Supporting Information

for

Scalable synthesis of 5,11-diethynylated indeno[1,2-*b*]fluorene-6,12-diones and exploration of their solid state packing

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Experimental procedures, computational details and xyz coordinates, X-ray information including CCDC numbers and copies of ¹H and ¹³C NMR spectra

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Experimental details

General methods. ¹H and ¹³C NMR spectra were recorded on a Bruker Avance III HD 600 with Prodigy BBO multinuclear Cryoprobe (¹H: 599.98 MHz, ¹³C: 150.88 MHz) or Varian Mercury 300 MHz (¹H: 300.09 MHz). Chemical shifts are reported in parts per million (ppm) relative to tetramethylsilane, which was referenced according to trace amounts of non-deuterated chloroform (7.26 ppm) or dimethylsulfoxide (2.5 ppm) for ¹H and CDCl₃ (77.23 ppm) and DMSO-*d*₆ (39.51 ppm) for ¹³C. Absorption spectra were recorded on HP 8453 UV–vis spectrometer. Glassware was dried in an oven at 100 °C and cooled under a stream of inert gas before use. Dry THF was distilled from potassium metal using benzophenone as an indicator under a nitrogen atmosphere. Sorbent Technologies silica G TLC plate w/UV254 aluminum backed, 200µm was used for TLC. Chromatography was performed using silica gel, tech grade, 60 Å, 230-400 mesh from Sigma-Aldrich. All commercial reagents were used as received unless otherwise noted. 5,11-Diiodoindeno[1,2-b]fluorene-6,12-dione (**2**),¹ (triisobutylsilyl)acetylene,² and (triphenylsilyl)acetylene³ were prepared according to literature procedures.



2,5-Dibromo-3,6-diiodo-*p*-xylene (12). 2,5-Dibromo-*p*-xylene (10 g, 37.9 mmol), $K_2S_2O_8$ (33.8 g, 125 mmol) and I_2 (31.7 g, 125 mmol) in CH_2Cl_2 (380 mL) were cooled in an ice bath and then a mixture of TFA (151 mL) and H_2SO_4 (6.8 mL) was added slowly. The reaction flaks was covered with Al foil and stirred at 60 °C. After 1 d an aliquot from the reaction was analyzed and if not complete, additional I_2 (6 g) and $K_2S_2O_8$ (6 g) were added. When complete the reaction was quenched by slowly pouring into cold H_2O (ca. 500 mL). The reaction was washed with H_2O several times and then the organic layer was reduced to half volume in vacuo. The resultant colored solid was collected and washed with acetone to yield **12** (9.77 g, 18.9 mmol,

50%) as a white solid. ¹H NMR (300 MHz, CDCl₃) δ 3.03 (s, 6H); ¹³C NMR (151 MHz, CDCl₃): δ 142.45, 131.02, 110.63, 37.61; HRMS (TOF MS ESI+) [M]⁺ calcd for C₈H₆Br₂I₂⁺ 513.6926; found 513.6906.



2,5-Dibromo-3,6-dimethyl-*p***-terphenyl (14)**. A flask was charged with diiodide **12** (3.68 g, 7.14 mmol), phenylboronic acid (2.61 g, 21.4 mmol), K₃PO₄ (5.61 g, 29 mmol) and Pd(dppf)Cl₂•CH₂Cl₂ (0.11 g, 0.14 mmol). Another flask was filled with dioxane (100 mL) and H₂O (27 mL). Both flasks were purged with N₂ or Ar for 45 min. The solvent was then transferred via cannula to the reaction flask and the mixture heated to 60 °C overnight. When complete, the cooled reaction was extracted with Et₂O and washed with H₂O, 10% HCl solution, H₂O and then dried over MgSO₄. The solvent was removed under reduced pressure and the white solid was used as collected (2.71 g, 6.52 mmol, 91%). Analytically pure crystals of **14** were obtained by recrystallization from Et₂O. ¹H NMR (600 MHz, CDCl₃) δ 7.47-7.52 (m, 4H), 7.40-7.44 (m, 2H), 7.20 (m, 4H), 2.20 (s, 6H); ¹³C NMR (151 MHz, CDCl₃): δ 143.34, 142.56, 135.73, 129.19, 128.71, 127.70, 126.80, 23.49; HRMS (TOF MS ESI+) [M]⁺ calcd for C₂₀H₁₇Br₂⁺ 414.9697; found 414.9704.



2,5-Dibromo-3,6-diphenylterephthalic acid (**15**). *p*-Terphenyl **14** (2.51 g, 6 mmol), KMnO₄ (12 g, 76 mmol), pyridine (150 mL) and H₂O (20 mL) were added to a flask equipped with a mechanical stirrer and condenser. The reaction was heated to reflux and four additional portions of KMnO₄ (12 g each) were added every hour after reaching reflux. The mixture was refluxed overnight until the purple color of KMnO₄ was no longer visible. After cooling, the solid salts were collected by filtration and washed with of boiling 10% KOH solution. The combined solutions were then reduced to approximately half volume. After cooling to rt, the resulting solution was acidified carefully with conc. HCl and then cooled on ice. The precipitate was collected, washed with H₂O (ca. 100 mL) and dried overnight at 70 °C to give **15** (2.38 g, 5.0 mmol, 83%) as a white solid. Analytically pure samples were obtained by recrystallization from EtOH. ¹H NMR (600 MHz, DMSO-*d*₆) δ 13.62 (br s, 2H), 7.42-7.50 (m, 6H), 7.29-7.32 (m, 4H); ¹³C NMR (151 MHz, DMSO-*d*₆): δ 166.73, 139.82, 139.39, 137.38, 129.39, 128.57, 128.15, 118.81; HRMS (TOF MS ESI+) [M]⁺ calcd for C₂₀H₁₂Br₂O₄⁺ 473.9103; found 473.9093.



5,11-Dibromoindeno[**1,2-***b*]**fluorene-6,12-dione** (**11**). Terephthalic acid **15** (1.97 g, 4.13 mmol) was slowly added to stirred conc. H₂SO₄ (130 mL) which resulted in a rapid color changed to opaque dark brown. After stirring at rt for 16 h, the reaction mixture was poured slowly onto ice (ca. 400 g). The precipitate was collected and washed sequentially with H₂O, satd NaHCO₃ solution, H₂O, and then acetone. The solid was dried overnight at 70 °C to yield **11** (1.36 g, 3.08 mmol, 75%) as a bright orange solid. ¹H NMR (600 MHz, CDCl₃) δ 8.67 (d, *J* = 7.7 Hz, 2H), 7.77 (d, *J* =7.2 Hz, 2H), 7.62 (dt, *J* = 7.6, 1.3 Hz, 2H), 7.44 (t, *J* = 7.5 Hz, 2H); ¹³C NMR (151 MHz, CDCl₃): δ 189.92, 147.02, 141.38, 137.30, 135.42, 134.22, 130.49, 124.95, 124.78, 115.14; HRMS (TOF MS ESI+) [M]⁺ calcd for C₂₀H₈Br₂O₂⁺ 437.8891; found 437.8871.



Cross-coupling with 5,11-diiodoindeno[1,2-*b***]fluorene-6,12-dione. A mixture of dione 9** (0.100 g, 0.187 mmol), Pd(PPh₃)₄ (0.025 g, 0.022 mmol) and CuI (0.002 g, 0.011 mmol) in THF (30 mL) and iPr_2NH (30 mL) was degassed with Ar for 45 min. The appropriate ethynylsilane (0.748 mmol) was then added via syringe if it was a liquid. Alternatively, solid triphenylsilylacetylene was dissolved in THF (6 mL), degassed by Ar bubbling for 30 min and then transferred via cannula under inert atmosphere. The reaction mixture was then heated to 55-60 °C and monitored via NMR until complete, typically 24-48 h. After removal of the solvent, the residue was purified as indicated to give product **8** as an orange solid. The spectral data for **8a-b,d-f,i** are given in reference 7.

Cross-coupling with 5,11-Dibromoindeno[1,2-*b***]fluorene-6,12-dione**. A pressure reaction vessel charged with dione **11** (0.73 g, 1.6 mmol), CuI (0.02 g, 0.08 mmol), Pd(PPh₃)₂Cl₂ (0.120 g, 0.17 mmol) in Et₃N (15 mL) and THF (10 mL) was degassed with by evacuating and backfilling the reaction vessel with Ar (3x). The appropriate ethynylsilane (8.3 mmol) was added and the sealed flask was stirred at 100 °C for 36 h. After cooling to rt, the solvent was removed in vacuo and the residue was purified by column chromatography on silica (see below for eluent conditions) to give product **8** as an orange solid. Analytical samples were obtained using a recycling HPLC with polystyrene beads eluting with CHCl₃.

8b (SiEt₃). 4:1 hexanes/CH₂Cl₂; 27% yield. NMR data matched those in reference 7.

8c (SiPr₃). 4:1 hexanes/CH₂Cl₂; 72% yield. ¹H NMR (600 MHz, CDCl₃) δ 8.59 (d, *J* = 7.6 Hz, 2H), 7.72 (d, *J* = 7.3 Hz, 2H), 7.51 (td, *J* = 7.5, 1.3 Hz, 2H), 7.39 (t, *J* = 7.4 Hz, 2H), 1.61

(m, 12H), 1.07 (t, J = 7.3 Hz, 18H), 0.86 (m, 12H); ¹³C NMR (151 MHz, CDCl₃): δ 190.42, 146.63, 142.34, 138.60, 134.71, 134.11, 129.91, 124.31, 123.66, 114.24, 108.45, 99.98, 18.58, 17.80, 16.09; UV/Vis (CHCl₃) λ_{max} 312, 332, 524 nm ; HRMS (TOF MS ESI+) for C₄₂H₅₁O₂Si₂⁺ [M⁺+H]: calcd 643.3428; found 643.3397.

8d (Si(iPr)₃). 9:1 hexanes/CH₂Cl₂; 48% yield. NMR data matched those listed above.

8g (SiMe₂(CH₂)₂CF₃). 4:1 hexanes/CH₂Cl₂ increasing polarity to 7:3 hexanes/CH₂Cl₂; 30% yield. ¹H NMR (600 MHz, CDCl₃) δ 8.45 (d, *J* = 7.6 Hz, 2H), 7.72 (d, *J* = 7.7 Hz, 2H), 7.54 (dt, *J* = 7.6, 1.2 Hz, 2H), 7.40 (dt, *J* = 7.5, 0.8 Hz, 2H), 2.39 (m, 4H), 1.08 (m, 4H), 0.45 (s, 12H); ¹³C NMR (151 MHz, CDCl₃): δ 190.28, 146.65, 142.08, 138.75, 135.06, 134.06, 130.25, 124.51, 123.39, 113.87, 106.74, 100.35, 29.0 (q, *J* = 30.1 Hz), 8.16 (q, *J* = 2.2 Hz), -2.06, -3.63; UV/Vis (CHCl₃) λ_{max} 308, 330, 516 nm; HRMS (TOF MS ESI+) for C₃₄H₂₉O₂F₆Si₂⁺ [M⁺+H]: calcd 639.1610; found 639.1606.

8h (SiMe₂iBu). 4:1 hexanes/CH₂Cl₂; 35% yield. ¹H NMR (600 MHz, CDCl₃) δ 8.54 (d, J = 7.7 Hz, 2H), 7.71 (d, J = 7.2 Hz, 2H), 7.53 (dt, J = 7.6, 1.3 HZ, 2H), 7.37 (dt, J = 7.4, 1.0 Hz, 2H), 2.03 (n, J = 6.7 Hz 2H), 1.08 (d, J = 6.6 Hz, 12H), 0.88 (d, J = 6.6 Hz, 4H), 0.43 (s, 12H); ¹³C NMR (151 MHz, CDCl₃): δ 190.51, 146.61, 142.29, 138.57, 134.86, 134.08, 129.96, 124.28, 123.62, 114.23, 109.54, 99.43, 26.64, 26.43, 25.36, 0.76; UV/Vis (CHCl₃) λ_{max} 311, 331, 523 nm; HRMS (TOF MS ESI+) for C₃₆H₃₉O₂Si₂⁺ [M⁺+H]: calcd 559.2489; found 559.2502.

8j (SiMe₂Ph). 4:1 hexanes/CH₂Cl₂; 24% yield. ¹H NMR (600 MHz, CDCl₃) δ 8.37 (m, 2H), 7.82 (m, 4H), 7.70 (m, 2H), 7.45 (m, 6H), 7.34 (m, 4H), 0.68 (s, 12H); ¹³C NMR (151 MHz, CDCl₃): δ 190.50, 146.82, 138.64, 136.06, 135.03, 134.20, 134.02, 130.01, 129.98, 128.34, 124.30, 123.73, 114.09, 107.53, 100.34, 10.7; UV/Vis (CHCl₃) λ_{max} 310, 331, 521 nm; HRMS (TOF MS ESI+) [M]⁺ for C₄₀H₃₁O₂Si₂⁺: calcd 599.1863; found 599.1870.

Electronic Absorption Spectra



Figure S1: Electronic absorption spectra of diones 8c, 8g, 8h and 8j.

Electrochemical details

All electrochemical experiments were conducted in a traditional 3-electrode geometry using a Solartron 1287 potentiostat. Electrolyte solutions (0.1 M) were prepared from HPLC-grade CH₂Cl₂ and anhydrous Bu₄NBF₄, and the solutions were freeze-pump-thaw degassed (3x) prior to analysis. Cyclic voltammetry was conducted under a nitrogen atmosphere. The working electrode was a glassy carbon electrode (3-mm diameter), with a Pt-coil counter electrode and Ag wire pseudo reference. The ferrocene/ferrocenium (Fc/Fc^{+}) couple was used as an internal standard following each experiment. Potential values were re-referenced to SCE using a value of 0.46 (V vs. SCE) for the Fc/Fc⁺ couple in CH₂Cl₂. When necessary, potentials were rereferenced to NHE using SCE = -0.24 (V vs. NHE). LUMO energy levels were approximated using SCE = -4.68 eV vs. vacuum.⁴ Cyclic voltammetry experiments were conducted at sweep rates of 50 (reported), 75, 100 and 125 mV s⁻¹. All scan rates show quasi-reversible kinetics with no alteration of peak splitting with scan rate. E_{1.2} values were calculated assuming $E_{1/2} \approx$ $E^{\circ} = (E_{anodic} + E_{cathodic})/2$ based on these observations. The $E_{a,c}$ peak splitting of the Fc/Fc⁺ couple was similar to that of the analyte (~100 mV). The anodic peak current increases linearly with the square root of the scan rate in the range 50 to 125 mV s^{-1} , indicating a diffusion-controlled process. Analyte concentrations were ca. 5-7 mM.



Figure S2: Cyclic voltammogtrams of 8c, 8g, 8h and 8j.

X-ray crystallography

Diffraction intensities for **8b**, **8e**, **8i**; **8c**, **8h** and **8g**, **8j** were collected at 173(2); 193(2) and 100(2) K, respectively, on a Bruker Apex2 CCD diffractometer using MoK α radiation $\lambda = 0.71073$ Å. Space groups were determined based on systematic absences (**8b**, **8e**, **8i**; **8g**, **8h**) and intensity statistics (**8c** and **8j**). Absorption corrections were applied by SADABS.⁵ Structures were solved by direct methods and Fourier techniques and refined on F^2 using full matrix least-squares procedures. All non-H atoms were refined with anisotropic thermal parameters. All H atoms in **8b**, **8e** and **8i** were found from the residual density map and refined with isotropic thermal parameters. H atoms in **8c**, **8g**, **8h** and **8j** were refined in calculated positions in a rigid group model. All calculations were performed by the Bruker SHELXTL (v. 6.10) package.⁶ These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif. The x-ray data for **8a** (CCDC 841548), **8d** (CCDC 787155) and **8f** (CCDC 841549) were reported in the original communication.⁷

Crystallographic data for **8b**: $C_{36}H_{38}O_2Si_2$, M = 558.84, 0.35 x 0.11 x 0.12 mm, T = 173(2) K, Monoclinic, space group $P2_1/c$, a = 17.3760(18) Å, b = 6.4393(7) Å, c = 15.6311(16) Å, $\beta = 116.306(2)^\circ$, V = 1567.8(3) Å³, Z = 2, $D_c = 1.184$ Mg/m³, $\mu = 0.143$ mm⁻¹, F(000) = 596, $2\theta_{max} = 54.00^\circ$, 12383 reflections, 3420 independent reflections [R_{int} = 0.0211], R1 = 0.0401, wR2 = 0.1106 and GOF = 1.034 for 3420 reflections (257 parameters) with I>2 σ (I), R1 = 0.0460, wR2 = 0.1169 and GOF = 1.034 for all reflections, max/min residual electron density +0.398/-0.214 eÅ⁻³. CCDC 1011434.

Crystallographic data for **8c**: $C_{42}H_{50}O_2Si_2$, M = 643.00, 0.46 x 0.24 x 0.03 mm, T = 193(2) K, Triclinic, space group *P*-1, *a* = 8.7419(11) Å, *b* = 12.1839(16) Å, *c* = 18.359(2) Å, *a* = 106.489(2)°, β = 92.556(2)°, γ = 94.239(2)°, *V* = 1865.5(4) Å³, *Z* = 2, *D*_c = 1.145 Mg/m³, μ = 0.129 mm⁻¹, *F*(000) = 692, $2\theta_{max}$ = 50.00°, 17919 reflections, 6560 independent reflections [R_{int} = 0.0345], R1 = 0.0682, wR2 = 0.1686 and GOF = 1.055 for 6560 reflections (411 parameters) with I>2 σ (I), R1 = 0.1071, wR2 = 0.2015 and GOF = 1.058 for all reflections, max/min residual electron density +0.697/-0.285 eÅ⁻³. CCDC 1011438.

Crystallographic data for **8e**: C₄₈H₆₂O₂Si₂, M = 727.16, 0.45 x 0.07 x 0.05 mm, T = 173(2) K, Monoclinic, space group $P2_1/n$, a = 6.1344(6) Å, b = 17.3347(17) Å, c = 20.190(2) Å, $\beta = 90.915(2)^{\circ}$, V = 2146.7(4) Å³, Z = 2, $D_c = 1.125$ Mg/m³, $\mu = 0.119$ mm⁻¹, F(000) = 788, $2\theta_{max} = 50.0^{\circ}$, 13428 reflections, 3784 independent reflections [R_{int} = 0.0513], R1 = 0.0462, wR2 = 0.1035 and GOF = 1.011 for 37845 reflections (359 parameters) with I>2 σ (I), R1 = 0.0723, wR2 = 0.1185 and GOF = 1.011 for all reflections, max/min residual electron density +0.315/-0.281 eÅ⁻³. CCDC 1011435.

Crystallographic data for **8g**: $C_{34}H_{28}F_6O_3Si_2$, M = 638.74, 0.14 x 0.12 x 0.09 mm, T = 100(2) K, Orthorhombic, space group *Pca2*₁, *a* = 15.7713(9) Å, *b* = 6.0958(4) Å, *c* = 32.7766(19) Å, *V* = 3151.1(3) Å³, *Z* = 4, *D*_c = 1.346 Mg/m³, μ = 0.178 mm⁻¹, *F*(000) = 1320, 2 θ_{max} = 56.00°, 15175 reflections, 7303 independent reflections [R_{int} = 0.0253], R1 = 0.0452, wR2 = 0.1040 and GOF = 1.059 for 7303 reflections (397 parameters) with I>2 σ (I), R1 = 0.0558, wR2 = 0.1088 and GOF = 1.059 for all reflections, the Flack = 0.03(11), max/min residual electron density +0.420/- 0.321 eÅ⁻³. CCDC 1011439.

Crystallographic data for **8h**: C₃₆H₃₈O₂Si₂, M = 558.84, 0.35 x 0.07 x 0.05 mm, T = 193(2) K, Monoclinic, space group $P2_1/c$, a = 16.489(6) Å, b = 5.976(2) Å, c = 16.259(5) Å, V = 1579.3(9) Å³, Z = 2, $D_c = 1.175$ Mg/m³, $\mu = 0.142$ mm⁻¹, F(000) = 596, $2\theta_{max} = 50.00^{\circ}$, 13905 reflections, 2775 independent reflections [R_{int} = 0.0697], R1 = 0.0568, wR2 = 0.1409 and GOF = 1.056 for 2775 reflections (181 parameters) with I>2 σ (I), R1 = 0.0919, wR2 = 0.1690 and GOF = 1.056 for all reflections, max/min residual electron density +0.307/-0.315 eÅ⁻³. CCDC 1011437.

Crystallographic data for **8i**: $C_{36}H_{38}O_2Si_2$, M = 558.84, 0.42 x 0.20 x 0.03 mm, T = 173(2) K, Monoclinic, space group $P2_1/c$, a = 16.742(4) Å, b = 6.3559(14) Å, c = 15.144(3) Å, $\beta = 100.795(4)^\circ$, V = 1582.9(6) Å³, Z = 2, $D_c = 1.173$ Mg/m³, $\mu = 0.142$ mm⁻¹, F(000) = 596, $2\theta_{max} = 100.795(4)^\circ$, V = 1582.9(6) Å³, Z = 2, $D_c = 1.173$ Mg/m³, $\mu = 0.142$ mm⁻¹, F(000) = 596, $2\theta_{max} = 100.795(4)^\circ$, V = 1582.9(6) Å³, Z = 2, $D_c = 1.173$ Mg/m³, $\mu = 0.142$ mm⁻¹, F(000) = 596, $2\theta_{max} = 0.142$ mm⁻¹, P(000) = 506, $2\theta_{max} = 0.142$ mm⁻¹, P(000) = 0.142 mm⁻¹, P(00) = 0.142 mm⁻¹ 54.00°, 14104 reflections, 3449 independent reflections [$R_{int} = 0.0386$], R1 = 0.0460, wR2 = 0.1169 and GOF = 1.097 for 3449 reflections (257 parameters) with I>2 σ (I), R1 = 0.0632, wR2 = 0.1371 and GOF = 1.097 for all reflections, max/min residual electron density +0.420/-0.278 eÅ⁻³. CCDC 1011436.

Crystallographic data for **8j**: $C_{40}H_{30}O_2Si_2$, M = 598.82, 0.32 x 0.12 x 0.04 mm, T = 100(2) K, Triclinic, space group *P*-1, *a* = 6.2923(12) Å, *b* = 15.615(3) Å, *c* = 16.303(3) Å, *α* = 103.724(2)°, *β* = 90.601(3)°, *γ* = 93.428(2)°, *V* = 1552.9(5) Å³, *Z* = 2, *D*_c = 1.281 Mg/m³, *μ* = 0.150 mm⁻¹, *F*(000) = 628, 2 θ_{max} = 50.00°, 18419 reflections, 5434 independent reflections [R_{int} = 0.0503], R1 = 0.0399, wR2 = 0.0891 and GOF = 1.014 for 5434 reflections (397 parameters) with I>2σ(I), R1 = 0.0632, wR2 = 0.0993 and GOF = 1.014 for all reflections, max/min residual electron density +0.281/-0.295 eÅ⁻³. CCDC 1011440.

Computational details

Calculations were performed in Gaussian 09^8 and results were visualized in Gaussview 5.⁹ All minimized geometries were verified as minima using analytically obtained frequencies ensuring that all frequencies were positive. Geometries were minimized using B3LYP^{10–12} functional with the 6-31G(d) basis set. Time dependent single point energies were then carried out using B3LYP functional and 6-311+G(d,p) basis set. Energies are given in Hartrees.

Fluorenone

E(RB3LYP) = -575.437041862

Zero-point correction = 0.169993 (Hartree/Particle)

Sum of electronic and zero-point Energies = -575.267049

Atomic Number	Х	Y	Ζ
6	3.031563	-1.393089	-0.000144
6	3.468261	-0.065168	-0.000144

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6	2.539066	0.983719	-0.000091
6	1.189461	0.665408	-0.000039
6	0.742036	-0.671224	-0.000038
6	1.664659	-1.710876	-0.00009
1	3.763676	-2.196219	-0.000186
1	4.532617	0.151689	-0.000185
1	2.854581	2.023303	-0.000091
1	1.345666	-2.74975	-0.00009
6	0	1.577717	0.000021
6	-1.189461	0.665408	0.000058
6	-2.539066	0.983719	0.000116
6	-3.468261	-0.065169	0.000142
6	-3.031563	-1.393089	0.000105
6	-1.664659	-1.710876	0.000046
6	-0.742036	-0.671224	0.000023
1	-2.854581	2.023303	0.000142
1	-4.532618	0.151689	0.00019
1	-3.763676	-2.196219	0.000123
1	-1.345666	-2.74975	0.00002
8	0	2.796303	0.000036

Benzophenone

E(RB3LYP) = -576.632267849

Zero-point correction = 0.192039 (Hartree/Particle)

Sum of electronic and zero-point Energies = -576.440229

Atomic Number	Х	Y	Ζ
6	0.000014	1.080491	-0.000004
8	0.000002	2.306866	-0.000052
6	-1.303858	0.337286	0.024491
6	-1.454265	-0.925657	0.617795
6	-2.434074	0.983323	-0.502109
6	-2.708843	-1.534408	0.67056
1	-0.596683	-1.421123	1.061536
6	-3.680729	0.36645	-0.466685
1	-2.310177	1.971543	-0.933156
6	-3.820701	-0.894964	0.120505
1	-2.817285	-2.506434	1.144026
1	-4.546443	0.868969	-0.88957
1	-4.795612	-1.374137	0.154485
6	1.303909	0.337347	-0.02443

6	1.454234	-0.925562	-0.617824
6	2.434141	0.983322	0.50218
6	2.708769	-1.534394	-0.670609
1	0.596592	-1.420922	-1.061583
6	3.680761	0.366374	0.466719
1	2.310287	1.971521	0.933288
6	3.820658	-0.895025	-0.120521
1	2.817163	-2.506407	-1.144111
1	4.54651	0.868823	0.889617
1	4.795543	-1.374249	-0.154517

Dione 7a

E(RB3LYP) = -1888.30699292

Zero-point correction = 0.462882 (Hartree/Particle)

Sum of electronic and zero-point Energies = -1887.844111

Atomic Number	Х	Y	Ζ
6	1.450667	0.032662	0.001002
6	0.664894	1.202577	0.000617
6	0.742202	-1.189641	0.000258
6	-0.664898	-1.202551	-0.000627
6	-1.450671	-0.032634	-0.001011
6	-0.742206	1.189668	-0.00027
6	1.130061	2.636739	0.00074
6	-1.234289	2.590735	-0.000334
6	-1.130065	-2.636713	-0.000742
8	-2.274835	-3.051807	-0.001258
8	2.274831	3.051832	0.001262
6	0.119251	-3.451679	-0.000121
6	1.234286	-2.590708	0.000319
6	-0.119255	3.451706	0.000116
6	2.518612	-3.128163	0.000464
1	3.392674	-2.488402	0.000495
6	2.657095	-4.524854	0.000355
1	3.655101	-4.955142	0.000374
6	-2.518616	3.12819	-0.000494
1	-3.392677	2.488429	-0.00054
6	-2.657099	4.52488	-0.000383
1	-3.655105	4.955169	-0.000412
6	-1.545073	5.370916	-0.000113
1	-1.685127	6.44813	-0.000034

6	1.545069	-5.370889	0.000099
1	1.685123	-6.448103	0.000021
6	0.252422	-4.83124	-0.000191
1	-0.630932	-5.46355	-0.000521
6	-0.252426	4.831267	0.000188
1	0.630928	5.463577	0.000526
6	-2.871701	-0.103024	-0.001918
6	2.871697	0.103048	0.001915
6	4.089686	0.189218	0.002527
6	-4.089689	-0.189205	-0.002525
14	-5.901489	-0.540714	0.000351
14	5.901495	0.540674	-0.000334
6	-6.260267	-1.701436	1.445344
1	-5.665448	-2.61764	1.363489
1	-6.018595	-1.229914	2.40459
1	-7.320318	-1.983516	1.46681
6	-6.338468	-1.36077	-1.64365
1	-7.405562	-1.613118	-1.681021
1	-6.119842	-0.701038	-2.490897
1	-5.767091	-2.285088	-1.781974
6	-6.846058	1.084896	0.202073
1	-6.576979	1.590873	1.136396
1	-6.641157	1.774037	-0.625407
1	-7.927729	0.903083	0.222316
6	6.26032	1.701408	-1.445306
1	6.018615	1.22992	-2.40456
1	5.665553	2.617644	-1.363426
1	7.320386	1.983431	-1.466776
6	6.846009	-1.084966	-0.202075
1	7.927688	-0.903194	-0.222291
1	6.641064	-1.774118	0.625384
1	6.57693	-1.590909	-1.136415
6	6.33849	1.360694	1.64368
1	5.767141	2.285029	1.78201
1	6.119836	0.70096	2.490918
1	7.405591	1.613008	1.681062

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