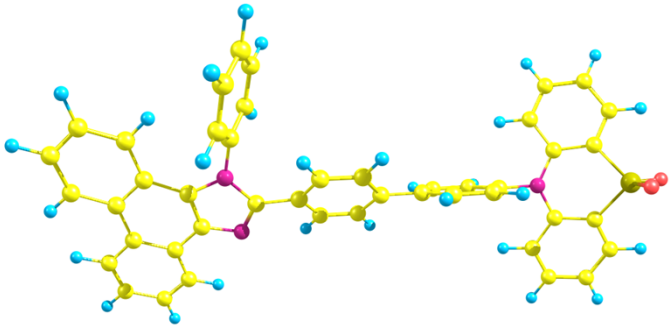
74	1	0	-9.551034	4.212283	-1.371191
75	7	0	-6.912506	-0.208924	-0.030600
76	7	0	4.047446	0.624869	0.029504
77	7	0	3.758742	-1.577959	-0.301588
78	1	0	-9.107195	-0.064786	-1.546691
79	1	0	-9.039503	-0.281479	1.584947

Optimized molecular coordinates of **PPI-TPA-SO2-1**:



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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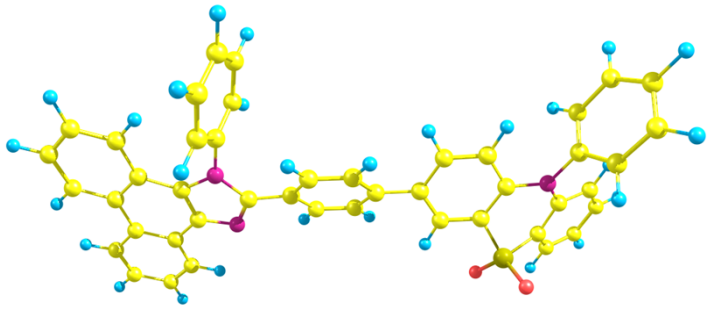
63	6	0	8.876858	2.572768	-0.641014
64	6	0	8.739725	-2.247894	1.024879
65	1	0	4.934543	-1.761047	1.570162
66	6	0	6.650834	-2.986392	1.946308
67	6	0	8.225691	3.799093	-0.628426
68	1	0	6.315295	4.775863	-0.413419
69	1	0	9.943644	2.496536	-0.823853
70	6	0	8.027494	-3.169510	1.780841
71	1	0	9.805446	-2.355689	0.851863
72	1	0	6.074815	-3.703520	2.523678
73	1	0	8.778744	4.717037	-0.795929
74	1	0	8.530085	-4.022253	2.224477
75	7	0	6.067723	0.231024	0.164310
76	7	0	-4.896360	-0.622006	-0.166903
77	7	0	-4.598328	1.583143	0.136351
78	16	0	8.964164	-0.152997	-0.708475
79	8	0	8.630202	-0.614386	-2.068480
80	8	0	10.381082	-0.058544	-0.31821148

Optimized molecular coordinates of **PPI-TPA-SO2-2**:



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.225308	-4.593459	-0.028924
2	6	0	-6.219642	-3.645579	-0.023309
3	6	0	-6.533999	-2.272110	-0.039678
4	6	0	-7.887475	-1.834734	-0.065592
5	6	0	-8.888683	-2.833794	-0.067818
6	6	0	-8.568643	-4.180621	-0.049972
7	6	0	-5.507364	-1.269853	-0.022811
8	6	0	-8.195432	-0.398716	-0.097565
9	6	0	-7.151282	0.588342	-0.084254
10	6	0	-5.802851	0.088694	-0.018472
11	6	0	-7.497330	1.958235	-0.151326
12	1	0	-6.717757	2.706843	-0.163800
13	6	0	-8.817831	2.364336	-0.210348
14	6	0	-9.843552	1.408980	-0.206911
15	6	0	-9.528914	0.062579	-0.155091
16	1	0	-6.980046	-5.651332	-0.014591
17	1	0	-5.173297	-3.931052	-0.002178
18	1	0	-9.936107	-2.556058	-0.082635
19	1	0	-9.363957	-4.920255	-0.051787
20	1	0	-9.054405	3.422997	-0.262098
21	1	0	-10.882977	1.720029	-0.251213
22	1	0	-10.341081	-0.654282	-0.164777
23	6	0	-3.596203	-0.289912	0.033315
24	6	0	-4.310534	2.135208	-0.000867
25	6	0	-4.456384	2.888793	1.168607
26	6	0	-3.920826	2.748437	-1.193579
27	6	0	-4.213037	4.261616	1.139249
28	1	0	-4.761054	2.394409	2.085349
29	6	0	-3.674168	4.121730	-1.214296
30	1	0	-3.815037	2.148100	-2.091010
31	6	0	-3.820651	4.879226	-0.051041
32	1	0	-4.328162	4.847609	2.045903
33	1	0	-3.370693	4.598674	-2.141138
34	1	0	-3.630334	5.947943	-0.070988
35	6	0	-2.134719	-0.114904	0.055206
36	6	0	-1.355169	-1.169835	-0.457346
37	6	0	-1.463669	0.996696	0.592003
38	6	0	0.030809	-1.107148	-0.448961
39	1	0	-1.863454	-2.036441	-0.863751
40	6	0	-0.073175	1.053427	0.598135
41	1	0	-2.017084	1.812611	1.037650
42	6	0	0.706316	0.009857	0.074921
43	1	0	0.599971	-1.925266	-0.879926

44	1	0	0.413839	1.910042	1.054232
45	7	0	-4.557619	0.723640	0.026853
46	7	0	-4.156712	-1.485471	0.003063
47	6	0	2.185396	0.079585	0.079156
48	6	0	2.969696	-1.062201	0.270387
49	6	0	2.867452	1.298823	-0.097417
50	6	0	4.360723	-0.983203	0.272599
51	1	0	2.513091	-2.028332	0.457682
52	6	0	4.252263	1.378542	-0.122502
53	1	0	2.296240	2.207201	-0.261903
54	6	0	5.045771	0.226082	0.041055
55	1	0	4.724550	2.336734	-0.295866
56	6	0	6.752270	-2.161452	-0.177208
57	6	0	7.478904	-3.283669	-0.580931
58	6	0	7.231539	-0.850946	-0.376356
59	6	0	8.732801	-3.127244	-1.156905
60	1	0	7.044503	-4.264967	-0.420885
61	6	0	8.516257	-0.715111	-0.938927
62	6	0	9.248034	-1.836414	-1.312648
63	1	0	9.306323	-3.993619	-1.468372
64	1	0	8.932829	0.271402	-1.094845
65	1	0	10.232597	-1.695336	-1.748615
66	6	0	7.093190	1.568313	-0.007121
67	6	0	7.560581	2.032653	1.224401
68	6	0	7.249249	2.344195	-1.160301
69	6	0	8.186277	3.277643	1.301703
70	1	0	7.429027	1.414293	2.106579
71	6	0	7.875379	3.588642	-1.076613
72	1	0	6.881073	1.969296	-2.110287
73	6	0	8.343850	4.055564	0.153235
74	1	0	8.549749	3.638296	2.258982
75	1	0	7.996958	4.191379	-1.971454
76	1	0	8.830962	5.023914	0.215743
77	7	0	6.448267	0.279006	-0.066598
78	16	0	5.283349	-2.408503	0.782484
79	8	0	4.597451	-3.636607	0.347251
80	8	0	5.629189	-2.250987	2.206965

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