Supporting Information

Through-Space Charge Transfer Hexaarylbenzene Dendrimers with Thermally Activated Delayed Fluorescence and Aggregation-Induced Emission for Efficient Solution-Processed OLEDs

Xingdong Wang, Shumeng Wang, Jianhong Lv, Shiyang Shao,* Lixiang Wang,* Xiabin Jing, and Fosong Wang

State Key Laboratory of Polymer Physics and Chemistry, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun 130022, P. R. China

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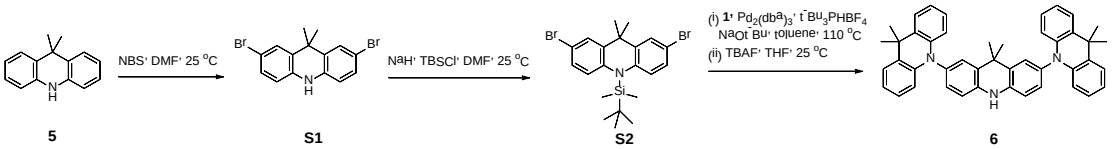
Experimental Procedures

General Information: The starting materials were purchased from commercial sources without further purification. Dioxane, tetrahydrofuran (THF), *N*,*N*-dimethylformamide (DMF) and toluene were dried by molecular sieve and then sodium before use. NMR spectra (^{1}H and ^{13}C) were recorded on a Bruker Avance 400 NMR spectrometer. MALDI-TOF mass spectra were recorded on an AXIMA CFR MS apparatus. Elemental analysis was performed on a Bio-Rad elemental analysis system. Thermal properties including thermal gravimetric analysis (TGA) and differential scanning calorimetry (DSC) were analyzed in N_2 at a heating rate of 10 ^{o}C/min with Perkin-Elmer-TGA 7 and PerkinElmer-DSC 7, respectively. UV–visible and PL spectra were recorded on Perkin-Elmer Lambda 35 UV–vis spectrometer and LS 50B spectrofluorometer, respectively. Phosphorescent spectra were measured in toluene at 77 K. PL decay curves were recorded using Edinburgh fluorescence spectrometer (FLSP-980). The photoluminescence quantum efficiencies were measured by integrating sphere on Hamamatsu Photonics C9920-2. Cyclic voltammetry characteristics were measured on a three-electrode system using ferrocene as the reference and n-Bu_4NClO_4 as the supporting electrolyte. The HOMO and LUMO energy levels were calculated from the onset of the oxidation ($E_{onset,\ ox}$) and reduction potential ($E_{onset,red}$), respectively, according to the equation of E_{HOMO} (or E_{LUMO}) = -e [$E_{onset,\ ox}$(or $E_{onset,\ red}$) + 4.8V].

Synthesis



2,7-dibromo-9,9-dimethylacridan (S1) A solution of *N*-bromosuccinimide (NBS) (18.7 g, 105.0 mmol) in DMF (50 mL) was added dropwisely to a mixture of 9,9-dimethylacridan (**5)** (10.5 g, 50.0 mmol) and DMF (30 mL) at 25 °C. After stirring for 12 h, the solution was poured into water and filtered. The filter cake was collected and purified by silica gel column chromatography (dichloromethane/hexane = 1:4, v/v) to give the product (13.2 g, 36 mmol, 72%) as a white solid. ^{1}H NMR (400 MHz, DMSO-d^6) δ 9.18 (s, 1H), 7.47 (d, *J* = 2.0 Hz, 2H), 7.23 (dd, *J* = 8.5, 2.0 Hz, 2H), 6.74 (d, *J* = 8.5 Hz, 2H), 1.48 (s, 6H).

2,7-dibromo-10-(*tert*-butyldimethylsilyl)-9,9-dimethylacridan (S2) S1 (11.0 g, 30.0 mmol) was dissolved in dry DMF and then NaH (60%, dispersed in Paraffin Liquid) (1.8 g, 45.0 mmol) was added in batches at room temperature. After that, a solution of *tert*-butyldimethylchlorosilane (6.8 g, 45.0 mmol) in dry DMF (50 mL) was added dropwisely. After stirring for 8 h, the mixture was poured into water and filtered to give the crude product, which was then purified by silica gel column chromatography (dichloromethane/hexane = 1:10, v/v) to give the pure product as a white solid (12.0 g) in yield of 82%. ^{1}H NMR (400 MHz, C_6D_6) δ 7.44 (d, *J* = 2.3 Hz, 2H), 7.24 (dd, *J* = 8.5, 2.3 Hz, 2H), 6.99 (d, *J* = 8.5 Hz, 2H), 1.23 (s, 9H), 1.48 (br, 6H), 0.15 (s, 6H).

9,9,9',9',9'',9''-hexamethyl-teracridan (6) A mixture of **S2** (4.8 g, 10.0 mmol), **5** (5.0 g, 24 mmol), tris(dibenzylideneacetone)dipalladium ($Pd_2(dba)_3$) (275 mg, 0.3 mmol), *t*-$Bu_3P{\cdot}HBF_4$ (348 mg, 1.2 mmol), and *t*-BuONa (2.9 g, 30 mmol) in dry toluene was heated at 110 °C for 24 h under an argon atmosphere. After cooling, the mixture was poured into ethanol and filtered to afford the filter cake as the crude product. This crude product was dissolved in dry THF, and then tetrabutylammonium fluoride (2.62 g, 10 mmol) was added. The mixture was stirred at 25 °C for 4h, followed by pouring into water for filtration. The residue was collected and applied on silica gel column chromatography (dichloromethane/hexane = 1/3, v/v) to give the product as a white solid (3.80 g, 61%).^{1}H NMR (400 MHz, C_6D_6) δ 7.42 (dd, *J* = 7.6, 1.7 Hz, 4H), 7.22 (d, *J* = 2.1 Hz, 2H), 7.00 – 6.90 (m, 10H), 6.59 (dd, *J* = 8.0, 1.4 Hz, 4H), 6.36 (d, *J* = 8.3 Hz, 2H), 5.63 (s, 1H), 1.69 (s, 18H).

2-(4-iodophenyl)-4,6-diphenyl-1,3,5-triazine (2) Under an argon atmosphere, 2-chloro-4,6-diphenyl-1,3,5-triazine **(1)** (16.1 g, 60.0 mmol), 4-trimethylsilylphenyl-boronic acid (14.0 g, 72.0 mmol), $Pd_2(dba)_3$ (1.65 g, 1.8 mmol) and

2-dicyclohexylphosphino-2',6'-dimethoxybiphenyl (S-Phos, 2.96 g, 7.2mmol) were added into a flask containing de-aerated toluene (300 mL) and potassium carbonate solution (0.18 mol, 90 mL). The mixture was heated at 100 °C for 24 h. After cooling to room temperature, the mixture was poured into water and the organic layer was extracted with toluene. The combined organic phase was concentrated under reduced pressure and then poured into ethanol. The mixture was filtered, and the residue was dried under vacuum. After redissolving the residue in dry THF, ICl (9.72 g, 60 mmol) was added, which was stirred at room temperature for 5h. The mixture was poured into water and the filter cake was collected, which was purified by silica gel column chromatography (dichloromethane/hexane = 1:4, v/v) to give the pure product as a white solid (17.2 g, 65%).^{1}H NMR (400 MHz, $CDCl_3$) δ 8.84 – 8.71 (m, 6H), 7.68 – 7.54 (m, 6H), 7.32 (d, *J* = 8.9 Hz, 2H)

2-(4-((4-bromophenyl)ethynyl)phenyl)-4,6-diphenyl-1,3,5-triazine (3) Under an argon atmosphere, **2** (8.71 g, 20.0 mmol), 4-bromophenylacetylene (4.35 g, 24.0 mmol), tetrakis(triphenylphosphine)palladium(0) ($Pd(PPh_3)_4$, 1.16 g, 1.0 mmol), CuI (0.38 g, 2 mmol) and triphenylphosphine (PPh_3) (0.53 g, 2 mmol) were added into a dry Schlenk flask where dry THF (100 mL) and freshly distilled triethylamine (100 mL) were introduced. The mixture was heated at 60 °C for 24 h, which was then poured into dilute hydrochloric acid. After filtration, the crude product was washed by water and dried under vacuum. Purification of the crude product by silica gel column chromatography (dichloromethane/n-hexane = 1:3, v/v) afforded the product as a light yellow solid (5.3 g, 54%).^{1}H NMR (400 MHz, $CDCl_3$) δ 8.79 (d, *J* = 7.1 Hz, 6H), 7.73 (d, *J* = 8.3 Hz, 2H), 7.68 – 7.58 (m, 6H), 7.54 (d, *J* = 8.3 Hz, 2H), 7.46 (d, *J* = 8.4 Hz, 2H).

6,6''-(2',4',6'-tris(4-bromophenyl)-5'-(4-(4,6-diphenyl-1,3,5-triazin-2-yl)phenyl)-[1,1':3',1''-terphenyl]-4,4''-diyl)bis(2,4-diphenyl-1,3,5-triazine) (4) To a Schlenk flask was added $Co_2(CO)_8$ (0.45 g, 1.3 mmol), **3** (3.2 g, 6.6 mmol) and dry 1,4-dioxane (50 mL). The mixture was degassed, and then heated at 120 °C for 48 h under an argon atmosphere. After cooling to room temperature, the solution was poured into water. After filtration, the residue was dried under vacuum and then purified by silica gel column chromatography (dichloromethane/n-hexane = 1:4, v/v) to give the desired symmetrical hexaarylbenzene derivative **4** (1.12 g, 0.8mmol, 36%) as well as an asymmetrical isomer (0.71 g, 0.71 mmol, 22%). ^{1}H NMR (400 MHz, $CDCl_3$) for **4:** δ 8.76 (dd, *J* = 32.8, 6.8 Hz, 12H), 8.51 (dd, *J* = 13.6, 8.3 Hz, 6H), 7.71 – 7.49 (m, 18H), 7.25 – 7.06 (m, 12H), 6.88 (ddd, *J* = 18.3, 8.4, 2.8 Hz, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) for **4:** δ 171.53, 171.38, 171.01, 170.91, 144.28, 144.25, 140.34, 139.58, 139.56, 139.53, 139.50, 138.54, 138.51, 136.18, 136.10, 133.77, 132.72, 132.42, 132.31, 131.59, 131.49, 130.47, 128.92, 128.82, 128.54, 128.44, 127.90, 120.47, 120.41. Anal. calcd for **4 (**$C_{87}H_{54}Br_3N_9$**)**: C, 71.32; H, 3.71; N, 8.60. found: C, 71.22; H, 3.65; N, 8.45.

Ac3TRZ3 A mixture of **4** (0.44 g, 0.3 mmol), **5** (0.4 g, 1.8 mmol), $Pd_2(dba)_3$ (83 mg, 0.09 mmol), *t*-$Bu_3P{\cdot}HBF_4$ (105 mg, 0.36 mmol) and *t*-BuONa (0.35 g, 3.6 mmol) in dry toluene was heated at 110 °C for 24 h under an argon atmosphere. After cooling to room temperature, the mixture was poured into water and the organic layer was extracted three times by dichloromethane. The combined organic phase was concentrated under reduced pressure, followed by purification by silica gel column chromatography (dichloromethane/cyclohexane = 1/5, v/v) to give the product as a white solid (0.25 g, 47%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.79 – 8.57 (m, 18H), 7.59 – 7.51 (m, 18H), 7.37 – 7.19 (m, 18H), 7.07 – 6.94 (m, 6H), 6.79 – 6.71 (m, 6H), 6.60 – 6.40 (m, 6H), 5.99 – 5.91 (m, 6H), 1.59 – 1.56 (m, 18H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.63, 171.53, 171.05, 171.01, 170.97, 170.94, 144.88, 144.69, 144.58, 140.54, 140.50, 140.47, 140.38, 140.33, 140.30, 140.20, 140.11, 139.18, 139.13, 138.96, 138.87, 136.19, 136.17, 136.14, 134.10, 133.99, 133.93, 133.86, 132.50, 132.43, 132.20, 132.14, 132.01, 130.35, 129.66, 129.62, 129.55, 128.96, 128.90, 128.62, 128.56, 127.90, 127.86, 127.68, 126.72, 126.43, 124.97, 124.92, 120.25, 113.80, 113.69, 35.82, 35.81, 35.78, 35.75, 31.26, 31.19, 31.16, 31.13. MALDI TOF-MS: calcd for $C_{132}H_{96}N_{12}$: 1850 found: 1851 $[M+H]^+$. Anal. calcd for $C_{132}H_{96}N_{12}$: C, 85.69; H, 5.23; N, 9.08. found: C, 85.45; H, 5.08; N, 8.98.

TAc3TRZ3 A mixture of **4** (0.44 g, 0.3 mmol), **6** (1.12 g, 1.8 mmol), $Pd_2(dba)_3$ (83 mg, 0.09 mmol), *t*-$Bu_3P{\cdot}HBF_4$ (105 mg, 0.36 mmol) and *t*-BuONa (0.35 g, 3.6 mmol) in dry toluene was heated at 110 °C for 24 h under an argon atmosphere. After cooling to room temperature, the mixture was poured into water and the organic layer was extracted by dichloromethane. The organic layer was concentrated under reduced pressure, and the residue was purified by silica gel column chromatography (dichloromethane/cyclohexane = 1/5, v/v) to afford the product as a white solid (0.32 g, 34%). ^{1}H NMR (400 MHz, C_6D_6) δ 8.95 – 8.81 (m, 6H), 8.51 – 8.41 (m, 12H), 7.59 – 7.52 (m, 12H), 7.27 (d, *J* = 7.6 Hz, 12H), 7.24 (d, *J* = 10.4 Hz, 6H), 7.12 – 6.97 (m, 24H), 6.90 (t, *J* = 7.5 Hz, 6H), 6.80 (dd, *J* = 13.2, 6.8 Hz, 12H), 6.70 – 6.62 (m, 18H), 6.35 – 6.27 (m, 12H), 1.55 (s, 36H), 1.51 (s, 18H). ^{13}C NMR (126 MHz, C_6D_6) δ 171.27, 171.23, 171.12, 171.08, 170.59, 170.57, 170.25, 170.20, 144.65, 144.42, 144.32, 141.18, 141.09, 140.86, 140.82, 140.75, 140.60, 140.57, 140.53, 140.33, 140.25, 140.04, 139.91, 139.86, 135.56, 135.06, 134.45, 134.39, 134.24, 134.17, 133.87, 133.62, 132.35, 132.28, 132.14, 132.10, 132.07, 131.98, 130.28, 130.24, 129.80, 129.75, 129.36, 129.02, 128.50, 128.45, 128.18, 127.91, 127.83, 127.62, 127.42, 127.09, 126.19, 126.02, 124.79, 124.40, 120.14, 120.05, 115.67, 115.29, 113.78, 113.66, 77.26, 77.01, 76.75, 36.32, 36.28, 35.74, 35.67, 30.87, 30.56, 30.42, 30.13. MALDI TOF-MS: calcd for $C_{222}H_{174}N_{18}$: 3094 found: 3095 $[M+H]^+$. Anal. calcd for $C_{222}H_{174}N_{18}$: C, 86.18; H, 5.67; N, 8.15. found: C, 85.99; H, 5.80; N, 8.01.

1,2-bis(4-(9,9-dimethylacridinyl)phenyl)ethyne (8) A mixture of **5** (5.02 g, 24.0 mmol),

bis(4-bromophenyl)acetylene **7** (2.70 g, 8.0 mmol), $Pd_2(dba)_3$ (0.73 g, 0.8 mmol), *t*-$Bu_3P{\cdot}HBF_4$ (0.93 g, 3.2 mmol) and *t*-BuONa (4.61 g, 48.0 mmol) in dry toluene was heated at 110 °C for 24 h under an argon atmosphere. After cooling to room temperature, the mixture was poured into ethanol. After filtration, the residue was collected and recrystallized from chloroform to give the desired product. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 (d, *J* = 8.3 Hz, 4H), 7.47 (dd, *J* = 7.6, 1.5 Hz, 4H), 7.37 (d, *J* = 8.3 Hz, 4H), 7.00 (td, *J* = 7.4, 1.2 Hz, 4H), 6.95 (td, *J* = 7.40, 1.2 Hz, 4H), 6.31 (dd, *J* = 8.1, 1.1 Hz, 4H), 1.70 (s, 12H).

Ac6 To a Schlenk flask was added **8** (4.7 g, 6.2 mmol), $Co_2(CO)_8$ (0.44 g, 1.3 mmol) and dry 1,4-dioxane (50 mL). The mixture was degassed, and then heated at 120 °C for 48 h under an argon atmosphere. After cooling to room temperature, the solution was poured into water. After filtration, the residue was dried under vacuum and then purified by silica gel column chromatography (dichloromethane/n-hexane = 1/3, v/v) to give the (2.60 g, 55%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41 (d, *J* = 7.5 Hz, 12H), 7.36 (d, *J* = 7.6 Hz, 12H), 7.16 (d, *J* = 7.5 Hz, 12H), 6.68 (t, *J* = 6.0 Hz, 12H), 6.43 (t, *J* = 6.4 Hz, 12H), 6.08 (d, *J* = 8.1 Hz, 12H), 1.65 (s, 36H).^{13}C NMR (126 MHz, $CDCl_3$) δ 140.66, 140.41, 140.36, 139.29, 134.19, 130.37, 129.92, 126.72, 124.44, 120.42, 113.74, , 35.94, 30.25. MALDI TOF-MS: calcd for $C_{132}H_{108}N_6$: 1778 found: 1778 $[M]^+$. Anal. calcd for $C_{132}H_{108}N_6$: C, 89.15; H, 6.12; N, 4.73. found: C, 88.98; H, 6.02; N, 4.63.

1,2-bis(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)ethyne (9) A mixture of bis(4-bromophenyl)acetylene (1.68 g, 5.0 mmol), bis(pinacolato)diboron (5.08 g, 20.0 mmol), [1,1'-Bis(diphenylphosphino)ferrocene]dichloropalladium(II) ($PdCl_2$(dppf)) (0.37 g, 0.5 mmol) and potassium acetate (2.94 g, 30 mmol) in dry DMF was heated at 90 °C for 24 h under an argon atmosphere. After cooling to temperature, the mixture was poured into water and filtered. The residue was purified by silica gel column chromatography (dichloromethane/n-hexane/methanol = 10/40/1, v/v/v) to give the product as a white solid (0.67 g, 31%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.2 Hz, 4H), 7.53 (d, *J* = 8.2 Hz, 4H), 1.35 (s, 24H).

TRZ6 Under an argon atmosphere, **1** (1.28 g, 4.8 mmol), **9** (0.66 g, 1.6 mmol), $Pd_2(dba)_3$ (147 mg, 0.16mmol) and S-Phos (263 mg, 0.64mmol) were added into a flask where de-aerated toluene (20 mL) and potassium carbonate solution (6.4 mmol, 3.2 mL) were then introduced. The mixture was heated at 100 °C for 24 h. After cooling to room temperature, the mixture was poured into ethanol and filtered. The residue was dried under vacuum and was directly used for the next step without further purification because of its poor solubility. Under argon, the crude product **10** and $Co_2(CO)_8$ 110 mg, 0.32 mmol) were dissolved in dry 1,4-dioxane, which was then stirred at 120 ^{o}C for 48h. After cooling to room temperature, the mixture was poured into water and filtered. The residue was purified by silica gel column chromatography (1,1,2,2-tetrachloroethane/cyclohexane = 1/3,

v/v) to give the product as a white solid (0.13 g, 13%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.83 – 7.78 (m, 36H), 7.80 (d, *J* = 8.4 Hz, 12H), 7.67 – 7.52 (m, 36H). ^{13}C NMR (101 MHz, $C_2Cl_4D_2$) δ 172.12, 171.30, 142.26, 141.13, 136.70, 136.51, 132.62, 132.57, 132.14, 129.20, 129.08, 128.78, 127.30. Anal. calcd for $C_{132}H_{84}N_{18}$: C, 82.48; H, 4.40; N, 13.12. found: C,82.28; H, 4.56; N, 12.98.

2-(4''-bromo-3',4',5',6'-tetraphenyl-[1,1':2',1''-terphenyl]-4-yl)-4,6-diphenyl-1,3,5-triazine (12) A mixture of **3** (0.29 g, 0.6 mmol), tetraphenylcyclopentadienone (**11**, 0.23 g, 0.6 mmol) in diphenyl ether (10 mL) was heated at 260 °C for 48 h under an argon atmosphere. After cooling to room temperature, the mixture was directly applied on silica gel column chromatography (dichloromethane/cyclohexane = 1/5, v/v) to afford the product as a white solid (0.25 g, 50%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.71 – 8.65 (m, 4H), 8.36 (d, *J* = 8.3 Hz, 2H), 7.58 – 7.46 (m, 6H), 7.35 – 7.27 (m, 2H), 7.11 – 7.05 (m, 2H), 7.00 (dd, *J* = 8.5, 2.0 Hz, 2H), 6.92 – 6.73 (m, 20H)

***o*-AcTRZ** A mixture of **12** (0.21 g, 0.25 mmol), **5** (0.11 g, 0.5 mmol), $Pd_2(dba)_3$ (27 mg, 0.03 mmol), *t*-$Bu_3P{\cdot}HBF_4$ (35 mg, 0.12 mmol) and *t*-BuONa (0.19 g, 2 mmol) in dry toluene was heated at 110 °C for 24 h under argon. After cooling to room temperature, the mixture was poured into water and the organic layer was extracted with dichloromethane. After the solvent was removed under reduced pressure, the residue was applied on silica gel column chromatography (dichloromethane / cyclohexane = 1/5, v/v) to give the product as a white solid (0.14 g, 56%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.72 (d, *J* = 7.1 Hz, 4H), 8.48 (d, *J* = 8.2 Hz, 2H), 7.64 – 7.48 (m, 6H), 7.26 (d, *J* = 6.1 Hz, 2H), 7.17 (d, *J* = 8.2 Hz, 2H), 7.12 (d, *J* = 8.2 Hz, 2H), 6.96 – 6.79 (m, 24H), 6.59 (t, *J* = 7.4 Hz, 2H), 5.86 (d, *J* = 8.1 Hz, 2H), 1.52 (s, 6H). MALDI TOF-MS: calcd for $C_{72}H_{52}N_4$: 973 found: 972 $[M-H]^+$. Anal. calcd for $C_{72}H_{52}N_4$: C, 88.86; H, 5.39; N, 5.76. found: C,88.47; H,5.21; N,5.65.

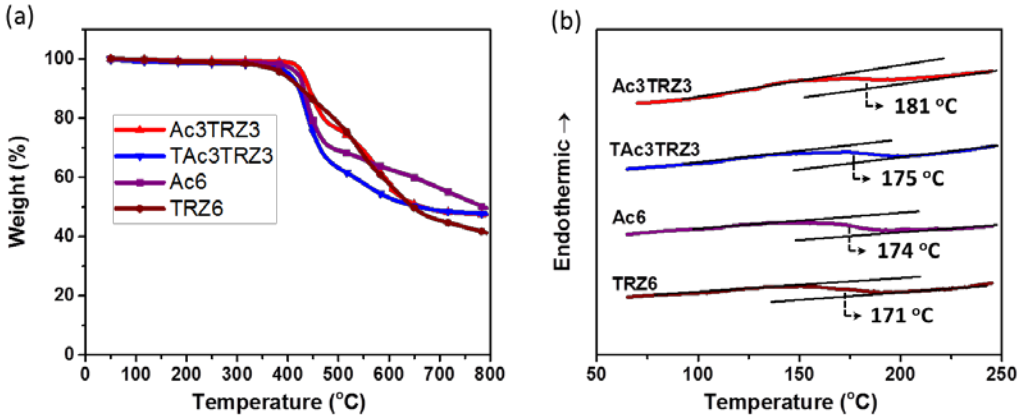


Figure S1. Thermogravimetric analysis (a) and differential scanning calorimetry (b) curves of the compounds.

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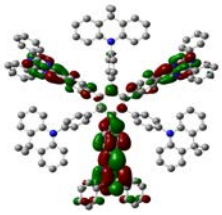
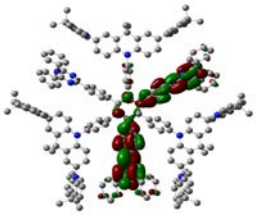
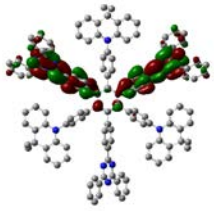
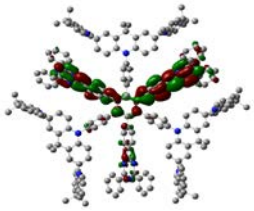
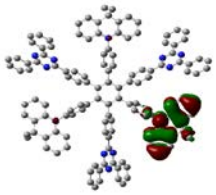
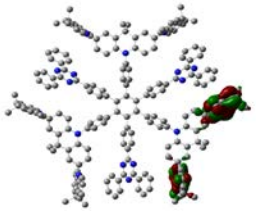
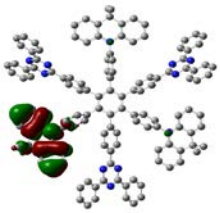
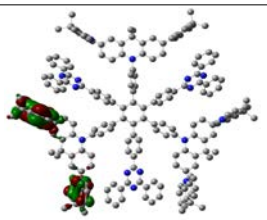
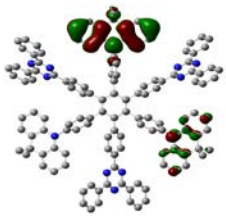
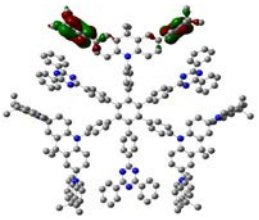
LUMO+1		
LUMO		
HOMO		
HOMO-1		
HOMO-2		

Figure S2. Calculated molecular orbitals of Ac3TRZ3 and TAc3TRZ3 at the b3lyp/6-31g(d) level. There are two degenerate unoccupied molecular orbitals (LUMO and LUMO+1) and three degenerate occupied molecular orbitals (HOMO, HOMO-1 and HOMO-2) for both Ac3TRZ3 and TAc3TRZ3 because of their approximately D3h symmetry.

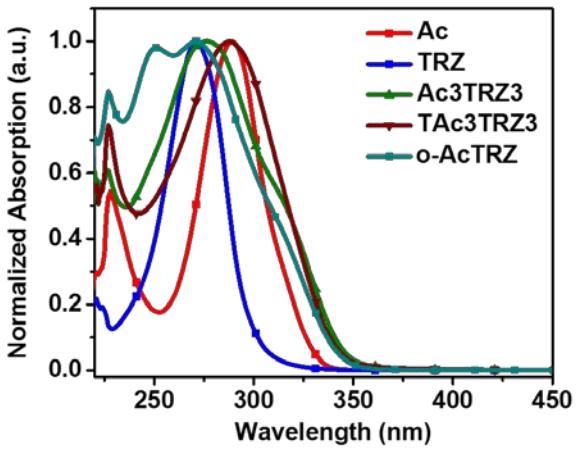


Figure S3. Absorption spectra of the TSCT-HABs and the *N*-phenyl-9,9-dimethyl arcidan (Ac) and 2,4,6-triphenyltriazine (TRZ) segments in toluene with concentration of 10^{-5} mol/L.

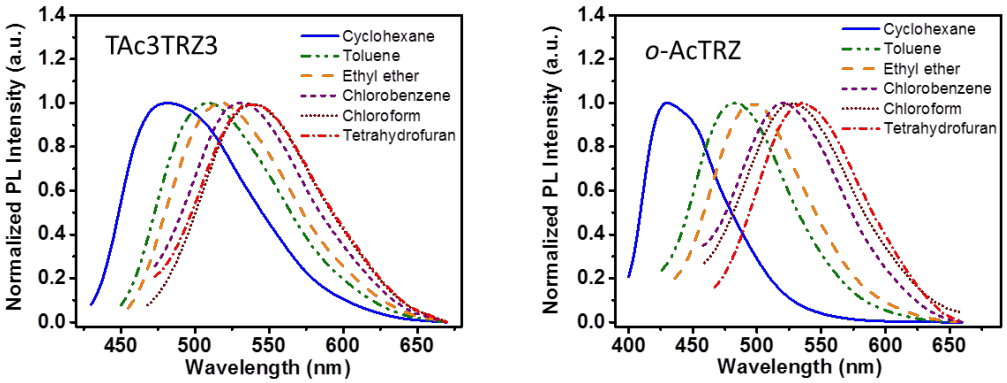


Figure S4. PL spectra of TAc3TRZ3 and o-AcTRZ in solvents with different polarity. Both TAc3TRZ3 and o-AcTRZ shows strong positive solvation effect with the $\lambda_{em,max}$ red-shifted by 60 nm and 76 nm respectively as the solvent goes from cyclohexane to THF, confirming the charge transfer character of their emission.

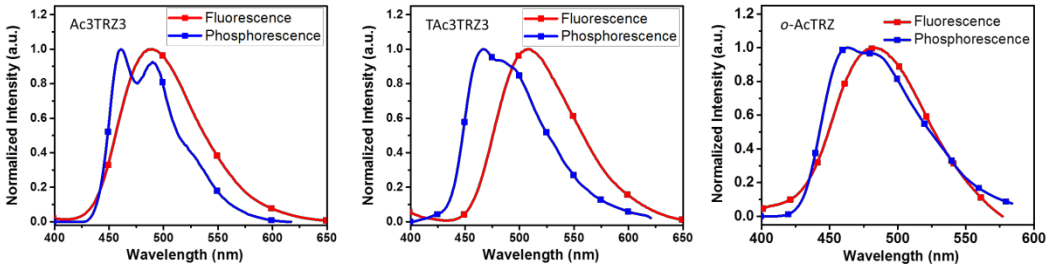
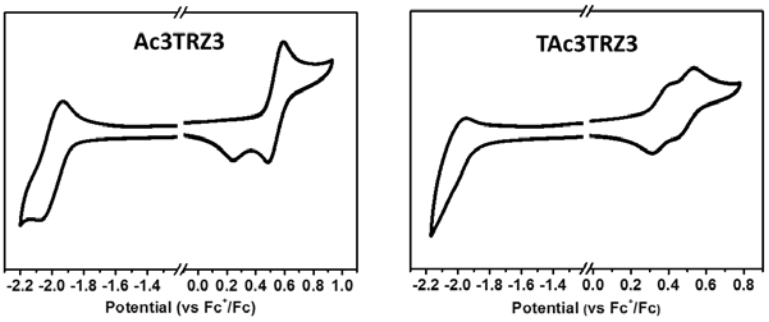


Figure S5. Phosphorescence (77 K) and fluorescence spectra (298 K) of Ac3TRZ3, TAc3TRZ3 and *o*-AcTRZ in toluene.



Polymer	$E_{onset, ox}$	$E_{onset, red}$	HOMO (eV)	LUMO (eV)
Ac6	0.50	--[a]	-5.30	--
TRZ6	--	-1.83	--	-2.97
Ac3TRZ3	0.48	-1.84	-5.28	-2.96
TAc3TRZ3	0.30	-1.86	-5.10	-2.94

[a] not detected.

Figure S6. Cyclic voltammetry characteristics of the compounds. The oxidation and reduction curves were recorded in dichloromethane and DMF, respectively, using ferrocene as the reference and n-Bu_4NClO_4 as the supporting electrolyte. The HOMO and LUMO energy levels were calculated according to the equation of E_{HOMO} (or E_{LUMO}) = -e [$E_{onset, ox}$(or $E_{onset, red}$) + 4.8V], where $E_{onset, ox}$ and $E_{onset,red}$ refer to the onset of the oxidation and reduction potentials, respectively.

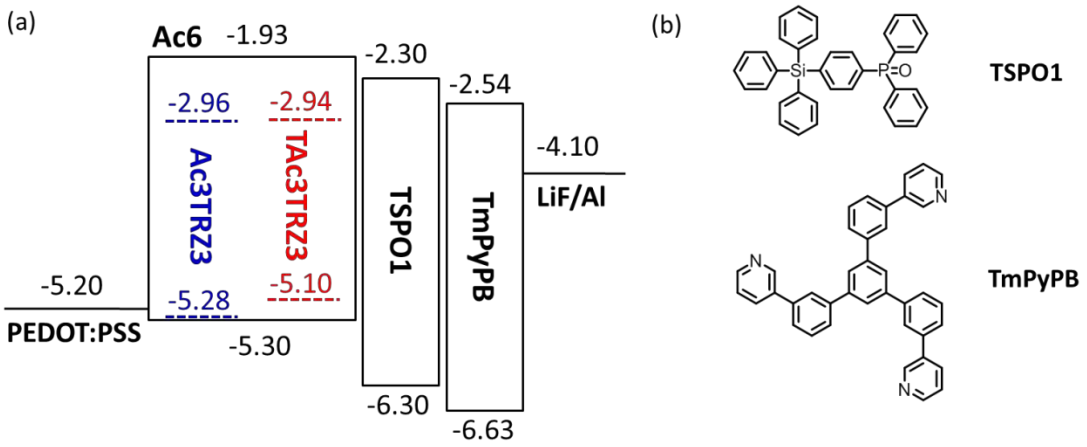


Figure S7. Device structure and schematic energy level alignment of the OLEDs (a), and the structures of the exciton-blocking material (TSPO1) and electron-transporting material TmPyPB (b).

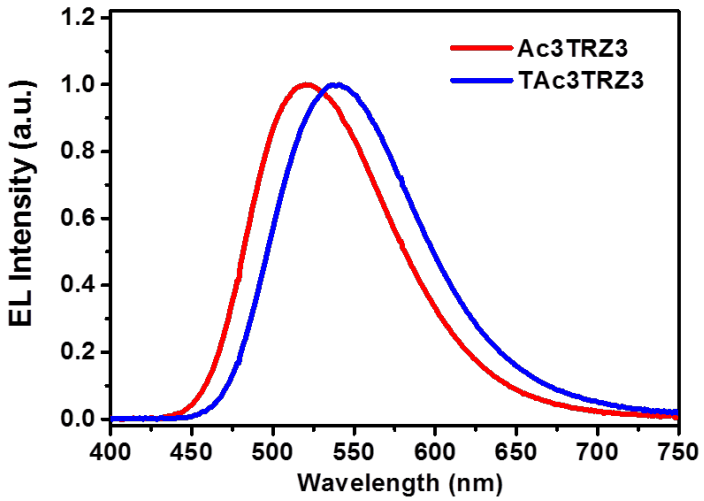


Figure S8. EL spectra of the nondoped OLEDs based on Ac3TRZ3 and TAc3TRZ3 neat films.

Table S1. Photophysical properties of Ac3TRZ3, TAc3TRZ3 and *o*-AcTRZ in solvents of different polarity.

Solvent	*f*	**Ac3TRZ3**			**TAc3TRZ3**			**o-AcTRZ**		
		$\lambda_{abs,\ max}$ (nm)	$\lambda_{em,\ max}$ (nm)	Stokes shift (cm^{-1})	$\lambda_{abs,\ max}$ (nm)	$\lambda_{em,\ max}$ (nm)	Stokes shift (cm^{-1})	$\lambda_{abs,\ max}$ (nm)	$\lambda_{em,\ max}$ (nm)	Stokes shift (cm^{-1})
Cyclohexane	0.0019	314	441	9171	324	478	9943	307	430	9317
Toluene	0.017	319	486	10771	329	508	10710	319	480	10514
Ethyl ether	0.16	313	504	12107	321	517	11810	311	497	12022
Chlorobenzene	0.14	322	525	12008	326	530	11806	316	520	12414
Chloroform	0.15	323	529	12056	329	539	11842	321	528	12213
Tetrahydrofuran	0.21	320	541	12765	323	540	12441	315	536	13089

Table S2. Theoretical computation details for Ac3TRZ3 and TAc3TRZ3. (The calculations were performed on Gaussian 09 program package. The ground-state (S_0) geometry was optimized via DFT calculations. The excited state (S_1/T_1) properties were calculated based on TD-DFT method. All the calculations were performed with the b3lyp functional and 6-31g(d) basis sets.)

Optimized S_0 geometry for Ac3TRZ3**:**

C	-1.41381094	0.13402463	-0.00222379
C	-0.82595005	-1.14959640	-0.00254953
C	0.57940597	-1.28391190	-0.00242069
C	1.39744135	-0.13330888	-0.00245365
C	0.81096410	1.15093993	-0.00235779
C	-0.59472511	1.28393686	-0.00185260
C	1.20304398	-2.64739860	-0.00176600
C	1.94327148	-3.10188118	-1.10434604
C	1.06411735	-3.50282424	1.10236373
C	2.52759726	-4.36414779	-1.10388613
H	2.06253477	-2.45755014	-1.97020866
C	1.64170757	-4.76812433	1.10577654
H	0.49685823	-3.17145524	1.96693199
C	2.38355060	-5.21522980	0.00214686
H	3.09604869	-4.70731811	-1.96079748
H	1.53183016	-5.42044659	1.96465266
C	3.00568382	-6.56026153	0.00561645
N	2.69682776	-7.39162947	1.01258695
N	3.84244984	-6.86650958	-0.99773984
C	3.28657023	-8.59731072	0.97593387
C	4.38454009	-8.09404278	-0.95194851
N	4.13588471	-8.99094414	0.01456718
C	2.97568451	-9.55577603	2.06396656
C	5.32167868	-8.48017194	-2.03448089
C	2.10550640	-9.19280118	3.10449841
C	3.54722693	-10.83799970	2.06502170
C	5.60605567	-7.58792406	-3.08076555
C	5.93717056	-9.74182522	-2.02411029
C	1.81222060	-10.09604504	4.12326712
H	1.66909489	-8.20054780	3.10170823
C	3.25228864	-11.73811195	3.08578425
H	4.21833402	-11.11284489	1.25943253
C	6.49019798	-7.95088399	-4.09384776
H	5.12580985	-6.61615217	-3.08701213
C	6.82001374	-10.10152743	-3.03919299
H	5.71415875	-10.42661482	-1.21402472
C	2.38429729	-11.37055506	4.11705934
H	1.13663746	-9.80568099	4.92317648

H	3.69931081	-12.72849759	3.07725971
C	7.09953849	-9.20788506	-4.07615274
H	6.70433511	-7.25254750	-4.89823339
H	7.29184992	-11.08021434	-3.02171610
H	2.15463893	-12.07451765	4.91263706
H	7.78939089	-9.48992960	-4.86722326
C	1.68048789	2.37244265	-0.00242791
C	1.70305139	3.24084227	-1.10494246
C	2.49470206	2.67766433	1.09939293
C	2.50750203	4.37555343	-1.10717903
H	1.08252755	3.02340840	-1.96908052
C	3.30519934	3.80807721	1.10010588
H	2.49213166	2.02064300	1.96391996
C	3.32156979	4.67345063	-0.00403849
H	2.52035913	5.03878758	-1.96462353
H	3.92911838	4.03689193	1.95660256
C	4.18409294	5.87848946	-0.00580560
N	5.06463116	6.02060615	0.99661680
N	4.03419822	6.75568240	-1.01009735
C	5.82612943	7.12544098	0.95251258
C	4.83838771	7.83013034	-0.97174544
N	5.74785210	8.05557567	-0.01135301
C	6.81995849	7.32737872	2.03441956
C	4.70945982	8.83322360	-2.05629178
C	6.93234060	6.39656023	3.07969507
C	7.66130158	8.45108756	2.02468930
C	3.78409118	8.64277107	-3.09513661
C	5.51060961	9.98601761	-2.05568081
C	7.86936772	6.58620116	4.09250276
H	6.27824339	5.53218512	3.08548896
C	8.59651971	8.63774542	3.03944286
H	7.57029796	9.16637158	1.21537978
C	3.66222432	9.58833879	-4.11042326
H	3.16961145	7.74976795	-3.09396147
C	5.38652829	10.92881504	-3.07297785
H	6.22340497	10.12788352	-1.25151082
C	8.70383331	7.70648681	4.07543462
H	7.94903753	5.85935525	4.89618538
H	9.24370189	9.51045829	3.02246969
C	4.46246287	10.73340396	-4.10253522
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C	-9.38809219	-1.05677666	-3.08332629
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H	-7.19249319	-9.19216183	-1.50361727
H	-6.48166759	-8.17586544	2.08081881
H	-7.72563625	-8.82817631	1.00038914
H	-6.33129182	-9.82204585	1.44173318
H	-9.29796902	-5.27025960	-1.19090419
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C	2.88967623	-0.27509944	-0.00208990
C	3.56378463	-0.75796127	1.12847603
C	3.64261651	0.07228893	-1.13259041
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C	7.29971704	1.67473071	0.62637037
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C	9.59606949	-3.35984810	-0.64226829
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C	8.05904988	2.79660778	0.93642609
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C	10.92954440	-1.35841086	1.22519618
C	8.77608431	-4.44278767	-0.94777237
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H	7.55487250	3.73158438	1.16653746
H	10.40382453	-0.42989682	-2.10301159
H	11.71401263	0.08185158	-1.02507121
H	11.55580525	-1.62098325	-1.47426098
H	10.29788642	-1.53066836	2.10277227
H	11.49111333	-2.27721230	1.02593400
H	11.65228675	-0.57483258	1.47600053
H	9.21002680	-5.40916369	-1.18738327
H	10.05738732	3.58470739	1.18687374
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C	-2.38315241	5.20910450	0.00479542
H	-2.98166454	4.77222185	-2.01157824
H	-1.65834188	5.36751141	2.02086118
N	-2.97668467	6.51432312	0.00779955
C	-4.34450348	6.64447257	0.31719111
C	-2.17698648	7.63216227	-0.29966306
C	-4.96233889	7.91232919	0.32696386

C	-5.10628174	5.49857649	0.62391164
C	-2.72685433	8.93097243	-0.30264119
C	-0.81340357	7.45495727	-0.61111070
C	-4.20204731	9.20802603	0.01525830
C	-6.32708222	7.97382800	0.63927121
C	-6.45889302	5.59688916	0.92740086
H	-4.63561677	4.52317909	0.62142095
C	-1.87741544	10.00142201	-0.61303226
C	0.00026057	8.54045555	-0.91273030
H	-0.38716709	6.45940421	-0.61364689
C	-4.28647709	10.15255911	1.24534151
C	-4.86178579	9.90043372	-1.20842976
C	-7.08319660	6.84321615	0.93687309
H	-6.81648137	8.94376608	0.64950834
H	-7.01932777	4.69335645	1.15300125
C	-0.52920973	9.82993509	-0.91540539
H	-2.28713330	11.00759498	-0.61761993
H	1.04889273	8.37004597	-1.14224907
H	-3.82634669	9.68606693	2.12253556
H	-3.76888572	11.09835956	1.05350766
H	-5.32724970	10.38712021	1.49242564
H	-4.81470408	9.25304743	-2.09017139
H	-5.91433280	10.13024789	-1.01224990
H	-4.35578489	10.84093055	-1.45047743
H	-8.13959410	6.93588509	1.17147222
H	0.09423439	10.68819565	-1.14844136

Optimized S_0 geometry for TAc3TRZ3:

C	4.15027757	-8.24229999	-0.90942136
N	3.45031332	-7.09571921	-0.95645156
C	3.67094105	-6.23943422	0.05139060
N	4.51535923	-6.46348189	1.06848281
C	5.15261050	-7.64685313	1.04560132
N	5.00375160	-8.56078638	0.07519945
C	3.96785111	-9.21451740	-2.01180700
C	6.07897064	-7.95986730	2.15813730
C	2.92881847	-4.95486902	0.04046538
C	6.40669365	-6.98023871	3.10905702
C	7.29346063	-7.27061541	4.14264555
C	7.84700565	-8.54865605	4.25035261
C	7.51524591	-9.53342093	3.31574393
C	6.64354270	-9.24038305	2.26982467
C	4.78085335	-10.35633961	-2.08916849
C	4.60889848	-11.27054463	-3.12551014
C	3.61509329	-11.06423361	-4.08637658
C	2.79939355	-9.93241259	-4.01383607
C	2.98036225	-9.00780473	-2.98851567
C	2.16264848	-4.58243729	-1.07386067
C	1.46462218	-3.37902452	-1.08048685
C	1.50826060	-2.51266628	0.02279019
C	2.27660153	-2.89083839	1.13474213
C	2.97797178	-4.09224978	1.14556469
C	-9.15261763	0.49942707	-0.97452185
N	-7.80965462	0.54673323	-1.01051607
C	-7.18054971	-0.04548757	0.01478782
N	-7.79902964	-0.64643094	1.04145434
C	-9.14255527	-0.61924822	1.00772585
N	-9.85734049	-0.06534314	0.01716820
C	-9.90098856	1.10978157	-2.09761831
C	-9.87950397	-1.24007567	2.13264520
C	-5.69700960	-0.03483087	0.01366889
C	-9.19462129	-1.97066738	3.11685753
C	-9.89213797	-2.56756869	4.16380770
C	-11.27907285	-2.42577642	4.25067041
C	-11.96642092	-1.68838983	3.28251664
C	-11.27379749	-1.10483409	2.22459812
C	-11.29315442	0.95281627	-2.18722210
C	-11.99680389	1.52680318	-3.24307154
C	-11.32292598	2.27647339	-4.21124222
C	-9.93823021	2.44011263	-4.12664083

C	-9.22950306	1.85265975	-3.08190107
C	-4.98683017	0.42484291	-1.10531196
C	-3.59560699	0.43250859	-1.10407789
C	-2.87186267	-0.01631631	0.01136999
C	-3.58785114	-0.47382468	1.12822682
C	-4.97900752	-0.48460229	1.13162262
C	5.05882534	7.70887133	-1.03792195
N	4.43652497	6.51752337	-1.05878023
C	3.59684985	6.28357131	-0.04001641
N	3.36694110	7.13792596	0.96738126
C	4.05174398	8.29353514	0.91789461
N	4.89951602	8.62192138	-0.06838900
C	5.97940589	8.03255212	-2.15217739
C	3.85842557	9.26476066	2.01931603
C	2.87068199	4.98993301	-0.02726460
C	2.87945161	9.04354362	3.00143721
C	2.68866769	9.96681393	4.02617669
C	3.48585078	11.11212701	4.09257222
C	4.47089316	11.33327759	3.12602259
C	4.65262818	10.42012478	2.09043291
C	6.52988151	9.31913500	-2.26429445
C	7.39592506	9.62226101	-3.31203900
C	7.73563426	8.64192825	-4.24844161
C	7.19598115	7.35798464	-4.14044261
C	6.31522140	7.05722934	-3.10470926
C	2.93008364	4.12675074	-1.13139016
C	2.24338007	2.91691535	-1.11920955
C	1.47942319	2.53084119	-0.00696699
C	1.42583004	3.39768099	1.09552862
C	2.10929492	4.60941372	1.08761440
C	-0.67348109	1.21893359	0.00297642
C	0.73832504	1.22799927	0.00208677
C	1.45027345	0.00875409	0.00820345
C	0.75212556	-1.21846111	0.01519368
C	-0.65957619	-1.22549712	0.01587948
C	-1.37283762	-0.00734638	0.01001246
H	5.96471534	-5.99420147	3.02098181
H	7.56675396	-6.49821841	4.85505203
H	8.54049968	-8.77244029	5.05619154
H	7.94106531	-10.52969871	3.39936453
H	6.38615173	-9.99295412	1.53335978
H	5.54281783	-10.50990880	-1.33368564
H	5.24766401	-12.14785315	-3.18193163
H	3.47059033	-11.78549786	-4.88596607

H	2.01353538	-9.78093465	-4.74754850
H	2.35843739	-8.12187565	-2.92735388
H	2.12882604	-5.24431131	-1.93192020
H	0.87800123	-3.10488421	-1.95240551
H	2.32201352	-2.23662860	2.00045774
H	3.56364642	-4.38114612	2.01101371
H	-8.11723837	-2.06735865	3.04448570
H	-9.35826819	-3.15579175	4.90402313
H	-11.82200903	-2.89419547	5.06691028
H	-13.04474027	-1.57210158	3.35012137
H	-11.79680770	-0.53765304	1.46322012
H	-11.80576636	0.37638149	-1.42572762
H	-13.07327160	1.39358651	-3.30893749
H	-11.87464147	2.73758070	-5.02576420
H	-9.41510357	3.03780166	-4.86694133
H	-8.15365492	1.96628193	-3.01136526
H	-5.53946486	0.76616300	-1.97339768
H	-3.06109062	0.78956241	-1.97953528
H	-3.04731812	-0.82337987	2.00302369
H	-5.52569413	-0.83318223	2.00059040
H	2.27198854	8.14733442	2.94499535
H	1.90941102	9.80361423	4.76438713
H	3.33360026	11.83229661	4.89168967
H	5.09521271	12.22122516	3.17749795
H	5.40805972	10.58482554	1.33075385
H	6.26610983	10.06845512	-1.52677040
H	7.81083908	10.62310744	-3.39590321
H	8.42441703	8.87382970	-5.05600888
H	7.47553613	6.58920863	-4.85430598
H	5.88406550	6.06643136	-3.01643356
H	3.51236092	4.42167623	-1.99710310
H	2.29701590	2.26230944	-1.98414241
H	0.84313617	3.11724615	1.96806234
H	2.06770464	5.27158213	1.94509821
C	-1.43381491	2.51195460	-0.00429100
C	-1.44887274	3.33066082	-1.14247647
C	-2.15074691	2.92723264	1.12704854
C	-2.16843733	4.52440054	-1.15540634
H	-0.89589428	3.02861239	-2.02707265
C	-2.85724701	4.12829446	1.12538849
H	-2.15507877	2.30415190	2.01655984
C	-2.87318598	4.93055287	-0.01903627
H	-2.18386977	5.15031060	-2.04271691
H	-3.40585826	4.44766919	2.00648649

N	-3.61058989	6.16337743	-0.02632414
C	-2.94556753	7.36303088	0.28853220
C	-4.98654694	6.13901564	-0.32126889
C	-3.64548438	8.58827968	0.31676519
C	-1.56640100	7.34940366	0.58214485
C	-5.74455454	7.32961503	-0.31929258
C	-5.62143182	4.91735717	-0.62674838
C	-5.14104373	8.70158277	0.00156246
C	-2.93169685	9.74498325	0.64417751
C	-0.88365304	8.51940017	0.89435681
H	-1.02027066	6.41460829	0.56208560
C	-7.10592646	7.24199783	-0.62549631
C	-6.97933482	4.86354390	-0.91939218
H	-5.04869664	3.99839819	-0.63085996
C	-5.32977594	9.63813590	-1.22289934
C	-5.87590390	9.30463639	1.22970358
C	-1.56748397	9.73547033	0.93227757
H	-3.44631327	10.70006198	0.67555301
H	0.18094052	8.48747686	1.10727450
C	-7.73765519	6.03515646	-0.92307314
H	-7.71174011	8.14251203	-0.63326994
H	-7.45032962	3.91039436	-1.14153974
H	-4.81933391	9.23341823	-2.10294286
H	-6.38990117	9.75578502	-1.46972602
H	-4.92213685	10.63445538	-1.02338042
H	-5.75884640	8.65981237	2.10678105
H	-5.47921961	10.29370889	1.48058689
H	-6.94674984	9.41770506	1.03248215
C	-1.40483081	-2.52724771	0.02121962
C	-2.11620067	-2.94920283	-1.11115758
C	-1.41027640	-3.34824562	1.15783486
C	-2.80765630	-4.15895148	-1.11206899
H	-2.12778464	-2.32468098	-1.99958160
C	-2.11512832	-4.55077281	1.16829873
H	-0.86126412	-3.04111104	2.04314312
C	-2.81427091	-4.96351213	0.03082373
H	-3.35193151	-4.48341177	-1.99400407
H	-2.12333919	-5.17842231	2.05447915
N	-3.53677778	-6.20512824	0.03510928
C	-4.91414331	-6.19672967	0.32446047
C	-2.85785818	-7.39636423	-0.28263303
C	-5.66008636	-7.39479844	0.31167766
C	-5.56261239	-4.98361661	0.63531919
C	-3.54526647	-8.62849879	-0.32060342

C	-1.47752662	-7.36770298	-0.56993162
C	-5.04132764	-8.75854161	-0.01478881
C	-7.02381646	-7.32286405	0.61150096
C	-6.92227936	-4.94537970	0.92217859
H	-4.99916879	-4.05901578	0.64819838
C	-2.81838678	-9.77641347	-0.64989768
C	-0.78168967	-8.52934108	-0.88462686
H	-0.94054390	-6.42780068	-0.54347821
C	-5.76332996	-9.36053042	-1.25103681
C	-5.22769730	-9.70515245	1.20231243
C	-7.66894549	-6.12442130	0.91435663
H	-7.62051117	-8.22945353	0.60978176
H	-7.40361560	-3.99847503	1.14883564
C	-1.45299639	-9.75206549	-0.93133282
H	-3.32361557	-10.73621124	-0.68889070
H	0.28342788	-8.48548699	-1.09281682
H	-5.64669030	-8.70941099	-2.12351325
H	-5.35649526	-10.34455811	-1.50544827
H	-6.83431861	-9.48406277	-1.06096350
H	-4.72610666	-9.30139465	2.08786926
H	-6.28794961	-9.83496090	1.44237595
H	-4.80925559	-10.69609294	0.99843329
C	2.95013300	0.01693155	0.00601745
C	3.66798103	-0.39974843	-1.12413781
C	3.66723067	0.44122877	1.13383723
C	5.06150114	-0.38377470	-1.13262440
H	3.13052380	-0.73709826	-2.00550550
C	5.06087358	0.44110765	1.13732122
H	3.12914638	0.77185093	2.01737370
C	5.76477773	0.03280837	0.00102082
H	5.61178942	-0.69997623	-2.01380982
H	5.61066184	0.76323600	2.01667296
N	7.20134812	0.04102539	-0.00178591
C	7.89529048	-1.14310949	0.30898439
C	7.88080192	1.23352054	-0.31270212
C	9.30634780	-1.16945969	0.31847801
C	7.18074910	-2.31908034	0.61770626
C	9.29153708	1.27631580	-0.32508327
C	7.15208812	2.40142871	-0.61891798
C	10.16519618	0.05809431	-0.00548724
C	9.93873811	-2.37476569	0.63842836
C	7.84010078	-3.50388379	0.92341535
H	6.09798175	-2.30862905	0.61384271
C	9.90920859	2.48912463	-0.64540143

C	7.79700094	3.59413075	-0.92478791
H	6.06951250	2.37855270	-0.61283532
C	11.06135081	-0.26038276	-1.23323699
C	11.06433812	0.38604968	1.21751211
C	9.23519997	-3.54045222	0.93875423
H	11.02292831	-2.42311929	0.65381235
H	7.27066627	-4.40119255	1.14768051
C	9.19156793	3.64684831	-0.94324770
H	10.99273684	2.55002747	-0.66338885
H	7.21667056	4.48500300	-1.14691522
H	10.44884439	-0.49461853	-2.11004224
H	11.70258801	0.59058207	-1.48467873
H	11.71112375	-1.11873079	-1.03457259
H	10.45403827	0.61303857	2.09775889
H	11.71654771	-0.45765498	1.46511724
H	11.70351540	1.25159316	1.01585395
N	-0.89989195	10.96602445	1.25307063
C	-0.82786330	11.38119856	2.59477665
C	-0.42617613	11.78153724	0.20692562
C	-0.33358722	12.65961057	2.93179157
C	-1.25421442	10.51250987	3.62028269
C	0.06816166	13.07700712	0.46583923
C	-0.44194545	11.29837713	-1.11687782
C	0.10885149	13.68029156	1.87546467
C	-0.28554557	13.00906430	4.28773687
C	-1.19241421	10.89298974	4.95570415
H	-1.63751206	9.53292880	3.36297852
C	0.51197933	13.84023438	-0.62220547
C	0.01024258	12.08172790	-2.17156359
H	-0.81010301	10.29957074	-1.31550521
C	1.55340575	14.15438411	2.18823954
C	-0.85110054	14.90113793	1.92736374
C	-0.70253088	12.15143303	5.30274218
H	0.08204394	13.99460629	4.55931982
H	-1.53388709	10.20157897	5.72202788
C	0.49057685	13.36787151	-1.93154675
H	0.88306155	14.84453252	-0.43869092
H	-0.01464765	11.67992907	-3.18118235
H	2.25134026	13.31215221	2.16306902
H	1.89056794	14.90032151	1.46162330
H	1.61227312	14.61672024	3.17898385
H	-1.87986703	14.59497682	1.71047200
H	-0.83831324	15.36910085	2.91795099
H	-0.56113012	15.65982797	1.19208051

H	-0.65360542	12.46567732	6.34138307
H	0.84315434	13.99388407	-2.74609802
N	-9.14329384	6.02156729	-1.21749899
C	-9.57049525	6.20140479	-2.54535405
C	-10.06468415	5.93390220	-0.15612636
C	-10.93896360	6.36402710	-2.85006061
C	-8.62240341	6.21933903	-3.58884887
C	-11.44747314	6.09565274	-0.38263216
C	-9.60208015	5.67923406	1.15055082
C	-12.02876424	6.39276084	-1.77063319
C	-11.29651189	6.53751759	-4.19352844
C	-9.01364653	6.39297389	-4.91118855
H	-7.57196762	6.09732139	-3.35541702
C	-12.30830403	6.00573732	0.71922558
C	-10.48520591	5.59291636	2.21968262
H	-8.54143405	5.54663108	1.32403634
C	-13.11599488	5.33722892	-2.10725450
C	-12.67738706	7.80463908	-1.75107504
C	-10.36232487	6.55335328	-5.22634328
H	-12.34533998	6.67536472	-4.44054371
H	-8.25753215	6.40674303	-5.69221377
C	-11.85331939	5.75906685	2.01163581
H	-13.37454777	6.14005711	0.56088839
H	-10.09712546	5.39418893	3.21531696
H	-12.68505966	4.33184305	-2.13095806
H	-13.92013702	5.34788655	-1.36466307
H	-13.57203635	5.53578522	-3.08265591
H	-11.93182686	8.57075195	-1.51358545
H	-13.11644590	8.04932138	-2.72462434
H	-13.47218753	7.86067424	-0.99905336
H	-10.68321165	6.69654954	-6.25419340
H	-12.55573921	5.69812844	2.83783052
N	-9.07589190	-6.12625062	1.20273699
C	-9.50707516	-6.32258352	2.52699909
C	-9.99343408	-6.03811816	0.13810859
C	-10.87535443	-6.49944329	2.82434275
C	-8.56326737	-6.34291605	3.57434441
C	-11.37586969	-6.21220953	0.35755613
C	-9.52750124	-5.77034743	-1.16477341
C	-11.96103384	-6.52347318	1.74076169
C	-11.23692092	-6.69063318	4.16434797
C	-8.95842461	-6.53398116	4.89310191
H	-7.51297404	-6.20943347	3.34669806
C	-12.23290606	-6.12027403	-0.74704654

C	-10.40692773	-5.68275357	-2.23685593
H	-8.46719694	-5.62844966	-1.33299383
C	-13.05322203	-5.47457936	2.08226151
C	-12.60421471	-7.93756200	1.70694477
C	-10.30688640	-6.70971642	5.20082713
H	-12.28562318	-6.83987143	4.40540230
H	-8.20544184	-6.54943297	5.67712206
C	-11.77462581	-5.86048092	-2.03569185
H	-13.29871492	-6.26366985	-0.59385605
H	-10.01627962	-5.47383942	-3.22939614
H	-12.62626806	-4.46768960	2.11426840
H	-13.85539653	-5.48299180	1.33746403
H	-13.51070798	-5.68196573	3.05517113
H	-11.85492285	-8.69888476	1.46585398
H	-13.04586451	-8.19200799	2.67677636
H	-13.39607570	-7.99042009	0.95161859
H	-10.63072918	-6.86690313	6.22570408
H	-12.47414575	-5.79842907	-2.86426004
N	-0.77214490	-10.97439133	-1.25558921
C	-0.69321350	-11.38316170	-2.59884741
C	-0.29087304	-11.78870314	-0.21195530
C	-0.18280277	-12.65402479	-2.94038889
C	-1.12835182	-10.51539679	-3.62145843
C	0.22004718	-13.07678174	-0.47561365
C	-0.31588186	-11.31196413	1.11404166
C	0.27107761	-13.67337183	-1.88768576
C	-0.12827169	-12.99720248	-4.29767854
C	-1.05959722	-10.88945081	-4.95836756
H	-1.52382501	-9.54156704	-3.36073788
C	0.67096716	-13.83938119	0.60991652
C	0.14392690	-12.09438836	2.16613296
H	-0.69720020	-10.31888613	1.31646267
C	1.72239093	-14.12677074	-2.20000656
C	-0.67241035	-14.90662989	-1.94654019
C	-0.55385244	-12.14040482	-5.30981992
H	0.25211317	-13.97694267	-4.57269679
H	-1.40809728	-10.19899505	-5.72238259
C	0.64101315	-13.37324530	1.92131310
H	1.05493508	-14.83812922	0.42263477
H	0.11165508	-11.69762941	3.17753431
H	2.40919366	-13.27561506	-2.16953678
H	2.06807660	-14.87167429	-1.47632499
H	1.78911687	-14.58342948	-3.19291528
H	-1.70554994	-14.61497136	-1.73047345

H	-0.65148045	-15.37037342	-2.93896606
H	-0.37396052	-15.66448124	-1.21376403
H	-0.49932525	-12.44964277	-6.34968221
H	0.99981793	-13.99845610	2.73375705
N	9.95195939	-4.74581683	1.24798264
C	10.29124297	-5.02275738	2.58431403
C	10.37455981	-5.58068877	0.19536735
C	11.11895535	-6.11903026	2.90889535
C	9.80323407	-4.19508951	3.61621180
C	11.21151788	-6.68898601	0.44217423
C	9.95638855	-5.30873357	-1.12279024
C	11.72243920	-7.04394922	1.84406871
C	11.41823700	-6.33874947	4.25985122
C	10.12077371	-4.44326092	4.94647289
H	9.17230519	-3.35094890	3.36729108
C	11.60291658	-7.47276932	-0.65128657
C	10.36164583	-6.10982284	-2.18322618
H	9.30663599	-4.46346419	-1.31214152
C	11.34729502	-8.51499471	2.16769396
C	13.26849948	-6.89294780	1.86840031
C	10.93452137	-5.52491259	5.28134001
H	12.06291062	-7.17286045	4.52219615
H	9.73248884	-3.78322946	5.71815351
C	11.19528494	-7.20319855	-1.95482072
H	12.25569651	-8.32335852	-0.47670107
H	10.02085393	-5.87436928	-3.18810788
H	10.26122566	-8.64735882	2.16116798
H	11.78069309	-9.20373319	1.43546131
H	11.72084188	-8.81098969	3.15344655
H	13.56073952	-5.86229145	1.64155973
H	13.67321223	-7.15110719	2.85322380
H	13.73889302	-7.54953056	1.12826852
H	11.19674012	-5.72830393	6.31566183
H	11.52343241	-7.83657620	-2.77388041
N	9.89394236	4.86031984	-1.25379571
C	10.22666144	5.14159890	-2.59089920
C	10.31190618	5.69820078	-0.20170749
C	11.04276161	6.24612186	-2.91695272
C	9.74401051	4.30993020	-3.62211640
C	11.13753143	6.81459972	-0.45006776
C	9.90044362	5.42100885	1.11745239
C	11.64082244	7.17567631	-1.85310777
C	11.33608281	6.46976603	-4.26857899
C	10.05540704	4.56217133	-4.95306024

H	9.12220195	3.45933931	-3.37222107
C	11.52510826	7.60087589	0.64296696
C	10.30154166	6.22480543	2.17743862
H	9.25943534	4.56933673	1.30791149
C	11.25098301	8.64356446	-2.17400790
C	13.18815482	7.03932299	-1.88207240
C	10.85749602	5.65204414	-5.28935966
H	11.97195955	7.31022200	-4.53211870
H	9.67157149	3.89884907	-5.72414565
C	11.12418257	7.32615818	1.94749442
H	12.16960006	8.45756903	0.46728122
H	9.96620950	5.98515175	3.18316214
H	10.16371602	8.76561205	-2.16548246
H	11.67897247	9.33551166	-1.44159557
H	11.62005361	8.94456535	-3.15993108
H	13.49091813	6.01143233	-1.65648738
H	13.58758119	7.30163372	-2.86796245
H	13.65433791	7.70010154	-1.14304109
H	11.11481380	5.85877501	-6.32424964
H	11.44907798	7.96169878	2.76617660

Optimized S_0 geometry for *o*-AcTRZ:

C	5.40786250	-2.39369114	1.01432383
N	4.11039567	-2.05444635	1.06460697
C	3.34314834	-2.52568009	0.06806936
N	3.80004192	-3.28655420	-0.93855188
C	5.11053294	-3.57299395	-0.90706190
N	5.95206139	-3.15053359	0.04938114
C	6.29798821	-1.89772744	2.09272757
C	5.66407842	-4.41325320	-1.99672678
C	1.90216153	-2.18343990	0.08152334
C	4.82562545	-4.90728056	-3.00848197
C	5.34696213	-5.69771732	-4.02962316
C	6.70992619	-6.00370973	-4.05435746
C	7.55039291	-5.51519668	-3.05095113
C	7.03237384	-4.72538197	-2.02769530
C	7.67119174	-2.18830272	2.06935574
C	8.50672669	-1.71825711	3.07946078
C	7.98302108	-0.95354967	4.12490543
C	6.61714215	-0.66218097	4.15626434
C	5.77837881	-1.13110028	3.14800221
C	1.34775573	-1.47053414	1.15578076
C	-0.00390761	-1.14463688	1.16382669
C	-0.84553799	-1.51713213	0.10344681
C	-0.28677070	-2.23700627	-0.96380126
C	1.06456515	-2.56585983	-0.97721421
C	-5.10629055	4.75450617	-0.25077867
C	-5.32999708	4.04508386	0.93019039
C	-4.98886997	2.69516127	1.01314997
C	-4.41273253	2.03129284	-0.07941597
C	-4.19256477	2.75487599	-1.26055124
C	-4.53839379	4.10372061	-1.34748280
C	-7.70785177	-4.81082403	0.51448736
C	-6.86288757	-4.55321952	1.59510327
C	-5.87470536	-3.57403561	1.49496967
C	-5.71745780	-2.83026007	0.31663578
C	-6.57439268	-3.09649739	-0.76115981
C	-7.55876931	-4.07986369	-0.66512741
C	-5.02615853	-0.41254115	0.11713735
C	-4.65758936	-1.77337755	0.21035322
C	-3.29261997	-2.13881927	0.20491530
C	-2.29737355	-1.14140326	0.10728029
C	-2.66717949	0.21822729	0.01256222
C	-4.03024284	0.58370359	0.01660726

H	3.76974205	-4.66388264	-2.97849459
H	4.68966422	-6.07619807	-4.80781025
H	7.11536873	-6.62040522	-4.85227472
H	8.61113378	-5.75063923	-3.06636549
H	7.67468696	-4.34150142	-1.24347505
H	8.06667479	-2.78135491	1.25278436
H	9.56853015	-1.94769020	3.05134534
H	8.63652545	-0.58654570	4.91201396
H	6.20490070	-0.06851840	4.96759716
H	4.71673953	-0.91311477	3.16518919
H	1.98813678	-1.18012354	1.98081906
H	-0.41516040	-0.59005702	2.00189619
H	-0.92067606	-2.54148882	-1.79123761
H	1.48763887	-3.11859357	-1.80823701
H	-5.77248234	4.54206195	1.78954876
H	-5.17277162	2.14734717	1.93298480
H	-3.74637946	2.25604414	-2.11630975
H	-4.36454506	4.64521202	-2.27384796
H	-6.97028235	-5.11684616	2.51824892
H	-5.21518752	-3.38451349	2.33704578
H	-6.46928680	-2.52554281	-1.67931380
H	-8.21133926	-4.27250835	-1.51274774
C	-6.47452211	-0.02172175	0.12875194
C	-7.25132606	-0.18080328	1.28536074
C	-7.08173470	0.51539155	-1.01552289
C	-8.59631608	0.18820320	1.29881709
H	-6.79749608	-0.60001482	2.17885573
C	-8.42810783	0.87941687	-1.00564611
H	-6.49265342	0.65055579	-1.91819742
C	-9.19022218	0.71844745	0.15245899
H	-9.18058317	0.05912518	2.20622058
H	-8.88064825	1.29158422	-1.90385531
C	-1.60753514	1.27515199	-0.08641922
C	-1.36342511	2.14516122	0.98601556
C	-0.82743976	1.40780373	-1.24368810
C	-0.35812755	3.10693550	0.91268902
H	-1.96293037	2.06286367	1.88785352
C	0.16982525	2.37813133	-1.32751358
H	-0.99942668	0.74145387	-2.08397585
C	0.41545083	3.22722715	-0.24514649
H	-0.16471718	3.76981509	1.75087142
H	0.77170689	2.47660075	-2.22607516
N	1.46147034	4.20704960	-0.31512679
C	2.77298208	3.83318151	0.03888469

C	1.14797817	5.52185230	-0.70454281
C	3.82129696	4.77638584	0.01717073
C	3.04422076	2.50358804	0.42079675
C	2.14553831	6.51909238	-0.74462752
C	-0.17557171	5.85003554	-1.06341973
C	3.60931065	6.24305702	-0.37850166
C	5.10326910	4.34105773	0.37902733
C	4.32865081	2.10618697	0.77219312
H	2.24309484	1.77521889	0.43970664
C	1.76797790	7.80986931	-1.13733492
C	-0.51251516	7.14174832	-1.44900363
H	-0.94408680	5.08720744	-1.03678801
C	4.50732294	6.57348927	-1.60193984
C	4.01353809	7.15175241	0.81459064
C	5.37427816	3.02799960	0.75397981
H	5.91969998	5.05790491	0.36664879
H	4.50415103	1.07205315	1.05647605
C	0.46132419	8.13818516	-1.48819576
H	2.52584120	8.58765493	-1.16863663
H	-1.54205268	7.36361853	-1.71789208
H	4.24196805	5.94276433	-2.45664930
H	4.39444127	7.61997559	-1.90451025
H	5.56489119	6.40634334	-1.37245627
H	3.39411541	6.93581386	1.69128587
H	5.06106435	6.99505467	1.09290147
H	3.89024657	8.21091629	0.56487021
H	6.38316236	2.73193878	1.02624346
H	0.21190807	9.15248285	-1.78612834
C	-2.89715552	-3.58205955	0.30863197
C	-2.22841415	-4.06148078	1.44440106
C	-3.18254163	-4.48196507	-0.72854054
C	-1.85705309	-5.40235323	1.54219424
H	-1.99642463	-3.37669031	2.25524636
C	-2.80633073	-5.82165413	-0.63509289
H	-3.70566345	-4.12848088	-1.61243888
C	-2.14293493	-6.28710415	0.50139225
H	-1.34109452	-5.75444290	2.43163964
H	-3.03380047	-6.50247431	-1.45124187
H	-1.85074667	-7.33121542	0.57516405
H	-10.23870890	1.00426125	0.16157165
H	-8.47653654	-5.57528095	0.59098744
H	-5.37352619	5.80579786	-0.31644404