Supporting Information

Inclusion of C_{60} into the hexagonal columnar space formed by intra- and intermolecular CH$\cdots\pi$ interactions

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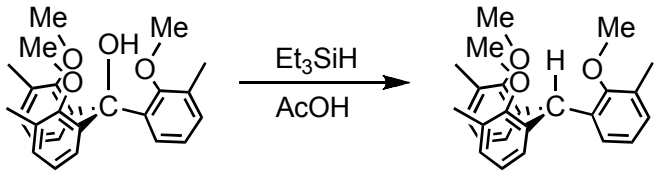
Experimental

Synthesis of Tris(2-methoxy-3-methylphenyl)methane **1**

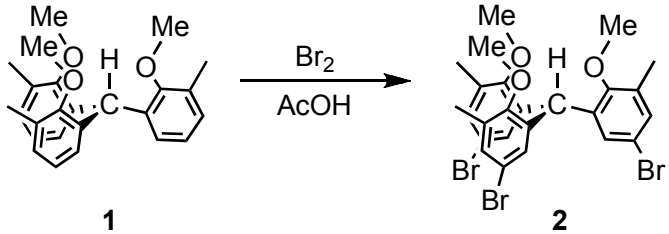


1

To the solution of tris(2-methoxy-3-methylphenyl)methanol (23.5 g, 59.8 mmol) in AcOH (750 mL) was added triethylsilane (13.0 mL, 81.4 mmol) and the mixture was stirred 80 ºC for overnight. After cooling to room temperature, the solution was neutralized with aq. NaOH. The solution was extracted with $CHCl_3$ and the organic layer was dried with $MgSO_4$. After filtration and evaporation, the crude product was purified by reprecipitation with $CHCl_3$-MeOH affording triarylmethane **1** as white solid; yield 19.1 g (85%).

1 : mp 138-139 ºC; ^{1}H NMR ($CDCl_3$, 500 MHz, r.t.) δ 2.28 (s, 9H), 3.58 (s, 9H), 6.54 (s, 1H), 6.68 (brd, 3H, J = 6.5 Hz), 6.88(t, 3H, J = 6.5 Hz), 7.04 (brd, 3H, J = 6.5 Hz); ^{13}C NMR ($CDCl_3$, 126 MHz, r.t.) δ 16.3 (q), 37.7 (d), 59.9 (q), 123.4 (d), 128.1 (d), 129.7 (d), 130.9 (s), 137.2 (s), 156.4 (s); Anal. Calcd for $C_{25}H_{28}O_3$: C, 79.75; H, 7.50, Found C, 79.53; H, 7.66.

Synthesis of Tris(3-bromo-6-methoxy-5-methylphenyl)methane **2**

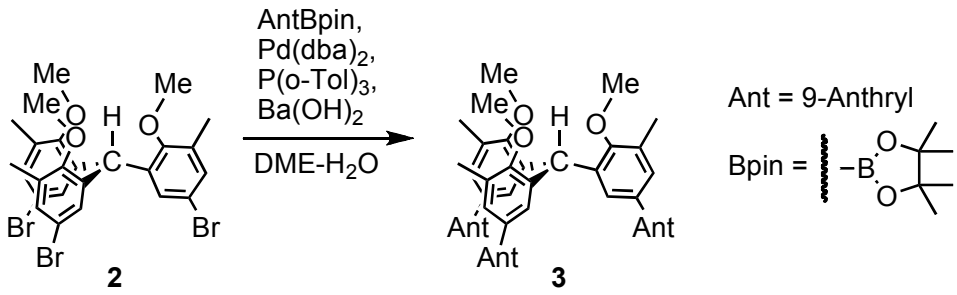


1 **2**

To the solution of **1** (4.00 g, 10.6 mmol) in AcOH (300 mL) was added bromine (3.2 mL, 63 mmol) in AcOH (50 mL) dropwise in the ice-water bath. After stirring at room temperature overnight, the reaction mixture was quenched with saturated aq. Na_2SO_3 and neutralized with saturated aq. NaOH. Then the solution was extracted with $CHCl_3$ and the organic layer was dried with $MgSO_4$. After filtration and evaporation, the crude product was purified by reprecipitation with $CHCl_3$-MeOH and pure **2** was obtained as white solid; yield 4.97 g (76%).

2; mp 212-213 ºC; ^{1}H NMR($CDCl_3$, 500 MHz, r.t.) δ 2.26 (s, 9H), 3.54 (s, 9H), 6.38 (s, 1H), 6.73 (d, 3H, J = 1.9 Hz), 7.23 (d, 3H, J = 1.9 Hz); ^{13}C NMR($CDCl_3$, 126 MHz, r.t.) δ 16.2 (q), 37.8 (d), 60.0 (q), 116.7 (s), 130.2 (d), 133.2 (d), 133.6 (s), 138.1 (s), 155.41 (s); Anal. Calcd for $C_{25}H_{25}Br_3O_3$: C, 48.97; H, 4.11, Found C, 48.77; H, 4.14.

Synthesis of Tris[3-(9-trianthryl)-6-methoxy-5-methylphenyl]methane **3**



2-Anthracen-9-yl-4,4,5,5-tetramethyl-[1,3,2]-dioxaborolane was prepared from 9-anthraceneylboronic acid and pinacol, and used without further purification. To the mixture of **2** (3.02 g, 4.93 mmol), 2-anthracen-9-yl-4,4,5,5,-tetramethyl-[1,3,2]-dioxaborolane (8.45 g, 22.4 mmol), and $Ba(OH)_2 \cdot 8H_2O$ (9.32 g, 29.5 mmol) in DME(180 mL) and H_2O (30 mL) which was bubbled with nitrogen gas, $Pd(dba)_2$ (566 mg, 0.984 mmol) and P(*o*-Tol)$_3$ (463 mg, 1.52 mmol) was added under argon. After heated at 85 ºC for 2 days and the reaction was quenched with water, the solution was extracted with $CHCl_3$. The organic layer was washed with water and brine, and then dried over $MgSO_4$. After filtration and evaporation, the crude product was subjected to column chromatography on silica gel with $CHCl_3$-hexane (2:1) to separate anthracene. Then **3** was further purified by reprecipitation with $CHCl_3$-hexane, affording **3** as pale yellow solid; yield 3.49g (78%).

3 : mp 172-173 ºC; ^{1}H NMR($CDCl_3$, 500 MHz, r.t.) δ 2.37 (s, 9H), 3.87 (s, 9H), 6.31 (br, 6H), 7.02-7.03 (m, 6H), 7.05 (s, 1H), 7.18-7.21 (m, 6H), 7.29-7.30 (m, 6H), 7.90-7.92 (m, 6H), 8.37 (s, 3H); ^{13}C NMR($CDCl_3$,126 MHz, r.t.) δ16.5 (q), 37.7 (d), 60.3 (q), 124.8 (d), 125.0 (d), 126.1 (d), 126.5 (d), 127.9 (d), 129.9 (s), 131.1 (s), 131.2 (s), 131.4 (d), 132.8 (d), 133.4 (s), 136.7 (s), 137.1 (s), 155.8 (s); Anal. Calcd. for $C_{67}H_{52}O_3$. C, 88.91; H, 5.79, Found C, 88.74; H, 5.93.