Supporting Information

Electron Transfer Reactions: KO*t*Bu (but not NaO*t*Bu) Photo-reduces Benzophenone, under Activation by Visible Light

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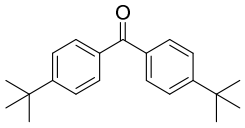
General information

All reagents were purchased from commercial sources and used without further purification, except where stated. Anhydrous diethyl ether, tetrahydrofuran, dichloromethane and hexane were dried using a Pure-Solv 400 solvent purification system (Innovative Technology Inc., U.S.A.). Tetrahydrofuran was further distilled over sodium "wire" using benzophenone as indicator using a still. The distilled THF was used for all the ketyl radical development. Anhydrous benzene was purchased from Sigma Aldrich and dried over 3Å molecular sieves, previously activated by microwave heating. Thin layer chromatography analyses were carried out on silica gel pre-coated aluminum foil sheets and were visualized using UV light (254 nm). Flash column chromatography was carried out using slurry packed silica gel (SiO_2), 35-75 μm particle size, 60 Å pore size, under a light positive pressure, eluting with the specified solvent system.

Where reactions were carried out in a glovebox, the atmosphere used was nitrogen and the glovebox was supplied by Innovative Technology Inc., USA. ^{1}H-NMR, ^{2}H-NMR and ^{13}C-NMR spectra were recorded on spectrometers operating at 400 MHz, 61 MHz and 101 MHz, respectively. All spectral data were acquired at 295 K. Chemical shifts (δ) are quoted in parts per million (ppm). Coupling constants (*J*) are reported in Hertz (Hz) to the nearest 0.1 Hz. The multiplicity abbreviations used are: s (singlet), d (doublet), t (triplet), q (quartet), qn (quintet), sextet (st), m (multiplet). Infrared (IR) spectra were recorded using an FTIR-ATR spectrometer. High resolution mass spectrometry was performed at the University of Swansea, in the EPSRC National Mass Spectrometry Centre. Accurate mass was obtained using a LTQ Orbitrap XL using Atmospheric Pressure Chemical Ionization (APCI) or High Resolution Nano-Electrospray (HNESP) using Electrospray Ionization (ESI). The mass spectra were recorded by gas-phase chromatography (GCMS) using electron ionization (EI). Low resolution GCMS data were recorded using an Agilent Technologies 7890A GC system coupled to a 5975C inert XL EI/CI MSD detector. Separation was performed using the DB5MS-UI column (30 m x 0.25 mm x 0.25 μm) at a temperature of 320 ^{o}C, using helium as the carrier gas.
All the UV reactions were carried out by using two focused UV lamps with filters (λ= 365 nm, each 100 watts) placed opposite to each other, around the reaction flask, at room temperature. All the Vis light reactions were carried out by using 60 LEDs in series (400 nm, 14.4 W total, SMD5050). The series internally lined a beaker and the reaction tubes were placed centrally in the beaker (2-3 cm of distance from the LEDs). When stated, the reactions were performed in direct sunlight. The 'dark' reactions were performed by covering the tube in foil to avoid any light exposure.
UV-visible absorption measurements were performed using a PerkinElmer Lambda 25 UV/VIS spectrophotometer.
Calculations of the yields of reactions using the internal standard 1,3,5-trimethoxybenzene (^{1}H-NMR internal standard) were performed as follows: 1,3,5-trimethoxybenzene (8.4 mg, 0.050 mmol, 10 mol%) was added as a solid to the reaction mixture. $CDCl_3$ (~1 mL) was added and the solution stirred for 5 min. A portion of the solution was taken and diluted for NMR analysis.

Preparation of the substrates

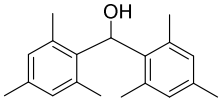
4,4'-Di-*tert*-butylbenzophenone, 27



4,4'-Di-tert-butylbenzophenone
Chemical Formula: $C_{21}H_{26}O$
Exact Mass: 294,1984

p-tert-Butylbenzoyl chloride (1.18 g, 1.17 ml, 6 mmol) was slowly added to *tert*-butylbenzene (1.93 mg, 2.22 mL, 14.4 mmol) and aluminium trichloride (2.22 g, 15.2 mmol) at RT. During the addition of *p-tert*-butylbenzoyl chloride, the reaction turned from a yellow suspension to a dark reddish brown solution. After the addition was complete, the reaction was warmed at 80 °C for 2.5 h. Vigorous bubbling was observed throughout the reaction. Afterwards, the hot reaction mixture was poured into crushed ice (30 g) and concentrated hydrochloric acid (10.5 mL). This yielded a tar-like substance which metamorphosed to a yellow solid after decomposition was complete (few minutes). This yellow solid was filtered, dissolved in toluene (15 mL), washed with water and 5% aqueous sodium hydroxide and dried over sodium sulfate. Recrystallisation from toluene produced a white powder which was washed with hexane to give **27** as a white solid (625 mg, 0.68 mmol, 35.5%).[1] Mp: 122-124 °C (lit: 123-124°C).[2] ν_{max} (neat, cm^{-1}) 2959, 2903, 2864, 1643, 1605, 1280, 1186, 1104, 932. ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.76 (4 H, d, *J* = 8.6, Ar*H*), 7.49 (4 H, d, *J* = 8.8, Ar*H*), 1.37 (18 H, s, CH_3) ppm. ^{13}C-NMR (101 MHz, $CDCl_3$) δ 195.7, 155.4, 134.7, 129.5, 124.7, 34.6, 30.7 ppm. GC-MS (EI) *m/z* 294.1. Data were consistent with the literature.[1]

Dimesitylmethanol, **38**

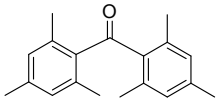


Dimesitylmethanol
Chemical Formula: $C_{19}H_{24}O$
Exact Mass: 268,1827

To a cooled (-78 °C) solution of mesityllithium, prepared by addition of *n*-butyllithium (2.2 mmol) to a solution of mesityl bromide (478 mg, 0.37 mL, 2.4 mmol) in 8 mL of THF, a solution of mesitylaldehyde (296 mg, 0.294 mL, 2.0 mmol) in 2 mL of THF. After 30 min, the solution was allowed to warm and was quenched with aqueous ammonium chloride. The product was extracted with diethyl ether, dried over sodium sulfate and concentrated. The crude was washed with pentane to give dimesitylmethanol **38** as a white solid (315 mg, 1.18

mol, 59%). Mp: 145-147 (lit: 149-150 °C)[3] IR ν_{max} (neat, cm^{-1}) 3472, 2908, 1608, 1476, 1420, 1375, 1126, 1045, 1003, 851, 694. ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.82–6.78 (4 H, s, Ar*H*), 6.37–6.33 (1 H, s, C*H*OH), 2.27–2.24 (6 H, s, CH_3), 2.23–2.19 (12 H, s, CH_3), 1.73–1.68 (1 H, s, O*H*) ppm. ^{13}C-NMR (101 MHz, $CDCl_3$) δ 136.7, 130.7, 73.5, 21.2, 20.8 ppm.[4] GC-MS (EI) *m/z* 268.1. Data were consistent with the literature. [4]

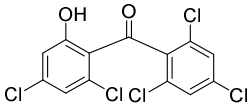
Dimesitylmethanone, 28



Dimesitylmethanone
Chemical Formula: $C_{19}H_{22}O$
Exact Mass: 266,1671

Pyridinium chlorochromate (2.53 g, 11.8 mmol) was added to a solution of dimesitylmethanol **38** (2.10 g, 7.8 mmol) in 35 mL of DCM and allowed to stir at RT for 3 h. The crude product was filtered on a celite pad, the solution concentrated and crystallised from methanol to give dimesitylmethanone, **28** as a white solid (1.4 g, 5.2 mmol, 67%). [4] Mp: 140-143 °C (lit: 138-140 °C)[4]. IR ν_{max} (neat, cm^{-1}) 2916, 1643, 1605, 1422, 1242, 887, 855, 696. ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.84 (4 H, s, Ar*H*), 2.29 (6 H, s, CH_3), 2.12 (12 H, s, CH_3) ppm. ^{13}C-NMR (101 MHz, $CDCl_3$) δ 202.8, 140.1, 138.6, 136.8, 129.9 21.3, 20.9 ppm. GC-MS (EI) *m/z* 266.1 (M^+).

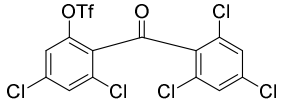
(2,4-Dichloro-6-hydroxyphenyl)(2,4,6-trichlorophenyl)methanone, 39



(2,4-dichloro-6-hydroxyphenyl)(2,4,6-trichlorophenyl)methanone
Chemical Formula: $C_{13}H_5Cl_5O_2$
Exact Mass: 367.8732

3,5-Dichloroanisole (2.8 mg, 16 mmol) and aluminium chloride (2.55 g, 19.2 mmol) were cooled to 0 °C in a flask under inert atmosphere. 2,4,6-Trichlorobenzoyl chloride (4.65 g, 19.2 mmol) was then added and the reaction mixture was stirred at 110 °C for 15 h. At the end of the reaction (monitored by TLC), water (15 mL) was added and the mixture stirred. The mixture was extracted with ethyl acetate, dried over sodium sulfate and concentrated *in vacuo*. Purification with silica gel chromatography (hexane) afforded (2,4-dichloro-6-hydroxyphenyl)(2,4,6-trichlorophenyl)methanone, **39** (1.7 g, 4.69 mmol, 58.6 %) as a white solid. Mp: 82-84 °C. IR ν_{max} (neat, cm^{-1}) 1626, 1543, 1386, 1365, 1298, 1224, 1184, 1089, 960, 916. ^{1}H NMR (400 MHz $CDCl_3$) δ 12.58 (1 H, s, O*H*), 7.38 (2 H, s, Ar*H*), 7.06 (1 H, d, *J* = 2.1, Ar*H*), 6.96 (1 H, d, *J* = 2.1, Ar*H*) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.7, 165.9, 143.0, 137.8, 136.6, 136.44, 132.2, 128.5, 123.0, 118.4, 117.0 ppm. *m/z* (APCI) calcd. for $C_{13}H_6Cl_5O_2$ $[M+H]^+$: 368.8805, found: 368.8798.

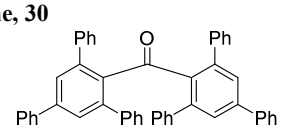
3,5-Dichloro-2-(2,4,6-trichlorobenzoyl)phenyl trifluoromethanesulfonate, **40**



3,5-dichloro-2-(2,4,6-trichlorobenzoyl)phenyl trifluoromethanesulfonate
Chemical Formula: $C_{14}H_4Cl_5F_3O_4S$
Exact Mass: 499.8225
Molecular Weight: 502.4872

Ketone **39** (1.61 g, 4,4 mmol), anhydrous DCM (8 mL) and pyridine (695.2 mg, 8,8 mmol) were added to a round-bottomed flask, under argon atmosphere. The mixture was cooled to 0° C in an ice bath, then was treated with dropwise addition of triflic anhydride (4.49 g, 5.28 mmol). The resulting mixture was allowed to warm up to RT and kept stirred for additional 4 h. The mixture was then filtered and concentrated *in vacuo*. The product was purified by chromatography (hexane), affording **40** (1.24 g, 2.48 mmol, 56.4 %). Mp: 110-112 °C. IR ν_{max} (neat, cm^{-1}) 1686, 1427, 1207, 1136, 1091, 953, 910, 798. ^{1}H NMR (400 MHz $CDCl_3$) δ 7.46 (1 H, d, *J* = 1.9, Ar*H*), 7.40 – 7.36 (3 H, m, Ar*H*) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ ppm 185.8, 148.5, 138.8, 137.9, 134.9, 134.6, 134.5, 130.4, 129.3, 121.5, 118.5 (q, *J* = 320.6, *C*F_3) ppm. *m/z* (APCI) calcd. for $C_{14}H_5Cl_5F_3O_4S$ $[M+H]^+$: 500.8298, found: 500.8287.

Bis(5'-phenyl-[1,1':3',1''-terphenyl]-2'-yl)methanone, 30

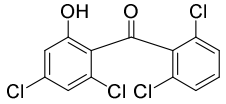


bis(5'-phenyl-[1,1':3',1''-terphenyl]-2'-yl)methanone
Chemical Formula: $C_{49}H_{34}O$
Exact Mass: 638.2610
Molecular Weight: 638.8100

Six different oven-dried microwave vials were charged, independently, with **40** (100,4 mg, 0,2 mmol), bis(acetonitrile)dichloropalladium(II) (2,6 mg, 0,01 mmol, 5%), Sphos (8,2 mg, 0,02 mmol, 10 %), phenylboric acid (292,8 mg, 2,4 mmol)

and K_3PO_4 (508,8 mg, 2,4 mmol). The mixture was then introduced into the glovebox and anhydrous toluene (10 mL) was added. The vial was then sealed inside the glovebox and transferred into the fumehood, where it was heated at 110 °C for 4 days. The six cooled reaction mixtures were then combined and diluted with water and extracted with toluene. The combined organic layers were combined, dried over sodium sulfate, filtered and concentrated *in vacuo*. The residue was purified by chromatography (hexane) affording a white solid which was recrystallised using a small amounts of toluene (very soluble) and hexane (almost insoluble) giving rise to ketone **30** (454 mg, 0.71 mmol, 59.3% combined yield from the 6 vials). The reaction was found to work better in a system under pressure such as a microwave vial. A bigger scale in a normal three-necked flask was tried, but only traces of product were detected.[5] Mp: 246-248 °C. IR ν_{max} (neat, cm^{-1}) 3053, 1665, 1590, 1491, 1229, 1074, 1029. ^{1}H NMR (400 MHz $CDCl_3$) δ 7.52 – 7.48 (4 H, m, Ar*H*), 7.43 (4 H, t, *J* = 7.3, Ar*H*), 7.39 – 7.35 (2 H, m, Ar*H*), 7.33 – 7.26 (12 H, m, Ar*H*), 7.20 – 7.17 (8 H, m, Ar*H*), 7.09 (4 H, s, Ar*H*) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.7, 143.4, 141.2, 140.9, 139.4, 136.2, 129.8, 128.7, 128.3, 127.3, 126.7, 126.7, 126.2 ppm. *m/z* (APCI) calcd. for $C_{49}H_{35}O$ $[M+H]^+$: 639.2682, found: 639.2678.

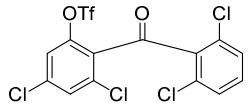
(2,4-Dichloro-6-hydroxyphenyl)(2,6-dichlorophenyl)methanone, 41



(2,4-dichloro-6-hydroxyphenyl)(2,6-dichlorophenyl)methanone
Chemical Formula: $C_{13}H_6Cl_4O_2$
Exact Mass: 333.9122
Molecular Weight: 335.9890

Aluminium chloride (1.8 g, 13.2 mmol) and 3,5-dichloroanisole (1.0 g, 6 mmol) were added to a flask under inert atmosphere and this was then cooled at 0 °C. 2,6-Dichlorobenzoyl chloride (1.5 g mg, 7.2 mmol) was then added. The reaction mixture was stirred at 110°C for 15 h. The mixture was extracted with ethyl acetate, dried over sodium sulfate and concentrated *in vacuo*. Purification with silica gel chromatography using pure hexane as eluent afforded **41** (1.91 g , 5.72 mmol, 72 % yield). Mp: 98-100 °C. IR ν_{max} (neat, cm^{-1}) 3080, 1618, 1593, 1545, 1425, 1396, 1296, 1223, 1175, 956, 912, 846, 804. ^{1}H NMR (400 MHz $CDCl_3$) δ 12.70 (1 H, s, O*H*), 7.37 – 7.31 (3 H, m, Ar*H*), 7.05 (1 H, d, *J* = 2.0, Ar*H*), 6.94 (1 H, d, *J* = 2.1, Ar*H*) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.0, 165.3, 142.1, 138.5, 136.1, 131.2, 130.9, 130.5, 127.7, 122.3, 120.3, 117.6, 116.5 pm. *m/z* (APCI) calcd. for $C_{13}H_7Cl_4O_2$ $[M+H]^+$: 334.9200, found 334.9209. Analogous demethylation of anisole using $AlCl_3$ was previously reported in the literature.[6]

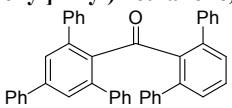
3,5-Dichloro-2-(2,6-dichlorobenzoyl)phenyl trifluoromethanesulfonate, 42



3,5-dichloro-2-(2,6-dichlorobenzoyl)phenyl
trifluoromethanesulfonate
Chemical Formula: $C_{14}H_5Cl_4F_3O_4S$
Exact Mass: 465.8615

Ketone **41** (1.6 g, 4.8 mmol), anhydrous DCM (8 mL) and pyridine (758.4 mg, 9.6 mmol) were added to a round-bottomed flask, under argon atmosphere. The solution was cooled to 0° C in an ice bath and then was treated with dropwise addition of triflic anhydride (1.62 g, 5.76 mmol). The resulting mixture was allowed to warm to RT and stirred for additional 4 h. At the end of the reaction (monitored by TLC), the mixture was filtered and concentrated *in vacuo*. The product was purified by chromatography (hexane), affording ketone **42** (2.0 g, 4.40 mmol, 92%) as a white solid. Mp: 95-97 °C. IR ν_{max} (neat, cm^{-1}) 1690, 1591, 1429, 1211, 1138, 955, 910, 868, 800, 781. ^{1}H NMR (400 MHz $CDCl_3$) δ 7.46 (1 H, d, *J* = 1.8, Ar*H*), 7.38 (1 H, d, *J* = 1.8, Ar*H*), 7.36 – 7.34 (3 H, m, Ar*H*) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 186.0, 147.9, 137.9, 135.8, 134.0, 133.2, 131.7, 129.9, 129.7, 128.6, 120.7, 117.9 (q, *J* = 320 Hz, *C*F_3) ppm. *m/z* (APCI) calcd. for $C_{14}H_9Cl_4F_3NO_4S$ $[M+NH_4]^+$: 483.8953, found 483.8950.

[1,1':3',1''-Terphenyl]-2'-yl(5'-phenyl-[1,1':3',1''-terphenyl]-2'-yl)methanone, 29

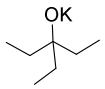


[1,1':3',1''-terphenyl]-2'-yl(5'-phenyl-[1,1':3',1''-terphenyl]-2'-yl)methanone
Chemical Formula: $C_{43}H_{30}O$
Exact Mass: 562.2297
Molecular Weight: 562.7120

Six oven-dried microwave vials were charged, independently, with ketone **42** (93.6 mg, 0.2 mmol), bis(acetonitrile)dichloropalladium(II) (2.59 mg, 0.01 mmol, 5%), Sphos (8.2 mg, 0.02 mmol, 10%) phenylboronic acid (244 mg, 2 mmol) and K_3PO_4 (424 mg, 2 mmol). The mixture was then introduced in the glovebox and anhydrous toluene (10 mL) was added. The vials were then closed, removed from the glovebox and placed in the fumehood, where they were heated at 110 °C for 5 days (monitored *via* NMR). The cooled reaction mixture was diluted with water and extracted with toluene. The combined organic layers were combined, dried over sodium sulfate, filtered and the filtrate was concentrated *in vacuo*. The mixture was purified *via* chromatography (hexane : ethyl acetate as 9.5 : 0.5), affording the product (420 mg, 0.75 mmol, 62 % combined yield) as a white powder. The reaction was found to work better in a system under pressure such as a microwave vial. A bigger scale in a normal three-necked flask was tried but only traces of product were detected. Reaction conditions were inspired by prior literature.[5] Mp: 90-93 °C. IR ν_{max} (neat/cm^{-1}) 3048, 1667, 1589, 1491, 1231, 926, 885, 756, 694. ^{1}H NMR (400 MHz

$CDCl_3$) δ 7.51 – 7.47 (2 H, m), 7.45 – 7.39 (2 H, m), 7.39 – 7.33 (1 H, m), 7.33 – 7.23 (13 H, m), 7.18 – 7.13 (4 H, m), 7.13 – 7.09 (4 H, m), 7.06 (2 H, s), 6.87 (2 H, d, *J* = 7.6) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.9, 143.4, 142.6, 141.1, 140.9, 140.9, 139.4, 137.3, 135.8, 130.2, 129.8, 128.8, 128.6, 128.30, 127.3, 126.8, 126.7, 126.6, 126.2, 126.0 ppm. *m*/*z* (APCI) calcd. for $C_{43}H_{31}O$ $[M+H]^+$: 563.2375, found 563.2388.

Potassium 3-ethylpentan-3-olate, 43



potassium 3-ethylpentan-3-olate
Chemical Formula: $C_7H_{15}KO$
Exact Mass: 154.0760

In the glovebox, previously washed potassium hydride (400 mg, 10 mmol) was added to a flame-dried three-necked flask, equipped with a vacuum tap. The flask was then sealed, removed from the glovebox and placed in a -78 ^{o}C bath in a fumehood. A solution of triethylcarbinol (1160 mg, 10 mmol) in anhydrous diethyl ether (20 mL) was added. The reaction mixture was stirred at -78 °C for 1 h, then at RT overnight. The solvent was removed on the house vacuum line and the crude material was dried for 3 h, put under an argon atmosphere and transferred into the glove box immediately giving rise to **43** (1.3 g, 8.4 mmol, 84 %). ^{1}H NMR (400 MHz, C_6D_6) δ 1.22 (6 H, q, *J* = 7.5, C*H*$_2$CH$_3$), 0.85 (9 H, t, *J* = 7.5, CH$_2$C*H*$_3$) ppm. ^{13}C NMR (101 MHz, C_6D_6) δ 71.8, 33.1, 8.1 ppm.

Qualitative evaluation of formation of ketyl radicals of aromatic ketones

General procedure for testing the reduction of benzophenone and benzophenone derivatives with Na or KO*t*Bu.

The aromatic ketone (1 eq, 0.77 mmol) was added to distilled THF (5 mL) into a pressure tube containing sodium (18 mg, 0.77 mmol) or KOIBu (172 mg 1.54 mmol) in the glovebox. The sealed pressure tube was then removed from the glovebox and placed on a stirrer hotplate in the fumehood. Where specified, the reaction was heated to 70°C behind a blast shield. The ketyl radical formation was detected through development of a blue coloration in the solution. The reaction was quenched with isopropyl alcohol and the blue coloration disappeared soon after the addition.

Figure S1 Above is a typical example of reaction performed under UV lamps (365 nm, 100 W x 2) at RT.
Left: THF + **17** (0.5 mmol) + KO*t*Bu (2eq). Right: blank reaction THF + **17** (0.5 mmol). Picture taken after 30 min.

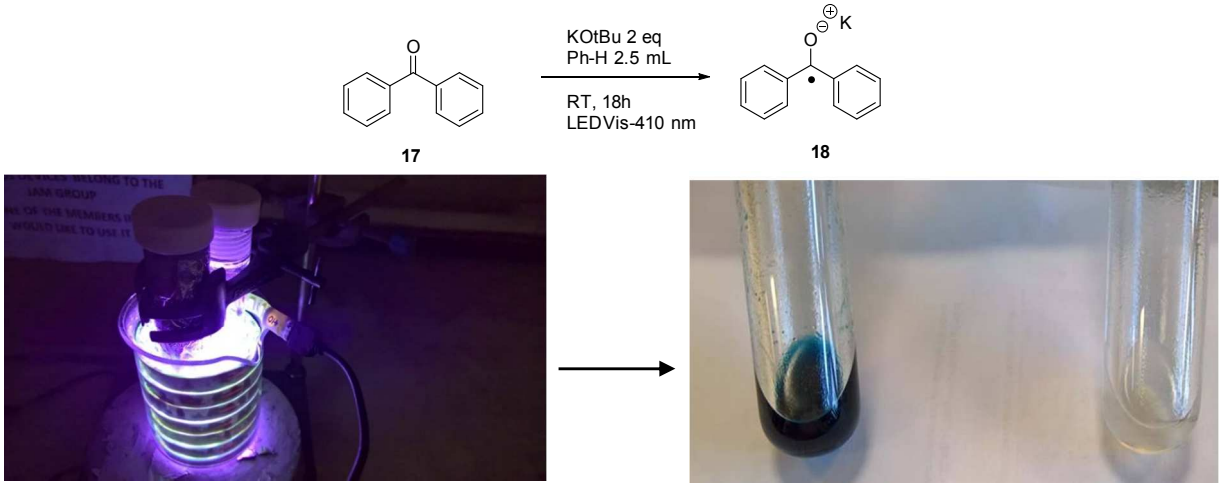


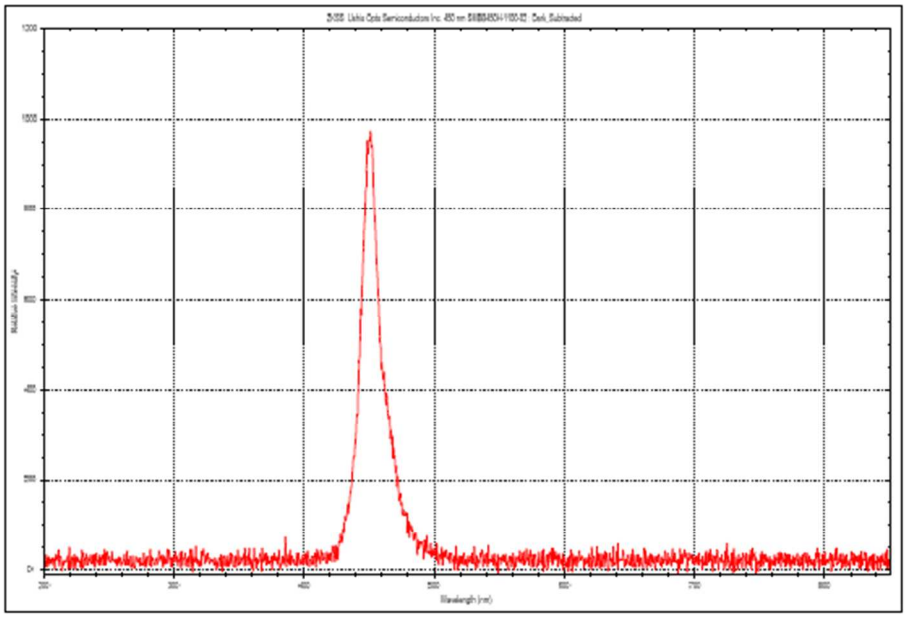
Figure S2. Above is a typical example of reaction **17** + KO*t*Bu 2 eq in benzene 2.5 mL performed under Vis LEDs light (400 nm, 14.4 W) at RT. Only the tube with a direct exposition to the light gives the typical blue coloration of the ketyl radical, afterwards confirmed by UV measurement.

LED Output Spectra

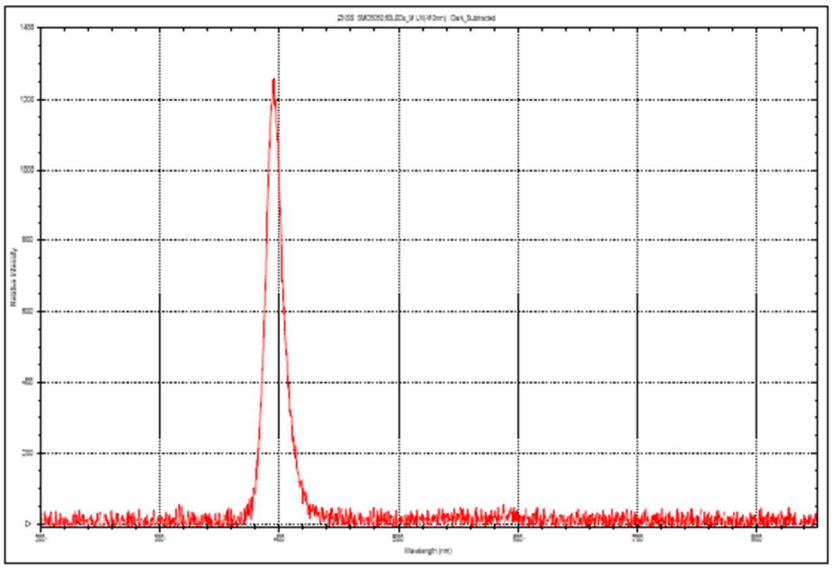
These spectra were produced using a BWTEK Inc, Exemplar LS (Low Straylight Smart CCD Spectrometer, http://bwtek.com/products/exemplar-ls/)

(i) Reference spectrum taken of a Ushio Opto Semiconductors Inc. **450 nm:** SMBB450H-1100-02

(Full details in SI of https://doi.org/10.1002/cptc.201800082 page S10)



(ii) Spectrumof SMD5050;60LEDs/M; Color: UV('410nm')



Luminous flux measurements

Luminous flux

Luminous flux measurements were taken with a Traceable® Dual-Display Light Meter (https://traceable.com/3252-traceable-dual-display-light-meter.html purchased from Fisher Scientific).

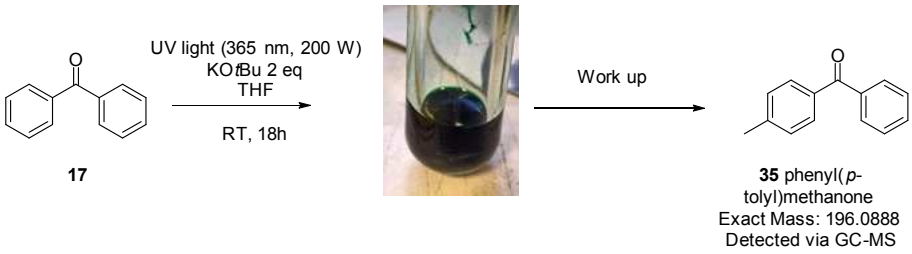
The Lux sensor was placed inside the coil of SMD5050;60LEDs Figure X, and the setup covered with tin foil to remove any external light.

Figure X Lux measurement set up

Traceable® Dual-Display Light Meter was set to F= fluorescent mode, the LEDs where turned on a LUX reading taken, 39 LUX.

Detection of methylated and ethylated benzophenone

Phenyl(*p*-tolyl)methanone, 35



Benzophenone **17** (91 mg, 0.5 mmol), KO*t*Bu (112 mg, 1 mmol) were loaded in a 15 mL pressure tube with THF (2.5 mL). The sealed tube was then moved out from the glovebox and placed under UV light for 18h. The dark green/blue colour gradually developed from the start of the reaction. After 18 h the tube was opened and water was added. The dark coloration disappear after few seconds of air exposure or water contact. The mixture was then extracted with ether, dried over sodium sulfate and concentrated *in vacuo*. The residue was analysed via TOF MS EI$^+$ (see spectrum below). The fragmentation pattern is consistent with the literature data for the ketone **35**. (lit: GCMS (EI) (%): 196 (M$^+$, 43), 181(9), 165 (4), 152(4), 119(100), 105(32), 91(46), 77(43)).[7]

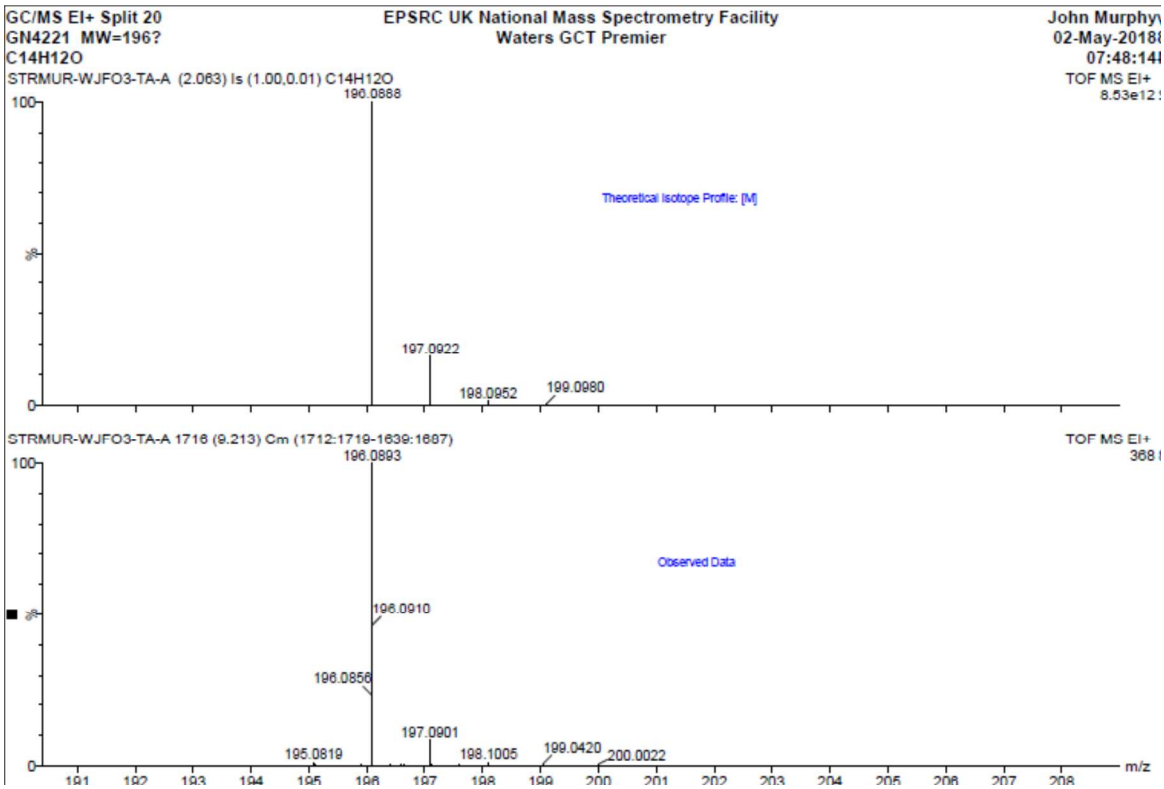


Figure S3 Calculated and observed high resolution mass spectra of phenyl(*p*-tolyl)methanone **35**

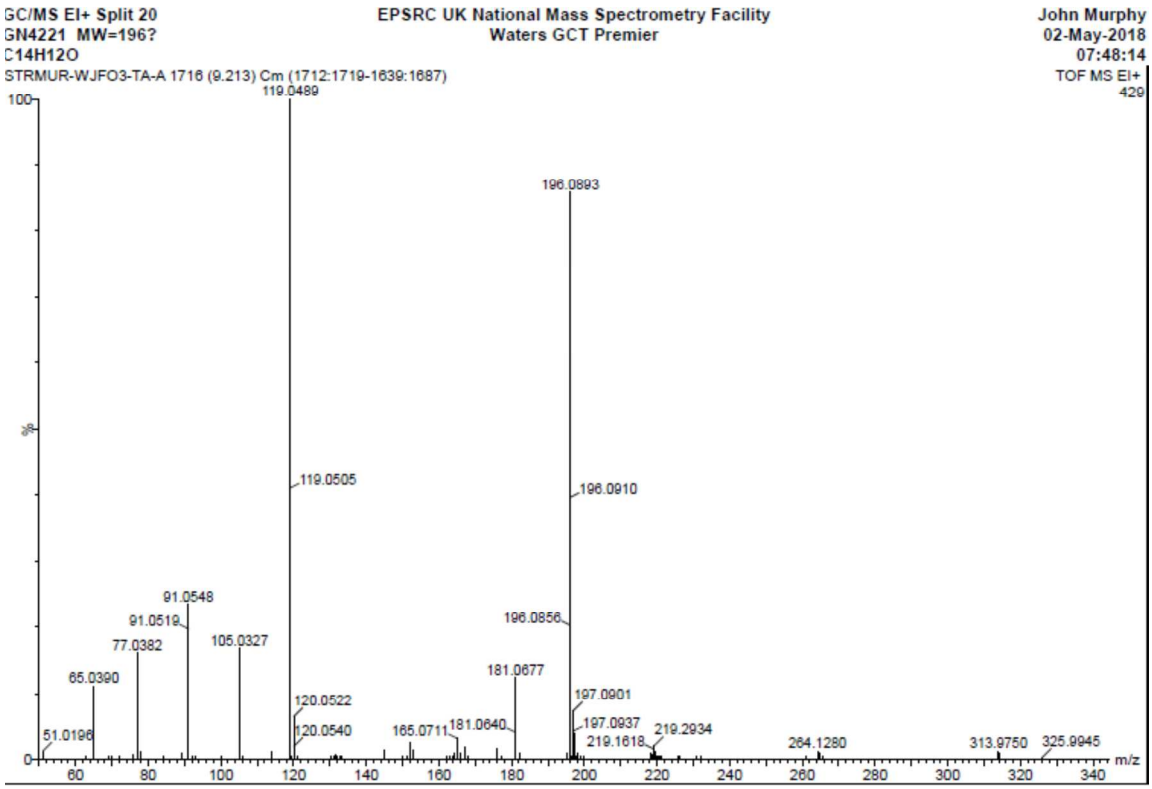
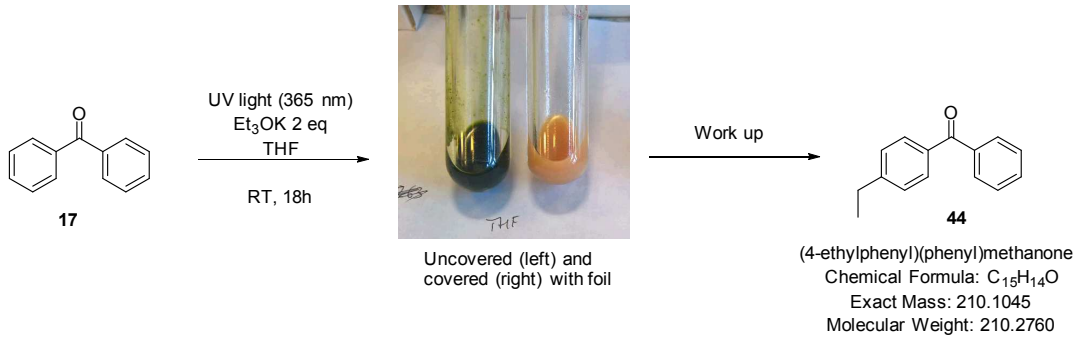


Figure S4. EI spectrum of phenyl(*p*-tolyl)methanone **35**

(4-Ethylphenyl)(phenyl)methanone, 44



Benzophenone **17** (91 mg, 0.5 mmol), $KOEt_3$ (154 mg, 1 mmol) were loaded in a 15 mL pressure tube with THF (2.5 mL). The sealed tube was then moved out from the glovebox and placed under UV light for 18h. The dark green/blue colour was gradually developed since the start of the reaction. The blank reaction (absence of any source of lights) does not give any blue/green colour throughout the entire course of the reaction. After 18 h the tube was opened and water was added. The dark coloration disappeared after few seconds of air exposure or water contact. The mixture was then extracted with ether, dried over sodium sulfate and concentrated *in vacuo*. The residue was analyzed via TOF MS EI^+ (see spectra below).

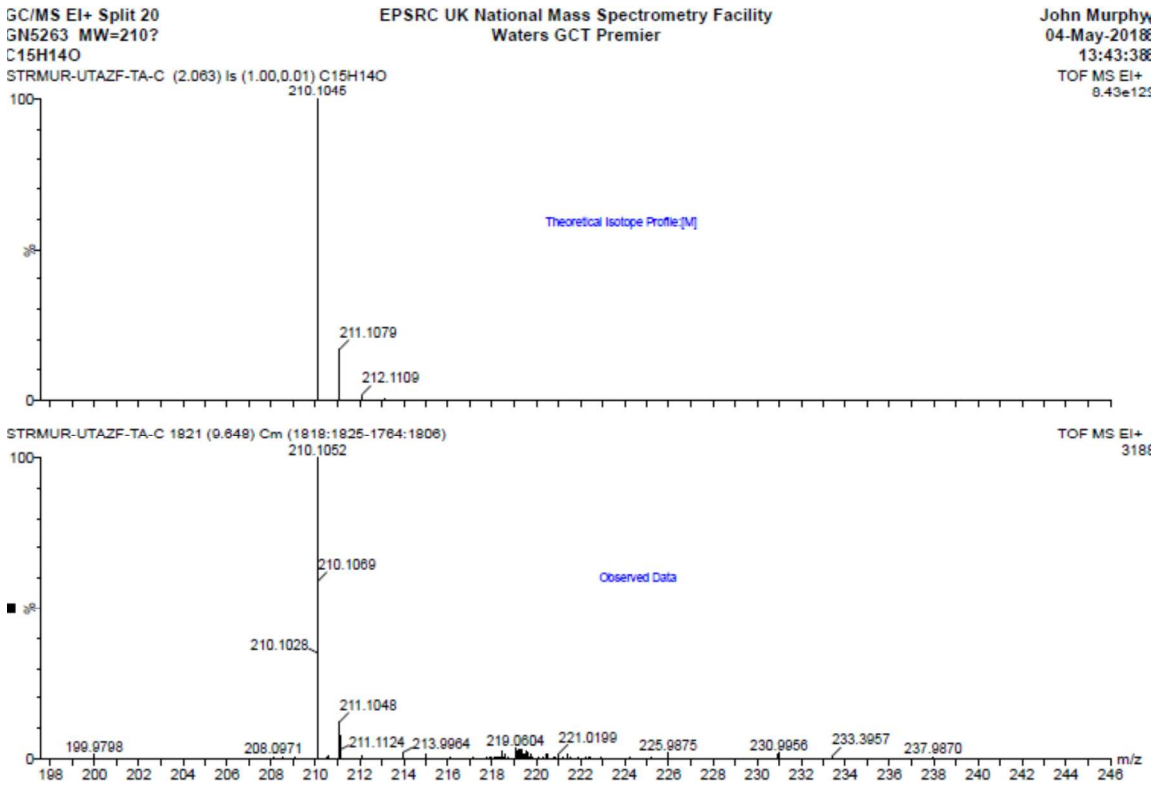


Figure S5. Calculated and observed high resolution mass spectra of of 4-ethylphenyl)(phenyl)methanone **44**

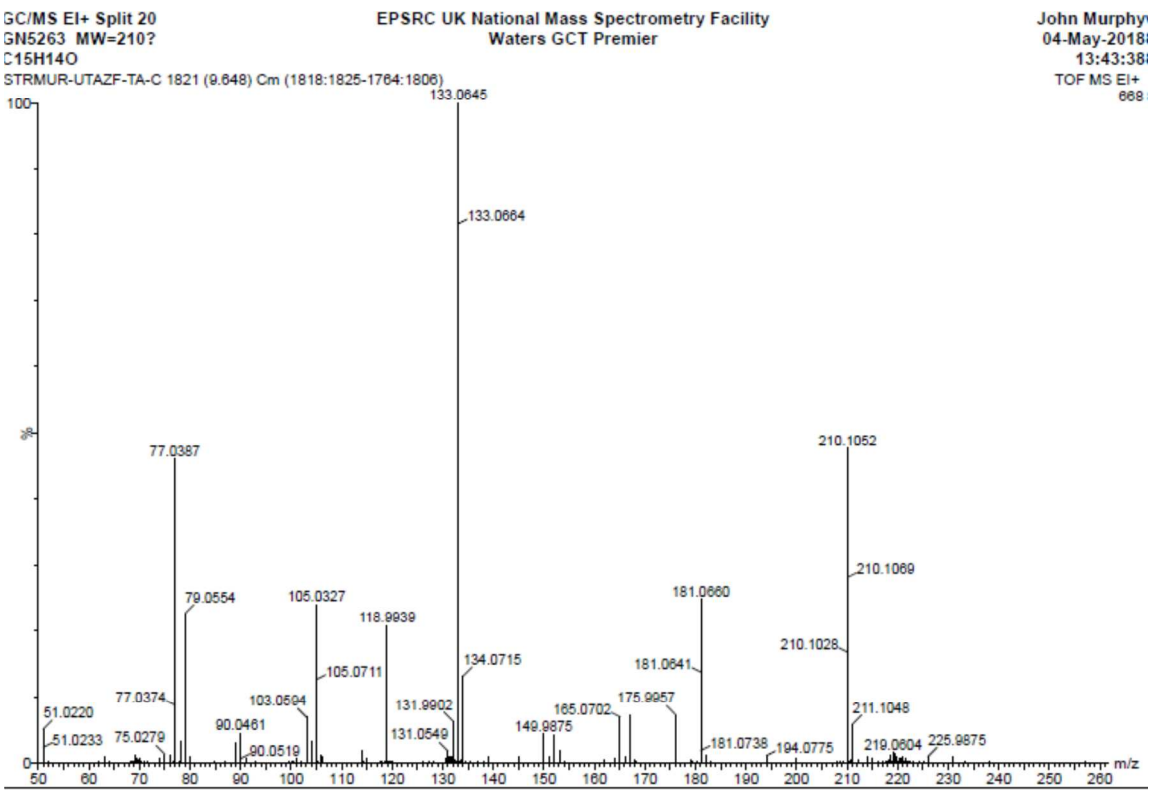


Figure S6. EI spectrum of 4-ethylphenyl)(phenyl)methanone **44**

UV measurements

Every solution was prepared in the glovebox using distilled THF (3 mL) and a quartz standard cuvette.

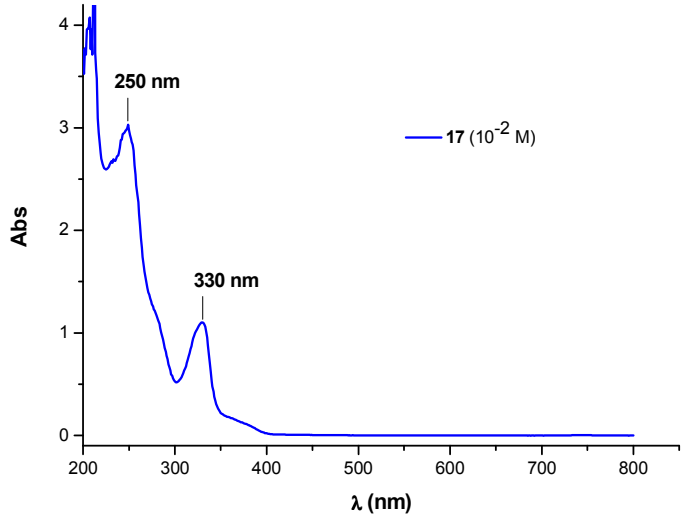


Figure S7. UV spectrum of benzophenone **17** (10^{-2} **M**) in THF

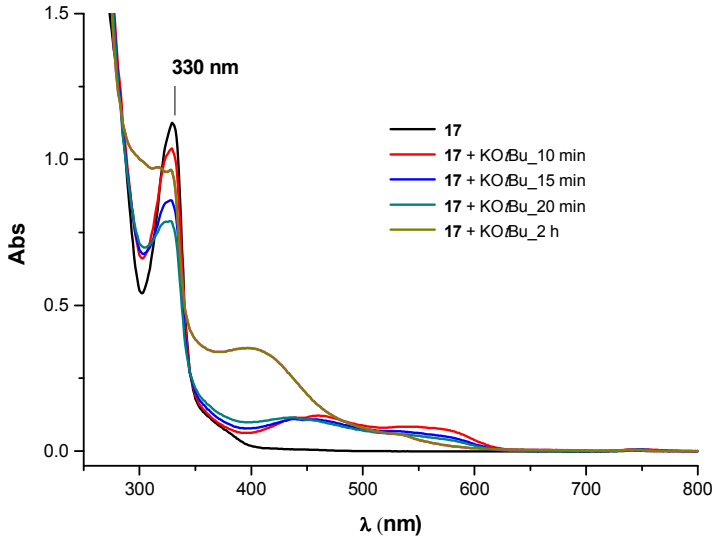


Figure S8. UV spectrum of benzophenone **17** (10^{-2} **M**) in THF; In the presence of KO*t*Bu, a bathochromic expansion of the absorption occurs with the time.

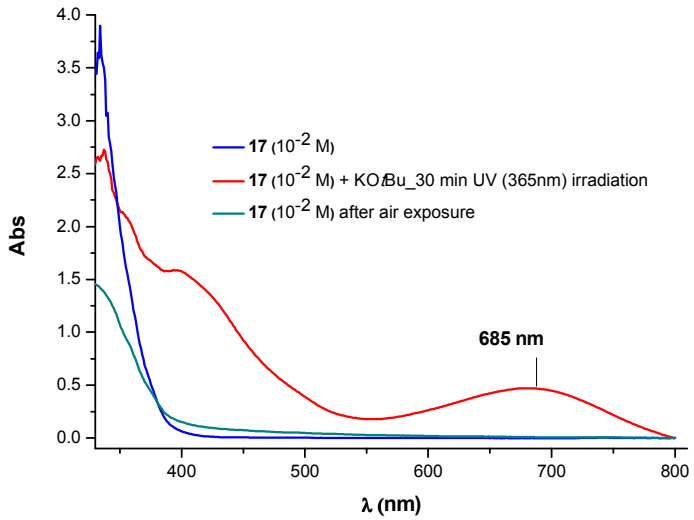


Figure S9. Formation of the ketyl radical **18** after irradiating the complex **17**+KO*t*Bu with UV light (365 nm, 100W x 2).

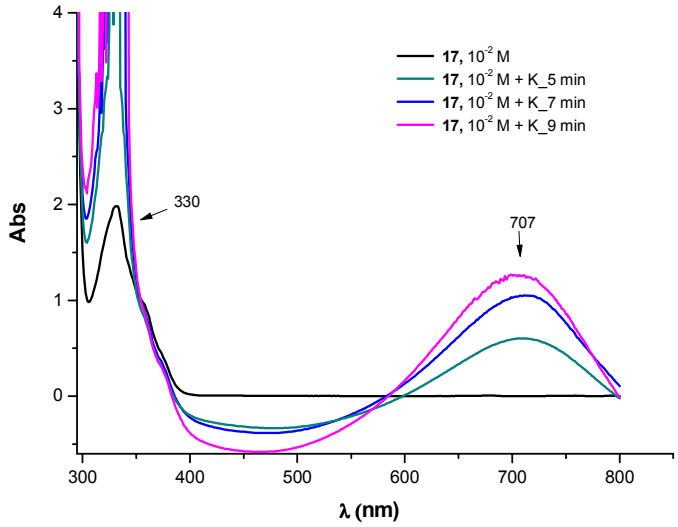


Figure S10. UV spectrum of **17** 10^{-2} **M** in presence of an excess of potassium metal. In the first 10 minutes formation of the ketyl radical peak around 700 nm was observed. The concentration of BZP used needs to be around 10^{-2}-10^{-3} **M** to make evident the development of the ketyl radical anion **18** peak. This spectrum is consistent with the literature.[8]

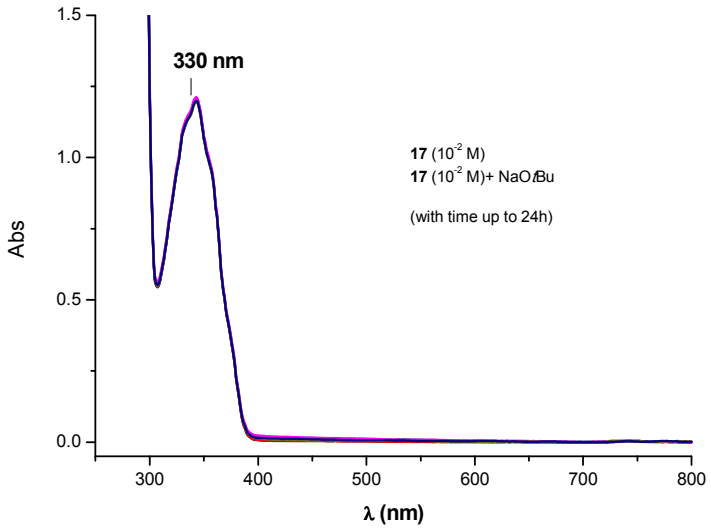


Figure S 11. UV measurements of **17** (10^{-2} **M**) before and after adding NaO*t*Bu. The cuvette was agitated and measurements were taken every 10 min for 1h. The cuvette was then left overnight and no shift was observed the following day. No colour change in the cuvette was observed.

NMR tests throughout the reaction

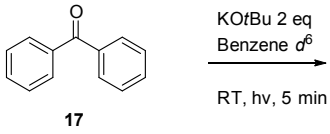
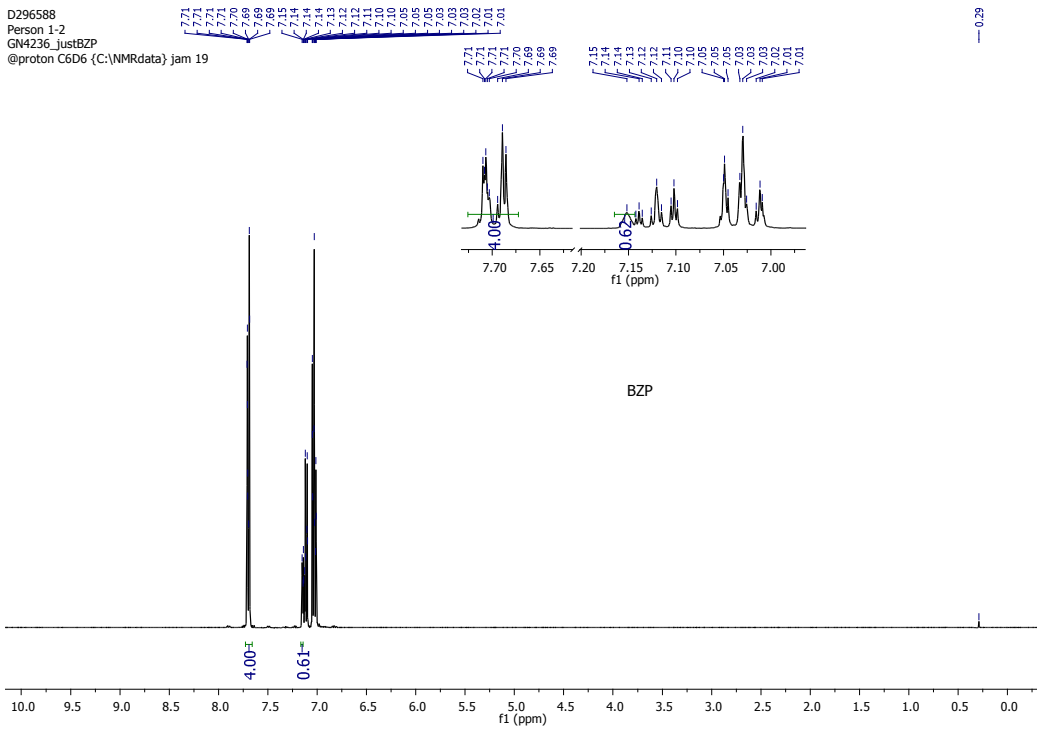


Figure S 12. The signals from structure **17** disappear just after 5 minutes UV exposure, indicating that radical species and macromolecular structures are formed in the reaction.[8]

^{1}H NMR spectrum of benzophenone **17**



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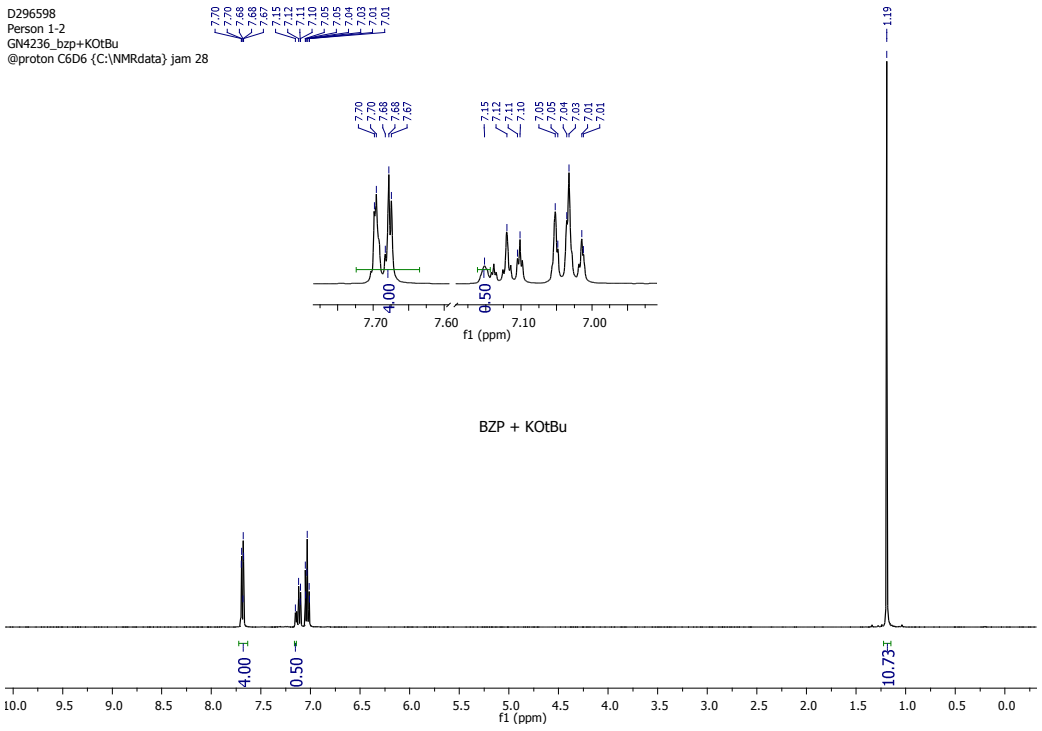
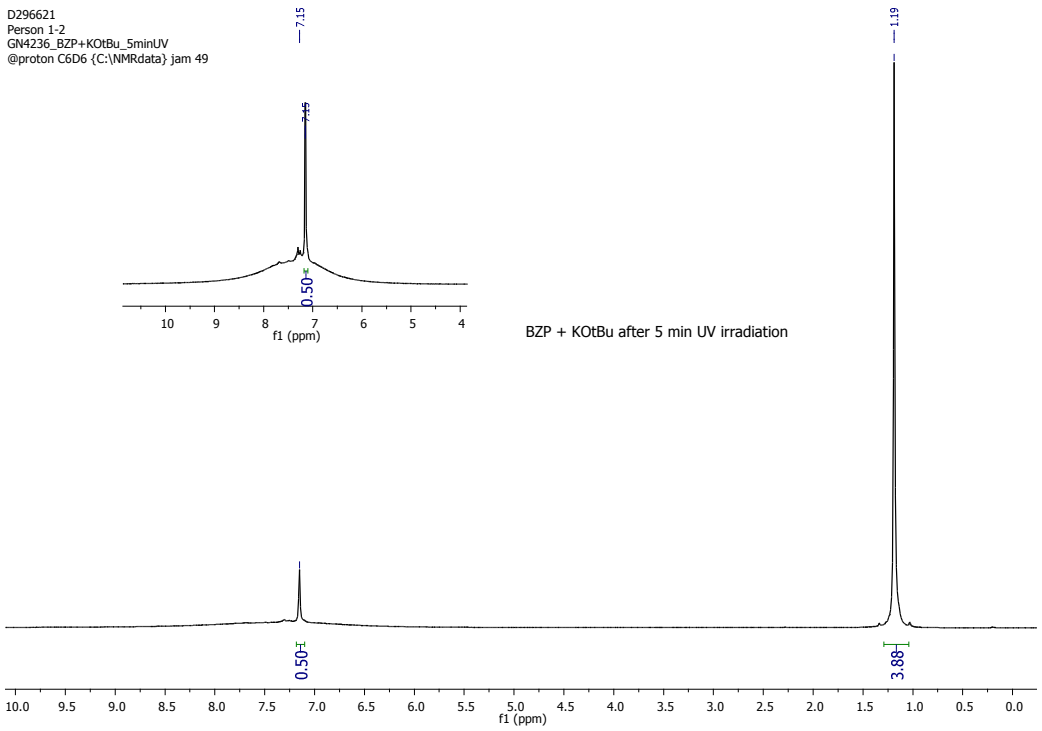
^{1}H NMR spectrum of benzophenone **17** + KO*t*Bu



^{1}H NMR spectrum of benzophenone **17** + KO*t*Bu after 5 min irradiation with UV (365 nm)



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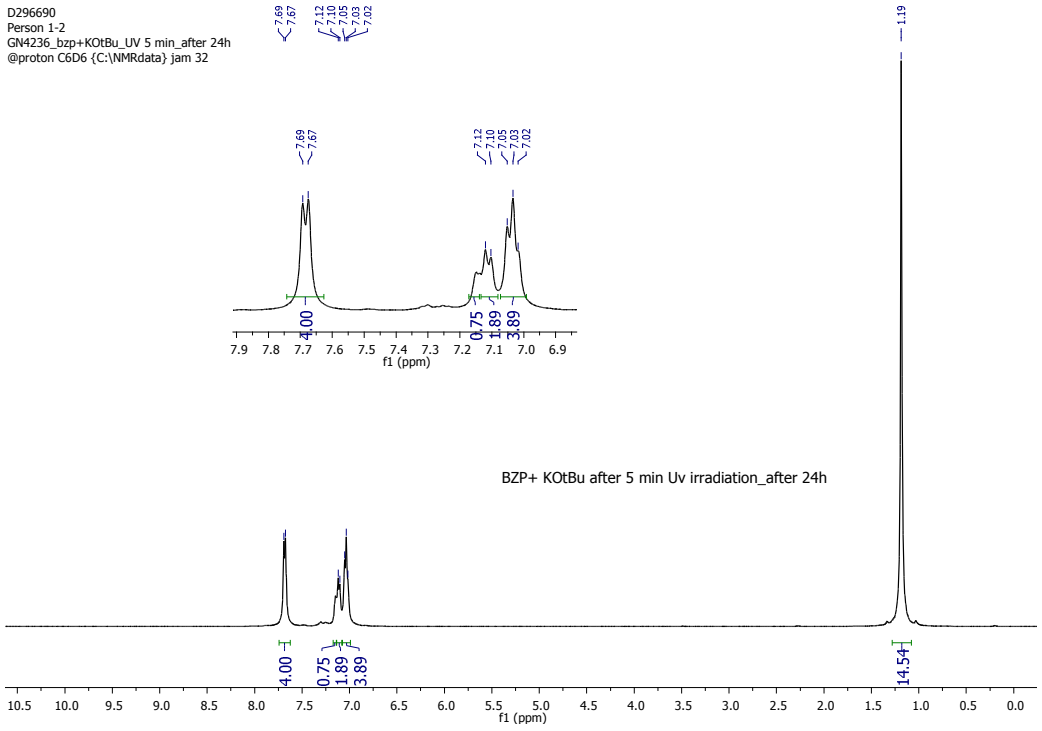
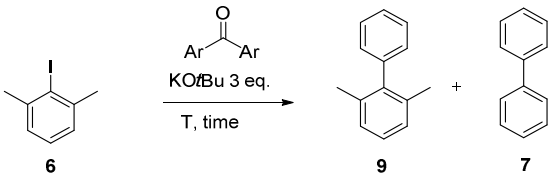
^{1}H NMR spectrum of benzophenone **17** + KO*t*Bu after 5 min irradiation with UV (365 nm), then standing for 24 h



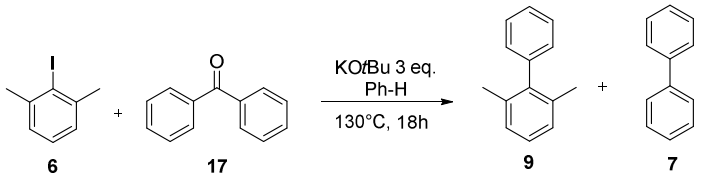
General conditions and yield calculations for cross coupling reactions

Reactions with iodo-*m*-xylene using the aromatic ketones as additives.



A mixture of iodo-*m*-xylene **6** (0.5 mmol), KO*t*Bu (3.0 eq.) and the desired aromatic ketone (0.2 eq) in benzene (5 mL) was sealed in a 15 mL pressure tube in a glovebox. The tube was removed from the glovebox and heated at 130 ºC for 18 h behind a blast shield. After cooling to room temperature, the reaction was quenched by water (15 mL) and acidified with 1N hydrochloric acid until neutral p*H*. The mixture was extracted with diethyl ether (3 x 15 mL). The organic layer was dried over sodium sulfate, filtered and concentrated to give rise to the residue. Since the coupled products **9** and **7** are inseparable, the yields were calculated from NMR spectra *via* internal standard. 1,3,5-trimethoxybenzene 8.4 mg, (0.050 mmol, 10 mol%) which was added as a solid to the reaction mixture, ~1 mL $CDCl_3$ was added to form a homogeneous solution and the solution stirred. A portion of the solution was taken and diluted for NMR analysis.

Cross coupling reaction using **17** as additive.



A mixture of 1-iodo-2,6-dimethylbenzene **6** (116 mg, 0.5 mmol), KO*t*Bu (168 mg, 1.5 mmol) and **17** (18.2 mg; 0.01 mmol) in benzene (5 mL) was sealed in a 15 mL pressure tube in a glovebox. The tube was removed from the glovebox and heated at 130 ºC for 18 h behind a blast shield. After cooling to room temperature, the reaction was quenched by water (15 mL) and acidified with 1N HCl until neutral pH. The mixture was extracted with diethyl ether (15 mL). The organic layer was dried over sodium sulfate, filtered and concentrated to give the residue as a dark yellow oil. The yield was calculated using 1,3,5-trimethoxybenzene (10%) as internal standard. The quantity of each product was determined as following (also see annotated example spectrum below):

For the recovered starting material **6** the integration of methoxy signal of the internal standard in the ^{1}H-NMR spectrum was set to 9 units. The integration of the methyl signal of **6** (2.50 ppm) was then measured and the following calculation gave the amount of **6** present:

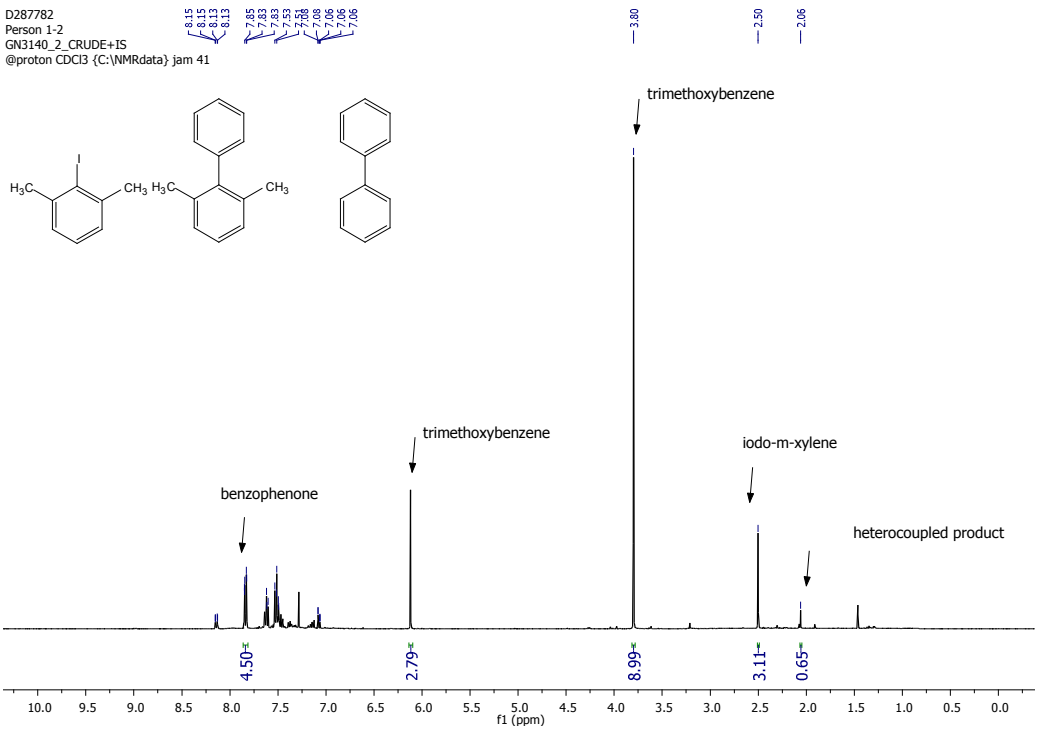
(3.11/6) × 10 = 5.2%

For the hetero-coupled product **9**, the integration of the methoxy signal of the internal standard in the ^{1}H-NMR spectrum was set to 9 units. The integration of the methyl signal of **9** (2.04 ppm) was then measured and the following calculation gave the amount of **9** present:

(0.65/6) × 10 = 1.1%

For the biphenyl product **7** the integration of the aromatic signal of the internal standard was set to 3 units. The integration of the aromatic signals of **7** at 7.64–7.59 ppm (4 H) was then measured and the following calculation gave the amount of **7** present:

(int/4) × 10 = yield % but see text below the next spectrum**

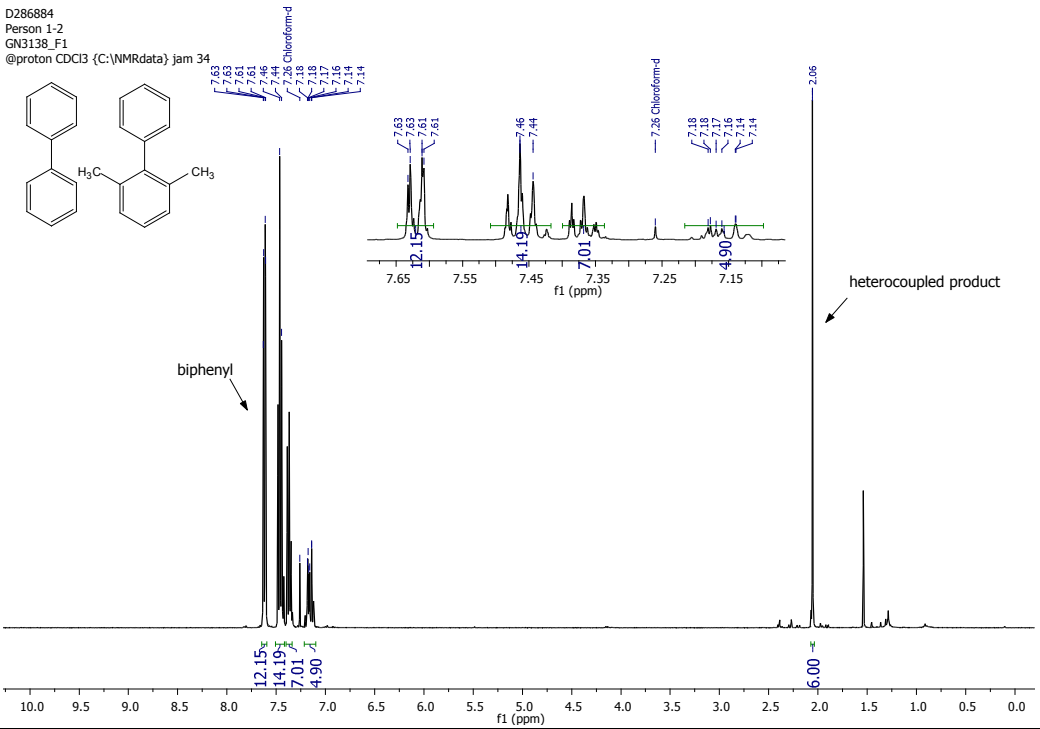


**In this particular case the diagnostic peak of biphenyl overlaps with one of the benzophenone peak. In the BHAS mediated mechanism the ratio between biphenyl and heterocoupled product is always 3:1. In fact, after purification by chromatography the inseparable mixture was indeed in 3:1 ratio. Integrating the methyl group (6H, 2.06 ppm) as 6 the ratio of biphenyl (4H, 7.62 ppm) is:

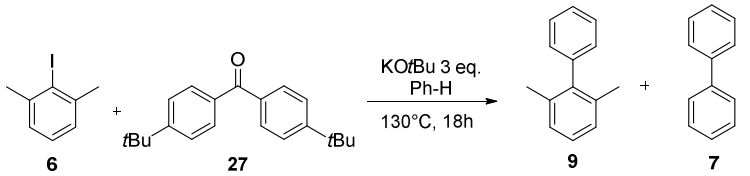
(12.15/4) = 3.0

Since the ratio was found to be 3:1, the tiled of biphenyl present in the mixture was 3.3%.
Number of runs: (a) Biphenyl 3.3 % ; 1,3-dimethylbiphenyl 1.1 %. (b) Biphenyl 3.6 % ; 1,3-dimethylbiphenyl 1.2%. (c) Biphenyl 3.6 % ; 1,3-dimethylbiphenyl 1.2%

Average of 3 runs: Biphenyl 3.5 % ; 1,3-dimethylbiphenyl 1.2%.

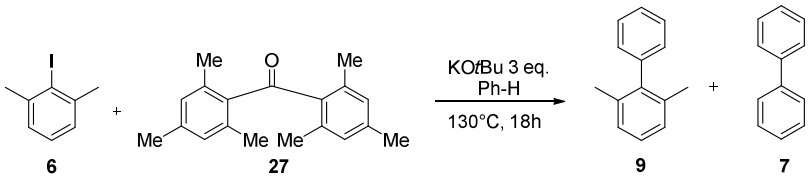


Cross coupling reaction using **27** as additive.



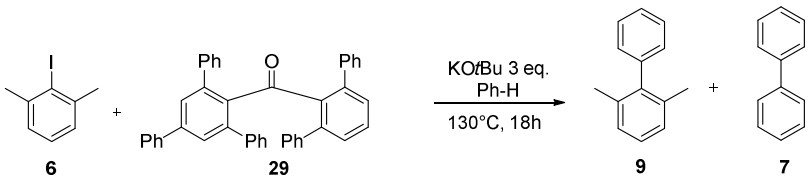
A mixture of 1-iodo-2,6-dimethylbenzene **6** (116 mg, 0.5 mmol), KO*t*Bu (168 mg, 1.5 mmol) and **27** (29.4 mg; 0.1 mmol) in benzene (5 mL) was sealed in a 15 mL pressure tube in a glovebox. The tube was removed from the glovebox and heated at 130 ºC for 18 h behind a blast shield. After cooling to room temperature, the reaction was quenched by water (15 mL) and acidified with 1N HCl until neutral pH. The mixture was extracted with diethyl ether (15 mL). The organic layer was dried over sodium sulfate, filtered and concentrated to give the residue as a dark yellow oil which yielded 1.0 % of **9** and 3.2 % of **7**. The yield was calculated using 1,3,5-trimethoxybenzene (10%) as internal standard.

Cross coupling reaction using **28** as additive.



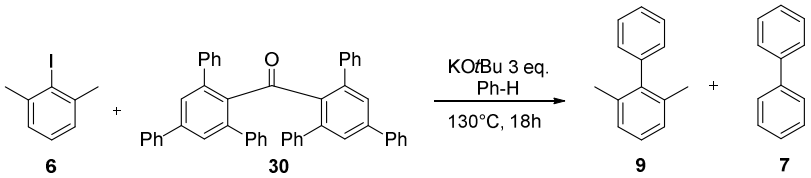
A mixture of 1-iodo-2,6-dimethylbenzene **6** (116 mg, 0.5 mmol), KO*t*Bu (168 mg, 1.5 mmol) and **28** (26.6 mg; 0.1 mmol) in benzene (5 mL) was sealed in a 15 mL pressure tube in a glovebox. The tube was removed from the glovebox and heated at 130 ºC for 18 h behind a blast shield. After cooling to room temperature, the reaction was quenched by water (15 mL) and acidified with 1N HCl until neutral pH. The mixture was extracted with diethyl ether (15 mL). The organic layer was dried over sodium sulfate, filtered and concentrated to give the residue as a dark yellow oil which yielded 0.7 % of **9** and 1.8 % of **7**. The yield was calculated using 1,3,5-trimethoxybenzene (10%) as internal standard.

Cross coupling reaction using **29** as additive.



A mixture of 1-iodo-2,6-dimethylbenzene **6** (116 mg, 0.5 mmol), KO*t*Bu (168 mg, 1.5 mmol) and **28** (56.2 mg; 0.1 mmol) in benzene (5 mL) was sealed in a 15 mL pressure tube in a glovebox. The tube was removed from the glovebox and heated at 130 ºC for 18 h behind a blast shield. After cooling to room temperature, the reaction was quenched by water (15 mL) and acidified with 1N HCl until neutral pH. The mixture was extracted with diethyl ether (15 mL). The organic layer was dried over sodium sulfate, filtered and concentrated to give the residue as a dark yellow oil which yielded 0.8 % of **9** and 2.4 % of **7**. The yield was calculated using 1,3,5-trimethoxybenzene (10%) as internal standard.

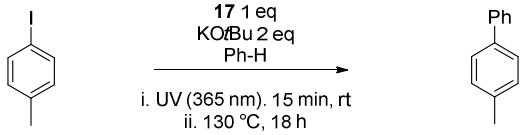
Cross coupling reaction using **30** as additive.



6 **30** **9** **7**

A mixture of 1-iodo-2,6-dimethylbenzene **6** (116 mg, 0.5 mmol), KO*t*Bu (168 mg, 1.5 mmol) and **28** (63.8 mg; 0.1 mmol) in benzene (5 mL) was sealed in a 15 mL pressure tube in a glovebox. The tube was removed from the glovebox and heated at 130 ºC for 18 h behind a blast shield. After cooling to room temperature, the reaction was quenched by water (15 mL) and acidified with 1N HCl until neutral pH. The mixture was extracted with diethyl ether (15 mL). The organic layer was dried over sodium sulfate, filtered and concentrated to give the residue as a dark yellow oil which yielded 0.4 % of **9** and 1.2 % of **7**. The yield was calculated using 1,3,5-trimethoxybenzene (10%) as internal standard.

Reactions with iodo-*para*-toluene using **17** as additive



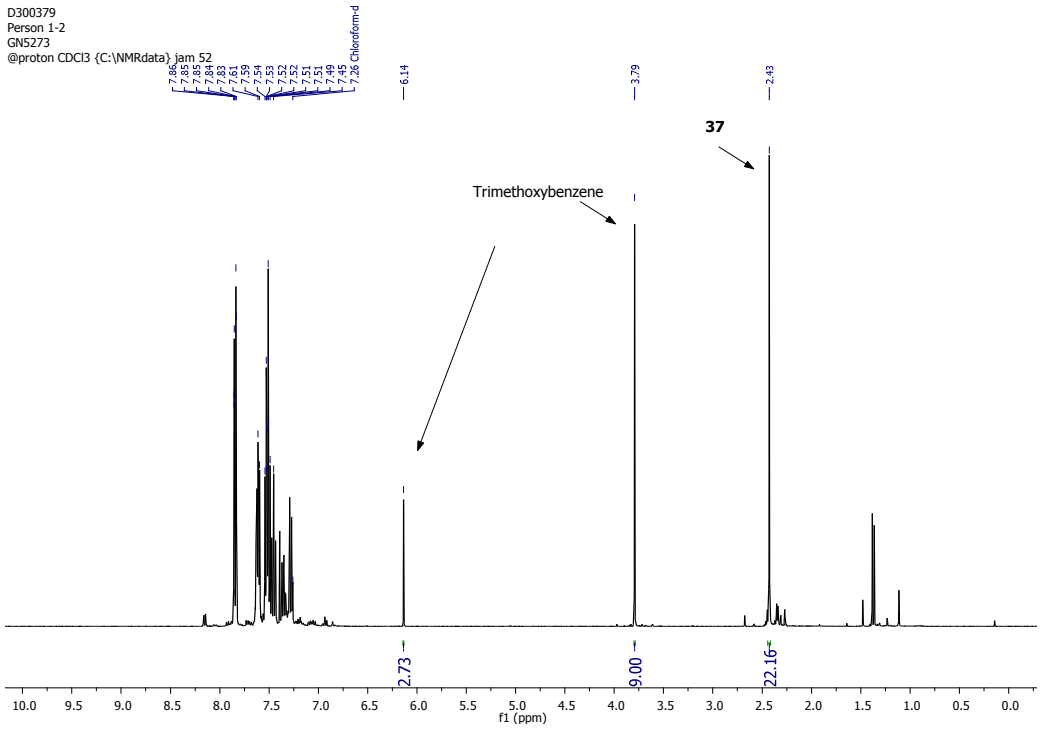
36 **37**

A mixture of iodo-*p*-toluene **36** (0.5 mmol), KO*t*Bu (112 mg, 1 mmol), **17** (91 mg, 0.5 mmol, if added) in benzene (2.5 mL) was sealed in a 15 mL pressure tube in glovebox. The tube was removed from the glovebox and placed RT for 15 min under UV (365 nm) irradiation and then transferred into an oil bath at 130 °C for 18h. After cooling to room temperature, the reaction was quenched by water (15 mL) and acidified with 1N HCl until neutral pH. The mixture was extracted with diethyl ether (3 x 15 mL). The organic layer was dried over sodium sulfate, filtered and concentrated to give rise to the residue. 1,3,5-Trimethoxybenzene 8.4 mg, (0.050 mmol, 10 mol%) was added as a solid to the reaction mixture, ~1 mL $CDCl_3$ was added and the solution stirred. A portion of the solution was taken and diluted for NMR analysis. The quantity of product was determined as following. For the recovered starting material the integration of methoxy signal (3.81 ppm) of the internal standard in the ^{1}H-NMR spectrum was set to 9 units. The integration of the methyl signal of **36** (3H, 2.33 ppm) was then measured and the following calculation gave the amount of **36** present:

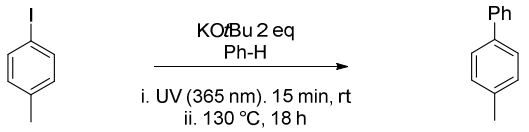
$(6.24/3) \times 10 = 21$ %

For the product **37** the integration of methoxy signal of the internal standard in the ^{1}H-NMR spectrum was set to 9. The integration of the methyl signal of **37** (3H, 2.46 ppm) was then measured and the following calculation gave the amount of **37** present.

$(22.25/3) \times 10 = 74$ %



Reactions with iodo-*p*-toluene with no additive (blank reaction)



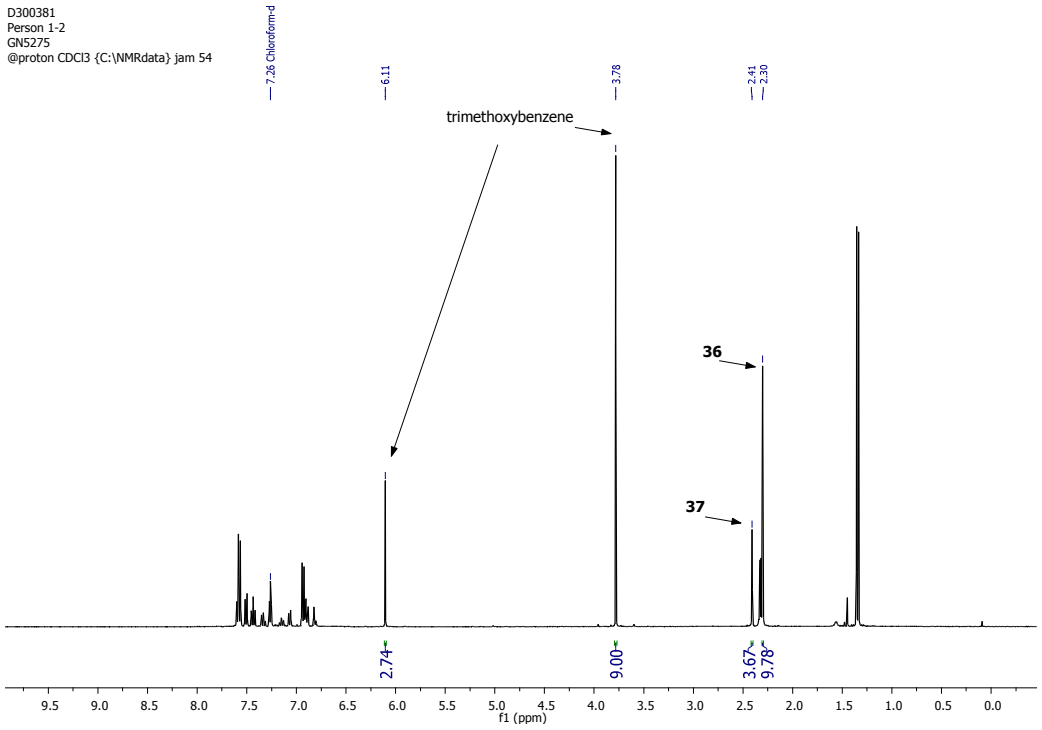
36 **37**

A mixture of iodo-*p*-toluene **36** (0.5 mmol), KO*t*Bu (112 mg, 1 mmol) in benzene (2.5 mL) was sealed in a 15 mL pressure tube in glovebox. The tube was removed from the glovebox and placed RT for 15 min under UV (365 nm) irradiation and then transferred into an oil bath at 130 °C for 18h. After cooling to room temperature, the reaction was quenched by water (15 mL) and acidified with 1N HCl until neutral pH. The mixture was extracted with diethyl ether (3 x 15 mL). The organic layer was dried over sodium sulfate, filtered and concentrated to give rise to the residue. 1,3,5-Trimethoxybenzene 8.4 mg, (0.050 mmol, 10 mol%) was added as a solid to the reaction mixture, ~1 mL $CDCl_3$ was added and the solution stirred. A portion of the solution was taken and diluted for NMR analysis. The quantity of product was determined as following. For the recovered starting material the integration of methoxy signal (3.81 ppm) of the internal standard in the ^{1}H-NMR spectrum was set to 9 units. The integration of the methyl signal of **36** (3H, 2.33 ppm) was then measured and the following calculation gave the amount of **36** present:

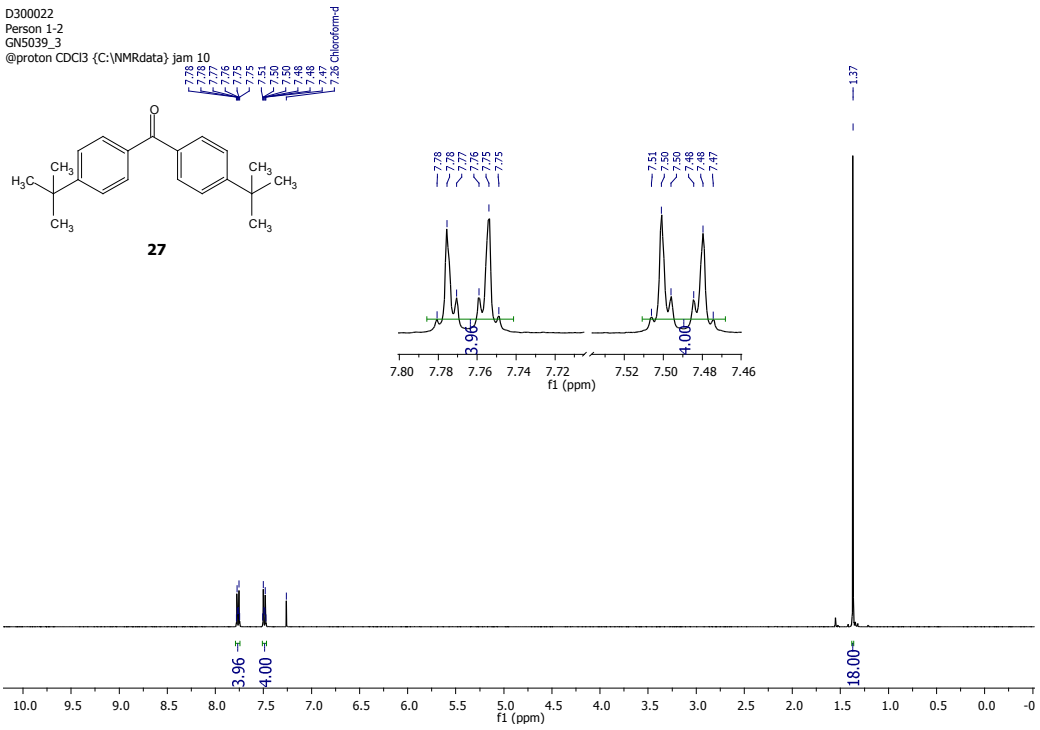
(9.78/3) × 10 = 33 %

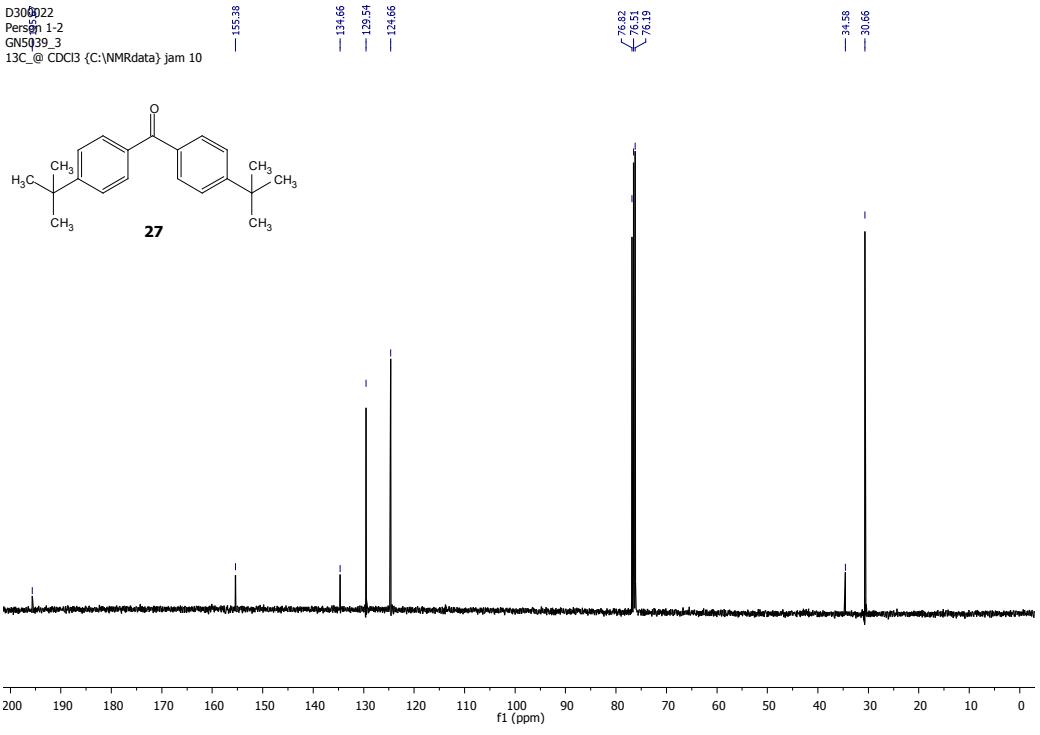
For the product **37** the integration of methoxy signal of the internal standard in the ^{1}H-NMR spectrum was set to 9 units. The integration of the methyl signal of **37** (3H, 2.46 ppm) was then measured and the following calculation gave the amount of **37** present.

(3.68/3) × 10 = 12 %


D300381
Person 1-2
GN5275
@proton CDCl3 {C:\NMRdata} jam 54
7.26 Chloroform-d
6.11
3.78
2.41
2.30
trimethoxybenzene
36
37
2.74
9.00
3.67
9.78
f1 (ppm)

NMR Spectra:


D300022
Person 1-2
GN5039_3
@proton CDCl3 {C:\NMRdata} jam 10
27
3.96
4.00
18.00
f1 (ppm)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GN5039_3
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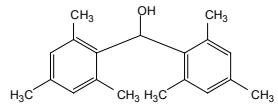
27
f1 (ppm)

D261691
Person 1-2
GN2077
@proton CDCl3 {C:\NMRdata} jam 28



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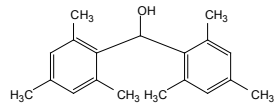

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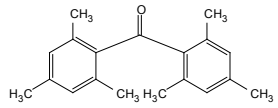
GN2078-CLEAN
@proton CDCl3 {C:\NMRdata} jam 91



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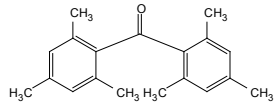
Person 1-2
GN2078-CLEAN
13C_@ CDCl3 {C:\NMRdata} jam 91



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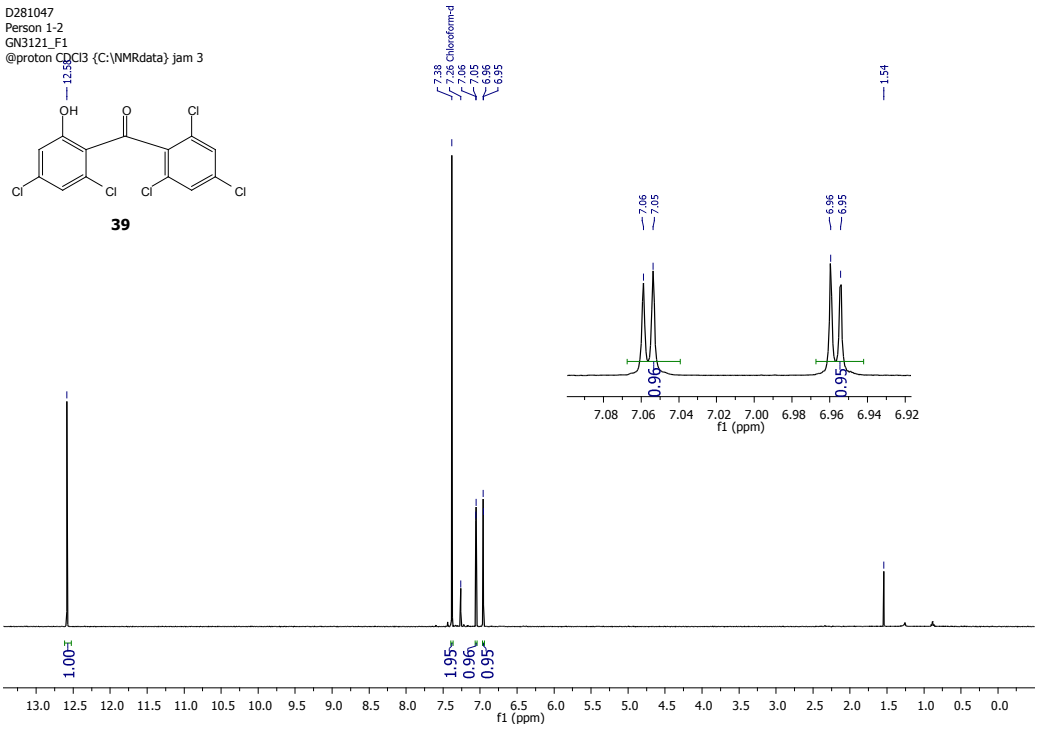
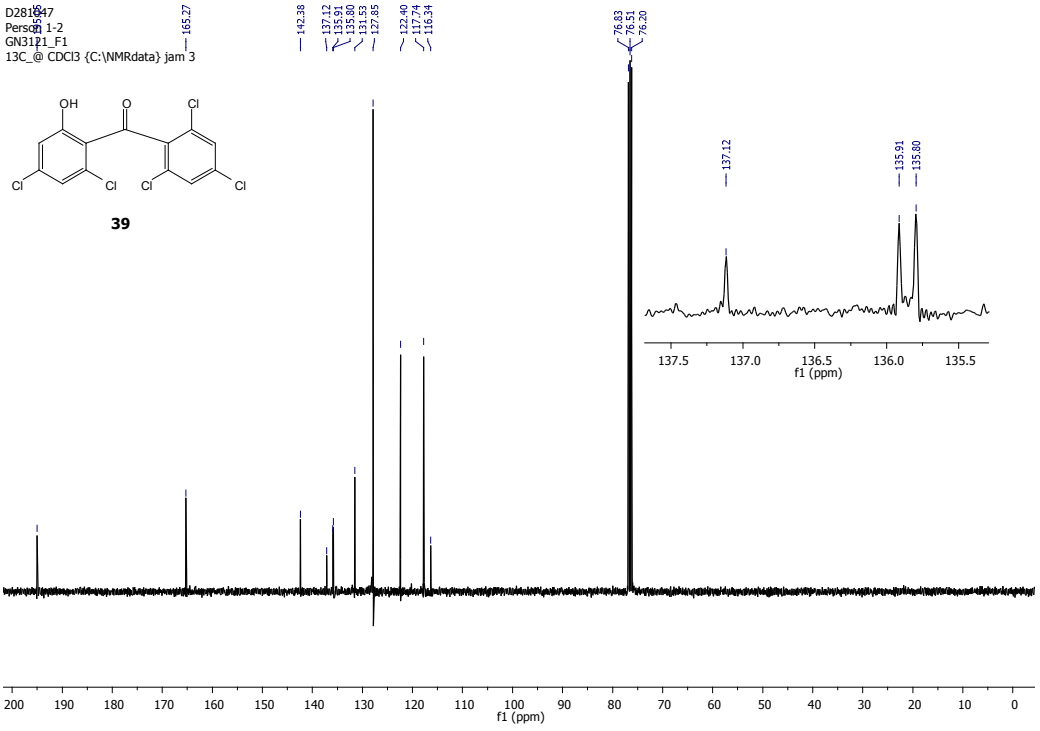

D281047
Person 1-2
GN3121_F1
@proton CDCl3 {C:\NMRdata} jam 3
12.56
7.38
7.26 Chloroform-d
7.06
7.05
6.96
6.95
1.54
OH
O
Cl
39
7.06
7.05
6.96
6.95
0.96
0.95
7.08 7.06 7.04 7.02 7.00 6.98 6.96 6.94 6.92
f1 (ppm)
1.00
1.95
0.96
0.95
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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GN3121_F1
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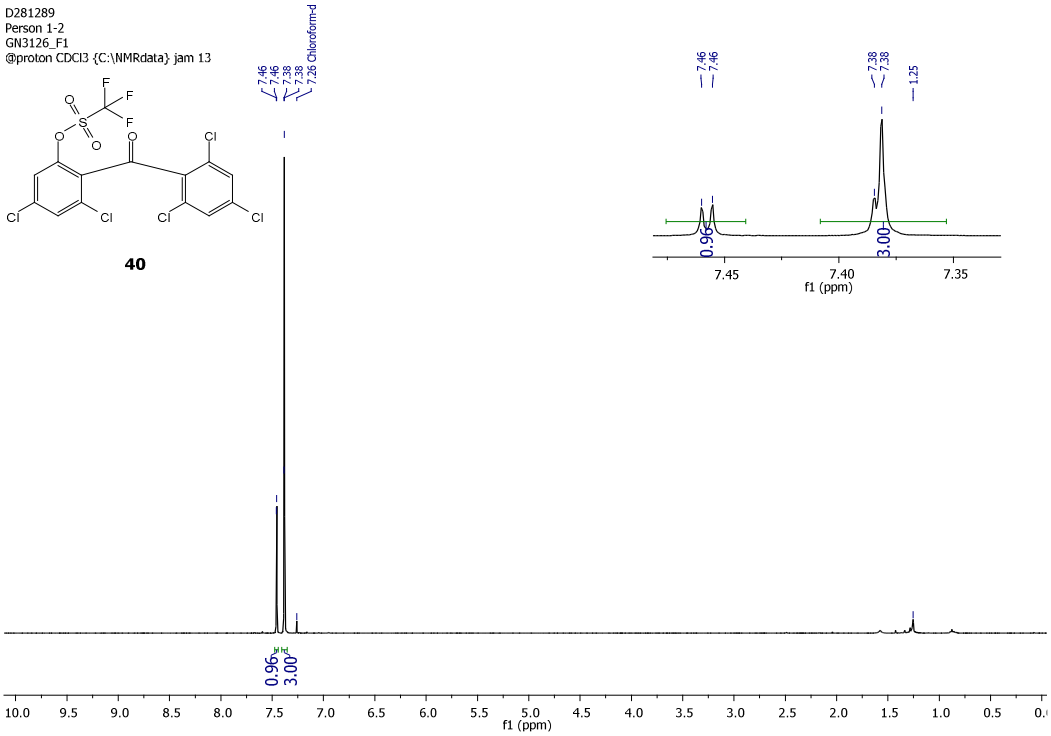
137.12
135.91
135.80
131.53
127.85
122.40
117.74
116.34
76.83
76.51
76.20
OH
O
Cl
39
137.12
135.91
135.80
137.5 137.0 136.5 136.0 135.5
f1 (ppm)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


D281289
Person 1-2
GN3126_F1
@proton CDCl3 {C:\NMRdata} jam 13
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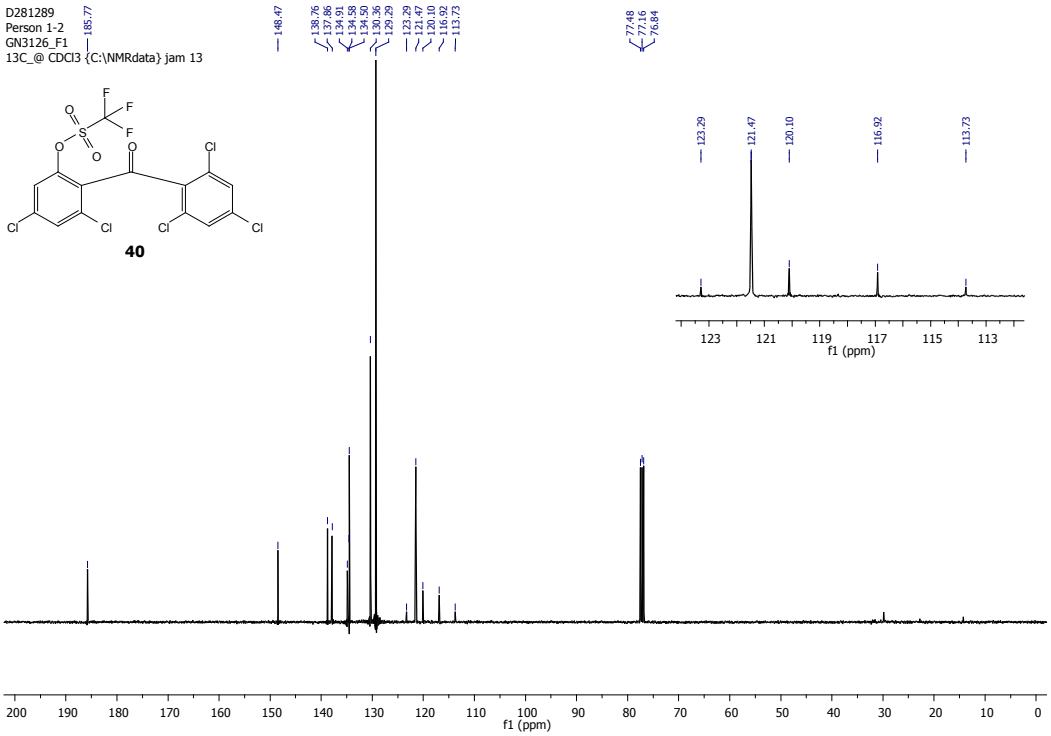
7.46
7.38
7.38
7.26 Chloroform-d
40
0.96
3.00
f1 (ppm)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GN3126_F1
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138.76
137.86
134.91
134.58
134.50
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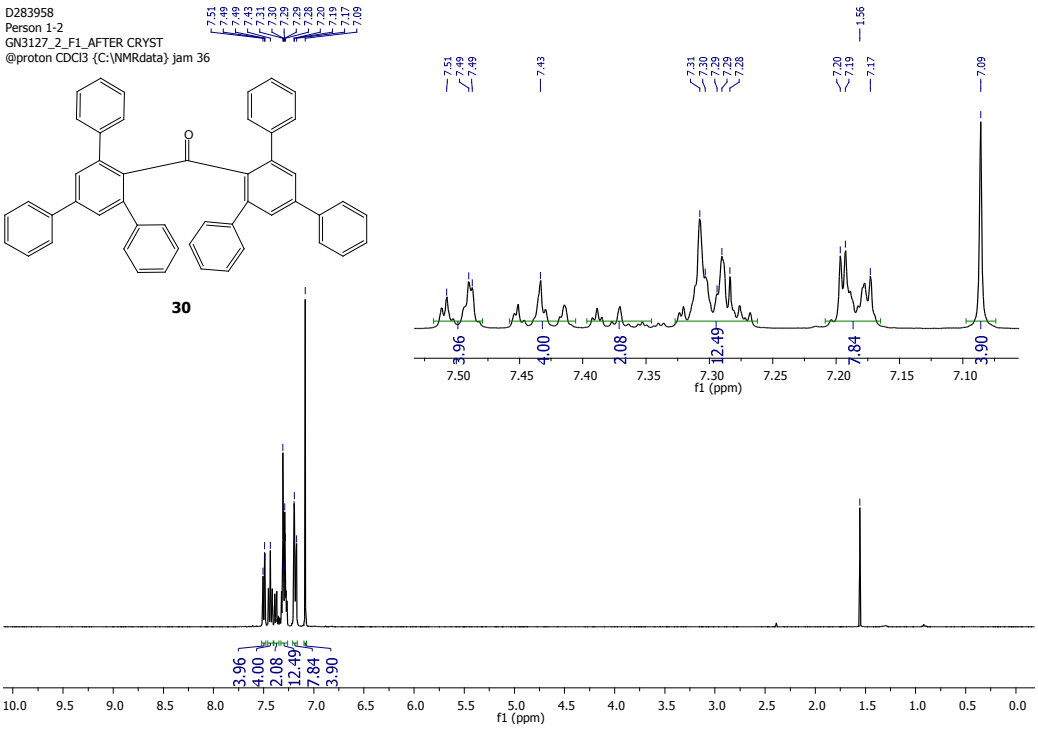
129.29
123.29
121.47
120.10
116.92
113.73
77.48
77.16
76.84
40
f1 (ppm)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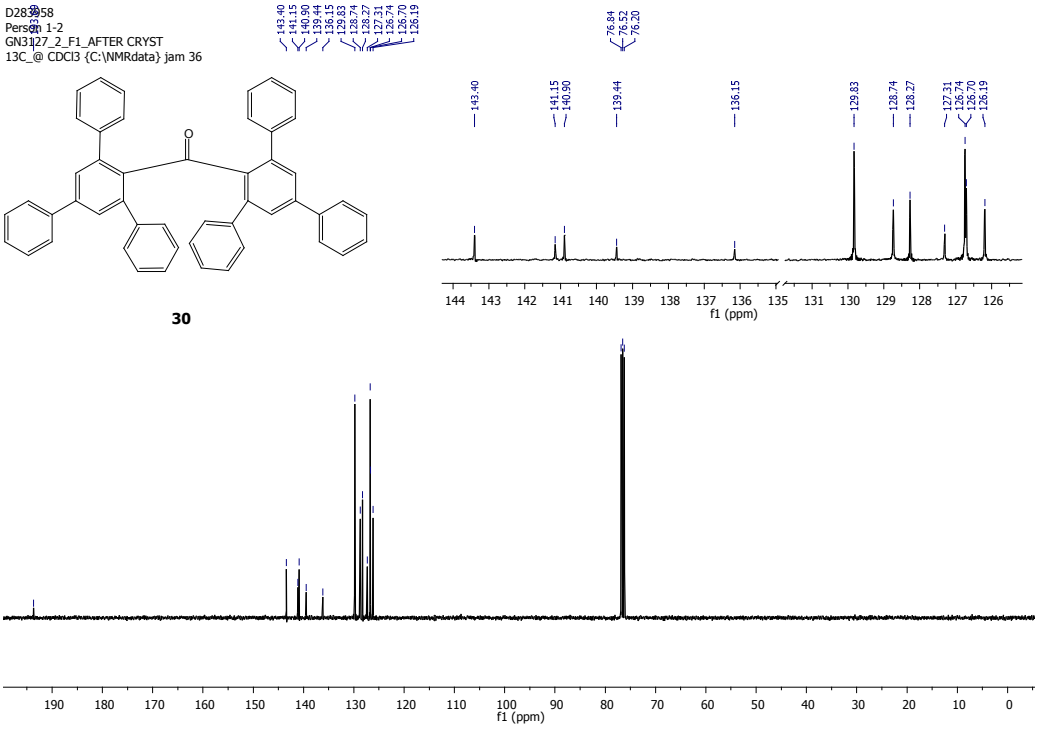
Person 1-2
GN3127_2_F1_AFTER CRYST
@proton CDCl3 {C:\NMRdata} jam 36
30
f1 (ppm)


D283958
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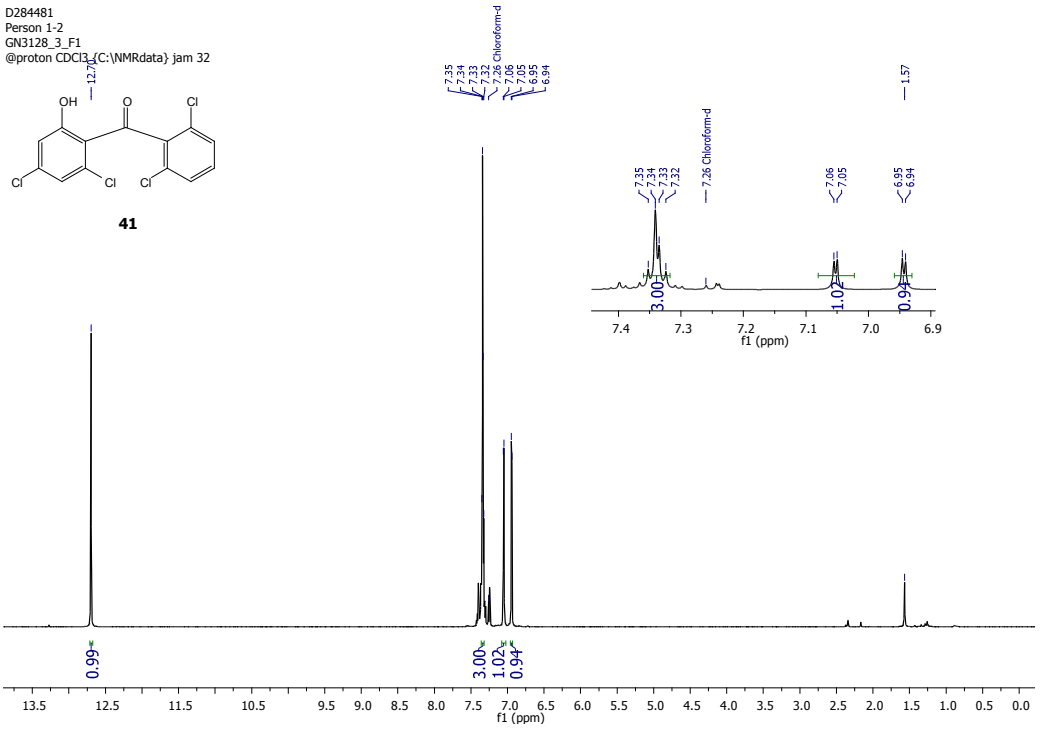
GN3127_2_F1_AFTER CRYST
13C_@ CDCl3 {C:\NMRdata} jam 36
30
f1 (ppm)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GN3128_3_F1
@proton CDCl3 {C:\NMRdata} jam 32
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OH
O
Cl
Cl
Cl
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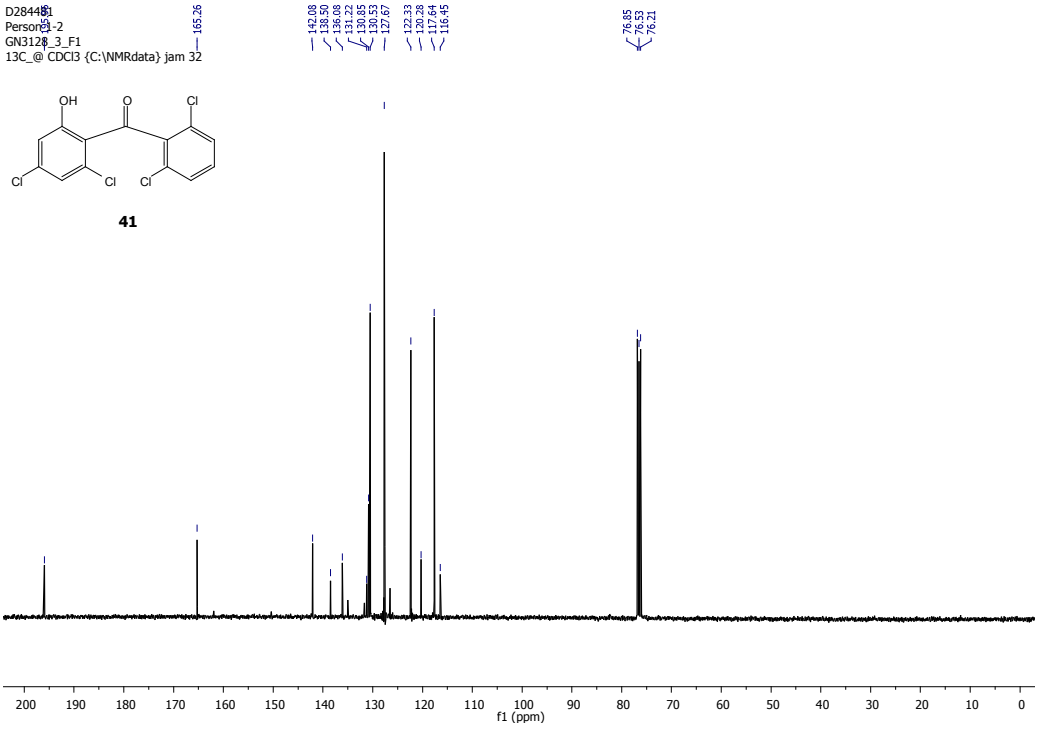
41
7.35
7.34
7.33
7.32
7.26 Chloroform-d
7.06
7.05
6.95
6.94
1.57
3.00
1.02
0.94
0.99
f1 (ppm)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136.08
131.22
130.55
130.53
127.67
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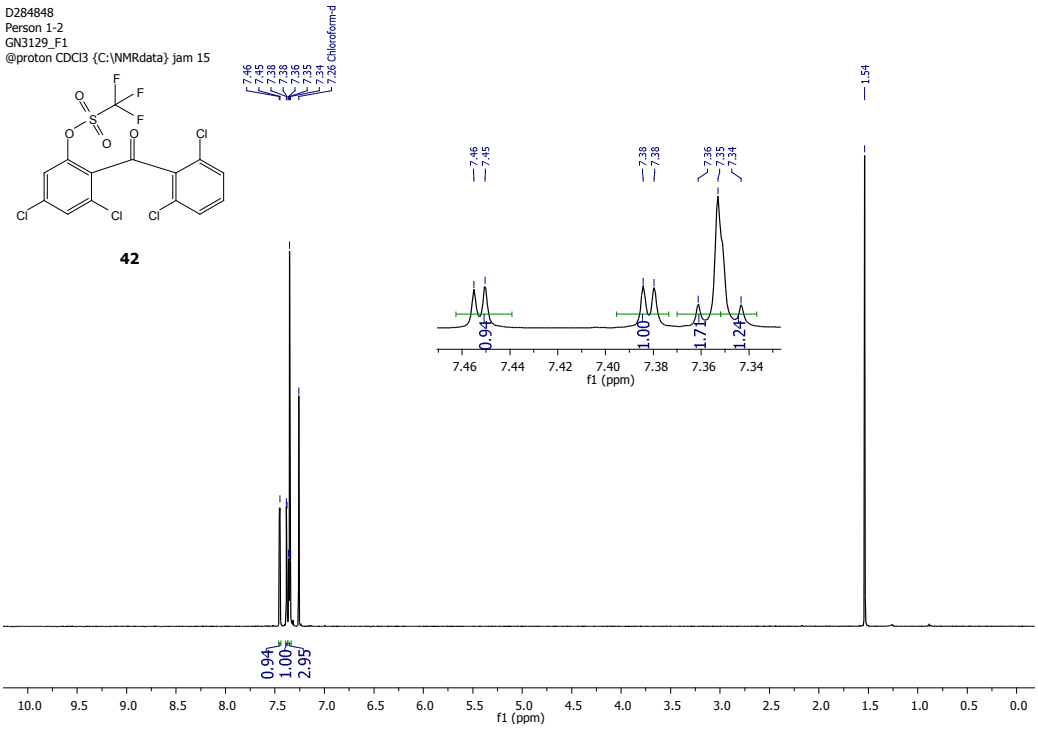
116.45
76.85
76.53
76.21
OH
O
Cl
Cl
Cl
Cl
41
f1 (ppm)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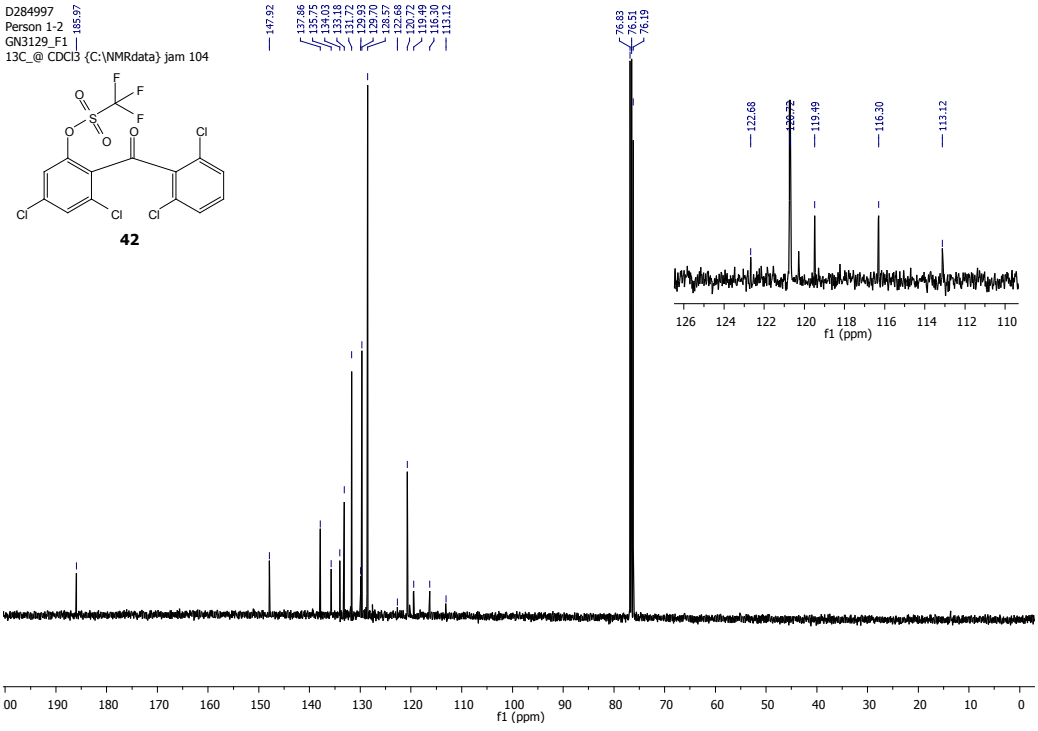
42
Chloroform-d
f1 (ppm)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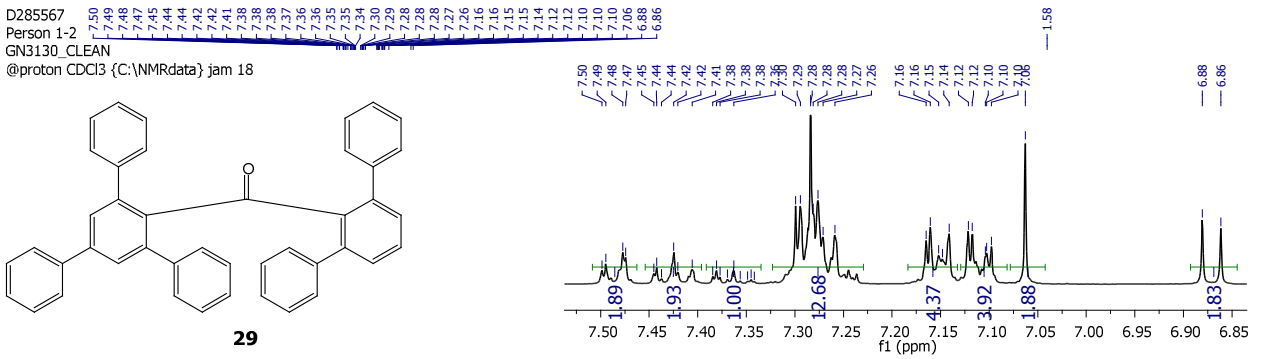
13C_@ CDCl3 {C:\NMRdata} jam 104
42
f1 (ppm)


D285567
Person 1-2
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@proton CDCl3 {C:\NMRdata} jam 18
29
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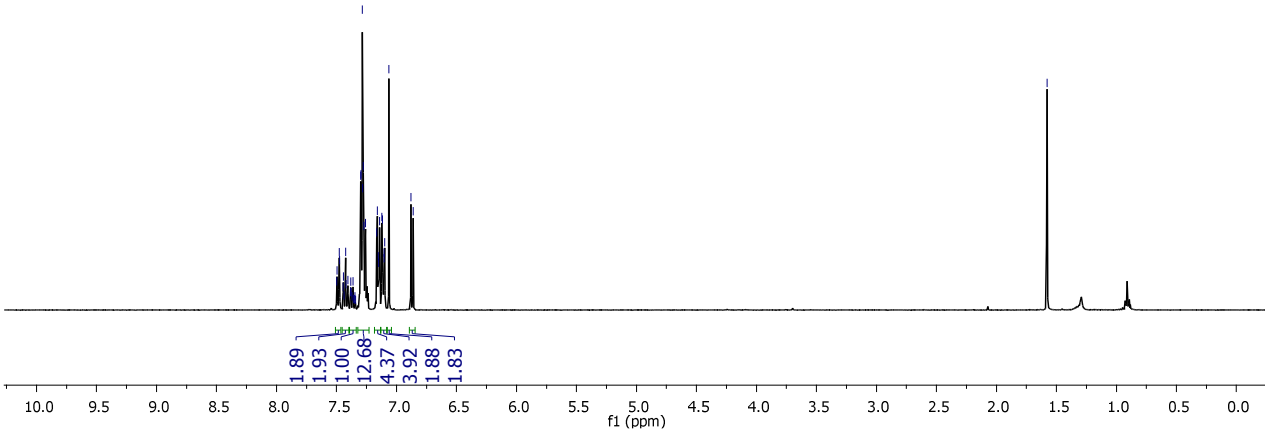
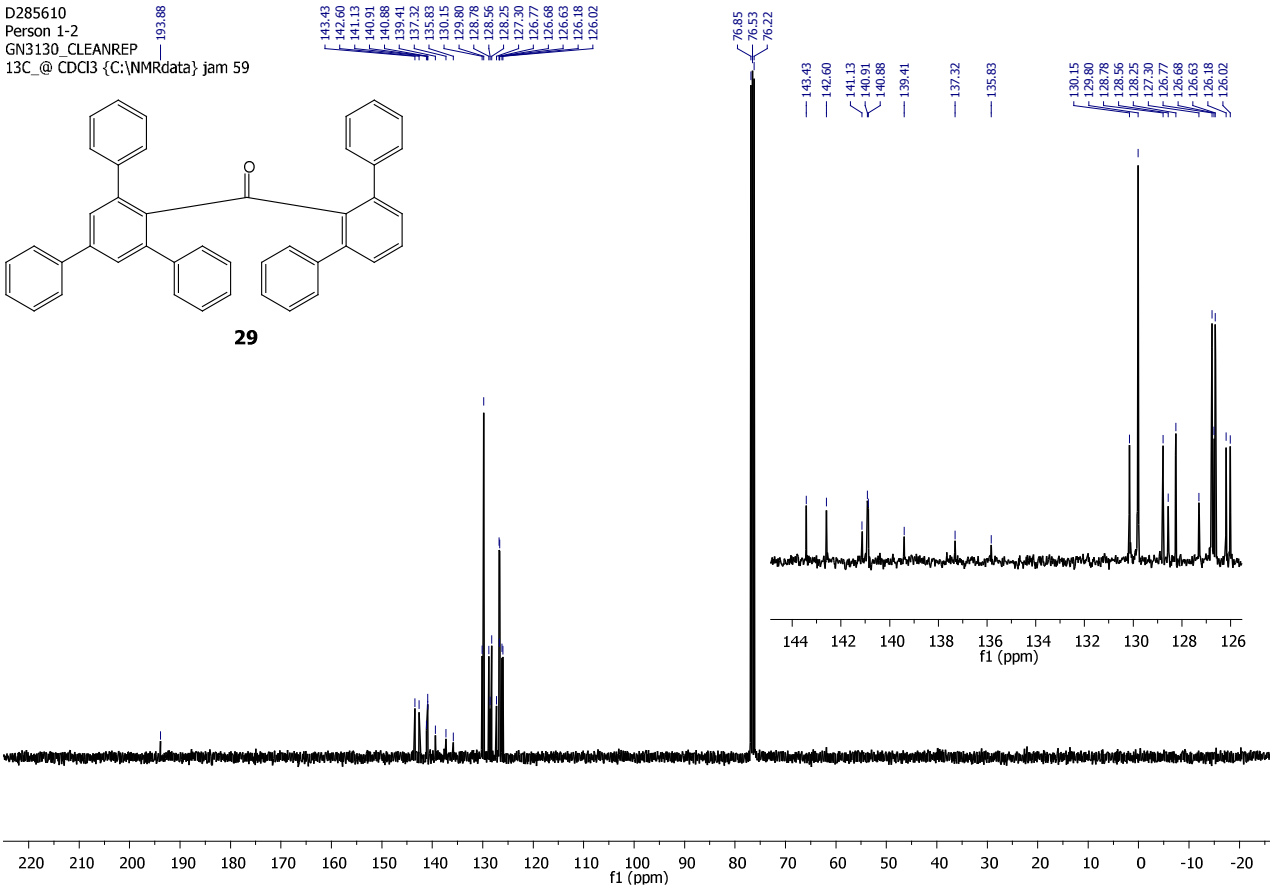
1.93
1.00
12.68
4.37
3.92
1.88
1.83
f1 (ppm)


1.89
1.93
1.00
12.68
4.37
3.92
1.88
1.83
f1 (ppm)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GN3130_CLEANREP
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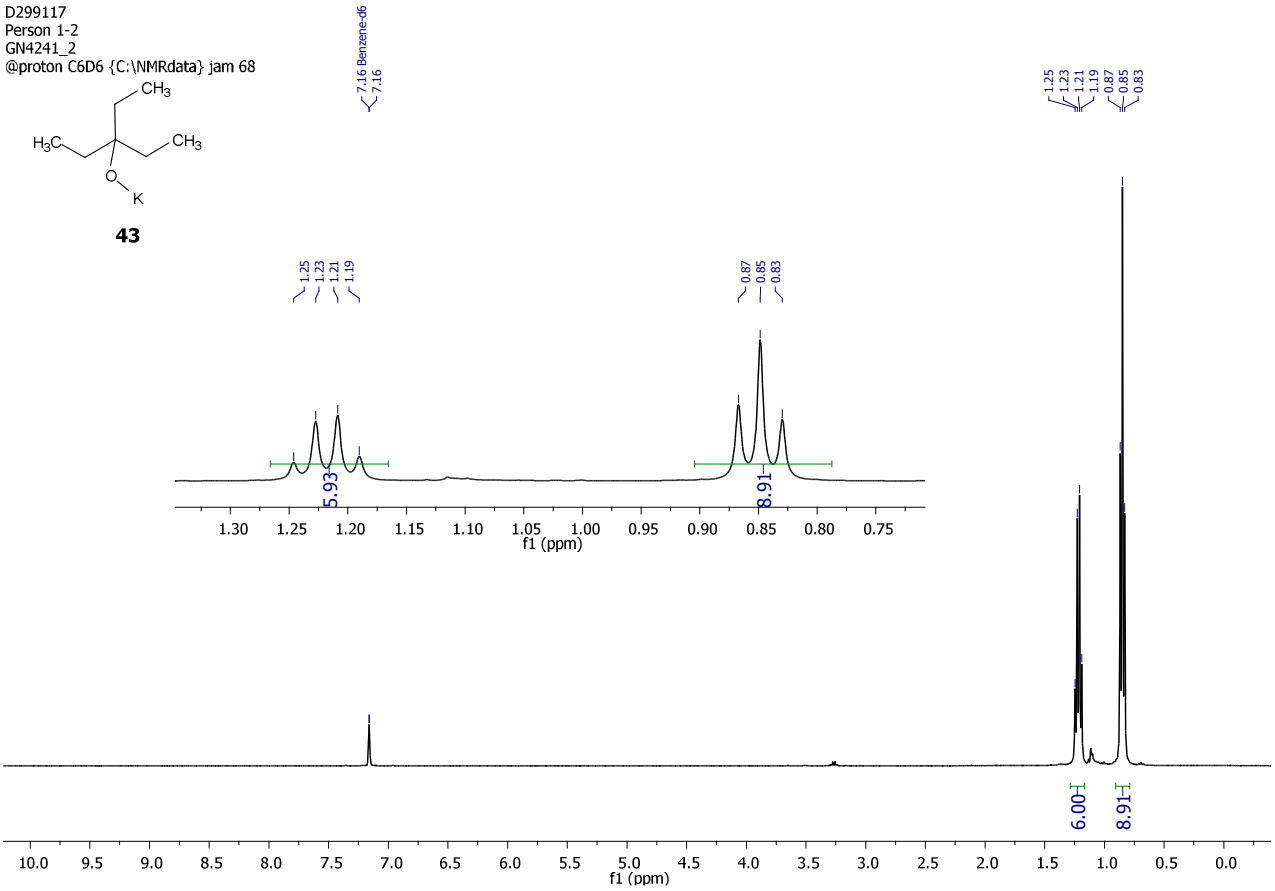
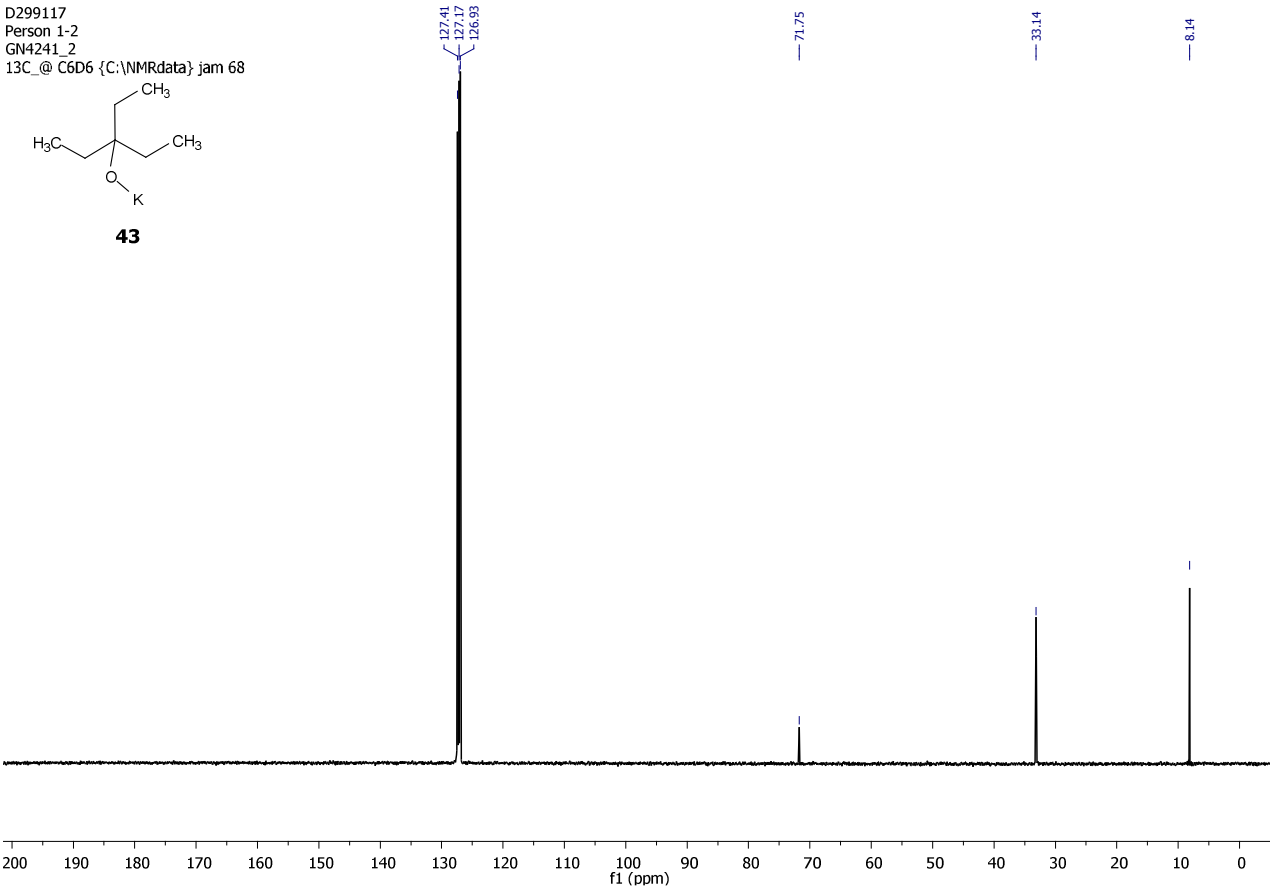
29
f1 (ppm)


D299117
Person 1-2
GN4241_2
@proton C6D6 {C:\NMRdata} jam 68
CH3
H3C
CH3
O
K
43
7.16 Benzene-d6
7.16
1.25
1.23
1.21
1.19
0.87
0.85
0.83
5.93
8.91
6.00
8.91
f1 (ppm)


D299117
Person 1-2
GN4241_2
13C_@ C6D6 {C:\NMRdata} jam 68
CH3
H3C
CH3
O
K
43
127.41
127.17
126.93
71.75
33.14
8.14
f1 (ppm)

Computational Results

Computational Methods

Density Functional Theory (DFT) was used for the geometry optimizations of all reactant complexes, transition states, intermediates and product complexes. The final optimized geometries were characterized as minima or transition states by performing frequency calculations, which also enabled calculation of the zero-point energies (ZPE), enthalpies (H), entropies (S) and Gibbs free energies (G) at 298 K. Geometry optimizations and frequency calculations were performed using the Gaussian 09[9] software package, using the M06-2X functional[10] and 6-31++G(d,p) basis set,[11] unless otherwise stated. Implicit solvation was modelled using the Conductor-Like Polarisable Continuum Model (CPCM)[12] with the associated parameters of THF solvent, unless otherwise stated. Gibbs free energy barriers and relative free energies were calculated between reactant complexes and transition states or reactant complexes and product complexes, respectively and are reported in kcal/mol throughout. Time dependent DFT (TD-DFT)[13] calculations were performed on the M06-2X/6-31++G(d,p) optimised geometries, with the CAM-B3LYP functional,[14] due to its good performance with intermolecular charge transfer (CT) excitations,[15] whilst maintaining the 6-31++G(d,p) basis set and CPCM solvent model.

Naked monomeric *tert*-butoxide anion is used throughout this work as a simple representation of tetrameric KO*t*Bu; see **Table S1** where it can be seen that the naked monomer is found to more closely reproduce the thermodynamics of the reaction utilising a KO*t*Bu tetramer, whilst underestimating the kinetics. This approach has also previously been utilised by Grubbs *et al*.,[16-17] after having shown that tetramer is the most stable structure in solution by DFT calculations.

Marcus Theory Calculations

In order to model a single electron transfer reaction computationally, Marcus-Hush Theory[18] is employed with the 4-point method of Nelsen et al.[19] or the complexation method of Anderson, Tuttle and co-workers[20] allowing calculation of the reorganisation energy (λ), ΔG_{rel} and ΔG^*. The Nelsen 4-point method requires optimisation of the individual electron donor and acceptor species, before and after single electron transfer. Single point energy calculations are then performed on these optimised geometries using the charge and multiplicity of their other state in the electron transfer reaction. The complexation method requires optimisation of the electron donor and acceptor as a complex in both the reactant and product electronic states. Single point energy calculations are then performed on these optimized geometries with the alternative electronic configuration.

KO*t*Bu Representation

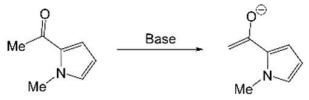


Figure S15. Deprotonation reaction studied using various forms of KO*t*Bu.

Table S1. Results of DFT Calculations for the reaction depicted in Figure S1, energies calculated relative to reactant and product complexes. (Computational Method: M06-2X/6-311++G(d,p), CPCM solvation method with parameters for benzene)

Base	ΔG^* (Kcal/mol)	ΔG_{rel} (Kcal/mol)
O*t*Bu anion	0.4	-12.1
KO*t*Bu monomer	4.8	-4.1
KO*t*Bu dimer	7.8	-3.0
KO*t*Bu tetramer	3.9	-14.5

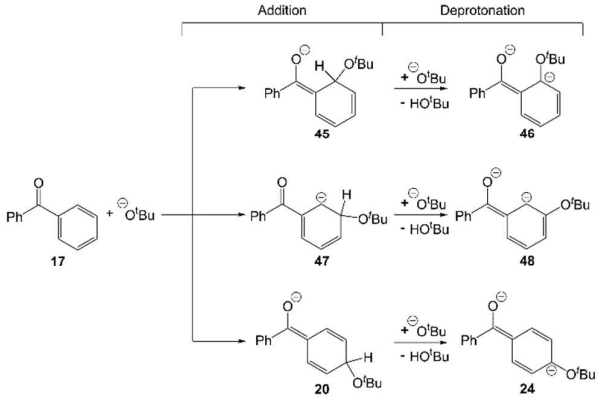
Feasibility of forming organic electron donors (**Scheme 3 (a)** main paper)

Given our group's previous evidence showing KO*t*Bu is a poor single electron donor, our initial investigations focused on the possible formation of *in situ* organic electron donor species resulting from reaction of KO*t*Bu with benzophenone (**17**). We proposed that *tert*-butoxide anion might add to the *ortho, meta* or *para* positions of a phenyl moiety in benzophenone generating anions **45, 47** and **20**, which could then be followed by a deprotonation, generating dianionic species **46, 48** and **24**. Dianions **46, 48** and **24** have the structural characteristics[21] to act as electron donors towards benzophenone, should they be accessible.

As shown in **Table S2**, addition in the *meta* position has an accessible free energy barrier (21.1 kcal/mol) but is highly endergonic (18.6 kcal/mol) thus disfavouring the addition reaction and we therefore disregarded any further reactivity through a *meta*-adduct. Addition in the *ortho* and *para* positions exhibits accessible free energy barriers at the reported

experimental conditions (room temperature),[22-25] whilst being endergonic by 5.8 and 5.0 kcal/mol, respectively. Subsequent deprotonation of *ortho* (**45**) and *para* (**20**) adducts to form dianions **46** and **24** respectively, occurs with accessible free energy barriers, with both reactions being endergonic (9.7 and 7.0 kcal/mol, calculated relative to reactant complex of **45** or **20** with *tert*-butoxide anion). Whilst bearing in mind the observation of 3% benzophenone ketyl radical anion **18**, by Ashby *et al.* these results suggest it is unlikely for even such a small amount of dianionic species such as **46** or **24** to be formed (<<1% of product would be formed in both addition and deprotonation steps).

Table S2. Calculated Gibbs free energies for addition and deprotonation.

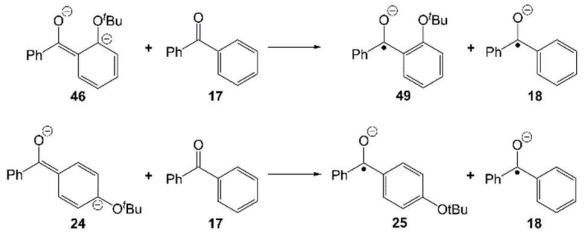


	ortho (kcal/mol)		*meta* (kcal/mol)		*para* (kcal/mol)	
	ΔG*	**ΔG_{rel}**	**ΔG***	**ΔG_{rel}**	**ΔG***	**ΔG_{rel}**
$^{\ominus}$O^{t}Bu Addition	15.6	5.8	21.1	18.6	15.1	5.0
Deprotonation by $^{\ominus}$O^{t}Bu	25.9	9.7	-	-	20.7	7.0

Despite the lack of possibility for forming dianions **46** and **24**, their ability to act as single electron donors to a molecule of neutral benzophenone was still examined. Marcus Theory calculations were performed to calculate the free energy of activation for SET, as well as the relative free energy, utilising the complexation method of Anderson *et al.*[20] and the Nelsen Four Point method.[19] Marcus Theory calculations utilising the method of Anderson *et al.* were carried out with and without potassium counter cations (see below for images of optimised complexes), and the results are presented in **Table S3**.

The calculated low activation energies and exergonic relative energies, from the complexation method, suggest that single electron transfer from a dianionic species such as **46** or **24** to benzophenone would occur readily. Results utilising the Nelsen 4-point method are also included and show similar overall exergonic SET reactions, however the predicted activation energy is higher for both **46** and **24**. Previous work in the group has shown the complexation method with counterions to be the most accurate for predicting SET energies,[20] (however, we include here the Nelsen 4-point results to allow comparison with results from later calculations which require the use of this methodology).

Table S3. Calculated Gibbs free energies for SET from dianions **46** and **24** to benzophenone (**17**).

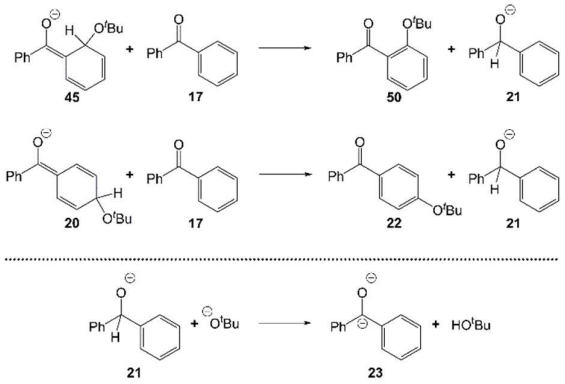


Complexation Method[20]	ΔG* (kcal/mol)	ΔG_{rel} (kcal/mol)
46 + **17** → **49** + **18**	0.3	-20.3
46 + **17** → **49** + **18** (with 2 potassium cations)	0.1	-26.5
24 + **17** → **25** + **18**	0.4	-17.8
24 + **17** → **25** + **18** (with 2 potassium cations)	3.3	-7.9

Nelsen 4-Point Method[19]	ΔG* (kcal/mol)	ΔG_{rel} (kcal/mol)
46 + **17** → **49** + **18**	9.1	-36.7
24 + **17** → **25** + **18**	8.3	-32.9

With these results in hand, we wanted to probe alternative mechanisms that could be operating. We therefore investigated the possibility of a hydride transfer from either species **45** or **20** to benzophenone, forming **21**. Hydride transfer from anion **45** to benzophenone (**17**) exhibited an unfavourable free energy barrier of 34.3 kcal/mol and was slightly exergonic (0.7 kcal/mol), **Table S4**. On the other hand, anion **20** exhibited a comparable barrier to deprotonation (22.4 kcal/mol) and was exergonic by 3.8 kcal/mol; these results suggest hydride transfer from **20** would be possible. In order to achieve an electron donor species from **21** it would be necessary to deprotonate and access dianion **23** (SET from **23** to benzophenone (**17**) has an activation free energy of 6.9 kcal/mol and is exergonic by 31.6 kcal/mol, see **Figure S16** for results); this exhibits an accessible barrier of 23.0 kcal/mol whilst being endergonic by 10.2 kcal/mol. The combination of hydride transfer followed by deprotonation of **21** to form electron donor **23** can also be dismissed, on the basis of unfavourable kinetics.

Table S4. Calculated Gibbs free energies for hydride transfer from anions **45** and **20** to benzophenone (**17**) and deprotonation of product **21**.



Reaction	ΔG* (kcal/mol)	ΔG_{rel} (kcal/mol)
45 + **17** → **50** + **21**	34.3	-0.7
20 + **17** → **22** + **21**	22.4	-3.8
21 + ⊖O*t*Bu → **23** + HO*t*Bu	23.0	10.2

The above computational data indicates *tert*-butoxy substitution could not occur; similarly there has been no experimental evidence for formation of such *tert*-butoxy (or other alkoxy) substituted benzophenone products.

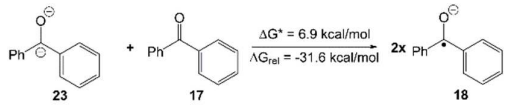
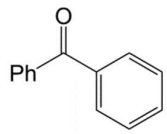


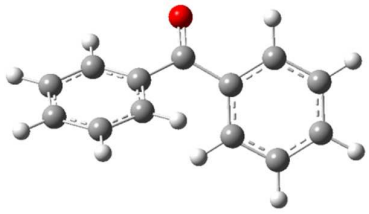
Figure S16. SET from 23 to 17 – Calculated using the Nelsen 4-point method

of this reaction and the ease of reverse reaction we decided not to further probe this as a route to potential electron donor species.

XYZ Coordinates of Optimised Geometries

Benzophenone (**17**)





24
-576.4217964

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C	-2.66005	-1.51373	0.72891
C	-1.41870	-0.88307	0.66828
C	-1.29468	0.35659	0.03049
C	-2.42112	0.95791	-0.54344
C	-3.65452	0.31666	-0.50056
H	-4.73880	-1.41734	0.17881
H	-2.75616	-2.46854	1.23558
H	-0.55385	-1.34456	1.13523
H	-2.31247	1.92559	-1.02326
H	-4.52237	0.77910	-0.95960
C	0.00001	1.10670	0.00012
C	1.29469	0.35658	-0.03038
C	1.41863	-0.88309	-0.66815
C	2.42119	0.95790	0.54342
C	2.65996	-1.51377	-0.72891
H	0.55373	-1.34459	-1.13500
C	3.65458	0.31663	0.50042
H	2.31261	1.92559	1.02323
C	3.77490	-0.91950	-0.13847
H	2.75601	-2.46859	-1.23556
H	4.52249	0.77908	0.95936
H	4.73877	-1.41739	-0.17902
O	0.00001	2.32919	-0.00004

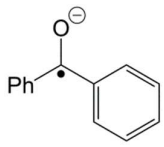
Single Point Radical Anion
using Optimised Geometry
17

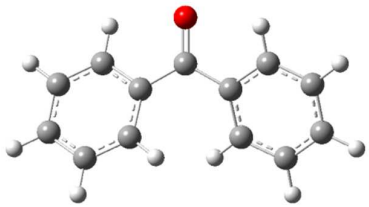
24
-576.4969276

C	-3.77491100	-0.91946000	0.13834000
C	-2.66004800	-1.51372800	0.72891100
C	-1.41869800	-0.88306600	0.66827600
C	-1.29467500	0.35658600	0.03049100
C	-2.42111600	0.95791000	-0.54343500
C	-3.65451800	0.31665800	-0.50055600
H	-4.73879700	-1.41733800	0.17880600
H	-2.75615900	-2.46854300	1.23557600
H	-0.55385200	-1.34456400	1.13522700
H	-2.31247100	1.92559200	-1.02325800
H	-4.52236900	0.77910400	-0.95959900
C	0.00000900	1.10669700	0.00012000
C	1.29468600	0.35657700	-0.03037700
C	1.41862700	-0.88308900	-0.66815100
C	2.42119400	0.95790000	0.54341800
C	2.65996300	-1.51376800	-0.72890500
H	0.55372600	-1.34458800	-1.13499700
C	3.65458400	0.31663200	0.50042000
H	2.31261200	1.92559200	1.02323500
C	3.77489600	-0.91949800	-0.13846700
H	2.75600900	-2.46859300	-1.23556100
H	4.52248800	0.77907700	0.95936400

H	4.73877200	-1.41738800	-0.17902500
O	0.00000900	2.32919400	-0.00003600

Benzophenone Radical Anion (**18**)





24
-576.5066700

C	3.87258	-0.87217	-0.07837
C	2.74326	-1.58592	-0.49682
C	1.47967	-1.00708	-0.46971
C	1.28461	0.32117	-0.01271
C	2.44758	1.03748	0.36951
C	3.70662	0.45123	0.34648
H	4.85658	-1.33022	-0.09921
H	2.85244	-2.60291	-0.86540
H	0.63747	-1.57669	-0.84842
H	2.32393	2.06687	0.68988
H	4.57160	1.03022	0.66107
C	0.00000	1.02918	0.00001
C	-1.28461	0.32117	0.01272
C	-1.47968	-1.00708	0.46972
C	-2.44758	1.03748	-0.36951
C	-2.74327	-1.58592	0.49682
H	-0.63748	-1.57669	0.84844
C	-3.70661	0.45123	-0.34649
H	-2.32392	2.06687	-0.68988
C	-3.87258	-0.87216	0.07835
H	-2.85245	-2.60291	0.86540
H	-4.57159	1.03023	-0.66109
H	-4.85658	-1.33021	0.09919
O	0.00000	2.31424	-0.00000

Single Point Singlet using
Optimised Geometry
Benzophenone Radical Anion

24
-576.4126038

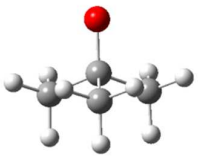
C	3.87257800	-0.87216700	-0.07836500
C	2.74326400	-1.58592400	-0.49682400
C	1.47967100	-1.00708400	-0.46970900
C	1.28460700	0.32116900	-0.01271100
C	2.44758200	1.03748100	0.36951200
C	3.70661900	0.45122700	0.34647600
H	4.85658400	-1.33021700	-0.09921400
H	2.85244400	-2.60290900	-0.86539600
H	0.63747300	-1.57669300	-0.84842200
H	2.32392700	2.06687100	0.68988000
H	4.57159700	1.03022500	0.66106700
C	0.00000100	1.02918100	0.00001100
C	-1.28460700	0.32116900	0.01272300
C	-1.47967500	-1.00708300	0.46972000
C	-2.44757700	1.03748100	-0.36951200
C	-2.74326900	-1.58592200	0.49682300
H	-0.63748100	-1.57669200	0.84844200
C	-3.70661400	0.45122900	-0.34648800
H	-2.32391800	2.06687200	-0.68988000
C	-3.87257900	-0.87216500	0.07835200
H	-2.85245300	-2.60290600	0.86539500
H	-4.57158900	1.03022700	-0.66108900
H	-4.85658500	-1.33021400	0.09919300
O	0.00000000	2.31423600	-0.00000200

Single Point Dianion using
Optimised Geometry
Benzophenone Radical Anion

24
-576.5350689

C	3.87257800	-0.87216700	-0.07836500
C	2.74326400	-1.58592400	-0.49682400
C	1.47967100	-1.00708400	-0.46970900
C	1.28460700	0.32116900	-0.01271100
C	2.44758200	1.03748100	0.36951200
C	3.70661900	0.45122700	0.34647600
H	4.85658400	-1.33021700	-0.09921400
H	2.85244400	-2.60290900	-0.86539600
H	0.63747300	-1.57669300	-0.84842200
H	2.32392700	2.06687100	0.68988000
H	4.57159700	1.03022500	0.66106700
C	0.00000100	1.02918100	0.00001100
C	-1.28460700	0.32116900	0.01272300
C	-1.47967500	-1.00708300	0.46972000
C	-2.44757700	1.03748100	-0.36951200
C	-2.74326900	-1.58592200	0.49682300
H	-0.63748100	-1.57669200	0.84844200
C	-3.70661400	0.45122900	-0.34648800
H	-2.32391800	2.06687200	-0.68988000
C	-3.87257900	-0.87216500	0.07835200
H	-2.85245300	-2.60290600	0.86539500
H	-4.57158900	1.03022700	-0.66108900
H	-4.85658500	-1.33021400	0.09919300
O	0.00000000	2.31423600	-0.00000200

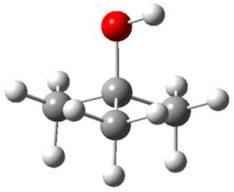
tert-Butoxide Anion



14
-233.0544325

C	1.44067	-0.06139	-0.43463
C	0.00048	-0.00003	0.12965
H	2.01123	0.80195	-0.07121
H	1.93541	-0.97065	-0.07217
H	1.47391	-0.06232	-1.53300
C	-0.77523	-1.21695	-0.43101
C	-0.66855	1.27897	-0.43026
H	-1.80900	-1.19007	-0.06549
H	-0.79611	-1.24637	-1.52932
H	-0.31234	-2.14272	-0.06828
H	-0.68742	1.30985	-1.52855
H	-1.70061	1.34069	-0.06418
H	-0.12759	2.16163	-0.06827
O	0.00353	-0.00071	1.49975

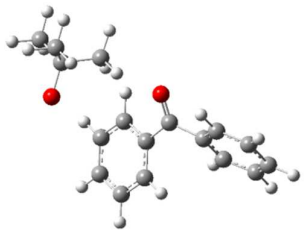
tert-Butanol (HO^{t}Bu)



15
-233.5806428

C	-1.49270	-0.00002	-0.31732
C	-0.00606	0.00000	0.01498
H	-1.97347	-0.88876	0.10226
H	-1.97350	0.88872	0.10223
H	-1.64200	-0.00005	-1.40068
C	0.67162	1.25791	-0.52689
C	0.67166	-1.25789	-0.52689
H	1.73360	1.27098	-0.25667
H	0.59949	1.29843	-1.61812
H	0.19631	2.15130	-0.11123
H	0.59956	-1.29840	-1.61812
H	1.73363	-1.27094	-0.25665
H	0.19636	-2.15130	-0.11124
O	0.05936	0.00000	1.44873
H	0.98799	0.00002	1.71513

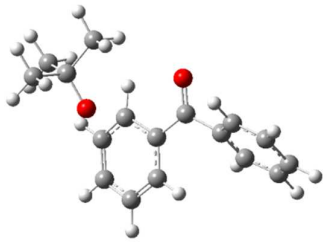
Reactant Complex for formation of **45** from **17** and **O*t*Bu anion**



38
-809.4818830

C	5.75012	-0.43125	0.87668
C	4.74081	0.27793	1.52733
C	3.43543	0.24017	1.03985
C	3.13285	-0.52599	-0.09143
C	4.14609	-1.25151	-0.72891
C	5.45254	-1.19473	-0.25437
H	6.76811	-0.39192	1.25185
H	4.96966	0.86115	2.41343
H	2.64934	0.78691	1.55171
H	3.89440	-1.85102	-1.59820
H	6.23842	-1.74576	-0.76103
C	1.73281	-0.65782	-0.60991
C	0.78155	0.48671	-0.48134
C	1.21869	1.81657	-0.52179
C	-0.58800	0.20876	-0.38002
C	0.28886	2.85304	-0.46424
H	2.27664	2.04065	-0.62171
C	-1.52047	1.24045	-0.29914
H	-0.90924	-0.82943	-0.35637
C	-1.07095	2.56398	-0.34541
H	0.62718	3.88358	-0.51076
H	-2.59293	1.02871	-0.19787
H	-1.79138	3.37533	-0.28890
O	1.37780	-1.70367	-1.13584
O	-4.65328	0.80218	0.05679
C	-4.81929	-0.54029	0.28655
C	-6.30695	-0.89171	0.52227
C	-4.32392	-1.37679	-0.91856
C	-4.02291	-0.99562	1.53466
H	-6.68252	-0.32872	1.38539
H	-6.89410	-0.59729	-0.35615
H	-6.47163	-1.96222	0.70755
H	-3.26540	-1.15830	-1.10670
H	-4.43264	-2.45923	-0.76507
H	-4.88899	-1.09369	-1.81492
H	-4.13618	-2.06713	1.74922
H	-2.95657	-0.78347	1.38792
H	-4.36193	-0.42757	2.40960

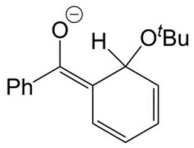
Transition State for formation of **45** from **17** and **O*t*Bu anion**

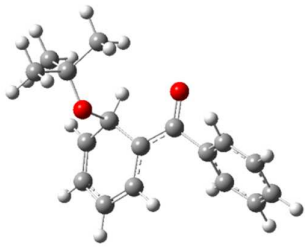


38
-809.4594074

C	-5.10676	-0.68944	0.37800
C	-4.63181	0.47287	-0.22909
C	-3.27433	0.60620	-0.51979
C	-2.38391	-0.43043	-0.22151
C	-2.87105	-1.60334	0.36448
C	-4.22292	-1.72792	0.67640
H	-6.16204	-0.78810	0.61365
H	-5.31740	1.27787	-0.47566
H	-2.90698	1.51233	-0.99330
H	-2.17865	-2.41309	0.57628
H	-4.58870	-2.63593	1.14617
C	-0.92247	-0.36473	-0.59182
C	-0.12721	0.80604	-0.22909
C	-0.61645	1.83045	0.61240
C	1.21147	0.87633	-0.70544
C	0.11949	2.97893	0.83758
H	-1.59007	1.72199	1.08120
C	1.87747	2.13091	-0.60911
H	1.50402	0.16378	-1.46708
C	1.35775	3.13917	0.17336
H	-0.26605	3.76395	1.47997
H	2.83408	2.26301	-1.10580
H	1.90255	4.07475	0.27689
O	-0.45147	-1.32119	-1.21422
O	2.25590	-0.23500	0.68946
C	3.27430	-1.06397	0.24335
C	4.09660	-1.54901	1.45419
C	2.70977	-2.30053	-0.48538
C	4.23711	-0.32453	-0.71331
H	4.54504	-0.69078	1.96782
H	3.43727	-2.06467	2.16129
H	4.89978	-2.23787	1.15997
H	2.07524	-1.98863	-1.32082
H	3.50411	-2.95851	-0.86174
H	2.08025	-2.87568	0.20412
H	5.08348	-0.95831	-1.00675
H	3.71812	-0.01269	-1.62712
H	4.62820	0.57417	-0.22244

45

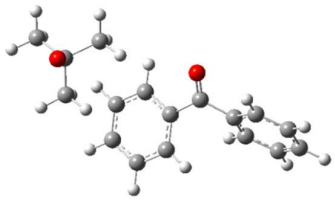




38
-809.4797478

C	-5.12994	-0.47372	0.29764
C	-4.55389	0.63735	-0.31762
C	-3.17948	0.67168	-0.55762
C	-2.36537	-0.40805	-0.19792
C	-2.95745	-1.52718	0.39929
C	-4.32617	-1.55756	0.65770
H	-6.19815	-0.49805	0.49134
H	-5.17387	1.47917	-0.61182
H	-2.73321	1.53784	-1.03822
H	-2.33063	-2.37550	0.65958
H	-4.76858	-2.42711	1.13509
C	-0.88442	-0.44785	-0.50926
C	-0.05308	0.63349	-0.12283
C	-0.50295	1.73619	0.65971
C	1.39830	0.57215	-0.49606
C	0.24269	2.88106	0.79872
H	-1.47689	1.67738	1.14149
C	1.96422	1.95531	-0.66761
H	1.50775	-0.03059	-1.40411
C	1.45213	3.00441	0.02430
H	-0.11460	3.71477	1.39453
H	2.84830	2.08534	-1.28761
H	1.93740	3.97758	-0.04007
O	-0.47819	-1.46891	-1.12563
O	2.13877	-0.11883	0.57171
C	3.19686	-1.00635	0.20197
C	3.91569	-1.31213	1.51473
C	2.62805	-2.29912	-0.39045
C	4.18524	-0.35931	-0.77590
H	4.33732	-0.39481	1.93763
H	3.21105	-1.73590	2.23667
H	4.72592	-2.03086	1.35353
H	2.01911	-2.09661	-1.27508
H	3.43918	-2.98411	-0.66131
H	1.98359	-2.79061	0.34545
H	5.02217	-1.04169	-0.95806
H	3.71743	-0.13960	-1.74067
H	4.57943	0.57305	-0.35974

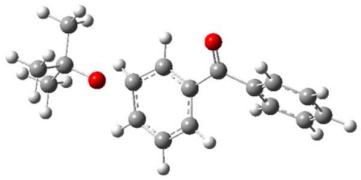
Reactant Complex for formation of **47** from **17** and **O*t*Bu anion**



38
-809.4818921

C	-1.31648	1.76606	-0.92637
C	-0.03380	2.31452	-0.89947
C	1.07756	1.48021	-0.79390
C	0.90251	0.09195	-0.73691
C	-0.38965	-0.44798	-0.78282
C	-1.50556	0.38170	-0.86543
H	-2.18186	2.41998	-0.99649
H	0.10334	3.38983	-0.95920
H	2.07665	1.90571	-0.77991
H	-0.50640	-1.52750	-0.74409
H	-2.52188	-0.03314	-0.88081
C	2.06432	-0.84605	-0.69612
C	3.33468	-0.43144	-0.01781
C	3.33729	0.40958	1.10063
C	4.54132	-0.96206	-0.48896
C	4.53736	0.71449	1.74085
H	2.40226	0.80736	1.48330
C	5.74043	-0.63909	0.13783
H	4.52346	-1.62137	-1.35119
C	5.73870	0.19825	1.25568
H	4.53369	1.35418	2.61743
H	6.67534	-1.04031	-0.24028
H	6.67335	0.44478	1.74993
O	1.98609	-1.95243	-1.21230
O	-4.52486	-0.58824	-0.87041
C	-4.97974	-0.37810	0.40732
C	-4.83469	1.10870	0.81535
C	-6.47280	-0.75910	0.54479
C	-4.18087	-1.22273	1.43026
H	-3.77873	1.40068	0.76436
H	-5.39521	1.73623	0.11157
H	-5.20186	1.31198	1.83089
H	-6.60596	-1.81573	0.28234
H	-6.86436	-0.60142	1.55923
H	-7.06879	-0.15929	-0.15382
H	-4.51751	-1.07363	2.46554
H	-4.28124	-2.28670	1.18351
H	-3.11761	-0.95969	1.36985

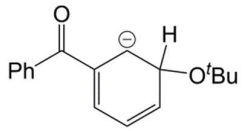
Transition State for formation of **47** from **17** and **O*t*Bu anion**

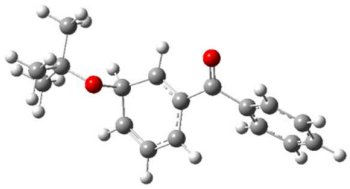


38
-809.4503761

C	1.57376	1.97195	-0.10672
C	0.40222	2.22196	0.59235
C	-0.64972	1.29731	0.61613
C	-0.50268	0.11478	-0.13691
C	0.67574	-0.15339	-0.83020
C	1.82982	0.68288	-0.68696
H	2.35085	2.73146	-0.15013
H	0.28245	3.17521	1.10364
H	-1.55871	1.50100	1.17075
H	0.73568	-1.05433	-1.43445
H	2.57021	0.63363	-1.47984
C	-1.60210	-0.88418	-0.22392
C	-3.03157	-0.44581	-0.06128
C	-3.49191	0.78414	-0.54450
C	-3.93695	-1.33773	0.52514
C	-4.84213	1.11643	-0.43828
H	-2.79483	1.47165	-1.01312
C	-5.28012	-0.99618	0.65143
H	-3.57127	-2.29560	0.88239
C	-5.73480	0.23233	0.16699
H	-5.19637	2.06625	-0.82651
H	-5.97391	-1.68663	1.12096
H	-6.78396	0.49705	0.25764
O	-1.37855	-2.07221	-0.43576
O	2.91253	-0.20338	0.52699
C	4.24769	-0.41629	0.17342
C	4.96905	0.91068	-0.14138
C	4.95597	-1.07608	1.36721
C	4.36537	-1.36281	-1.03875
H	4.52435	1.41057	-1.00867
H	4.88542	1.58632	0.71744
H	6.03252	0.74779	-0.35500
H	4.46147	-2.02167	1.61427
H	6.01264	-1.28021	1.15112
H	4.89895	-0.42013	2.24250
H	5.41299	-1.57285	-1.28705
H	3.86496	-2.31068	-0.81152
H	3.88901	-0.93407	-1.92689

47

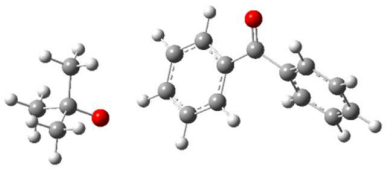




38
-809.4555653

C	1.61390	1.90790	-0.10802
C	0.45450	2.16663	0.59449
C	-0.59546	1.23259	0.69188
C	-0.45718	0.03794	-0.05718
C	0.70163	-0.25512	-0.75955
C	1.94230	0.53414	-0.57169
H	2.36441	2.68717	-0.22758
H	0.32333	3.15108	1.04453
H	-1.50052	1.45464	1.24452
H	0.73321	-1.14513	-1.38372
H	2.54842	0.54320	-1.48351
C	-1.58237	-0.93088	-0.14808
C	-3.00188	-0.44084	-0.04375
C	-3.39821	0.79133	-0.57520
C	-3.96148	-1.28320	0.52927
C	-4.73861	1.17447	-0.52987
H	-2.65650	1.43992	-1.03008
C	-5.29534	-0.89061	0.59581
H	-3.64474	-2.24464	0.92243
C	-5.68574	0.33996	0.06285
H	-5.04307	2.12580	-0.95540
H	-6.03097	-1.54317	1.05596
H	-6.72709	0.64491	0.10583
O	-1.39886	-2.13293	-0.32434
O	2.81151	-0.16256	0.44710
C	4.18080	-0.37290	0.11834
C	4.89188	0.94380	-0.22498
C	4.80495	-0.96647	1.38065
C	4.32103	-1.37697	-1.03469
H	4.49315	1.39636	-1.13818
H	4.76796	1.65937	0.59420
H	5.96237	0.76698	-0.37765
H	4.29258	-1.89510	1.65049
H	5.86717	-1.18406	1.22497
H	4.70838	-0.26266	2.21318
H	5.37707	-1.59675	-1.22694
H	3.81114	-2.31028	-0.77467
H	3.88414	-0.99446	-1.96206

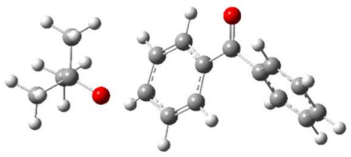
Reactant Complex for formation of **20** from **17** and **O*t*Bu anion**



38
-809.4824518

C	5.90193	-1.42010	0.02160
C	4.79318	-1.73406	-0.76399
C	3.66907	-0.90974	-0.74735
C	3.65923	0.24456	0.04389
C	4.78326	0.56600	0.81397
C	5.89572	-0.26930	0.81297
H	6.77226	-2.06887	0.01567
H	4.80152	-2.62126	-1.38880
H	2.80972	-1.15419	-1.36418
H	4.76749	1.47110	1.41317
H	6.75856	-0.02337	1.42362
C	2.50307	1.19815	0.04776
C	1.11253	0.68398	-0.12574
C	0.73332	-0.59745	0.29423
C	0.14899	1.54451	-0.66902
C	-0.59270	-1.00795	0.16686
H	1.46582	-1.26323	0.74098
C	-1.16774	1.12001	-0.80902
H	0.45199	2.53944	-0.98113
C	-1.55131	-0.15970	-0.39218
H	-0.88248	-1.99785	0.50725
H	-1.90793	1.78775	-1.24142
O	2.70894	2.39553	0.19672
H	-2.59566	-0.48531	-0.49750
O	-4.54872	-1.03841	-0.73092
C	-5.37456	-0.33290	0.10741
C	-6.84924	-0.41518	-0.35246
C	-5.29875	-0.87962	1.55316
C	-4.97885	1.16412	0.15015
H	-6.93694	-0.01654	-1.37043
H	-7.16895	-1.46412	-0.37135
H	-7.53362	0.14473	0.29990
H	-4.26500	-0.81113	1.91369
H	-5.94771	-0.33615	2.25379
H	-5.59002	-1.93705	1.55871
H	-5.63203	1.76183	0.80071
H	-3.94814	1.26411	0.51111
H	-5.02358	1.58126	-0.86369

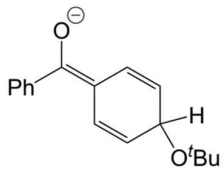
Transition State for formation of **20** from **17** and **O*t*Bu anion**

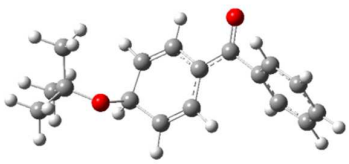


38
-809.4600997

C	5.54083	-0.87473	0.67246
C	4.70913	-1.43198	-0.29855
C	3.49667	-0.82040	-0.61415
C	3.11460	0.36270	0.02706
C	3.96482	0.92910	0.98288
C	5.16588	0.30683	1.31482
H	6.48066	-1.35642	0.92465
H	5.00346	-2.34258	-0.81114
H	2.85111	-1.25270	-1.37314
H	3.67065	1.85855	1.46169
H	5.81284	0.74436	2.06903
C	1.85371	1.09626	-0.35089
C	0.62102	0.34939	-0.58157
C	0.41122	-0.96918	-0.11147
C	-0.42354	0.95545	-1.31889
C	-0.78423	-1.62289	-0.31925
H	1.20499	-1.47992	0.42688
C	-1.61291	0.30095	-1.54958
H	-0.24791	1.94090	-1.74326
C	-1.88447	-0.95768	-0.93565
H	-0.91840	-2.63474	0.05073
H	-2.37668	0.77053	-2.16339
O	1.91654	2.32615	-0.46613
H	-2.70292	-1.55677	-1.31458
O	-3.02614	-0.64814	0.70359
C	-4.26385	-0.02389	0.59785
C	-5.12218	-0.41166	1.81777
C	-4.11003	1.51117	0.58044
C	-5.02550	-0.45663	-0.67361
H	-5.26698	-1.49780	1.83918
H	-4.60656	-0.11668	2.73845
H	-6.10752	0.07279	1.79911
H	-3.50731	1.81781	-0.28012
H	-5.07922	2.02472	0.53059
H	-3.59067	1.83540	1.48975
H	-6.03563	-0.03003	-0.69919
H	-4.50195	-0.12898	-1.57884
H	-5.11221	-1.54942	-0.70414

20

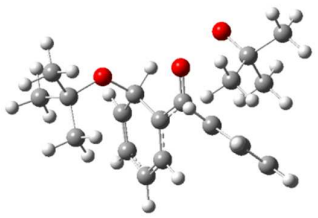




38
-809.4795644

C	5.43204	-1.12117	0.51928
C	4.72102	-1.30372	-0.66650
C	3.54569	-0.58682	-0.89767
C	3.07364	0.32988	0.04798
C	3.80682	0.52124	1.22452
C	4.97006	-0.20569	1.46723
H	6.34284	-1.68347	0.70223
H	5.08192	-2.00419	-1.41407
H	2.99547	-0.72991	-1.82409
H	3.45228	1.24944	1.94865
H	5.51918	-0.05602	2.39232
C	1.85189	1.19115	-0.18644
C	0.61265	0.58761	-0.51060
C	0.36875	-0.83273	-0.54524
C	-0.50916	1.41761	-0.86879
C	-0.85493	-1.36055	-0.79822
H	1.19955	-1.51501	-0.37942
C	-1.74431	0.92285	-1.12673
H	-0.32092	2.48341	-0.98296
C	-2.09349	-0.52104	-0.90262
H	-0.98624	-2.43947	-0.83873
H	-2.52909	1.59199	-1.47339
O	2.02509	2.43361	-0.05019
H	-2.74414	-0.89353	-1.70586
O	-2.82505	-0.76348	0.34530
C	-4.14885	-0.24466	0.52930
C	-4.79432	-1.20422	1.53041
C	-4.09057	1.15913	1.14439
C	-4.97243	-0.22886	-0.76125
H	-4.86294	-2.20881	1.10176
H	-4.18798	-1.25561	2.44001
H	-5.80003	-0.86611	1.80037
H	-3.66558	1.88407	0.44734
H	-5.09577	1.49311	1.42530
H	-3.46622	1.14060	2.04316
H	-5.99919	0.06868	-0.52567
H	-4.57909	0.48289	-1.49330
H	-5.00134	-1.22320	-1.21880

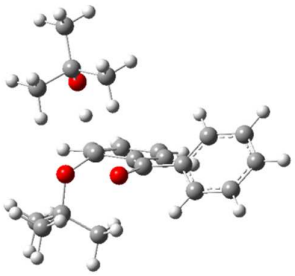
Reactant Complex for formation of **46** from **45** and **O*t*Bu anion**



52
-1042.5207433

C	1.07281	5.10002	0.36101
C	1.68861	3.98540	0.93030
C	1.23665	2.70132	0.62325
C	0.17238	2.51272	-0.26521
C	-0.42299	3.63716	-0.84853
C	0.01229	4.92224	-0.52979
H	1.41922	6.09989	0.60542
H	2.52172	4.11439	1.61530
H	1.71598	1.83406	1.06937
H	-1.23300	3.49181	-1.55827
H	-0.47041	5.78514	-0.97972
C	-0.29778	1.13567	-0.68885
C	-0.68291	0.18653	0.28928
C	-0.71291	0.49054	1.67968
C	-0.99605	-1.20924	-0.19207
C	-0.85428	-0.47171	2.64813
H	-0.61717	1.53019	1.98694
C	-0.95642	-2.20762	0.92822
H	-0.25661	-1.48103	-0.95873
C	-0.92092	-1.85193	2.23437
H	-0.86948	-0.21203	3.70175
H	-0.96816	-3.25983	0.64851
H	-0.91888	-2.63041	2.99682
O	-0.30219	0.92201	-1.93067
O	-2.20986	-1.33190	-1.01793
C	-3.53968	-1.30445	-0.49775
C	-4.39441	-0.94070	-1.71511
C	-3.96176	-2.69222	0.00739
C	-3.75453	-0.25994	0.59827
H	-4.10082	0.04189	-2.09758
H	-4.25112	-1.67882	-2.51083
H	-5.45678	-0.91492	-1.44955
H	-3.43306	-2.95731	0.92527
H	-5.03948	-2.71068	0.20812
H	-3.73806	-3.44585	-0.75525
H	-4.81339	-0.25578	0.88240
H	-3.15692	-0.47942	1.48609
H	-3.48241	0.73740	0.23934
O	3.40051	-3.28512	-0.99105
C	3.88156	-2.12610	-0.43806
C	2.73857	-1.14255	-0.09320
C	4.66464	-2.41500	0.86680
C	4.84563	-1.40351	-1.41089
H	2.17864	-0.88050	-1.00003
H	2.03181	-1.61457	0.60078
H	3.10172	-0.21112	0.36481
H	5.49227	-3.10173	0.64867
H	5.07740	-1.50881	1.33184
H	4.00039	-2.90402	1.58978
H	5.25244	-0.46897	-0.99977
H	5.68289	-2.06836	-1.65737
H	4.31267	-1.17017	-2.34048

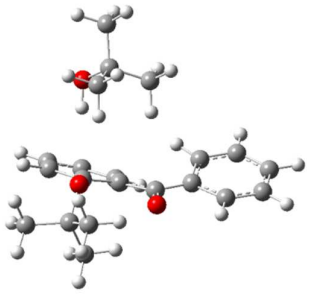
Transition State for formation of **46** from **45** and **O*t*Bu anion**



52
-1042.4790474

C	-5.37397	0.13865	-0.18284
C	-4.54667	0.80351	0.72458
C	-3.16229	0.64500	0.66699
C	-2.55514	-0.18413	-0.29411
C	-3.40535	-0.81563	-1.22026
C	-4.78969	-0.67198	-1.16019
H	-6.45229	0.26163	-0.13906
H	-4.98015	1.46138	1.47380
H	-2.53238	1.18868	1.36620
H	-2.94952	-1.42352	-1.99679
H	-5.41783	-1.19014	-1.88081
C	-1.06324	-0.32483	-0.46547
C	-0.23878	-0.46391	0.65471
C	-0.79431	-0.76309	1.96065
C	1.28272	-0.35874	0.60340
C	-0.05937	-0.94428	3.09580
H	-1.86645	-0.93080	2.03297
C	1.98694	-0.70780	1.83577
H	1.59283	1.03005	0.58765
C	1.39234	-0.88904	3.04372
H	-0.55935	-1.20275	4.02686
H	3.07599	-0.71482	1.76298
H	1.98059	-1.01851	3.94955
O	-0.66675	-0.33243	-1.70247
O	1.96121	-0.84414	-0.56368
C	2.05422	-2.24805	-0.84641
C	2.13176	-2.31453	-2.37125
C	3.33795	-2.82143	-0.23075
C	0.84841	-3.05714	-0.36653
H	1.21788	-1.87238	-2.77949
H	2.99499	-1.74124	-2.72850
H	2.23187	-3.34909	-2.71925
H	3.27342	-2.83860	0.86106
H	3.50743	-3.84692	-0.58110
H	4.19916	-2.20883	-0.51947
H	0.99612	-4.10928	-0.63972
H	0.73334	-2.98957	0.72024
H	-0.06238	-2.67916	-0.83822
O	1.93276	2.20597	0.74563
C	1.63442	3.04320	-0.33396
C	0.13173	2.98967	-0.65760
C	2.01345	4.48271	0.04252
C	2.44658	2.62211	-1.57193
H	-0.16843	1.96337	-0.89485
H	-0.43952	3.31822	0.22011
H	-0.12636	3.64276	-1.50156
H	3.08126	4.53961	0.28285
H	1.80312	5.18473	-0.77485
H	1.44594	4.79723	0.92570
H	2.20323	3.23144	-2.45163
H	3.51768	2.72971	-1.36111
H	2.25170	1.56989	-1.80049

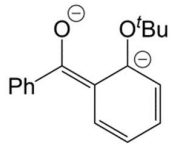
Product Complex of **46** and
HO^{t}Bu

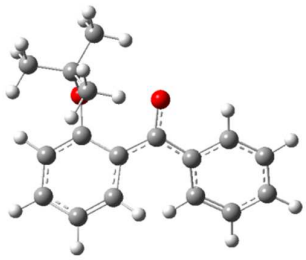


52
-1042.5068018

C	-5.05918800	-1.34905200	-0.00939100
C	-4.38141500	-0.34867000	0.71092300
C	-2.99614900	-0.27772900	0.74411700
C	-2.15624800	-1.21411700	0.04601900
C	-2.88548000	-2.17942800	-0.73318200
C	-4.27158800	-2.25087600	-0.74113300
H	-6.14356400	-1.40435800	-0.01725900
H	-4.95197200	0.40676300	1.25004900
H	-2.55223100	0.55562500	1.27622300
H	-2.29723900	-2.87065800	-1.32609700
H	-4.75472400	-3.02528200	-1.33671500
C	-0.70863100	-1.21775700	-0.07930200
C	0.12580400	-0.45412800	0.80250300
C	-0.31116900	0.02650900	2.10004300
C	1.52528800	-0.12723100	0.55037400
C	0.44222000	0.83522300	2.93312500
H	-1.26982900	-0.31410400	2.47309900
C	2.25682500	0.70335600	1.38587700
H	0.67576600	2.41094300	0.69156000
C	1.74356700	1.23778500	2.58402000
H	0.01441000	1.14300200	3.88673900
H	3.26749700	0.95014100	1.06574500
H	2.33460400	1.89923500	3.20827600
O	-0.19708200	-1.97709400	-1.04903800
O	2.17370100	-0.56027600	-0.59764000
C	2.92431600	-1.79654400	-0.53190100
C	2.84133600	-2.36823200	-1.94296000
C	4.37273600	-1.46693800	-0.16054400
C	2.32926500	-2.78432400	0.46946100
H	1.78893000	-2.56909200	-2.15959400
H	3.23072400	-1.64146300	-2.66512900
H	3.43187400	-3.28762200	-2.02386900
H	4.42556500	-1.04541200	0.84831600
H	4.98893100	-2.37281500	-0.18576900
H	4.79033300	-0.74033400	-0.86608500
H	2.87601700	-3.73191400	0.40278500
H	2.41781400	-2.40687700	1.49404200
H	1.27513700	-2.93226300	0.21505700
O	0.46961700	3.30050100	0.35630900
C	-0.07679800	3.19688000	-0.96365400
C	-1.40681500	2.44755500	-0.91058200
C	-0.28060800	4.63423600	-1.42888200
C	0.91000200	2.46457100	-1.87326100
H	-1.25406300	1.42533200	-0.54356000
H	-2.10324400	2.96316800	-0.24033000
H	-1.86098200	2.38955300	-1.90625400
H	0.67481200	5.16866800	-1.44478700
H	-0.70882300	4.65360400	-2.43572900
H	-0.96167200	5.15797400	-0.75027700
H	0.52421200	2.41107800	-2.89709000
H	1.87046200	2.99161900	-1.88838200
H	1.07776000	1.44390000	-1.51203100

46





37
-808.9107073

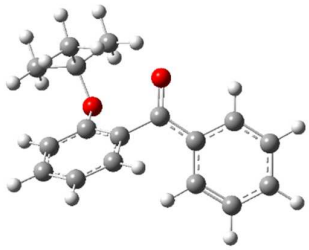
C	-5.09273	-0.40979	-0.11715
C	-4.36586	0.77381	-0.36630
C	-2.98319	0.81716	-0.30598
C	-2.18053	-0.34127	0.01404
C	-2.95579	-1.54818	0.19609
C	-4.34177	-1.56767	0.14772
H	-6.17765	-0.42811	-0.15316
H	-4.90106	1.68619	-0.62911
H	-2.49893	1.75416	-0.55951
H	-2.40064	-2.46135	0.38060
H	-4.85764	-2.51342	0.31667
C	-0.74659	-0.46026	0.03630
C	0.09885	0.71198	0.02797
C	-0.33415	1.98764	0.54559
C	1.47571	0.74059	-0.42306
C	0.41382	3.15243	0.48422
H	-1.29254	2.02962	1.05221
C	2.20425	1.91917	-0.50513
C	1.69919	3.15968	-0.07928
H	-0.00436	4.06722	0.90265
H	3.20258	1.85078	-0.93248
H	2.28966	4.06697	-0.15735
O	-0.22876	-1.69128	0.06450
O	2.09847	-0.40260	-0.90163
C	2.91605	-1.17213	0.01309
C	2.79152	-2.60737	-0.48613
C	4.36247	-0.68120	-0.09312
C	2.42404	-1.07492	1.45548
H	1.74084	-2.89765	-0.40297
H	3.10504	-2.66740	-1.53479
H	3.42389	-3.28037	0.10349
H	4.44950	0.34781	0.26968
H	5.02376	-1.31293	0.51069
H	4.70099	-0.71585	-1.13444
H	3.02221	-1.74771	2.08072
H	2.53560	-0.05638	1.84266
H	1.36937	-1.36845	1.47553

Single Point Radical Anion
using Optimised Geometry
46

37
-808.8706291

C	-5.09273100	-0.40979100	-0.11715000
C	-4.36585900	0.77381000	-0.36630500
C	-2.98319200	0.81716000	-0.30597700
C	-2.18053100	-0.34126600	0.01404400
C	-2.95578500	-1.54817800	0.19608700
C	-4.34176800	-1.56767000	0.14771600
H	-6.17765200	-0.42811000	-0.15316300
H	-4.90106100	1.68619100	-0.62911300
H	-2.49893200	1.75416200	-0.55951500
H	-2.40064000	-2.46134800	0.38059500
H	-4.85764100	-2.51342200	0.31667100
C	-0.74659400	-0.46026300	0.03629600
C	0.09885300	0.71197600	0.02796500
C	-0.33415200	1.98763800	0.54559200
C	1.47570900	0.74058600	-0.42306000
C	0.41382500	3.15243300	0.48421600
H	-1.29254200	2.02962200	1.05221200
C	2.20424600	1.91916700	-0.50513000
C	1.69918900	3.15967600	-0.07928100
H	-0.00436100	4.06722000	0.90265500
H	3.20258300	1.85078400	-0.93248100
H	2.28966200	4.06696900	-0.15735400
O	-0.22875800	-1.69128000	0.06449700
O	2.09846900	-0.40259600	-0.90163000
C	2.91604600	-1.17213500	0.01308800
C	2.79151900	-2.60737400	-0.48612900
C	4.36246900	-0.68119800	-0.09312000
C	2.42403600	-1.07492500	1.45548100
H	1.74084000	-2.89764900	-0.40297300
H	3.10504100	-2.66739600	-1.53479200
H	3.42389100	-3.28037300	0.10348900
H	4.44950100	0.34781400	0.26967800
H	5.02376100	-1.31293000	0.51069300
H	4.70099300	-0.71584700	-1.13444500
H	3.02220900	-1.74771000	2.08072100
H	2.53560000	-0.05637700	1.84266200
H	1.36937300	-1.36845300	1.47553300

49



37
-808.8808189

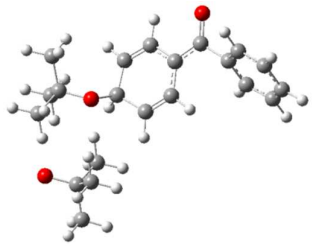
C	-4.87949000	-0.42050500	-0.63585500
C	-4.04384100	0.63688300	-1.03822500
C	-2.71673200	0.69602200	-0.64534400
C	-2.13944000	-0.31170400	0.18834400
C	-3.00330300	-1.38500700	0.57242400
C	-4.32935800	-1.42858500	0.17128400
H	-5.91823900	-0.45902000	-0.94804000
H	-4.44040300	1.42271500	-1.67747200
H	-2.09965400	1.51890000	-0.99476400
H	-2.58828100	-2.17165800	1.19452000
H	-4.95281800	-2.26164500	0.48971600
C	-0.76400200	-0.33218600	0.61315400
C	0.11345500	0.84941900	0.33623000
C	-0.25291600	2.13361900	0.77352600
C	1.35792900	0.71827200	-0.31305500
C	0.56972200	3.24199600	0.59024400
H	-1.20829900	2.25054400	1.27979900
C	2.17770200	1.83077300	-0.51814600
C	1.79583700	3.09073600	-0.05944500
H	0.25641300	4.21671500	0.95243900
H	3.11088200	1.70057200	-1.05765800
H	2.44568700	3.94567100	-0.22073000
O	-0.26809100	-1.32522900	1.25366100
O	1.70715200	-0.49604100	-0.84827500
C	2.75596700	-1.29979000	-0.23306200
C	2.25650900	-2.73285900	-0.38164200
C	4.04916500	-1.09201300	-1.02039700
C	2.94716600	-0.95676600	1.24069700
H	1.32098100	-2.83808100	0.17436900
H	2.07483600	-2.95816000	-1.43767600
H	2.99908800	-3.43952800	0.00230600
H	4.43118800	-0.07468600	-0.89482200
H	4.81834000	-1.78716100	-0.66788300
H	3.87657200	-1.27432000	-2.08555700
H	3.65718100	-1.66631100	1.67713600
H	3.35217800	0.05142700	1.37168300
H	1.98563000	-1.03564500	1.75515300

Single Point Dianion using
Optimised Geometry **49**

37
-808.9011778

C	-4.87949000	-0.42050500	-0.63585500
C	-4.04384100	0.63688300	-1.03822500
C	-2.71673200	0.69602200	-0.64534400
C	-2.13944000	-0.31170400	0.18834400
C	-3.00330300	-1.38500700	0.57242400
C	-4.32935800	-1.42858500	0.17128400
H	-5.91823900	-0.45902000	-0.94804000
H	-4.44040300	1.42271500	-1.67747200
H	-2.09965400	1.51890000	-0.99476400
H	-2.58828100	-2.17165800	1.19452000
H	-4.95281800	-2.26164500	0.48971600
C	-0.76400200	-0.33218600	0.61315400
C	0.11345500	0.84941900	0.33623000
C	-0.25291600	2.13361900	0.77352600
C	1.35792900	0.71827200	-0.31305500
C	0.56972200	3.24199600	0.59024400
H	-1.20829900	2.25054400	1.27979900
C	2.17770200	1.83077300	-0.51814600
C	1.79583700	3.09073600	-0.05944500
H	0.25641300	4.21671500	0.95243900
H	3.11088200	1.70057200	-1.05765800
H	2.44568700	3.94567100	-0.22073000
O	-0.26809100	-1.32522900	1.25366100
O	1.70715200	-0.49604100	-0.84827500
C	2.75596700	-1.29979000	-0.23306200
C	2.25650900	-2.73285900	-0.38164200
C	4.04916500	-1.09201300	-1.02039700
C	2.94716600	-0.95676600	1.24069700
H	1.32098100	-2.83808100	0.17436900
H	2.07483600	-2.95816000	-1.43767600
H	2.99908800	-3.43952800	0.00230600
H	4.43118800	-0.07468600	-0.89482200
H	4.81834000	-1.78716100	-0.66788300
H	3.87657200	-1.27432000	-2.08555700
H	3.65718100	-1.66631100	1.67713600
H	3.35217800	0.05142700	1.37168300
H	1.98563000	-1.03564500	1.75515300

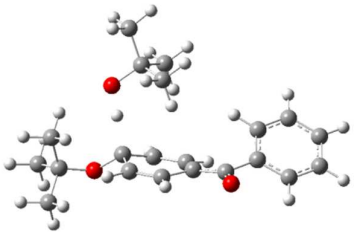
Reactant Complex for formation of **24** from **20** and **O*t*Bu anion**



52
-1042.5299146

C	-6.20090	2.02091	0.95151
C	-5.19761	2.46783	0.09198
C	-4.28256	1.56288	-0.44871
C	-4.36398	0.19923	-0.14634
C	-5.38998	-0.24139	0.69773
C	-6.29448	0.66087	1.25402
H	-6.90877	2.72568	1.37753
H	-5.12643	3.52212	-0.15948
H	-3.50269	1.91441	-1.11911
H	-5.46938	-1.30313	0.91434
H	-7.07479	0.30444	1.92037
C	-3.44191	-0.82747	-0.76705
C	-2.04136	-0.66037	-0.67696
C	-1.37771	0.37039	0.08652
C	-1.16865	-1.55071	-1.40276
C	-0.02888	0.45577	0.18812
H	-1.98010	1.11828	0.59737
C	0.18263	-1.49162	-1.32579
H	-1.63867	-2.26372	-2.07765
C	0.90073	-0.58472	-0.36468
H	0.42866	1.25979	0.76077
H	0.78485	-2.14027	-1.95880
O	-4.01354	-1.80342	-1.33251
H	1.76196	-0.10513	-0.84957
O	1.43592	-1.28049	0.80248
C	2.52872	-2.20309	0.66497
C	3.26009	-2.12434	2.00580
C	1.98152	-3.62213	0.46637
C	3.50246	-1.83778	-0.45827
H	3.67462	-1.12117	2.14607
H	2.56427	-2.33586	2.82428
H	4.07780	-2.85177	2.04539
H	1.47434	-3.72085	-0.49612
H	2.79579	-4.35454	0.50723
H	1.26249	-3.85544	1.25855
H	4.32616	-2.56061	-0.45066
H	3.03020	-1.89102	-1.44525
H	3.93604	-0.84016	-0.31397
O	5.58503	1.05348	-0.00816
C	4.64513	2.04276	-0.13615
C	3.52141	1.89341	0.91913
C	5.27489	3.44660	0.04408
C	3.98281	2.00556	-1.53588
H	3.03578	0.91566	0.81142
H	3.95883	1.94288	1.92462
H	2.75033	2.67275	0.83733
H	6.06435	3.59104	-0.70388
H	4.54455	4.26143	-0.05983
H	5.73315	3.51698	1.03845
H	3.20385	2.77007	-1.66479
H	4.74909	2.15586	-2.30653
H	3.53006	1.02023	-1.69831

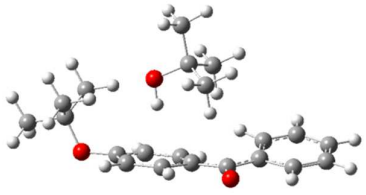
Transition State for formation of **24** from **20** and **O*t*Bu anion**



52
-1042.4942279

C	5.78637	0.41966	-1.15973
C	4.56433	1.09537	-1.12938
C	3.45989	0.52878	-0.49443
C	3.54209	-0.72998	0.12591
C	4.78754	-1.37928	0.11420
C	5.89113	-0.82260	-0.52953
H	6.64696	0.86117	-1.65393
H	4.47336	2.07521	-1.59114
H	2.52083	1.07533	-0.45775
H	4.87148	-2.33317	0.62678
H	6.83861	-1.35550	-0.53509
C	2.40167	-1.34314	0.89360
C	1.09680	-1.21430	0.42137
C	0.69680	-0.74582	-0.90622
C	-0.02799	-1.65507	1.24430
C	-0.60051	-0.51529	-1.22599
H	1.45891	-0.60327	-1.66954
C	-1.32037	-1.40514	0.91038
H	0.20836	-2.16514	2.17533
C	-1.71768	-0.58995	-0.26193
H	-0.85226	-0.19495	-2.23840
H	-2.10194	-1.74913	1.58809
O	2.73043	-1.95449	1.99021
H	-1.95906	0.86199	0.04933
O	-2.85772	-1.13635	-1.01053
C	-4.17420	-1.15363	-0.46491
C	-5.10196	-0.84028	-1.64300
C	-4.48334	-2.56798	0.04975
C	-4.40909	-0.12815	0.64475
H	-4.90798	0.17237	-2.01144
H	-4.91907	-1.54706	-2.45926
H	-6.15469	-0.91260	-1.34847
H	-3.82996	-2.83337	0.88502
H	-5.52382	-2.64088	0.38755
H	-4.32648	-3.29685	-0.75223
H	-5.46138	-0.17348	0.94828
H	-3.79028	-0.33289	1.52296
H	-4.17283	0.88118	0.30269
O	-2.18940	2.00964	0.18741
C	-1.05391	2.79682	0.43933
C	-0.27656	3.06761	-0.85974
C	-1.52813	4.13292	1.02495
C	-0.12562	2.10050	1.44538
H	0.06092	2.11871	-1.28925
H	-0.92741	3.56992	-1.58522
H	0.59992	3.70365	-0.68066
H	-2.07412	3.95806	1.95870
H	-0.68639	4.80463	1.23490
H	-2.20363	4.63186	0.32062
H	0.74611	2.72357	1.68328
H	-0.67109	1.89911	2.37540
H	0.22686	1.14490	1.04235

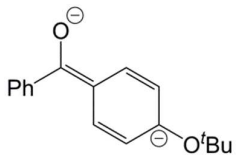
Product Complex of **24** and **HO^{t}Bu**

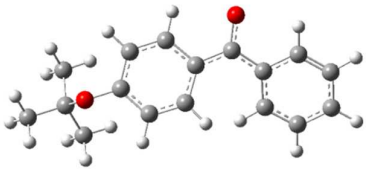


52
-1042.5214805

C	5.49302	-0.79425	-1.43145
C	4.20920	-0.89572	-1.99563
C	3.05680	-0.89344	-1.22192
C	3.09117	-0.79258	0.21819
C	4.42263	-0.62602	0.75421
C	5.56122	-0.64100	-0.03494
H	6.38653	-0.80790	-2.04793
H	4.10231	-0.96489	-3.07795
H	2.11436	-0.91082	-1.75274
H	4.50156	-0.49598	1.82758
H	6.53317	-0.52680	0.44514
C	1.99714	-0.76605	1.14669
C	0.62852	-1.03036	0.79838
C	0.10469	-1.60502	-0.41591
C	-0.37866	-0.78054	1.80242
C	-1.25479	-1.78303	-0.63008
H	0.77325	-1.98197	-1.17803
C	-1.73696	-0.96430	1.57161
H	-0.03239	-0.42849	2.76729
C	-2.20602	-1.42824	0.33729
H	-1.59857	-2.22838	-1.56239
H	-2.45703	-0.74471	2.35854
O	2.26235	-0.46806	2.42553
H	-0.90555	1.06098	0.42430
O	-3.56237	-1.65624	0.11620
C	-4.34686	-0.56858	-0.42872
C	-5.73157	-1.17724	-0.61933
C	-4.40247	0.59667	0.55793
C	-3.77347	-0.10513	-1.76664
H	-5.68089	-2.02227	-1.31304
H	-6.12096	-1.53592	0.33863
H	-6.42544	-0.43372	-1.02272
H	-3.41176	1.03992	0.69266
H	-5.07634	1.37210	0.17843
H	-4.77642	0.25391	1.52850
H	-4.42880	0.65413	-2.20594
H	-2.77958	0.33136	-1.63162
H	-3.70010	-0.94768	-2.46234
O	-1.13420	1.94238	0.08095
C	0.07747	2.68807	-0.09801
C	0.89043	2.06543	-1.23180
C	-0.36498	4.10152	-0.45783
C	0.88604	2.67634	1.19923
H	1.16678	1.04069	-0.96327
H	0.30232	2.05121	-2.15609
H	1.81176	2.63134	-1.41114
H	-0.95763	4.53402	0.35488
H	0.50563	4.74093	-0.63391
H	-0.97615	4.08778	-1.36633
H	1.79709	3.27542	1.08775
H	0.29105	3.10003	2.01607
H	1.18036	1.65198	1.46223

24





37
-808.9229047

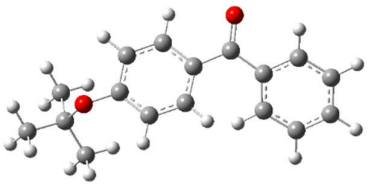
C	-5.45312	-1.52396	0.16393
C	-4.14562	-2.04807	0.18962
C	-3.02194	-1.23778	0.14052
C	-3.10816	0.20324	0.04794
C	-4.46341	0.70752	0.11245
C	-5.57214	-0.12124	0.14823
H	-6.32499	-2.17024	0.19022
H	-4.00160	-3.12561	0.27037
H	-2.05665	-1.71947	0.24091
H	-4.58352	1.78516	0.11932
H	-6.56393	0.33148	0.17049
C	-2.04132	1.15131	0.00044
C	-0.66494	0.79507	-0.23020
C	-0.15238	-0.44020	-0.76060
C	0.34119	1.80300	-0.02021
C	1.20558	-0.66735	-0.94157
H	-0.83434	-1.20969	-1.10126
C	1.69674	1.55944	-0.19495
H	-0.00109	2.78330	0.29223
C	2.15884	0.30900	-0.62223
H	1.54398	-1.61360	-1.36116
H	2.42273	2.34918	-0.00618
O	-2.32538	2.44767	0.19524
O	3.51722	0.08234	-0.84345
C	4.29390	-0.46312	0.24760
C	5.70195	-0.57785	-0.32562
C	4.28068	0.48492	1.44587
C	3.76810	-1.84055	0.64863
H	5.70008	-1.23520	-1.20055
H	6.06596	0.40772	-0.63187
H	6.38874	-0.98882	0.42031
H	3.27107	0.58597	1.85373
H	4.93602	0.09939	2.23356
H	4.63670	1.47685	1.14915
H	4.41575	-2.27786	1.41535
H	2.75367	-1.77041	1.05073
H	3.75300	-2.50849	-0.21887

Single Point Radical Anion
using Optimised Geometry
24

37
-808.8795541

C	-5.45312300	-1.52395700	0.16393200
C	-4.14562400	-2.04807000	0.18961700
C	-3.02194000	-1.23777500	0.14052100
C	-3.10815800	0.20323700	0.04794100
C	-4.46341400	0.70752300	0.11245500
C	-5.57214000	-0.12123600	0.14823300
H	-6.32499400	-2.17024000	0.19022300
H	-4.00160300	-3.12561300	0.27037100
H	-2.05664600	-1.71946800	0.24090800
H	-4.58352000	1.78515800	0.11932000
H	-6.56393000	0.33148000	0.17049200
C	-2.04131600	1.15130600	0.00043700
C	-0.66493800	0.79507300	-0.23020100
C	-0.15237800	-0.44020200	-0.76060000
C	0.34119000	1.80300400	-0.02020800
C	1.20558300	-0.66735400	-0.94156900
H	-0.83434000	-1.20969200	-1.10125900
C	1.69674500	1.55943900	-0.19494600
H	-0.00108600	2.78330500	0.29223300
C	2.15883800	0.30899900	-0.62222600
H	1.54397900	-1.61360500	-1.36116000
H	2.42272800	2.34918400	-0.00618200
O	-2.32537900	2.44767000	0.19524300
O	3.51721500	0.08233500	-0.84344800
C	4.29390000	-0.46311900	0.24759600
C	5.70195200	-0.57784900	-0.32562000
C	4.28068300	0.48492200	1.44586800
C	3.76809600	-1.84055500	0.64863000
H	5.70008300	-1.23520100	-1.20055400
H	6.06595800	0.40772000	-0.63186500
H	6.38874400	-0.98882400	0.42031400
H	3.27106600	0.58597100	1.85373100
H	4.93602000	0.09939500	2.23355800
H	4.63669800	1.47685100	1.14915000
H	4.41574600	-2.27786000	1.41534800
H	2.75367300	-1.77041300	1.05072700
H	3.75300200	-2.50848700	-0.21887200

25



37
-808.8876265

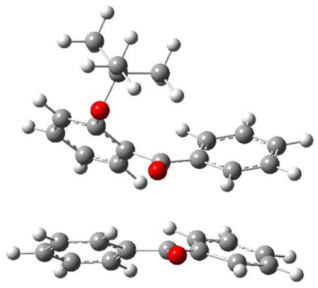
C	-5.30743	-1.62581	0.17207
C	-3.99279	-2.06245	0.37983
C	-2.92481	-1.17485	0.32528
C	-3.12072	0.20545	0.05412
C	-4.46551	0.63123	-0.11331
C	-5.52643	-0.26318	-0.06608
H	-6.13713	-2.32466	0.21071
H	-3.79923	-3.10925	0.60150
H	-1.92848	-1.54746	0.53913
H	-4.64224	1.68750	-0.28737
H	-6.53949	0.10311	-0.21541
C	-2.06691	1.21913	0.02667
C	-0.65164	0.87227	-0.17069
C	-0.18503	-0.28980	-0.83136
C	0.33238	1.80812	0.23030
C	1.17155	-0.52334	-1.02520
H	-0.89504	-0.99982	-1.24217
C	1.68896	1.57348	0.04174
H	-0.00343	2.73013	0.69363
C	2.12369	0.39390	-0.56941
H	1.50662	-1.41146	-1.55445
H	2.42668	2.30495	0.36151
O	-2.38155	2.45535	0.18532
O	3.46756	0.18562	-0.81997
C	4.25410	-0.50302	0.18762
C	5.64306	-0.58312	-0.43291
C	4.29070	0.30567	1.48268
C	3.69597	-1.90172	0.44023
H	5.60734	-1.14729	-1.36953
H	6.02074	0.42176	-0.64399
H	6.33625	-1.08139	0.25094
H	3.29670	0.37913	1.93278
H	4.95647	-0.18061	2.20230
H	4.66471	1.31627	1.29044
H	4.34861	-2.43833	1.13560
H	2.69440	-1.85476	0.87740
H	3.64378	-2.46727	-0.49542

Single Point Dianion using
Optimised Geometry **25**

37
-808.9145670

C	-5.30742700	-1.62580700	0.17206800
C	-3.99279400	-2.06244900	0.37983400
C	-2.92480900	-1.17485200	0.32528100
C	-3.12072300	0.20545400	0.05411800
C	-4.46550700	0.63122500	-0.11330900
C	-5.52643200	-0.26318000	-0.06607900
H	-6.13712800	-2.32465700	0.21071100
H	-3.79923400	-3.10924700	0.60150300
H	-1.92847900	-1.54745800	0.53912700
H	-4.64224300	1.68750100	-0.28737300
H	-6.53948900	0.10310600	-0.21541000
C	-2.06691500	1.21912500	0.02667200
C	-0.65163700	0.87226800	-0.17069000
C	-0.18503000	-0.28979700	-0.83135800
C	0.33237800	1.80811600	0.23030000
C	1.17154600	-0.52334500	-1.02519600
H	-0.89503900	-0.99982400	-1.24217300
C	1.68895600	1.57348300	0.04174400
H	-0.00342600	2.73012600	0.69363400
C	2.12368600	0.39389800	-0.56941200
H	1.50662200	-1.41145600	-1.55444600
H	2.42668500	2.30494800	0.36151300
O	-2.38155300	2.45535000	0.18532500
O	3.46755600	0.18561600	-0.81997300
C	4.25409700	-0.50301600	0.18762400
C	5.64306000	-0.58312200	-0.43290800
C	4.29069900	0.30567500	1.48267700
C	3.69596900	-1.90172300	0.44023200
H	5.60733700	-1.14728500	-1.36953300
H	6.02073500	0.42176300	-0.64399300
H	6.33625400	-1.08139100	0.25094000
H	3.29669800	0.37913000	1.93278400
H	4.95646900	-0.18060800	2.20229700
H	4.66471100	1.31626600	1.29044100
H	4.34861500	-2.43833300	1.13560500
H	2.69439500	-1.85475600	0.87739500
H	3.64377700	-2.46727400	-0.49542400

Singlet Complex between **46** and **17** (no counterions)



61
-1385.3661018

C	2.10253	-3.76954	0.78342
C	1.39720	-3.00080	1.72273
C	0.58367	-1.94848	1.32329
C	0.42428	-1.61693	-0.05019
C	1.14512	-2.40603	-0.98594
C	1.96408	-3.44836	-0.57520
H	2.72950	-4.59784	1.09980
H	1.47877	-3.23342	2.78256
H	0.02522	-1.40803	2.08153
H	1.03270	-2.16232	-2.03662
H	2.50757	-4.02313	-1.32283
C	-0.54220	-0.64943	-0.56822
C	-1.33043	0.18656	0.39015
C	-0.69362	0.90351	1.41773
C	-2.72927	0.35487	0.27123
C	-1.37441	1.77149	2.26102
H	0.38173	0.79607	1.51077
C	-3.41303	1.25139	1.09826
C	-2.74772	1.96717	2.09105
H	-0.82826	2.32412	3.02049
H	-4.48245	1.36991	0.94749
H	-3.29392	2.66292	2.72134
O	-0.85046	-0.63462	-1.78819
O	-3.47182	-0.30979	-0.68268
C	-4.02768	-1.60594	-0.34906
C	-4.73116	-2.03086	-1.63259
C	-2.93220	-2.60635	0.01316
C	-5.03665	-1.48084	0.79314
H	-5.50158	-1.30159	-1.90179
H	-4.00888	-2.09630	-2.45131
H	-5.20366	-3.00871	-1.50055
H	-2.39539	-2.30264	0.91785
H	-3.38481	-3.58650	0.19637
H	-2.20668	-2.68921	-0.80039
H	-5.51561	-2.44970	0.96600
H	-4.54850	-1.17105	1.72186
H	-5.81166	-0.74873	0.54353
C	5.07151	-0.86219	0.95012
C	4.13341	-0.07029	1.63389
C	3.09671	0.56066	0.95986
C	2.94245	0.45461	-0.45052
C	3.88111	-0.38842	-1.11248
C	4.91927	-1.01292	-0.43371
H	5.88549	-1.34689	1.48111
H	4.20139	0.03735	2.71461
H	2.37985	1.12279	1.54733
H	3.76668	-0.51360	-2.18370
H	5.61832	-1.63657	-0.98826
C	1.90285	1.06991	-1.27272
C	1.13047	2.23977	-0.82753
C	1.50163	3.12910	0.21229
C	-0.02384	2.59422	-1.57454

C	0.74713	4.26017	0.51103
H	2.42179	2.96797	0.76281
C	-0.78115	3.71489	-1.26184
H	-0.31533	1.92808	-2.37993
C	-0.41194	4.56615	-0.20943
H	1.07918	4.92107	1.30922
H	-1.67474	3.93398	-1.84338
H	-0.99893	5.44877	0.02744
O	1.77896	0.69448	-2.49333

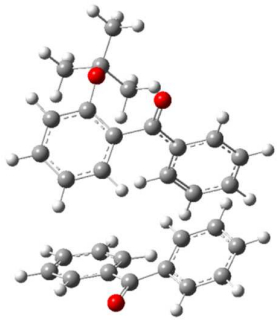
Single Point Triplet, Using Singlet Complex (of **46** and **17**, no counterions) Optimised Geometry

61
-1385.3661697

C	2.10253	-3.76954	0.78342
C	1.39720	-3.00080	1.72273
C	0.58367	-1.94848	1.32329
C	0.42428	-1.61693	-0.05019
C	1.14512	-2.40603	-0.98594
C	1.96408	-3.44836	-0.57520
H	2.72950	-4.59784	1.09980
H	1.47877	-3.23342	2.78256
H	0.02522	-1.40803	2.08153
H	1.03270	-2.16232	-2.03662
H	2.50757	-4.02313	-1.32283
C	-0.54220	-0.64943	-0.56822
C	-1.33043	0.18656	0.39015
C	-0.69362	0.90351	1.41773
C	-2.72927	0.35487	0.27123
C	-1.37441	1.77149	2.26102
H	0.38173	0.79607	1.51077
C	-3.41303	1.25139	1.09826
C	-2.74772	1.96717	2.09105
H	-0.82826	2.32412	3.02049
H	-4.48245	1.36991	0.94749
H	-3.29392	2.66292	2.72134
O	-0.85046	-0.63462	-1.78819
O	-3.47182	-0.30979	-0.68268
C	-4.02768	-1.60594	-0.34906
C	-4.73116	-2.03086	-1.63259
C	-2.93220	-2.60635	0.01316
C	-5.03665	-1.48084	0.79314
H	-5.50158	-1.30159	-1.90179
H	-4.00888	-2.09630	-2.45131
H	-5.20366	-3.00871	-1.50055
H	-2.39539	-2.30264	0.91785
H	-3.38481	-3.58650	0.19637
H	-2.20668	-2.68921	-0.80039
H	-5.51561	-2.44970	0.96600
H	-4.54850	-1.17105	1.72186
H	-5.81166	-0.74873	0.54353
C	5.07151	-0.86219	0.95012
C	4.13341	-0.07029	1.63389
C	3.09671	0.56066	0.95986
C	2.94245	0.45461	-0.45052
C	3.88111	-0.38842	-1.11248
C	4.91927	-1.01292	-0.43371
H	5.88549	-1.34689	1.48111
H	4.20139	0.03735	2.71461
H	2.37985	1.12279	1.54733
H	3.76668	-0.51360	-2.18370
H	5.61832	-1.63657	-0.98826
C	1.90285	1.06991	-1.27272
C	1.13047	2.23977	-0.82753
C	1.50163	3.12910	0.21229
C	-0.02384	2.59422	-1.57454
C	0.74713	4.26017	0.51103
H	2.42179	2.96797	0.76281
C	-0.78115	3.71489	-1.26184
H	-0.31533	1.92808	-2.37993
C	-0.41194	4.56615	-0.20943
H	1.07918	4.92107	1.30922
H	-1.67474	3.93398	-1.84338
H	-0.99893	5.44877	0.02744

O	1.77896	0.69448	-2.49333

Triplet Complex between **46** and **17** (no counterions)



61
-1385.3909734

C	-0.32054	3.28662	2.37139
C	-0.21122	1.88413	2.36881
C	0.39681	1.21017	1.32235
C	0.92311	1.90722	0.19123
C	0.82347	3.33348	0.22639
C	0.21881	3.99367	1.28554
H	-0.80278	3.80620	3.19335
H	-0.61023	1.30982	3.20335
H	0.46433	0.12627	1.36772
H	1.23526	3.89132	-0.60891
H	0.15728	5.08017	1.26766
C	1.60460	1.27876	-0.91153
C	1.68977	-0.21477	-0.97196
C	0.52507	-1.00170	-0.93673
C	2.91599	-0.89452	-1.13417
C	0.55465	-2.38759	-1.06306
H	-0.43464	-0.50595	-0.81708
C	2.94817	-2.28208	-1.29677
C	1.77543	-3.03493	-1.25676
H	-0.37480	-2.94828	-1.01394
H	3.91111	-2.76044	-1.45031
H	1.81777	-4.11354	-1.37701
O	2.15890	1.96505	-1.83958
O	4.10772	-0.20402	-1.19966
C	4.87802	-0.01866	0.01465
C	6.04037	0.85665	-0.43789
C	4.05891	0.69584	1.08674
C	5.39105	-1.35991	0.53914
H	6.61915	0.34636	-1.21391
H	5.65930	1.79716	-0.84634
H	6.70095	1.07858	0.40540
H	3.18492	0.10576	1.38202
H	4.68180	0.85172	1.97370
H	3.70637	1.66420	0.72194
H	6.05863	-1.18935	1.38962
H	4.56742	-1.99607	0.87595
H	5.94849	-1.88855	-0.24073
C	-4.01173	3.08433	-1.04743
C	-2.85430	2.49392	-0.52758
C	-2.79134	1.12157	-0.31013
C	-3.88740	0.27074	-0.59621
C	-5.03641	0.88767	-1.15233
C	-5.09821	2.26017	-1.36384
H	-4.06107	4.15610	-1.21480
H	-1.97805	3.09540	-0.29241
H	-1.85756	0.71881	0.06180
H	-5.87739	0.25218	-1.40981
H	-6.00332	2.69515	-1.78153
C	-3.89504	-1.19199	-0.44141

C	-2.95486	-1.90242	0.43006
C	-2.21782	-1.32408	1.49677
C	-2.82561	-3.30787	0.26513
C	-1.37371	-2.08785	2.29391
H	-2.32699	-0.27031	1.72871
C	-1.98050	-4.06436	1.06663
H	-3.40515	-3.77845	-0.52241
C	-1.23025	-3.46490	2.08523
H	-0.82706	-1.60059	3.09874
H	-1.89836	-5.13515	0.89356
H	-0.56497	-4.05538	2.70773
O	-4.76940	-1.87314	-1.09315

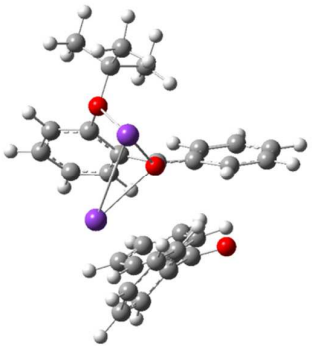
Single Point Singlet, Using Triplet Complex (of **46** and **17**, no counterions) Optimised Geometry

61
-1385.3505837

C	-0.32054	3.28662	2.37139
C	-0.21122	1.88413	2.36881
C	0.39681	1.21017	1.32235
C	0.92311	1.90722	0.19123
C	0.82347	3.33348	0.22639
C	0.21881	3.99367	1.28554
H	-0.80278	3.80620	3.19335
H	-0.61023	1.30982	3.20335
H	0.46433	0.12627	1.36772
H	1.23526	3.89132	-0.60891
H	0.15728	5.08017	1.26766
C	1.60460	1.27876	-0.91153
C	1.68977	-0.21477	-0.97196
C	0.52507	-1.00170	-0.93673
C	2.91599	-0.89452	-1.13417
C	0.55465	-2.38759	-1.06306
H	-0.43464	-0.50595	-0.81708
C	2.94817	-2.28208	-1.29677
C	1.77543	-3.03493	-1.25676
H	-0.37480	-2.94828	-1.01394
H	3.91111	-2.76044	-1.45031
H	1.81777	-4.11354	-1.37701
O	2.15890	1.96505	-1.83958
O	4.10772	-0.20402	-1.19966
C	4.87802	-0.01866	0.01465
C	6.04037	0.85665	-0.43789
C	4.05891	0.69584	1.08674
C	5.39105	-1.35991	0.53914
H	6.61915	0.34636	-1.21391
H	5.65930	1.79716	-0.84634
H	6.70095	1.07858	0.40540
H	3.18492	0.10576	1.38202
H	4.68180	0.85172	1.97370
H	3.70637	1.66420	0.72194
H	6.05863	-1.18935	1.38962
H	4.56742	-1.99607	0.87595
H	5.94849	-1.88855	-0.24073
C	-4.01173	3.08433	-1.04743
C	-2.85430	2.49392	-0.52758
C	-2.79134	1.12157	-0.31013
C	-3.88740	0.27074	-0.59621
C	-5.03641	0.88767	-1.15233
C	-5.09821	2.26017	-1.36384
H	-4.06107	4.15610	-1.21480
H	-1.97805	3.09540	-0.29241
H	-1.85756	0.71881	0.06180
H	-5.87739	0.25218	-1.40981
H	-6.00332	2.69515	-1.78153
C	-3.89504	-1.19199	-0.44141
C	-2.95486	-1.90242	0.43006
C	-2.21782	-1.32408	1.49677
C	-2.82561	-3.30787	0.26513
C	-1.37371	-2.08785	2.29391
H	-2.32699	-0.27031	1.72871
C	-1.98050	-4.06436	1.06663
H	-3.40515	-3.77845	-0.52241
C	-1.23025	-3.46490	2.08523
H	-0.82706	-1.60059	3.09874
H	-1.89836	-5.13515	0.89356
H	-0.56497	-4.05538	2.70773

O	-4.76940	-1.87314	-1.09315

Singlet Complex between **46** and **17** (counterions)



63
-2585.0745194

C	0.84795900	-3.29825300	-3.26774500
C	0.53231300	-3.64211700	-1.94275600
C	0.11927600	-2.68372500	-1.03084300
C	-0.00776500	-1.30897600	-1.39430500
C	0.32516300	-0.98573300	-2.74259900
C	0.72775200	-1.95809900	-3.64906200
H	1.16959900	-4.05471600	-3.97717700
H	0.60425900	-4.67898600	-1.62069300
H	-0.15424200	-3.00602300	-0.03094700
H	0.22719500	0.04712500	-3.05826500
H	0.96615300	-1.66527300	-4.66968300
C	-0.54563700	-0.28369100	-0.54555900
C	-0.98688900	-0.57553800	0.82709100
C	-0.16853800	-1.24201200	1.77087800
C	-2.21947800	-0.05441700	1.33195900
C	-0.47472000	-1.27824100	3.12826300
H	0.76111100	-1.67785400	1.42422300
C	-2.49964300	-0.05477600	2.69481700
C	-1.62647700	-0.65061100	3.61227400
H	0.21376800	-1.76853400	3.81188300
H	-3.43550500	0.38649800	3.02764800
H	-1.85587200	-0.64080600	4.67279800
O	-0.84456000	0.90260600	-1.02369300
O	-3.19201100	0.43687900	0.46729900
C	-4.18303800	-0.52993500	-0.00412500
C	-5.00347800	0.24401300	-1.02947400
C	-3.50988300	-1.72790700	-0.66849900
C	-5.08052700	-0.97928000	1.14740400
H	-5.38824400	1.17301500	-0.59471500
H	-4.40635000	0.46540700	-1.92032700
H	-5.85773000	-0.35529500	-1.35489500
H	-2.92351100	-2.30722000	0.05108600
H	-4.27879700	-2.38205200	-1.09141600
H	-2.83795300	-1.40058700	-1.46728600
H	-5.87329200	-1.62500600	0.75809400
H	-4.51766300	-1.54588500	1.89326600
H	-5.54358600	-0.11515600	1.63472000
C	3.16934700	-2.79780400	2.26519700
C	3.10285200	-1.45203100	2.64281700
C	2.98854400	-0.45040400	1.68605400
C	2.96587100	-0.75369800	0.30232100
C	3.03834200	-2.12033500	-0.06020400
C	3.12931000	-3.11733500	0.90312700
H	3.25026000	-3.57848500	3.01522000
H	3.11491400	-1.18063300	3.69511400
H	2.89779000	0.57007200	2.03803300
H	2.98918600	-2.37117300	-1.11418800
H	3.16159200	-4.15796500	0.58967900
C	2.83845900	0.22276500	-0.79799400
C	2.64539800	1.67569400	-0.54236800

C	3.30126700	2.41416400	0.46651300
C	1.78955400	2.37505400	-1.41902300
C	3.05268000	3.77460200	0.63446500
H	4.04192200	1.93545500	1.09773800
C	1.53549900	3.73295900	-1.24081900
H	1.30154100	1.81714200	-2.20891500
C	2.15176300	4.44145400	-0.20409400
H	3.57739200	4.32109100	1.41255400
H	0.85278400	4.24369700	-1.91486500
H	1.95604900	5.50020000	-0.06701800
O	2.88215200	-0.15624000	-1.98904300
K	-2.70145800	2.54503200	-1.26602500
K	0.25361200	2.03240300	1.21810700

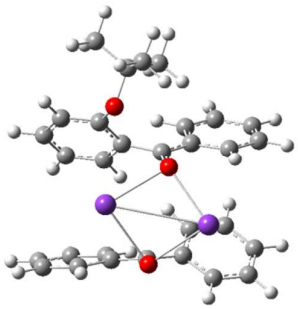
Single Point Triplet, Using Singlet Complex (of **46** and **17**, counterions) Optimised Geometry

63
-2585.0749126

C	0.84795900	-3.29825300	-3.26774500
C	0.53231300	-3.64211700	-1.94275600
C	0.11927600	-2.68372500	-1.03084300
C	-0.00776500	-1.30897600	-1.39430500
C	0.32516300	-0.98573300	-2.74259900
C	0.72775200	-1.95809900	-3.64906200
H	1.16959900	-4.05471600	-3.97717700
H	0.60425900	-4.67898600	-1.62069300
H	-0.15424200	-3.00602300	-0.03094700
H	0.22719500	0.04712500	-3.05826500
H	0.96615300	-1.66527300	-4.66968300
C	-0.54563700	-0.28369100	-0.54555900
C	-0.98688900	-0.57553800	0.82709100
C	-0.16853800	-1.24201200	1.77087800
C	-2.21947800	-0.05441700	1.33195900
C	-0.47472000	-1.27824100	3.12826300
H	0.76111100	-1.67785400	1.42422300
C	-2.49964300	-0.05477600	2.69481700
C	-1.62647700	-0.65061100	3.61227400
H	0.21376800	-1.76853400	3.81188300
H	-3.43550500	0.38649800	3.02764800
H	-1.85587200	-0.64080600	4.67279800
O	-0.84456000	0.90260600	-1.02369300
O	-3.19201100	0.43687900	0.46729900
C	-4.18303800	-0.52993500	-0.00412500
C	-5.00347800	0.24401300	-1.02947400
C	-3.50988300	-1.72790700	-0.66849900
C	-5.08052700	-0.97928000	1.14740400
H	-5.38824400	1.17301500	-0.59471500
H	-4.40635000	0.46540700	-1.92032700
H	-5.85773000	-0.35529500	-1.35489500
H	-2.92351100	-2.30722000	0.05108600
H	-4.27879700	-2.38205200	-1.09141600
H	-2.83795300	-1.40058700	-1.46728600
H	-5.87329200	-1.62500600	0.75809400
H	-4.51766300	-1.54588500	1.89326600
H	-5.54358600	-0.11515600	1.63472000
C	3.16934700	-2.79780400	2.26519700
C	3.10285200	-1.45203100	2.64281700
C	2.98854400	-0.45040400	1.68605400
C	2.96587100	-0.75369800	0.30232100
C	3.03834200	-2.12033500	-0.06020400
C	3.12931000	-3.11733500	0.90312700
H	3.25026000	-3.57848500	3.01522000
H	3.11491400	-1.18063300	3.69511400
H	2.89779000	0.57007200	2.03803300
H	2.98918600	-2.37117300	-1.11418800
H	3.16159200	-4.15796500	0.58967900
C	2.83845900	0.22276500	-0.79799400
C	2.64539800	1.67569400	-0.54236800
C	3.30126700	2.41416400	0.46651300
C	1.78955400	2.37505400	-1.41902300
C	3.05268000	3.77460200	0.63446500
H	4.04192200	1.93545500	1.09773800
C	1.53549900	3.73295900	-1.24081900
H	1.30154100	1.81714200	-2.20891500
C	2.15176300	4.44145400	-0.20409400
H	3.57739200	4.32109100	1.41255400
H	0.85278400	4.24369700	-1.91486500
H	1.95604900	5.50020000	-0.06701800

O	2.88215200	-0.15624000	-1.98904300
K	-2.70145800	2.54503200	-1.26602500
K	0.25361200	2.03240300	1.21810700

Triplet Complex between **46** and **17** (counterions)



63
-2585.1100546

C	-0.00789200	4.27420500	-2.22961300
C	-0.47176300	3.11282900	-2.86804400
C	-0.78548100	1.97159500	-2.14556000
C	-0.62693800	1.92397100	-0.72995600
C	-0.18540000	3.12361700	-0.10134000
C	0.11424600	4.26231900	-0.83471300
H	0.23528200	5.16331100	-2.80221100
H	-0.59710400	3.10501400	-3.94806900
H	-1.16137300	1.10048800	-2.67455400
H	-0.10962900	3.14464000	0.98085800
H	0.44939300	5.15675600	-0.31433600
C	-0.92076400	0.77163700	0.07370600
C	-1.48707200	-0.47045300	-0.53914300
C	-0.77228900	-1.19743500	-1.50802300
C	-2.69427300	-1.03677300	-0.07018400
C	-1.21140100	-2.42956500	-1.98644200
H	0.17403500	-0.80086200	-1.86441600
C	-3.12466100	-2.28436800	-0.53209900
C	-2.39211200	-2.98252000	-1.48975500
H	-0.61287700	-2.96710900	-2.71591300
H	-4.04065000	-2.69889900	-0.12249200
H	-2.73678800	-3.95183100	-1.83590400
O	-0.72149500	0.76699900	1.35523900
O	-3.41730900	-0.42351200	0.92619800
C	-4.52085800	0.45417500	0.56212000
C	-5.03655400	0.94439600	1.90884200
C	-4.02540900	1.62338800	-0.28330800
C	-5.60623800	-0.32487400	-0.17791900
H	-5.37672100	0.09989900	2.51558000
H	-4.23999700	1.46642300	2.44680200
H	-5.87392700	1.63306000	1.76536600
H	-3.57859000	1.27665800	-1.22107700
H	-4.86918800	2.27623100	-0.52795500
H	-3.27235700	2.20223000	0.25870200
H	-6.46930600	0.32604600	-0.34659300
H	-5.25277500	-0.67675200	-1.15142000
H	-5.93200800	-1.18661700	0.41302000
C	3.87552600	2.95228000	-0.53037400
C	2.97627800	2.22818400	-1.31470000
C	2.54826300	0.96581800	-0.91544200
C	2.99773900	0.38586400	0.28520100
C	3.89315200	1.13945700	1.07325900
C	4.32998200	2.39922700	0.66964400
H	4.20395700	3.93957100	-0.84021700
H	2.56917700	2.66229800	-2.22398700
H	1.80314500	0.45493500	-1.51460600
H	4.24950100	0.71096100	2.00709500
H	5.02966300	2.95054900	1.29187100
C	2.51863400	-0.91761600	0.81032900
C	2.41340700	-2.09702700	-0.02462300
C	2.69141400	-2.13652100	-1.42175200

C	2.06698200	-3.34034400	0.58085100
C	2.54477000	-3.30314000	-2.15525400
H	3.04108100	-1.24534000	-1.93045400
C	1.92364400	-4.50352600	-0.16586800
H	1.96273900	-3.37889800	1.66148900
C	2.13764800	-4.50056600	-1.54746300
H	2.76046000	-3.28549700	-3.22059400
H	1.65652500	-5.42877700	0.33877100
H	2.02018500	-5.40784200	-2.13101800
O	2.28697900	-0.99744700	2.08591200
K	1.33593900	1.43415900	2.77617500
K	-0.29345100	-1.82670600	1.87715200

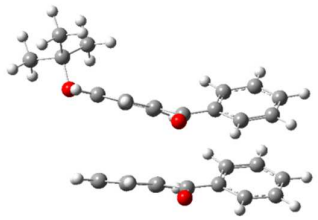
Single Point Singlet, Using Triplet Complex (of **46** and **17**, counterions) Optimised Geometry

63
-2585.0741665

C	0.00789200	-4.27420500	-2.22961300
C	0.47176300	-3.11282900	-2.86804400
C	0.78548100	-1.97159500	-2.14556000
C	0.62693800	-1.92397100	-0.72995600
C	0.18540000	-3.12361700	-0.10134000
C	-0.11424600	-4.26231900	-0.83471300
H	-0.23528200	-5.16331100	-2.80221100
H	0.59710400	-3.10501400	-3.94806900
H	1.16137300	-1.10048800	-2.67455400
H	0.10962900	-3.14464000	0.98085800
H	-0.44939300	-5.15675600	-0.31433600
C	0.92076400	-0.77163700	0.07370600
C	1.48707200	0.47045300	-0.53914300
C	0.77228900	1.19743500	-1.50802300
C	2.69427300	1.03677300	-0.07018400
C	1.21140100	2.42956500	-1.98644200
H	-0.17403500	0.80086200	-1.86441600
C	3.12466100	2.28436800	-0.53209900
C	2.39211200	2.98252000	-1.48975500
H	0.61287700	2.96710900	-2.71591300
H	4.04065000	2.69889900	-0.12249200
H	2.73678800	3.95183100	-1.83590400
O	0.72149500	-0.76699900	1.35523900
O	3.41730900	0.42351200	0.92619800
C	4.52085800	-0.45417500	0.56212000
C	5.03655400	-0.94439600	1.90884200
C	4.02540900	-1.62338800	-0.28330800
C	5.60623800	0.32487400	-0.17791900
H	5.37672100	-0.09989900	2.51558000
H	4.23999700	-1.46642300	2.44680200
H	5.87392700	-1.63306000	1.76536600
H	3.57859000	-1.27665800	-1.22107700
H	4.86918800	-2.27623100	-0.52795500
H	3.27235700	-2.20223000	0.25870200
H	6.46930600	-0.32604600	-0.34659300
H	5.25277500	0.67675200	-1.15142000
H	5.93200800	1.18661700	0.41302000
C	-3.87552600	-2.95228000	-0.53037400
C	-2.97627800	-2.22818400	-1.31470000
C	-2.54826300	-0.96581800	-0.91544200
C	-2.99773900	-0.38586400	0.28520100
C	-3.89315200	-1.13945700	1.07325900
C	-4.32998200	-2.39922700	0.66964400
H	-4.20395700	-3.93957100	-0.84021700
H	-2.56917700	-2.66229800	-2.22398700
H	-1.80314500	-0.45493500	-1.51460600
H	-4.24950100	-0.71096100	2.00709500
H	-5.02966300	-2.95054900	1.29187100
C	-2.51863400	0.91761600	0.81032900
C	-2.41340700	2.09702700	-0.02462300
C	-2.69141400	2.13652100	-1.42175200
C	-2.06698200	3.34034400	0.58085100
C	-2.54477000	3.30314000	-2.15525400
H	-3.04108100	1.24534000	-1.93045400
C	-1.92364400	4.50352600	-0.16586800
H	-1.96273900	3.37889800	1.66148900
C	-2.13764800	4.50056600	-1.54746300
H	-2.76046000	3.28549700	-3.22059400
H	-1.65652500	5.42877700	0.33877100
H	-2.02018500	5.40784200	-2.13101800

O	-2.28697900	0.99744700	2.08591200
K	-1.33593900	-1.43415900	2.77617500
K	0.29345100	1.82670600	1.87715200

Singlet Complex between **24** and **17** (no counterions)



61
-1385.3732444

C	-5.10017	0.10807	-1.78301
C	-3.76676	0.02184	-2.21120
C	-2.73692	0.57166	-1.46555
C	-2.98117	1.25385	-0.24409
C	-4.33016	1.27894	0.19597
C	-5.36184	0.73713	-0.56205
H	-5.90346	-0.32088	-2.37523
H	-3.52580	-0.52089	-3.12278
H	-1.71899	0.41086	-1.80230
H	-4.53687	1.75243	1.15040
H	-6.38324	0.79465	-0.19061
C	-1.96905	1.85084	0.63146
C	-0.64410	2.26220	0.14329
C	-0.28313	2.45291	-1.21365
C	0.33815	2.61285	1.10695
C	0.97589	2.92314	-1.57549
H	-1.01203	2.28629	-1.99862
C	1.59841	3.06167	0.73998
H	0.07742	2.50569	2.15480
C	1.94118	3.22136	-0.60815
H	1.20241	3.06709	-2.62992
H	2.33019	3.28548	1.51370
H	2.92740	3.57442	-0.89550
O	-2.29962	2.16431	1.82861
C	-3.90161	-3.09579	-0.56226
C	-2.60549	-3.07430	-1.08985
C	-1.58218	-2.37755	-0.45570
C	-1.80414	-1.67092	0.75355
C	-3.11929	-1.73718	1.28822
C	-4.13827	-2.41630	0.63972
H	-4.69982	-3.63426	-1.06498
H	-2.38472	-3.61527	-2.00771
H	-0.58568	-2.43308	-0.87966
H	-3.30901	-1.22314	2.22497
H	-5.13775	-2.41244	1.07023
C	-0.77718	-0.99086	1.54770
C	0.57383	-0.72137	1.01895
C	0.89696	-0.52239	-0.34298
C	1.62604	-0.55506	1.94589
C	2.19377	-0.25619	-0.75409
H	0.10644	-0.50421	-1.08494
C	2.93156	-0.29645	1.53748
H	1.39098	-0.64142	3.00193
C	3.23064	-0.16716	0.18172
H	2.41038	-0.06828	-1.80251
H	3.72869	-0.18154	2.26794
O	-0.99641	-0.77195	2.78427
O	4.51887	0.14295	-0.22581
C	5.41036	-0.95125	-0.55668
C	6.71110	-0.25486	-0.93742
C	5.62259	-1.85762	0.65446
C	4.86605	-1.75178	-1.73842
H	6.54752	0.41004	-1.79080
H	7.08034	0.33965	-0.09642
H	7.47270	-0.99227	-1.20752

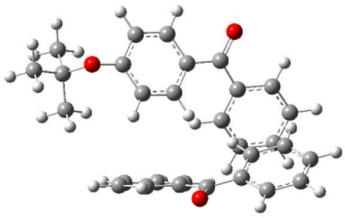
H	4.69266	-2.35546	0.94392
H	6.36369	-2.62667	0.41511
H	5.98640	-1.27568	1.50731
H	5.59255	-2.51558	-2.03318
H	3.92875	-2.25181	-1.47912
H	4.68559	-1.09284	-2.59372

Single Point Triplet, Using Singlet Complex (of **24** and **17**, no counterions) Optimised Geometry

61
-1385.3745736

C	-5.10016900	0.10807000	-1.78300600
C	-3.76676100	0.02184000	-2.21120200
C	-2.73691900	0.57166000	-1.46554700
C	-2.98116900	1.25384800	-0.24408700
C	-4.33016200	1.27893900	0.19597200
C	-5.36183500	0.73712800	-0.56204600
H	-5.90346300	-0.32088200	-2.37522800
H	-3.52579900	-0.52089200	-3.12278300
H	-1.71898600	0.41086400	-1.80230200
H	-4.53687400	1.75243200	1.15039700
H	-6.38323800	0.79464800	-0.19061300
C	-1.96905300	1.85083600	0.63146300
C	-0.64409600	2.26219800	0.14329100
C	-0.28312700	2.45290600	-1.21364600
C	0.33815300	2.61285400	1.10695300
C	0.97589500	2.92314400	-1.57549000
H	-1.01203300	2.28629400	-1.99861500
C	1.59841000	3.06166700	0.73997900
H	0.07741700	2.50569000	2.15479900
C	1.94117600	3.22136300	-0.60815100
H	1.20240600	3.06709200	-2.62991500
H	2.33018500	3.28548500	1.51369600
H	2.92739700	3.57442400	-0.89550200
O	-2.29962500	2.16431100	1.82861300
C	-3.90160600	-3.09578900	-0.56225800
C	-2.60548900	-3.07429500	-1.08984700
C	-1.58218300	-2.37754700	-0.45569800
C	-1.80413600	-1.67091700	0.75355500
C	-3.11928900	-1.73717900	1.28821800
C	-4.13826600	-2.41629700	0.63972500
H	-4.69981900	-3.63426100	-1.06497600
H	-2.38472200	-3.61526900	-2.00770500
H	-0.58567900	-2.43308300	-0.87966200
H	-3.30901400	-1.22313600	2.22497200
H	-5.13774800	-2.41244400	1.07022800
C	-0.77717600	-0.99086500	1.54770300
C	0.57383100	-0.72136800	1.01894900
C	0.89696400	-0.52239300	-0.34297700
C	1.62604300	-0.55505700	1.94588500
C	2.19377100	-0.25618800	-0.75409500
H	0.10643600	-0.50421300	-1.08493700
C	2.93156300	-0.29645200	1.53748100
H	1.39098500	-0.64142000	3.00192700
C	3.23064000	-0.16715900	0.18171800
H	2.41038400	-0.06827600	-1.80251200
H	3.72868800	-0.18154300	2.26794300
O	-0.99641100	-0.77195300	2.78427000
O	4.51886800	0.14294900	-0.22581200
C	5.41035600	-0.95124500	-0.55667900
C	6.71109800	-0.25485600	-0.93742300
C	5.62259100	-1.85761900	0.65445900
C	4.86605000	-1.75178300	-1.73842300
H	6.54751600	0.41004400	-1.79080000
H	7.08034300	0.33965200	-0.09642500
H	7.47270300	-0.99227200	-1.20752200
H	4.69266200	-2.35546400	0.94391600
H	6.36368800	-2.62667300	0.41511200
H	5.98640200	-1.27568000	1.50730600
H	5.59254500	-2.51558200	-2.03318000
H	3.92874600	-2.25181000	-1.47912300

H	4.68559100	-1.09283700	-2.59371600



Triplet Complex between **24** and **17** (no counterions)

61
-1385.3969055

C	-5.18824500	-0.51908900	-1.54246600
C	-4.06327300	0.06402900	-0.94806600
C	-2.96486300	-0.71104200	-0.59161900
C	-2.94200600	-2.11075800	-0.80562900
C	-4.07861300	-2.67333100	-1.43751500
C	-5.17712500	-1.89676100	-1.78860500
H	-6.04617200	0.08651400	-1.81862800
H	-4.02590200	1.13550600	-0.76201700
H	-2.10498400	-0.20374200	-0.16970800
H	-4.07005500	-3.73958700	-1.63950200
H	-6.03542900	-2.36869700	-2.26117900
C	-1.80497300	-2.99490200	-0.50637800
C	-0.78170800	-2.65136000	0.48241000
C	-0.93801500	-1.70815100	1.53194900
C	0.43825100	-3.38012200	0.46460000
C	0.07292500	-1.48052000	2.45830200
H	-1.87148900	-1.16578300	1.64174400
C	1.44197800	-3.14854100	1.39538600
H	0.56712500	-4.12911900	-0.30988100
C	1.28123300	-2.18590700	2.40003500
H	-0.08770600	-0.74601500	3.24501300
H	2.36593400	-3.71982900	1.33745200
H	2.07057700	-1.99781200	3.12156600
O	-1.71610100	-4.11542800	-1.13051400
C	-3.64670400	2.36329500	2.21569500
C	-2.43072100	1.68621800	2.38093100
C	-1.37236400	1.88417400	1.50429300
C	-1.47981400	2.76876200	0.39583400
C	-2.70995300	3.47311600	0.27093900
C	-3.76254000	3.26841800	1.15283500
H	-4.47236100	2.19785300	2.90071200
H	-2.30271000	0.99827300	3.21447400
H	-0.43879200	1.36685600	1.69848000
H	-2.80768700	4.17830800	-0.54804000
H	-4.69182700	3.81549400	1.00916000
C	-0.40755100	3.07059500	-0.54713300
C	0.78378700	2.21087800	-0.68046100
C	0.82183600	0.82805900	-0.38847700
C	1.96297900	2.77354900	-1.22190300
C	1.97271500	0.06945600	-0.56993800
H	-0.06762500	0.31341900	-0.04424300
C	3.11819900	2.02057300	-1.39985700
H	1.94670700	3.82291900	-1.49825400
C	3.13957000	0.66598100	-1.05621300
H	1.95967700	-0.99405300	-0.34086500
H	4.01798500	2.47295300	-1.80916100
O	-0.48044700	4.13198500	-1.26896900
O	4.27575900	-0.08917000	-1.28713500
C	5.21309700	-0.26131100	-0.19241000
C	6.32828300	-1.10129900	-0.80256600
C	5.75037600	1.09295200	0.26696400
C	4.55534700	-1.00388800	0.96817900
H	5.93079600	-2.05784400	-1.15455200

H	6.77742800	-0.57569800	-1.65058900
H	7.10634900	-1.29660500	-0.05892500
H	4.95601000	1.70797600	0.69990800
H	6.52185500	0.94521000	1.02891600
H	6.19184300	1.63405000	-0.57606800
H	5.30007200	-1.20540200	1.74486200
H	3.74623500	-0.41663900	1.41183700
H	4.13783100	-1.95604400	0.62573800

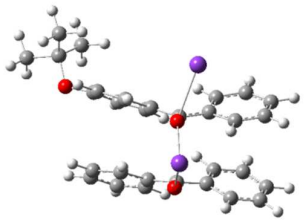
Single Point Singlet, Using Triplet Complex (of **24** and **17**, no counterions) Optimised Geometry

61
-1385.3571770

C	-5.18824500	-0.51908900	-1.54246600
C	-4.06327300	0.06402900	-0.94806600
C	-2.96486300	-0.71104200	-0.59161900
C	-2.94200600	-2.11075800	-0.80562900
C	-4.07861300	-2.67333100	-1.43751500
C	-5.17712500	-1.89676100	-1.78860500
H	-6.04617200	0.08651400	-1.81862800
H	-4.02590200	1.13550600	-0.76201700
H	-2.10498400	-0.20374200	-0.16970800
H	-4.07005500	-3.73958700	-1.63950200
H	-6.03542900	-2.36869700	-2.26117900
C	-1.80497300	-2.99490200	-0.50637800
C	-0.78170800	-2.65136000	0.48241000
C	-0.93801500	-1.70815100	1.53194900
C	0.43825100	-3.38012200	0.46460000
C	0.07292500	-1.48052000	2.45830200
H	-1.87148900	-1.16578300	1.64174400
C	1.44197800	-3.14854100	1.39538600
H	0.56712500	-4.12911900	-0.30988100
C	1.28123300	-2.18590700	2.40003500
H	-0.08770600	-0.74601500	3.24501300
H	2.36593400	-3.71982900	1.33745200
H	2.07057700	-1.99781200	3.12156600
O	-1.71610100	-4.11542800	-1.13051400
C	-3.64670400	2.36329500	2.21569500
C	-2.43072100	1.68621800	2.38093100
C	-1.37236400	1.88417400	1.50429300
C	-1.47981400	2.76876200	0.39583400
C	-2.70995300	3.47311600	0.27093900
C	-3.76254000	3.26841800	1.15283500
H	-4.47236100	2.19785300	2.90071200
H	-2.30271000	0.99827300	3.21447400
H	-0.43879200	1.36685600	1.69848000
H	-2.80768700	4.17830800	-0.54804000
H	-4.69182700	3.81549400	1.00916000
C	-0.40755100	3.07059500	-0.54713300
C	0.78378700	2.21087800	-0.68046100
C	0.82183600	0.82805900	-0.38847700
C	1.96297900	2.77354900	-1.22190300
C	1.97271500	0.06945600	-0.56993800
H	-0.06762500	0.31341900	-0.04424300
C	3.11819900	2.02057300	-1.39985700
H	1.94670700	3.82291900	-1.49825400
C	3.13957000	0.66598100	-1.05621300
H	1.95967700	-0.99405300	-0.34086500
H	4.01798500	2.47295300	-1.80916100
O	-0.48044700	4.13198500	-1.26896900
O	4.27575900	-0.08917000	-1.28713500
C	5.21309700	-0.26131100	-0.19241000
C	6.32828300	-1.10129900	-0.80256600
C	5.75037600	1.09295200	0.26696400
C	4.55534700	-1.00388800	0.96817900
H	5.93079600	-2.05784400	-1.15455200
H	6.77742800	-0.57569800	-1.65058900
H	7.10634900	-1.29660500	-0.05892500
H	4.95601000	1.70797600	0.69990800
H	6.52185500	0.94521000	1.02891600
H	6.19184300	1.63405000	-0.57606800
H	5.30007200	-1.20540200	1.74486200
H	3.74623500	-0.41663900	1.41183700

H	4.13783100	-1.95604400	0.62573800

Singlet Complex between **24** and **17** (counterions)



63
-2585.0928644

C	-4.73708400	1.40014600	-2.21282300
C	-3.39034100	1.39343500	-2.59219900
C	-2.38698500	1.51316500	-1.64156800
C	-2.69281300	1.64917600	-0.27261000
C	-4.05103800	1.61541600	0.09634100
C	-5.05841400	1.50649100	-0.85917300
H	-5.51901500	1.30872200	-2.96091000
H	-3.12166600	1.26196800	-3.63685500
H	-1.35175300	1.44189800	-1.95786100
H	-4.29806000	1.69274600	1.15077600
H	-6.09902800	1.49874200	-0.54522000
C	-1.68316700	1.75116300	0.80379600
C	-0.34491400	2.34876500	0.56987400
C	-0.02348800	3.17589200	-0.52115500
C	0.64245400	2.15361900	1.55528700
C	1.23955800	3.75606700	-0.63345500
H	-0.77246200	3.40447800	-1.27165500
C	1.90529200	2.71748000	1.43412700
H	0.39629000	1.52449100	2.40393400
C	2.21644900	3.52319700	0.33535000
H	1.45730900	4.40013500	-1.48110800
H	2.65717500	2.52347400	2.19451400
H	3.20323600	3.96663900	0.23908000
O	-2.03314700	1.51475700	1.99187000
C	-3.54913600	-2.21212900	-2.53144000
C	-2.22524300	-1.93009200	-2.89647100
C	-1.28912300	-1.50001100	-1.96583900
C	-1.61680700	-1.32794200	-0.58581300
C	-2.96540900	-1.65989600	-0.23804000
C	-3.89445500	-2.07345800	-1.18237700
H	-4.27643300	-2.54140000	-3.26690200
H	-1.91233200	-2.05579400	-3.93109300
H	-0.27314800	-1.34150000	-2.30782200
H	-3.25943700	-1.56435000	0.80255200
H	-4.91277300	-2.28731300	-0.86227800
C	-0.70350700	-0.97468700	0.47928700
C	0.70747400	-0.66421200	0.24783800
C	1.22856600	0.00038100	-0.89262300
C	1.63924700	-0.94267200	1.27686200
C	2.57401600	0.31119200	-1.01107600
H	0.55442700	0.35550200	-1.66401200
C	2.99479300	-0.64593400	1.15273500
H	1.26461800	-1.39009500	2.19208700
C	3.47874100	-0.02844100	0.00139500
H	2.93376300	0.86212400	-1.87642600
H	3.68708800	-0.87268500	1.96032600
O	-1.06086300	-1.27052800	1.71778400
O	4.80780500	0.34876800	-0.09109300
C	5.74151400	-0.57455100	-0.70839000
C	7.07041900	0.16889500	-0.65679900
C	5.81904800	-1.87057300	0.09595500
C	5.34328300	-0.86060600	-2.15478500
H	6.99915700	1.10863000	-1.21249100
H	7.33599800	0.39546100	0.38002200
H	7.86524800	-0.43944000	-1.09775100

H	4.86453300	-2.40457300	0.07640300
H	6.58650700	-2.52502400	-0.32854400
H	6.07990700	-1.65684300	1.13728500
H	6.10647000	-1.48532300	-2.62907800
H	4.38757000	-1.39003900	-2.20634100
H	5.25750500	0.07292700	-2.71973400
K	-0.86901500	-3.79725000	0.94225600
K	-2.36701700	-0.35660300	3.66392100

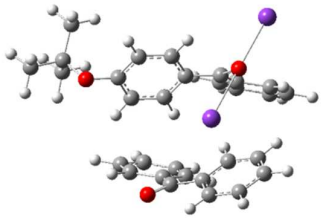
Single Point Triplet, Using Singlet Complex (of **24** and **17**, counterions) Optimised Geometry

63
-2585.0809371

C	-4.73708400	1.40014600	-2.21282300
C	-3.39034100	1.39343500	-2.59219900
C	-2.38698500	1.51316500	-1.64156800
C	-2.69281300	1.64917600	-0.27261000
C	-4.05103800	1.61541600	0.09634100
C	-5.05841400	1.50649100	-0.85917300
H	-5.51901500	1.30872200	-2.96091000
H	-3.12166600	1.26196800	-3.63685500
H	-1.35175300	1.44189800	-1.95786100
H	-4.29806000	1.69274600	1.15077600
H	-6.09902800	1.49874200	-0.54522000
C	-1.68316700	1.75116300	0.80379600
C	-0.34491400	2.34876500	0.56987400
C	-0.02348800	3.17589200	-0.52115500
C	0.64245400	2.15361900	1.55528700
C	1.23955800	3.75606700	-0.63345500
H	-0.77246200	3.40447800	-1.27165500
C	1.90529200	2.71748000	1.43412700
H	0.39629000	1.52449100	2.40393400
C	2.21644900	3.52319700	0.33535000
H	1.45730900	4.40013500	-1.48110800
H	2.65717500	2.52347400	2.19451400
H	3.20323600	3.96663900	0.23908000
O	-2.03314700	1.51475700	1.99187000
C	-3.54913600	-2.21212900	-2.53144000
C	-2.22524300	-1.93009200	-2.89647100
C	-1.28912300	-1.50001100	-1.96583900
C	-1.61680700	-1.32794200	-0.58581300
C	-2.96540900	-1.65989600	-0.23804000
C	-3.89445500	-2.07345800	-1.18237700
H	-4.27643300	-2.54140000	-3.26690200
H	-1.91233200	-2.05579400	-3.93109300
H	-0.27314800	-1.34150000	-2.30782200
H	-3.25943700	-1.56435000	0.80255200
H	-4.91277300	-2.28731300	-0.86227800
C	-0.70350700	-0.97468700	0.47928700
C	0.70747400	-0.66421200	0.24783800
C	1.22856600	0.00038100	-0.89262300
C	1.63924700	-0.94267200	1.27686200
C	2.57401600	0.31119200	-1.01107600
H	0.55442700	0.35550200	-1.66401200
C	2.99479300	-0.64593400	1.15273500
H	1.26461800	-1.39009500	2.19208700
C	3.47874100	-0.02844100	0.00139500
H	2.93376300	0.86212400	-1.87642600
H	3.68708800	-0.87268500	1.96032600
O	-1.06086300	-1.27052800	1.71778400
O	4.80780500	0.34876800	-0.09109300
C	5.74151400	-0.57455100	-0.70839000
C	7.07041900	0.16889500	-0.65679900
C	5.81904800	-1.87057300	0.09595500
C	5.34328300	-0.86060600	-2.15478500
H	6.99915700	1.10863000	-1.21249100
H	7.33599800	0.39546100	0.38002200
H	7.86524800	-0.43944000	-1.09775100
H	4.86453300	-2.40457300	0.07640300
H	6.58650700	-2.52502400	-0.32854400
H	6.07990700	-1.65684300	1.13728500
H	6.10647000	-1.48532300	-2.62907800
H	4.38757000	-1.39003900	-2.20634100

H	5.25750500	0.07292700	-2.71973400
K	-0.86901500	-3.79725000	0.94225600
K	-2.36701700	-0.35660300	3.66392100

Triplet Complex between **24** and **17** (counterions)



63
-2585.0997061

C	-3.60714300	-1.40758700	-2.73856900
C	-3.33312300	-1.13632800	-1.38890600
C	-2.19402800	-1.63499300	-0.76767500
C	-1.26500400	-2.45774500	-1.46841800
C	-1.54481100	-2.68628200	-2.84860000
C	-2.68759100	-2.18487800	-3.45851200
H	-4.50295400	-1.02002500	-3.21248200
H	-4.00434500	-0.50468300	-0.81380100
H	-2.00187700	-1.33697900	0.25824400
H	-0.83555200	-3.28167900	-3.41323300
H	-2.86853800	-2.40057300	-4.50870600
C	-0.02336500	-3.00173200	-0.92958200
C	0.23808700	-3.09935500	0.52019900
C	-0.75061500	-3.12748300	1.52975900
C	1.58192800	-3.23186500	0.93881800
C	-0.40660500	-3.20651000	2.87670200
H	-1.80161200	-3.12240700	1.26228800
C	1.92282600	-3.30220100	2.28431000
H	2.34945900	-3.26620300	0.17189300
C	0.93235700	-3.27418400	3.27150700
H	-1.19491400	-3.22513200	3.62499500
H	2.96934900	-3.38081200	2.56840600
H	1.19649200	-3.32607800	4.32317600
O	0.88225900	-3.40504600	-1.74160800
C	-3.63633400	0.51136500	3.36572800
C	-2.23763700	0.48017400	3.45143500
C	-1.44403900	0.86384900	2.37965400
C	-2.01904300	1.29076900	1.15153100
C	-3.43922400	1.34022300	1.09669900
C	-4.22410400	0.95483600	2.17721900
H	-4.24889000	0.20591000	4.20755500
H	-1.76007800	0.15816900	4.37318800
H	-0.36577000	0.85592900	2.49815800
H	-3.90763400	1.65503000	0.16822200
H	-5.30695400	0.99042500	2.08844400
C	-1.25868500	1.71741100	-0.00874500
C	0.18717100	1.46324000	-0.15501000
C	0.83423600	0.30249900	0.32030100
C	0.95570800	2.35910400	-0.93092400
C	2.18261200	0.07487500	0.06947800
H	0.26912200	-0.46192100	0.84710000
C	2.30834500	2.13942800	-1.17020300
H	0.46795300	3.23776700	-1.34291600
C	2.93544100	1.00153000	-0.65711100
H	2.64918200	-0.84341200	0.41187300
H	2.89122300	2.84111900	-1.76026700
O	-1.85761900	2.35885000	-0.97254000
O	4.25433000	0.75163100	-0.96054000
C	5.27120000	1.14359300	0.00412000
C	6.57744500	0.77711400	-0.68757100
C	5.19893800	2.64574900	0.26499600
C	5.11175900	0.35764200	1.30348100
H	6.60425800	-0.29562700	-0.89941100
H	6.67214600	1.32304400	-1.63067700
H	7.42787900	1.02987300	-0.04841600

H	4.25789200	2.91946400	0.75167900
H	6.02148800	2.94474500	0.92130000
H	5.28367400	3.20081000	-0.67450700
H	5.94709500	0.58600000	1.97219900
H	4.18342800	0.61925600	1.81932200
H	5.11135400	-0.71818900	1.10201200
K	-2.70453200	4.39399100	0.43847800
K	-1.01835400	0.49754200	-2.77767800

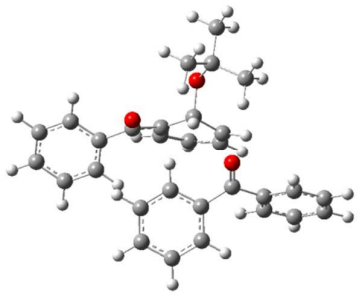
Single Point Singlet, Using Triplet Complex (of **24** and **17**, counterions) Optimised Geometry

63
-2585.0715682

C	-3.60714300	-1.40758700	-2.73856900
C	-3.33312300	-1.13632800	-1.38890600
C	-2.19402800	-1.63499300	-0.76767500
C	-1.26500400	-2.45774500	-1.46841800
C	-1.54481100	-2.68628200	-2.84860000
C	-2.68759100	-2.18487800	-3.45851200
H	-4.50295400	-1.02002500	-3.21248200
H	-4.00434500	-0.50468300	-0.81380100
H	-2.00187700	-1.33697900	0.25824400
H	-0.83555200	-3.28167900	-3.41323300
H	-2.86853800	-2.40057300	-4.50870600
C	-0.02336500	-3.00173200	-0.92958200
C	0.23808700	-3.09935500	0.52019900
C	-0.75061500	-3.12748300	1.52975900
C	1.58192800	-3.23186500	0.93881800
C	-0.40660500	-3.20651000	2.87670200
H	-1.80161200	-3.12240700	1.26228800
C	1.92282600	-3.30220100	2.28431000
H	2.34945900	-3.26620300	0.17189300
C	0.93235700	-3.27418400	3.27150700
H	-1.19491400	-3.22513200	3.62499500
H	2.96934900	-3.38081200	2.56840600
H	1.19649200	-3.32607800	4.32317600
O	0.88225900	-3.40504600	-1.74160800
C	-3.63633400	0.51136500	3.36572800
C	-2.23763700	0.48017400	3.45143500
C	-1.44403900	0.86384900	2.37965400
C	-2.01904300	1.29076900	1.15153100
C	-3.43922400	1.34022300	1.09669900
C	-4.22410400	0.95483600	2.17721900
H	-4.24889000	0.20591000	4.20755500
H	-1.76007800	0.15816900	4.37318800
H	-0.36577000	0.85592900	2.49815800
H	-3.90763400	1.65503000	0.16822200
H	-5.30695400	0.99042500	2.08844400
C	-1.25868500	1.71741100	-0.00874500
C	0.18717100	1.46324000	-0.15501000
C	0.83423600	0.30249900	0.32030100
C	0.95570800	2.35910400	-0.93092400
C	2.18261200	0.07487500	0.06947800
H	0.26912200	-0.46192100	0.84710000
C	2.30834500	2.13942800	-1.17020300
H	0.46795300	3.23776700	-1.34291600
C	2.93544100	1.00153000	-0.65711100
H	2.64918200	-0.84341200	0.41187300
H	2.89122300	2.84111900	-1.76026700
O	-1.85761900	2.35885000	-0.97254000
O	4.25433000	0.75163100	-0.96054000
C	5.27120000	1.14359300	0.00412000
C	6.57744500	0.77711400	-0.68757100
C	5.19893800	2.64574900	0.26499600
C	5.11175900	0.35764200	1.30348100
H	6.60425800	-0.29562700	-0.89941100
H	6.67214600	1.32304400	-1.63067700
H	7.42787900	1.02987300	-0.04841600
H	4.25789200	2.91946400	0.75167900
H	6.02148800	2.94474500	0.92130000
H	5.28367400	3.20081000	-0.67450700
H	5.94709500	0.58600000	1.97219900
H	4.18342800	0.61925600	1.81932200

H	5.11135400	-0.71818900	1.10201200
K	-2.70453200	4.39399100	0.43847800
K	-1.01835400	0.49754200	-2.77767800

Reactant Complex for formation of **50** and **21** from **45** and **17**

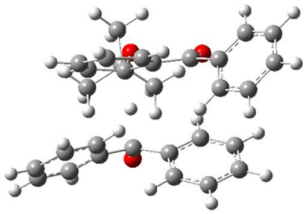


62
-1385.9139884

C	0.86878	-3.78018	-1.19840
C	-0.42615	-4.16450	-0.84843
C	-1.44850	-3.21782	-0.81251
C	-1.18074	-1.88340	-1.14343
C	0.11634	-1.50752	-1.51285
C	1.13858	-2.45061	-1.52912
H	1.66733	-4.51631	-1.21387
H	-0.64083	-5.19968	-0.60257
H	-2.45612	-3.52239	-0.54676
H	0.33284	-0.47311	-1.76423
H	2.14656	-2.14061	-1.78958
C	-2.25407	-0.84279	-1.17875
C	-3.46490	-0.98529	-0.30734
C	-3.39445	-1.54138	0.97482
C	-4.68062	-0.47524	-0.77530
C	-4.53191	-1.58753	1.77814
H	-2.44404	-1.90202	1.35670
C	-5.82133	-0.54128	0.02022
H	-4.71833	-0.03194	-1.76577
C	-5.74699	-1.09589	1.29902
H	-4.46793	-2.00292	2.77886
H	-6.76512	-0.15648	-0.35299
H	-6.63392	-1.13886	1.92367
O	-2.15847	0.11797	-1.93011
C	5.97406	-1.62733	0.58832
C	4.74793	-2.14881	1.00079
C	3.57041	-1.43439	0.77608
C	3.60034	-0.19533	0.12548
C	4.83421	0.30717	-0.30449
C	6.01432	-0.39388	-0.06509
H	6.89140	-2.17959	0.76953
H	4.70608	-3.11417	1.49716
H	2.61560	-1.84712	1.09061
H	4.85616	1.25639	-0.83260
H	6.96477	0.01704	-0.39315
C	2.34422	0.57543	-0.21963
C	1.36077	0.81369	0.77125
C	1.52335	0.46217	2.14394
C	0.10078	1.51725	0.35673
C	0.46758	0.43982	3.02104
H	2.51113	0.17847	2.50096
C	-1.05364	1.10480	1.22809
H	-0.10419	1.30732	-0.69854
C	-0.85579	0.67524	2.49922
H	0.60737	0.16300	4.06101
H	-2.06367	1.23008	0.84484
H	-1.71724	0.46154	3.13167
O	2.23926	0.94471	-1.42120
O	0.30083	2.96856	0.46853
C	-0.29047	3.80634	-0.52930
C	-0.10122	5.22450	0.00556
C	0.44300	3.65551	-1.86570

C	-1.78645	3.52293	-0.71186
H	-0.62155	5.33980	0.96159
H	0.96270	5.42751	0.16253
H	-0.49694	5.96066	-0.70172
H	0.37585	2.63273	-2.24527
H	0.01683	4.33899	-2.60846
H	1.50422	3.88998	-1.73735
H	-2.21294	4.24545	-1.41616
H	-1.96235	2.51846	-1.11101
H	-2.31124	3.61771	0.24440

Transition State for formation of **50** and **21** from **45** and **17**

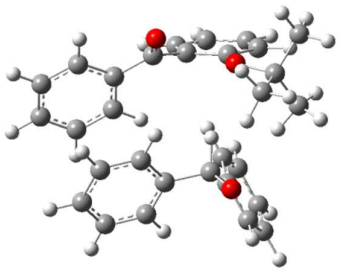


62
-1385.8589518

C	2.45915000	-2.09826200	-2.49545400
C	1.53473500	-2.98577500	-1.94950100
C	0.29762000	-2.52224100	-1.49212100
C	-0.03656300	-1.16606600	-1.58088400
C	0.90204200	-0.28651300	-2.13301700
C	2.13825700	-0.74176700	-2.58042000
H	3.42322900	-2.45669300	-2.84421800
H	1.76820200	-4.04473300	-1.88321200
H	-0.41797100	-3.23329000	-1.09083300
H	0.65489000	0.76887100	-2.19715600
H	2.85735000	-0.03517600	-2.98566200
C	-1.44632800	-0.63863200	-1.30801300
C	-2.30644500	-1.45850000	-0.36824000
C	-1.79394500	-2.09017100	0.76773300
C	-3.67690400	-1.55895900	-0.63118100
C	-2.62259000	-2.83389400	1.60490900
H	-0.74094900	-1.97704400	1.01752300
C	-4.51319500	-2.29269700	0.20959800
H	-4.06478200	-1.05804800	-1.51300900
C	-3.98578300	-2.94132300	1.32770500
H	-2.20479500	-3.31314200	2.48622100
H	-5.57455600	-2.36497700	-0.01070600
H	-4.63257400	-3.51958200	1.98114500
O	-2.02501400	-0.12339200	-2.32980700
C	5.55160700	-0.66090500	0.85989100
C	4.41034300	-1.43896900	0.66049100
C	3.15881400	-0.83333200	0.56267600
C	3.03931400	0.55723700	0.64539000
C	4.18900300	1.33319400	0.81699100
C	5.43902000	0.72807000	0.93899700
H	6.52535600	-1.13377700	0.94645500
H	4.49432600	-2.51864100	0.57469800
H	2.26940200	-1.43622700	0.38799400
H	4.09395500	2.41483800	0.85496900
H	6.32455400	1.33828000	1.09030700
C	1.71166600	1.25621500	0.43706400
C	0.55592800	0.80285700	1.20600300
C	0.76665800	0.00854900	2.35775400
C	-0.80943900	1.19416700	0.84583100
C	-0.24389200	-0.35784000	3.22306300
H	1.78573400	-0.26977000	2.60595300
C	-1.83197900	0.82534100	1.81924400
H	-1.11702900	0.37889700	-0.33478100
C	-1.55743600	0.08413900	2.93562500
H	-0.02891300	-0.92855000	4.11975000
H	-2.83874800	1.18989400	1.65301600
H	-2.36812100	-0.14510800	3.62388400
O	1.69896200	2.17506900	-0.38907900
O	-0.90626500	2.50612700	0.37805600
C	-1.81659900	3.02382500	-0.61283500
C	-1.92298400	4.50281800	-0.24135400
C	-1.18045600	2.88084200	-1.99485000
C	-3.20129800	2.37944200	-0.58348000
H	-2.33354400	4.61620800	0.76670000
H	-0.93374400	4.97018200	-0.27203800

H	-2.57673700	5.02299700	-0.94827600
H	-1.21855100	1.83993000	-2.32468400
H	-1.73388200	3.48987600	-2.71949700
H	-0.14304000	3.22317400	-1.95095200
H	-3.79124100	2.79431500	-1.40779400
H	-3.14327400	1.29815600	-0.73570700
H	-3.72594600	2.60159800	0.35085400

Product Complex for formation of **50** and **21** from **45** and **17**

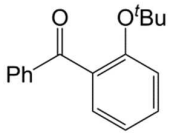


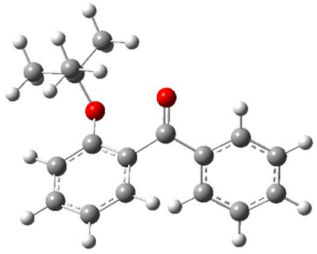
62
-1385.9151685

C	-4.11678	1.54675	-1.24331
C	-3.49056	2.54731	-0.50260
C	-2.09579	2.58914	-0.41347
C	-1.30488	1.63799	-1.06364
C	-1.95056	0.63811	-1.80280
C	-3.33833	0.58721	-1.89575
H	-5.20084	1.50537	-1.30320
H	-4.08690	3.29488	0.01440
H	-1.61894	3.37172	0.17252
H	-1.34255	-0.11404	-2.30493
H	-3.81694	-0.20733	-2.46262
C	0.23418	1.69117	-1.11272
C	0.78802	2.36661	0.15399
C	0.95410	1.66295	1.35234
C	1.15720	3.71371	0.12303
C	1.45868	2.28750	2.49360
H	0.71077	0.60176	1.38491
C	1.65533	4.34973	1.26164
H	1.05533	4.24130	-0.82127
C	1.80704	3.63937	2.45380
H	1.58971	1.71694	3.40974
H	1.93354	5.39967	1.21895
H	2.20346	4.12916	3.33859
O	0.65855	2.26451	-2.27077
C	-4.54212	-1.22490	1.08090
C	-3.46337	-0.45419	1.51391
C	-2.16289	-0.82974	1.18817
C	-1.93595	-1.96861	0.40742
C	-3.02303	-2.72611	-0.04096
C	-4.32165	-2.36305	0.30397
H	-5.55556	-0.93273	1.33999
H	-3.63451	0.44699	2.09422
H	-1.32835	-0.21569	1.51271
H	-2.83353	-3.60032	-0.65638
H	-5.16114	-2.96243	-0.03467
C	-0.56221	-2.38299	-0.03195
C	0.60638	-2.05841	0.84603
C	0.46239	-2.18140	2.23195
C	1.87233	-1.71964	0.30302
C	1.53878	-1.99883	3.09459
H	-0.51202	-2.44212	2.63470
C	2.95762	-1.56326	1.17611
H	0.54516	0.61728	-1.01589
C	2.78507	-1.69695	2.55173
H	1.40854	-2.10268	4.16616
H	3.94186	-1.33767	0.79419
H	3.64466	-1.56296	3.20185
O	-0.42545	-3.02485	-1.06261
O	1.91556	-1.55853	-1.02871
C	3.02181	-1.00598	-1.79549
C	4.09912	-2.07592	-1.95973
C	2.34958	-0.70006	-3.13283
C	3.57043	0.30218	-1.21867

H	4.53438	-2.37546	-1.00265
H	3.67573	-2.96235	-2.44109
H	4.90410	-1.68753	-2.59092
H	1.63553	0.12377	-3.00577
H	3.10464	-0.40211	-3.86680
H	1.83116	-1.58993	-3.50268
H	4.08167	0.83430	-2.02656
H	2.75019	0.93709	-0.87271
H	4.29184	0.16797	-0.41191

50

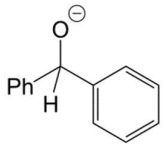


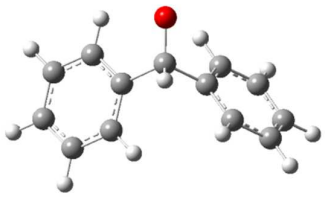


37
-808.7992613

C	-4.86776	-0.41049	-0.62905
C	-3.99293	0.51453	-1.19720
C	-2.65544	0.54093	-0.80544
C	-2.18694	-0.36987	0.14844
C	-3.06787	-1.30496	0.70652
C	-4.40471	-1.32032	0.32511
H	-5.91089	-0.42490	-0.92954
H	-4.35116	1.21556	-1.94399
H	-1.97460	1.25867	-1.25243
H	-2.68843	-2.00890	1.44032
H	-5.08748	-2.03906	0.76667
C	-0.74922	-0.41085	0.56538
C	0.09460	0.80873	0.33964
C	-0.35465	2.05514	0.79162
C	1.34508	0.71075	-0.29143
C	0.43543	3.19110	0.64976
H	-1.32773	2.12635	1.27053
C	2.11583	1.86214	-0.47485
C	1.67039	3.09009	0.00769
H	0.08488	4.14802	1.02109
H	3.05647	1.78948	-1.00923
H	2.28448	3.97414	-0.13380
O	-0.28676	-1.40700	1.09710
O	1.72581	-0.49265	-0.80881
C	2.84571	-1.23020	-0.22039
C	2.99364	-0.92671	1.26669
C	2.46376	-2.68941	-0.43602
C	4.12182	-0.88977	-0.98687
H	3.30212	0.10864	1.44016
H	2.04948	-1.11245	1.78515
H	3.76383	-1.58197	1.68376
H	2.30426	-2.88256	-1.50120
H	3.26215	-3.34595	-0.07827
H	1.54229	-2.91432	0.10699
H	4.93112	-1.55521	-0.67041
H	3.96323	-1.02140	-2.06117
H	4.44317	0.13809	-0.79853

21

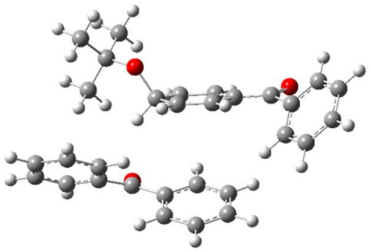




25
-577.1054866

C	3.47966	-1.04717	0.60152
C	2.59326	-1.70582	-0.25566
C	1.48398	-1.03222	-0.76370
C	1.23797	0.30637	-0.43256
C	2.13210	0.95578	0.41825
C	3.24405	0.28613	0.93617
H	4.34569	-1.56867	0.99906
H	2.77060	-2.74328	-0.52675
H	0.79519	-1.55130	-1.42924
H	1.93106	1.99761	0.65045
H	3.93092	0.80718	1.59844
C	0.00695	1.06832	-0.98244
C	-1.23648	0.38687	-0.37454
C	-1.59424	0.66649	0.94976
C	-2.03258	-0.49984	-1.10202
C	-2.70770	0.06886	1.53418
H	-0.98334	1.37057	1.50958
C	-3.15487	-1.10272	-0.52457
H	-1.77602	-0.71805	-2.13735
C	-3.49535	-0.82211	0.79713
H	-2.96745	0.29586	2.56490
H	-3.76504	-1.78471	-1.11080
H	-4.36693	-1.28601	1.24959
O	0.04618	2.40220	-0.76372
H	-0.02470	0.78953	-2.06733

Reactant Complex for formation of **22** and **21** from **20** and **17**

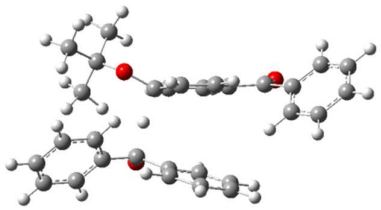


62
-1385.9144795

C	-6.46454	-0.56985	-1.69885
C	-5.30953	-1.29211	-1.39933
C	-4.32036	-0.72919	-0.59210
C	-4.47476	0.55828	-0.06552
C	-5.64935	1.26405	-0.35177
C	-6.63128	0.71305	-1.17248
H	-7.23180	-1.00443	-2.33268
H	-5.17811	-2.29619	-1.79273
H	-3.42252	-1.29432	-0.35726
H	-5.78238	2.25219	0.07966
H	-7.52951	1.28020	-1.39887
C	-3.46540	1.17460	0.87828
C	-2.09106	1.17147	0.54095
C	-1.55147	0.75794	-0.73099
C	-1.11878	1.59763	1.51559
C	-0.22534	0.77634	-1.00947
H	-2.23261	0.41947	-1.50834
C	0.21477	1.62300	1.27868
H	-1.49209	1.85889	2.50415
C	0.81308	1.29405	-0.05944
H	0.13079	0.44849	-1.98461
H	0.89751	1.87019	2.08935
O	-3.93884	1.66770	1.94111
H	1.62116	0.55831	0.05483
O	1.42558	2.43833	-0.73226
C	2.65093	3.00336	-0.24451
C	3.32006	3.58270	-1.49209
C	2.35194	4.13847	0.74228
C	3.58308	1.96964	0.39249
H	3.55240	2.78051	-2.20007
H	2.64579	4.29276	-1.98107
H	4.24732	4.10338	-1.23200
H	1.90557	3.76070	1.66460
H	3.27336	4.67306	0.99853
H	1.65325	4.84762	0.28754
H	4.52335	2.46087	0.66364
H	3.16094	1.53025	1.30271
H	3.81035	1.16096	-0.31099
C	5.23823	-1.15398	-1.81266
C	3.89354	-1.17497	-2.18376
C	2.90849	-1.40003	-1.22400
C	3.26510	-1.58644	0.11681
C	4.61447	-1.55010	0.48509
C	5.59882	-1.34626	-0.47737
H	6.00457	-0.98330	-2.56246
H	3.61046	-1.00922	-3.21835
H	1.86088	-1.38921	-1.51141
H	4.87589	-1.67513	1.53135
H	6.64469	-1.32748	-0.18765
C	2.23681	-1.70206	1.20173
C	0.89312	-2.28310	0.90087
C	0.71319	-3.28382	-0.06201
C	-0.20257	-1.82822	1.64379
C	-0.55454	-3.81879	-0.28186

H	1.56280	-3.65889	-0.62486
C	-1.47091	-2.34825	1.40753
H	-0.05275	-1.04447	2.37815
C	-1.64702	-3.34468	0.44512
H	-0.68949	-4.60215	-1.02068
H	-2.32258	-1.97009	1.96536
H	-2.63690	-3.75392	0.26288
O	2.49792	-1.30172	2.32807

Transition State for formation of **22** and **21** from **20** and **17**

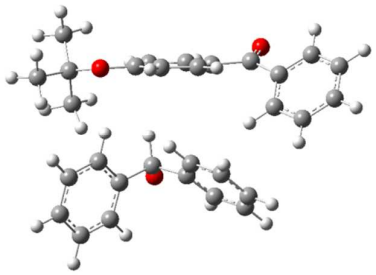


62
-1385.8777800

C	-6.58335800	-0.72169400	-1.34930600
C	-5.38328800	-1.39153200	-1.11275800
C	-4.34502500	-0.75194500	-0.43513000
C	-4.50276800	0.55969300	0.02545000
C	-5.71930600	1.21622700	-0.19495400
C	-6.74893600	0.58643600	-0.88980900
H	-7.38845900	-1.21790500	-1.88273700
H	-5.25325900	-2.41450000	-1.45369200
H	-3.41521200	-1.27972200	-0.24503100
H	-5.84498800	2.22541700	0.18599800
H	-7.68268100	1.11113000	-1.06828300
C	-3.44474200	1.27204700	0.83140600
C	-2.05581700	1.20072200	0.43594400
C	-1.59694900	0.69744000	-0.81446900
C	-1.06827300	1.74230700	1.29908300
C	-0.27392800	0.71587700	-1.15541000
H	-2.31136600	0.33539200	-1.54837600
C	0.26432500	1.79562000	0.98112000
H	-1.39986200	2.15032100	2.25063300
C	0.75846600	1.20774900	-0.25428600
H	0.05352600	0.36349500	-2.12985500
H	0.96269400	2.20679300	1.69813600
O	-3.83047100	1.91667000	1.82363900
H	1.37658400	0.08215100	0.23094700
O	1.82005500	1.73650500	-0.99417800
C	2.82242900	2.62885900	-0.46580200
C	3.78547700	2.78143900	-1.64250300
C	2.21290100	3.99808100	-0.14120600
C	3.57211600	2.02929400	0.72629800
H	4.15534000	1.79666800	-1.94413000
H	3.28115500	3.24837900	-2.49419500
H	4.63718700	3.40452800	-1.35336500
H	1.61314400	3.99442700	0.76931600
H	3.01922700	4.72735800	-0.01252200
H	1.58076300	4.32559200	-0.97242400
H	4.17665400	2.81064100	1.19917900
H	2.90407000	1.59760400	1.47667700
H	4.24131800	1.23205300	0.38994700
C	5.63616600	-1.60899000	-0.94659100
C	4.52376100	-1.24800400	-1.70983900
C	3.28898400	-1.04654800	-1.09569500
C	3.14483600	-1.20367000	0.28746300
C	4.26499400	-1.55914900	1.04450600
C	5.50189200	-1.76565600	0.43347800
H	6.60020100	-1.75963000	-1.42322000
H	4.62217100	-1.10797000	-2.78270500
H	2.43726200	-0.72225600	-1.68865000
H	4.15209300	-1.64969800	2.12082300
H	6.36354800	-2.04111600	1.03491600
C	1.83566300	-0.94037200	1.01533000
C	0.66977900	-1.85877000	0.67276400
C	0.64358600	-2.72832400	-0.42366300
C	-0.46101600	-1.78505300	1.49588900
C	-0.48813500	-3.50161700	-0.69248900
H	1.50906300	-2.81940700	-1.07175700

C	-1.58930600	-2.55419400	1.22969800
H	-0.43255500	-1.10698900	2.34210800
C	-1.60984200	-3.41588700	0.12984800
H	-0.48808700	-4.17392000	-1.54564600
H	-2.45938500	-2.47873600	1.87698100
H	-2.49178400	-4.01404000	-0.08230400
O	1.90460500	-0.51922400	2.22266700

Product Complex for formation of **22** and **21** from **20** and **17**

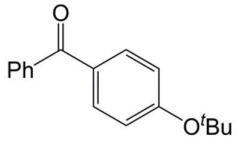


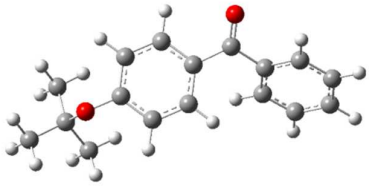
62
-1385.9218525

C	5.95010	0.77914	-1.00308
C	4.64208	1.21209	-0.78994
C	3.68860	0.34245	-0.26061
C	4.05525	-0.96734	0.07071
C	5.37518	-1.39134	-0.12476
C	6.31788	-0.52633	-0.67103
H	6.68363	1.46006	-1.42393
H	4.35746	2.22984	-1.03407
H	2.67299	0.69598	-0.08887
H	5.64620	-2.40571	0.15169
H	7.33590	-0.86587	-0.83424
C	3.09771	-1.93392	0.69871
C	1.67646	-1.96645	0.26529
C	1.24570	-1.51159	-0.99164
C	0.73839	-2.56143	1.11480
C	-0.07893	-1.64668	-1.36983
H	1.95145	-1.06618	-1.68613
C	-0.59646	-2.68913	0.75406
H	1.06927	-2.92595	2.08225
C	-1.02166	-2.21778	-0.49724
H	-0.42266	-1.29491	-2.33736
H	-1.28397	-3.14040	1.45308
O	3.50619	-2.70841	1.55701
H	-1.07133	0.17644	0.52593
O	-2.28106	-2.24582	-0.98271
C	-3.45740	-2.67544	-0.24523
C	-4.58709	-2.32630	-1.21171
C	-3.41940	-4.18649	-0.02187
C	-3.64173	-1.87753	1.04748
H	-4.62846	-1.24370	-1.36560
H	-4.42439	-2.81579	-2.17610
H	-5.54451	-2.66065	-0.80347
H	-2.60209	-4.49900	0.63029
H	-4.35860	-4.50422	0.44056
H	-3.31423	-4.70143	-0.98136
H	-4.67328	-2.00447	1.38949
H	-2.98656	-2.19213	1.86040
H	-3.47091	-0.81359	0.85698
C	-4.74981	2.92631	-0.76349
C	-4.14499	1.82096	-1.36080
C	-3.00419	1.25268	-0.78748
C	-2.45007	1.77419	0.38585
C	-3.07359	2.87548	0.98213
C	-4.20841	3.45152	0.41375
H	-5.63778	3.37003	-1.20421
H	-4.56466	1.39595	-2.26921
H	-2.54677	0.37588	-1.24670
H	-2.65687	3.26291	1.90854
H	-4.67795	4.30888	0.88884
C	-1.18677	1.16507	1.03110
C	0.01271	1.99802	0.51186
C	0.30932	2.10106	-0.85479
C	0.81857	2.68703	1.41865

C	1.35871	2.90009	-1.30488
H	-0.29795	1.55508	-1.57483
C	1.87311	3.49113	0.97512
H	0.58841	2.57530	2.47431
C	2.13864	3.61154	-0.38795
H	1.56997	2.97100	-2.36887
H	2.48583	4.02786	1.69499
H	2.94981	4.24600	-0.73476
O	-1.25206	1.08132	2.37987

22

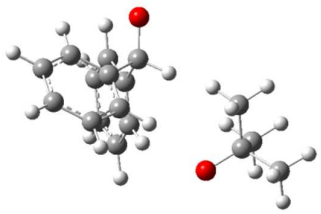




37
-808.8042505

C	-5.12732	-1.71741	0.14505
C	-3.85453	-2.02500	0.62451
C	-2.84443	-1.06537	0.58859
C	-3.11192	0.21369	0.08763
C	-4.39700	0.52341	-0.37266
C	-5.39819	-0.44222	-0.35537
H	-5.90995	-2.46966	0.16485
H	-3.64782	-3.01149	1.02689
H	-1.85694	-1.30524	0.97139
H	-4.59371	1.52318	-0.74744
H	-6.38912	-0.20279	-0.72771
C	-2.08051	1.29930	0.08730
C	-0.64158	0.95759	-0.11928
C	-0.23732	-0.14893	-0.87643
C	0.32901	1.82256	0.40201
C	1.11436	-0.39340	-1.09637
H	-0.97752	-0.80832	-1.31892
C	1.68006	1.57389	0.19888
H	0.00928	2.69203	0.96771
C	2.07628	0.45632	-0.54458
H	1.43726	-1.23528	-1.69986
H	2.43658	2.24170	0.59759
O	-2.42057	2.46247	0.25412
O	3.40163	0.24156	-0.81192
C	4.18985	-0.54608	0.13244
C	5.55449	-0.63359	-0.53621
C	4.28721	0.17725	1.47232
C	3.57881	-1.93378	0.30347
H	5.46855	-1.12827	-1.50782
H	5.96780	0.36767	-0.68676
H	6.24312	-1.20689	0.09041
H	3.31053	0.25320	1.95913
H	4.95317	-0.37923	2.13837
H	4.69474	1.18343	1.33520
H	4.23188	-2.54288	0.93488
H	2.59666	-1.88321	0.78300
H	3.47332	-2.42937	-0.66638

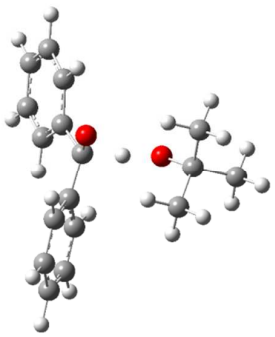
Reactant Complex for formation of **23** and **HO^{t}Bu** from **21** and **OtBu anion**



39
-810.1530973

C	0.79226	3.75659	-1.07679
C	-0.26555	2.85112	-1.15924
C	-0.24264	1.66189	-0.42304
C	0.84350	1.36498	0.40881
C	1.89558	2.28386	0.49314
C	1.87702	3.46695	-0.24387
H	0.77098	4.68055	-1.64813
H	-1.12077	3.07048	-1.79422
H	-1.08963	0.97471	-0.50194
H	2.72420	2.05641	1.15931
H	2.70461	4.16803	-0.16783
C	0.91269	0.06144	1.23394
C	1.70065	-0.96116	0.37797
C	1.20028	-1.45244	-0.83571
C	2.94456	-1.41753	0.81577
C	1.92711	-2.36922	-1.59343
H	0.22748	-1.11171	-1.18756
C	3.68201	-2.33175	0.05831
H	3.30620	-1.04234	1.76898
C	3.17729	-2.81160	-1.15012
H	1.51975	-2.74221	-2.52956
H	4.65007	-2.67534	0.41464
H	3.74587	-3.52586	-1.73901
O	1.41894	0.23330	2.47841
H	-0.13505	-0.32907	1.22354
O	-3.09021	-0.10940	-1.13593
C	-3.63866	-0.67787	-0.01520
C	-3.44313	0.22523	1.22696
C	-5.15979	-0.91057	-0.19015
C	-2.98813	-2.04847	0.29664
H	-2.37264	0.38524	1.40148
H	-3.90533	1.20343	1.04314
H	-3.88301	-0.20079	2.13956
H	-5.33215	-1.56598	-1.05294
H	-5.63040	-1.36665	0.69221
H	-5.65363	0.04864	-0.38947
H	-3.40858	-2.52871	1.19138
H	-3.12865	-2.72289	-0.55734
H	-1.90957	-1.91573	0.45002

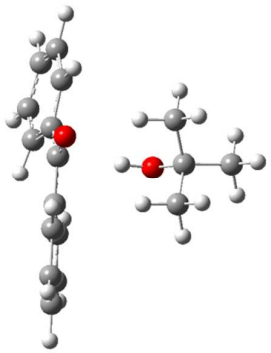
Transition State for
formation of **23** and **HO^{t}Bu**
from **21** and **OtBu anion**



39
-810.1171016

C	2.45006	-3.33827	-0.37560
C	1.74524	-2.63590	-1.36125
C	0.83272	-1.64369	-1.01452
C	0.56171	-1.31193	0.33497
C	1.31259	-2.00875	1.30656
C	2.22684	-3.00411	0.96231
H	3.16774	-4.10741	-0.64707
H	1.92720	-2.84994	-2.41244
H	0.35810	-1.06934	-1.80508
H	1.15741	-1.72466	2.34241
H	2.77529	-3.52242	1.74691
C	-0.32282	-0.18568	0.75624
C	-1.73069	-0.23462	0.27966
C	-2.23227	-0.96422	-0.82969
C	-2.68280	0.56855	0.96076
C	-3.55724	-0.86196	-1.24474
H	-1.58341	-1.64562	-1.36867
C	-4.00524	0.67509	0.53739
H	-2.33663	1.10544	1.83800
C	-4.46485	-0.03048	-0.57886
H	-3.88857	-1.45161	-2.09766
H	-4.69083	1.31410	1.09147
H	-5.49616	0.05009	-0.90987
O	-0.16335	0.21862	2.05690
H	0.09301	0.80810	-0.08321
O	0.46724	1.79918	-0.85988
C	1.60256	2.42403	-0.34244
C	2.66572	1.37890	0.04528
C	2.18833	3.36655	-1.40392
C	1.23453	3.23144	0.91511
H	2.25666	0.71613	0.81557
H	2.92106	0.76622	-0.82823
H	3.58160	1.85200	0.42384
H	1.44272	4.11837	-1.68828
H	3.08504	3.88635	-1.04099
H	2.45733	2.79533	-2.30014
H	2.10961	3.71622	1.36884
H	0.50354	4.00798	0.65701
H	0.78180	2.54251	1.63794

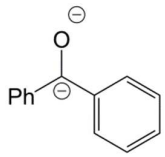
Product Complex for formation of **23** and **HO^{t}Bu** from **21** and **OtBu anion**

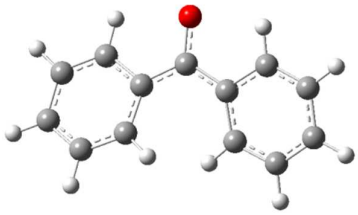


39
-810.1414320

C	3.90670	-1.50900	-0.66151
C	2.78043	-1.46925	-1.50330
C	1.49937	-1.27112	-1.00955
C	1.23461	-1.09289	0.39383
C	2.41468	-1.08113	1.21856
C	3.68709	-1.29462	0.70921
H	4.90363	-1.67282	-1.05904
H	2.91055	-1.57667	-2.57964
H	0.69797	-1.17516	-1.73281
H	2.26949	-0.89402	2.27689
H	4.53519	-1.28956	1.39360
C	-0.03128	-0.82710	1.02674
C	-1.30076	-1.05212	0.39255
C	-1.56893	-1.79970	-0.81205
C	-2.48864	-0.58337	1.06507
C	-2.85182	-1.96517	-1.31275
H	-0.76305	-2.31094	-1.32447
C	-3.76041	-0.74641	0.54034
H	-2.34617	-0.07146	2.01044
C	-3.98072	-1.42224	-0.67337
H	-2.98020	-2.55235	-2.22179
H	-4.61050	-0.34356	1.09107
H	-4.97867	-1.54927	-1.08130
O	-0.02326	-0.40095	2.29593
H	-0.32754	0.81138	-0.62721
O	-0.36025	1.63671	-1.15173
C	0.07129	2.69408	-0.29127
C	1.54649	2.49225	0.06176
C	-0.12454	3.98122	-1.08356
C	-0.78028	2.68970	0.97897
H	1.67479	1.54357	0.59493
H	2.15026	2.46012	-0.85223
H	1.91188	3.30833	0.69525
H	-1.17897	4.10400	-1.35202
H	0.18797	4.84797	-0.49245
H	0.46812	3.95553	-2.00413
H	-0.47183	3.49709	1.65356
H	-1.83580	2.83545	0.72155
H	-0.66880	1.72756	1.49811

23





24
-576.5430630

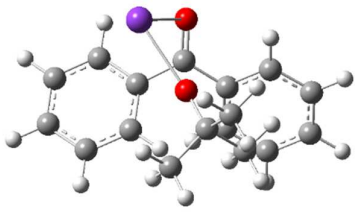
C	3.93409	-0.84781	-0.02633
C	2.79551	-1.61869	-0.33036
C	1.51843	-1.07963	-0.32629
C	1.26328	0.30324	-0.00469
C	2.45815	1.07902	0.22642
C	3.72613	0.51879	0.23161
H	4.92888	-1.28262	-0.02361
H	2.91443	-2.66815	-0.59902
H	0.70416	-1.72072	-0.64286
H	2.32613	2.14010	0.40878
H	4.58259	1.16105	0.43767
C	0.00001	0.98227	0.00018
C	-1.26319	0.30325	0.00508
C	-1.51856	-1.07953	0.32690
C	-2.45813	1.07912	-0.22641
C	-2.79571	-1.61860	0.33027
H	-0.70468	-1.72063	0.64433
C	-3.72602	0.51893	-0.23204
H	-2.32593	2.14023	-0.40850
C	-3.93412	-0.84784	0.02560
H	-2.91455	-2.66807	0.59896
H	-4.58245	1.16119	-0.43816
H	-4.92902	-1.28243	0.02271
O	0.00016	2.32310	0.00001

Single Point Radical Anion
using Optimised Geometry
23

24
-576.4988415

C	0.06673400	2.46635100	1.08064200
C	-0.08552000	1.26026900	0.30293700
C	-0.41975100	1.49579300	-1.08046400
C	-0.49679400	2.77062600	-1.61962100
C	-0.26265800	3.92476600	-0.84791600
C	0.00000000	3.73242900	0.52022600
H	0.25336500	2.34506100	2.14221700
H	-0.68576700	0.66372800	-1.72182000
H	-0.76913400	2.87357200	-2.66984700
H	-0.31816800	4.91798700	-1.28284000
H	0.15032900	4.59960000	1.16364400
C	0.00000000	0.00000000	0.98163000
C	0.08552000	-1.26026900	0.30293700
C	0.41975100	-1.49579300	-1.08046400
C	-0.06673400	-2.46635100	1.08064200
C	0.49679400	-2.77062600	-1.61962100
H	0.68576700	-0.66372800	-1.72182000
C	0.00000000	-3.73242900	0.52022600
H	-0.25336500	-2.34506100	2.14221700
C	0.26265800	-3.92476600	-0.84791600
H	0.76913400	-2.87357200	-2.66984700
H	-0.15032900	-4.59960000	1.16364400
H	0.31816800	-4.91798700	-1.28284000
O	0.00000000	0.00000000	2.32223400

Singlet Complex KO^{t}Bu + Benzophenone



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-1409.2932637

C	3.56791700	-1.28791300	-1.59990700
C	2.37991400	-0.72238500	-2.06753500
C	1.25181200	-0.69279900	-1.25195800
C	1.31337600	-1.21906600	0.04243400
C	2.51048800	-1.76844600	0.51559100
C	3.63351200	-1.81196700	-0.30847600
H	4.44420900	-1.31428500	-2.24015600
H	2.33476800	-0.29657600	-3.06508000
H	0.33720400	-0.21548000	-1.58723500
H	2.54864400	-2.16558900	1.52597400
H	4.55657200	-2.25122300	0.05616400
C	0.14690100	-1.15169200	0.97677400
C	-1.23124500	-1.42876900	0.48090900
C	-1.46852700	-2.15435600	-0.69164100
C	-2.31240900	-0.98445500	1.25121300
C	-2.77623500	-2.41532200	-1.09767400
H	-0.63731600	-2.52790100	-1.28113200
C	-3.61545400	-1.23857300	0.84186700
H	-2.11074900	-0.42225800	2.15759400
C	-3.84863200	-1.95111900	-0.33709900
H	-2.95706000	-2.98072000	-2.00618300
H	-4.45093600	-0.87778200	1.43339500
H	-4.86666000	-2.14822500	-0.65908300
O	0.34485800	-0.91198800	2.16459100
C	-0.73007700	2.57544700	-0.63723600
C	0.08225100	2.90717200	-1.90974700
H	0.95072300	3.52032400	-1.63983200
H	0.45284000	1.98152500	-2.36601700
H	-0.50633400	3.45079700	-2.66045200
C	-1.25231200	3.90618200	-0.05016500
H	-1.88416500	4.46484900	-0.75334600
H	-1.83763600	3.69930100	0.85397400
H	-0.40405900	4.54148200	0.23248700
C	-1.95665400	1.73479700	-1.05600600
H	-1.63305200	0.77473300	-1.47700200
H	-2.57197900	1.51395700	-0.17636700
H	-2.58043700	2.24794000	-1.79990700
O	0.04823300	1.90833600	0.28024700
K	1.76331200	1.43441800	1.96239100

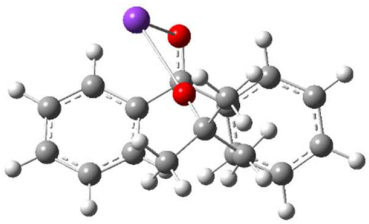
Single Point Triplet using Optimised Geometry of Singlet Complex KO*t*Bu + Benzophenone

39
-1409.2035039

C	3.56791700	-1.28791300	-1.59990700
C	2.37991400	-0.72238500	-2.06753500
C	1.25181200	-0.69279900	-1.25195800
C	1.31337600	-1.21906600	0.04243400
C	2.51048800	-1.76844600	0.51559100
C	3.63351200	-1.81196700	-0.30847600
H	4.44420900	-1.31428500	-2.24015600
H	2.33476800	-0.29657600	-3.06508000

H	0.33720400	-0.21548000	-1.58723500
H	2.54864400	-2.16558900	1.52597400
H	4.55657200	-2.25122300	0.05616400
C	0.14690100	-1.15169200	0.97677400
C	-1.23124500	-1.42876900	0.48090900
C	-1.46852700	-2.15435600	-0.69164100
C	-2.31240900	-0.98445500	1.25121300
C	-2.77623500	-2.41532200	-1.09767400
H	-0.63731600	-2.52790100	-1.28113200
C	-3.61545400	-1.23857300	0.84186700
H	-2.11074900	-0.42225800	2.15759400
C	-3.84863200	-1.95111900	-0.33709900
H	-2.95706000	-2.98072000	-2.00618300
H	-4.45093600	-0.87778200	1.43339500
H	-4.86666000	-2.14822500	-0.65908300
O	0.34485800	-0.91198800	2.16459100
C	-0.73007700	2.57544700	-0.63723600
C	0.08225100	2.90717200	-1.90974700
H	0.95072300	3.52032400	-1.63983200
H	0.45284000	1.98152500	-2.36601700
H	-0.50633400	3.45079700	-2.66045200
C	-1.25231200	3.90618200	-0.05016500
H	-1.88416500	4.46484900	-0.75334600
H	-1.83763600	3.69930100	0.85397400
H	-0.40405900	4.54148200	0.23248700
C	-1.95665400	1.73479700	-1.05600600
H	-1.63305200	0.77473300	-1.47700200
H	-2.57197900	1.51395700	-0.17636700
H	-2.58043700	2.24794000	-1.79990700
O	0.04823300	1.90833600	0.28024700
K	1.76331200	1.43441800	1.96239100

Triplet Complex KO*t*Bu + Benzophenone



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-1409.2222485

C	3.63296200	-0.45756700	-1.77428500
C	2.34970700	-0.07100200	-2.18334200
C	1.22615500	-0.42428800	-1.44769900
C	1.33001100	-1.19261300	-0.25680500
C	2.64404800	-1.55249400	0.15084500
C	3.76273500	-1.19774400	-0.59444100
H	4.50647600	-0.18073400	-2.35543400
H	2.22689600	0.52723400	-3.08300500
H	0.25398900	-0.07304300	-1.77642900
H	2.75438100	-2.13583600	1.06054100
H	4.74815500	-1.50784700	-0.25598600
C	0.21217900	-1.52023000	0.62335000
C	-1.18173800	-1.51550100	0.16200800
C	-1.58022300	-1.73491100	-1.17567500
C	-2.20720000	-1.34821100	1.12057400
C	-2.92268700	-1.72526200	-1.53895300
H	-0.83192900	-1.94260600	-1.93427900
C	-3.54785600	-1.33680700	0.75357400
H	-1.91886300	-1.21691100	2.15868600
C	-3.92082100	-1.51134100	-0.58277900
H	-3.19463900	-1.90041600	-2.57653100
H	-4.31074500	-1.18916000	1.51360300
H	-4.96752400	-1.50173200	-0.87070200

O	0.45664400	-1.76516200	1.86940600
C	-0.74974500	2.57995100	-0.25854800
C	0.15573100	3.25602300	-1.28973600
H	0.96802700	3.79135700	-0.79015100
H	0.58940900	2.50260400	-1.95432300
H	-0.41807500	3.96451600	-1.89442700
C	-1.28439300	3.62538100	0.75910200
H	-1.86284400	4.36399300	0.19742000
H	-1.93210900	3.14491400	1.49554900
H	-0.45818200	4.12838200	1.26640900
C	-1.92290000	1.84412500	-0.91174200
H	-1.56172500	1.13209800	-1.65881300
H	-2.49169000	1.28547500	-0.16244900
H	-2.58147800	2.56176100	-1.41046700
O	-0.01759300	1.73108200	0.55644000
K	1.63127800	0.53755500	2.33112300

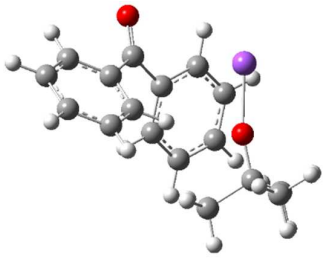
Single Point Singlet using Optimised Geometry of Triplet Complex KO*t*Bu + Benzophenone

39

-1409.2708159

C	3.63296200	-0.45756800	-1.77428500
C	2.34970700	-0.07100200	-2.18334200
C	1.22615500	-0.42428800	-1.44769900
C	1.33001100	-1.19261300	-0.25680500
C	2.64404800	-1.55249500	0.15084500
C	3.76273500	-1.19774500	-0.59444100
H	4.50647600	-0.18073500	-2.35543400
H	2.22689600	0.52723400	-3.08300500
H	0.25398900	-0.07304300	-1.77642900
H	2.75438100	-2.13583700	1.06054100
H	4.74815500	-1.50784800	-0.25598600
C	0.21217900	-1.52023000	0.62335000
C	-1.18173800	-1.51550100	0.16200800
C	-1.58022300	-1.73491100	-1.17567500
C	-2.20720000	-1.34821100	1.12057400
C	-2.92268700	-1.72526200	-1.53895300
H	-0.83192900	-1.94260600	-1.93427900
C	-3.54785600	-1.33680600	0.75357400
H	-1.91886300	-1.21691100	2.15868600
C	-3.92082100	-1.51134000	-0.58277900
H	-3.19463900	-1.90041500	-2.57653100
H	-4.31074500	-1.18915900	1.51360300
H	-4.96752400	-1.50173100	-0.87070200
O	0.45664400	-1.76516200	1.86940600
C	-0.74974500	2.57995100	-0.25854800
C	0.15573100	3.25602300	-1.28973600
H	0.96802800	3.79135700	-0.79015100
H	0.58940900	2.50260400	-1.95432300
H	-0.41807400	3.96451600	-1.89442700
C	-1.28439200	3.62538100	0.75910200
H	-1.86284300	4.36399300	0.19742000
H	-1.93210900	3.14491400	1.49554900
H	-0.45818100	4.12838200	1.26640900
C	-1.92290000	1.84412500	-0.91174200
H	-1.56172500	1.13209800	-1.65881300
H	-2.49169000	1.28547500	-0.16244900
H	-2.58147800	2.56176100	-1.41046700
O	-0.01759300	1.73108200	0.55644000
K	1.63127800	0.53755500	2.33112300

Benzophenone complex with NaO*t*Bu



39
-971.7183487

C	1.75878	3.01639	-1.07029
C	1.04574	2.10808	-1.85180
C	-0.12554	1.53527	-1.36098
C	-0.59872	1.88760	-0.09223
C	0.10943	2.81591	0.68025
C	1.29221	3.36836	0.19807
H	2.68089	3.44779	-1.44761
H	1.40675	1.83618	-2.83869
H	-0.67616	0.82272	-1.96775
H	-0.27567	3.09088	1.65782
H	1.84947	4.07383	0.80611
C	-1.87998	1.33464	0.44584
C	-2.31700	-0.03488	0.03283
C	-1.39267	-1.07007	-0.16243
C	-3.68875	-0.28193	-0.10037
C	-1.85437	-2.34562	-0.48891
H	-0.32059	-0.90834	-0.02255
C	-4.13824	-1.55008	-0.45425
H	-4.39067	0.52989	0.06523
C	-3.21929	-2.58443	-0.64698
H	-1.14129	-3.15381	-0.62131
H	-5.20067	-1.73494	-0.57717
H	-3.56913	-3.57617	-0.91713
O	-2.56374	1.99739	1.21437
O	1.73406	-1.13754	0.93557
C	2.65690	-1.56193	0.00418
C	3.72705	-0.47802	-0.23993
C	3.36609	-2.84330	0.48772
C	1.96886	-1.86779	-1.34288
H	3.24383	0.44005	-0.59543
H	4.24375	-0.25101	0.70030
H	4.47633	-0.78615	-0.98056
H	2.62509	-3.63425	0.65293
H	4.11037	-3.21063	-0.23034
H	3.87206	-2.64606	1.44034
H	2.67877	-2.20545	-2.10860
H	1.21336	-2.65065	-1.20438
H	1.46257	-0.96728	-1.71207
Na	0.73503	-0.37133	2.58857

References

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