SUPPLEMENTARY INFORMATION

Steric Effects which Determine the Conformational Preferences and Stereodynamic Processes of Aryl Fluorenyl Ketones.

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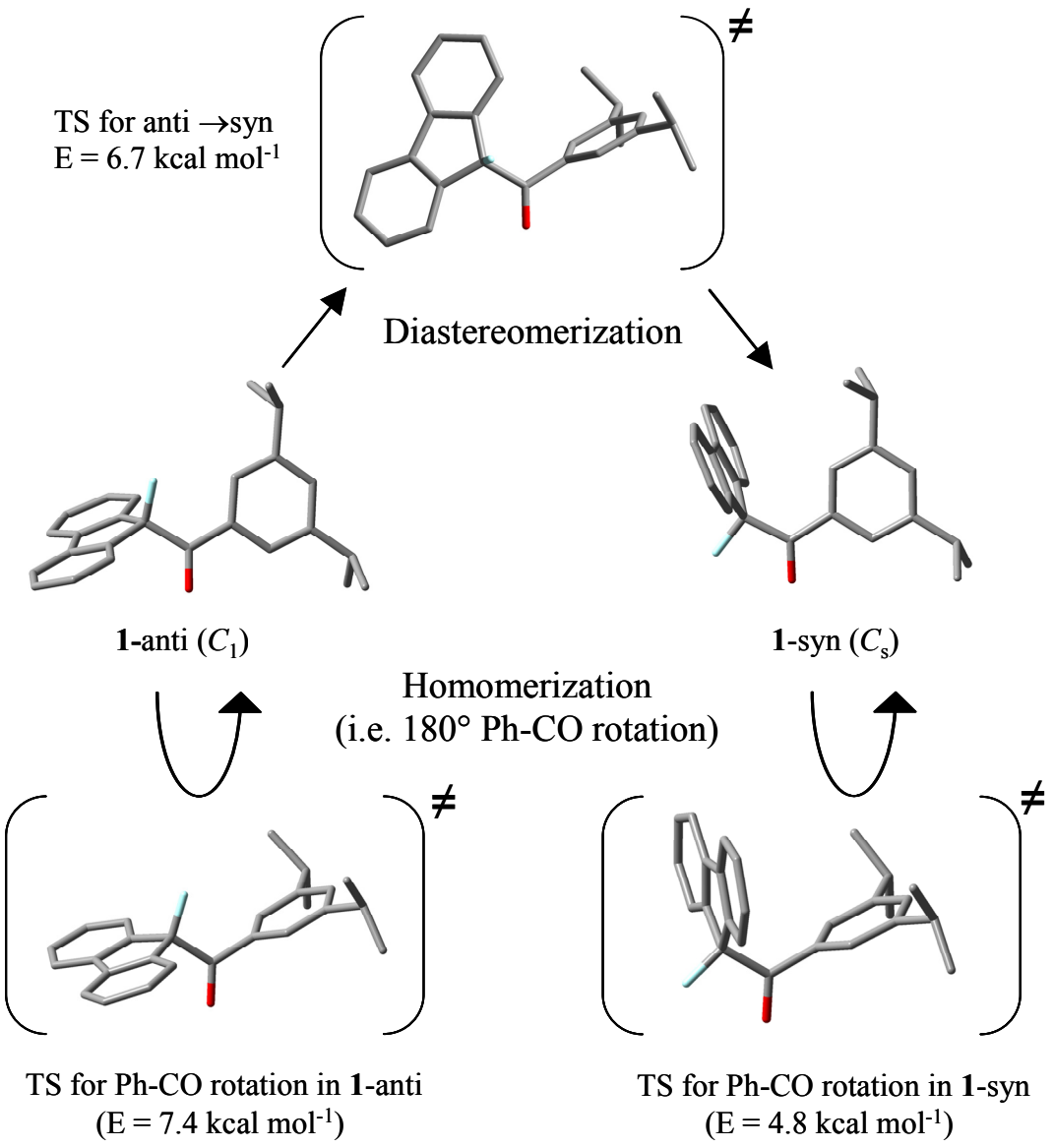


FIGURE S-1. Centre: DFT computed ground state conformations **1**-anti (C_1) and **1**-syn (C_s).Top: Calculated transition state for the anti to syn interconversion (diastereomerization). Bottom: transition states calculated for the Ph-CO bond rotation (homomerization) in **1**-anti (left) and **1**-syn (right)

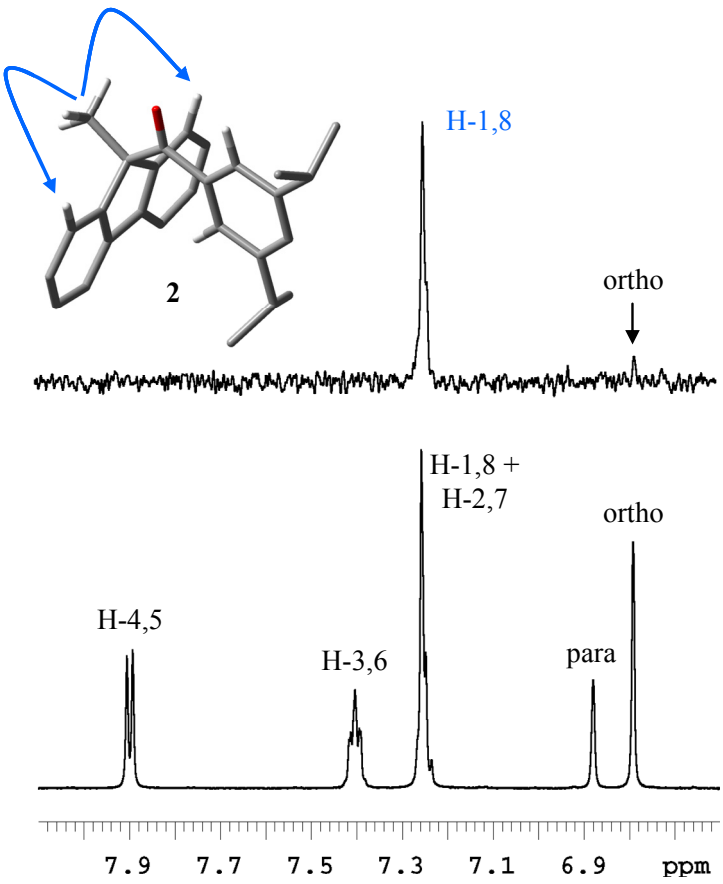


FIGURE S-2. Bottom: ^{1}H spectrum (600 MHz in CD_2Cl_2) of the aromatic region of **2** at –80 °C. Top: NOE effect observed by irradiation of the line of the methyl bonded to C-9 (1.62 ppm).

In the **2**-anti conformer the averaged computed distances [a)] are 3.08 Å (between Me-9 and H-1,8) and 2.63 Å (between Me-9 and H-ortho). In **2**-syn the same distances are 3.17 and 4.94 Å, respectively. Their ratios elevated to the 6th power are $(2.63 / 3.08)^6 = 0.39$ in **2**-anti and $(4.94 / 3.17)^6 = 14.3$ in **2**-syn. Thus the distance ratio in **2**-syn agrees with the observation of an almost negligible NOE effect for the H-ortho with respect to the H-1,8 signal, whereas the ratio in **2**-anti does not (in the latter, in fact, the NOE experienced by the H-ortho should be higher than that experienced by the H-1,8 signal). Except for those relevant to NOE analysis, all the hydrogens have been removed in the 3D structure.

[a)] determined as $\langle r^{-6} \rangle^{-1/6}$, according to: Claridge, T. D. W. *High-Resolution NMR Techniques in Organic Chemistry*, Pergamon, Oxford, 1999 p 303.

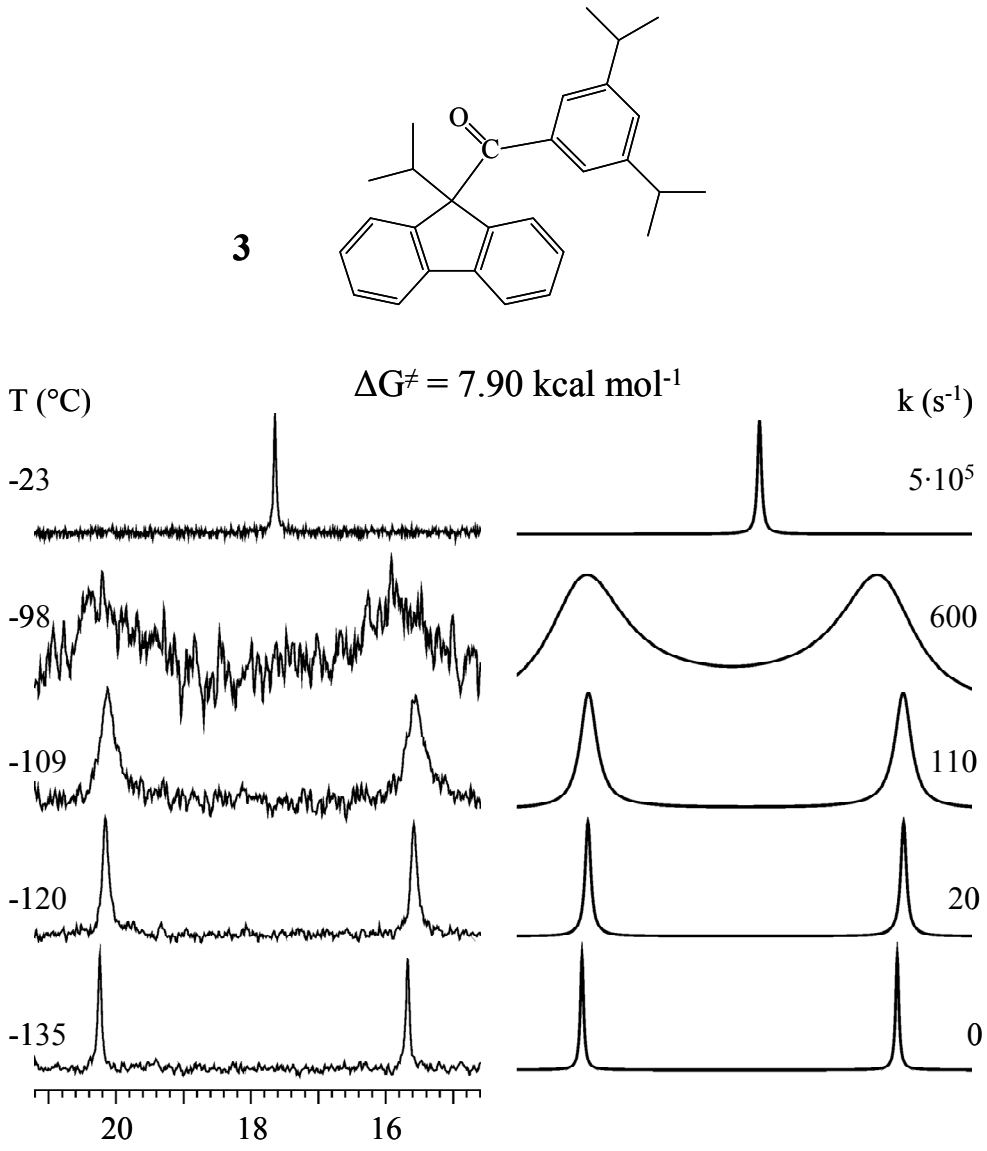


FIGURE S-3. Temperature dependence of the ^{13}C NMR (150.8 MHz in $CHF_2Cl/CHFCl_2$) methyl signal of the isopropyl bonded to C-9 of compound **3** (left). On the right the simulation obtained with the rate constants reported.

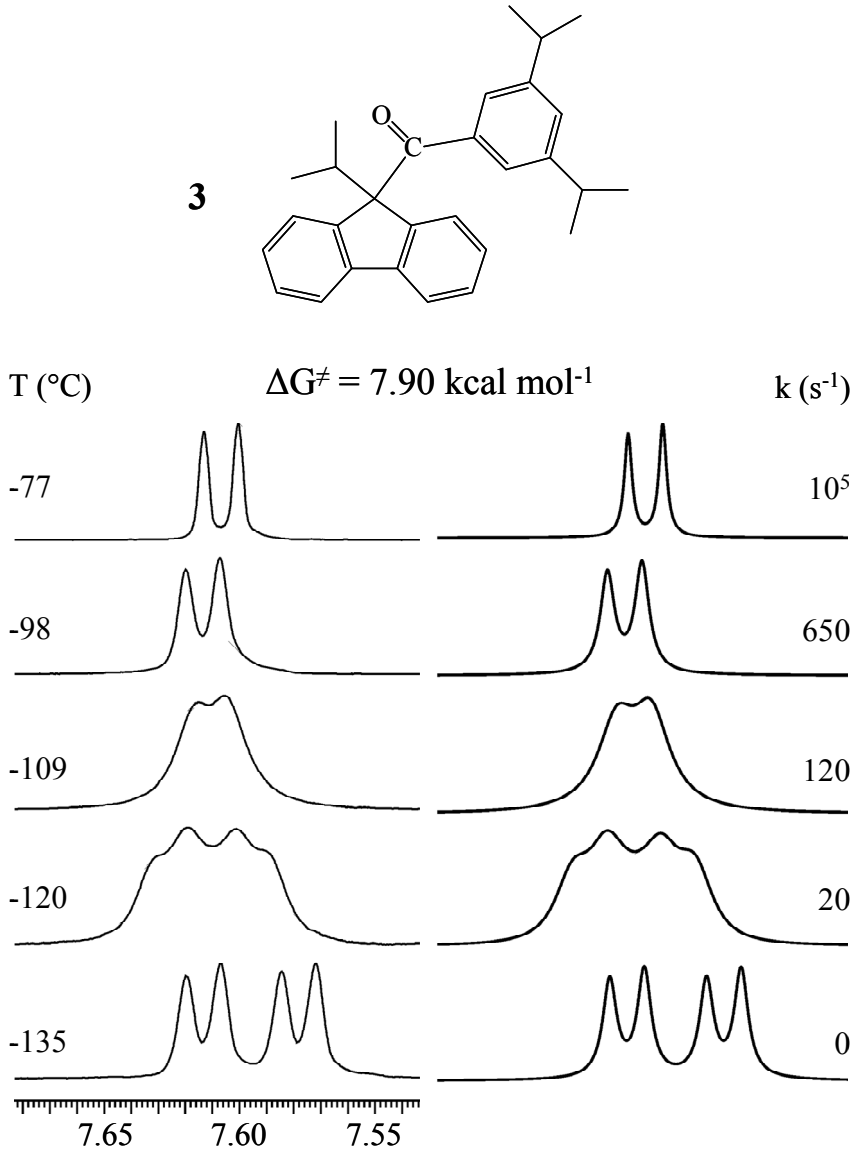


FIGURE S-4. Temperature dependence of the ^{1}H NMR (600 MHz in $CHF_2Cl/CHFCl_2$) signal of the hydrogens in position 1,8 of the fluorenyl moiety of **3** (left). On the right the simulation obtained with the rate constants reported.

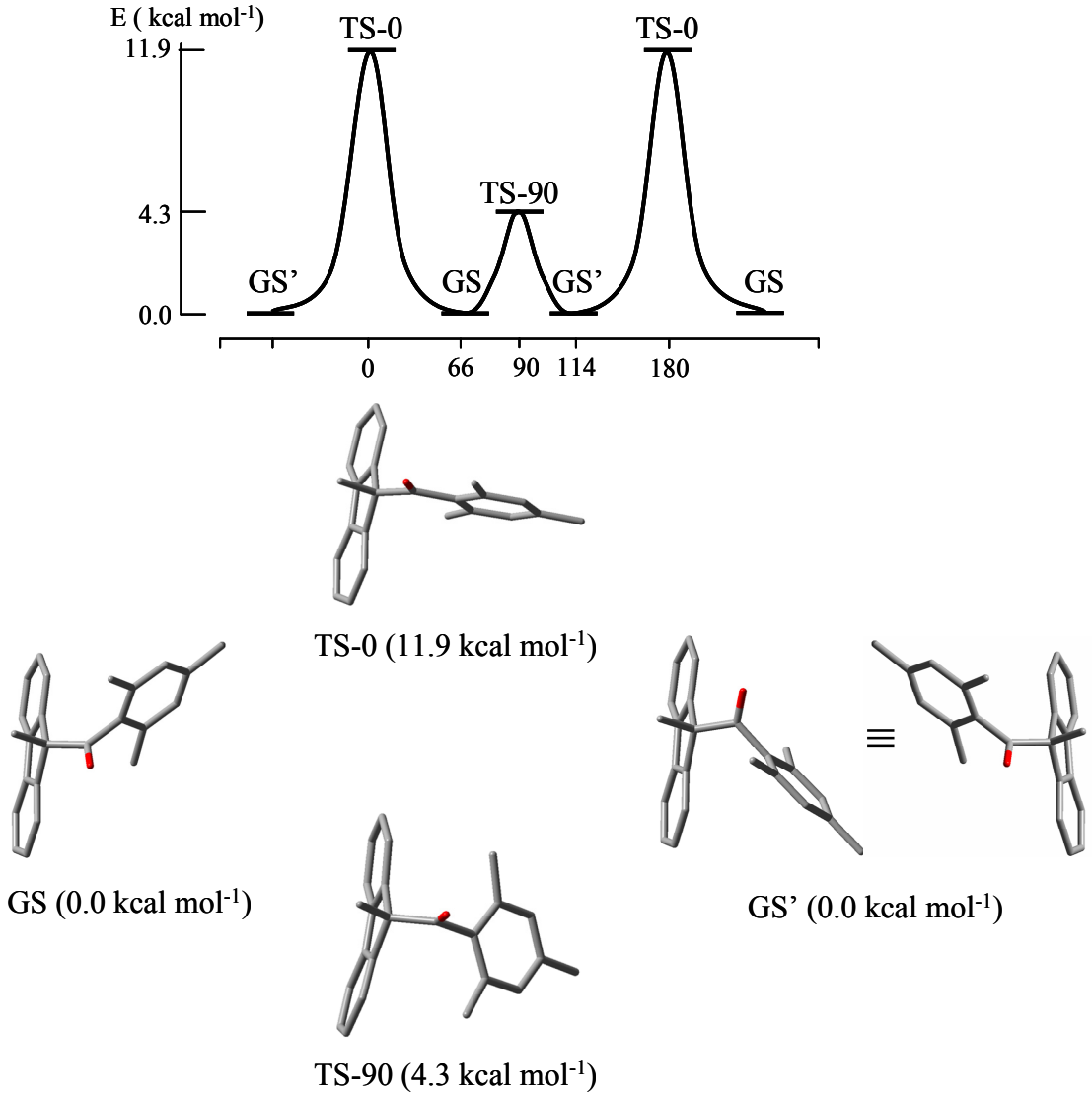


FIGURE S-5. Schematic representation of the pathway for the mesityl rotation interconverting the two enantiomers (GS and GS') of **4**; the abscissa scale represent the torsion angle between the plane of C=O and that of the mesityl ring (i.e. the dihedral angle O-C-Cq-C_{ortho}). Underneath are displayed the 3D computed structures for the enantiomeric ground states (GS and GS') and the two transition states (TS-0 and TS-90).

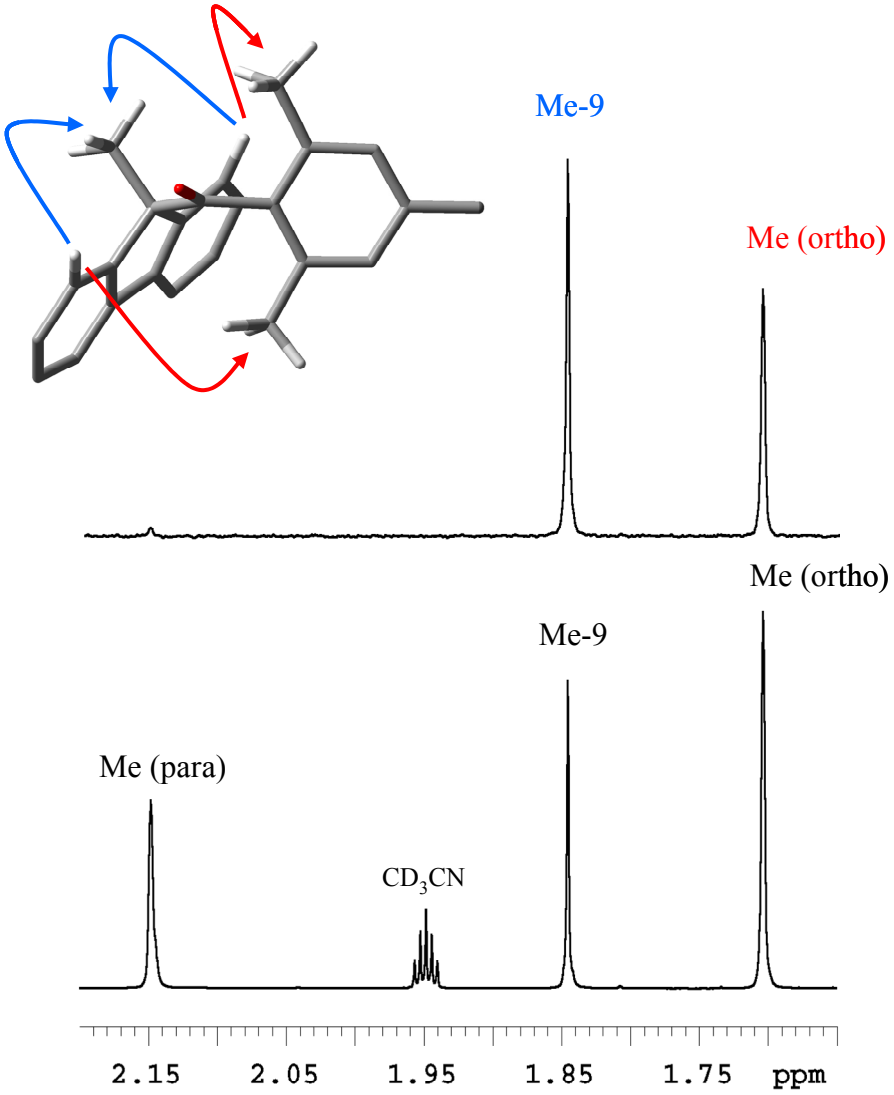
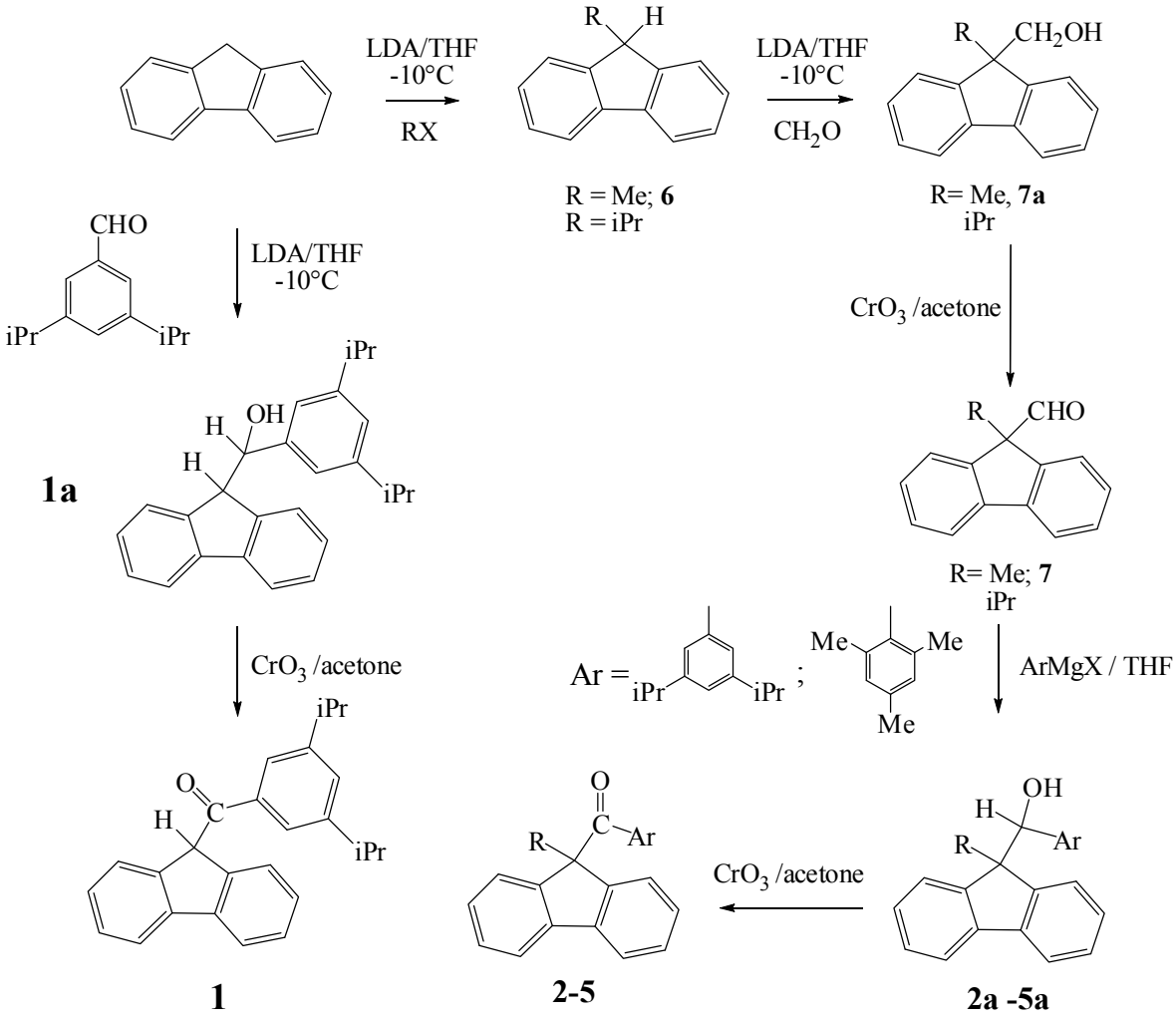


FIGURE S-6. Bottom: ^{1}H spectrum of the methyl signals of **4** (600 MHZ in CD_3CN at +25°C). Top: NOE spectrum obtained by saturation of the 1,8 hydrogens of the fluorene moiety (at 7.49 ppm).

In the syn conformation, the averaged computed distance [a)] between H-1,8 and Me-9 hydrogens is 3.17 Å, that between H-1,8 and the two ortho methyl groups is 3.94 Å. Thus the NOE experienced by Me-9 is expected to be larger than that experienced by the ortho methyls, in agreement with the experimental result (Figure S-6, top). Except for those relevant to NOE analysis, all the hydrogens have been removed in the 3D structure.

[a)] determined as $\langle r^{-6} \rangle^{-1/6}$, according to: Claridge, T. D. W. *High-Resolution NMR Techniques in Organic Chemistry*, Pergamon, Oxford, 1999 p 303.

Experimental procedures for the preparation of the intermediates.



(3,5-diisopropylphenyl)(9-H-fluoren-9-yl)methanol (1a). To a stirred solution of N,N-diisopropylammine (1.1 mL, 8mmol in 30 mL of anhydrous THF) kept at -10°C under nitrogen, 5.5 mL (8.5 mmol, 1.6M solution) of *n*-BuLi were slowly added. The mixture was allowed to react at -10°C for 30 min and then slowly transferred by a double-tipped needle into a solution of 9-fluorene (1.0 g, 6 mmol in 25 mL of anhydrous THF) kept at -15°C. The orange solution was stirred at -15°C for additional 20 min before adding in 10 min a solution of 3,5-diisopropyl benzaldehyde (10 mmol in 10 mL of dry THF).[21] The solution discharged in short time, and after 15 min of stirring at RT the reaction was quenched with 20 mL of H_2O. The extracted organic layer (Et_2O) was dried (Na_2SO_4) and evaporated. The crude was purified by a silica gel

chromatography column (petroleum ether/EtAc 90:10) to give the intermediate alchool (yield 74%) as white solid that was used in the next step. ^{1}H-NMR ($CDCl_3$, 600 MHz) δ 1.19 (6H, d, J = 6.9 Hz), 2.10 (1H, d, J =3.5 Hz), 2.85 (2H, m, J = 6.9 Hz), 4.37 (1H, d, J = 6.3 Hz), 5.03 (1H, dd, J = 6.3, 3.5 Hz), 6.94 (2H, d, J =1.7 Hz), 6.98 (1H, t, J = 1.7 Hz), 7.05 (1H, d, J = 7.5 Hz), 7.18 (1H, dt, J = 7.5, 1.1 Hz), 7.25 (1H, dt, J = 7.5, 1.1 Hz), 7.34 (1H , t. J = 7.6 Hz), 7.37(1H, t, J = 7.6 Hz), 7.45 (1H, d, J = 7.6 Hz), 7.67 (1H, d, J = 7.6 Hz), 7.69 (1H, d, J = 7.6 Hz). ^{13}C-NMR ($CDCl_3$, 150.8 MHz) δ 23.9 ($2CH_3$), 24.0 ($2CH_3$), 34.2 (2CH), 54.9 (CH), 76.9 (OCH), 119.6 (CH), 119.7 (CH), 122.3 (2CH), 124.3 (CH), 125.9 (CH), 126.3 (CH), 126.4 (CH), 126.5 (CH), 127.4 (CH), 127.5 (CH), 141.7 (2Cq), 141.8 (Cq), 143.4 (Cq), 143.9 (Cq), 148.6 (2Cq).

(3,5-Diisopropylphenyl)(9-H-fluoren-9-yl)methanone (1).

To a solution of **1a** (0.1 g, 10 mmol) in aceton, solid CrO_3 (0.4g, 10 mmol) [22] was added in small quotes under fast stirring, and the temperature was kept below 25°C. The reaction was monitored by TLC until the alcohol disappeared, then the solvent was evaporated at reduced pressure and ambient temperature. The crude was purified by a silica gel chromatography column (petroleum ether/EtAc 95:5) to give the desired product (yield 68%) as a white solid. Analytically pure samples were obtained by semipreparative HPLC on a C18 column (t_r = 14.38 min, Luna C18(2), 5 μm, 250 × 10 mm, Acetonitrile/H_2O 90:10 v:v, 5 mL/min).

(9-Methyl-fluorene-9-yl)methanol (7a)[23]: as for **1a**, a stirred solution of LDA was prepared and slowly added to fluorene (2.7 g, 16.3 mmol in 15 mL of anhydrous THF). After stirring for 20 min at -10°C a solution of methyl iodide (1 mL, 16.5 mmol in 5 mL of dry THF) was dropped in 10 min to the orange solution and the color turned in short time to pale yellow. A small quote of the mixture was purified by chromatography on silica gel to isolate 9-methyl-9H-fluorene **6** (yield 85% by GC-MS).[24] The remaining reaction mixture was cooled again to -10°C, and a solution of *n*-BuLi (11 mL, 17.5 mmol) 1.6 M in hexane was slowly added. After 15 min at -10°C, solid CH_2O (0.6 g, 20 mmol) was added in one pot to the reddish-wine solution. The reaction resulted slightly exothermic and the temperature raised slowly to +30°C, while the wine-red color turned to yellow in a short time. The reaction was the quenched with 40 mL of H_2O, and extracted with Et_2O (3 x 15 mL). The collected organic layers were dried (Na_2SO_4) and evaporated. The crude was purified by a silica gel chromatography column (petroleum ether /EtAc 90:10) to give 2.7 g of (9-methyl-fluorene-9-yl) methanol (total yield 80%) as a white solid. ^{1}H-NMR ($CDCl_3$, 600 MHz) δ 1.40 (1H, br s), 1.47 (3H, s), 3.78 (2H, s), 7.32 (2H, dt, J = 7.5, 1.1 Hz), 7.37 (2H, dt, J = 7.5, 1.1

Hz), 7.47 (2H, d, J = 7.7 Hz), 7.74 (2H, d, J = 7.7 Hz). ^{13}C-NMR ($CDCl_3$, 150.8 MHz) δ 21.0 (CH_3), 52.6 (Cq), 70.0 (OCH_2), 120.1 (2CH), 123.2 (2CH), 127.3 (2CH), 127.6 (2CH), 140.4 (2Cq), 149.3 (2Cq).

9-Methyl-fluorene-9-carboxyaldehyde (7)[25]: to a solution of (9-Methyl-fluorene-9-yl)methanol (1.3 g, 6.2 mmol) in 30 mL of acetone solid CrO_3 (1.3 g, 13 mmol) was added in small quotes , keeping the temperature below + 35°C. The end of the reaction was monitored by TLC; then the solvent was evaporated at ambient temperature and reduced pressure. The crude was purified by a silica gel chromatography column (petroleum ether/EtAc 95:5) to give 0.9 g of white solid (yield 71%). ^{1}H-NMR ($CDCl_3$, 600 MHz) δ 1.68 (3H, s), 7.37 (2H, dt, J = 7.4, 1.0 Hz), 7.40 (2H, d, J = 7.4, 1.0 Hz), 7.46 (2H, dt, J = 7.5, 1.2 Hz), 7.81 (2H, d, J = 7.5 Hz), 8.78 (1H, s). ^{13}C-NMR ($CDCl_3$, 150.8 MHz) δ 17.1 ($2CH_3$), 63.3 (Cq), 120.6 (CH), 124.9 (CH), 128.2 (CH), 129.0 (CH), 142.1 (2Cq), 144.1 (2Cq), 197.3 (CH).

(3,5-Diisopropylphenyl-)(9-methyl-fluoren-9-yl)methanol (2a): To a suspension of Mg (0.044 g, 1.8 m mol) in 25 ml of dry THF was slowly dropped (20 min) a solution of 1-Bromo-3,5-diisopropylbenzene (0.45g, 1.8 mmol) in 10 ml of dry THF). After refluxing for 2h, the mixture was cooled to room temperature and a solution of 9-methyl-fluorene-9-carboxyaldehyde (0.31 g, 1.45 mmol) in 10 ml of dry THF was slowly added in 10 min. After 1h of additional stirring at +25°C the end of the reaction was checked by GC-MS. The mixture was treated with H_2O (40 mL), extracted with Et_2O (3x15 mL) and dried (Na_2SO_4). After removing the solvent, the crude was purified by a silica gel chromatography column (petroleum ether/EtAc 9:1) to give 0.44 g of the alcohol as a white solid (yield 80%). ^{1}H-NMR ($CDCl_3$, 600 MHz) δ 0.99 (12H, d, J = 7.0 Hz), 1.54 (1H, s), 1.68 (3H,s), 2.61 (2H, septet, J = 7.0 Hz), 7.22 (2H, m), 7.28 (2H, m), 7.34 (1H, d, J = 6.1 Hz), 7.48 (1H, d, J = 6.1 Hz), 7.52 (1H, d, J = 6.1 Hz), 7.57 (1H, d, J = 6.1 Hz).^{13}C-NMR ($CDCl_3$, 150.8 MHz) δ 21.5 (CH_3), 23.8 ($2CH_3$), 23.9 ($2CH_3$), 33.9 (2CH), 55.8 (Cq), 80.9 (CH), 119.5 (CH), 119.6 (CH), 122.7 (2CH), 124.1 (CH), 124.4 (CH), 125.1 (CH), 126.4 (CH), 126.7 (CH), 127.2 (CH), 127.3 (CH), 139.8 (Cq), 140.5 (Cq), 140.8 (Cq), 147.2 (2Cq), 148.5 (Cq), 149.2 (Cq).

(3,5-Diisopropylphenyl-)(9-methyl-fluoren-9-yl)methanone(2): To a solution of **2a** (0.44 g, 1.2 mmol) in acetone (25 mL), solid CrO_3 was added in small quotes (0.25 g, 2.5 mmol) under rapid stirring, keeping the temperature below +25°C. The reaction was monitored by TLC until the alcohol disappeared, then the solvent was evaporated at reduced pressure and ambient temperature.

The crude was purified by a silica gel chromatography column (petroleum ether/EtAc 95:5) to give 0.26 g of pale yellow solid. (yield 60%). Analytically pure samples of **2** were obtained by semipreparative HPLC on a C18 column (t_r = 18.42 min, Luna C18(2), 5 μm, 250 × 10 mm, Acetonitrile/H_2O 90:10 v:v, 5 mL/min).

Compound **3** was prepared following the same procedure use in the preparation of **2**, using 9-isopropyl-fluorene-9-carboxyaldehyde[5b]. Analytically pure samples of **3** were obtained by semipreparative HPLC on a C18 column (t_r = 19.90 min, Luna C8(2), 5 μm, 250 × 10 mm, Acetonitrile/H_2O 90:10 v:v, 5 mL/min). Crystals suitable for X-ray diffraction analysis were obtained by slow evaporation of an hexane solution.

(3,5-Diisopropylphenyl)(9-isopropyl-fluoren-9-yl)methanol (3a): ^{1}H-NMR ($CDCl_3$, 600 MHz) δ 0.32 (3H, d, J = 6.7 Hz), 0.850 (6H, d, J = 6.9 Hz), 0.847 (6H, d, J = 6.9 Hz), 1.46 (3H, d, J = 6.7 Hz), 2.02 (1H, d, J = 2.6 Hz), 2.45 (2H, septet, J = 6.9 Hz), 2.98 (1H, septet, J = 6.7 Hz), 5.49 (1H, d, J = 2.6 Hz), 6.20 (2H,d, J = 1.7 Hz), 6.50 (1H, t, J = 1.7 Hz), 7.16 (1H, dt, J = 7.6, 1.2 Hz), 7.21 (1H, dt, J = 7.6, 1.2 Hz), 7.24 (1H, dt, J = 7.6, 1.2 Hz), 7.31(1H, dt, J = 7.6, 1.2 Hz), 7.35 (1H, d, J = 7.4 Hz), 7.37 (1H, d, J = 7.4 Hz), 7.55 (1H, d, J = 7.4 Hz), 7.86 (1H, d, J = 7.4 Hz). ^{13}C-NMR ($CDCl_3$, 150.8 MHz) δ 18.1 (CH_3), 18.6 (CH_3), 23.99 ($2CH_3$), 24.01 ($2CH_3$), 32.4 (CH), 34.0 (2CH), 63.5 (Cq), 77.7 (CH), 119.2 (CH), 119.7 (CH), 122.7 (2CH), 123.9 (CH), 125.7 (CH), 125.9 (CH), 126.1 (CH), 126.7 (CH), 127.19 (CH), 127.21 (CH), 140.3 (Cq), 141.8 (Cq), 142.3 (Cq), 146.0 (Cq), 146.9 (2Cq), 147.9 (Cq).

Compound **4** was prepared following the same procedure use in the preparation of **2**, using mesityl bromide to prepare the Grignard reagent. Analytically pure samples of **4** were obtained by semipreparative HPLC on a C18 column (t_r = 10.55 min, Luna C18(2), 5 μm, 250 × 10 mm, Acetonitrile/H_2O 90:10 v:v, 5 mL/min).

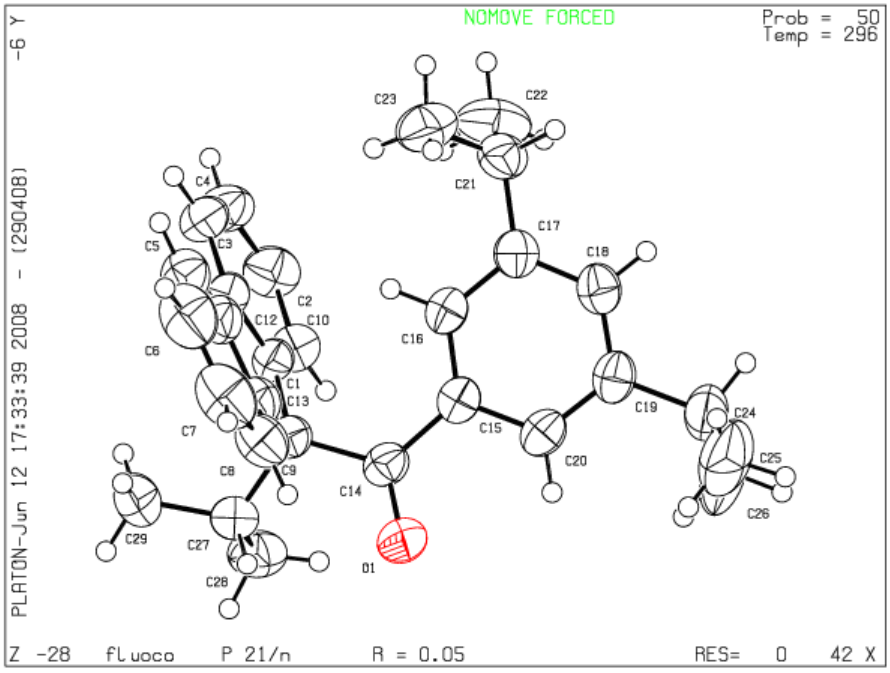
Mesityl(9-methyl-fluoren-9-yl)methanol (4a): ^{1}H-NMR ($CDCl_3$, 600 MHz) δ 1.44 (3H, s), 1.60 (3H, s), 1.95 (1H, d, J = 3.7 Hz), 2.27 (3H, s), 2.53 (3H, s), 4.93 (1H, d, J = 3.7 Hz), 6.52 (1H, d, J = 7.6 Hz), 6.64 (1H, s), 6.90 (1H, s), 7.03 (1H, dt, J = 7.5, 1.1 Hz), 7.28 (1H, dt, J = 7.5, 1.1 Hz), 7.29 (1H, dt, J = 7.5, 1.1 Hz), 7.38 (1H, dt, J = 7.5, 1.1 Hz), 7.61 (1H, d, J = 7.5 Hz), 7.69 (1H, d, J = 7.5 Hz), 7.74 (1H, d, J = 7.5 Hz).^{13}C-NMR ($CDCl_3$, 150.8 MHz) δ 20.4 (CH_3), 20.9 (CH_3), 21.2

(CH_3), 22.7 (CH_3), 57.5 (Cq), 76.5 (CH), 119.8 (CH), 120.1 (CH), 125.0 (CH), 125.4 (CH), 126.9 (CH), 127.1 (CH), 127.6 (CH), 127.7 (CH), 129.1 (CH), 131.9 (CH), 133.6 (Cq), 136.8 (Cq), 138.20 Cq), 138.25 (Cq), 139.8 (Cq), 140.8 (Cq), 149.2 (Cq), 152.2 (Cq).

Compound **5** was prepared following the same procedure use in the preparation of **2**, using mesityl bromide to prepare the Grignard reagent and 9-isopropyl-fluorene-9-carboxyaldehyde[5b]. Analytically pure samples of **5** were obtained by semipreparative HPLC on a C18 column (t_r = 16.80 min, Luna C18(2), 5 μm, 250 × 10 mm, Acetonitrile/H_2O 90:10 v:v, 5 mL/min). Crystals suitable for X-ray diffraction analysis were obtained by slow evaporation of an hexane solution.

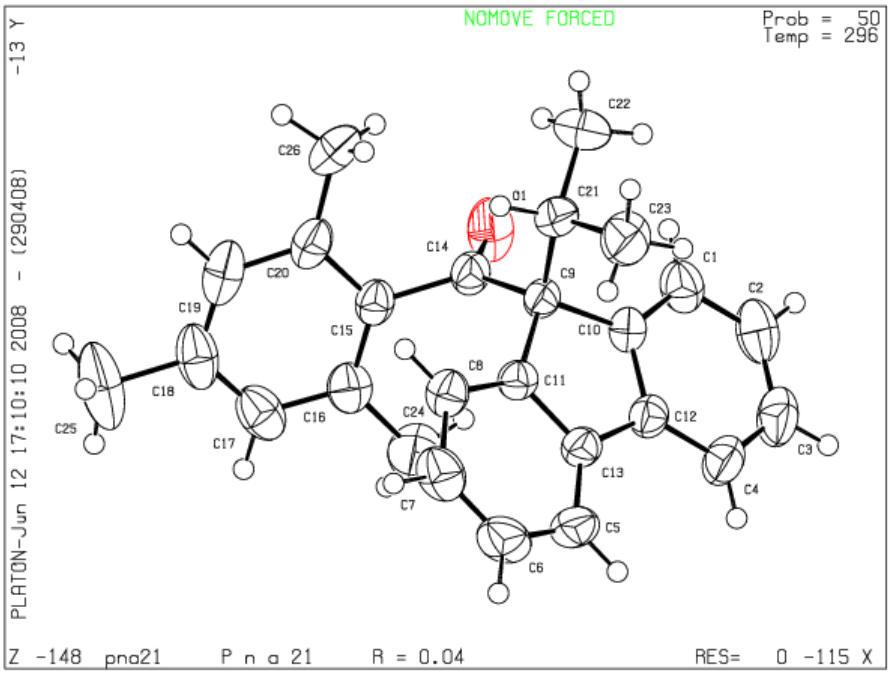
Mesityl(9-isopropyl-fluoren-9-yl)methanol (5a): ^{1}H-NMR ($CDCl_3$, 600 MHz) δ 0.63 (3H, d, J = 6.7 Hz), 0.99 (6H, d, J = 6.7 Hz), 1.60 (3H, s), 1.78 (1H, d, J = 4.2 Hz), 2.16 (3H, s), 2.29 (3H, s), 2.60 (1H, septet, J = 6.7 Hz), 5.86 (1H, d, J = 4.2 Hz), 6.55 (1H, s), 6.69 (1H, s), 6.93 (1H, d, J = 7.6 Hz), 6.99 (1H, dt, J = 7.6, 1.2 Hz), 7.22 (1H, dt, J = 7.6, 1.2 Hz), 7.25 (1H, dt, J = 7.6, 1.2 Hz), 7.36(1H, dt, J = 7.6, 1.2 Hz), 7.50 (1H, d, J = 7.6 Hz), 7.60 (1H, d, J = 7.6 Hz), 7.69 (1H, d, J = 7.6 Hz). ^{13}C-NMR ($CDCl_3$, 150.8 MHz) δ 18.9 (CH_3), 19.6 (CH_3), 20.6 (CH_3), 21.0 (CH_3), 22.0 (CH_3), 35.0 (CH), 64.4 (Cq), 75.1 (CH), 119.1 (CH), 119.6 (CH), 125.8 (CH), 126.1 (CH), 126.3 (CH), 126.8 (CH), 127.3 (CH), 127.4 (CH), 128.8 (CH), 131.3 (CH), 135.1 (Cq), 136.4 (2Cq), 138.3 (Cq), 141.1 (Cq), 142.4 (Cq), 146.5 (Cq), 148.1 (Cq).

Crystal Data for 3



Crystals obtained from hexane, molecular formula: $C_{29}H_{22}O$, M_r = 396.55, monoclinic, space group $P2_1/n$ (No. 14), a = 11.5913(16), b = 9.2125(13), c = 22.2062(32) Å, β = 99.490(2), V = 2338.8(6) Å^3, T = 298(2) K, Z = 4, ρ_c = 1.126 g cm^{-3}, F(000) = 856, graphite-monochromated Mo$_{K\alpha}$ radiation (λ = 0.71073 Å), μ(Mo$_{K\alpha}$) = 0.066 mm^{-1}, colourless brick (0.4 × 0.4 × 0.2 mm^3), empirical absorption correction with SADABS (transmission factors: 0.9741 – 0.9869), 2400 frames, exposure time 10 s, $1.86 \leq \theta \leq 27.50$, $-15 \leq h \leq 14$, $-11 \leq k \leq 11$, $-28 \leq l \leq 28$, 25573 reflections collected, 5625 independent reflections (R_{int} = 0.0229), solution by direct methods (SHELXS97[a]) and subsequent Fourier syntheses, full-matrix least-squares on F_o^2 (SHELX97), hydrogen atoms refined with a riding model, data / restraints / parameters = 5325/ 0 / 277, $S(F^2)$ = 1.054, $R(F)$ = 0.0723 and $wR(F^2)$ = 0.1737 on all data, $R(F)$ = 0.0539 and $wR(F^2)$ = 0.1563 for 3888 reflections with $I > 2\sigma(I)$, weighting scheme $w = 1/[\sigma^2(F_o^2) + (0.0849P)^2 + 0.5106P]$ where $P = (F_o^2 + 2F_c^2)/3$, largest difference peak and hole 0.803 and –0.202 e Å^{-3}. Crystallographic data (excluding structure factors) for the structure reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC-XXXXXX. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: (+44) 1223-336-033; e-mail: deposit@ccdc.cam.ac.uk).

Crystal Data for 5



Crystals obtained from hexane, molecular formula: $C_{26}H_{26}O$, M_r = 354.47, orthorhombic, space group $Pna_2/1$ (No. 33), a = 17.0726(14), b = 7.4102(6), c = 16.2202(14) Å, V = 2052.0 (3) Å^3, T = 298(2) K, Z = 4, ρ_c = 1.147 g cm^{-3}, $F(000)$ = 760, graphite-monochromated $Mo_{K\alpha}$ radiation (λ = 0.71073 Å), $\mu(Mo_{K\alpha})$ = 0.068 mm^{-1}, colourless block (0.5 × 0.3 × 0.2 mm^3), empirical absorption correction with SADABS (transmission factors: 0.9866 – 0.9669), 2400 frames, exposure time 10 s, $2.39 \leq \theta \leq 28.72$, $-21 \leq h \leq 22$, $-10 \leq k \leq 9$, $-21 \leq l \leq 20$, 22311 reflections collected, 4980 independent reflections (R_{int} = 0.0186), solution by direct methods (SHELXS97[a]) and subsequent Fourier syntheses, full-matrix least-squares on F_o^2 (SHELX97), hydrogen atoms refined with a riding model, data / restraints / parameters = 4980/ 1 / 250, $S(F^2)$ = 1.029, $R(F)$ = 0.0420 and $wR(F^2)$ = 0.1059 on all data, $R(F)$ = 0.0374 and $wR(F^2)$ = 0.11016 for 4652 reflections with $I > 2\sigma(I)$, weighting scheme $w = 1/[\sigma^2(F_o^2) + (0.0374P)^2 + 0.1375P]$ where $P = (F_o^2 + 2F_c^2)/3$, largest difference peak and hole 0.170 and –0.162 e Å^{-3}. Flack parameter = 0.1 (14). Crystallographic data (excluding structure factors) for the structure reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC-XXXXXX. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: (+44) 1223-336-033; e-mail: deposit@ccdc.cam.ac.uk).

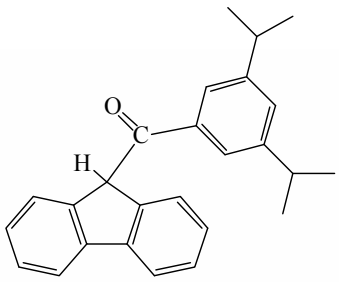
fluorene-chetone-isopropile
Inova600-Triple H1-s2pul-CDCl3 Apr 13 2007

Archive directory:
Sample directory:

Pulse Sequence: s2pul

Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: fluorene-chetone-diisopropile-protone
INOVA-300 "blade"

Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 2.995 sec
Width 9611.9 Hz
16 repetitions
OBSERVE H1, 599.7347464 MHz
DATA PROCESSING
FT size 65536
Total time 1 min, 20 sec



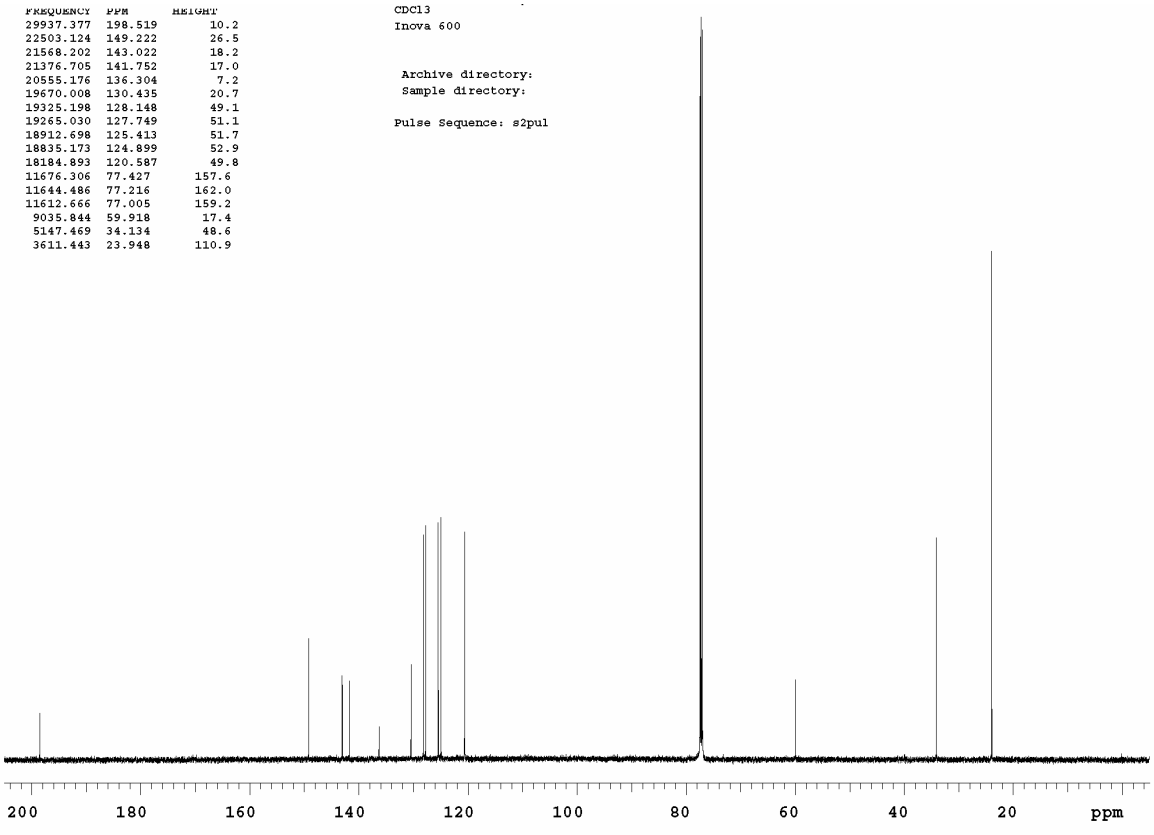
1

INDEX	FREQUENCY	PPM	HEIGHT
1	29937.377	198.519	10.2
2	22503.124	149.222	26.5
3	21568.202	143.022	18.2
4	21376.705	141.752	17.0
5	20555.176	136.304	7.2
6	19670.008	130.435	20.7
7	19325.198	128.148	49.1
8	19265.030	127.749	51.1
9	18912.698	125.413	51.7
10	18835.173	124.899	52.9
11	18184.893	120.587	49.8
12	11676.306	77.427	157.6
13	11644.486	77.216	162.0
14	11612.666	77.005	159.2
15	9035.844	59.918	17.4
16	5147.469	34.134	48.6
17	3611.443	23.948	110.9

CDCl3
Inova 600

Archive directory:
Sample directory:

Pulse Sequence: s2pul



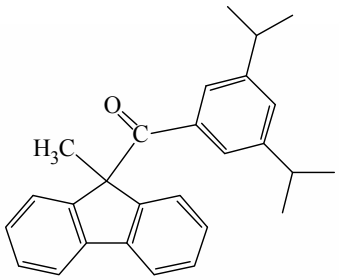
fluorene 9Me CO-35iPr2Ph
Inova600-Triple H1-s2pul-cd3cn May 14 2008

Archive directory:
Sample directory:

Pulse Sequence: s2pul

Solvent: cd3cn
Temp. 25.0 C / 298.1 K
File: 9MeFL-CO-35ipr2ph-protone-HPLC
INOVA-300 "blade"

Pulse 45.0 degrees
Acq. time 2.995 sec
Width 9611.9 Hz
4 repetitions
OBSERVE H1, 599.7379258 MHz
DATA PROCESSING
FT size 131072
Total time 0 min, 12 sec



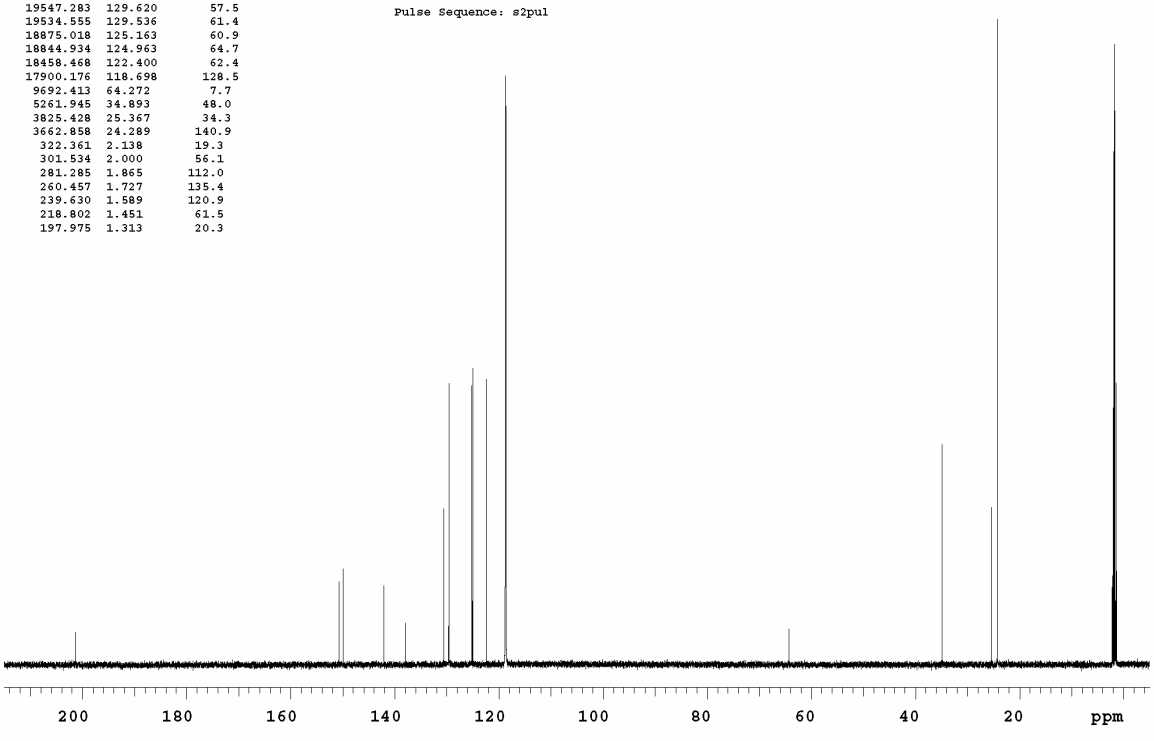
2

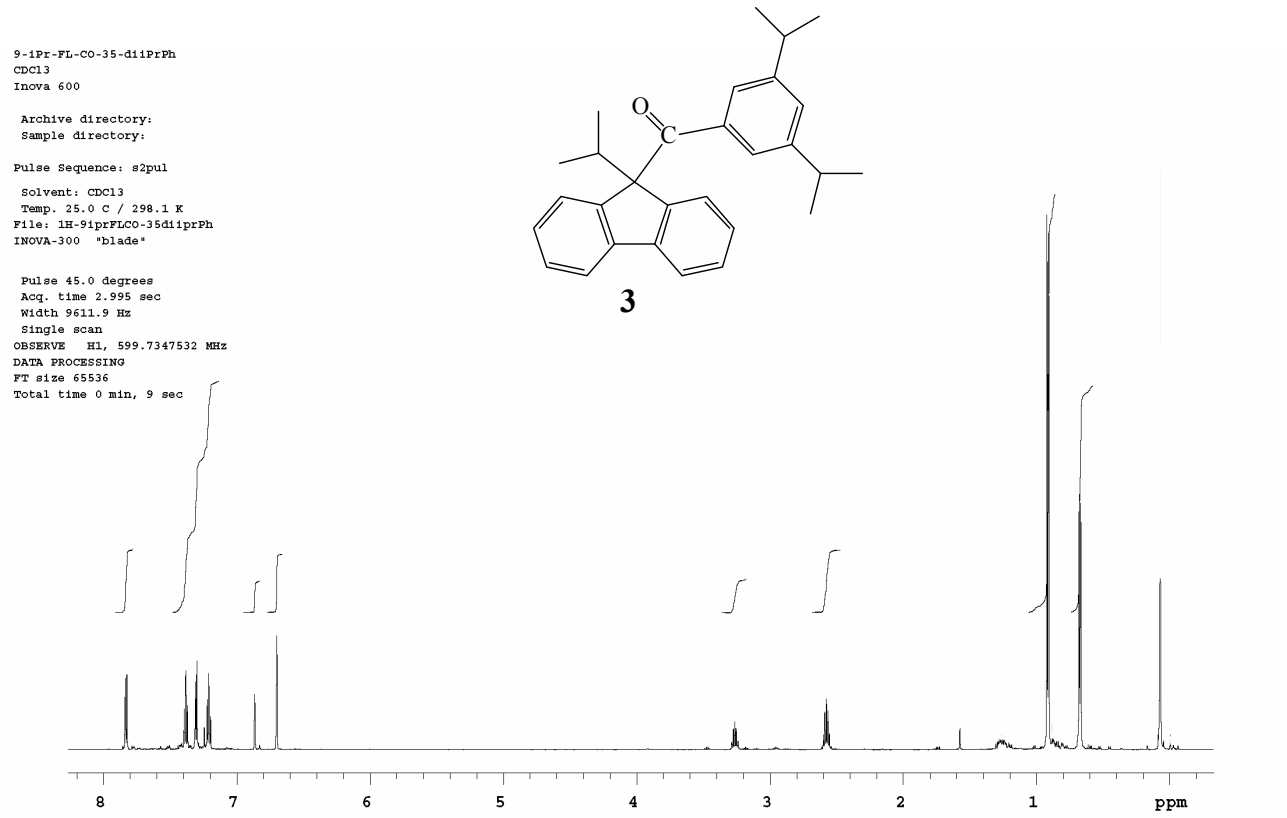
INDEX	FREQUENCY	PPM	HEIGHT
1	30361.952	201.334	6.9
2	22717.688	150.644	18.0
3	22605.451	149.900	20.8
4	21428.698	142.096	17.1
5	20802.138	137.942	8.9
6	19694.232	130.595	34.1
7	19547.283	129.620	57.5
8	19534.555	129.536	61.4
9	18875.018	125.163	60.9
10	18844.934	124.963	64.7
11	18458.468	122.400	62.4
12	17900.176	118.698	128.5
13	9692.413	64.272	7.7
14	5261.945	34.893	48.0
15	3825.428	25.367	34.3
16	3662.858	24.289	140.9
17	322.361	2.138	19.3
18	301.534	2.000	56.1
19	281.285	1.865	112.0
20	260.457	1.727	135.4
21	239.630	1.589	120.9
22	218.802	1.451	61.5
23	197.975	1.313	20.3

Inova600-Triple C13-s2pul
cd3cn May 14 2008

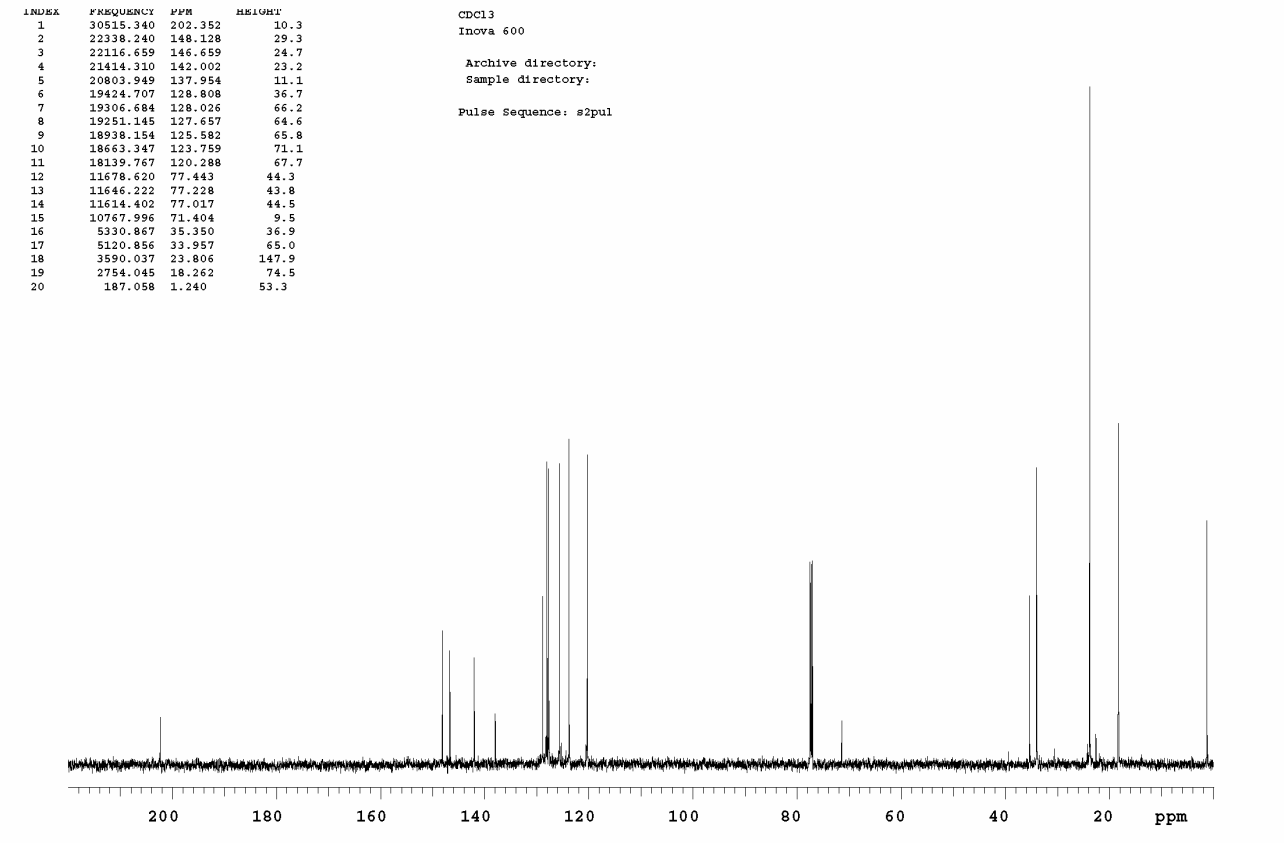
Archive directory:
Sample directory:

Pulse Sequence: s2pul





INDEX	FREQUENCY	PPM	HEIGHT
1	30515.340	202.352	10.3
2	22338.240	148.128	29.3
3	22116.659	146.659	24.7
4	21414.310	142.002	23.2
5	20803.949	137.954	11.1
6	19424.707	128.808	36.7
7	19306.684	128.026	66.2
8	19251.145	127.657	64.6
9	18938.154	125.582	65.8
10	18663.347	123.759	71.1
11	18139.767	120.288	67.7
12	11678.620	77.443	44.3
13	11646.222	77.228	43.8
14	11614.402	77.017	44.5
15	10767.996	71.404	9.5
16	5330.867	35.350	36.9
17	5120.856	33.957	65.0
18	3590.037	23.806	147.9
19	2754.045	18.262	74.5
20	187.058	1.240	53.3



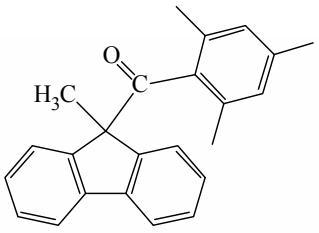
Fluorene 9Me-9CO-mesitile
Inova 600-Triple H1-s2pul
cd3cn Apr 15 2008

Archive directory:
Sample directory:

Pulse Sequence: s2pul

Solvent: cd3cn
Temp. 25.0 C / 298.1 K
File: 1H-9Me-FLCOMes
INOVA-300 "blade"

Pulse 30.0 degrees
Acq. time 2.995 sec
Width 9611.9 Hz
4 repetitions
OBSERVE H1, 599.7379258 MHz
DATA PROCESSING
FT size 131072
Total time 0 min, 12 sec



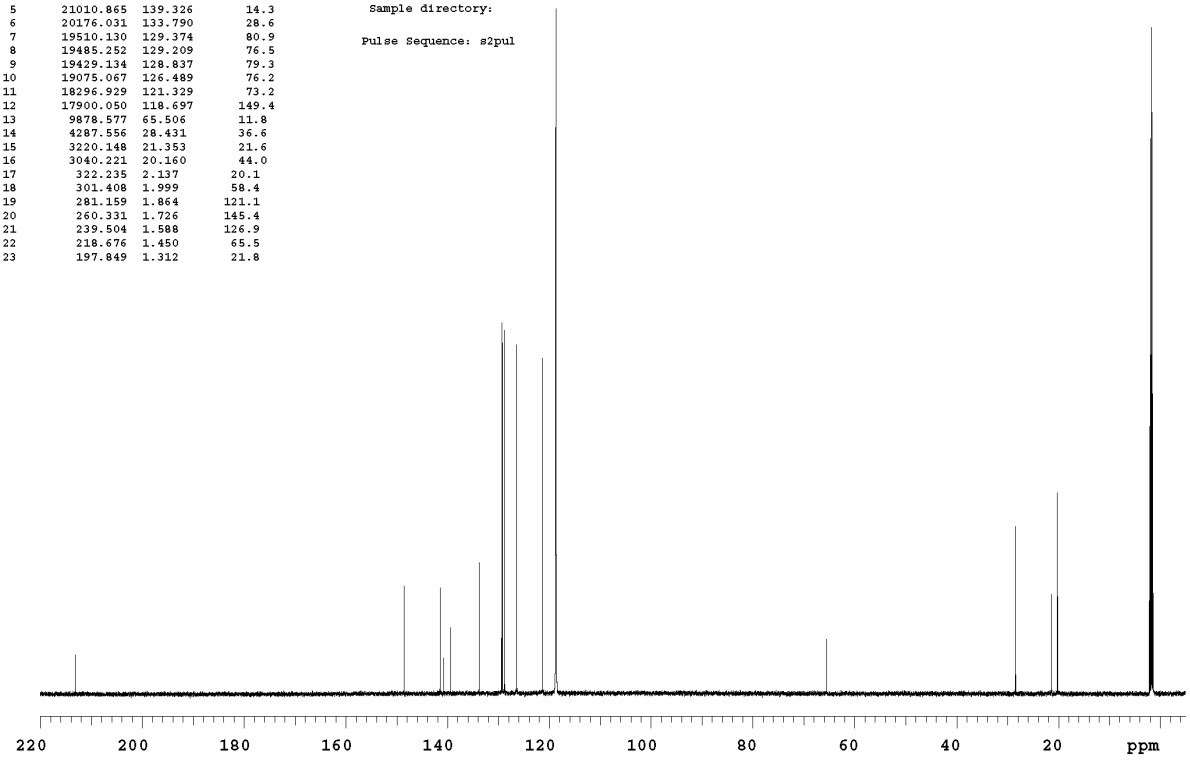
4

INDEX	FREQUENCY	PPM	HEIGHT
1	32146.625	213.168	8.3
2	22397.050	148.518	23.3
3	21339.477	141.505	23.0
4	21227.240	140.760	7.7
5	21010.865	139.326	14.3
6	20176.031	133.790	28.6
7	19510.130	129.374	80.9
8	19485.252	129.209	76.5
9	19429.134	128.837	79.3
10	19075.067	126.489	76.2
11	18296.929	121.329	73.2
12	17900.050	118.697	149.4
13	9878.577	65.506	11.8
14	4287.556	28.431	36.6
15	3220.148	21.353	21.6
16	3040.221	20.160	44.0
17	322.235	2.137	20.1
18	301.408	1.999	58.4
19	281.159	1.864	121.1
20	260.331	1.726	145.4
21	239.504	1.588	126.9
22	218.676	1.450	65.5
23	197.849	1.312	21.8

Inova600-Triple C13-s2pul
cd3cn Apr 15 2008

Archive directory:
Sample directory:

Pulse Sequence: s2pul



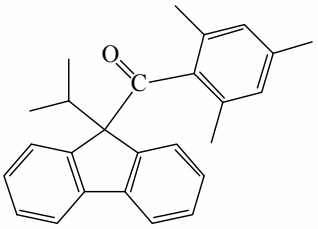
9-iPr-FL-9-COMes
HPLC
CD3CN Inova 600

Archive directory:
Sample directory:

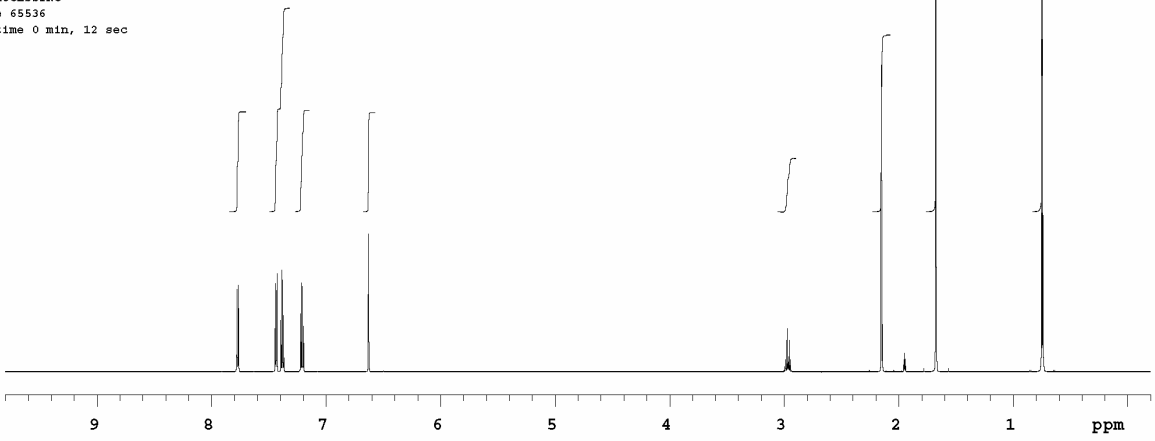
Pulse Sequence: s2pul

Solvent: cd3cn
Temp. 25.0 C / 298.1 K
File: 1H-9ipr-FLCOMes
INOVA-300 "blade"

Pulse 45.0 degrees
Acq. time 2.995 sec
Width 9611.9 Hz
4 repetitions
OBSERVE H1, 599.7379258 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 12 sec



5

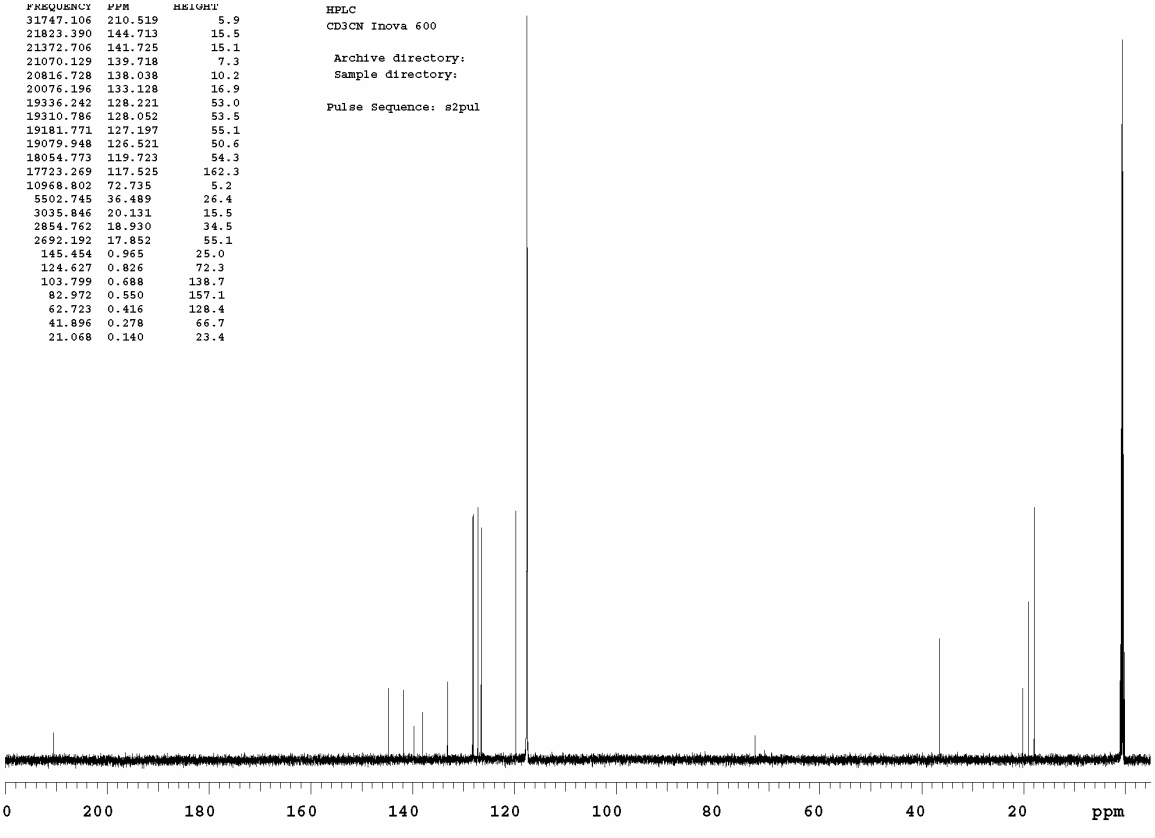


INDEX	FREQUENCY	PPM	HEIGHT
1	31747.106	210.519	5.9
2	21823.390	144.713	15.5
3	21372.706	141.725	15.1
4	21070.129	139.718	7.3
5	20816.728	138.038	10.2
6	20076.196	133.128	16.9
7	19336.242	128.221	53.0
8	19310.786	128.052	53.5
9	19181.771	127.197	55.1
10	19079.948	126.521	50.6
11	18054.773	119.723	54.3
12	17723.269	117.525	162.3
13	10968.802	72.735	5.2
14	5502.745	36.489	26.4
15	3035.846	20.131	15.5
16	2854.762	18.930	34.5
17	2692.192	17.852	55.1
18	145.454	0.965	25.0
19	124.627	0.826	72.3
20	103.799	0.688	138.7
21	82.972	0.550	157.1
22	62.723	0.416	128.4
23	41.896	0.278	66.7
24	21.068	0.140	23.4

HPLC
CD3CN Inova 600

Archive directory:
Sample directory:

Pulse Sequence: s2pul



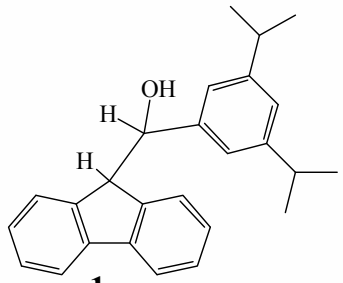
Fluorene-9-(CH(OH)-3,5-iPr2Ph
CDCl3
Inova600

Archive directory:
Sample directory:

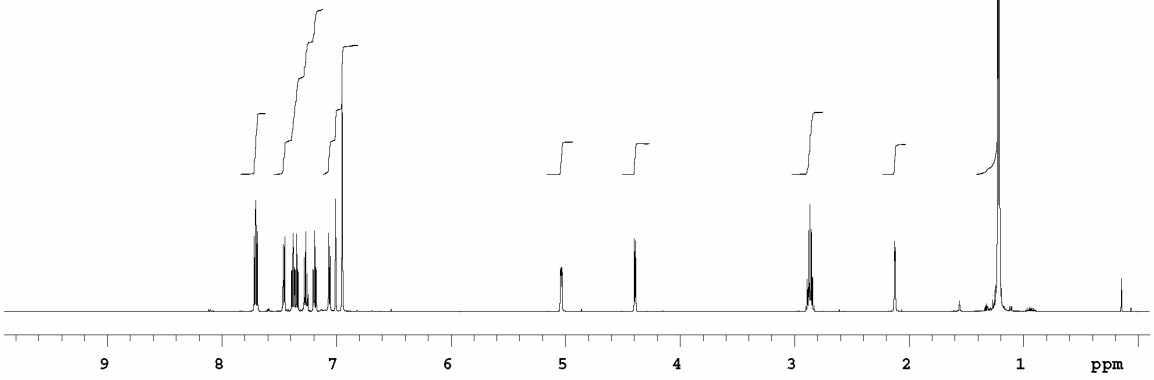
Pulse Sequence: s2pul

Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: 1H-9FLCHOH-35PhiPr2
INOVA-300 "blade"

Pulse 45.0 degrees
Acq. time 2.995 sec
Width 9611.9 Hz
4 repetitions
OBSERVE H1, 599.7347494 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 18 sec



1a

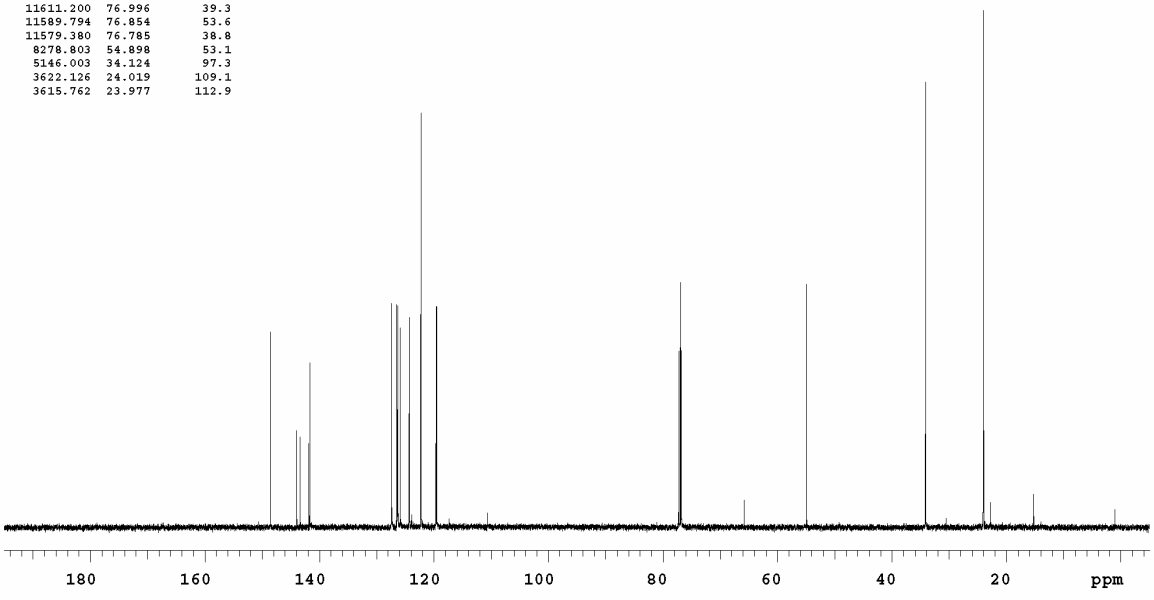


INDEX	FREQUENCY	PPM	HEIGHT
1	22402.728	148.556	42.9
2	21708.478	143.952	21.0
3	21616.490	143.342	19.6
4	21384.495	141.804	18.3
5	21360.775	141.646	36.0
6	19213.809	127.410	44.4
7	19206.288	127.360	49.0
8	19070.909	126.462	48.7
9	19066.281	126.431	47.3
10	19044.296	126.286	48.5
11	18977.186	125.841	43.7
12	18741.719	124.279	46.0
13	18434.514	122.242	90.5
14	18042.263	119.641	48.4
15	18023.171	119.514	48.2
16	11643.020	77.207	38.6
17	11611.200	76.996	39.3
18	11589.794	76.854	53.6
19	11579.380	76.785	38.8
20	8278.803	54.898	53.1
21	5146.003	34.124	97.3
22	3622.126	24.019	109.1
23	3615.762	23.977	112.9

CDCl3
Inova 600

Archive directory:
Sample directory:

Pulse Sequence: s2pul



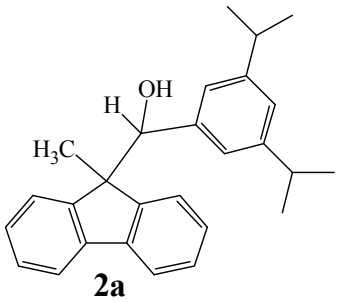
9-Me-FL-CHOH-Ph35di1Pr
CDCl3 Inova 600

Archive directory:
Sample directory:

Pulse Sequence: s2pul

Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: 1H-9Me-FL-CHOH-PH351Pr
INOVA-300 "blade"

Pulse 29.0 degrees
Acq. time 3.000 sec
Width 9595.8 Hz
4 repetitions
OBSERVE H1, 599.7347567 MHz
DATA PROCESSING
Resol. enhancement 0.6 Hz
Gauss apodization 0.700 sec
FT size 65536
Total time 0 min, 18 sec



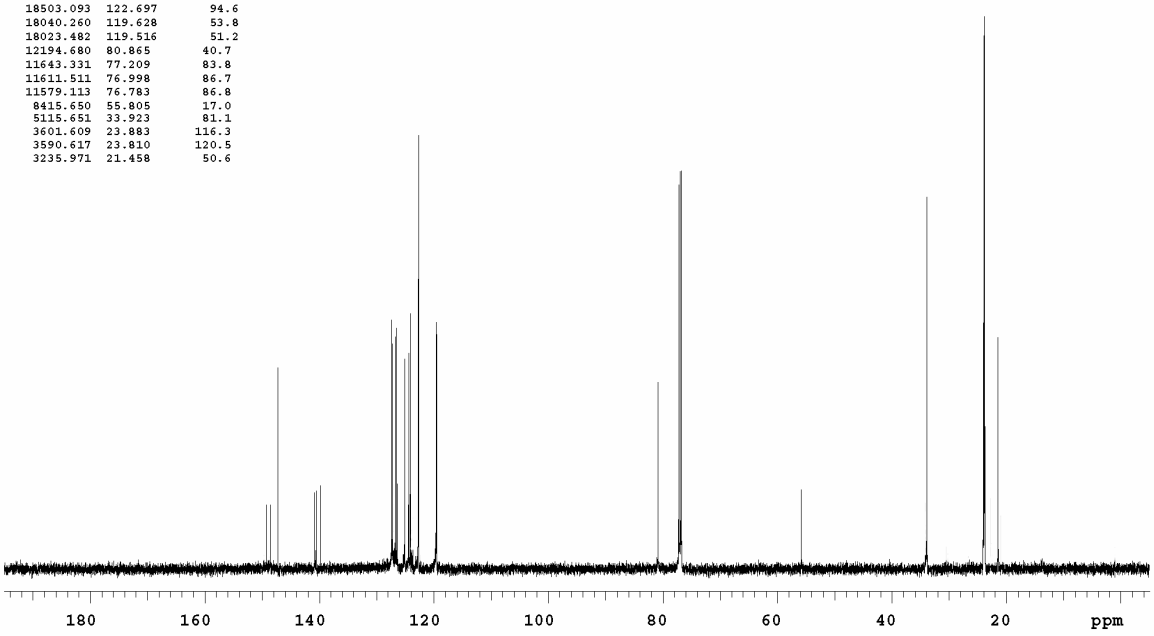
2a

INDEX	FREQUENCY	PPM	HEIGHT
1	22501.969	149.214	13.8
2	22401.881	148.550	13.8
3	22201.128	147.219	43.9
4	21239.592	140.843	16.4
5	21193.309	140.536	16.9
6	21085.122	139.819	18.0
7	19204.863	127.350	54.4
8	19186.928	127.231	49.2
9	19103.618	126.679	50.6
10	19066.592	126.433	52.5
11	18866.995	125.110	45.8
12	18757.651	124.385	47.1
13	18711.368	124.078	55.7
14	18503.093	122.697	94.6
15	18040.260	119.628	53.8
16	18023.482	119.516	51.2
17	12194.680	80.865	40.7
18	11643.331	77.209	83.8
19	11611.511	76.998	86.7
20	11579.113	76.783	86.8
21	8415.650	55.805	17.0
22	5115.651	33.923	81.1
23	3601.609	23.883	116.3
24	3590.617	23.810	120.5
25	3235.971	21.458	50.6

CDCl3 Inova 600

Archive directory:
Sample directory:

Pulse Sequence: s2pul



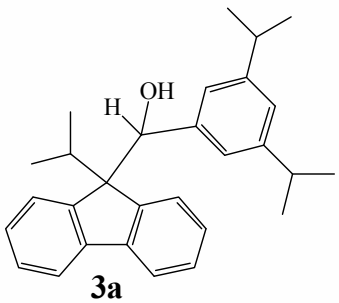
9-iPr-FL-CHOH-35-di1PrPh
CDCl3
Inova 600

Archive directory:
Sample directory:

Pulse Sequence: s2pul

Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: 1H-9iprFL-CHOH-35di1prPh
INOVA-300 "blade"

Pulse 45.0 degrees
Acq. time 2.995 sec
Width 9611.9 Hz
4 repetitions
OBSERVE H1, 599.7347532 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 18 sec



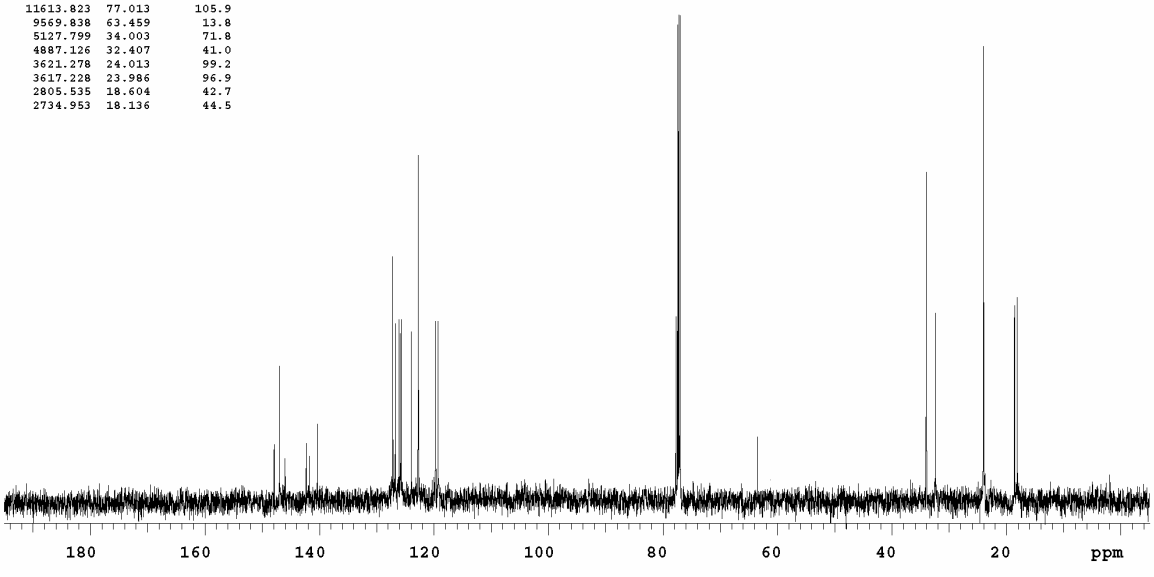
3a

INDEX	FREQUENCY	PPM	HEIGHT
1	22302.370	147.890	12.1
2	22161.206	146.954	29.5
3	22013.678	145.976	9.1
4	21457.700	142.289	12.4
5	21377.862	141.760	9.6
6	21162.066	140.329	16.6
7	19181.141	127.193	53.3
8	19114.030	126.748	38.7
9	19017.992	126.111	39.7
10	18979.809	125.858	36.6
11	18958.981	125.720	39.6
12	18688.224	123.924	36.9
13	18505.984	122.716	75.3
14	18047.200	119.674	39.1
15	17981.825	119.240	39.3
16	11719.696	77.715	40.2
17	11678.041	77.439	103.8
18	11645.643	77.224	106.0
19	11613.823	77.013	105.9
20	9569.838	63.459	13.8
21	5127.799	34.003	71.8
22	4887.126	32.407	41.0
23	3621.278	24.013	99.2
24	3617.228	23.986	96.9
25	2805.535	18.604	42.7
26	2734.953	18.136	44.5

CDCl3
Inova 600

Archive directory:
Sample directory:

Pulse Sequence: s2pul



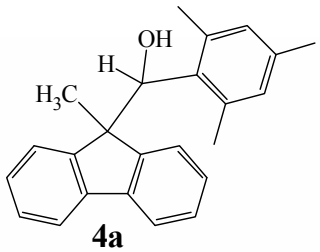
9-Me-FL-CHOH-Mes HPLC
CDCl3 Inova 600 triple

Archive directory:
Sample directory:

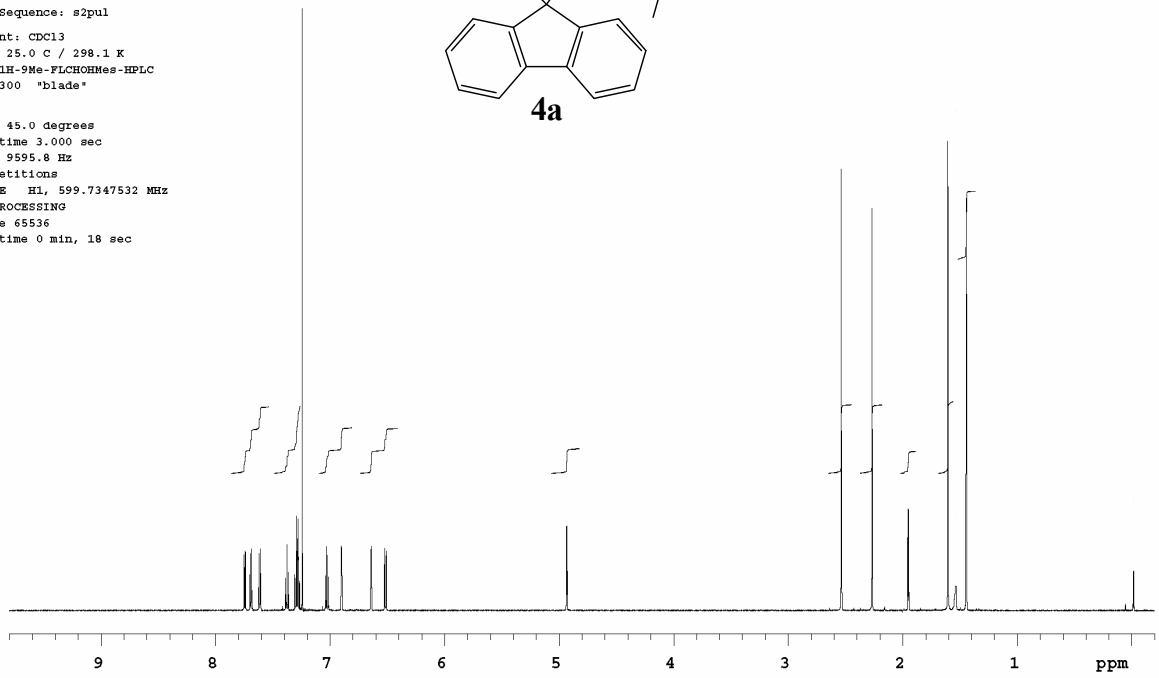
Pulse Sequence: s2pul

Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: 1H-9Me-FLCHOHMes-HPLC
INOVA-300 "blade"

Pulse 45.0 degrees
Acq. time 3.000 sec
Width 9595.8 Hz
4 repetitions
OBSERVE H1, 599.7347532 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 18 sec



4a

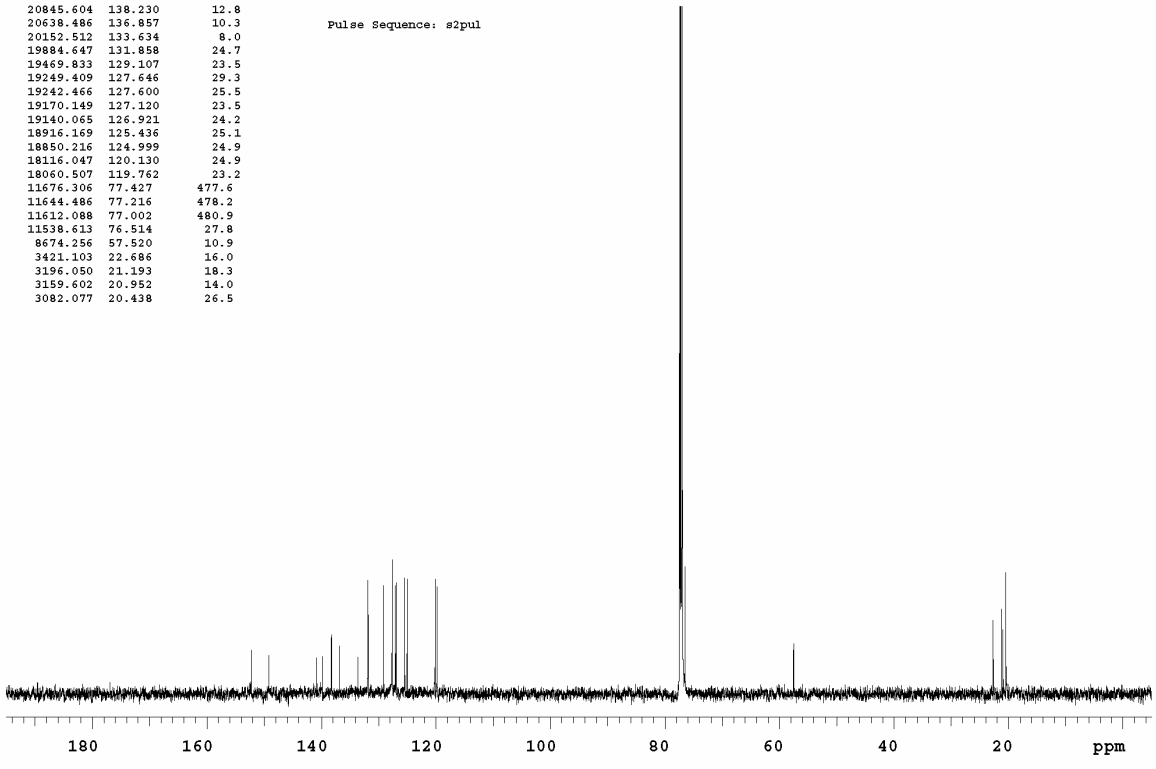


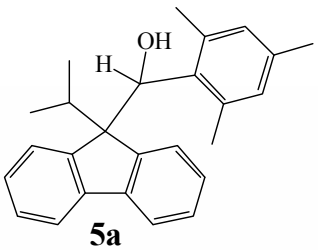
INDEX	FREQUENCY	PPM	HEIGHT
1	22954.386	152.214	9.5
2	22494.446	149.164	8.4
3	21231.491	140.789	7.8
4	21084.541	139.815	8.1
5	20845.604	138.230	12.8
6	20638.486	136.857	10.3
7	20152.512	133.634	8.0
8	19884.647	131.858	24.7
9	19469.833	129.107	23.5
10	19249.409	127.646	29.3
11	19242.466	127.600	25.5
12	19170.149	127.120	23.5
13	19140.065	126.921	24.2
14	18916.169	125.436	25.1
15	18850.216	124.999	24.9
16	18116.047	120.130	24.9
17	18060.507	119.762	23.2
18	11676.306	77.427	477.6
19	11644.486	77.216	478.2
20	11612.088	77.002	480.9
21	11538.613	76.514	27.8
22	8674.256	57.520	10.9
23	3421.103	22.686	16.0
24	3196.050	21.193	18.3
25	3159.602	20.952	14.0
26	3082.077	20.438	26.5

CDCl3 Inova 600 triple

Archive directory:
Sample directory:

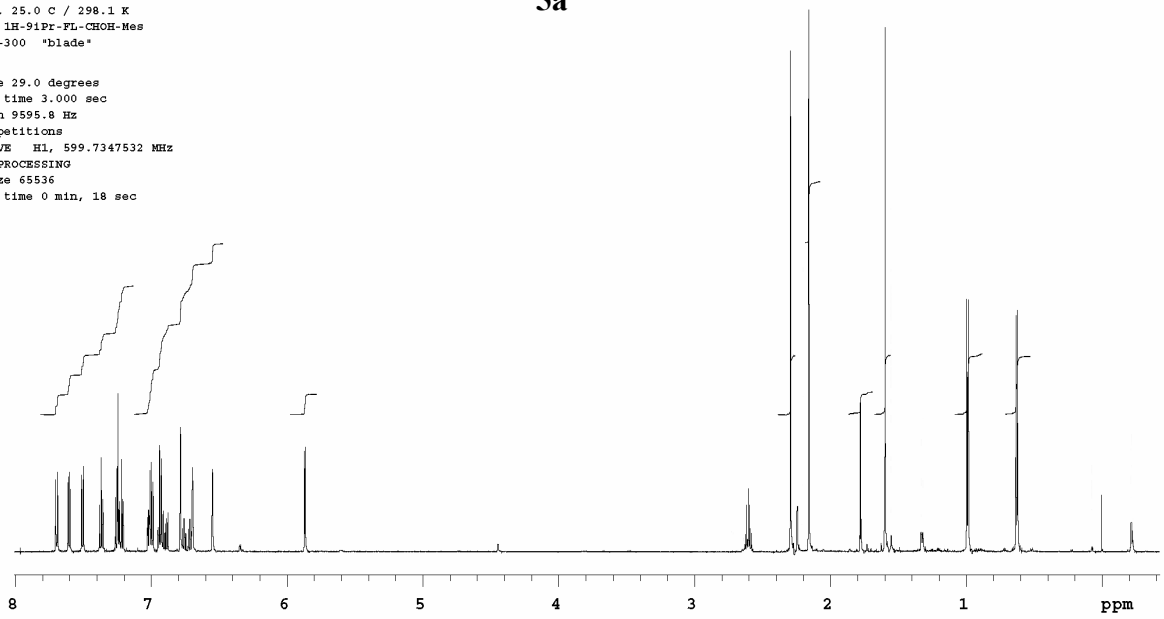
Pulse Sequence: s2pul



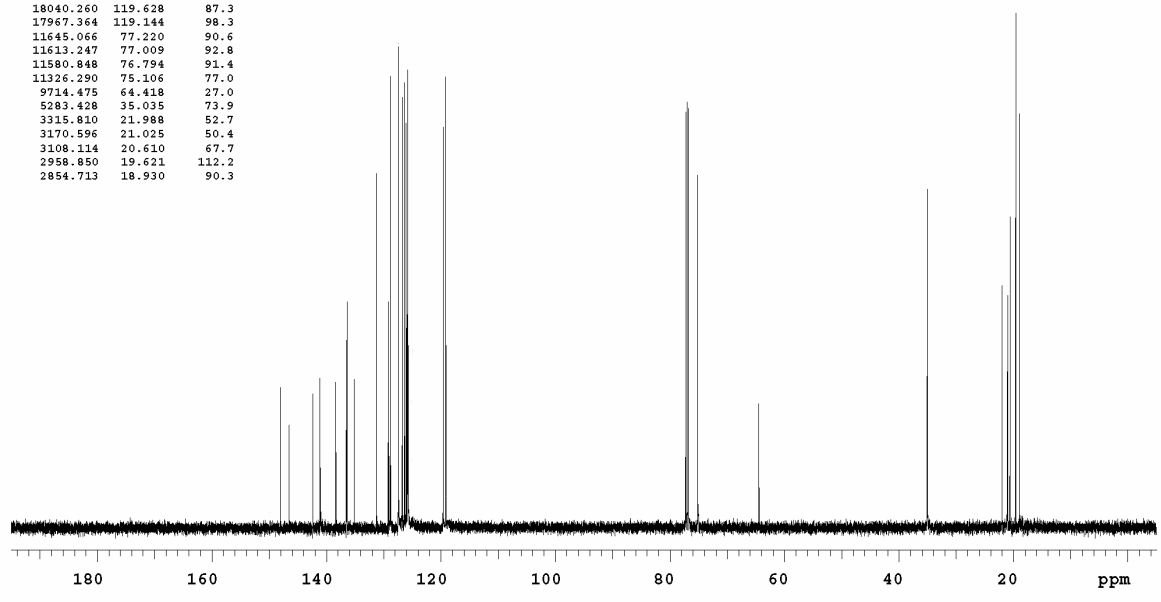


5a

```
9-iPr-FL-CHOH-Mes
CDCl3
Inova 600

 Archive directory:
 Sample directory:

Pulse Sequence: s2pul
 Solvent: CDCl3
 Temp. 25.0 C / 298.1 K
File: 1H-9iPr-FL-CHOH-Mes
INOVA-300  "blade"

 Pulse 29.0 degrees
 Acq. time 3.000 sec
 Width 9595.8 Hz
 4 repetitions
OBSERVE   H1, 599.7347532 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 18 sec
```



INDEX	FREQUENCY	PPM	HEIGHT
1	22331.878	148.086	30.4
2	22331.878	148.086	30.4
3	21475.059	142.404	29.1
4	21276.040	141.085	32.4
5	20863.541	138.349	31.6
6	20564.435	136.366	49.2
7	20379.880	135.142	32.2
8	19797.868	131.283	77.4
9	19425.866	128.816	98.4
10	19213.541	127.408	88.9
11	19209.492	127.381	105.5
12	19116.346	126.763	93.8
13	19049.814	126.322	97.0
14	19019.730	126.123	88.2
15	18971.133	125.800	99.8
16	18040.260	119.628	87.3
17	17967.364	119.144	98.3
18	11645.066	77.220	90.6
19	11613.247	77.009	92.8
20	11580.848	76.794	91.4
21	11326.290	75.106	77.0
22	9714.475	64.418	27.0
23	5283.428	35.035	73.9
24	3315.810	21.988	52.7
25	3170.596	21.025	50.4
26	3108.114	20.610	67.7
27	2958.850	19.621	112.2
28	2854.713	18.930	90.3



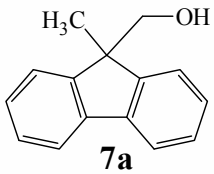
grezzo 9-Me-9-CH2OH-Fluorene
Inova 600 CDCl3

Archive directory:
Sample directory:

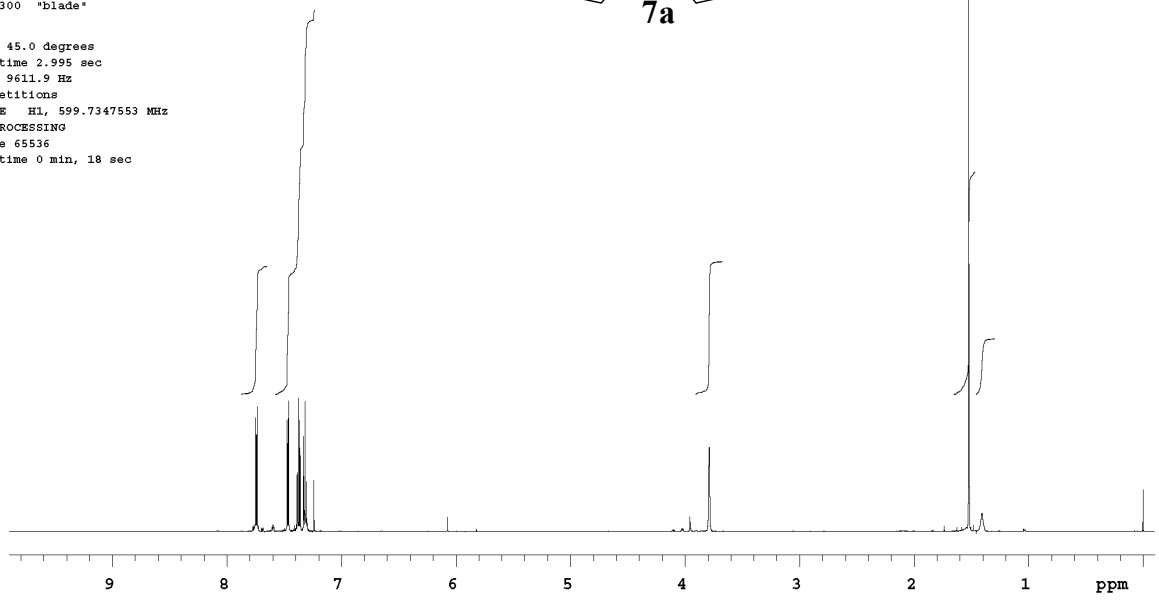
Pulse Sequence: s2pul

Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: 1H-9-Me-9CH2OH-FL
INOVA-300 "blade"

Pulse 45.0 degrees
Acq. time 2.995 sec
Width 9611.9 Hz
4 repetitions
OBSERVE H1, 599.7347553 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 18 sec



7a

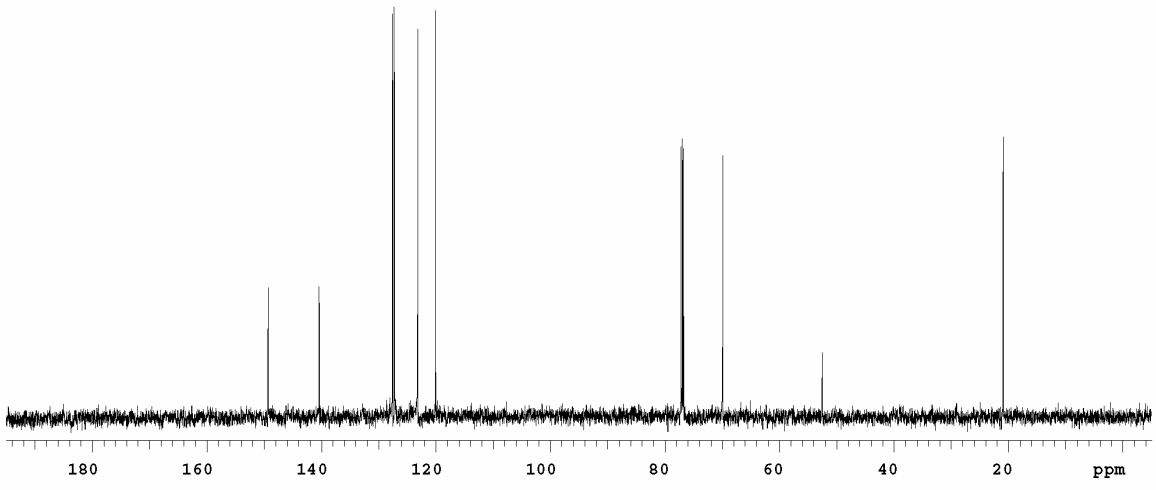


INDEX	FREQUENCY	PPM	HEIGHT
1	22514.775	149.299	28.4
2	21170.246	140.383	28.7
3	19236.761	127.562	88.2
4	19193.949	127.278	89.6
5	18577.224	123.188	84.7
6	18110.920	120.096	88.8
7	11636.467	77.163	59.1
8	11604.647	76.952	61.0
9	11572.827	76.741	58.8
10	10544.760	69.924	57.3
11	7923.390	52.541	14.0
12	3154.475	20.918	61.3

Inova 600 CDCl3

Archive directory:
Sample directory:

Pulse Sequence: s2pul



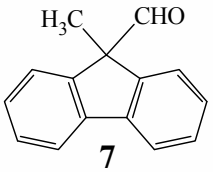
9Me-Fluorene-9CHO
CDCl3
Inova 600

Archive directory:
Sample directory:

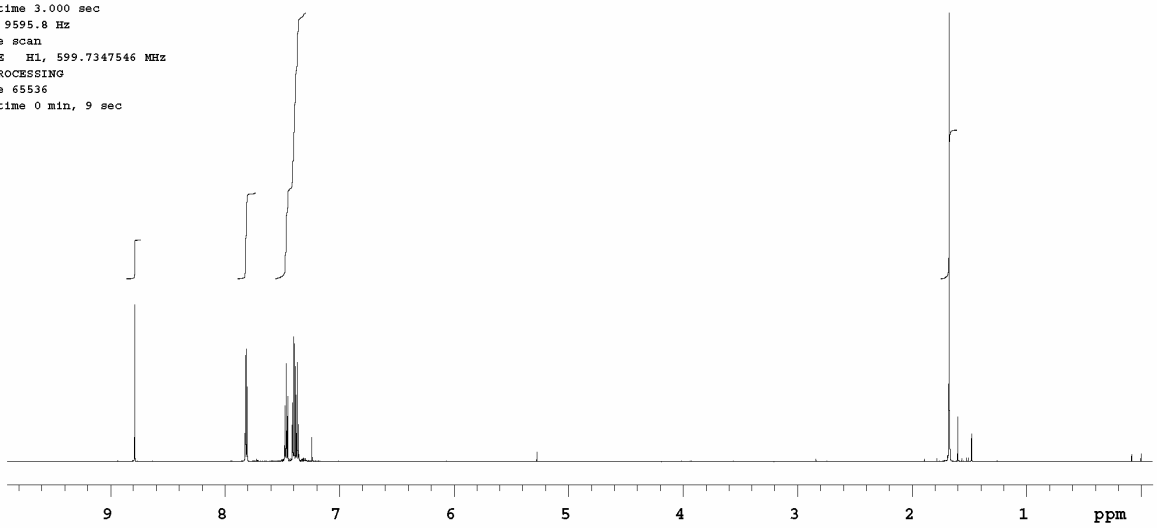
Pulse Sequence: s2pul

Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: 1H-9Me-FLCHO
INOVA-300 "blade"

Pulse 45.0 degrees
Acq. time 3.000 sec
Width 9595.8 Hz
Single scan
OBSERVE H1, 599.7347546 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 9 sec



7

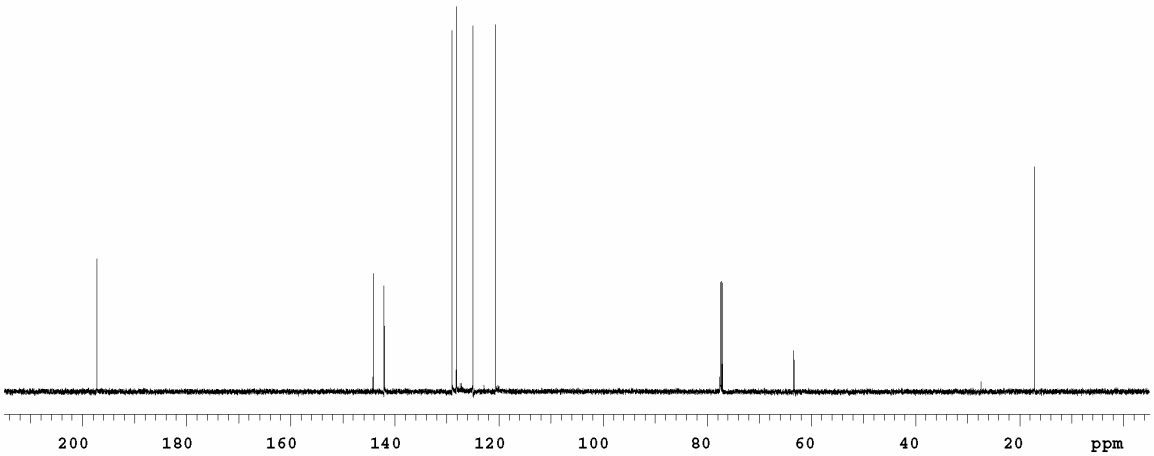


INDEX	FREQUENCY	PPM	HEIGHT
1	29749.930	197.276	29.0
2	21739.450	144.158	25.7
3	21422.988	142.059	23.0
4	19456.527	129.019	78.9
5	19330.983	128.187	84.1
6	18842.116	124.945	79.8
7	18193.571	120.644	80.1
8	11683.827	77.477	23.7
9	11652.007	77.266	24.0
10	11620.187	77.055	23.5
11	9551.903	63.340	8.8
12	2581.639	17.119	49.1

CDCl3
Inova 600

Archive directory:
Sample directory:

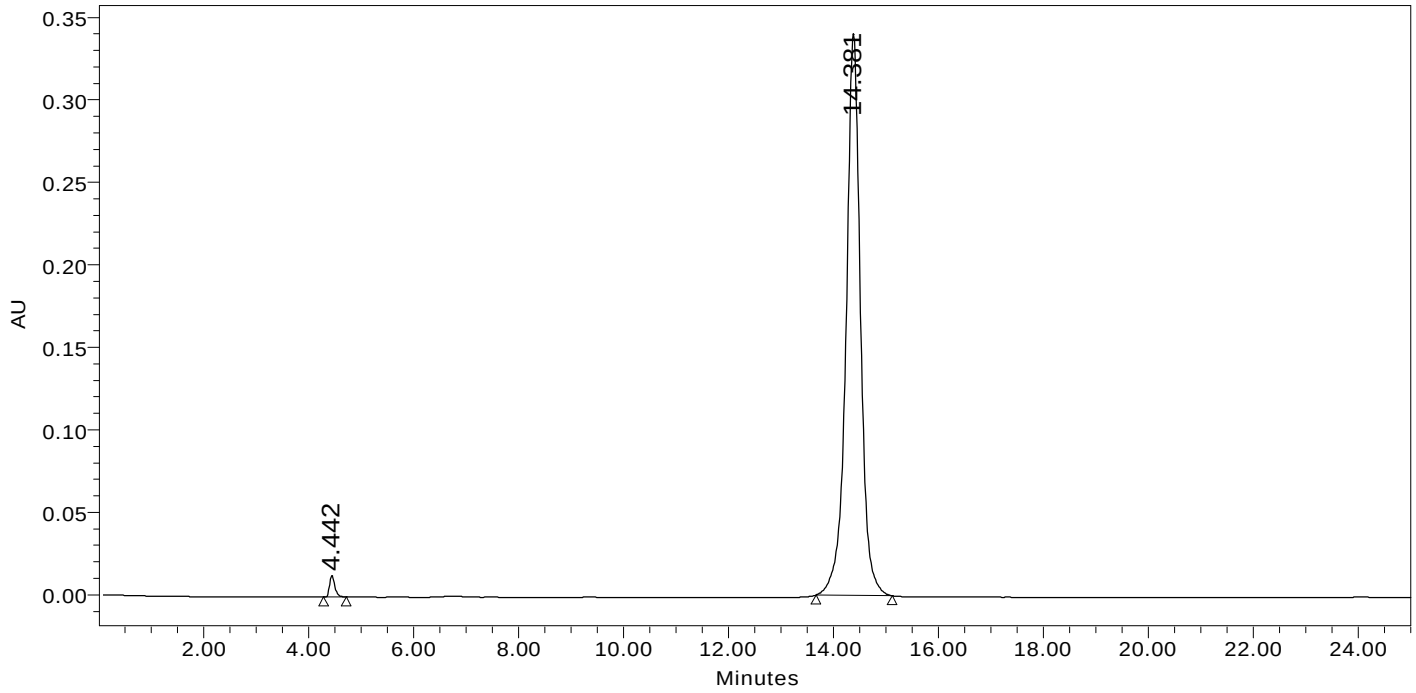
Pulse Sequence: s2pul



Reported by User: System Project Name: LunaC18

SAMPLE INFORMATION

Sample Name:	9H-fluo-CO-35ipr2ph-anal	Acquired By:	System
Vial:	4	Date Acquired:	5/28/2008 1:02:38 PM
Injection #:	1	Flow (ml / min) :	5.0
Injection Volume:	100.00 ul	Solvent 1:	**ACN** 90.0 %
Run Time:	25.0 Minutes	Solvent 2:	**Water** 10.0 %
Acq. Method Set:	azeo_0_5	Column:	Luna C18
Compound Name:	compound 1	Channel Name:	2487Channel 1

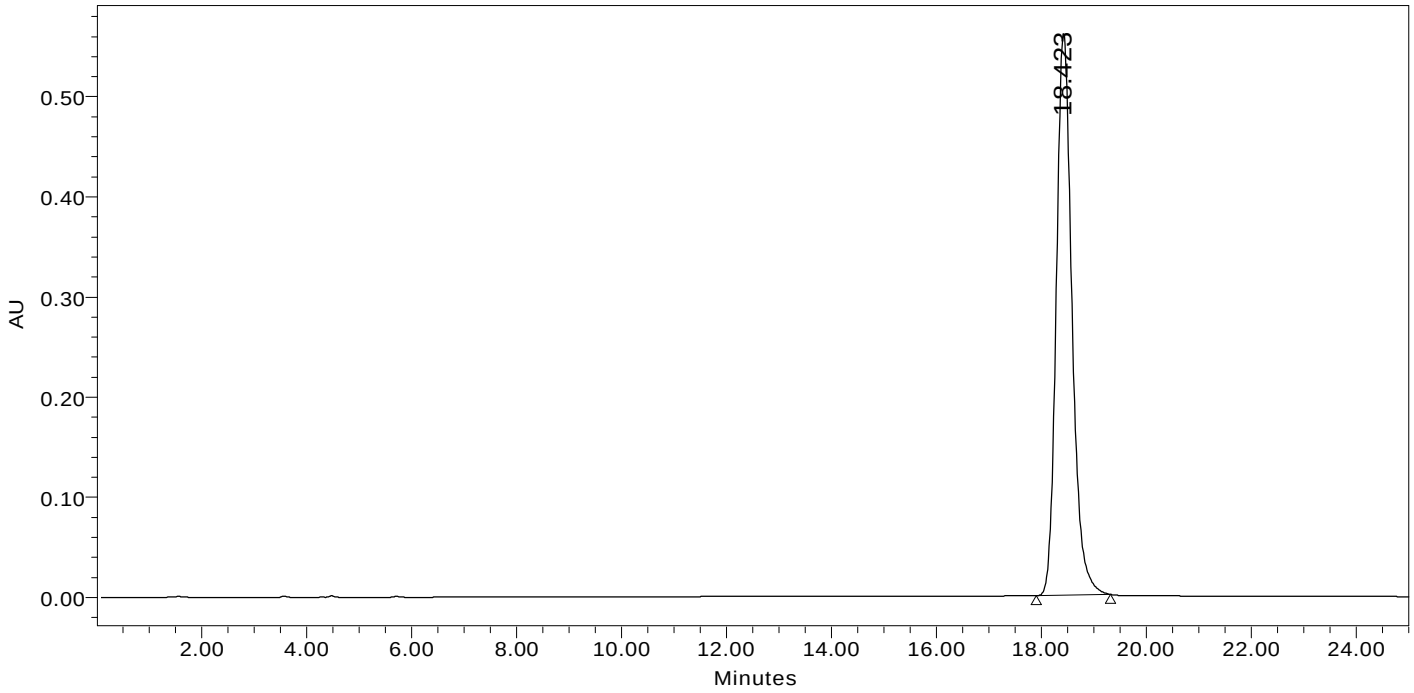


	RT	Area	% Area	Height
1	4.442	90953	1.38	13173
2	14.381	6499332	98.62	340480

Reported by User: System Project Name: LunaC18

SAMPLE INFORMATION

Sample Name:	fluorene-CO-9Me-35ipr2-anal	Acquired By:	System
Vial:	7	Date Acquired:	5/14/2008 9:28:06 AM
Injection #:	1	Flow (ml / min) :	5.0
Injection Volume:	100.00 ul	Solvent 1:	**ACN** 90.0 %
Run Time:	25.0 Minutes	Solvent 2:	**Water** 10.0 %
Acq. Method Set:	azeo_0_5	Column:	Luna C18
Compound Name:	Compound 2	Channel Name:	2487Channel 1

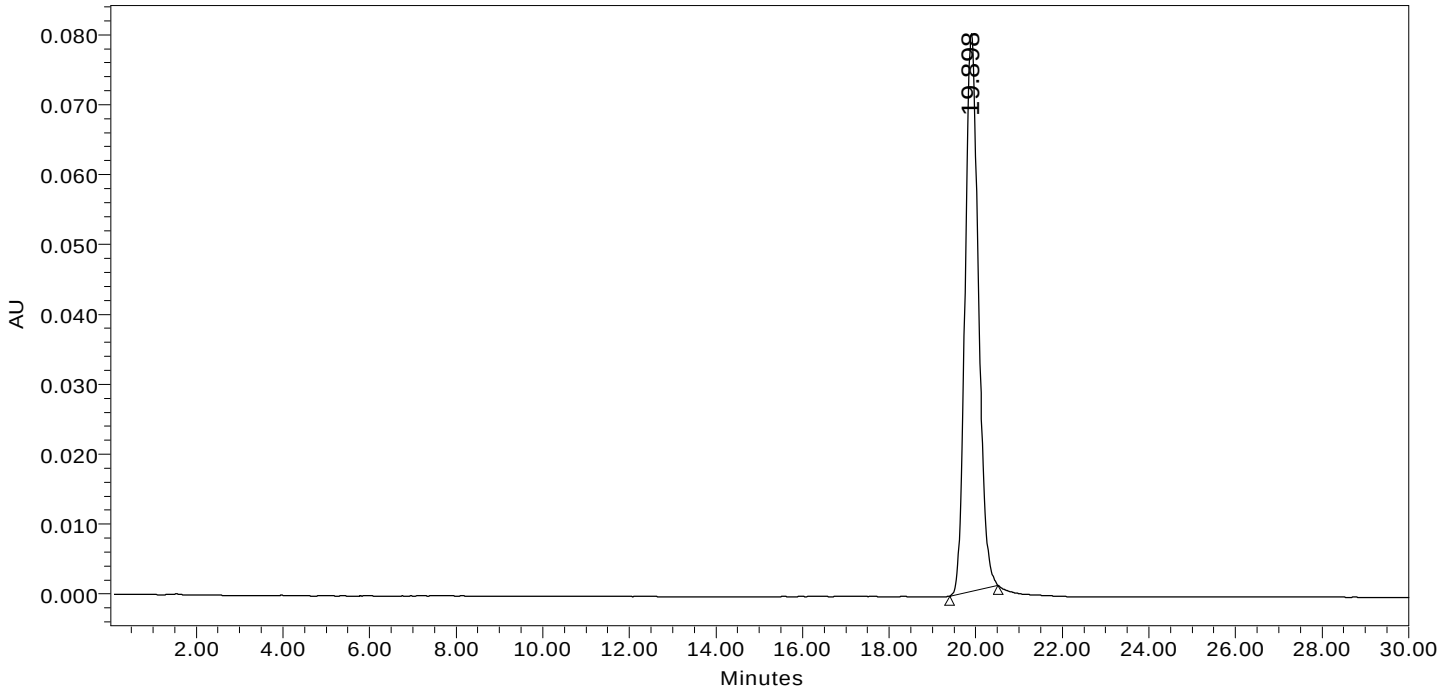


	RT	Area	% Area	Height
1	18.423	11697428	100.00	561290

Reported by User: System Project Name: LunaC8

SAMPLE INFORMATION

Sample Name:	fluorene-9ipr-CO-35ipr2PH-anal	Acquired By:	System
Vial:	2	Date Acquired:	5/14/2008 12:35:17 PM
Injection #:	1	Flow (ml / min) :	5.0
Injection Volume:	100.00 ul	Solvent 1:	**ACN** 90.0 %
Run Time:	30.0 Minutes	Solvent 2:	**Water** 10.0 %
Acq. Method Set:	azeo_0_5	Column:	Luna C8
Compound Name:	compound 3	Channel Name:	2487Channel 1

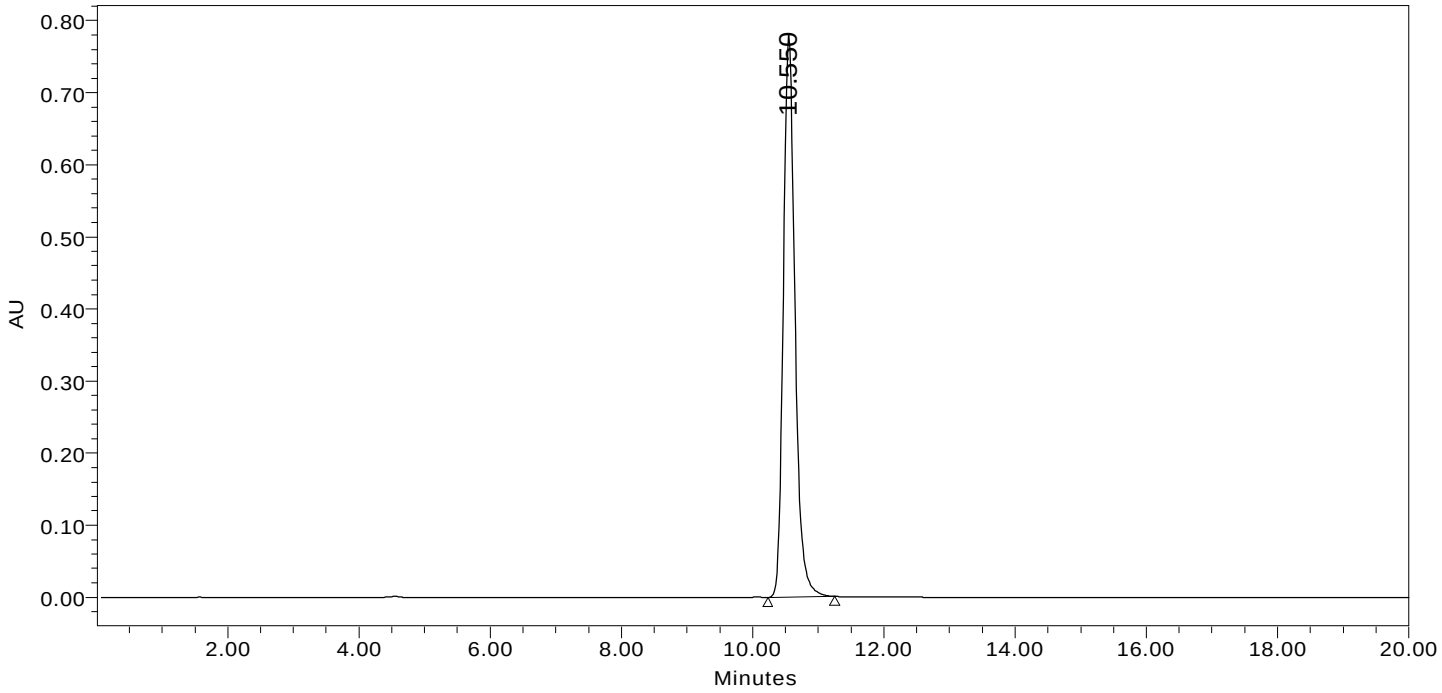


	RT	Area	% Area	Height
1	19.898	1717934	100.00	79795

Reported by User: System Project Name: LunaC18

SAMPLE INFORMATION

Sample Name:	fluorene-CO-9me-mes-anal	Acquired By:	System
Vial:	6	Date Acquired:	4/15/2008 2:30:59 PM
Injection #:	1	Flow (ml / min) :	5.0
Injection Volume:	100.00 ul	Solvent 1:	**ACN** 90.0 %
Run Time:	20.0 Minutes	Solvent 2:	**Water** 10.0 %
Acq. Method Set:	azeo_0_5	Column:	Luna C18
Compound Name:	compound 4	Channel Name:	2487Channel 1

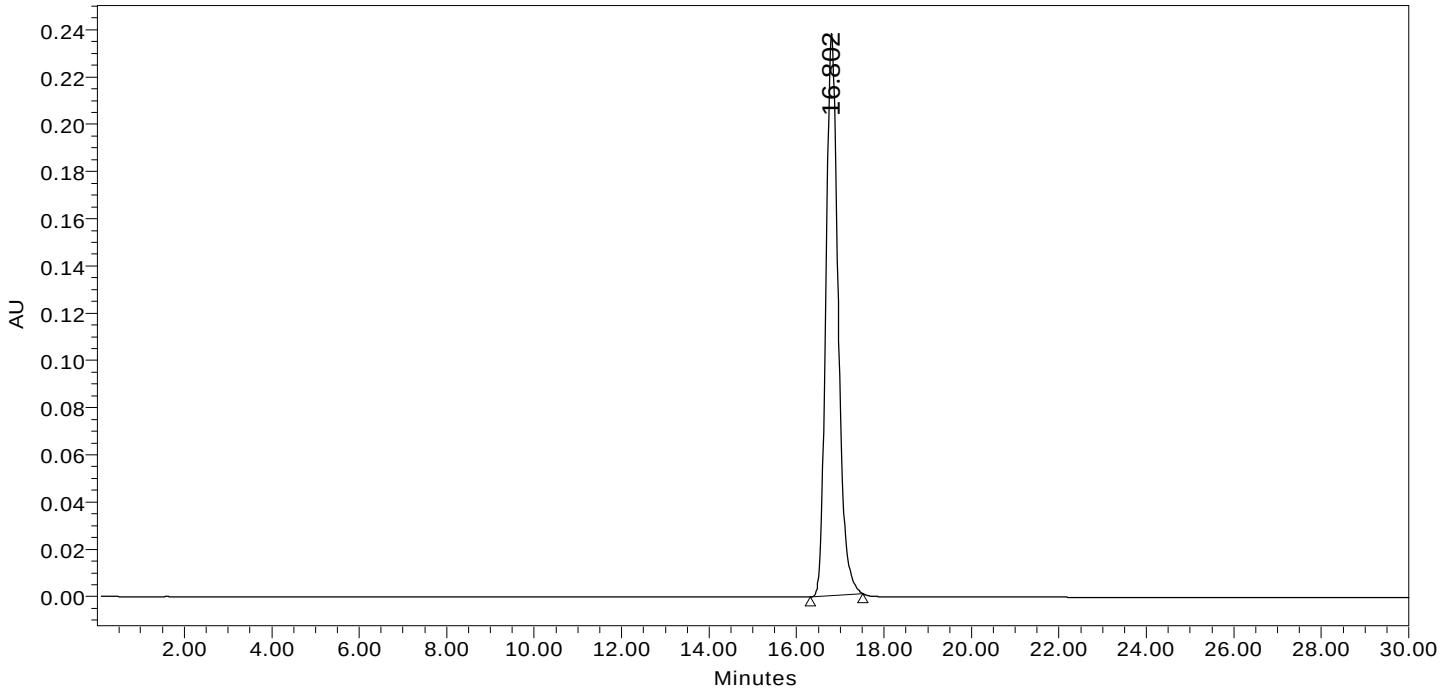


	RT	Area	% Area	Height
1	10.550	9595503	100.00	781032

Reported by User: System Project Name: LunaC18

SAMPLE INFORMATION

Sample Name:	9ipr-flo-comesitile-anal	Acquired By:	System
Vial:	4	Date Acquired:	6/12/2008 1:50:46 PM
Injection #:	1	Flow (ml / min) :	5.0
Injection Volume:	100.00 ul	Solvent 1:	**ACN** 90.0 %
Run Time:	30.0 Minutes	Solvent 2:	**Water** 10.0 %
Acq. Method Set:	azeo_0_5	Column:	Luna C18
Compound Name:	compound 5	Channel Name:	2487Channel 1



	RT	Area	% Area	Height
1	16.802	4640718	100.00	238105

COMPUTATIONAL SECTION

Compound 1 Chemical shift calculations
(only aliphatic signals are tabulated)

^{1}H chemical Shift indicated in Figure 1 are moved upfield by 0.35 ppm

Compound **1** - syn
B3LYP/6-311++G(2d,p)

	Abs. Shield.	C.S. vs TMS	mean value	
C	112,36	70,10	**70,10**	C9
H	26,40	5,42	**5,42**	H9
C	139,91	42,54	**42,21**	CH
C	140,58	41,88		
H	29,21	2,61	**2,46**	CH
H	29,50	2,32		
C	156,14	26,32	**17,08**	Me
C	156,60	25,86		
C	157,21	25,25		
C	156,69	25,77		
H	30,54	1,28	**0,99**	Me_a-1
H	30,54	1,28		
H	30,72	1,10		
H	30,44	1,38		Me_a-2
H	30,69	1,13		
H	30,69	1,13		
H	31,65	0,17		Me_b-1
H	31,07	0,75		
H	31,24	0,58		
H	31,22	0,60		Me_b-2
H	31,07	0,75		
H	31,53	0,29		

Compound **1** - anti
B3LYP/6-311++G(2d,p)

	Abs. Shield.	C.S. vs TMS	mean value	
C	122,07	60,39	**60,39**	C9
H	25,64	6,18	**6,18**	H9
C	139,39	43,07	**43,07**	CH_a
H	28,89	2,93	**2,93**	
C	140,01	42,44	**42,44**	CH_b
H	29,00	2,82	**2,82**	
C	156,41	26,05	**26,34**	Me_a
C	155,83	26,63		
H	30,50	1,32	**1,39**	Me_a-1
H	30,49	1,33		
H	30,50	1,32		
H	30,34	1,48		Me_a-2
H	30,35	1,47		
H	30,38	1,44		
C	156,25	26,21	**26,12**	Me_b
C	156,42	26,04		
H	30,52	1,30	**1,26**	Me_b-1
H	30,59	1,23		
H	30,63	1,19		
H	30,60	1,22		Me_b-2
H	30,56	1,26		
H	30,46	1,36		

Compound 4 Chemical shift calculations

(only aliphatic signals are tabulated)

^{1}H chemical Shift indicated in Figure 5 are moved upfield by 0.46 ppm

Compound **4**
B3LYP/6-311++G(2d,p)

		Abs. Shield.	C.S. vs TMS	mean value	
	C	110,82	71,64	**71,64**	C9
	C	148,27	34,19	**34,19**	Me-9
	H	29,12	2,70	**1,82**	
	H	29,84	1,98		
	H	31,04	0,78		
	C	159,41	23,05	**23,05**	Me-ortho
	H	29,34	2,48	**2,49**	
	H	28,77	3,05		
	H	29,87	1,95		
	C	161,45	21,01	**21,01**	Me-ortho'
	H	30,88	0,93	**1,02**	
	H	30,82	1,00		
	H	30,70	1,12		
	C	159,68	22,78	**22,78**	Me-para
	H	29,43	2,39	**2,16**	
	H	29,69	2,13		
	H	29,87	1,95		

Compound 5 Chemical shift calculations

(only aliphatic signals are tabulated)

^{1}H chemical Shift indicated in Figure 6 are moved upfield by 0.27 ppm

Compound **5** - syn (cis)
B3LYP/6-311++G(2d,p)

	Abs. Shield.	C.S. vs TMS	mean value	
C	102.49	80.96	**80.96**	C9
C	134.27	49.19	**49.19**	CH_9
H	28.52	3.43	**3.43**	
C	161.30	22.15	**22.15**	Me_9-1
H	30.95	1.00	**1.35**	
H	29.98	1.97		
H	30.86	1.09		
C	165.19	18.26	**18.26**	Me_9-2
H	32.24	-0.29	**-0.01**	
H	31.91	0.04		
H	31.72	0.23		
C	160.12	23.33	**23.33**	Me-ortho
H	30.88	1.07	**1.02**	
H	31.09	0.86		
H	30.81	1.14		
C	159.05	24.40	**24.40**	Me-ortho'
H	29.84	2.11	**2.66**	
H	28.70	3.25		
H	29.32	2.63		
C	160.90	22.55	**22.55**	Me-para
H	29.43	2.52	**2.16**	
H	29.94	2.01		
H	30.01	1.94		

Compound **5** - syn (trans)
B3LYP/6-311++G(2d,p)

	Abs. Shield.	C.S. vs TMS	mean value	
C	104.98	78.47	**78.47**	C9
C	136.41	47.04	**47.04**	CH_9
H	29.19	2.76	**2.76**	
C	162.28	21.17	**21.17**	Me_9-1
H	30.33	1.62	**1.69**	
H	29.51	2.44		
H	30.94	1.01		
C	165.22	18.23	**18.23**	Me_9-2
H	31.61	0.34	**0.12**	
H	31.81	0.14		
H	32.09	-0.14		
C	163.03	20.42	**20.42**	Me-ortho
H	31.08	0.88	**0.95**	
H	31.13	0.82		
H	30.79	1.16		
C	160.37	23.08	**23.08**	Me-ortho'
H	29.87	2.08	**2.60**	
H	28.80	3.15		
H	29.38	2.57		
C	160.05	23.40	**23.40**	Me-para
H	29.60	2.35	**2.36**	
H	29.32	2.63		
H	29.84	2.11		

Note: H chemical shift relative to TMS (calculated at the same level of theory) have been shifted upfield by 0.27 ppm.

Compound 1	Method/ basis set	Total Energy (a.u.)	Rel. E. (kcal/mol)	
GS syn	B3LYP/6-31G(d)	-1081.68890321	**0.000**	**full opt.**
GS anti	B3LYP/6-31G(d)	-1081.68721229	**1.061**	**full opt.**
GS syn	B3LYP/6-311++G(2d,p)	-1081.98760557	**0.000**	**full opt.**
GS anti	B3LYP/6-311++G(2d,p)	-1081.98637494	**0.772**	**full opt.**
GS syn, CH2Cl2	B3LYP/6-311++G(2d,p)	-1082.00072525	**0.000**	**single point**
GS anti,CH2Cl2	B3LYP/6-311++G(2d,p)	-1082.00054937	**0.110**	**single point**
GS syn	M05-2X/6-31G(d)	-1081.57963156	**0.000**	**full opt.**
GS anti	M05-2X/6-31G(d)	-1081.57577163	**2.422**	**full opt.**
GS syn	PBE1PBE/6-31G(d)	-1080.41645902	**0.000**	**full opt.**
GS anti	PBE1PBE/6-31G(d)	-1080.41387963	**1.619**	**full opt.**
GS syn	HF(full)/6-31G(d)	-1074.60973184	**0.000**	**full opt.**
GS anti	HF(FULL)/6-31G(d)	-1074.60967200	**0.038**	**full opt.**
GS syn	HF/cc-pVDZ	-1074.69927418	**0.000**	**full opt.**
GS anti	HF/cc-pVDZ	-1074.69714115	**1.338**	**full opt.**
GS syn	MP2(full)/6-31G(d)	-1078.12895150	**0.000**	**single point**
GS anti	MP2(full)/6-31G(d)	-1078.12371878	**3.284**	**single point**
GS syn	CISD(full)/6-31G(d)	-1076.83280110	**0.000**	**single point**
GS anti	CISD(FULL)/6-31G(d)	-1076.83071840	**1.307**	**single point**

Summary of DFT calculated energies for 1-5

	Method/ basis set	Total Energy (a.u.)	**Rel. E. (kcal/mol)**	**G° after ZPE corr.**	img freq
Compound 1					
GS syn	B3LYP/6-311++G(2d,p)	-1081.98760557	**0.00**	**0.00**	0
GS anti	B3LYP/6-311++G(2d,p)	-1081.98637494	**0.77**	**0.42**	0
TS Fluorene-CO rotation	B3LYP/6-311++G(2d,p)	-1081.97696372	**6.68**	**7.37**	1
TS Ph-CO rotation on syn	B3LYP/6-311++G(2d,p)	-1081.97997975	**4.79**	**5.59**	1
TS Ph-CO rotation on anti	B3LYP/6-311++G(2d,p)	-1081.97585029	**7.38**	**7.00**	1
Compound 2					
GS syn	B3LYP/6-31G(d)	-1121.00145471	**0.00**	**0.00**	0
GS anti	B3LYP/6-31G(d)	-1120.99053083	**6.85**	**6.01**	0
TS Ph-CO rotation on syn	B3LYP/6-31G(d)	-1120.99435692	**4.45**	**4.78**	1
TS Fluorene-CO rotation	B3LYP/6-31G(d)	-1120.98969011	**7.38**	**7.36**	1
Compound 3					
GS syn	B3LYP/6-31G(d)	-1199.62296792	**0.00**	**0.00**	0
GS anti	B3LYP/6-31G(d)	-1199.61376777	**5.77**	**5.09**	0
TS Ph-CO rotation on syn	B3LYP/6-31G(d)	-1199.61636314	**4.14**	**4.66**	1
TS isopropyl rotation	B3LYP/6-31G(d)	-1199.61049457	**7.83**	**9.04**	1
Compound 4					
GS syn	B3LYP/6-31G(d)	-1003.05385494	**0.00**	**0.00**	0
correlated TS 0°-90°	B3LYP/6-31G(d)	-1003.03483411	**11.94**	**13.68**	1
correlated TS 90°-90°	B3LYP/6-31G(d)	-1003.04706022	**4.26**	**6.50**	1
Compound 5					
GS syn(trans)	B3LYP/6-31G(d)	-1081.67340926	**0.00**	**0.00**	0
GS syn(cis)	B3LYP/6-31G(d)	-1081.67311416	**0.19**	**0.15**	0
correlated TS 0°-90°	B3LYP/6-31G(d)	-1081.65277085	**12.95**	**15.59**	1
correlated TS 90°-90°	B3LYP/6-31G(d)	-1081.66573106	**4.82**	**7.19**	1

Compound 1 – Ground State syn

Method: b3lyp/6-311++g(2d,p)
SCF Done: E(RB+HF-LYP) = -1081.98760557 A.U. after 16 cycles
Imaginary frequencies: 0 (9.7)

This molecule is an asymmetric top.
Rotational symmetry number 1.
Warning -- assumption of classical behavior for rotation
may cause significant error
Rotational temperatures (Kelvin) 0.01267 0.00643 0.00639
Rotational constants (GHZ): 0.26398 0.13404 0.13315
Zero-point vibrational energy 1169314.4 (Joules/Mol)
279.47286 (Kcal/Mol)
Warning -- explicit consideration of 39 degrees of freedom as
vibrations may cause significant error

Zero-point correction= 0.445368 (Hartree/Particle)
Thermal correction to Energy= 0.469870
Thermal correction to Enthalpy= 0.470814
Thermal correction to Gibbs Free Energy= 0.388954
Sum of electronic and zero-point Energies= -1081.542237
Sum of electronic and thermal Energies= -1081.517736
Sum of electronic and thermal Enthalpies= -1081.516792
Sum of electronic and thermal Free Energies= -1081.598651

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.770040	-1.737368	-2.266456
2	1	0	1.037862	-1.765052	-3.065528
3	6	0	2.537276	-2.865139	-1.975636
4	1	0	2.395947	-3.773336	-2.549167
5	6	0	3.487681	-2.833391	-0.955075
6	1	0	4.077384	-3.717909	-0.745289
7	6	0	3.686635	-1.678022	-0.204687
8	1	0	4.429745	-1.661174	0.584270
9	6	0	3.632206	1.313486	1.181544
10	1	0	4.384810	0.722197	1.690367
11	6	0	3.389017	2.626543	1.574309
12	1	0	3.953672	3.055283	2.393731
13	6	0	2.425664	3.397577	0.923711
14	1	0	2.250001	4.417940	1.242707
15	6	0	1.304024	0.774006	-1.668033
16	6	0	1.689139	2.868113	-0.135559
17	1	0	0.946494	3.474296	-0.641941
18	6	0	1.962660	-0.586888	-1.518396
19	6	0	1.925272	1.559759	-0.525920
20	6	0	2.917671	-0.551877	-0.486885
21	6	0	2.894194	0.778873	0.128593
22	6	0	-1.118712	0.298620	-0.683231
23	6	0	-0.629673	-0.257165	0.500582
24	1	0	0.435840	-0.342206	0.655822
25	6	0	-2.500821	0.399092	-0.875463
26	1	0	-2.849788	0.832411	-1.803880
27	6	0	-0.233788	0.800460	-1.781413

28	6	0	-1.499895	-0.711591	1.490977
29	6	0	-2.871437	-0.594105	1.266085
30	1	0	-3.558419	-0.944116	2.031356
31	6	0	-3.394652	-0.043667	0.092805
32	6	0	-4.898643	0.060322	-0.107666
33	1	0	-5.367469	-0.342554	0.796408
34	6	0	-0.978902	-1.323060	2.782426
35	1	0	-1.855546	-1.576769	3.387679
36	1	0	1.627290	1.216636	-2.615728
37	6	0	-0.133814	-0.326157	3.591891
38	1	0	0.769131	-0.035935	3.049330
39	1	0	0.176603	-0.770141	4.541401
40	1	0	-0.697134	0.583628	3.810149
41	6	0	-0.203929	-2.625937	2.525322
42	1	0	-0.817058	-3.350983	1.985792
43	1	0	0.107346	-3.079732	3.469911
44	1	0	0.694901	-2.443018	1.931387
45	6	0	-5.377792	-0.792082	-1.294074
46	1	0	-4.952269	-0.435343	-2.235305
47	1	0	-6.466385	-0.748422	-1.383208
48	1	0	-5.088330	-1.838130	-1.172530
49	6	0	-5.357960	1.519953	-0.254673
50	1	0	-4.935741	1.979058	-1.151910
51	1	0	-5.049869	2.120397	0.603994
52	1	0	-6.446836	1.573810	-0.334454
53	8	0	-0.716367	1.253378	-2.803229

Compound 1 – Ground State anti

Method: b3lyp/6-311++g(2d,p)
SCF Done: E(RB+HF-LYP) = -1081.98637494 A.U. after 15 cycles
Imaginary frequencies: 0 (9.6)

This molecule is an asymmetric top.
Rotational symmetry number 1.
Warning -- assumption of classical behavior for rotation
may cause significant error
Rotational temperatures (Kelvin) 0.01272 0.00543 0.00496
Rotational constants (GHZ): 0.26506 0.11320 0.10337
Zero-point vibrational energy 1168741.5 (Joules/Mol)
279.33592 (Kcal/Mol)
Warning -- explicit consideration of 39 degrees of freedom as
vibrations may cause significant error

Zero-point correction= 0.445150 (Hartree/Particle)
Thermal correction to Energy= 0.469692
Thermal correction to Enthalpy= 0.470636
Thermal correction to Gibbs Free Energy= 0.388397
Sum of electronic and zero-point Energies= -1081.541225
Sum of electronic and thermal Energies= -1081.516683
Sum of electronic and thermal Enthalpies= -1081.515739
Sum of electronic and thermal Free Energies= -1081.597978

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.877678	-1.728887	-1.877227
2	1	0	2.039638	-2.076903	-2.470270
3	6	0	4.149780	-2.259673	-2.085000
4	1	0	4.299029	-3.015436	-2.846887
5	6	0	5.231827	-1.830279	-1.316508
6	1	0	6.213760	-2.254569	-1.489849
7	6	0	5.061483	-0.865045	-0.329222
8	1	0	5.906497	-0.537013	0.265059
9	6	0	3.999212	1.407100	1.795473
10	1	0	5.061218	1.259908	1.954098
11	6	0	3.296792	2.329351	2.566086
12	1	0	3.815624	2.900210	3.327106
13	6	0	1.931246	2.523826	2.369185
14	1	0	1.396978	3.242781	2.978715
15	6	0	1.443477	-0.028302	-0.498369
16	6	0	1.243501	1.798348	1.395196
17	1	0	0.180493	1.953414	1.256113
18	6	0	2.705335	-0.766665	-0.896158
19	6	0	1.940447	0.881276	0.624339
20	6	0	3.791167	-0.334386	-0.121175
21	6	0	3.317527	0.680105	0.824456
22	6	0	-1.117761	-0.469010	-0.119339
23	6	0	-2.104581	-1.264997	0.470897
24	1	0	-1.785044	-2.169965	0.971516
25	6	0	-1.491062	0.706379	-0.776542
26	1	0	-0.739544	1.332780	-1.238634
27	6	0	0.302167	-0.947756	-0.021199
28	6	0	-3.446558	-0.907146	0.415087
29	6	0	-3.784712	0.273201	-0.253731
30	1	0	-4.830164	0.563181	-0.307439
31	6	0	-2.829823	1.091816	-0.855593
32	6	0	-3.247353	2.363848	-1.577613
33	1	0	-4.336538	2.431914	-1.489994
34	6	0	-4.523713	-1.765939	1.059030
35	1	0	-5.482164	-1.274218	0.861510
36	1	0	1.093148	0.576781	-1.338822
37	6	0	-4.352207	-1.846539	2.584881
38	1	0	-3.413642	-2.338050	2.852550
39	1	0	-5.168113	-2.420072	3.032194
40	1	0	-4.348500	-0.852177	3.036614
41	6	0	-4.586998	-3.169097	0.434485
42	1	0	-4.745114	-3.115580	-0.644806
43	1	0	-5.406996	-3.745425	0.870386
44	1	0	-3.661385	-3.722880	0.609132
45	6	0	-2.909742	2.311342	-3.076739
46	1	0	-1.830030	2.261919	-3.239614
47	1	0	-3.280233	3.205037	-3.585238
48	1	0	-3.359130	1.437784	-3.553593
49	6	0	-2.653937	3.621081	-0.921192
50	1	0	-1.563166	3.630676	-0.992667
51	1	0	-2.920356	3.679120	0.136318
52	1	0	-3.024672	4.522919	-1.414899
53	8	0	0.553657	-2.037479	0.447545

Compound 1 – Transition State Fluorene-CO rotation

Method: b3lyp/6-311++g(2d,p)
SCF Done: E(RB+HF-LYP) = -1081.97696372 A.U. after 9 cycles
Imaginary frequencies: 1 (-35.7)

This molecule is an asymmetric top.
Rotational symmetry number 1.
Warning -- assumption of classical behavior for rotation
may cause significant error
Rotational temperatures (Kelvin) 0.01303 0.00597 0.00532
Rotational constants (GHZ): 0.27152 0.12448 0.11086
1 imaginary frequencies ignored.
Zero-point vibrational energy 1166819.3 (Joules/Mol)
278.87652 (Kcal/Mol)
Warning -- explicit consideration of 38 degrees of freedom as
vibrations may cause significant error

Zero-point correction= 0.444418 (Hartree/Particle)
Thermal correction to Energy= 0.468202
Thermal correction to Enthalpy= 0.469146
Thermal correction to Gibbs Free Energy= 0.390014
Sum of electronic and zero-point Energies= -1081.532546
Sum of electronic and thermal Energies= -1081.508762
Sum of electronic and thermal Enthalpies= -1081.507818
Sum of electronic and thermal Free Energies= -1081.586950

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.537830	0.889311	1.858118
2	1	0	-0.431179	0.428901	2.002653
3	6	0	0.818628	2.117809	2.456152
4	1	0	0.063494	2.602243	3.063554
5	6	0	2.061151	2.725096	2.282664
6	1	0	2.262963	3.679975	2.753643
7	6	0	3.047959	2.108197	1.520272
8	1	0	4.019337	2.574672	1.403790
9	6	0	4.953911	0.132282	-0.264645
10	1	0	5.519801	1.021377	-0.011430
11	6	0	5.547008	-0.892534	-0.995087
12	1	0	6.578307	-0.798423	-1.314370
13	6	0	4.826513	-2.042022	-1.316706
14	1	0	5.302790	-2.832082	-1.885016
15	6	0	1.489985	-1.060889	0.356684
16	6	0	3.497869	-2.186586	-0.917548
17	1	0	2.940613	-3.074835	-1.181224
18	6	0	1.510744	0.279034	1.080327
19	6	0	2.902429	-1.164857	-0.193118
20	6	0	2.771892	0.880217	0.925473
21	6	0	3.628399	-0.008691	0.136053
22	6	0	-0.972542	-0.686917	-0.516486
23	6	0	-1.972249	-1.406029	0.133560
24	1	0	-1.749493	-2.393064	0.523750
25	6	0	-1.243581	0.572135	-1.044456
26	1	0	-0.454711	1.119801	-1.547115

27	6	0	0.385599	-1.311652	-0.700273
28	6	0	-3.255316	-0.873076	0.268755
29	6	0	-3.502892	0.388947	-0.271881
30	1	0	-4.498896	0.811613	-0.178638
31	6	0	-2.519323	1.125175	-0.934698
32	6	0	-2.842120	2.490705	-1.520635
33	1	0	-3.897647	2.685035	-1.303208
34	6	0	-4.363657	-1.645193	0.967240
35	1	0	-5.254271	-1.008642	0.941755
36	1	0	1.310440	-1.861825	1.090490
37	6	0	-4.036102	-1.917803	2.444377
38	1	0	-3.161233	-2.565372	2.545478
39	1	0	-4.874631	-2.416015	2.937685
40	1	0	-3.829023	-0.989961	2.982028
41	6	0	-4.707442	-2.948299	0.227355
42	1	0	-4.972797	-2.753794	-0.813752
43	1	0	-5.552085	-3.450188	0.706508
44	1	0	-3.863057	-3.642223	0.231351
45	6	0	-2.676010	2.511104	-3.048877
46	1	0	-1.635857	2.341501	-3.338357
47	1	0	-2.979655	3.479761	-3.454231
48	1	0	-3.283638	1.737690	-3.523258
49	6	0	-2.022028	3.609581	-0.858302
50	1	0	-0.952973	3.485541	-1.046980
51	1	0	-2.168324	3.619667	0.223758
52	1	0	-2.318526	4.585484	-1.251431
53	8	0	0.585040	-2.062140	-1.625417

Compound 1 – Transition State Phenyl-CO rotation of syn conformer

Method: b3lyp/6-311++g(2d,p)
SCF Done: E(RB+HF-LYP) = -1081.97997975 A.U. after 9 cycles
Imaginary frequencies: 1 (-30.1)

This molecule is an asymmetric top.
Rotational symmetry number 1.
Warning -- assumption of classical behavior for rotation
may cause significant error
Rotational temperatures (Kelvin) 0.01015 0.00931 0.00633
Rotational constants (GHZ): 0.21141 0.19402 0.13193
1 imaginary frequencies ignored.
Zero-point vibrational energy 1176973.9 (Joules/Mol)
281.30350 (Kcal/Mol)
Warning -- explicit consideration of 38 degrees of freedom as
vibrations may cause significant error

Zero-point correction= 0.444666 (Hartree/Particle)
Thermal correction to Energy= 0.468490
Thermal correction to Enthalpy= 0.469434
Thermal correction to Gibbs Free Energy= 0.390233
Sum of electronic and zero-point Energies= -1081.535314
Sum of electronic and thermal Energies= -1081.511490
Sum of electronic and thermal Enthalpies= -1081.510546
Sum of electronic and thermal Free Energies= -1081.589746

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.406269	2.261241	1.013307
2	1	0	2.142581	2.626998	1.999643
3	6	0	2.895838	3.137734	0.045315
4	1	0	3.010960	4.189011	0.280642
5	6	0	3.242674	2.670983	-1.222739
6	1	0	3.620748	3.365790	-1.963311
7	6	0	3.116629	1.322696	-1.543663
8	1	0	3.398669	0.967788	-2.528110
9	6	0	2.684133	-1.945682	-1.606647
10	1	0	3.055004	-1.639155	-2.577835
11	6	0	2.453965	-3.291621	-1.338238
12	1	0	2.642762	-4.032093	-2.106473
13	6	0	1.992339	-3.700093	-0.086844
14	1	0	1.831123	-4.753531	0.108403
15	6	0	1.784952	-0.225390	1.566688
16	6	0	1.741774	-2.763708	0.915628
17	1	0	1.389390	-3.086947	1.889109
18	6	0	2.273035	0.919218	0.693765
19	6	0	1.959011	-1.421100	0.647933
20	6	0	2.632329	0.443986	-0.578483
21	6	0	2.438653	-1.008739	-0.606519
22	6	0	-0.782169	0.098084	1.069994
23	6	0	-1.466077	-1.044432	0.659721
24	1	0	-1.152208	-2.013441	1.027498
25	6	0	-1.183211	1.351498	0.611619
26	1	0	-0.648444	2.233583	0.941867
27	6	0	0.344029	-0.010127	2.068998
28	6	0	-2.553683	-0.949003	-0.208442
29	6	0	-2.932406	0.317144	-0.654352
30	1	0	-3.777936	0.403060	-1.330652
31	6	0	-2.265769	1.477000	-0.259097
32	6	0	-2.714061	2.836478	-0.772112
33	1	0	-3.599371	2.662296	-1.392670
34	6	0	-3.311830	-2.186597	-0.663187
35	1	0	-4.123296	-1.838251	-1.310659
36	1	0	2.394035	-0.323096	2.469497
37	6	0	-3.953939	-2.935363	0.516075
38	1	0	-3.195840	-3.322702	1.201387
39	1	0	-4.541614	-3.784273	0.156972
40	1	0	-4.615012	-2.280551	1.087597
41	6	0	-2.425527	-3.125265	-1.498201
42	1	0	-2.004571	-2.606693	-2.362086
43	1	0	-3.005241	-3.978175	-1.861215
44	1	0	-1.592719	-3.513980	-0.907089
45	6	0	-1.646412	3.488936	-1.666034
46	1	0	-0.731011	3.693122	-1.105299
47	1	0	-2.010669	4.437518	-2.069632
48	1	0	-1.383201	2.840888	-2.504661
49	6	0	-3.132305	3.778163	0.368367
50	1	0	-2.287069	4.019077	1.017924
51	1	0	-3.910051	3.327396	0.988281
52	1	0	-3.518810	4.718302	-0.033757
53	8	0	0.127794	0.088976	3.255939

Compound 1 – Transition State Phenyl-CO rotation of anti conformer

Method: b3lyp/6-311++g(2d,p)
SCF Done: E(RB+HF-LYP) = -1081.97585029 A.U. after 9 cycles
Imaginary frequencies: 1 (-26.9)

This molecule is an asymmetric top.
Rotational symmetry number 1.
Warning -- assumption of classical behavior for rotation
may cause significant error
Rotational temperatures (Kelvin) 0.01218 0.00624 0.00441
Rotational constants (GHZ): 0.25373 0.12998 0.09196
1 imaginary frequencies ignored.
Zero-point vibrational energy 1166571.9 (Joules/Mol)
278.81737 (Kcal/Mol)
Warning -- explicit consideration of 38 degrees of freedom as
vibrations may cause significant error

Zero-point correction= 0.444324 (Hartree/Particle)
Thermal correction to Energy= 0.468278
Thermal correction to Enthalpy= 0.469222
Thermal correction to Gibbs Free Energy= 0.388355
Sum of electronic and zero-point Energies= -1081.531527
Sum of electronic and thermal Energies= -1081.507572
Sum of electronic and thermal Enthalpies= -1081.506628
Sum of electronic and thermal Free Energies= -1081.587495

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.165699	-2.573076	-0.293648
2	1	0	1.172307	-2.987954	-0.423073
3	6	0	3.264834	-3.422817	-0.173024
4	1	0	3.121274	-4.496064	-0.208966
5	6	0	4.547195	-2.901970	-0.004562
6	1	0	5.390469	-3.575691	0.090692
7	6	0	4.754044	-1.526655	0.040074
8	1	0	5.754313	-1.129289	0.167534
9	6	0	4.565738	1.757078	-0.003557
10	1	0	5.604346	1.478445	0.131603
11	6	0	4.205796	3.098841	-0.086080
12	1	0	4.967772	3.865500	-0.010675
13	6	0	2.874001	3.466508	-0.270669
14	1	0	2.610397	4.515033	-0.340462
15	6	0	1.348238	-0.080998	-0.348317
16	6	0	1.877969	2.494845	-0.367909
17	1	0	0.846736	2.791719	-0.519315
18	6	0	2.367740	-1.203576	-0.246176
19	6	0	2.231318	1.158323	-0.277201
20	6	0	3.658322	-0.677186	-0.082557
21	6	0	3.573871	0.785639	-0.100609
22	6	0	-1.145854	-0.064210	0.434625
23	6	0	-1.851968	-1.249856	0.245824
24	1	0	-1.341812	-2.198302	0.371450
25	6	0	-1.790876	1.162075	0.297737
26	1	0	-1.235916	2.077965	0.464556

27	6	0	0.315377	-0.122411	0.808042
28	6	0	-3.208525	-1.224732	-0.079852
29	6	0	-3.831076	0.016851	-0.212646
30	1	0	-4.886755	0.048516	-0.465123
31	6	0	-3.147388	1.218567	-0.025897
32	6	0	-3.872289	2.547394	-0.169098
33	1	0	-4.914366	2.313013	-0.409800
34	6	0	-3.999467	-2.508453	-0.275766
35	1	0	-5.026138	-2.211665	-0.513888
36	1	0	0.808429	-0.121275	-1.298258
37	6	0	-4.050822	-3.353394	1.007682
38	1	0	-3.055558	-3.701058	1.295929
39	1	0	-4.680530	-4.234635	0.860364
40	1	0	-4.457360	-2.779961	1.843190
41	6	0	-3.474306	-3.334777	-1.461278
42	1	0	-3.472083	-2.748963	-2.382953
43	1	0	-4.100128	-4.216693	-1.620034
44	1	0	-2.453176	-3.681818	-1.283218
45	6	0	-3.311276	3.386472	-1.329020
46	1	0	-2.272023	3.671711	-1.146249
47	1	0	-3.889776	4.305609	-1.452208
48	1	0	-3.345243	2.834393	-2.270661
49	6	0	-3.872531	3.348549	1.143237
50	1	0	-2.859453	3.637489	1.434442
51	1	0	-4.300543	2.766902	1.962186
52	1	0	-4.459373	4.264029	1.032220
53	8	0	0.663951	-0.208641	1.959322

Compound 2 – Ground State syn

Method: B3LYP/6-31g(d)
SCF Done: E(RB+HF-LYP) = -1121.00145471 A.U. after 7 cycles
Imaginary frequencies: 0 (11.4)

This molecule is an asymmetric top.
Rotational symmetry number 1.
Warning -- assumption of classical behavior for rotation
may cause significant error
Rotational temperatures (Kelvin) 0.01161 0.00646 0.00622
Rotational constants (GHZ): 0.24193 0.13450 0.12968
Zero-point vibrational energy 1252775.0 (Joules/Mol)
299.42042 (Kcal/Mol)
Warning -- explicit consideration of 43 degrees of freedom as
vibrations may cause significant error

Zero-point correction= 0.477157 (Hartree/Particle)
Thermal correction to Energy= 0.502966
Thermal correction to Enthalpy= 0.503911
Thermal correction to Gibbs Free Energy= 0.420359
Sum of electronic and zero-point Energies= -1120.524298
Sum of electronic and thermal Energies= -1120.498488
Sum of electronic and thermal Enthalpies= -1120.497544
Sum of electronic and thermal Free Energies= -1120.581096

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.696611	-1.150753	-2.541733
2	1	0	-1.035150	-1.940105	-2.890370
3	6	0	-2.356927	-0.325950	-3.459909
4	1	0	-2.204372	-0.476489	-4.525135
5	6	0	-3.211239	0.689969	-3.018128
6	1	0	-3.718013	1.320479	-3.743757
7	6	0	-3.419783	0.902192	-1.652809
8	1	0	-4.086259	1.692423	-1.316365
9	6	0	-3.419763	0.902108	1.652890
10	1	0	-4.086273	1.692340	1.316513
11	6	0	-3.211180	0.689823	3.018195
12	1	0	-3.717941	1.320297	3.743864
13	6	0	-2.356836	-0.326099	3.459910
14	1	0	-2.204251	-0.476680	4.525127
15	6	0	-1.345268	-1.735588	-0.000052
16	6	0	-1.696533	-1.150853	2.541682
17	1	0	-1.035055	-1.940224	2.890243
18	6	0	-1.897753	-0.939857	-1.182618
19	6	0	-1.897727	-0.939891	1.182586
20	6	0	-2.758965	0.083741	-0.734253
21	6	0	-2.758956	0.083708	0.734279
22	6	0	1.122403	-0.674950	-0.000025
23	6	0	0.682209	0.655309	-0.000062
24	1	0	-0.376287	0.874110	-0.000074
25	6	0	2.502132	-0.938257	-0.000033
26	1	0	2.817033	-1.976572	0.000035
27	6	0	0.209296	-1.868807	0.000041

28	6	0	1.594402	1.716461	-0.000091
29	6	0	2.960931	1.415494	-0.000119
30	1	0	3.679149	2.234409	-0.000142
31	6	0	3.437572	0.097184	-0.000108
32	6	0	4.935132	-0.184911	-0.000123
33	1	0	5.446154	0.787809	-0.000297
34	6	0	1.116448	3.163583	-0.000044
35	1	0	2.013358	3.798281	-0.000261
36	6	0	0.312974	3.500979	1.270546
37	1	0	-0.605788	2.906285	1.332569
38	1	0	0.026986	4.559762	1.274960
39	1	0	0.899453	3.302382	2.174334
40	6	0	0.312359	3.500878	-1.270258
41	1	0	0.898357	3.302168	-2.174335
42	1	0	0.026391	4.559666	-1.274648
43	1	0	-0.606452	2.906200	-1.331748
44	6	0	5.375591	-0.937651	-1.269734
45	1	0	4.911209	-1.929162	-1.324727
46	1	0	6.463149	-1.077798	-1.277657
47	1	0	5.095672	-0.387018	-2.174547
48	6	0	5.375708	-0.937261	1.269663
49	1	0	4.911310	-1.928748	1.325022
50	1	0	5.095905	-0.386348	2.174344
51	1	0	6.463265	-1.077431	1.277507
52	8	0	0.691829	-2.992192	0.000234
53	6	0	-1.957258	-3.157870	-0.000055
54	1	0	-1.635608	-3.716062	-0.882934
55	1	0	-1.635691	-3.716030	0.882874
56	1	0	-3.049015	-3.086790	-0.000104

Compound 2 – Ground State anti

Method: B3LYP/6-31g(d)
SCF Done: E(RB+HF-LYP) = -1120.99053083 A.U. after 8 cycles
Imaginary frequencies: 0 (12.3)

This molecule is an asymmetric top.
Rotational symmetry number 1.
Warning -- assumption of classical behavior for rotation
may cause significant error
Rotational temperatures (Kelvin) 0.01200 0.00567 0.00449
Rotational constants (GHZ): 0.25006 0.11805 0.09354
Zero-point vibrational energy 1251193.4 (Joules/Mol)
299.04241 (Kcal/Mol)
Warning -- explicit consideration of 42 degrees of freedom as
vibrations may cause significant error

Zero-point correction= 0.476554 (Hartree/Particle)
Thermal correction to Energy= 0.502616
Thermal correction to Enthalpy= 0.503560
Thermal correction to Gibbs Free Energy= 0.419017
Sum of electronic and zero-point Energies= -1120.513976
Sum of electronic and thermal Energies= -1120.487915
Sum of electronic and thermal Enthalpies= -1120.486970
Sum of electronic and thermal Free Energies= -1120.571514

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.587655	-2.277454	1.298973
2	1	0	-1.690515	-2.665927	1.774504
3	6	0	-3.769454	-3.025718	1.315813
4	1	0	-3.787607	-3.992005	1.812691
5	6	0	-4.926753	-2.542184	0.695634
6	1	0	-5.837282	-3.135134	0.716500
7	6	0	-4.920683	-1.305234	0.048870
8	1	0	-5.821248	-0.933436	-0.433249
9	6	0	-4.254776	1.626980	-1.273438
10	1	0	-5.290334	1.373216	-1.484959
11	6	0	-3.719123	2.835446	-1.724068
12	1	0	-4.341405	3.524469	-2.288884
13	6	0	-2.387460	3.161927	-1.456411
14	1	0	-1.977823	4.101912	-1.816073
15	6	0	-1.432378	-0.034604	0.549525
16	6	0	-1.571020	2.285391	-0.730904
17	1	0	-0.535192	2.553391	-0.547801
18	6	0	-2.578892	-1.045571	0.656020
19	6	0	-2.098195	1.081835	-0.274501
20	6	0	-3.740000	-0.559609	0.032067
21	6	0	-3.441814	0.751751	-0.552559
22	6	0	1.185851	-0.310103	-0.094955
23	6	0	2.113231	-1.298244	-0.465339
24	1	0	1.723259	-2.242682	-0.829969
25	6	0	1.664388	0.930327	0.349543
26	1	0	0.971966	1.717285	0.618735
27	6	0	-0.266932	-0.682413	-0.270507
28	6	0	3.488643	-1.078735	-0.376810
29	6	0	3.927976	0.173406	0.073201
30	1	0	4.998227	0.362305	0.143311
31	6	0	3.037834	1.191508	0.430270
32	6	0	3.559428	2.545185	0.898022
33	1	0	4.656122	2.493691	0.864159
34	6	0	4.490359	-2.159211	-0.765315
35	1	0	5.493658	-1.742229	-0.601418
36	6	0	4.381921	-2.528248	-2.256985
37	1	0	3.402435	-2.961724	-2.489854
38	1	0	5.146788	-3.265987	-2.527355
39	1	0	4.516587	-1.647487	-2.894275
40	6	0	4.358590	-3.408801	0.125282
41	1	0	4.475096	-3.155710	1.184879
42	1	0	5.123755	-4.149640	-0.135108
43	1	0	3.378638	-3.884223	0.000420
44	6	0	3.158845	2.843897	2.355231
45	1	0	2.070615	2.931745	2.460258
46	1	0	3.600893	3.789253	2.691578
47	1	0	3.496146	2.049998	3.030400
48	6	0	3.125501	3.687218	-0.040074
49	1	0	2.036428	3.817478	-0.034398
50	1	0	3.433433	3.491918	-1.072891
51	1	0	3.572605	4.636938	0.276622
52	8	0	-0.546403	-1.557839	-1.072921
53	6	0	-1.052538	0.434176	1.976111
54	1	0	-0.542557	-0.364842	2.525510

55	1	0	-0.405423	1.312030	1.981711
56	1	0	-1.965418	0.690601	2.522144

Compound 2 – Transition State Fluorene-CO rotation

Method: b3lyp/6-31g(d)
SCF Done: E(RB+HF-LYP) = -1120.98969011 A.U. after 8 cycles
Imaginary frequencies: 1 (-25.7)

This molecule is an asymmetric top.
Rotational symmetry number 1.
Warning -- assumption of classical behavior for rotation
may cause significant error
Rotational temperatures (Kelvin) 0.01227 0.00582 0.00527
Rotational constants (GHZ): 0.25568 0.12118 0.10977
1 imaginary frequencies ignored.
Zero-point vibrational energy 1250457.5 (Joules/Mol)
298.86652 (Kcal/Mol)
Warning -- explicit consideration of 41 degrees of freedom as
vibrations may cause significant error

Zero-point correction= 0.476274 (Hartree/Particle)
Thermal correction to Energy= 0.501548
Thermal correction to Enthalpy= 0.502492
Thermal correction to Gibbs Free Energy= 0.420329
Sum of electronic and zero-point Energies= -1120.513416
Sum of electronic and thermal Energies= -1120.488142
Sum of electronic and thermal Enthalpies= -1120.487198
Sum of electronic and thermal Free Energies= -1120.569361

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.462193	0.634302	1.956320
2	1	0	-0.489534	0.116597	2.020871
3	6	0	0.694546	1.763222	2.751246
4	1	0	-0.081488	2.110268	3.428203
5	6	0	1.913097	2.444938	2.683352
6	1	0	2.078102	3.319922	3.306578
7	6	0	2.923548	2.003356	1.826817
8	1	0	3.875606	2.526284	1.785188
9	6	0	4.894421	0.449889	-0.285801
10	1	0	5.428007	1.303981	0.123527
11	6	0	5.518589	-0.399530	-1.201213
12	1	0	6.543111	-0.203482	-1.506537
13	6	0	4.835675	-1.500732	-1.727843
14	1	0	5.332843	-2.151600	-2.442090
15	6	0	1.482378	-1.013068	0.149255
16	6	0	3.515968	-1.771779	-1.349124
17	1	0	2.987598	-2.616853	-1.776295
18	6	0	1.459279	0.198400	1.088328
19	6	0	2.891018	-0.928477	-0.436044
20	6	0	2.694359	0.877305	1.034596
21	6	0	3.578277	0.180115	0.093603
22	6	0	-0.995415	-0.496934	-0.666152

23	6	0	-1.937796	-1.342494	-0.071556
24	1	0	-1.656238	-2.355747	0.200834
25	6	0	-1.365929	0.793830	-1.057188
26	1	0	-0.626844	1.435330	-1.529229
27	6	0	0.405340	-0.974239	-0.977758
28	6	0	-3.251000	-0.904810	0.148948
29	6	0	-3.587916	0.398046	-0.234596
30	1	0	-4.603609	0.750781	-0.062297
31	6	0	-2.666335	1.261799	-0.839829
32	6	0	-3.077358	2.671236	-1.246025
33	1	0	-4.137643	2.784295	-0.981455
34	6	0	-4.292397	-1.819707	0.781311
35	1	0	-5.225664	-1.244232	0.848342
36	6	0	-3.903743	-2.232480	2.213598
37	1	0	-2.983312	-2.828548	2.221904
38	1	0	-4.695319	-2.839512	2.668698
39	1	0	-3.739857	-1.354953	2.848818
40	6	0	-4.576044	-3.055884	-0.093261
41	1	0	-4.887121	-2.764582	-1.102197
42	1	0	-5.373200	-3.665432	0.348564
43	1	0	-3.686614	-3.689996	-0.188655
44	6	0	-2.955308	2.889874	-2.765923
45	1	0	-1.913509	2.811303	-3.097905
46	1	0	-3.317620	3.887504	-3.041086
47	1	0	-3.539222	2.148431	-3.321899
48	6	0	-2.290143	3.742236	-0.467195
49	1	0	-1.219089	3.695006	-0.695979
50	1	0	-2.404319	3.610846	0.614333
51	1	0	-2.643568	4.746605	-0.729407
52	8	0	0.670557	-1.342587	-2.104993
53	6	0	1.280527	-2.336461	0.939496
54	1	0	0.308427	-2.355784	1.441572
55	1	0	1.347550	-3.200850	0.270351
56	1	0	2.059073	-2.426604	1.703021

Compound 2 – Transition State Phenyl-CO rotation of syn conformer

Method: B3LYP/6-31g(d)
SCF Done: E(RB+HF-LYP) = -1120.99435692 A.U. after 11 cycles
Imaginary frequencies: 1 (-27.1)

This molecule is an asymmetric top.
Rotational symmetry number 1.
Warning -- assumption of classical behavior for rotation
may cause significant error
Rotational temperatures (Kelvin) 0.00967 0.00887 0.00630
Rotational constants (GHZ): 0.20144 0.18472 0.13122
1 imaginary frequencies ignored.
Zero-point vibrational energy 1250848.5 (Joules/Mol)
298.95996 (Kcal/Mol)
Warning -- explicit consideration of 41 degrees of freedom as
vibrations may cause significant error

Zero-point correction= 0.476423 (Hartree/Particle)
Thermal correction to Energy= 0.501614
Thermal correction to Enthalpy= 0.502558

Thermal correction to Gibbs Free Energy= 0.420887
Sum of electronic and zero-point Energies= -1120.517934
Sum of electronic and thermal Energies= -1120.492743
Sum of electronic and thermal Enthalpies= -1120.491799
Sum of electronic and thermal Free Energies= -1120.573470

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.056514	2.540256	0.654118
2	1	0	1.953164	2.889906	1.678737
3	6	0	2.203723	3.458555	-0.391893
4	1	0	2.216028	4.523529	-0.176366
5	6	0	2.340608	3.015304	-1.712500
6	1	0	2.453357	3.740450	-2.513978
7	6	0	2.342274	1.650851	-2.009798
8	1	0	2.457315	1.313902	-3.036814
9	6	0	2.340801	-1.652510	-2.010004
10	1	0	2.456177	-1.315531	-3.036973
11	6	0	2.337925	-3.016997	-1.712880
12	1	0	2.450057	-3.742141	-2.514447
13	6	0	2.200635	-3.460293	-0.392330
14	1	0	2.212014	-4.525303	-0.176935
15	6	0	1.912195	-0.000850	1.319888
16	6	0	2.054212	-2.541994	0.653792
17	1	0	1.950563	-2.891688	1.678366
18	6	0	2.049684	1.180495	0.360548
19	6	0	2.048558	-1.182189	0.360399
20	6	0	2.199335	0.732707	-0.967489
21	6	0	2.198656	-0.734373	-0.967580
22	6	0	-0.724136	0.000331	1.072851
23	6	0	-1.312437	-1.209422	0.690479
24	1	0	-0.854299	-2.144509	0.997681
25	6	0	-1.311568	1.210474	0.690359
26	1	0	-0.852745	2.145256	0.997472
27	6	0	0.495608	0.000040	1.968664
28	6	0	-2.477373	-1.224629	-0.085694
29	6	0	-3.038515	0.001091	-0.462091
30	1	0	-3.942717	0.001390	-1.068977
31	6	0	-2.476472	1.226444	-0.085837
32	6	0	-3.112758	2.539020	-0.525134
33	1	0	-4.026248	2.283240	-1.079508
34	6	0	-3.114669	-2.536793	-0.524769
35	1	0	-4.027778	-2.280387	-1.079482
36	6	0	-3.534900	-3.408191	0.673444
37	1	0	-2.666050	-3.725274	1.262270
38	1	0	-4.049672	-4.313158	0.329030
39	1	0	-4.210306	-2.864121	1.342523
40	6	0	-2.196795	-3.319281	-1.483987
41	1	0	-1.935618	-2.716345	-2.360537
42	1	0	-2.692141	-4.233861	-1.832124
43	1	0	-1.260907	-3.609851	-0.992418
44	6	0	-2.194453	3.320384	-1.484864
45	1	0	-1.258220	3.610372	-0.993603
46	1	0	-2.689119	4.235239	-1.833246
47	1	0	-1.933964	2.716898	-2.361240

48	6	0	-3.531882	3.411187	0.672904
49	1	0	-2.662604	3.727611	1.261451
50	1	0	-4.207675	2.867978	1.342292
51	1	0	-4.045850	4.316548	0.328324
52	8	0	0.369707	0.000701	3.178093
53	6	0	2.987219	-0.001445	2.420112
54	1	0	2.886271	-0.882507	3.059955
55	1	0	3.984219	-0.001923	1.969470
56	1	0	2.887146	0.879629	3.060067

Compound 3 – Ground State syn

Method: B3LYP/6-31g(d)
SCF Done: E(RB+HF-LYP) = -1199.62296792 A.U. after 6 cycles
Imaginary frequencies: 0 (13.5)

This molecule is an asymmetric top.
Rotational symmetry number 1.
Warning -- assumption of classical behavior for rotation
may cause significant error
Rotational temperatures (Kelvin) 0.00998 0.00606 0.00545
Rotational constants (GHZ): 0.20794 0.12629 0.11352
Zero-point vibrational energy 1402039.9 (Joules/Mol)
335.09559 (Kcal/Mol)
Warning -- explicit consideration of 47 degrees of freedom as
vibrations may cause significant error

Zero-point correction= 0.534009 (Hartree/Particle)
Thermal correction to Energy= 0.562572
Thermal correction to Enthalpy= 0.563516
Thermal correction to Gibbs Free Energy= 0.474469
Sum of electronic and zero-point Energies= -1199.088959
Sum of electronic and thermal Energies= -1199.060396
Sum of electronic and thermal Enthalpies= -1199.059452
Sum of electronic and thermal Free Energies= -1199.148499

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.114526	-0.363216	2.498385
2	1	0	0.460803	-1.169509	2.815779
3	6	0	1.474934	0.638914	3.407093
4	1	0	1.108823	0.592552	4.429107
5	6	0	2.295294	1.699817	3.011579
6	1	0	2.568923	2.467874	3.729992
7	6	0	2.755101	1.785955	1.695153
8	1	0	3.379536	2.620173	1.385326
9	6	0	3.367349	1.493004	-1.528997
10	1	0	3.855590	2.396950	-1.173494
11	6	0	3.432524	1.141660	-2.879866
12	1	0	3.974726	1.777219	-3.574864
13	6	0	2.801788	-0.016390	-3.347353
14	1	0	2.854826	-0.270424	-4.402492
15	6	0	1.379653	-1.270518	0.030852
16	6	0	2.098465	-0.849244	-2.468899
17	1	0	1.602659	-1.745029	-2.833352
18	6	0	1.582931	-0.296175	1.188822
19	6	0	2.038059	-0.504394	-1.123475
20	6	0	2.392271	0.790158	0.786391
21	6	0	2.664134	0.666239	-0.650440
22	6	0	-1.200155	-0.568770	-0.249820
23	6	0	-0.997498	0.817246	-0.213148
24	1	0	0.007545	1.216525	-0.244694
25	6	0	-2.510758	-1.071812	-0.235079
26	1	0	-2.641686	-2.147872	-0.286570
27	6	0	-0.095510	-1.579747	-0.375473

28	6	0	-2.082068	1.700352	-0.166748
29	6	0	-3.373945	1.162751	-0.133944
30	1	0	-4.224183	1.842029	-0.087740
31	6	0	-3.612811	-0.217909	-0.164348
32	6	0	-5.036488	-0.759822	-0.126113
33	1	0	-5.710170	0.107899	-0.102265
34	6	0	-1.869601	3.209213	-0.146564
35	1	0	-2.865191	3.673602	-0.166786
36	6	0	2.138923	-2.639746	0.261318
37	1	0	1.957687	-3.211892	-0.653987
38	6	0	1.579718	-3.463618	1.432594
39	1	0	2.032879	-4.461868	1.422611
40	1	0	0.496586	-3.595893	1.366302
41	1	0	1.823528	-3.007472	2.398289
42	6	0	3.655735	-2.465042	0.431840
43	1	0	3.897241	-1.889156	1.332551
44	1	0	4.116549	-1.965325	-0.424871
45	1	0	4.125534	-3.450145	0.535147
46	6	0	-1.107932	3.701952	-1.391326
47	1	0	-0.091905	3.291940	-1.428451
48	1	0	-1.024799	4.795349	-1.382731
49	1	0	-1.620759	3.405968	-2.313043
50	6	0	-1.173201	3.669515	1.148484
51	1	0	-1.739491	3.359044	2.033491
52	1	0	-1.081212	4.762306	1.168302
53	1	0	-0.165830	3.246059	1.233365
54	6	0	-5.298301	-1.582441	1.149589
55	1	0	-4.660483	-2.473566	1.184652
56	1	0	-6.341801	-1.917569	1.186065
57	1	0	-5.097501	-0.992332	2.050587
58	6	0	-5.376077	-1.574237	-1.388491
59	1	0	-4.746109	-2.467854	-1.467195
60	1	0	-5.226197	-0.979725	-2.296278
61	1	0	-6.421494	-1.904381	-1.364465
62	8	0	-0.353374	-2.678456	-0.847546

Compound 3 – Ground State anti

Method: B3LYP/6-31g(d)
SCF Done: E(RB+HF-LYP) = -1199.61376777 A.U. after 10 cycles
Imaginary frequencies: 0 (14.0)

This molecule is an asymmetric top.
Rotational symmetry number 1.
Warning -- assumption of classical behavior for rotation
may cause significant error
Rotational temperatures (Kelvin) 0.01047 0.00525 0.00491
Rotational constants (GHZ): 0.21813 0.10932 0.10226
Zero-point vibrational energy 1400976.4 (Joules/Mol)
334.84141 (Kcal/Mol)
Warning -- explicit consideration of 47 degrees of freedom as
vibrations may cause significant error

Zero-point correction= 0.533604 (Hartree/Particle)
Thermal correction to Energy= 0.562329
Thermal correction to Enthalpy= 0.563274

Thermal correction to Gibbs Free Energy= 0.473391
Sum of electronic and zero-point Energies= -1199.080164
Sum of electronic and thermal Energies= -1199.051438
Sum of electronic and thermal Enthalpies= -1199.050494
Sum of electronic and thermal Free Energies= -1199.140377

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.337359	-0.292505	-2.076270
2	1	0	2.797818	0.025902	-2.960526
3	6	0	4.598769	-0.882961	-2.209431
4	1	0	5.037171	-0.990115	-3.198044
5	6	0	5.292959	-1.348745	-1.088442
6	1	0	6.270712	-1.807663	-1.209362
7	6	0	4.730212	-1.238034	0.183354
8	1	0	5.262112	-1.611790	1.054640
9	6	0	2.916151	-0.721040	2.850220
10	1	0	3.841365	-1.213503	3.138384
11	6	0	1.969513	-0.376857	3.817227
12	1	0	2.156542	-0.607636	4.862672
13	6	0	0.785850	0.267077	3.447673
14	1	0	0.055926	0.534171	4.207159
15	6	0	1.442014	0.467414	-0.386139
16	6	0	0.526578	0.571669	2.105545
17	1	0	-0.400842	1.067600	1.839663
18	6	0	2.779088	-0.155727	-0.807379
19	6	0	1.460147	0.221007	1.134013
20	6	0	3.473396	-0.644357	0.315569
21	6	0	2.658175	-0.418922	1.512575
22	6	0	-1.169306	-0.203014	-0.622702
23	6	0	-1.883744	-1.408853	-0.553793
24	1	0	-1.356058	-2.329757	-0.780596
25	6	0	-1.842546	1.000375	-0.372298
26	1	0	-1.319617	1.945035	-0.459158
27	6	0	0.271252	-0.320502	-1.067324
28	6	0	-3.235453	-1.434160	-0.202991
29	6	0	-3.876219	-0.212893	0.042600
30	1	0	-4.932739	-0.215882	0.306500
31	6	0	-3.205943	1.011281	-0.049410
32	6	0	-3.950843	2.320384	0.184388
33	1	0	-4.984986	2.057403	0.445003
34	6	0	-4.001842	-2.746846	-0.099363
35	1	0	-5.031690	-2.496118	0.189956
36	6	0	-3.423407	-3.661425	0.996791
37	1	0	-2.394826	-3.960120	0.763293
38	1	0	-4.022530	-4.574816	1.091816
39	1	0	-3.411728	-3.157629	1.969511
40	6	0	-4.067658	-3.478591	-1.453459
41	1	0	-4.514789	-2.843822	-2.226221
42	1	0	-4.670481	-4.390634	-1.368993
43	1	0	-3.068578	-3.769639	-1.798070
44	6	0	-4.003637	3.183508	-1.090719
45	1	0	-3.000019	3.497940	-1.401304
46	1	0	-4.597395	4.089230	-0.919181
47	1	0	-4.453153	2.632666	-1.923922

48	6	0	-3.368928	3.116905	1.367268
49	1	0	-2.336574	3.430546	1.170190
50	1	0	-3.368431	2.519744	2.285850
51	1	0	-3.959164	4.022633	1.550226
52	8	0	0.520012	-1.122059	-1.951536
53	6	0	1.371905	2.019481	-0.687153
54	1	0	0.538691	2.401924	-0.087079
55	6	0	1.087469	2.353401	-2.160022
56	1	0	0.957936	3.435904	-2.276343
57	1	0	1.920135	2.054760	-2.804713
58	1	0	0.180964	1.866977	-2.536042
59	6	0	2.629837	2.760733	-0.205717
60	1	0	3.507694	2.483774	-0.797860
61	1	0	2.481750	3.842264	-0.308545
62	1	0	2.847813	2.550311	0.845723

Compound 3 – Transition State Phenyl-CO rotation of syn conformer

Method: B3LYP/6-31g(d)
SCF Done: E(RB+HF-LYP) = -1199.61636314 A.U. after 7 cycles
Imaginary frequencies: 1 (-16.4)

This molecule is an asymmetric top.
Rotational symmetry number 1.
Warning -- assumption of classical behavior for rotation
may cause significant error
Rotational temperatures (Kelvin) 0.00904 0.00721 0.00564
Rotational constants (GHZ): 0.18830 0.15022 0.11748
1 imaginary frequencies ignored.
Zero-point vibrational energy 1400289.0 (Joules/Mol)
334.67711 (Kcal/Mol)
Warning -- explicit consideration of 45 degrees of freedom as
vibrations may cause significant error

Zero-point correction= 0.533342 (Hartree/Particle)
Thermal correction to Energy= 0.561263
Thermal correction to Enthalpy= 0.562207
Thermal correction to Gibbs Free Energy= 0.475289
Sum of electronic and zero-point Energies= -1199.083021
Sum of electronic and thermal Energies= -1199.055100
Sum of electronic and thermal Enthalpies= -1199.054156
Sum of electronic and thermal Free Energies= -1199.141074

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.023694	-2.627469	0.590850
2	1	0	0.825456	-3.253170	-0.273387
3	6	0	0.851455	-3.152898	1.876457
4	1	0	0.533087	-4.185071	1.995192
5	6	0	1.082960	-2.363045	3.007043
6	1	0	0.943935	-2.785223	3.998680
7	6	0	1.486572	-1.034586	2.868721
8	1	0	1.658954	-0.418835	3.747795

9	6	0	2.384702	1.974170	1.896371
10	1	0	2.358217	1.961203	2.982920
11	6	0	2.737398	3.140801	1.214195
12	1	0	2.988369	4.036913	1.775429
13	6	0	2.770596	3.167653	-0.185052
14	1	0	3.046187	4.083530	-0.700679
15	6	0	1.719838	-0.507701	-0.832959
16	6	0	2.449465	2.024534	-0.926121
17	1	0	2.464103	2.050467	-2.012742
18	6	0	1.438823	-1.305295	0.440823
19	6	0	2.103375	0.859936	-0.247238
20	6	0	1.662564	-0.511007	1.586584
21	6	0	2.065706	0.831559	1.159428
22	6	0	-0.870034	0.037946	-0.994264
23	6	0	-1.243291	1.349403	-0.683348
24	1	0	-0.555364	2.161571	-0.897795
25	6	0	-1.752347	-1.015870	-0.738489
26	1	0	-1.460979	-2.030375	-0.994540
27	6	0	0.450814	-0.212902	-1.688753
28	6	0	-2.487564	1.619206	-0.101055
29	6	0	-3.348230	0.544917	0.150543
30	1	0	-4.318948	0.742728	0.602734
31	6	0	-3.005254	-0.775799	-0.162409
32	6	0	-3.970849	-1.917004	0.131757
33	1	0	-4.889162	-1.465194	0.531190
34	6	0	-2.898251	3.043477	0.250628
35	1	0	-3.913226	2.991930	0.668177
36	6	0	2.868523	-1.078523	-1.736354
37	1	0	2.969523	-0.353000	-2.551329
38	6	0	2.540758	-2.434420	-2.383434
39	1	0	3.298429	-2.667881	-3.140541
40	1	0	1.568676	-2.429250	-2.883733
41	1	0	2.560353	-3.246959	-1.649193
42	6	0	4.211636	-1.165400	-0.994991
43	1	0	4.162664	-1.878475	-0.163990
44	1	0	4.525880	-0.197489	-0.593274
45	1	0	4.992145	-1.511685	-1.682566
46	6	0	-2.958556	3.948803	-0.994104
47	1	0	-1.969337	4.063456	-1.452609
48	1	0	-3.318603	4.949351	-0.725945
49	1	0	-3.631454	3.535180	-1.753082
50	6	0	-1.984045	3.649303	1.332837
51	1	0	-1.979654	3.031368	2.237479
52	1	0	-2.324991	4.655036	1.606973
53	1	0	-0.948787	3.730307	0.981419
54	6	0	-3.416166	-2.864734	1.212612
55	1	0	-2.489381	-3.347055	0.880421
56	1	0	-4.142128	-3.653451	1.444384
57	1	0	-3.191675	-2.322136	2.137235
58	6	0	-4.357068	-2.693934	-1.140705
59	1	0	-3.487891	-3.194298	-1.583974
60	1	0	-4.780535	-2.027408	-1.899818
61	1	0	-5.100868	-3.465798	-0.909297
62	8	0	0.532959	-0.093378	-2.897370

Compound 3 – Transition State isopropyl rotation

Method: B3LYP/6-31g(d)
SCF Done: E(RB+HF-LYP) = -1199.61049457 A.U. after 8 cycles
Imaginary frequencies: 1 (-76.4)

This molecule is an asymmetric top.
Rotational symmetry number 1.
Warning -- assumption of classical behavior for rotation
may cause significant error
Rotational temperatures (Kelvin) 0.00994 0.00608 0.00551
Rotational constants (GHZ): 0.20708 0.12677 0.11486
1 imaginary frequencies ignored.
Zero-point vibrational energy 1402700.7 (Joules/Mol)
335.25351 (Kcal/Mol)
Warning -- explicit consideration of 47 degrees of freedom as
vibrations may cause significant error

Zero-point correction= 0.534260 (Hartree/Particle)
Thermal correction to Energy= 0.561805
Thermal correction to Enthalpy= 0.562750
Thermal correction to Gibbs Free Energy= 0.476399
Sum of electronic and zero-point Energies= -1199.076234
Sum of electronic and thermal Energies= -1199.048689
Sum of electronic and thermal Enthalpies= -1199.047745
Sum of electronic and thermal Free Energies= -1199.134096

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.073832	-0.428120	2.539088
2	1	0	0.436178	-1.260976	2.822831
3	6	0	1.387654	0.560035	3.478681
4	1	0	0.997928	0.482150	4.489953
5	6	0	2.194498	1.646873	3.127146
6	1	0	2.435780	2.402920	3.869470
7	6	0	2.675400	1.777735	1.822146
8	1	0	3.278335	2.638254	1.543147
9	6	0	3.206324	1.663778	-1.421007
10	1	0	3.689194	2.554669	-1.027396
11	6	0	3.173179	1.430022	-2.798136
12	1	0	3.643937	2.137077	-3.475895
13	6	0	2.520635	0.304893	-3.311773
14	1	0	2.480016	0.147902	-4.386135
15	6	0	1.413115	-1.277733	0.058845
16	6	0	1.913559	-0.620215	-2.454609
17	1	0	1.398096	-1.485999	-2.861209
18	6	0	1.572016	-0.321016	1.244011
19	6	0	1.969308	-0.408404	-1.080702
20	6	0	2.351153	0.798000	0.881538
21	6	0	2.591149	0.747805	-0.565257
22	6	0	-1.187147	-0.635497	-0.202792
23	6	0	-1.002145	0.753657	-0.219240
24	1	0	-0.003339	1.164793	-0.269152
25	6	0	-2.493042	-1.150585	-0.161107
26	1	0	-2.612285	-2.228987	-0.166087

27	6	0	-0.074453	-1.646911	-0.272424
28	6	0	-2.096334	1.625612	-0.198537
29	6	0	-3.382216	1.075900	-0.142092
30	1	0	-4.239870	1.746945	-0.117584
31	6	0	-3.604691	-0.307345	-0.119854
32	6	0	-5.021737	-0.864306	-0.057796
33	1	0	-5.704940	-0.003796	-0.045094
34	6	0	-1.900150	3.136756	-0.224709
35	1	0	-2.900243	3.589068	-0.275366
36	6	0	2.250521	-2.643099	0.258193
37	1	0	1.505710	-3.433173	0.140659
38	6	0	2.890051	-2.813302	1.646815
39	1	0	3.383451	-3.791648	1.687960
40	1	0	2.159326	-2.784995	2.458866
41	1	0	3.648843	-2.050095	1.853406
42	6	0	3.330372	-2.895493	-0.807615
43	1	0	4.114500	-2.129905	-0.792658
44	1	0	2.921773	-2.937380	-1.819845
45	1	0	3.805980	-3.863039	-0.607782
46	6	0	-1.123353	3.599963	-1.471310
47	1	0	-0.101745	3.202501	-1.479900
48	1	0	-1.054136	4.694122	-1.495067
49	1	0	-1.617378	3.269519	-2.391609
50	6	0	-1.230656	3.644038	1.067135
51	1	0	-1.810737	3.357758	1.951384
52	1	0	-1.146350	4.737560	1.053672
53	1	0	-0.222386	3.230245	1.183402
54	6	0	-5.264506	-1.664971	1.235376
55	1	0	-4.617702	-2.548970	1.282452
56	1	0	-6.304217	-2.009723	1.286774
57	1	0	-5.062515	-1.055584	2.123167
58	6	0	-5.362270	-1.706258	-1.301781
59	1	0	-4.721398	-2.593050	-1.369618
60	1	0	-5.227968	-1.126744	-2.221669
61	1	0	-6.403158	-2.049065	-1.262439
62	8	0	-0.346134	-2.786653	-0.621505

Compound 4 – Ground State syn

Method: B3LYP/6-31g(d)
SCF Done: E(RB+HF-LYP) = -1003.05385494 A.U. after 9 cycles
Imaginary frequencies: 0 (23.5)

This molecule is an asymmetric top.
Rotational symmetry number 1.
Warning -- assumption of classical behavior for rotation
may cause significant error
Rotational temperatures (Kelvin) 0.01730 0.00871 0.00769
Rotational constants (GHZ): 0.36050 0.18145 0.16017
Zero-point vibrational energy 1024271.0 (Joules/Mol)
244.80664 (Kcal/Mol)
Warning -- explicit consideration of 36 degrees of freedom as
vibrations may cause significant error

Zero-point correction= 0.390124 (Hartree/Particle)
Thermal correction to Energy= 0.412485
Thermal correction to Enthalpy= 0.413429
Thermal correction to Gibbs Free Energy= 0.338468
Sum of electronic and zero-point Energies= -1002.663731
Sum of electronic and thermal Energies= -1002.641370
Sum of electronic and thermal Enthalpies= -1002.640426
Sum of electronic and thermal Free Energies= -1002.715387

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.923028	-1.788262	-0.222846
2	1	0	-2.565762	-2.763889	0.091147
3	6	0	-4.086953	-1.663041	-0.990913
4	1	0	-4.645350	-2.553238	-1.267717
5	6	0	-4.537216	-0.404951	-1.405148
6	1	0	-5.444105	-0.325678	-1.998810
7	6	0	-3.829812	0.750729	-1.066016
8	1	0	-4.181685	1.725556	-1.394278
9	6	0	-1.726616	3.034520	0.034752
10	1	0	-2.518088	3.533781	-0.518455
11	6	0	-0.694465	3.776276	0.612736
12	1	0	-0.682228	4.857630	0.504956
13	6	0	0.322131	3.139157	1.331973
14	1	0	1.119287	3.728653	1.776664
15	6	0	-0.958731	-0.498584	0.977234
16	6	0	0.322771	1.748147	1.484402
17	1	0	1.120118	1.265064	2.042356
18	6	0	-2.220390	-0.637969	0.119010
19	6	0	-0.696902	1.001358	0.902723
20	6	0	-2.665768	0.629841	-0.304634
21	6	0	-1.724892	1.645883	0.182765
22	6	0	1.483266	-0.936052	-0.059465
23	6	0	1.577617	-0.338178	-1.329965
24	6	0	2.644372	-1.153613	0.715414
25	6	0	0.166208	-1.455170	0.471881
26	6	0	2.836023	0.065325	-1.790802
27	6	0	3.992888	-0.093240	-1.026829

28	6	0	3.873664	-0.711092	0.222360
29	8	0	-0.013415	-2.656642	0.576167
30	6	0	-1.269826	-0.913047	2.444254
31	1	0	-1.499900	-1.980031	2.488370
32	1	0	-0.413904	-0.712835	3.098417
33	1	0	-2.125149	-0.341370	2.815824
34	1	0	4.766108	-0.869012	0.825015
35	1	0	2.909036	0.511751	-2.780770
36	6	0	2.592378	-1.865358	2.051007
37	1	0	1.893226	-1.389648	2.749672
38	1	0	2.263574	-2.902918	1.932860
39	1	0	3.578997	-1.869353	2.523678
40	6	0	0.372323	-0.144416	-2.222579
41	1	0	-0.336936	-0.974903	-2.150246
42	1	0	-0.171729	0.772103	-1.966569
43	1	0	0.681008	-0.060842	-3.269476
44	6	0	5.332438	0.393333	-1.527558
45	1	0	5.554912	1.400789	-1.150809
46	1	0	6.146598	-0.261531	-1.198222
47	1	0	5.357593	0.442422	-2.621143

Compound 4 – Transition State Phenyl-CO rotation 0° (correlated)

Method: B3LYP/6-31g(d)
SCF Done: E(RB+HF-LYP) = -1003.03483411 A.U. after 16 cycles
Imaginary frequencies: 1 (-80.0)

This molecule is an asymmetric top.
Rotational symmetry number 1.
Warning -- assumption of classical behavior for rotation
may cause significant error
Rotational temperatures (Kelvin) 0.01585 0.00809 0.00757
Rotational constants (GHZ): 0.33020 0.16863 0.15771
1 imaginary frequencies ignored.
Zero-point vibrational energy 1027861.6 (Joules/Mol)
245.66481 (Kcal/Mol)
Warning -- explicit consideration of 36 degrees of freedom as
vibrations may cause significant error

Zero-point correction= 0.391492 (Hartree/Particle)
Thermal correction to Energy= 0.412262
Thermal correction to Enthalpy= 0.413206
Thermal correction to Gibbs Free Energy= 0.341260
Sum of electronic and zero-point Energies= -1002.643342
Sum of electronic and thermal Energies= -1002.622573
Sum of electronic and thermal Enthalpies= -1002.621628
Sum of electronic and thermal Free Energies= -1002.693574

standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.801465	-1.068019	-2.527831
2	1	0	-0.965787	-1.677386	-2.863087
3	6	0	-2.631128	-0.431330	-3.459371

4	1	0	-2.432065	-0.543295	-4.521716
5	6	0	-3.715466	0.343344	-3.034513
6	1	0	-4.352567	0.826704	-3.770305
7	6	0	-3.986421	0.504483	-1.672950
8	1	0	-4.828932	1.111062	-1.350277
9	6	0	-3.992490	0.566312	1.631790
10	1	0	-4.832827	1.161568	1.283339
11	6	0	-3.727532	0.455772	2.999573
12	1	0	-4.366811	0.967230	3.714175
13	6	0	-2.646730	-0.304917	3.457552
14	1	0	-2.452640	-0.378194	4.524192
15	6	0	-1.390436	-1.569195	0.024053
16	6	0	-1.814303	-0.977017	2.553666
17	1	0	-0.981328	-1.574999	2.915192
18	6	0	-2.062839	-0.902374	-1.173100
19	6	0	-2.068512	-0.859828	1.192468
20	6	0	-3.153875	-0.116650	-0.740691
21	6	0	-3.156783	-0.089863	0.726872
22	6	0	1.227921	-0.543529	0.011187
23	6	0	0.977482	0.862705	0.008253
24	6	0	2.606607	-0.968947	0.003877
25	6	0	0.188786	-1.655417	0.020981
26	6	0	2.051407	1.761887	-0.007938
27	6	0	3.381062	1.358954	-0.022196
28	6	0	3.624496	-0.011843	-0.011708
29	8	0	0.603775	-2.807941	0.021025
30	6	0	-1.920885	-3.038952	0.050940
31	1	0	-1.575734	-3.593327	-0.824039
32	1	0	-1.572188	-3.561251	0.944402
33	1	0	-3.014701	-3.019848	0.053220
34	1	0	4.654891	-0.359440	-0.014854
35	1	0	1.827135	2.825800	-0.008700
36	6	0	3.108461	-2.401229	0.014926
37	1	0	2.764323	-2.956491	0.891028
38	1	0	2.763226	-2.970334	-0.851874
39	1	0	4.204035	-2.396503	0.014058
40	6	0	-0.377825	1.526208	0.027050
41	1	0	-0.255689	2.612046	-0.016245
42	1	0	-0.993827	1.235411	-0.824257
43	1	0	-0.936122	1.298516	0.936687
44	6	0	4.511204	2.357043	-0.067505
45	1	0	5.340403	2.052072	0.580668
46	1	0	4.914733	2.448787	-1.084724
47	1	0	4.180586	3.352476	0.245672

Compound 4 – Transition State Phenyl-CO rotation 90° (correlated)

Method: B3LYP/6-31g(d)
SCF Done: E(RB+HF-LYP) = -1003.04706022 A.U. after 17 cycles
Imaginary frequencies: 1 (-20.0)

This molecule is an asymmetric top.
Rotational symmetry number 1.
Warning -- assumption of classical behavior for rotation
may cause significant error

```
Rotational temperatures (Kelvin)      0.01335     0.01089     0.00897
Rotational constants (GHZ):           0.27819     0.22689     0.18691
   1 imaginary frequencies ignored.
Zero-point vibrational energy    1025675.4 (Joules/Mol)
                                 245.14230 (Kcal/Mol)
Warning -- explicit consideration of  36 degrees of freedom as
          vibrations may cause significant error

Zero-point correction=                           0.390659 (Hartree/Particle)
Thermal correction to Energy=                    0.411789
Thermal correction to Enthalpy=                  0.412733
Thermal correction to Gibbs Free Energy=         0.342031
Sum of electronic and zero-point Energies=         -1002.656401
Sum of electronic and thermal Energies=            -1002.635272
Sum of electronic and thermal Enthalpies=          -1002.634327
Sum of electronic and thermal Free Energies=       -1002.705029

                         Input orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          6             0        2.248366    2.530396    0.596734
   2          1             0        2.224964    2.882727    1.624421
   3          6             0        2.436829    3.440829   -0.449699
   4          1             0        2.559021    4.497534   -0.227685
   5          6             0        2.472962    3.000677   -1.777082
   6          1             0        2.614462    3.719813   -2.579468
   7          6             0        2.356260    1.642078   -2.077743
   8          1             0        2.419930    1.300708   -3.107715
   9          6             0        2.354463   -1.644263   -2.077738
  10          1             0        2.418523   -1.302962   -3.107709
  11          6             0        2.469589   -3.002997   -1.777083
  12          1             0        2.610287   -3.722292   -2.579467
  13          6             0        2.432922   -3.443106   -0.449703
  14          1             0        2.553920   -4.499947   -0.227684
  15          6             0        1.938771   -0.000861    1.263502
  16          6             0        2.245441   -2.532465    0.596732
  17          1             0        2.221638   -2.884773    1.624417
  18          6             0        2.100136    1.179167    0.301758
  19          6             0        2.098772   -1.181065    0.301763
  20          6             0        2.186731    0.731908   -1.032817
  21          6             0        2.185940   -0.733907   -1.032812
  22          6             0       -0.753304    0.000512    1.094051
  23          6             0       -1.381198   -1.218661    0.758069
  24          6             0       -1.379831    1.220143    0.757300
  25          6             0        0.513089   -0.000034    1.940754
  26          6             0       -2.532987   -1.191797   -0.035025
  27          6             0       -3.107217    0.001323   -0.475122
  28          6             0       -2.531654    1.194062   -0.035813
  29          8             0        0.434189    0.000114    3.154764
  30          6             0        3.010942   -0.001455    2.367215
  31          1             0        2.910146   -0.881566    3.008058
  32          1             0        4.008111   -0.001974    1.916848
  33          1             0        2.911091    0.878722    3.008117
  34          6             0       -0.916256   -2.563458    1.276462
  35          1             0       -1.785157   -3.170226    1.554864
  36          1             0       -0.353735   -3.121811    0.521508
```

37	1	0	-0.287117	-2.469775	2.164667
38	6	0	-0.913548	2.564776	1.274932
39	1	0	-0.351172	3.122488	0.519398
40	1	0	-1.781829	3.172243	1.553758
41	1	0	-0.283860	2.470976	2.162726
42	6	0	-4.325424	0.001696	-1.368011
43	1	0	-4.039377	0.000803	-2.428504
44	1	0	-4.947004	-0.884330	-1.199550
45	1	0	-4.945643	0.888883	-1.200667
46	1	0	-3.005200	2.140040	-0.293242
47	1	0	-3.007610	-2.137398	-0.291851

Compound 5 – Ground State syn (cis)

Method: B3LYP/6-31g(d)
SCF Done: E(RB+HF-LYP) = -1081.67311416 A.U. after 8 cycles
Imaginary frequencies: 0 (15.6)

This molecule is an asymmetric top.
Rotational symmetry number 1.
Warning -- assumption of classical behavior for rotation
may cause significant error
Rotational temperatures (Kelvin) 0.01383 0.00776 0.00754
Rotational constants (GHZ): 0.28808 0.16170 0.15705
Zero-point vibrational energy 1174915.0 (Joules/Mol)
280.81143 (Kcal/Mol)
Warning -- explicit consideration of 42 degrees of freedom as
vibrations may cause significant error

Zero-point correction= 0.447501 (Hartree/Particle)
Thermal correction to Energy= 0.472405
Thermal correction to Enthalpy= 0.473349
Thermal correction to Gibbs Free Energy= 0.392805
Sum of electronic and zero-point Energies= -1081.225613
Sum of electronic and thermal Energies= -1081.200709
Sum of electronic and thermal Enthalpies= -1081.199765
Sum of electronic and thermal Free Energies= -1081.280310

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.191221	-0.242912	2.243503
2	1	0	0.940391	0.531956	2.370913
3	6	0	0.139949	-1.311014	3.147105
4	1	0	0.840886	-1.344798	3.976714
5	6	0	-0.798166	-2.335111	2.988437
6	1	0	-0.826539	-3.156604	3.699351
7	6	0	-1.691299	-2.315416	1.915290
8	1	0	-2.410914	-3.119792	1.785269
9	6	0	-3.422607	-1.749454	-0.823136
10	1	0	-3.781743	-2.673919	-0.377751
11	6	0	-3.965541	-1.288503	-2.025376
12	1	0	-4.751481	-1.858139	-2.514116
13	6	0	-3.503160	-0.103530	-2.607438
14	1	0	-3.929759	0.237818	-3.546773
15	6	0	-0.898993	0.855482	0.099254
16	6	0	-2.493919	0.647956	-1.992326
17	1	0	-2.128011	1.563867	-2.446884
18	6	0	-0.705131	-0.205112	1.177916
19	6	0	-1.955659	0.190965	-0.794737
20	6	0	-1.637991	-1.253426	1.011099
21	6	0	-2.411337	-1.006733	-0.211358
22	6	0	1.662895	0.452053	-0.680497
23	6	0	1.770935	-0.881651	-1.133584
24	6	0	2.822534	1.129700	-0.229401
25	6	0	0.354300	1.221908	-0.764148
26	6	0	3.010603	-1.526162	-1.061596
27	6	0	4.150743	-0.899616	-0.560350

28	6	0	4.031653	0.431757	-0.158379
29	6	0	-1.531263	2.200795	0.669221
30	1	0	-1.712122	2.809142	-0.223552
31	6	0	-0.598330	2.999971	1.588689
32	1	0	-1.097219	3.927486	1.893316
33	1	0	0.330704	3.281792	1.089910
34	1	0	-0.356035	2.447862	2.503575
35	6	0	-2.873039	1.972101	1.382845
36	1	0	-2.747114	1.369660	2.289484
37	1	0	-3.608690	1.477219	0.743745
38	1	0	-3.290792	2.939622	1.684489
39	8	0	0.268753	2.179496	-1.515971
40	1	0	3.082205	-2.550781	-1.421859
41	1	0	4.912293	0.955752	0.208108
42	6	0	0.619284	-1.647817	-1.745679
43	1	0	0.010454	-2.142512	-0.981639
44	1	0	-0.046358	-1.008549	-2.331133
45	1	0	1.001547	-2.427563	-2.412310
46	6	0	2.823400	2.584055	0.194240
47	1	0	3.848978	2.963680	0.232049
48	1	0	2.255050	3.208551	-0.498304
49	1	0	2.394930	2.720003	1.195032
50	6	0	5.479450	-1.616186	-0.510074
51	1	0	6.028925	-1.501041	-1.454074
52	1	0	6.117940	-1.220929	0.287116
53	1	0	5.349257	-2.690334	-0.340038

Compound 5 – Ground State syn (trans)

Method: B3LYP/6-31g(d)
SCF Done: E(RB+HF-LYP) = -1081.67340926 A.U. after 6 cycles
Imaginary frequencies: 0 (21.4)

This molecule is an asymmetric top.
Rotational symmetry number 1.
Warning -- assumption of classical behavior for rotation
may cause significant error
Rotational temperatures (Kelvin) 0.01454 0.00784 0.00701
Rotational constants (GHZ): 0.30288 0.16331 0.14606
Zero-point vibrational energy 1174023.0 (Joules/Mol)
280.59823 (Kcal/Mol)
Warning -- explicit consideration of 41 degrees of freedom as
vibrations may cause significant error

Zero-point correction= 0.447162 (Hartree/Particle)
Thermal correction to Energy= 0.472173
Thermal correction to Enthalpy= 0.473117
Thermal correction to Gibbs Free Energy= 0.392852
Sum of electronic and zero-point Energies= -1081.226248
Sum of electronic and thermal Energies= -1081.201236
Sum of electronic and thermal Enthalpies= -1081.200292
Sum of electronic and thermal Free Energies= -1081.280557

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-0.405477	1.275999	1.710421
2	1	0	-1.189556	0.621859	2.080202
3	6	0	-0.405386	2.629558	2.066978
4	1	0	-1.189432	3.013678	2.713868
5	6	0	0.591551	3.490517	1.596892
6	1	0	0.578855	4.538808	1.883303
7	6	0	1.605277	3.011146	0.764915
8	1	0	2.382996	3.680270	0.405648
9	6	0	3.655327	1.313944	-1.147734
10	1	0	3.988927	2.347721	-1.104479
11	6	0	4.345652	0.381987	-1.925016
12	1	0	5.225523	0.690847	-2.483262
13	6	0	3.903199	-0.942000	-2.000256
14	1	0	4.437893	-1.654499	-2.622694
15	6	0	0.853472	-0.635721	0.390281
16	6	0	2.773757	-1.363093	-1.287608
17	1	0	2.418659	-2.382768	-1.376131
18	6	0	0.595337	0.793232	0.872023
19	6	0	2.094385	-0.443257	-0.491537
20	6	0	1.603666	1.661418	0.407108
21	6	0	2.527014	0.898481	-0.438820
22	6	0	-1.688662	-0.660991	-0.488090
23	6	0	-1.946847	0.442432	-1.322077
24	6	0	-2.742699	-1.286900	0.213157
25	6	0	-0.302479	-1.274416	-0.442536
26	6	0	-3.254939	0.934764	-1.401642
27	6	0	-4.305311	0.370628	-0.677642
28	6	0	-4.027078	-0.746602	0.117060
29	6	0	1.134919	-1.557547	1.665676
30	1	0	0.201644	-1.533576	2.246323
31	6	0	2.242926	-0.971568	2.559675
32	1	0	2.366160	-1.605292	3.445338
33	1	0	2.014615	0.040805	2.901260
34	1	0	3.202832	-0.947681	2.032379
35	6	0	1.464113	-3.026899	1.363186
36	1	0	2.426955	-3.115849	0.849278
37	1	0	0.708640	-3.520437	0.750726
38	1	0	1.547800	-3.572242	2.310912
39	8	0	-0.097109	-2.309435	-1.053098
40	1	0	-3.453844	1.780593	-2.057266
41	1	0	-4.837568	-1.225116	0.663726
42	6	0	-0.866298	1.097874	-2.154104
43	1	0	-0.380513	1.914298	-1.606812
44	1	0	-0.084658	0.392764	-2.452420
45	1	0	-1.293888	1.523750	-3.067794
46	6	0	-2.524362	-2.538230	1.036784
47	1	0	-3.468049	-2.884190	1.468802
48	1	0	-2.114142	-3.347212	0.423397
49	1	0	-1.824839	-2.376595	1.866090
50	6	0	-5.700901	0.944864	-0.747561
51	1	0	-6.461579	0.156821	-0.718043
52	1	0	-5.898042	1.615880	0.099343
53	1	0	-5.849469	1.525129	-1.664119

Compound 5 – Transition State Phenyl-CO rotation 0° (correlated)

Method: B3LYP/6-31g(d)
SCF Done: E(RB+HF-LYP) = -1081.65277086 A.U. after 10 cycles
Imaginary frequencies: 1 (-71.2)

This molecule is an asymmetric top.
Rotational symmetry number 1.
Warning -- assumption of classical behavior for rotation
may cause significant error
Rotational temperatures (Kelvin) 0.01333 0.00724 0.00716
Rotational constants (GHZ): 0.27770 0.15080 0.14909
1 imaginary frequencies ignored.
Zero-point vibrational energy 1177902.0 (Joules/Mol)
281.52533 (Kcal/Mol)
Warning -- explicit consideration of 41 degrees of freedom as
vibrations may cause significant error

Zero-point correction= 0.448639 (Hartree/Particle)
Thermal correction to Energy= 0.471948
Thermal correction to Enthalpy= 0.472892
Thermal correction to Gibbs Free Energy= 0.397065
Sum of electronic and zero-point Energies= -1081.204132
Sum of electronic and thermal Energies= -1081.180823
Sum of electronic and thermal Enthalpies= -1081.179878
Sum of electronic and thermal Free Energies= -1081.255705

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.937557	1.219037	2.290179
2	1	0	-0.260853	2.068393	2.240757
3	6	0	-1.489188	0.824204	3.515318
4	1	0	-1.230631	1.365843	4.421143
5	6	0	-2.370360	-0.260078	3.583079
6	1	0	-2.792170	-0.551613	4.541214
7	6	0	-2.709352	-0.976266	2.431777
8	1	0	-3.389899	-1.821822	2.492954
9	6	0	-2.973717	-2.290164	-0.581184
10	1	0	-3.602891	-2.860769	0.097381
11	6	0	-2.838284	-2.683909	-1.914896
12	1	0	-3.370959	-3.559870	-2.275270
13	6	0	-2.013922	-1.965354	-2.786336
14	1	0	-1.906740	-2.289613	-3.817932
15	6	0	-0.890731	0.795362	-0.307210
16	6	0	-1.323496	-0.829779	-2.343421
17	1	0	-0.681688	-0.283931	-3.028518
18	6	0	-1.272390	0.508604	1.143348
19	6	0	-1.455984	-0.429880	-1.016843
20	6	0	-2.153915	-0.591471	1.210440
21	6	0	-2.275414	-1.168538	-0.133403
22	6	0	1.896724	0.321550	-0.170502
23	6	0	1.954325	-1.072849	0.137366
24	6	0	3.153208	1.030533	-0.239452
25	6	0	0.651178	1.161103	-0.450781
26	6	0	3.195518	-1.698743	0.312330

27	6	0	4.408171	-1.028364	0.216479
28	6	0	4.351102	0.337415	-0.044890
29	8	0	0.846274	2.323650	-0.780969
30	6	0	-1.728662	2.078070	-0.782936
31	1	0	-1.267573	2.918465	-0.258258
32	1	0	5.281625	0.897463	-0.098836
33	1	0	3.202924	-2.761593	0.541353
34	6	0	3.344904	2.515633	-0.492157
35	1	0	3.018403	2.813487	-1.491654
36	1	0	2.776312	3.136271	0.204778
37	1	0	4.407421	2.761532	-0.387014
38	6	0	0.778325	-2.001829	0.317957
39	1	0	1.132151	-2.969453	0.684971
40	1	0	0.063275	-1.623089	1.047240
41	1	0	0.244389	-2.184439	-0.616262
42	6	0	5.725305	-1.744598	0.381405
43	1	0	6.164924	-1.989296	-0.594830
44	1	0	6.453772	-1.125101	0.916129
45	1	0	5.605422	-2.683709	0.931127
46	6	0	-1.635199	2.362797	-2.291832
47	1	0	-2.230977	1.648808	-2.870883
48	1	0	-2.041128	3.361684	-2.491608
49	1	0	-0.607488	2.348493	-2.658491
50	6	0	-3.213874	2.033662	-0.383596
51	1	0	-3.360144	1.992966	0.698606
52	1	0	-3.702690	2.944144	-0.749891
53	1	0	-3.735260	1.180661	-0.831899

Compound 5 – Transition State Phenyl-CO rotation 90° (correlated)

Method: B3LYP/6-31g(d)
SCF Done: E(RB+HF-LYP) = -1081.66573106 A.U. after 7 cycles
Imaginary frequencies: 1 (-19.9)

This molecule is an asymmetric top.
Rotational symmetry number 1.
Warning -- assumption of classical behavior for rotation
may cause significant error
Rotational temperatures (Kelvin) 0.01222 0.00894 0.00813
Rotational constants (GHZ): 0.25460 0.18624 0.16939
1 imaginary frequencies ignored.
Zero-point vibrational energy 1175847.4 (Joules/Mol)
281.03426 (Kcal/Mol)
Warning -- explicit consideration of 40 degrees of freedom as
vibrations may cause significant error

Zero-point correction= 0.447857 (Hartree/Particle)
Thermal correction to Energy= 0.471588
Thermal correction to Enthalpy= 0.472532
Thermal correction to Gibbs Free Energy= 0.396635
Sum of electronic and zero-point Energies= -1081.217874
Sum of electronic and thermal Energies= -1081.194143
Sum of electronic and thermal Enthalpies= -1081.193199
Sum of electronic and thermal Free Energies= -1081.269096

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.578458	2.694497	0.174317
2	1	0	-0.591593	3.152614	-0.810318
3	6	0	-0.304078	3.475932	1.302299
4	1	0	-0.097781	4.536314	1.183808
5	6	0	-0.299815	2.905590	2.579741
6	1	0	-0.080748	3.524159	3.445923
7	6	0	-0.597276	1.552942	2.750827
8	1	0	-0.621064	1.117955	3.746665
9	6	0	-1.582178	-1.556964	2.512677
10	1	0	-1.399752	-1.321352	3.557969
11	6	0	-2.094563	-2.803069	2.149402
12	1	0	-2.307357	-3.544398	2.915023
13	6	0	-2.344628	-3.098447	0.805606
14	1	0	-2.751039	-4.068423	0.532108
15	6	0	-1.216926	0.295012	-0.731028
16	6	0	-2.069465	-2.160168	-0.195579
17	1	0	-2.247078	-2.421322	-1.232591
18	6	0	-0.848714	1.338406	0.335070
19	6	0	-1.556013	-0.912232	0.154981
20	6	0	-0.884123	0.777164	1.625925
21	6	0	-1.326534	-0.613571	1.515735
22	6	0	1.421286	-0.229660	-0.979156
23	6	0	1.814575	-1.523949	-0.576500
24	6	0	2.354424	0.830944	-0.902659
25	6	0	0.065017	0.038510	-1.626011
26	6	0	3.062511	-1.697050	0.032048
27	6	0	3.951575	-0.639994	0.226146
28	6	0	3.587069	0.607352	-0.281211
29	8	0	-0.003895	0.148500	-2.836092
30	6	0	-2.409092	0.801946	-1.623008
31	1	0	-1.993333	1.637695	-2.200081
32	6	0	0.999780	-2.768650	-0.856679
33	1	0	1.667421	-3.578671	-1.171571
34	1	0	0.454747	-3.116982	0.026098
35	1	0	0.273812	-2.615601	-1.658428
36	6	0	2.126117	2.200840	-1.509040
37	1	0	1.970527	2.961059	-0.736096
38	1	0	3.010521	2.497371	-2.084594
39	1	0	1.275334	2.224893	-2.190942
40	6	0	5.271294	-0.843836	0.931540
41	1	0	5.177040	-0.656095	2.009662
42	1	0	5.636619	-1.869477	0.811940
43	1	0	6.039941	-0.162650	0.550614
44	1	0	4.292123	1.434611	-0.216818
45	1	0	3.354558	-2.700494	0.337316
46	6	0	-2.957410	-0.214440	-2.642960
47	1	0	-3.590200	-0.964741	-2.157372
48	1	0	-3.589828	0.314742	-3.365579
49	1	0	-2.166632	-0.715365	-3.203068
50	6	0	-3.584086	1.334435	-0.783203
51	1	0	-3.299389	2.170464	-0.139367
52	1	0	-4.383214	1.680849	-1.449044
53	1	0	-4.004209	0.545601	-0.148210

Compound 5 – Transition State isopropyl rotation

Method: B3LYP/6-31g(d)
SCF Done: E(RB+HF-LYP) = -1081.66350201 A.U. after 10 cycles
Imaginary frequencies: 1 (-76.6)

This molecule is an asymmetric top.
Rotational symmetry number 1.
Warning -- assumption of classical behavior for rotation
may cause significant error
Rotational temperatures (Kelvin) 0.01398 0.00776 0.00743
Rotational constants (GHZ): 0.29140 0.16179 0.15476
1 imaginary frequencies ignored.
Zero-point vibrational energy 1173639.5 (Joules/Mol)
280.50657 (Kcal/Mol)
Warning -- explicit consideration of 40 degrees of freedom as
vibrations may cause significant error

Zero-point correction= 0.447016 (Hartree/Particle)
Thermal correction to Energy= 0.471219
Thermal correction to Enthalpy= 0.472163
Thermal correction to Gibbs Free Energy= 0.393653
Sum of electronic and zero-point Energies= -1081.216486
Sum of electronic and thermal Energies= -1081.192283
Sum of electronic and thermal Enthalpies= -1081.191339
Sum of electronic and thermal Free Energies= -1081.269849

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.410930	0.949787	1.933772
2	1	0	-1.194209	0.245634	2.195404
3	6	0	-0.436232	2.239074	2.476639
4	1	0	-1.231999	2.515052	3.163108
5	6	0	0.547153	3.173824	2.140087
6	1	0	0.517640	4.170214	2.573010
7	6	0	1.556392	2.839192	1.235911
8	1	0	2.306680	3.573368	0.953578
9	6	0	3.477698	1.558744	-1.082008
10	1	0	3.811457	2.571451	-0.870270
11	6	0	4.066109	0.823242	-2.112851
12	1	0	4.871951	1.260638	-2.696259
13	6	0	3.608357	-0.463408	-2.413159
14	1	0	4.054356	-1.017098	-3.234974
15	6	0	0.885740	-0.740729	0.353982
16	6	0	2.576131	-1.047359	-1.669428
17	1	0	2.208709	-2.036994	-1.919514
18	6	0	0.605889	0.595343	1.049531
19	6	0	2.009622	-0.331335	-0.618306
20	6	0	1.574188	1.555433	0.687273
21	6	0	2.440155	0.981976	-0.347541
22	6	0	-1.641478	-0.661306	-0.573648
23	6	0	-1.854302	0.458499	-1.398825
24	6	0	-2.720439	-1.251718	0.120432
25	6	0	-0.288733	-1.336330	-0.481351
26	6	0	-3.145976	0.990297	-1.488406

27	6	0	-4.222045	0.454067	-0.780049
28	6	0	-3.986797	-0.672215	0.014828
29	6	0	1.348490	-1.911246	1.386756
30	1	0	0.647389	-2.735163	1.225437
31	6	0	1.263174	-1.518265	2.870389
32	1	0	1.555570	-2.380692	3.481072
33	1	0	0.256703	-1.225670	3.179572
34	1	0	1.938747	-0.691598	3.114921
35	6	0	2.748761	-2.482051	1.111425
36	1	0	3.530339	-1.722232	1.221075
37	1	0	2.833612	-2.913894	0.112616
38	1	0	2.953401	-3.280313	1.834894
39	8	0	-0.118526	-2.410076	-1.034628
40	1	0	-3.311343	1.848107	-2.137447
41	1	0	-4.815570	-1.123217	0.557417
42	6	0	-0.741269	1.089039	-2.204693
43	1	0	-0.118424	1.741949	-1.582774
44	1	0	-0.079794	0.340995	-2.652930
45	1	0	-1.152694	1.700151	-3.014192
46	6	0	-2.540554	-2.498898	0.960473
47	1	0	-3.485465	-2.786639	1.430805
48	1	0	-2.191646	-3.338985	0.351173
49	1	0	-1.804574	-2.358300	1.762736
50	6	0	-5.597500	1.073559	-0.861090
51	1	0	-6.384141	0.312289	-0.816347
52	1	0	-5.771008	1.767296	-0.027397
53	1	0	-5.727108	1.640967	-1.788547