Supplementary information

The lithiation and acyl transfer reactions of phosphines oxides, sulfides and boranes in the synthesis of cyclopropanes

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General

For reactions conducted under anhydrous conditions, glassware was dried overnight in an oven at 130 °C and was allowed to cool in a dessicator over anhydrous KOH. Anhydrous reactions were carried out under an atmosphere of argon. Solvents were BOC standard reagent grade and distilled prior to use. Reagents/solvents for anhydrous reactions were dried as follows: THF was dried over Na wire and distilled from a mixture of CaH_2 and $LiAlH_4$ with triphenylmethane as indicator. Dichloromethane, methanol, *n*-hexane, acetonitrile and toluene were distilled from CaH_2. Triethylamine, was dried and stored over 4 Å molecular sieves. Flash column chromatography was carried out using Merck Kiselgel 60 (230-400 mesh). TLC was run on commercially available pre-coated plates (Merck Kieselgel $60F_{254}$). ^{1}H, ^{13}C, APT, DEPT, HMQC, and COSY NMR spectra were recorded on Bruker Avance 400 (5 mm QNP probe) and Bruker Avance 500 (5 mm dual 13C-1H cryo probe) Fourier transform spectrometers using an internal deuterium lock. ^{31}P NMR spectra was recorded on a Bruker Avance 400 (5 mm QNP probe) Fourier transform spectrometer using 85% H_3PO_4 as external standard.

Solvents were used as internal standard when assigning NMR spectra (δ_H: $CDCl_3$ 7.26 ppm; δ_C: $CDCl_3$ 77.0 ppm; δ_H: DMSO-d_6 2.50 ppm; δ_C: DMSO-d_6 39.4 ppm). *J* values are given in Hz and were rounded to the nearest 0.5 Hz. EI and LSIMS mass spectra were recorded on a Kratos concept 1H double focusing magnetic sector instrument using a MACH 3 data system. +ESI mass spectra were recorded using a Bruker Bio-Apex II FT-ICR instrument or a Micromass Q-Tof 1 machine. Microanalyses were carried out in duplicate using a CE440 Elemental Analyser from Exeter Analytical, INC. and the averages of the two determinations were compared to the theoretical value. The calculated values were adjusted for residual solvents. Melting points were measured on a microscope hot stage melting point apparatus (C. Reichert Optische Werke AG) and are uncorrected. Infra-red spectra were recorded using a Perkin Elmer Spectrum One (FT-IR) spectrometer with a universal ATR sampling accessory.

Diphenylmethylphosphine borane 10

Method 1

To a mixture of sodium borohydride (2.3 g, 60 mmol) and diphenylmethylphosphine (10 g, 50 mmol) in dry THF (195 cm^3), stirred at 0 °C under a stream of nitrogen, was added a solution of iodine (7.6 g, 30 mmol) in dry THF (130 cm^3) dropwise. On completion of addition the resulting colourless solution was stirred for 1 h at room temperature. The THF was evaporated *in vacuo* and the residue partitioned between water (250 cm^3) and EtOAc (2 × 250 cm^3). The organic layer was dried (Na_2SO_4) and the THF evaporated under reduced pressure to yield the phosphine-borane **10** (10 g, 95%) as prisms mp 44-5 °C (from EtOAc) (lit.,[1] 55 °C); R_f(EtOAc-hexane, 1:1) 0.50; $\nu_{max}(CH_2Cl_2)/cm^{-1}$ 3081 (C-H), 2382 (B-H) and 1439 (P-Ph); δ_H(400 MHz; $CDCl_3$) 7.65 (4H, ddd, *J* 11.0, 8.0 and 1.5, Ph_2P *ortho*), 7.47-7.43 (6H, m, Ph_2P), 1.86 (3H, d, *J* 10.5, Me) and 0.99 (3H, m, BH_3); δ_C(100 MHz; $CDCl_3$) 131.7 (d, *J* 9.0, Ph_2P CH *ortho*), 131.1 (d, *J* 1.0, Ph_2P CH *para*), 130.5 (d, *J* 56.0, Ph_2P C *ipso*), 128.8 (d, *J* 10.0, Ph_2P CH *meta*) and 11.9 (d, *J* 40.0, Me); δ_P(162 MHz; $CDCl_3$) 10.7 (m); *m/z* (ES) 214 (7%, M) and 201 (100%, M-BH_3) (Found: M^+, 214.10827. $C_{13}H_{16}PB$ requires *M*, 214.10826). The spectroscopic data are consistent with that reported in the literature.[1]

Method 2

To a solution of diphenylmethylphosphine oxide (1.1 g, 5.0 mmol) in dry THF (25 cm^3), stirred at 0 °C under a stream of nitrogen, was added sodium borohydride (0.38 g, 10 mmol) and lithium aluminium hydride (0.38 g, 10 mmol). To the resulting mixture was added a solution of iodine (2.5 g, 10 mmol) in dry THF (25 cm^3) dropwise. On completion of addition the resultant mixture was heated at reflux for 18 h before allowing to cool to room temperature. The mixture was poured onto a mixture of ice (250 cm^3), saturated aqueous sodium potassium tartrate (50 cm^3) and sodium hydroxide (2.5M, 25 cm^3) and the resulting slurry stirred until the colour had dissipated. The mixture was extracted with diethyl ether (2 × 200 cm^3), the combined organic extracts dried (Na_2SO_4) and the solvents removed *in vacuo.* The residue was purified by flash chromatography (SiO_2, EtOAc-hexane 1:1) to give the phosphine borane **10** (0.80 g, 75%) as an oil. The spectroscopic data are consistent with that for the phosphine borane **10** prepared by Method 1.

Diphenylmethylphosphine sulfide 11

A solution of diphenylmethylphosphine (0.81 g, 4.0 mmol) in dry THF (20 cm^3), stirred at room temperature under argon, was treated with sulfur flowers (0.22 g, 0.86 mmol). The resulting mixture was left to stir until no more sulfur would dissolve, filtered and evaporated to yield the phosphine sulfide **11** (0.86 g, 92%) as a colourless oil; R_f 0.35 (EtOAc-hexane 1:3), $\nu_{max}(CH_2Cl_2)/cm^{-1}$ 3044 (C-H), 1437 (P-Ph) and 610 (P=S); δ_H(400 MHz; $CDCl_3$) 7.80 (4H, ddd, *J* 13.5, 8.0 and 1.5, Ph_2P *ortho*), 7.48-7.25 (6H, m, Ph_2P) and 2.27 (3H, d, *J* 13.0, Me); δ_C(100 MHz; $CDCl_3$) 133.8 (d, *J* 82.0, Ph C *ipso*), 131.5 (d, *J* 2.0, Ph CH *para*), 130.7 (d, *J* 10.5, Ph CH *ortho*), 128.7 (d, *J* 12.0, Ph CH *meta*) and 21.7 (d, *J* 59.5, Me); δ_P(162 MHz; $CDCl_3$) 36.5; *m/z* (ES) 232 (100%, M^+) (Found: 232.04682, M^+. $C_{13}H_{13}SP$ requires *M*, 232.04756). The spectroscopic data are consistent with that reported in the literature.[2]

Diphenyl(3-hydroxy-3-phenylpropyl)phosphine oxide 12

To a solution of diphenylmethylphosphine oxide (0.22 g, 1.0 mmol) in dry THF (5 cm^3), stirred at 0 ^oC under argon, was added butyllithium (2.0 mol dm^{-3} solution in hexane, 0.58 cm^3, 1.2 mmol) dropwise over 5 min to give a yellow solution. After 15 min, styrene oxide (0.14 cm^3, 1.2 mmol) was added dropwise. The resulting dark brown solution was allowed to warm to room temperature and stirred for a further 18 h, the colour fading. The reaction was quenched with saturated ammonium chloride (5 cm^3) and the resulting mixture washed with dichloromethane (3 × 10 cm^3). The combined organic layers were dried (Na_2SO_4) and the solvent removed *in vacuo*. The residue was purified using flash chromatography (SiO_2, EtOAc-MeOH, 9:1) to yield the phosphine oxide **12** (0.22 g, 65%) as prisms, mp 133-4 °C (from EtOAc) (lit.,[3] 141-3 °C); $\nu_{max}(CH_2Cl_2)/cm^{-1}$ 3600 (O-H), 3282 (O-H, br, H bonded), 3042 (C-H), 1603 (C=C, Ph) and 1438 (P-Ph); δ_H(400 MHz; $CDCl_3$) 7.72-7.66 (4H, m, PPh_2 *ortho*), 7.54-7.41 (6H, m, Ph), 7.32-7.20 (5H, m, Ph), 4.82 (1H, dt, 7.5 and 4.0, C*H*OH), 4.04 (1H, d, *J* 4.5, OH), 2.46-2.30 (2H, m, PCH_2) and 2.16-1.96 (2H, m, PCH_2CH_2); δ_C(100 MHz; $CDCl_3$) 144.0 (PhCH), 132.5 (d, *J* 99.0, PPh_2 C *ipso*), 132.3 (d, *J* 99.0, PPh_2 C *ipso*), 131.8 (Ph CH), 130.8 (d, *J* 9.0, PPh_2 CH *ortho*), 130.8 (d, *J* 9.0, PPh_2 CH *ortho*), 128.7 (d, *J* 11.5, PPh_2 CH *meta*), 128.4, 127.3 and 125.8 (Ph CH), 73.5 (d, *J* 9.5, CHOH), 31.4 (d, *J* 3.5, PCH_2CH_2) and 26.0 (d, *J* 71.5, PCH_2CH_2); δ_P(162 MHz; $CDCl_3$) 35.1; *m/z* (ES) 359 (100%, M) (Found: MNa^+, 359.11770. $C_{21}H_{21}O_2PNa$ requires *M*, 359.11768). The spectroscopic data are consistent with that reported in the literature.[3]

Diphenyl(3-hydroxy-3-phenylpropyl)phosphine borane 13

To a solution of diphenylmethylphosphine borane **10** (0.21 g, 1.0 mmol) in dry THF (5 cm^3), stirred at 0 °C under argon, was added butyllithium (2.0 mol dm^{-3} solution in hexane, 0.58 cm^3, 1.2 mmol) dropwise over 5 min to give a yellow solution. After 15 min, styrene oxide (0.14 cm^3, 1.2 mmol) was added dropwise. The resulting pale yellow solution was allowed to warm to room temperature and stirred for a further 18 h, the colour fading. The reaction was quenched with saturated NH_4Cl (5 cm^3) and the resulting mixture washed with dichloromethane (3 × 10 cm^3). The combined organic layers were dried (Na_2SO_4) and the solvent removed *in vacuo*. The residue was purified using flash chromatography (SiO_2, EtOAc-hexane, 1:4) to give the phosphine

borane **13** (0.27 g, 81%) as an oil; $\nu_{max}(CH_2Cl_2)/cm^{-1}$ 3597 (O-H), 3032 (C-H), 2386 (B-H), 1603 (C=C, Ph) and 1437 (P-Ph); δ_H(400 MHz; $CDCl_3$) 7.65-7.59 (4H, m, PPh_2 *ortho*), 7.49-7.39 (6H, m, Ph), 7.35-7.26 (5H, m, Ph), 4.76-4.72 (1H, m, C*H*OH), 2.46-2.35 (1H, m, PCH_AH$_B$), 2.26-2.15 (1H, m, PCH$_A$$H_B$), 2.02-1.87 (2H, m, PCH$_2CH_2$) 1.83 (1 H, d, *J* 3.5, OH) 1.4-0.5 (3H, br m, BH_3); δ_C(100 MHz; $CDCl_3$) 143.4 (Ph C *ipso*), 132.2, 132.1, 132.0, 131.1, 129.7, 128.8, 128.7, 128.6, 127.9 and 125.8 (Ph CH), 74.3 (d, *J* 13.5, CHOH), 32.0 (PCH$_2$*C*H$_2$) and 21.5 (d, *J* 38.0, P*C*H$_2$CH$_2$); δ_P(162 MHz; $CDCl_3$) 16.9 (m); *m/z* (ES) 357 (89%, MNa) and 343 (100%, MNa – BH_3) (Found: MNa^+, 357.15450. $C_{21}H_{24}OPBNa$ requires *M*, 357.15555).

Diphenyl(3-hydroxy-3-phenylpropyl)phosphine sulfide 14

To a solution of diphenylmethylphosphine sulfide **11** (0.23 g, 1.0 mmol) in dry THF (5 cm^3), stirred at 0 °C under argon, was added butyllithium (2.0 mol dm^{-3} solution in hexane, 0.58 cm^3, 1.2 mmol) dropwise over 5 min to give a yellow solution. After 15 min, styrene oxide (0.14 cm^3, 1.2 mmol) was added dropwise. The resulting red solution was allowed to warm to room temperature and stirred for a further 18 h, the colour fading. The reaction was quenched with saturated ammonium chloride (5 cm^3) and the resulting mixture washed with dichloromethane (3 × 10 cm^3). The combined organic layers were dried (Na_2SO_4) and the solvent removed *in vacuo*. The residue was purified using flash chromatography (SiO_2, EtOAc-hexane, 1:4) to yield the phosphine sulfide **14** (0.22 g, 61%) as an oil; $\nu_{max}(CH_2Cl_2)/cm^{-1}$ 3597 (O-H), 3391 (O-H, br, H bonded), 3042 (C-H), 1603 (C=C, Ph), 1437 (P-Ph) and 606 (P=S); δ_H(400 MHz; $CDCl_3$) 7.81-7.75 (4H, m, PPh_2 *ipso*), 7.50-7.40 (6H, m, Ph), 7.36-7.23 (5H, m, Ph), 4.79 (1H, dd, *J* 7.5 and 5.0, C*H*OH), 2.72-2.71 (1H, m, PCH_AH$_B$), 2.54-2.43 (1H, m, PCH$_A$$H_B$), 2.18-1.95 (2H, m, PCH$_2CH_2$) and 1.56 (1H, br s, OH); δ_C(125 MHz; $CDCl_3$) 143.5 (Ph C *ipso*), 133.0 (d, *J* 59.5, PPh_2 C *ipso*), 132.3 (d, *J* 59.5, PPh_2 C *ipso*), 131.4 (Ph CH), 131.1 (d, *J* 10.5, PPh_2 CH *ortho*), 131.0 (d, *J* 10.5, PPh_2 CH *ortho*), 128.6, 128.5, 127.7 and 125.7 (Ph CH), 73.8 (d, *J* 15.0, CHOH), 31.5 (PCH$_2$*C*H$_2$) and 28.5 (d, *J* 57.5, P*C*H$_2$CH$_2$); δ_P(162 MHz; $CDCl_3$) 43.7; *m/z* (ES) 375 (44%, MNa) (Found: MNa^+, 375.09470. $C_{21}H_{21}OPSNa$ requires *M*, 375.09484).

(3-Benzoyloxy-3-phenylpropyl)diphenylphosphine oxide 15

Method 1

To a solution of diphenyl(3-hydroxy-3-phenylpropyl)phosphine oxide **12** (0.17 g, 0.50 mmol) and DMAP (0.050 g, 0.40 mmol) in dry dichloromethane (5 cm^3), stirred at room temperature under argon, was added triethylamine (0.24 cm^3, 1.0 mmol) and benzoyl chloride (0.12 cm^3, 1.0 mmol). After 18 h the resulting yellow solution was quenched with water (1 cm^3), washed with water (10 cm^3) and the aqueous layer washed with EtOAc (2×25 cm^3). The combined organic layers were dried (Na_2SO_4) and evaporated under reduced pressure. The residue was purified *via* flash chromatography (SiO_2, EtOAc-MeOH 98:2) to give the ester **15** (0.19 g, 86%) as needles, mp 183-85 °C (from EtOAc); ν_{max} (CH_2Cl_2)/cm^{-1} 3068 (C-H), 1718 (C=O) and 1282 (P=O); δ_H(400 MHz; $CDCl_3$) 8.04 (2H, dd, *J* 8.5 and 1.5, Ph), 7.71-7.64 (4H, m, Ph), 7.56 (1H, tt, *J* 7.5 and 1.5, Ph), 7.53-7.40 (8H, m, Ph), 7.37-7.26 (5H, m, Ph), 6.02 (1H, dd, *J* 7.0 and 5.5, CHPh) and 2.44-2.19 (4H, m, C*H*$_2$C*H*$_2$); δ_C(100 MHz; $CDCl_3$) 165.6 (Ph*C*O_2), 139.4 (*Ph*CO_2 C *ipso*), 133.1 (Ph CH), 132.6 (d, *J* 98.5, PPh_2 C *ipso*), 132.4 (d, *J* 98.5, PPh_2 C *ipso*), 131.8 (Ph CH), 130.8 (d, *J* 9.0, PPh_2 CH *ortho*), 130.0 (Ph C *ipso*), 129.7 (Ph CH), 128.8-128.2 (m, Ph CH), 126.4 (Ph CH), 28.5 (PCH_2*C*H_2) and 25.8 (d, *J* 72.0, P*C*H_2); δ_P(162 MHz; $CDCl_3$) 32.7; *m/z* (ES) 463 (69%, MNa) (Found: MNa^+, 463.14580. $C_{28}H_{25}O_3PNa$ requires *M*, 463.14390). The spectroscopic data are consistent with that reported in the literature.[4]

Method 2

To a solution of diphenylmethylphosphine oxide (2.2 g, 10 mmol) in dry THF (50 cm^3), stirred at 0 °C under nitrogen, was added butyllithium (3.0 mol dm^{-3} solution in hexane, 3.3 cm^3, 10 mmol) dropwise and the resulting mixture stirred for 2 h before the addition of styrene oxide (1.4 cm^3, 12 mmol). The resulting mixture was allowed to warm to room temperature and stirred for a further 18 h before the addition of benzoyl chloride (2.9 cm^3, 25 mmol). The resulting mixture was allowed to stir for a further 48 h and then quenched with saturated ammonium chloride (2 cm^3). The solvent was removed *in vacuo* and the residue partitioned between water (50 cm^3) and dichloromethane (2×100 cm^3). The combined organic extracts were dried (Na_2SO_4), the solvents removed *in vacuo* and the residue purified by flash chromatography (SiO_2, CH_2Cl_2-MeOH 98:2) to

give the ester **15** (4.3 g, 97%) as needles. The spectroscopic data are consistent with that for the phosphine oxide **15** prepared by Method 1.

(3-Benzoyloxy-3-phenylpropyl)diphenylphosphine borane 16

Method 1

To a solution of diphenyl(3-hydroxy-3-phenylpropyl)phosphine borane **13** (0.17 g, 0.5 mmol) and DMAP (0.05 g, 0.4 mmol) in dry dichloromethane (5 cm^3), stirred at room temperature under argon, was added triethylamine (0.24 cm^3, 1.0 mmol) and benzoyl chloride (0.12 cm^3, 1.0 mmol). After 18 h the resulting yellow solution was quenched with water (1 cm^3), washed with water (10 cm^3) and the aqueous layer washed with EtOAc (2 × 25 cm^3). The combined organic layers were dried (Na_2SO_4) and evaporated under reduced pressure. The residue was purified *via* flash chromatography (SiO_2, EtOAc-hexane 1:3) to give the phosphine borane **16** (0.16 g, 73%) as prisms, mp 99-100 °C; $\nu_{max}(CH_2Cl_2)/cm^{-1}$ 3058 (C-H), 2384 (B-H) and 1719 (C=O); δ_H(400 MHz; $CDCl_3$)) 8.06 (2H, dd, *J* 8.5 and 1.5, COPh CH *ortho*), 7.64-7.55 (5H, m, Ph), 7.51-7.27 (13H, m, Ph), 6.02 (1H, dd, *J* 7.0 and 5.5, C*H*Ph), 2.38-2.11 (4H, m, CH_2CH_2), 1.4-0.6 (3H, br m, BH_3); δ_C(125 MHz; $CDCl_3$) 165.6 (Ph*C*O), 139.4 (Ph C *ipso*), 132.1 (d, *J* 9.0, PPh_2 CH *ortho*), 132.1 (d, *J* 9.0, PPh_2 CH *ortho*), 131.3 (Ph CH), 130.0 (Ph C *ipso*), 129.7 (Ph CH), 129.0 (d, *J* 55.0, PPh_2 C *ipso*), 128.9 (d, *J* 54.5, PPh_2 C *ipso*), 128.9 (d, *J* 10.0, PPh_2 CH *meta*), 128.7 (Ph CH), 128.5 (Ph CH), 128.3 (Ph CH), 126.4 (Ph CH), 76.3 (d, *J* 15.0, Ph*C*H), 29.9 (PCH_2*C*H_2) and 21.7 (d, *J* 38.0, P*C*H_2CH_2); δ_P(162 MHz; $CDCl_3$) 17.0 (m); *m/z* (ES) 461 (100%, MNa) (Found: MNa^+, 461.18230. $C_{28}H_{28}O_2PBNa$ requires *M*, 461.18177).

Method 2

To a solution of diphenylmethylphosphine borane **10** (2.1 g, 10 mmol) in dry THF (50 cm^3), stirred at 0 °C under nitrogen, was added butyllithium (3.0 mol dm^{-3} solution in hexane, 3.3 cm^3, 10 mmol) dropwise and the resulting mixture stirred for 2 h before the addition of styrene oxide (1.4 cm^3, 12 mmol). The resulting mixture was allowed to warm to room temperature and stirred for a further 18 h before the addition of benzoyl chloride (2.9 cm^3, 25 mmol). The resulting mixture was allowed to stir for a further 48 h and then quenched with

saturated ammonium chloride (2 cm^3). The solvent was removed *in vacuo* and the residue partitioned between water (50 cm^3) and dichloromethane (2 × 100 cm^3). The combined organic extracts were dried (Na_2SO_4), the solvents removed *in vacuo* and the residue purified by flash chromatography (SiO_2, EtOAc-hexane 1:4) and trituration with hexane to give the ester **16** (3.5 g, 81%) as an amorphous solid. The spectroscopic data are consistent with that for the phosphine borane **16** prepared by Method 1.

(3-Benzoyloxy-3-phenylpropyl)diphenylphosphine sulfide 17

Method 1

To a solution of diphenyl(3-hydroxy-3-phenylpropyl)phosphine sulfide **14** (0.18 g, 0.50 mmol) and DMAP (0.050 g, 0.40 mmol) in dry dichloromethane (5 cm^3), stirred at room temperature under argon, was added triethylamine (0.24 cm^3, 1.0 mmol) and benzoyl chloride (0.12 cm^3, 1.0 mmol). After 18 h the resulting yellow solution was quenched with water (1 cm^3), washed with water (10 cm^3) and the aqueous layer washed with EtOAc (2 × 25 cm^3). The combined organic layers were dried (Na_2SO_4) and evaporated under reduced pressure. The residue was purified *via* flash chromatography (SiO_2, EtOAc-hexane 1:3) to give the phosphine sulfide **17** (0.21 g, 92%) as prisms, mp 124-6 °C; $\nu_{max}(CH_2Cl_2)/cm^{-1}$ 3058 (C-H) and 1719 (C=O); δ_H(400 MHz; $CDCl_3$) 8.04 (2H, dd, *J* 8.5 and 1.0, CH *ortho* COPh), 7.79-7.71 (4H, m, Ph), 7.57 (1H, tt, *J* 7.5 and 1.5, CH *para*), 7.51-7.38 (8H, m, Ph), 7.36-7.26 (5H, m, Ph), 6.03 (1H, dd, *J* 7.5 and 5.5, C*H*Ph), 2.58-2.42 (2H, m, PCH_2) and 2.42-2.22 (2H, m, CH_2); δ_C(125 MHz; $CDCl_3$) 165.6 (Ph*C*O), 139.4 (Ph C *ipso*), 133.1 (Ph CH), 132.5 (d, *J* 79.5, PPh_2 C *ipso*), 132.3 (d, *J* 79.5, PPh_2 C *ipso*), 131.6 (Ph CH), 131.0 (d, *J* 10.0, PPh_2 CH), 130.0 (Ph C *ipso*), 129.7, 128.7, 128.6, 128.4, 128.3 and 126.4 (Ph CH), 76.1 (d, *J* 17.5, Ph*C*H), 29.3 (PCH_2CH_2) and 28.6 (d, *J* 59.5, PCH_2CH_2); δ_P(162 MHz; $CDCl_3$) 43.1; *m/z* (ES) 479 (100%, MNa), 335 (33%, M - $PhCO_2$) (Found: MNa^+, 479.12150. $C_{28}H_{25}O_2SPNa$ requires *M*, 479.12106).

Method 2

To a solution of diphenylmethylphosphine sulfide **11** (2.3 g, 10 mmol) in dry THF (50 cm^3), stirred at 0 °C under nitrogen, was added butyllithium (3.0 mol dm^{-3} solution in hexane, 3.3 cm^3, 10 mmol) dropwise and the

resulting mixture stirred for 2 h before the addition of styrene oxide (1.4 cm^3, 12 mmol). The resulting mixture was allowed to warm to room temperature and stirred for a further 18 h before the addition of benzoyl chloride (2.9 cm^3, 25 mmol). The resulting mixture was allowed to stir for a further 48 h and then quenched with saturated ammonium chloride (2 cm^3). The solvent was removed *in vacuo* and the residue partitioned between water (50 cm^3) and dichloromethane (2 × 100 cm^3). The combined organic extracts were dried (Na_2SO_4), the solvents removed *in vacuo* and the residue purified by trituration with ethyl acetate:hexane to give the ester **17** (2.9 g, 64%) as prisms. The spectroscopic data are consistent with that for the phosphine sulfide **17** prepared by Method 1.

(2*RS*,3*RS*,5*SR*)-2,5-Diphenyl-3-diphenylphosphinoyl-2-trimethylsilyloxytetrahydrofuran 18

A solution of LDA was prepared by the addition of *n*-butyllithium (2.5 mol dm^{-3} solution in hexane, 0.80 cm^3, 2.0 mmol) to a solution of di*iso*propylamine (0.31 cm^3, 2.2 mmol) in dry THF (5 cm^3), stirred at −78 °C under argon. After 30 min a solution of (3-benzoyloxy-3-phenylpropyl)diphenylphosphine oxide **15** (0.44 g, 1.0 mmol) and chlorotrimethylsilane (0.51 cm^3, 4.0 mmol) in dry THF (15 cm^3) was added *via* cannula. The resulting solution was allowed to warm to room temperature over 4 h and then stir at this temperature for a further 14 h. The mixture was quenched with silica (~2 g) and the THF evaporated *in vacuo*. The residue was purified by flash chromatography (SiO_2, EtOAc:hexane 3:1) to give the tetrahydrofuran **18** (0.43 g, 83%) as a white foam; $\nu_{max}(CH_2Cl_2)/cm^{-1}$ 3060 (C-H), 1605 (aryl-H), 1282 (P=O), 896 (Si-O) and 847 (Si-C); δ_H(400 MHz; $CDCl_3$) 7.76-7.67 (4H, m, Ph), 7.55-6.96 (16H, m, Ph), 5.69 (1H, dd, *J* 10.0 and 5.5, PhCH), 3.39 (1H, dt, *J* 11.0 and 3.5, PCH), 2.85 (1H, ddd, *J* 16.0, 13.0, 6.0 and 3.0, PCHC$H_A$$CH_B$), 2.40-2.26 (1H, m, PCHCH_ACH_B) and −0.04 (9H, s, $SiMe_3$); δ_C(125 MHz; $CDCl_3$) 145.7 (d, *J* 2.0, $PhCO_2$ C *ipso*), 140.7 (PhCH C *ipso*), 135.1 (d, *J* 96.5, P$Ph_A$$Ph_B$ C *ipso*), 134.1 (d, *J* 102.5, P$Ph_A$$Ph_B$ C *ipso*), 131.2 (d, *J* 9.5, P$Ph_A$$Ph_B$ CH *ortho*), 131.1 (d, *J* 2.5, P$Ph_A$$Ph_B$ CH *para*), 130.9 (d, *J* 3.0, P$Ph_A$$Ph_B$ CH *para*), 130.7 (d, *J* 8.0, P$Ph_A$$Ph_B$ CH *ortho*), 128.47 (d, *J* 11.0, P$Ph_A$$Ph_B$ CH *meta*), 128.46 (Ph CH), 127.9 (d, *J* 12.0, P$Ph_A$$Ph_B$ CH *meta*), 127.8 (Ph CH), 127.68 and 127.67 (Ph CH *para*), 126.1 and 125.6 (Ph CH), 108.1 (d, *J* 4.5, CO_2), 80.1 (d, *J* 2.5, Ph*C*H),

52.9 (d, *J* 72.0, PCH), 36.6 (CH_2) and 1.2 (Me); δ_P(162 MHz; $CDCl_3$) 27.6; m/z (ES) 535 (100%, M + Na), 423 (65%, M – $OSiMe_3$) (Found: MNa^+, 535.18460. $C_{31}H_{33}O_3PSiNa$ requires M, 535.18343).

(3-Benzoyloxy-3-phenyl-3-trimethylsilylpropyl)diphenylphosphine borane 19

A solution of LDA was prepared by the addition of butyllithium (3.0 mol dm^{-3} solution in hexane, 0.67 cm^3, 2.0 mmol) to a solution of di*iso*propylamine (0.31 cm^3, 2.2 mmol) in dry THF (5 cm^3), stirred at −78 °C under argon. After 1 h a solution of (3-benzoyloxy-3-phenylpropyl)diphenylphosphine borane **16** (0.44 g, 1.0 mmol) and chlorotrimethylsilane (0.51 cm^3, 4.0 mmol) in dry THF (15 cm^3) was added *via* cannula. The resulting solution was allowed to warm slowly to 0 °C over 18 h. The mixture was quenched with silica (~2 g) and the THF evaporated *in vacuo*. The residue was purified by flash chromatography (SiO_2, EtOAc:hexane 1:3) to give the silane **19** (0.14 g, 27%) as an oil; ν_{max}(film)/cm^{-1} 2954 (C-H), 2380 (B-H), 1712 (C=O), 1601 (C=C, Ph) and 1437 (P-Ph); δ_H(500 MHz; $CDCl_3$) 8.10-8.08 (2H, m, $PhCO_2$ *ortho*), 7.61 (1H, tt, *J* 7.5 and 2.0, $PhCO_2$ *para*), 7.59-7.48 (6H, m, PPh_2 *ortho* and $PhCO_2$), 7.46-7.41 (2H, m, PPh_2 *para*), 7.38-7.31 (6H, m, PPh_2 *meta* and PhCSi), 7.21 (1H, tt, *J* 7.5 and 1.0, PhCSi *para*), 7.13-7.11 (2H, m, PhCSi), 2.75 (1H, dddd, *J* 15.0, 12.5, 6.0 and 4.0, $PCH_2CH_AH_B$), 2.41 (1H, dddd, *J* 15.0, 12.5, 7.5 and 3.0, $PCH_2CH_AH_B$), 2.31-2.20 (1H, m, PCH_AH_B), 2.16-2.09 (1H, m, PCH_AH_B), 1.42-0.75 (3H, m, BH_3) and −5.52 (9H, Me); δ_C(125 MHz; $CDCl_3$) 165.9 (CO_2), 141.3 ($PhCO_2$ C *ipso*), 133.1 ($PhCO_2$ CH *para*), 132.1 (d, *J* 9.0, PPh_APh_B CH *ortho*), 132.0 (d, *J* 9.0, PPh_APh_B CH *ortho*), 131.2 (d, *J* 2.5, PPh_APh_B CH *para*), 131.1 (d, *J* 2.5, PPh_APh_B CH *para*), 130.4 (PhCSi C *ipso*), 129.6 ($PhCO_2$ CH *ortho*), 129.3 (d, *J* 55.0, PPh_APh_B C *ipso*), 129.0 (d, *J* 54.5, PPh_APh_B C *ipso*), 128.8 (d, *J* 10.0, PPh_APh_B CH *meta*), 128.7 (d, *J* 10.0, PPh_APh_B CH *meta*), 128.6 ($PhCO_2$ CH *meta*), 128.3 (PhCSi CH), 126.0 (PhCSi CH *para*), 125.0 (PhCSi CH), 83.2 (d, *J* 12.0, Ph*C*Si), 28.4 (d, *J* 2.0, PCH_2CH_2), 19.6 (d, *J* 37.0, PCH_2) and −1.5 (Me); δ_P(162 MHz; $CDCl_3$) 17.4-17.1 (m); *m/z* (ESI) 533 (100%, MNa^+) (Found: MNa^+, 533.22090. $C_{31}H_{36}O_2PBSiNa$ requires *M*, 533.22129).

(3-Benzoyloxy-3-phenyl-3-trimethylsilylpropyl)diphenylphosphine sulfide 20

A solution of LDA was prepared by the addition on butyllithium (3.0 mol dm^{-3} solution in hexane, 0.67 cm^3, 2.0 mmol) to a solution of di*iso*propylamine (0.31 cm^3, 2.2 mmol) in dry THF (5 cm^3), stirred at −78 °C under argon. After 1 h a solution of (3-benzoyloxy-3-phenylpropyl)diphenylphosphine sulfide **17** (0.46 g, 1.0 mmol) and chlorotrimethylsilane (0.51 cm^3, 4.0 mmol) in dry THF (15 cm^3) was added *via* cannula. The resulting solution was allowed to warm slowly to 0 °C over 18 h. The mixture was quenched with silica (~2 g) and the THF evaporated *in vacuo*. The residue was purified by flash chromatography (SiO_2, EtOAc:hexane 1:7) to give the silane **20** (0.14 g, 26%) as an oil; ν_{max}(film)/cm^{-1} 2955 (C-H), 1713 (C=O), 1601 (C=C, Ph) and 1437 (P-Ph); δ_H(500 MHz; $CDCl_3$) 8.11-8.09 (2H, m, $PhCO_2$ *ortho*), 7.75-7.65 (4H, m, PPh_2 *ortho*), 7.62 (2H, tt, *J* 7.5 and 1.5, $PhCO_2$ *para*), 7.48-7.20 (9H, m, PPh_2 *para*, PhCSi, PPh_2 *meta* and PhCSi *para*), 7.18-7.16 (2H, m, PhCSi), 2.90-2.83 (1H, m, $PCH_2CH_AH_B$), 2.62-2.35 (3H, m, PCH_2 and $PCH_2CH_AH_B$) and 0.01 (9H, Me); δ_C(125 MHz; $CDCl_3$) 165.9 (CO_2), 141.3 ($PhCO_2$ C *ipso*), 133.2 ($PhCO_2$ CH *para*), 132.8 (d, *J* 80.0, PPh_APh_B C *ipso*), 132.4 (d, *J* 79.5, PPh_APh_B C *ipso*), 131.5 (d, *J* 3.0, PPh_APh_B CH *para*), 131.4 (d, *J* 3.0, PPh_APh_B CH *para*), 131.0 (d, *J* 10.0, PPh_2 CH *ortho*), 130.5 (PhCSi C *ipso*), 129.7 ($PhCO_2$ CH *ortho*), 128.61 (d, *J* 12.0, PPh_APh_B CH *meta*), 128.62 ($PhCO_2$ CH *meta*), 128.58 (d, *J* 12.0, PPh_APh_B CH *meta*), 128.3 (PhCSi CH), 126.1 (PhCSi CH *para*), 125.1 (PhCSi CH), 83.1 (d, *J* 13.5, Ph*C*Si), 27.7 (PCH_2CH_2), 26.5 (d, *J* 56.5, PCH_2) and −1.5 (Me); δ_P(162 MHz; $CDCl_3$) 44.2; *m/z* (ESI) 551 (100%, M^+) (Found: MNa^+, 551.16000. $C_{31}H_{33}O_2PSSiNa$ requires *M*, 551.16058).

Diphenyl(3-hydroxypropyl)phosphine borane 22

Method 1

Lithium borohydride (2.0 mol dm^{-3} solution in THF, 0.55 cm^3, 1.1 mmol) was added to a stirred solution of methyl 3-(boronatodiphenylphosphinyl)propionate **21** (0.29 g, 1.0 mmol) in dry diethyl ether (20 cm^3) under argon at 0 °C. After 18 h at room temperature the mixture was treated with 2.5N sodium hydroxide (5 cm^3) and stirred until both layers were clear. The mixture was partitioned between Et_2O (2 × 50 cm^3) and water (30 cm^3) and the organic layer dried (Na_2SO_4) and evaporated give the alcohol **22** (0.27 g, >95%) as an oil; R_f(EtOAc-

hexane, 1:1) 0.30; ν_{max}(film)/cm^{-1} 3379 (br, O-H), 2941 (C-H), 2384 (B-H) and 1436 (P-Ph); δ_H(500 MHz; $CDCl_3$) 7.70-7.65 (4H, m, Ph *ortho*), 7.49-7.41 (6H, m, Ph), 3.67 (2H, t, *J* 6.0, CH_2O), 2.35-2.29 (2H, m, PCH_2), 1.76 (2H, qt, *J* 8.5 and 6.0, PCH_2CH_2) and 1.28-0.64 (3H, m, BH_3); δ_C(125 MHz; $CDCl_3$) 132.1 (d, *J* 9.0, Ph CH *ortho*), 131.2 (d, *J* 2.5, Ph CH *para*), 129.3 (d, *J* 55.0, Ph C *ipso*), 128.8 (d, *J* 10.0, Ph CH *meta*), 62.8 (d, *J* 14.5, CH_2O), 26.2 (PCH_2CH_2) and 22.0 (d, *J* 38.0, PCH_2); δ_P(162 MHz; $CDCl_3$) 16.9-16.5 (m); *m/z* (ES) 258 (70%, M), 244 (62, M − BH_3), 226 (34, M − BH_3 − H_2O), 199 (100, Ph_2PCH_2), 185 (62, Ph_2P) and 108 (61, PPh) (Found: M^+, 258.13335. $C_{15}H_{20}OPB$ requires *M*, 258.13448). The spectroscopic data are consistent with that reported in the literature.[5]

Method 2

To a solution of methyl 3-diphenylphosphinoyl-propionate **21** (7.2 g, 25 mmol) in dry THF (125 cm^3), stirred at 0 °C under a stream of nitrogen, was added lithium aluminium hydride (0.95 g, 25 mmol) and the resulting mixture stirred for 1 h before the addition of further lithium aluminium hydride (1.9 g, 50 mmol) and sodium borohydride (1.9 g, 50 mmol). A solution of iodine (13 g, 50 mmol) in dry THF (125 cm^3) was added dropwise and, on completion of addition, the mixture was heated at reflux for 84 h. The cooled solution was poured onto a mixture of ice (500 cm^3), saturated aqueous sodium potassium tartrate (100 cm^3) and sodium hydroxide (2.5 M, 50 cm^3) and the resulting mixture stirred until the colour had dissipated. The mixture was extracted with diethyl ether (2 × 500 cm^3), the combined organic extracts dried (Na_2SO_4) and the solvents removed *in vacuo*. The residue was purified by flash chromatography (SiO_2, EtOAc-hexane 1:1) to give the alcohol **22** (2.9 g, 44%) as an amorphous solid, mp 48-9 °C. The spectroscopic data are consistent with that for the phosphine borane **22** prepared by Method 1.

Diphenyl(3-hydroxypropyl)phosphine oxide 24

To a mixture of triphenylphosphine (6.6 g, 25 mmol) and sodium iodide (3.7 g, 25 mmol) in acetonitrile (100 cm^3) was added 3-chloropropan-1-ol (2.1 cm^3, 25 mmol). The resultant mixture was heated at reflux for 15 h and the solvent removed *in vacuo*. The residue was treated with potassium hydroxide (30%, 50 cm^3) and

methanol (20 cm^3) and the resulting solution heated at reflux for 24 h. The mixture was treated with saturated aqueous ammonium chloride (30 cm^3) and dilute HCl (3N, 5 cm^3) and extracted with ethyl acetate (2 × 200 cm^3). The combined organic extracts were dried (Na_2SO_4) and the solvents removed *in vacuo* to give an oil. The oil was triturated with diethyl ether to give the alcohol **24** (3.9 g, 60%) as prisms mp 95-6 °C (from EtOAc) (lit.,[6] 99.5-100.5 °C). The mother liquors were filtered through a pad of silica (EtOAc) to yield a further batch of the alcohol (1.8 g, 27%, 87% overall); ν_{max}(film)/cm^{-1} 3338 (br, O-H), 2933 (C-H), 1591 (C=C, Ph) and 1437 (P-Ph); δ_H(500 MHz; $CDCl_3$) 7.76-7.71 (4H, m, Ph *ortho*), 7.52 (2H, tq, *J* 7.5 and 1.5, Ph *para*), 7.48-7.44 (4H, m, Ph *meta*), 3.70 (2H, t, *J* 5.5, CH_2O), 2.41 (2H, dt, *J* 11.5 and 7.0, PCH_2) and 1.88 (2H, dtt, *J* 15.5, 7.5 and 5.5, PCH_2CH_2), OH peak not observed; δ_C(125 MHz; $CDCl_3$) 132.3 (d, *J* 99.0, Ph C *ipso*), 131.9 (d, *J* 3.0, Ph CH *para*), 130.8 (d, *J* 9.5, Ph CH *ortho*), 128.7 (d, *J* 11.5, Ph CH *meta*), 62.5 (d, *J* 9.0, CH_2O), 27.7 (d, *J* 71.5, PCH_2) and 25.5 (d, *J* 4.5, PCH_2CH_2); δ_P(162 MHz; $CDCl_3$) 35.3; *m/z* (EI) 260 (30%, M^+), 242 (16, M - H_2O), 215 (100, $Ph_2P(O)CH_2$), 202 (90, Ph_2POH), 201 (88, Ph_2PO) and 183 (38, M – Ph) (Found: M^+, 260.09749. $C_{15}H_{17}O_2P$ requires *M*, 260.09667). The spectroscopic data are consistent with that reported in the literature.[6]

Diphenyl(3-hydroxypropyl)phosphine sulfide 23

By a modification of the method of Pellon,[7] a mixture of diphenyl(3-hydroxypropyl)phosphine borane **22** (2.4 g, 9.3 mmol), DABCO (1.0 g, 9.3 mmol) and sulfur flowers (0.30 g, 1.2 mmol) was treated with toluene (50 cm^3) and the resulting mixture stirred at 40 °C for 4 h. The mixture was treated with ethyl acetate (50 cm^3) and washed with pH2 buffer (0.5 M H_2SO_4, 1.5 M Na_2SO_4 in water, 50 cm^3). The organic layer was dried (Na_2SO_4), the solvent removed *in vacuo* and the residue recrystallised from ethyl acetate to give the phosphine sulfide **420c** (1.6 g, 64%) as needles mp 100-2 °C (from EtOAc) (lit.,[8] 105-107 °C); ν_{max}(film)/cm^{-1} 3411 (br, O-H), 2939 (C-H) and 1436 (P-Ph); δ_H(500 MHz; $CDCl_3$) 7.82-7.78 (4H, m, Ph *ortho*), 7.47-7.39 (6H, m, Ph), 3.62 (2 H, t, *J* 6.0, CH_2O), 2.58-2.52 (2H, m, PCH_2) and 1.85-1.77 (2H, m, PCH_2CH_2); δ_C(125 MHz; $CDCl_3$) 132.6 (d, *J* 89.0, Ph C *ipso*), 131.5 (d, *J* 3.0, Ph CH *para*), 131.1 (d, *J* 10.0, Ph CH *ortho*), 128.7 (d, *J* 12.0, Ph

CH *meta*), 62.2 (d, *J* 16.0, CH_2O), 29.2 (d, *J* 57.5, PCH_2) and 25.5 (d, *J* 2.5, PCH_2CH_2); δ_P(162 MHz; $CDCl_3$) 43.7; *m/z* (EI) 276 (20%, M^+), 258 (50, M - H_2O), 231 (65, $Ph_2P(S)CH_2$), 218 (100, Ph_2PSH), 199 (55, M - Ph), 185 (74, Ph_2P) and 140 (PhPS) (Found: M^+, 276.07434. $C_{15}H_{17}OPS$ requires *M*, 276.07377). The ^{31}P NMR spectrum is consistent with that reported in the literature.[8]

(3-Benzoyloxypropyl)diphenylphosphine oxide 25

To a solution of diphenyl(3-hydroxypropyl)phosphine oxide **24** (2.6 g, 10 mmol) in dry THF (50 cm^3) stirred at 0 °C under nitrogen, was added butyllithium (3.5 mol dm^{-3} solution in hexane, 2.9 cm^3, 10 mmol) dropwise. Benzoyl chloride (1.2 cm^3, 10 mmol) was added dropwise and the resulting mixture stirred for 2 h. The THF was removed *in vacuo*, the residue partitioned between ethyl acetate (100 cm^3) and water (50 cm^3). The organic layer was dried (Na_2SO_4) and the solvent removed *in vacuo* to give an amorphous solid. The solid was recrystallised from ethyl acetate to give the ester **25** (2.8 g, 76%) as needles mp 124-5 °C (from EtOAc) (lit.,[6] 127-8.5 °C); ν_{max}(film)/cm^{-1} 2959 (C-H), 1714 (C=O), 1602 (C=C, Ph) and 1438 (P-Ph); δ_H(400 MHz; $CDCl_3$) 8.01-7.98 (2H, m, $PhCO_2$ *ortho*), 7.78-7.72 (4H, m, PPh_2), 7.57-7.41 (9H, m, Ph), 4.36 (2H, t, *J* 6.5, CH_2O), 2.44-2.37 (2H, m, PCH_2) and 2.15-2.06 (2H, m, PCH_2CH_2); δ_C(100 MHz; $CDCl_3$) 166.4 (CO_2), 133.0 ($PhCO_2$ CH *para*), 132.7 (d, *J* 98.5, PPh_2 C *ipso*), 131.8 (d, *J* 3.0, PPh_2 CH *para*), 130.8 (d, *J* 9.5, PPh_2 CH *ortho*), 130.0 ($PhCO_2$ C *ipso*), 129.5 ($PhCO_2$ CH), 128.7 (d, *J* 11.5, PPh_2 CH *meta*), 128.4 ($PhCO_2$ CH), 64.8 (d, *J* 15.5, CH_2O), 26.5 (d, *J* 72.5, PCH_2) and 21.4 (d, *J* 3.0, PCH_2CH_2); δ_P(162 MHz; $CDCl_3$) 32.4; *m/z* (ESI) 387 (100%, MNa^+) (Found: MNa^+, 387.11260. $C_{22}H_{21}O_3PNa$ requires *M*, 387.11260). The spectroscopic data are consistent with that reported in the literature.[6]

(3-Benzoyloxypropyl)diphenylphosphine borane 26

Method 1

Benzoyl chloride (0.21 cm^3, 1.8 mmol) was added to a stirred solution of diphenyl(3-hydroxypropyl)phosphine borane **22** (0.24 g, 0.92 mmol), DMAP (0.05 g, 0.4 mmol) and triethylamine (0.26 cm^3, 1.8 mmol) in

dichloromethane (10 cm^3) at room temperature under argon. After 18 h the mixture was quenched with water (1 cm^3) and washed with water (20 cm^3). The aqueous layer was extracted with EtOAc (2 × 50 cm^3) and the combined organic layers dried (Na_2SO_4) and evaporated under reduced pressure. The residue was purified *via* flash chromatography (SiO_2, EtOAc-hexane, 2:3) to give the ester **26** (0.23 g, 69%) as an oil; R_f(EtOAc-hexane, 1:1) 0.55; ν_{max}(film)/cm^{-1} 2925 (C-H), 2381 (B-H), 1716 (C=O), 1602 and 1585 (C=C, Ph) and 1437 (P-Ph); δ_H(500 MHz; $CDCl_3$) 8.02-8.00 (2H, m, COPh *ortho*), 7.70-7.66 (4H, m, PPh_2 *ortho*), 7.56 (1H, tt, *J* 7.5 and 1.0, Ph *para*), 7.50-7.41 (8H, m, Ph), 4.33 (2H, t, *J* 6.0, CH_2O), 2.38-2.33 (2H, m, PCH_2), 2.04-1.97 (2H, m, PCH_2CH_2) and 1.32-0.71 (3H, m, BH_3); δ_C(125 MHz; $CDCl_3$) 166.4 (CO_2), 133.1 ($PhCO_2$ CH *para*), 132.1 (d, *J* 9.0, PPh_2 CH *ortho*), 131.3 (d, *J* 2.5, PPh_2 CH *para*), 130.0 ($PhCO_2$ C *ipso*), 129.6 ($PhCO_2$ CH), 129.0 (d, *J* 55.0, PPh_2 C *ipso*), 128.9 (d, *J* 10.0, PPh_2 CH *meta*), 128.4 ($PhCO_2$ CH), 64.8 (d, *J* 15.0, CH_2O), 22.8 (PCH_2CH_2) and 22.5 (d, *J* 38.0, PCH_2); δ_P(162 MHz; $CDCl_3$) 17.0-16.6 (m); *m/z* (ESI) 385 (75%, MNa) and 371 (100, MNa - BH_3) (Found: MNa^+, 385.15120. $C_{22}H_{24}O_2PBNa$ requires *M*, 385.15047).

Method 2

To a solution of diphenyl(3-hydroxypropyl)phosphine borane **22** (2.9 g, 11 mmol) in dry THF, stirred at 0 °C under argon, was added *n*-butyllithium (3.5 mol dm^{-3} solution in hexane, 3.2 cm^3, 11 mmol). Benzoyl chloride (1.3 cm^3, 11 mmol) was added and the resulting mixture stirred for 16 h. The THF was removed *in vacuo* and the residue partitioned between ethyl acetate (100 cm^3) and water (50 cm^3). The organic layer was dried (Na_2SO_4), the solvent removed *in vacuo* and the residue purified by flash chromatography (SiO_2, EtOAc-hexane 1:4) to give the ester **26** (3.4 g, 83%) as an amorphous solid mp 68-9 °C. The spectroscopic data are consistent with that for the phosphine borane **26** prepared by Method 1.

(3-Benzoyloxypropyl)diphenylphosphine sulfide 27

To a solution of diphenyl(3-hydroxypropyl)phosphine sulfide **27** (1.4 g, 5.0 mmol) in dry THF (25 cm^3) stirred at 0 °C under nitrogen, was added *n*-butyllithium (3.5 mol dm^{-3} solution in hexane, 1.4 cm^3, 5.0 mmol) dropwise. Benzoyl chloride (0.58 cm^3, 10 mmol) was added dropwise and the resulting mixture stirred for 2 h.

The THF was removed *in vacuo*, the residue partitioned between ethyl acetate (50 cm^3) and water (25 cm^3). The organic layer was dried (Na_2SO_4) and the solvent removed *in vacuo*. The solid was purified by flash chromatography (SiO_2, EtOAc-hexane 1:4) to give the *ester* **27** (1.6 g, 83%) as an amorphous solid mp 94-5 °C; ν_{max}(film)/cm^{-1} 2958 (C-H), 1714 (C=O), 1601 and 1585 (C=C, Ph)) and 1436 (P-Ph); δ_H(500 MHz; $CDCl_3$) 8.00-7.98 (2H, m, $PhCO_2$ *ortho*), 7.85-7.81 (4H, m, PPh_2), 7.57-7.53 (1H, m, $PhCO_2$ *para*), 7.50-7.41 (8H, m, Ph), 4.35 (2H, t, *J* 6.5, CH_2O), 2.62-2.55 (2H, m, PCH_2) and 2.15-2.07 (2H, m, PCH_2CH_2); δ_C(125 MHz; $CDCl_3$) 166.4 (CO_2), 133.1 ($PhCO_2$ CH *para*), 132.5 (d, *J* 80.0, PPh_2 C *ipso*), 131.6 (d, *J* 3.0, PPh_2 CH *para*), 131.0 (d, *J* 10.0, PPh_2 CH *ortho*), 130.0 ($PhCO_2$ C *ipso*), 129.5 ($PhCO_2$ CH), 128.7 (d, *J* 12.0, PPh_2 CH *meta*), 128.4 ($PhCO_2$ CH), 64.6 (d, *J* 17.5, CH_2O), 29.4 (d, *J* 57.5, PCH_2) and 22.2 (d, *J* 1.5, PCH_2CH_2); δ_P(162 MHz; $CDCl_3$) 43.1; *m/z* (EI) 380 (32%, M^+), 275 (9, M − PhCO), 218 (100, Ph_2PSH), 185 (51, Ph_2P), 140 (43, PhPS) and 105 (68, PhCO) (Found: M^+, 380.10015. $C_{22}H_{21}O_2PS$ requires *M*, 380.09999).

(2*RS*,3*RS*)-3-Diphenylphosphinoyl-2-phenyl-2-trimethylsilyloxytetrahydrofuran 28 and

4,5-Dihydro-3-diphenylphosphinoyl-2-phenyl-4-trimethylsilyl-furan 29

A solution of LDA (1.8 mol dm^{-3} solution in heptane:THF:ethylbenzene, 1.1 cm^3, 2.0 mmol) was added to a solution of (3-benzoyloxypropyl)diphenylphosphine oxide **25** (0.36 g, 1.0 mmol) and chlorotrimethylsilane (0.51 cm^3, 4.0 mmol) in dry THF (20 cm^3), stirred at −78 °C under argon, *via* cannula. The resulting solution was allowed to warm to room temperature over 4 h and then stirred at this temperature for a further 14 h. The mixture was quenched with silica (~2 g) and the THF evaporated *in vacuo*. The residue was purified by flash chromatography (SiO_2, EtOAc:hexane 3:1) to give the phosphine oxide **28** (0.16 g, 37%) as an oil; R_f(EtOAc-hexane, 3:1) 0.35; ν_{max}(film)/cm^{-1} 2963 (C-H), 1594 (C=C, Ph) and 1438 (P-Ph); δ_H(500 MHz; $CDCl_3$) 7.72-7.68 (2H, m, Ph), 7.62-7.58 (2H, m, Ph), 7.44-7.35 (4H, m, PPh_2), 7.30-7.27 (2H, m, Ph), 7.16 (1H, tt, *J* 6.5 and 1.5, Ph *para*), 7.13-7.08 (2H, m, PPh_2), 7.02-7.00 (2H, m, Ph), 4.38 (1H, td, *J* 7.5 and 6.0, CH_AH_BO), 4.17 (1H, q, *J* 7.5, CH_AH_BO), 3.16 (1H, td, *J* 8.5 and 4.5, PCH), 2.64 (1H, ddq, *J* 14.5, 13.0 and 7.0, $PhCHCH_AH_B$), 2.32-2.23 (1H, m, $PhCHCH_AH_B$) and −0.01 (9H, Me); δ_C(125 MHz; $CDCl_3$) 145.0 (PhC C *ipso*), 134.6 (d, *J* 97.5,

P*Ph*$_A$Ph$_B$ C *ipso*), 133.0 (d, *J* 101.0, PPh$_A$*Ph*$_B$ C *ipso*), 131.3 (d, *J* 9.5, P*Ph*$_A$Ph$_B$ CH *ortho*), 131.1 (d, *J* 2.5, P*Ph*$_A$Ph$_B$ CH *para*), 130.9 (d, *J* 3.0, PPh$_A$*Ph*$_B$ CH *para*), 130.8 (d, *J* 8.5, PPh$_A$*Ph*$_B$ CH *ortho*), 128.4 (d, *J* 11.0, P*Ph*$_A$Ph$_B$ CH *meta*), 127.8 (d, *J* 12.0, PPh$_A$*Ph*$_B$ CH *meta*), 127.6 (PhC CH), 127.4 (PhC CH *para*), 125.7 (PhC CH), 108.1 (d, *J* 2.5, CO_2), 68.6 (d, *J* 8.5, CH_2O), 52.6 (d, *J* 74.0, PCH), 28.0 (PCH*C*H$_2$) and 1.1 (SiMe$_3$); δ_P(162 MHz; $CDCl_3$) 22.3; *m/z* (EI) 459 (100%, MNa^+), 387 (47, MHNa – SiMe$_3$) and 369 (100, MHNa – OSiMe$_3$) (Found: MNa^+, 459.15490. $C_{25}H_{29}O_3PSiNa$ requires *M*, 459.15213) and the vinyl phosphine oxide **29** (0.080 g, 19%) as an amorphous solid mp 175-6 °C; R_f(EtOAc-hexane, 3:1) 0.55; ν_{max}(film)/cm^{-1} 2957 (C-H), 1587 and 1567 (C=C, Ph) and 1437 (P-Ph); δ_H(500 MHz; $CDCl_3$) 7.88-7.84 (2H, m, P*Ph*$_A$Ph$_B$ *ortho*), 7.65-7.61 (2H, m, PPh$_A$*Ph*$_B$ *ortho*), 7.47-7.46 (2H, m, PhC), 7.42-7.39 (3H, m, P*Ph*$_A$Ph$_B$ *meta* and *para*), 7.08-6.95 (6H, m, PhC and PPh$_A$*Ph*$_B$ *meta* and *para*), 4.72 (1H, dd, *J* 10.0 and 8.0, C*H*$_A$H$_B$O), 4.62 (1H, ddd, *J* 8.0, 3.0 and 1.0, CH$_A$*H*$_B$O), 2.34 (1 H, dt, *J* 10.0 and 3.5, C*H*SiMe$_3$) and 0.05 (9H, SiMe$_3$); δ_C(125 MHz; $CDCl_3$) 165.8 (d, *J* 20.0, Ph*C*O), 134.6 (d, *J* 107.5, P*Ph*$_A$Ph$_B$ C *ipso*), 133.6 (d, *J* 107.0, PPh$_A$*Ph*$_B$ C *ipso*), 131.5 (d, *J* 9.0, PPh$_A$*Ph*$_B$ CH *ortho*), 131.4 (d, *J* 9.0, P*Ph*$_A$Ph$_B$ CH *ortho*), 130.9 (d, *J* 2.5, P*Ph*$_A$Ph$_B$ CH *para*), 130.4 (d, *J* 2.5, PPh$_A$*Ph*$_B$ CH *para*), 130.0 (d, *J* 0.5, Ph C *ipso*), 129.8 (Ph CH *para*), 129.3 (Ph CH), 128.3 (d, *J* 12.0, P*Ph*$_A$Ph$_B$ CH *meta*), 127.5 (d, *J* 12.5, PPh$_A$*Ph*$_B$ CH *meta*), 127.4 (Ph CH), 103.2 (d, J 118.5, P*C*=C), 73.6 (d, *J* 11.0, CH_2O), 36.6 (d, *J* 10.5, CHSi) and -2.9 (SiMe$_3$); δ_P(162 MHz; $CDCl_3$) 17.7; *m/z* (ESI) 441 (100%, MNa^+) and 419 (37, MH^+) (Found: MNa^+, 441.14300. $C_{25}H_{27}O_2PSiNa$ requires *M*, 441.14156).

N,*N*-Di*iso*propylbenzamide **30**

To a mixture of potassium carbonate (0.14 g, 1.0 mmol) and di*iso*propylamine (0.14 cm^3, 1.0 mmol) in dichloromethane (10 cm^3), stirred at room temperature under argon, was added benzoyl chloride (0.12 cm^3, 1.0 mmol). After 22 h the mixture was washed with water (10 cm^3), dried (Na_2SO_4), the solvent removed and the residue recrystallised from ethyl acetate to give the benzamide **30** (0.082 g, 40%) as plates, mp 64-5 °C (lit.,[9] 67-8 °C); ν_{max}(film)/cm^{-1} 2969 (C-H), 1625 (C=O) and 1599 (C=C, Ph); δ_H(400 MHz; $CDCl_3$) 7.38-7.34 (3H, m, Ph), 7.31-7.28 (2H, m, Ph), 3.89-3.46 (2H, br m, NCH) and 1.62-1.07 (12H, br m, Me); δ_C(100 MHz;

$CDCl_3$) 171.0 (CO), 138.9 (Ph C *ipso*), 128.6 (Ph CH *para*), 128.4 and 125.6 (Ph CH) and 20.7 (Me); δ_P(162 MHz; $CDCl_3$); *m/z* (EI) 205 (22%, M), 190 (5, M – Me), 162 (22, M – ^iPr), 119 (22, PhCON), 105 (100, PhCO) and 77 (7, Ph) (Found: M^+, 205.14679. $C_{13}H_{19}NO$ requires *M*, 205.14666). The spectroscopic data are consistent with that reported in the literature,[9] although N*C*Me_2 carbons were not observed in the ^{13}C NMR spectrum, presumably due to slow OC-N rotation.

(2*RS*,3*RS*)-3-Diphenylphosphinothioyl-2-phenyl-2-trimethylsilyloxytetrahydrofuran 31 and Diphenyl(1-trimethylsilyl-3-trimethylsilyloxypropyl)phosphine sulfide 32

A solution of LDA (1.8 mol dm^{-3} solution in heptane:THF:ethylbenzene, 1.1 cm^3, 2.0 mmol) was added to a solution of (3-benzoyloxypropyl)diphenylphosphine sulfide **27** (0.38 g, 1.0 mmol) and chlorotrimethylsilane (0.51 cm^3, 4.0 mmol) in dry THF (20 cm^3), stirred at −78 °C under argon, *via* cannula. The resulting solution was allowed to warm to room temperature over 4 h and then stir at this temperature for a further 14 h. The mixture was quenched with silica (~2 g) and the THF evaporated *in vacuo*. The residue was purified by flash chromatography (SiO_2, EtOAc:hexane 1:6) to give the phosphine sulfide **31** (0.15 g, 34%) as prisms mp 113-4 °C (from heptane); ν_{max}(film)/cm^{-1} 2956 (C-H) 1628 (C=C, Ph) and 1437 (P-Ph); δ_H(500 MHz; $CDCl_3$) 7.79-7.74 (2H, m, PPh_A*Ph*$_B$ *ortho*), 7.72-7.68 (2H, m, P*Ph*$_A$$Ph_B$ *ortho*), 7.41-7.32 (4H, m, PPh_A*Ph*$_B$ *meta* and PPh_2 *para*), 7.25 (2H, td, *J* 7.5 and 3.0, P*Ph*$_A$$Ph_B$ *meta*), 7.14 (1H, tt, *J* 7.5 and 1.5, Ph *para*), 7.07 (2H, t, *J* 7.5, Ph *meta*), 6.90-6.87 (2H, m, Ph *ortho*), 4.47 (1H, dt, *J* 8.0 and 7.0, C*H*$_A$$H_B$O), 4.21 (1H, dt, *J* 7.5 and 7.0, CH_A*H*$_B$O), 3.49 (1H, dt, *J* 9.0 and 6.5, PCH), 2.82 (1H, ddq, *J* 16.0, 13.0 and 7.0, PCHC*H*$_A$$H_B$), 2.35 (1H, dddt, *J* 13.5, 12.5, 9.0 and 7.0, $PCHCH_A$*H*$_B$) and 0.00 (9H, Me); δ_C(125 MHz; $CDCl_3$) 145.1 (Ph C *ipso*), 135.1 (d, *J* 80.0, P*Ph*$_A$$Ph_B$ C *ipso*), 132.4 (d, *J* 10.5, P*Ph*$_A$$Ph_B$ CH *ortho*), 131.4 (d, *J* 81.5, PPh_A*Ph*$_B$ C *ipso*), 130.9 (d, *J* 9.0, PPh_A*Ph*$_B$ CH *ortho*), 130.8 (d, *J* 2.5, PPh_2 CH *para*), 128.4 (d, *J* 11.5, PPh_A*Ph*$_B$ CH *meta*), 127.61 (Ph CH), 127.60 (d, *J* 12.5, P*Ph*$_A$$Ph_B$ CH *meta*), 127.4 (Ph CH *para*), 125.5 (Ph CH), 108.2 (d, *J* 2.0, CO_2), 68.7 (d, *J* 8.0, CH_2O), 51.9 (d, *J* 58.0, PCH), 29.5 (PCH*C*H_2) and 1.1 (Me); δ_P(162 MHz; $CDCl_3$) 43.5; *m/z* (ESI) 475 (77%, MNa^+) (Found: MNa^+, 475.13010. $C_{25}H_{29}O_2PSSiNa$ requires *M*, 475.12928) and the phosphine sulfide **32**

(0.043 g, 10%) as an amorphous solid; ν_{max}(film)/cm^{-1} 2955 (C-H), 1589 (C=C, Ph) and 1437 (P-Ph); δ_H(500 MHz; $CDCl_3$) 8.06-8.02 (2H, m, P*Ph*$_A$Ph$_B$ *ortho*), 7.99-7.95 (2H, m, PPh$_A$*Ph*$_B$ *ortho*), 7.45-7.43 (3H, m, P*Ph*$_A$Ph$_B$), 7.39-7.36 (3H, m, PPh$_A$*Ph*$_B$), 3.34-3.25 (2H, m, CH_2O), 2.38 (1H, dt, *J* 14.5 and 5.5, PCH), 2.01-1.93 (2H, m, PCHC*H*$_2$), 0.00 ($OSiMe_3$) and –0.02 (CHSi*Me*$_3$); δ_C(125 MHz; $CDCl_3$) 134.4 (d, *J* 78.0, P*Ph*$_A$Ph$_B$ *ipso*), 134.2 (d, *J* 73.5, PPh$_A$*Ph*$_B$ *ipso*), 131.3 (d, *J* 10.0, PPh$_A$*Ph*$_B$ *ortho*), 131.2 (d, *J* 9.5, P*Ph*$_A$Ph$_B$ *ortho*), 131.1 (d, *J* 3.0, P*Ph*$_A$Ph$_B$ *para*), 130.8 (d, *J* 3.0, PPh$_A$*Ph*$_B$ *para*), 128.4 (d, *J* 12.0, P*Ph*$_A$Ph$_B$ *meta*), 128.2 (d, *J* 11.5, PPh$_A$*Ph*$_B$ *meta*), 61.8 (d, *J* 10.5, CH_2O), 28.7 (d, *J* 2.0, *C*H_2CH_2O), 23.2 (d, *J* 44.0, PCH), 0.1 (d, *J* 2.5, CHSi*Me*$_3$) and –0.5 ($OSiMe_3$); δ_P(162 MHz; $CDCl_3$) 48.8; *m/z* (ESI) 443 (100%, MNa$^+$) (Found: M$^+$, 443.14250. $C_{21}H_{33}OPSSi_2Na$ requires *M*, 443.14260).

(3-Benzoyloxy-3,3-dimethylpropyl)diphenylphosphine oxide 37

To a solution of diphenylmethylphosphine oxide (1.1 g, 5.0 mmol) in dry THF (25 cm^3), stirred at 0 °C under nitrogen, was added *n*-butyllithium (2.9 mol dm^{-3} solution in hexane, 1.8 cm^3, 5.0 mmol) dropwise and the resulting mixture stirred for 2 h before the addition of 1,2-epoxy-2-methylpropane (0.53 cm^3, 6.0 mmol). The resulting mixture was allowed to warm to room temperature and stirred for a further 18 h before the addition of benzoyl chloride (0.81 cm^3, 7.0 mmol). The resulting mixture was allowed to stir for a further 18 h and then quenched with saturated ammonium chloride (1 cm^3). The solvent was removed *in vacuo* and the residue partitioned between water (25 cm^3) and dichloromethane (2 × 50 cm^3). The combined organic extracts were dried (Na_2SO_4), the solvents removed *in vacuo* and the residue purified by flash chromatography (SiO_2, CH_2Cl_2-MeOH 98:2). The ice-cooled residue was treated with 1,2-diaminoethane (~1 cm^3) and partitioned between pH2 buffer (0.5M H_2SO_4, 1.5M Na_2SO_4 in water, 2 × 50 cm^3) and ethyl acetate (50 cm^3). The organic layer was dried (Na_2SO_4) and the solvent removed *in vacuo* to give the *ester* **37** (1.5 g, 76%) as an amorphous solid mp 114-6 °C (from EtOAc); ν_{max}(film)/cm^{-1} 2924 (C-H), 1709 (C=O), 1601 (C=C, Ph) and 1438 (P-Ph); δ_H(400 MHz; $CDCl_3$) 7.94-7.90 (2H, m, $PhCO_2$ *ortho*), 7.77-7.71 (4H, m, PPh_2 *ortho*), 7.55-7.38 (9H, m, Ph), 2.43-2.36 (2H, m, PCH_2), 2.19-2.13 (2H, m, PCH_2CH_2) and 1.57 (6H, Me); δ_C(100 MHz; $CDCl_3$) 165.4 (CO_2),

132.7 ($PhCO_2$ CH *para*), 132.5 (d, *J* 98.5, PPh_2 C *ipso*), 131.9 (d, *J* 2.5, PPh_2 CH *para*), 131.5 ($PhCO_2$ C *ipso*), 130.8 (d, *J* 9.5, PPh_2 CH *ortho*), 129.4 ($PhCO_2$ CH *ortho*), 128.7 (d, *J* 11.5, PPh_2 CH *meta*), 128.3 ($PhCO_2$ CH *meta*), 82.1 (d, *J* 14.5, O*C*Me_2), 33.3 (PCH_2CH_2), 25.7 (Me) and 24.4 (d, *J* 72.0, PCH_2); δ_P(162 MHz; $CDCl_3$) 34.0; *m/z* (ESI) 415 (100%, MNa^+) and 293 (46, MNa - $PhCO_2H$) (Found: MNa^+, 415.14470. $C_{24}H_{25}O_3PNa$ requires *M*, 415.14390).

(3-Benzoyloxy-3,3-dimethylpropyl)diphenylphosphine borane 38

To a solution of diphenylmethylphosphine borane **10** (1.1 g, 5.0 mmol) in dry THF (25 cm^3), stirred at 0 °C under nitrogen, was added *n*-butyllithium (2.9 mol dm^{-3} solution in hexane, 1.8 cm^3, 5.0 mmol) dropwise and the resulting mixture stirred for 2 h before the addition of 1,2-epoxy-2-methylpropane (0.53 cm^3, 6.0 mmol). The resulting mixture was allowed to warm to room temperature and stirred for a further 18 h before the addition of benzoyl chloride (0.81 cm^3, 7.0 mmol). The resulting mixture was allowed to stir for a further 18 h and then quenched with saturated ammonium chloride (1 cm^3). The solvent was removed *in vacuo* and the residue partitioned between water (25 cm^3) and dichloromethane (2 × 50 cm^3). The combined organic extracts were dried (Na_2SO_4), the solvents removed *in vacuo* and the residue purified by flash chromatography (SiO_2, EtOAc-hexane 1:4). The ice-cooled residue was treated with 1,2-diaminoethane (~1 cm^3) and partitioned between pH2 buffer (0.5M H_2SO_4, 1.5M Na_2SO_4 in water, 2 × 50 cm^3) and ethyl acetate (50 cm^3). The organic layer was dried (Na_2SO_4) and the solvent removed *in vacuo* to give the *ester* **38** (1.5 g, 75%) as prisms mp 74-6 °C (from EtOAc); ν_{max}(film)/cm^{-1} 2979 (C-H), 2381 (B-H), 1709 (C=O) and 1437 (P-Ph); δ_H(500 MHz; $CDCl_3$) 7.96-7.94 (2H, m, $PhCO_2$ *ortho*), 7.70-7.66 (4H, m, PPh_2 *ortho*), 7.56-7.41 (9H, m, Ph), 2.37-2.31 (2H, m, PCH_2), 2.08-2.04 (2H, m, PCH_2CH_2), 1.59 (6H, Me) and 1.30-0.73 (3H, m, BH_3); δ_C(125 MHz; $CDCl_3$) 165.4 (CO_2), 132.7 ($PhCO_2$ CH *para*), 132.1 (d, *J* 9.0, PPh_2 CH *ortho*), 131.5 ($PhCO_2$ C *ipso*), 131.3 (d, *J* 2.5, PPh_2 CH *para*), 129.4 ($PhCO_2$ CH *ortho*), 129.1 (d, *J* 55.0, PPh_2 C *ipso*), 128.9 (d, *J* 10.0, PPh_2 CH *meta*), 128.3 ($PhCO_2$ CH *meta*), 82.1 (d, *J* 14.0, O*C*Me_2), 34.8 (PCH_2CH_2), 25.7 (Me) and 20.4 (d, *J* 38.5, PCH_2);

δ_P(162 MHz; $CDCl_3$) 17.4-17.0 (m); *m/z* (ESI) 413 (100%, MNa^+) and 399 (23, MNa – BH_3) (Found: MNa^+, 431.18280. $C_{24}H_{28}O_2PBNa$ requires *M*, 413.18177).

(3-Benzoyloxy-3,3-dimethylpropyl)diphenylphosphine sulfide 39

To a solution of diphenylmethylphosphine sulfide **11** (1.2 g, 5.0 mmol) in dry THF (25 cm^3), stirred at 0 °C under nitrogen, was added *n*-butyllithium (2.9 mol dm^{-3} solution in hexane, 1.8 cm^3, 5.0 mmol) dropwise and the resulting mixture stirred for 2 h before the addition of 1,2-epoxy-2-methylpropane (0.53 cm^3, 6.0 mmol). The resulting mixture was allowed to warm to room temperature and stirred for a further 18 h before the addition of benzoyl chloride (0.81 cm^3, 7.0 mmol). The resulting mixture was allowed to stir for a further 18 h and then quenched with saturated ammonium chloride (1 cm^3). The solvent was removed *in vacuo* and the residue partitioned between water (25 cm^3) and dichloromethane (2 × 50 cm^3). The combined organic extracts were dried (Na_2SO_4), the solvents removed *in vacuo* and the residue purified by flash chromatography (SiO_2, EtOAc-hexane 1:4) to give the *ester* **39** (1.7 g, 84%) as a gum; ν_{max}(film)/cm^{-1} 2976 (C-H), 1709 (C=O), 1600 and 1584 (C=C, Ph) and 1436 (P-Ph); δ_H(500 MHz; $CDCl_3$) 7.95-7.92 (2H, m, $PhCO_2$ *ortho*), 7.85-7.80 (4H, m, PPh_2 *ortho*), 7.55-7.40 (9H, m, Ph), 2.60-2.54 (2H, m, PCH_2), 2.18-2.13 (2H, m, PCH_2CH_2) and 1.59 (6H, Me); δ_C(125 MHz; $CDCl_3$) 165.4 (CO_2), 132.7 ($PhCO_2$ CH *para*), 132.5 (d, *J* 80.0, PPh_2 C *ipso*), 131.6 (d, *J* 3.0, PPh_2 CH *para*), 131.5 ($PhCO_2$ C *ipso*), 131.1 (d, *J* 10.0, PPh_2 CH *ortho*), 129.4 ($PhCO_2$ CH *ortho*), 128.7 (d, *J* 12.0, PPh_2 CH *meta*), 128.3 ($PhCO_2$ CH *meta*), 82.2 (d, *J* 16.0, O*C*Me_2), 34.2 (d, *J* 1.0, PCH_2CH_2), 27.4 (d, *J* 57.5, PCH_2) and 25.8 (Me); δ_P(162 MHz; $CDCl_3$) 44.0; *m/z* (ESI) 431 (100%, MNa^+) and 309 (49, MNa – Ph CO_2H) (Found: MNa^+, 431.12140. $C_{24}H_{25}O_2PSNa$ requires *M*, 431.12106).

(2*RS*,3*RS*)-5,5-Dimethyl-3-diphenylphosphinoyl-2-phenyl-2-trimethylsilyloxytetrahydrofuran 40

A solution of LDA (1.8 mol dm^{-3} solution in heptane:THF:ethylbenzene, 1.1 cm^3, 2.0 mmol) was added to a solution of (3-benzoyloxy-3,3-dimethylpropyl)diphenylphosphine oxide **37**

(0.39 g, 1.0 mmol) and chlorotrimethylsilane (0.51 cm^3, 4.0 mmol) in dry THF (20 cm^3), stirred at −78 °C under argon, *via* cannula. The resulting solution was allowed to warm to room temperature over 4 h and then stir at this temperature for a further 14 h. The mixture was quenched with silica (~2 g) and the THF evaporated *in vacuo*. The residue was purified by flash chromatography (SiO_2, EtOAc:hexane 3:1) to give the phosphine oxide **40** (0.26 g, 55%) as an oil mp 105-6 °C (prisms from EtOAc); R_f(EtOAc-hexane, 3:1) 0.25; ν_{max}(film)/cm^{-1} 2969 (C-H) and 1438 (P-Ph); δ_H(500 MHz; $CDCl_3$) 7.72-7.68 (2H, m, P*Ph*$_A$Ph$_B$ *ortho*), 7.61-7.58 (2H, m, PPh$_A$*Ph*$_B$ *ortho*), 7.46-7.35 (4H, m, Ph), 7.33-7.26 (2H, m, Ph), 7.13-7.04 (5H, m, Ph), 3.31 (1H, dt, *J* 12.5 and 7.0, PCH), 2.63 (1H, q, *J* 12.5, C*H*$_A$H$_B$), 2.05 (1H, ddd, *J* 12.5, 7.5 and 3.0, CH$_A$*H*$_B$), 1.52 (3H, Me$_A$), 1.45 (3H, Me$_B$) and −0.02 (9H, $SiMe_3$); δ_C(125 MHz; $CDCl_3$) 144.7 ($PhCO_2$ C *ipso*), 134.1 (d, *J* 99.0, P*Ph*$_A$Ph$_B$ C *ipso*), 132.9 (d, *J* 100.0, PPh$_A$*Ph*$_B$ C *ipso*), 131.6 (d, *J* 9.5, P*Ph*$_A$Ph$_B$ CH *ortho*), 131.3 (d, *J* 8.5, PPh$_A$*Ph*$_B$ CH *ortho*), 131.2 (d, *J* 3.0, P*Ph*$_A$Ph$_B$ CH *para*), 131.1 (d, *J* 3.0, PPh$_A$*Ph*$_B$ CH *para*), 128.2 (d, *J* 11.5, P*Ph*$_A$Ph$_B$ CH *meta*), 128.0 (d, *J* 12.0, PPh$_A$*Ph*$_B$ CH *meta*), 127.4 ($PhCO_2$ CH), 127.3 ($PhCO_2$ CH *para*), 126.4 ($PhCO_2$ CH) 108.6 (d, *J* 2.5, CO_2), 82.2 (d, *J* 13.0, *C*Me_2), 53.1 (d, *J* 75.5, PCH), 40.2 (CH_2), 29.4 and 28.6 (Me) and 1.9 ($SiMe_3$); δ_P(162 MHz; $CDCl_3$) 25.5; *m/z* (ESI) 487 (100%, MNa^+) and 375 (46, M - $OSiMe_3$) (Found: MNa^+, 487.18390. $C_{27}H_{33}O_3PSiNa$ requires *M*, 487.18343).

Cyclopropyl phenyl ketone 41

To a mixture of 3-diphenylphosphinothioyl-2-phenyl-2-trimethylsilyloxytetrahydrofuran **31** (45 mg, 0.10 mmol) and potassium *tert*-butoxide (34 mg, 0.30 mmol) was added 2-methylpropan-2-ol (3 cm^3) and the resulting solution stirred at 40 °C for 18 h. The mixture was partitioned between water (10 cm^3) and dichloromethane (3 × 15 cm^3). The combined organic extracts were dried (Na_2SO_4), the solvents removed *in vacuo* and the residue purified by flash chromatography (SiO_2, hexane). The residue was partitioned between diethyl ether (2 × 10 cm^3) and water (10 cm^3), the combined organic extracts dried (Na_2SO_4) and the solvents removed *in vacuo* to give the cyclopropane **41** (11 mg, 77%) as an oil; ν_{max}(film)/cm^{-1} 3009 (C-H), 1666 (C=O), and 1597 and 1579 (C=C, Ph); δ_H(500 MHz; $CDCl_3$) 8.02-8.00 (2H, m, Ph *ortho*), 7.56 (1H, tt, *J* 7.5

and 1.5, Ph *para*), 7.48-7.45 (2H, m, Ph *meta*), 2.67 (1H, tt, *J* 8.0 and 4.5, CH), 1.24 (1H, ddd, *J* 7.0, 4.5 and 3.5, C*H*$_A$H$_B$C*H*$_A$H$_B$) and 1.04 (1H, ddd, *J* 8.0, 7.0 and 3.5, CH$_A$*H*$_B$CH$_A$*H*$_B$); δ_C(125 MHz; $CDCl_3$) 200.7 (CO), 138.0 (Ph C *ipso*), 132.7 (Ph CH *para*), 128.5 and 128.0 (Ph CH), 17.1 (*C*HCO) and 11.6 (CH_2); *m/z* (EI) 146 (100%, M^+), 105 (82, PhCO), 77 (39, Ph) and 69 (73, M - Ph) (Found: M^+, 146.07319. $C_{10}H_{10}O$ requires *M*, 146.07316). The spectroscopic data are consistent with that reported in the literature.[10]

Diphenyl([1′-hydroxycyclobutyl]methyl)phosphine oxide 45

A solution of LDA was prepared by the addition on *n*-butyllithium (2.5 mol dm^{-3} solution in hexane, 2.1 cm^3, 5.3 mmol) to a solution of di*iso*propylamine (0.77 cm^3, 5.5 mmol) in dry THF (7.1 cm^3), stirred at −78 °C under argon. The resulting solution was allowed to stir for 30 min. A solution of diphenylmethylphosphine oxide (0.22 g, 1.0 mmol) in dry THF (8.0 cm^3), stirred under argon, was cooled to −78 °C and a slight excess of LDA added (2.0 cm^3, 1.05 mmol). After 30 min cyclobutanone (0.075 cm^3, 1.0 mmol) was added and the resulting mixture allowed to stir at −78 °C for a further 30 min. The mixture was quenched with methanol (0.25 cm^3) and allowed to warm to room temperature. Saturated aqueous NH_4Cl (2.5 cm^3) was added, the THF evaporated under reduced pressure and the residue extracted with dichloromethane (2×25 cm^3). The combined organic layers were dried (Na_2SO_4) and the dichloromethane evaporated *in vacuo*. The residue was purified by flash chromatography (SiO_2, EtOAc) to give the alcohol **45** (0.19 g, 67%) as needles, mp 76-78 °C; R_f 0.25 (EtOAc); $\nu_{max}(CH_2Cl_2)/cm^{-1}$ 3368 (O-H), 2965 (C-H), 1589 (C=C), 1438 (P-Ph) and 1284 (P=O); δ_H(400 MHz; $CDCl_3$) 7.76-7.70 (4H, m, Ph *ortho*), 7.50-7.41 (6H, m, Ph), 5.32 (1H, s, OH), 2.71 (2H, d, *J* 10.0, PCH_2), 2.11-2.03 (2H, m, C$_A$*H*$_A$H$_B$), 1.87-1.80 (2H, m, C$_A$H$_A$*H*$_B$), 1.78-1.68 (1H, m, C$_B$*H*$_A$H$_B$) and 1.51-1.40 (1H, m, C$_B$H$_A$*H*$_B$); δ_C(100 MHz; $CDCl_3$) 133.5 (d, *J* 97.5, Ph C *ipso*), 132.0 (d, *J* 1.5, Ph CH *para*), 130.5 (d, *J* 9.5, Ph CH *ortho*), 128.8 (d, *J* 11.5, Ph CH *meta*), 74.6 (d, *J* 6.5, COH), 38.5 (d, *J* 69.0, PCH_2), 36.9 (d, *J* 9.5, *C*H$_2$CH$_2$*C*H$_2$), 13.0 (CH_2); δ_P(162 MHz; $CDCl_3$) 33.1; *m/z* (ES) 286 (17%, M), 258 (65%, M – CH_2=CH_2), 215 (100%, $CH_2P(O)Ph_2$) and 201 (80%, $P(O)Ph_2$) (Found: M^+, 286.11264. $C_{17}H_{19}O_2P$ requires *M*, 286.11227).

Diphenyl([1′-hydroxycyclobutyl]methyl)phosphine borane 46

A solution of LDA was prepared by the addition of *n*-butyllithium (2.5 mol dm^{-3} solution in hexane, 2.1 cm^3, 5.3 mmol) to a solution of di*iso*propylamine (0.77 cm^3, 5.5 mmol) in dry THF (7.1 cm^3), stirred at −78 °C under argon. The resulting solution was allowed to stir for 30 min. A solution of diphenylmethylphosphine borane **43** (0.21 g, 1.0 mmol) in dry THF (8.0 cm^3), stirred under argon, was cooled to −78 °C and a slight excess of LDA added (2.0 cm^3, 1.1 mmol). After 30 min cyclobutanone (0.075 cm^3, 1.0 mmol) was added and the resulting mixture allowed to stir at −78 °C for a further 30 min. The mixture was quenched with methanol (0.25 cm^3) and allowed to warm to room temperature. Saturated aqueous NH_4Cl (2.5 cm^3) was added, the THF evaporated under reduced pressure and the residue extracted with dichloromethane (2 × 25 cm^3). The combined organic layers were dried (Na_2SO_4) and the dichloromethane evaporated *in vacuo*. The residue was purified by flash chromatography (SiO_2, EtOAc-hexane 1:4) to give the alcohol **46** (0.11 g, 37%) as prisms, mp 61-63 °C; R_f 0.30 (EtOAc-hexane 1:3); $\nu_{max}(CH_2Cl_2)/cm^{-1}$ 3507 (O-H), 2940 (C-H), 2388 (B-H), and 1437 (P-Ph); δ_H(400 MHz; $CDCl_3$) 7.75-7.62 (4H, m, Ph *ortho*), 7.50-7.40 (6H, m, Ph), 3.35 (1H, s, OH), 2.78 (2H, d, *J* 10.5, PCH_2), 2.12-2.04 (2H, m, $C_AH_AH_BH_B$), 1.98-1.92 (2H, m, $C_AH_AH_BH_B$), 1.83-1.74 (1H, m, $C_BH_AH_BH_B$), 1.56-1.45 (1H, m, $C_BH_AH_BH_B$) and 1.60-0.55 (3H, br m, BH_3); δ_C(100 MHz; $CDCl_3$) 132.1 (d, *J* 9.0, Ph CH *ortho*), 131.3 (Ph CH *para*), 130.0 (d, *J* 56.5, Ph C *ipso*), 128.9 (d, *J* 10.0, Ph CH *meta*), 74.6 (COH), 37.2 (d, *J* 38.5, PCH_2), 36.9 (d, *J* 13.0, $CH_2CH_2CH_2$) and 13.1 (CH_2); δ_P(162 MHz; $CDCl_3$) 9.0 (m); *m/z* (ES) 284 (70%, M) (Found: M^+, 284.15078. $C_{17}H_{22}OPB$ requires *M*, 284.15013).

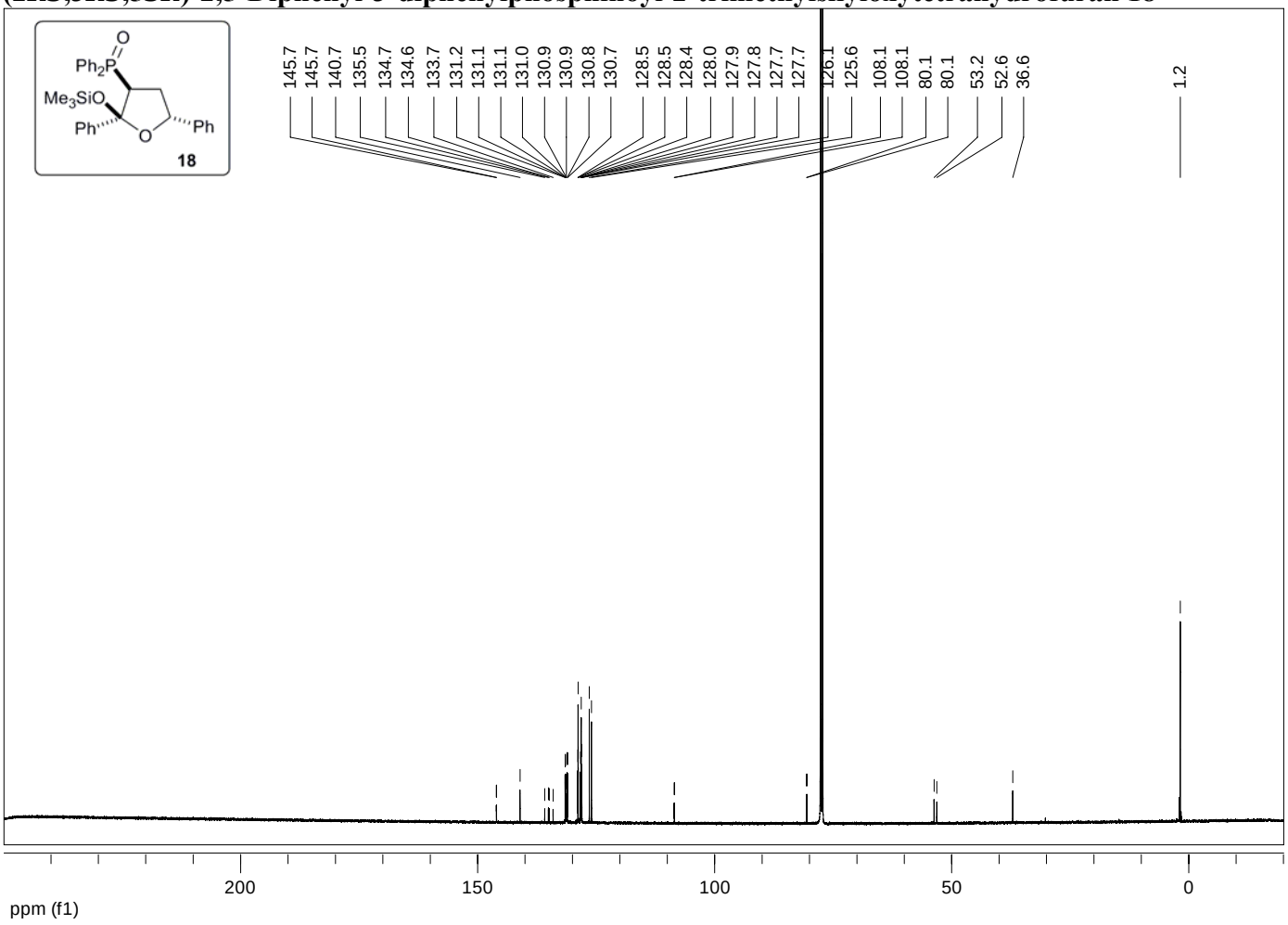
Diphenyl([1′-hydroxycyclobutyl]methyl)phosphine sulfide 47

A solution of LDA was prepared by the addition of *n*-butyllithium (2.5 mol dm^{-3} solution in hexane, 2.1 cm^3, 5.3 mmol) to a solution of di*iso*propylamine (0.77 cm^3, 5.5 mmol) in dry THF (7.1 cm^3), stirred at −78 °C under argon. The resulting solution was allowed to stir for 30 min. A solution of diphenylmethylphosphine sulfide **44** (0.21 g, 1.0 mmol) in dry THF (8.0 cm^3), stirred under argon, was cooled to -78 °C and a slight excess of LDA added (2.0 cm^3, 1.05 mmol). After 30 min cyclobutanone (0.075 cm^3, 1.0 mmol) was added and

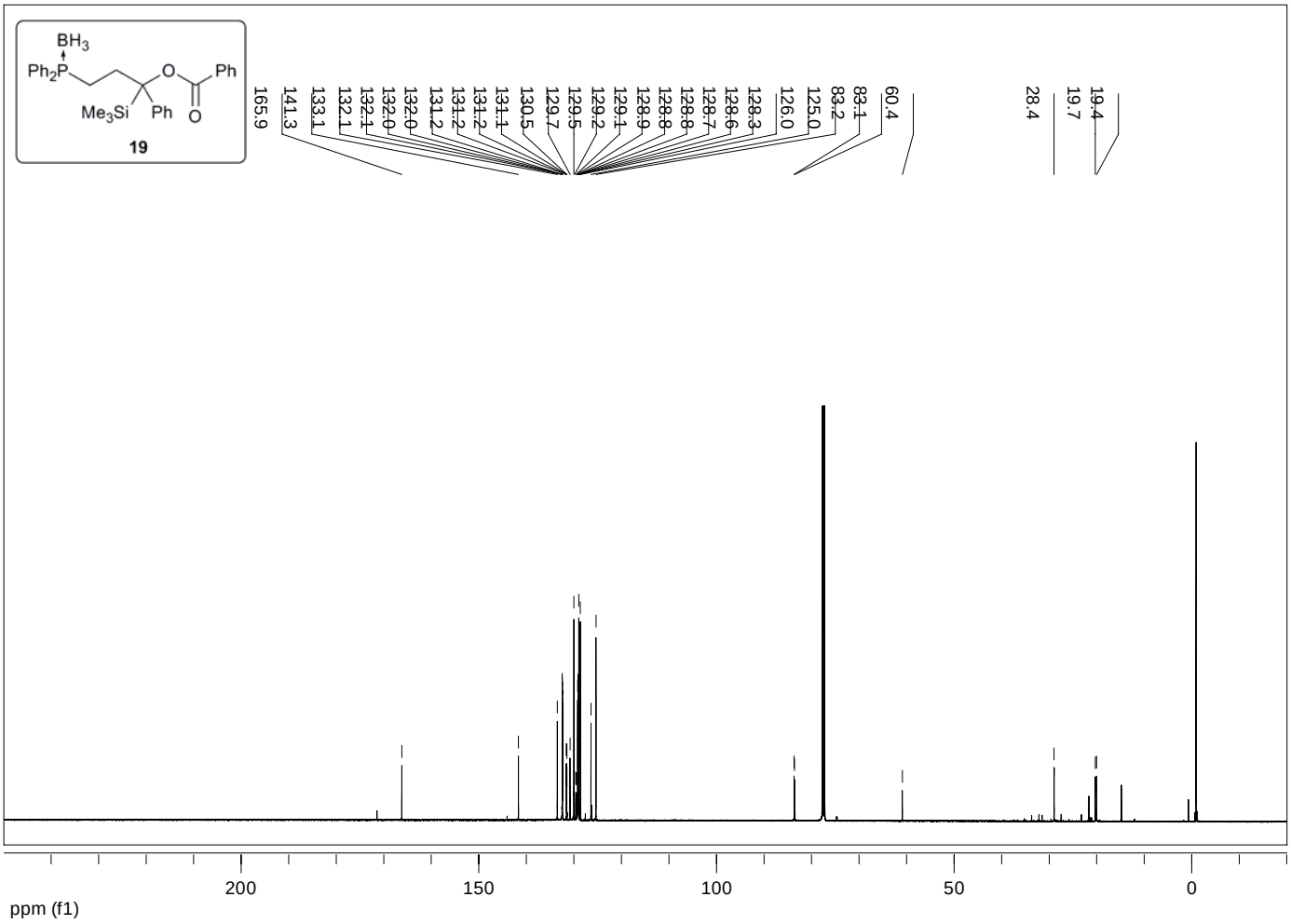
the resulting mixture allowed to stir at −78 °C for a further 30 min. The mixture was quenched with methanol (0.25 cm^3) and allowed to warm to room temperature. Saturated aqueous NH_4Cl (2.5 cm^3) was added, the THF evaporated under reduced pressure and the residue extracted with dichloromethane (2×25 cm^3). The combined organic layers were dried (Na_2SO_4) and the dichloromethane evaporated *in vacuo*. The residue was purified by flash chromatography (SiO_2, EtOAc-hexane 1:4) to give the alcohol **47** (0.22 g, 66%) as needles, mp 81-83 °C; R_f 0.25 (EtOAc-hexane 1:3); $\nu_{max}(CH_2Cl_2)/cm^{-1}$ 3379 (O-H), 2932 (C-H), 1436 (P-Ph) and 603 (P=S); δ_H(400 MHz; $CDCl_3$) 7.90-7.83 (4H, m, Ph *ortho*), 7.56-7.44 (6H, m, Ph), 5.07 (1H, s, OH), 2.99 (2H, d, *J* 10.5, PCH_2), 2.14-2.05 (2H, m, $C_AH_AH_B$), 1.90-1.83 (2H, m, $C_AH_AH_B$), 1.82-1.73 (1H, m, $C_BH_AH_B$) and 1.51-1.42 (1H, m, $C_BH_AH_B$); δ_C(100 MHz; $CDCl_3$) 133.4 (d, *J* 79.5, C Ph *ipso*), 131.6 (d, *J* 4.0, CH Ph *para*), 130.9 (d, *J* 10.5, CH Ph *ortho*), 128.7 (d, *J* 12.0 CH Ph *meta*), 74.8 (COH), 40.6 (d, *J* 55.5, PCH_2), 36.9 (d, *J* 10.0, CH_2COH), 13.4 (CH_2); δ_P(162 MHz; $CDCl_3$) 35.1; *m/z* (ES) 325 (100%, MNa) (Found: MNa^+, 325.08000. $C_{17}H_{19}OPSNa$ requires *M*, 325.07919).

Carbon NMR spectra (125 MHz, Bruker cryoprobe) for final tetrahydrofuran and cyclopropane products:

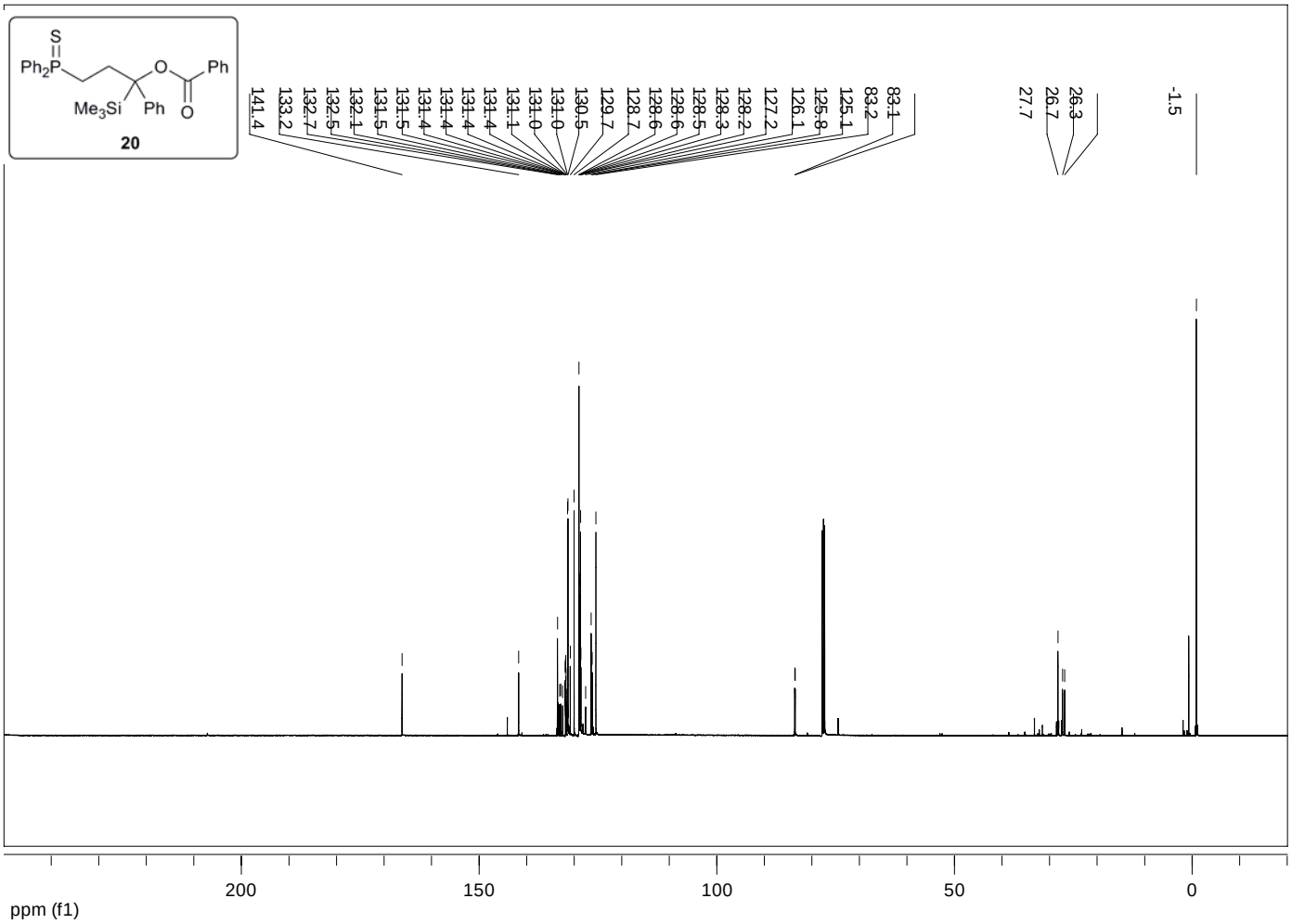
(2*RS*,3*RS*,5*SR*)-2,5-Diphenyl-3-diphenylphosphinoyl-2-trimethylsilyloxytetrahydrofuran 18



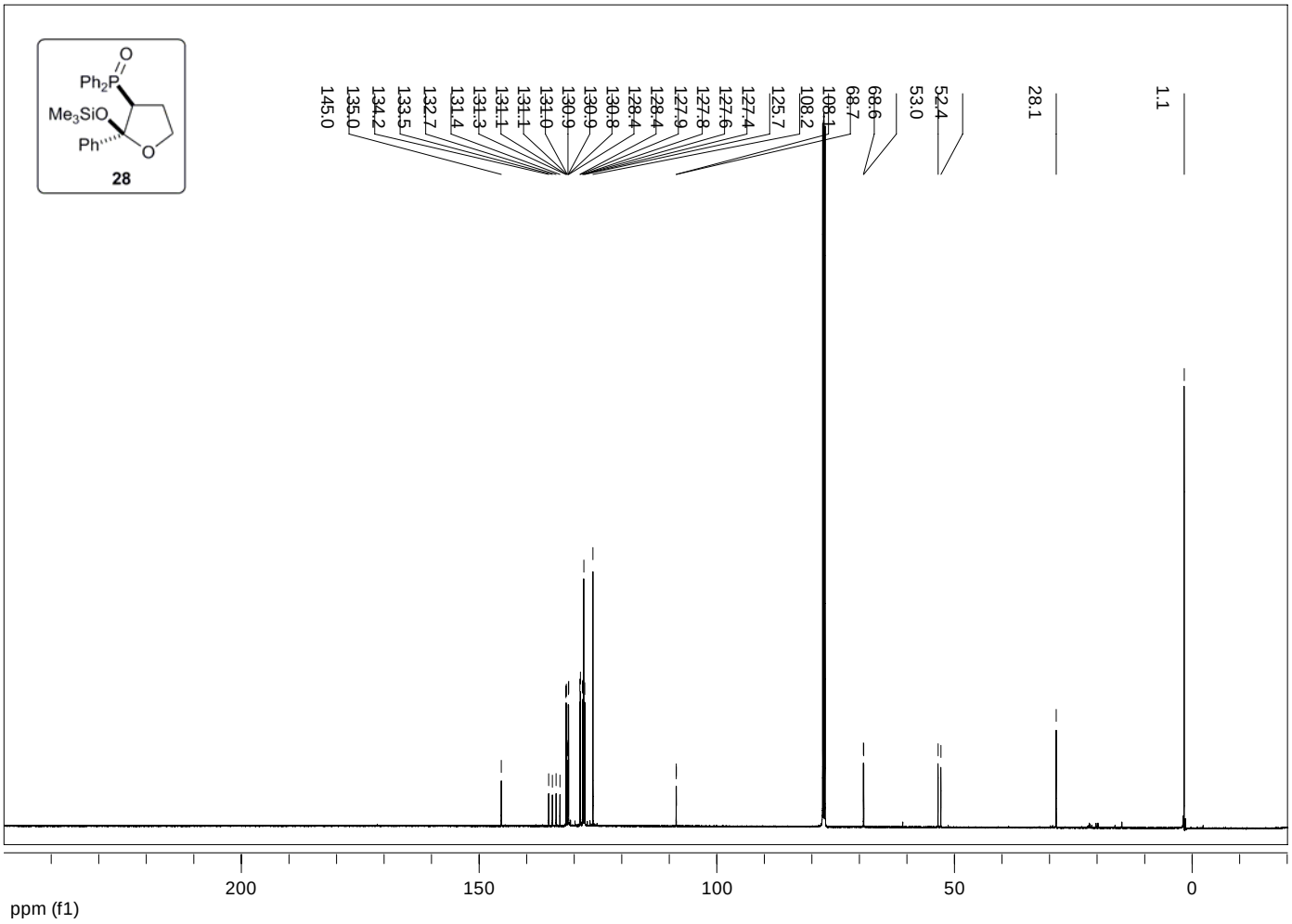
(3-Benzoyloxy-3-phenyl-3-trimethylsilylpropyl)diphenylphosphine borane 19



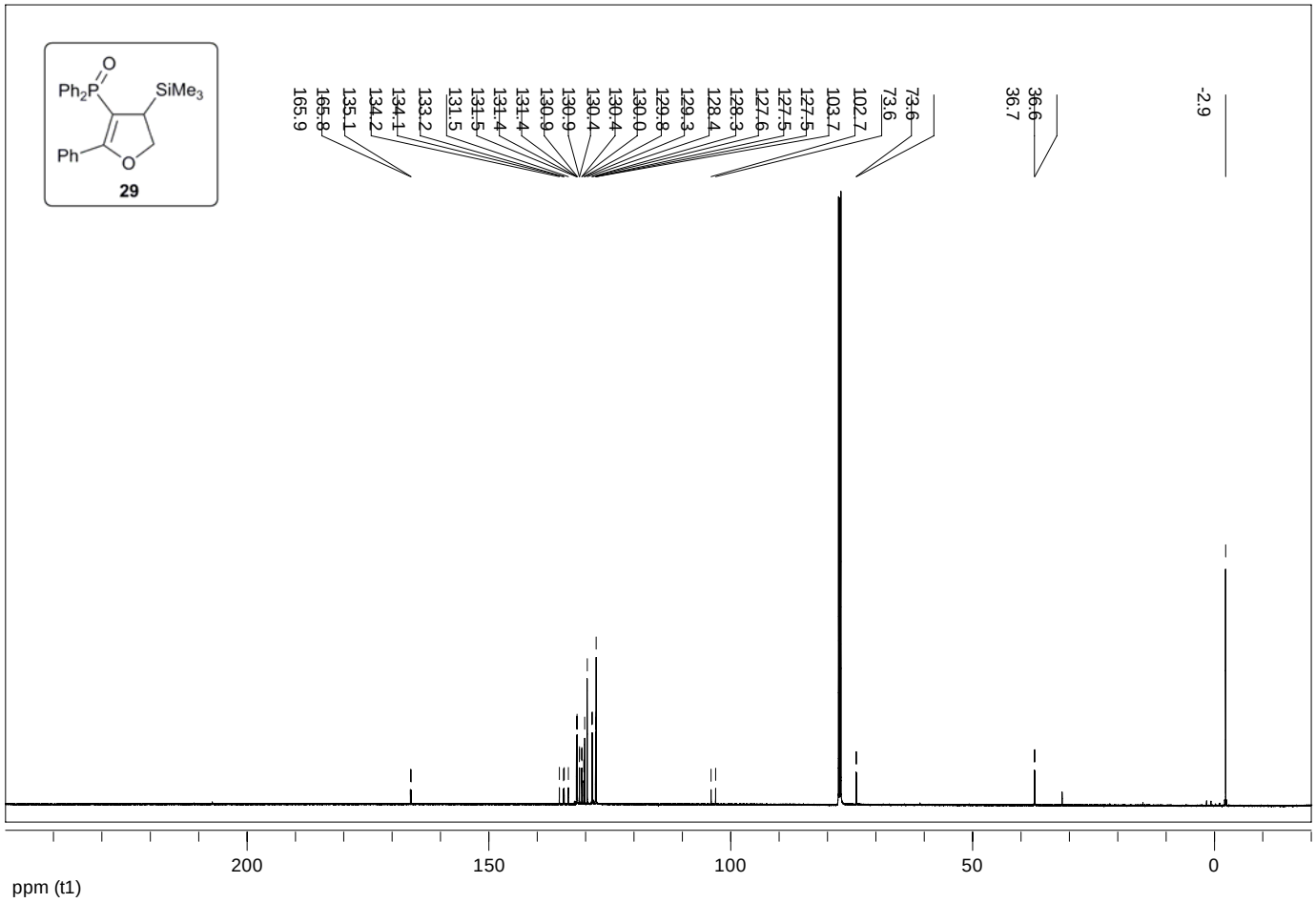
(3-Benzoyloxy-3-phenyl-3-trimethylsilylpropyl)diphenylphosphine sulfide 20



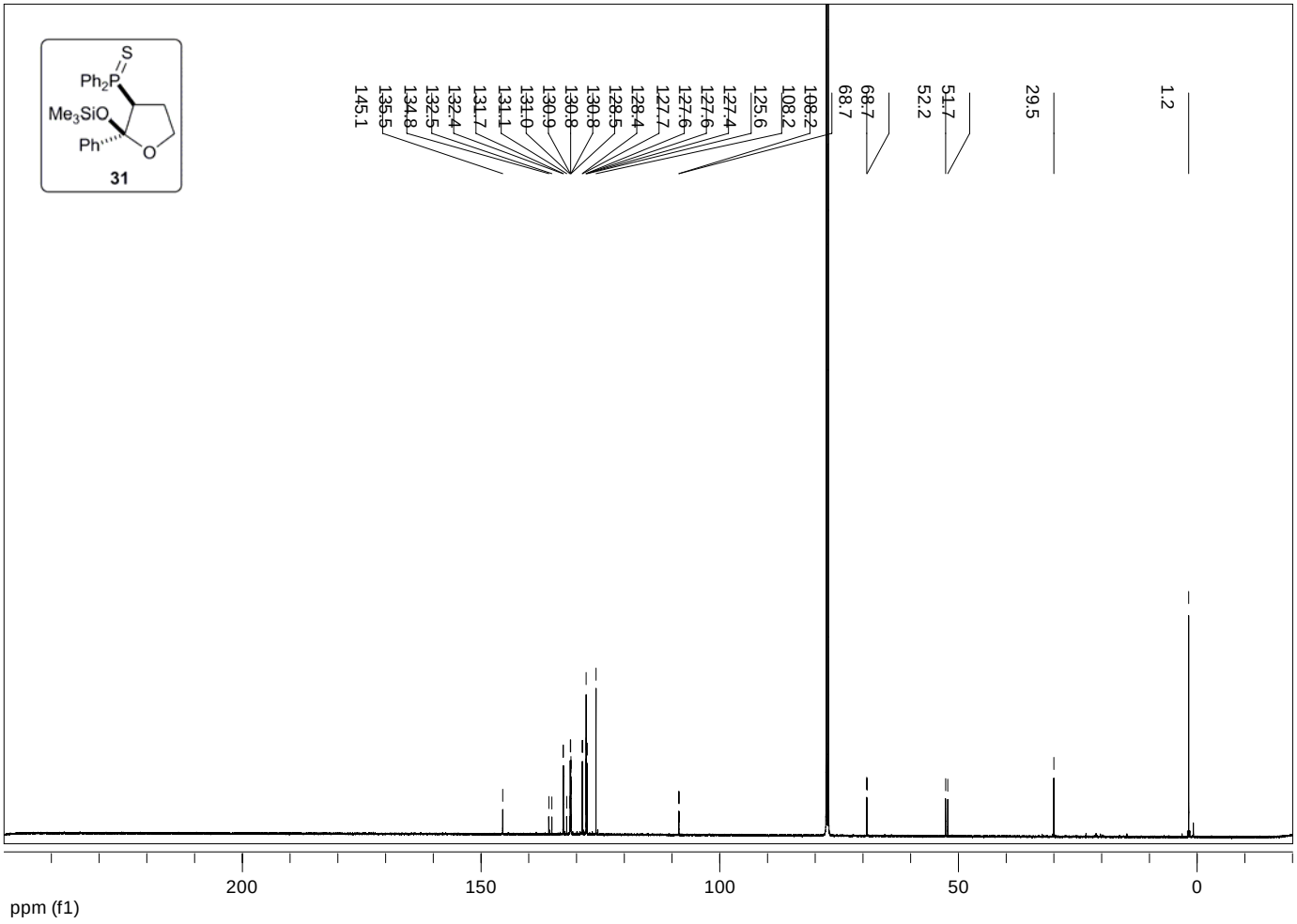
(2*RS*,3*RS*)-3-Diphenylphosphinoyl-2-phenyl-2-trimethylsilyloxytetrahydrofuran 28



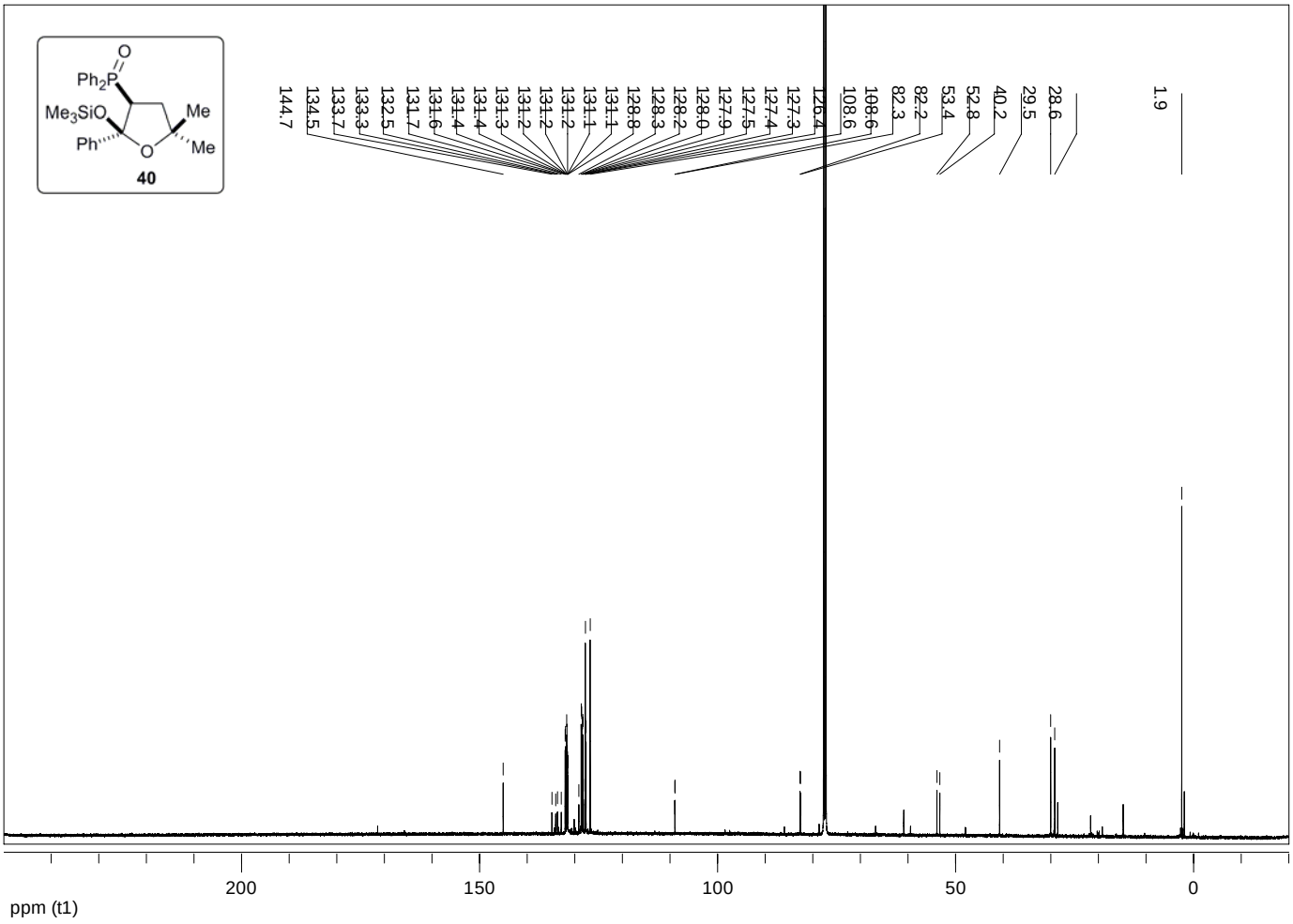
4,5-Dihydro-3-diphenylphosphinoyl-2-phenyl-4-trimethylsilyl-furan 29



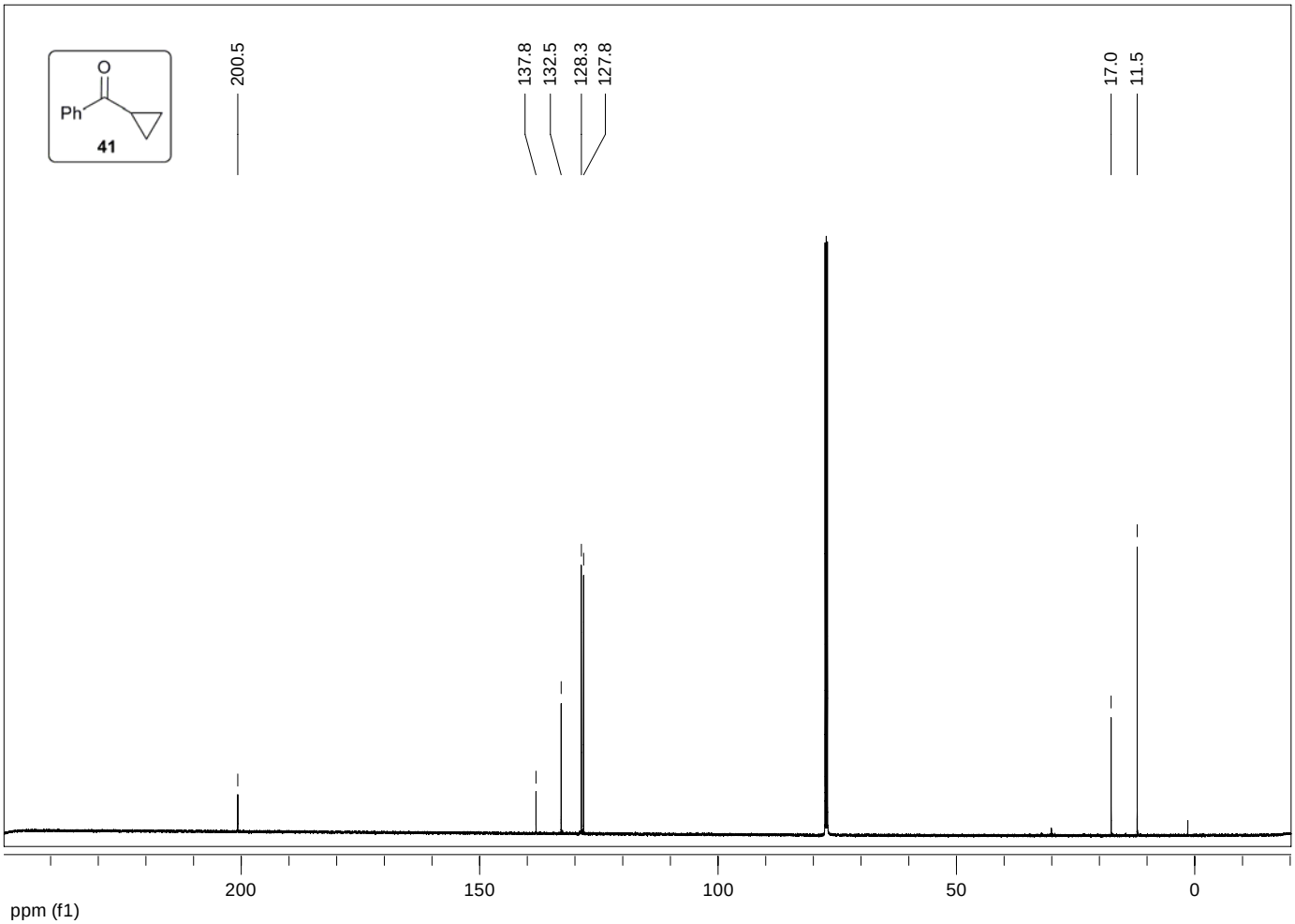
(2*RS*,3*RS*)-3-Diphenylphosphinothioyl-2-phenyl-2-trimethylsilyloxytetrahydrofuran 31



(2*RS*,3*RS*)-5,5-Dimethyl-3-diphenylphosphinoyl-2-phenyl-2-trimethylsilyloxytetrahydrofuran 40



Cyclopropyl(phenyl)methanone 41



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DFT calculations
DFT calculations were performed using PC-GAMESS at the B3LYP/6-31G(d) level. Ground-state and transition-state energy structures have an RMS gradient less than $2x10^{-5}$ Hartree/Bohr.

Energies and zero point energies (Hartrees/molecule), final gradients (Hartrees/Bohr), imaginary frequencies (cm^{-1}) and the associated reduced mass (atomic units) for transition states, and Cartesian coordinates (Ångstroms) are given for structures **49** to **78** (see main paper). Zero-point energies are based on unscaled vibrational frequencies, and do not include imaginary frequencies for the transition structures.

UNCOMPLEXED PHOSPHINE DERIVATIVES

49

ENERGY= -536.3529912
MAXIMUM GRADIENT = 0.0000083 RMS GRADIENT = 0.0000030
ZERO-POINT ENERGY = 0.117985

P	-0.0001294595	-0.0011491176	-0.1062085645
C	1.4895840114	0.7616714555	0.6462054338
C	-1.4049738412	0.9090061778	0.6457232823
C	-0.0848050920	-1.6706620078	0.6502765904
O	-0.0004446927	-0.0035392147	-1.6074445401
H	2.3798426652	0.2224614025	0.3077235406
H	1.4540663735	0.7415275968	1.7408842256
H	1.5720500549	1.7999188864	0.3099368436
H	-1.3833615762	1.9489877317	0.3053183017
H	-1.3703572299	0.8903533117	1.7404551504
H	-2.3452661658	0.4605756199	0.3100943059
H	0.7694050818	-2.2642812355	0.3099883268
H	-1.0003450317	-2.1702063657	0.3184486137
H	-0.0772326515	-1.6276348682	1.7448168600

50

ENERGY= -859.3223340
MAXIMUM GRADIENT = 0.0000092 RMS GRADIENT = 0.0000038
ZERO-POINT ENERGY = 0.116538

P	0.2525596504	-0.0002183673	0.0002194636
C	1.0189809120	0.2888683576	-1.6479995481
C	1.0172619034	1.2837490796	1.0745703221
C	1.0165721786	-1.5729436241	0.5743610351
S	-1.7192944054	0.0003365711	-0.0006576693
H	0.6837093997	-0.4893288677	-2.3392857063
H	2.1129750994	0.2761745360	-1.5865696102
H	0.6861978219	1.2574647664	-2.0312832770
H	0.6837866037	2.2707280172	0.7420093260
H	2.1114460834	1.2364439160	1.0376665780
H	0.6800555763	1.1346781561	2.1040911193
H	0.6767960223	-2.3897050213	-0.0684978096
H	0.6855809748	-1.7778698158	1.5962955729
H	2.1107268520	-1.5186680179	0.5485978683

51

```
ENERGY=    -487.7658694
MAXIMUM GRADIENT =  0.0000079    RMS GRADIENT = 0.0000033
ZERO-POINT ENERGY = 0.144925
 P           -0.0867527662  -0.0005064315  -0.0003077978
 C            0.6735319016  -1.3976522907  -0.9251052700
 C            0.6711934654   1.4999255997  -0.7481087600
 C            0.6722565764  -0.1019684553   1.6724763935
 B           -2.0198953660  -0.0003393874   0.0007380156
 H            0.3331507245  -2.3424624852  -0.4906246700
 H            1.7676392358  -1.3617715033  -0.8983573092
 H            0.3376085289  -1.3636112089  -1.9659463919
 H            0.3355384312   1.5922600410  -1.7854477245
 H            1.7652987601   1.4622889601  -0.7245628559
 H            0.3294347199   2.3843260848  -0.2019131786
 H            0.3424581489  -1.0241721587   2.1604161195
 H            0.3254641657   0.7425172185   2.2756329579
 H            1.7662841322  -0.0887235862   1.6287076712
 H           -2.3377109732  -1.0487967609   0.5229043444
 H           -2.3391013751   0.0727369592  -1.1679220014
 H           -2.3356675037   0.9762221721   0.6485049765
```

LITHIUM AMIDE DIMER COMPLEXES
PRE-LITHIATION COMPLEXES
52
ENERGY= -975.7018444
MAXIMUM GRADIENT = 0.0000082 RMS GRADIENT = 0.0000032
ZERO-POINT ENERGY = 0.364622

Li	-2.1224387978	0.0590528631	-0.0941291006
N	-1.4350635980	-1.7510791018	0.1186360751
O	-4.0152695832	0.4542060871	-0.2506542499
N	-0.5897394765	1.3059336998	-0.0981550780
C	-0.5212369153	2.2289137026	1.0115916676
C	-0.3422859152	2.0310804695	-1.3227316075
C	-1.6698541995	-2.4787398315	1.3484703739
Li	0.1916649856	-0.5672388408	0.1248509071
C	-1.4904278327	-2.6789878064	-0.9920352766
O	2.0476054560	-0.9501089180	0.2385459328
C	-4.9409045066	-0.6276820819	-0.2089425840
C	-4.6251803318	1.7297084479	-0.3873835626
P	3.3024688803	-0.1030132992	0.1474756893
C	4.8109922608	-1.1125981369	0.3565711479
C	3.3915625851	1.2014934546	1.4216507480
C	3.4862857614	0.7455301593	-1.4588113071
H	-0.7059522995	1.7113498839	1.9658105051
H	-1.2576385659	3.0644799339	0.9516496426
H	0.4673084723	2.7409114612	1.1143868596
H	-1.0661933312	2.8577068705	-1.5145968281
H	-0.3909564653	1.3597585721	-2.1943341480
H	0.6583275226	2.5296057874	-1.3592189141
H	-2.6616681027	-2.9883218293	1.3872052474
H	-1.6324715313	-1.8014475506	2.2168819659
H	-0.9257491585	-3.2845263101	1.5392979583
H	-1.3125191847	-2.1575703971	-1.9465416456
H	-2.4717608521	-3.1997673116	-1.0944630696
H	-0.7367978026	-3.4959573188	-0.9290230638
H	-4.3470221946	-1.5368117866	-0.1013791830
H	-5.5289338665	-0.6702613863	-1.1363809384
H	-5.6227691312	-0.5216833318	0.6464056741
H	-5.2023910538	1.7887039886	-1.3209451726
H	-3.8199820469	2.4665429064	-0.4076010133
H	-5.2929234015	1.9363969223	0.4609229904
H	4.8383875943	-1.8825102926	-0.4205141626
H	4.7776384052	-1.6096432723	1.3308508676
H	5.7187188776	-0.5036304649	0.2934319992
H	2.5222187194	1.8587898925	1.3200295925
H	4.3084829608	1.7929599362	1.3287882876
H	3.3610090556	0.7385898610	2.4130229414
H	2.6250178313	1.4027987691	-1.6153321538
H	3.5038082372	-0.0009521751	-2.2591350955
H	4.4065981144	1.3376393042	-1.4991116356

53
ENERGY=   -1298.6559598
MAXIMUM GRADIENT = 0.0000069   RMS GRADIENT = 0.0000025
ZERO-POINT ENERGY = 0.363696

Li	2.2972444239	0.1514737982	0.0913315855
N	1.7132408443	-1.7069167275	0.1073070838
O	4.1561348731	0.6820014325	0.0033156159
N	0.6561163874	1.2788152923	0.2903019441
C	0.3941625189	2.2497841624	-0.7513765533
C	0.7794310897	1.9731089398	1.5590033586
C	1.9097209536	-2.5450383304	-1.0592961366
Li	0.0439089341	-0.6310453044	0.1375100172
C	1.9692331052	-2.4934787347	1.2985719395
S	-2.2416419216	-1.5774344999	-0.3019314535
C	5.1349648227	-0.3549495516	-0.0032599608
C	4.7090715918	1.9912789725	0.0102160422
P	-3.3550787944	0.0786657249	-0.2778161108
C	-5.1398883360	-0.2798299795	-0.0460343968
C	-3.2689128212	1.0547569577	-1.8292569070
C	-2.8979754326	1.2468903686	1.0531036121
H	0.3265347265	1.7584998802	-1.7346007610
H	1.1810255960	3.0341206551	-0.8423177231
H	-0.5528353366	2.8223203926	-0.6110501157
H	1.5849974311	2.7437213112	1.5680496524
H	1.0053569401	1.2648225047	2.3710056060
H	-0.1375940662	2.5242259585	1.8695292597
H	2.9442665044	-2.9519273650	-1.1474008606
H	1.7146345363	-1.9796246684	-1.9841798773
H	1.2455536564	-3.4362286158	-1.0840374193
H	1.8218121126	-1.8873672744	2.2069479496
H	3.0066142441	-2.8989985337	1.3527518116
H	1.3071884357	-3.3816771637	1.3960482420
H	4.5862977574	-1.2979935837	-0.0006049528
H	5.7725538928	-0.2894655812	0.8891465655
H	5.7625321671	-0.2878604093	-0.9025325477
H	5.3318715975	2.1466248014	0.9021898322
H	3.8724638613	2.6924554065	0.0231722049
H	5.3187003511	2.1614400057	-0.8881309830
H	-5.2786899854	-0.8085237288	0.9009535944
H	-5.4884459090	-0.9238730995	-0.8581907036
H	-5.7253972585	0.6459371640	-0.0368053625
H	-2.2416637442	1.3996607230	-1.9745845407
H	-3.9386548576	1.9204789354	-1.7825416338
H	-3.5516519197	0.4175644913	-2.6717170253
H	-1.8274534968	1.4574741524	0.9543536255
H	-3.0759643038	0.7732032625	2.0230079500
H	-3.4774691979	2.1739417238	0.9852335962

54
ENERGY= -927.0977104
MAXIMUM GRADIENT = 0.0000093 RMS GRADIENT = 0.0000032
ZERO-POINT ENERGY = 0.392399

C	4.8558427068	0.2424020103	-1.4331332915
P	3.7485278685	0.0332075520	0.0177529035
B	2.2940828276	1.3091755501	0.0539138750
C	4.8557143060	0.1698179565	1.4771091955
C	3.2305515663	-1.7246489225	-0.0271401976
Li	-2.3635336942	-0.0756980071	0.1194872532
N	-1.6936831579	1.7596474879	0.1987414004
C	-5.2101267588	0.4973621247	0.2576053123
N	-0.7798454453	-1.2635237096	0.0050910640
C	-0.6496312949	-2.0298754380	-1.2154837536
C	-0.5991581515	-2.1472277326	1.1367212085
C	-1.8398134720	2.5089034319	1.4310378430
Li	-0.0774385014	0.6076789374	0.0747358395
O	-4.2412375558	-0.5420158125	0.1560164575
C	-4.8018796258	-1.8444820933	0.0622603584
C	-1.9436273518	2.6462796010	-0.9203806834
H	5.6786763937	-0.4793860418	-1.4175284824
H	5.2648488513	1.2570839328	-1.4343702493
H	4.2759999131	0.1064852341	-2.3510276078
H	1.6525793911	1.1118028453	-0.9610176584
H	2.8024420289	2.4059131616	0.0718777067
H	1.6733241003	1.0715413902	1.0731605355
H	4.2763756426	-0.0163533260	2.3864372127
H	5.2599360905	1.1849592928	1.5317075602
H	5.6820270677	-0.5462632562	1.4242889537
H	4.0942207325	-2.3973842794	-0.0450827132
H	2.6128991889	-1.8995220076	-0.9128376273
H	-4.6543974534	1.4345755426	0.3167897541
H	-5.8637040168	0.5051996137	-0.6256731220
H	-5.8235382505	0.3679236029	1.1601058575
H	-0.7922583921	-1.3875788742	-2.0984574023
H	-1.3859033682	-2.8629594131	-1.3033136839
H	0.3441502341	-2.5216460310	-1.3375394935
H	-1.3334521818	-2.9858358528	1.1737048334
H	-0.7010459287	-1.5959500200	2.0845610912
H	0.3970693692	-2.6480716740	1.1661638084
H	-1.6520073536	1.8648679998	2.3050524144
H	-2.8567022249	2.9450563889	1.5713379683
H	-1.1423169380	3.3713428025	1.5138377415
H	-3.9681116500	-2.5453483637	-0.0100889560
H	-5.4361715423	-1.9325528975	-0.8309702352
H	-5.4019569741	-2.0758491600	0.9534220265
H	-2.9667470636	3.0905497799	-0.9191696557
H	-1.8362969749	2.1092777059	-1.8763832242
H	-1.2521031654	3.5164508817	-0.9633806354
H	2.6140097620	-1.9450691908	0.8490196385

LITHIATION TRANSITION STRUCTURE COMPLEXES
55
ENERGY=   -975.6754241
MAXIMUM GRADIENT = 0.0000099   RMS GRADIENT = 0.0000030
ZERO-POINT ENERGY = 0.361253
IMAGINARY FREQUENCY = 1198.75 REDUCED MASS = 1.07492

C	-4.6887286604	0.4116021994	0.6197500813
P	-3.0877498960	-0.0890263319	-0.1329189062
O	-2.3710062997	1.1932771315	-0.6096082979
C	-3.5739335622	-1.1276343345	-1.5617161486
C	-2.0782592396	-1.0750616150	0.9279430908
Li	1.7167116036	0.0399615803	0.1060364614
N	1.2129115463	1.9543841381	-0.0015144478
C	4.2569245274	-1.5624740946	-0.3341242630
N	0.4993139292	-1.5486463676	0.0930035174
Li	-0.6389766683	1.5499844006	-0.3408048923
O	3.6580467544	-0.3568592483	0.1241561804
C	4.6128937424	0.6378245278	0.4797042900
C	1.8511182576	2.6915594840	-1.0820901577
C	1.3427325644	2.7182329323	1.2309118065
C	0.8462455144	-2.5433836495	1.1039092589
C	0.3133828986	-2.2068895060	-1.1942833825
H	-5.2643201864	-0.4629672945	0.9402191586
H	-5.2811679611	0.9959138139	-0.0926473045
H	-4.4843119241	1.0376334688	1.4941844717
H	-2.6737393801	-1.4911915630	-2.0652352210
H	-4.1580198559	-0.5309179525	-2.2690992967
H	-4.1696591304	-1.9883013896	-1.2399200206
H	-2.5054583796	-2.0753784503	1.0683140247
H	-1.9889176175	-0.5911805529	1.9095892608
H	3.4465460457	-2.2487848577	-0.5820689196
H	4.8705193958	-1.3759720371	-1.2268855072
H	4.8875086985	-2.0073050306	0.4481389460
H	4.0525663559	1.5183856676	0.7945666757
H	5.2459660052	0.8946139603	-0.3807795727
H	5.2497123022	0.2853897530	1.3031922283
H	1.7704454753	2.1390938295	-2.0304834492
H	2.9342229322	2.8794276161	-0.9130842121
H	1.4079048518	3.6961087475	-1.2557436927
H	2.3983815345	2.9023427586	1.5332819076
H	0.8639773224	2.1900345393	2.0695878220
H	0.8810094951	3.7282906447	1.1790414533
H	0.9818890924	-2.0577968708	2.0799262220
H	1.7802470407	-3.0867045823	0.8735778358
H	0.0613668728	-3.3157557576	1.2308616474
H	1.2185694858	-2.7346539618	-1.5470386918
H	0.0502420218	-1.4682196792	-1.9647812223
H	-0.4962034550	-2.9656577333	-1.1754481318
H	-0.7680201091	-1.2278289841	0.4534240133

56
ENERGY= -1298.6300007
MAXIMUM GRADIENT = 0.0000089 RMS GRADIENT = 0.0000026
ZERO-POINT ENERGY = 0.359745
IMAGINARY FREQUENCY = 1222.88 REDUCED MASS = 1.07028

C	-4.6243650326	0.1229902615	-0.5720297485
P	-2.9624925955	0.5558535130	0.1019692273
S	-2.2414718227	-0.9876995527	1.1960846976
C	-3.3075922491	2.0374169718	1.1342469578
C	-1.7974978110	1.0547630386	-1.1476944219
Li	2.1950027087	-0.0088090912	-0.0611700259
N	1.4277018690	-1.7431489311	-0.4264073927
C	4.7770622135	1.3970373286	0.8249310602
N	0.7663868891	1.4404791793	-0.2045231680
Li	-0.1865947477	-0.7069868343	-0.0380732619
O	4.0733740089	0.2629404323	0.3333863844
C	4.9019435848	-0.8907745599	0.1756919622
C	1.6239295070	-2.8977455191	0.4325844744
C	1.5527075085	-2.1610309097	-1.8131830851
C	1.3063154919	2.2030703739	-1.3345711147
C	0.6309656378	2.3092872336	0.9639240751
H	-5.0348776779	0.9640806165	-1.1417789514
H	-5.3077355599	-0.1383305646	0.2421606976
H	-4.5217249620	-0.7425994458	-1.2324214174
H	-2.3749348214	2.3933602319	1.5781448698
H	-4.0021694035	1.7714662631	1.9358677503
H	-3.7441206339	2.8357574728	0.5234401796
H	-2.0904207080	2.0096531363	-1.6021358231
H	-1.7669447300	0.2910296749	-1.9372105267
H	4.0579588622	2.2141533165	0.9083204833
H	5.2092705689	1.1874102209	1.8128324383
H	5.5804678165	1.6864918076	0.1339714524
H	4.2539371546	-1.6925062201	-0.1803609144
H	5.3513533366	-1.1743644429	1.1366521654
H	5.6978486074	-0.6937746092	-0.5549502295
H	1.5230381627	-2.6175654989	1.4914576503
H	2.6263437121	-3.3704446125	0.3188468524
H	0.8946693629	-3.7132778346	0.2453376006
H	2.5498160009	-2.5914274610	-2.0597121054
H	1.4013784736	-1.3086608379	-2.4952141939
H	0.8186049887	-2.9410331044	-2.1087897400
H	1.3740344729	1.5603936018	-2.2223438691
H	2.3156786234	2.6017423014	-1.1321298660
H	0.6737628336	3.0692120073	-1.6051947229
H	1.5989409288	2.7220972854	1.2981223773
H	0.2062412931	1.7440226400	1.8026891810
H	-0.0279005041	3.1786211128	0.7738099461
H	-0.4705323114	1.2395390380	-0.6098966180

57
ENERGY= -927.0684295
MAXIMUM GRADIENT = 0.0000091 RMS GRADIENT = 0.0000021
ZERO-POINT ENERGY = 0.388419
IMAGINARY FREQUENCY = 1253.90 REDUCED MASS = 1.06206

P	-3.2415591924	0.0652006408	-0.1130757070
B	-2.3743755856	1.2396883197	-1.3932561890
C	-3.7818405057	-1.5246633659	-0.8627359084
C	-2.0660615686	-0.3374274940	1.1783887544
C	-4.8136242494	0.7820421857	0.5427396424
H	-5.5178177293	0.9680298160	-0.2754313694
H	-4.5920164286	1.7366594767	1.0298849634
H	-1.9501519334	2.1757833094	-0.7298888973
H	-3.1325218773	1.6022185306	-2.2578105734
H	-1.4486843169	0.5797097667	-1.8537217477
H	-2.9153244561	-2.0387778026	-1.2868739191
H	-4.5009691809	-1.3310849719	-1.6644516739
H	-4.2466576595	-2.1737368557	-0.1130333881
H	-2.4410615204	-1.1204793528	1.8486946476
H	-1.8900581933	0.5626057606	1.7873450374
Li	1.9265830207	-0.0439816080	0.0488461614
N	1.3446455448	1.8021266029	0.0446441133
C	4.7386085478	0.4905048960	-0.2075865622
N	0.3825178405	-1.3218706386	0.3588307730
C	0.7791432015	-1.9731534256	1.6098501330
C	0.1233779054	-2.3316351882	-0.6645052954
C	1.6981075199	2.7178602304	-1.0265606880
Li	-0.3833885844	0.9356929084	-0.1974671252
O	3.7798767297	-0.5678884079	-0.1889718014
C	4.3495736855	-1.8475336537	-0.4352869438
C	1.4831557593	2.4905880798	1.3177703105
H	4.1864685512	1.4141342142	-0.0300647347
H	5.4899401218	0.3416281834	0.5795760090
H	5.2392175328	0.5385486781	-1.1838990874
H	0.9347132331	-1.2190296600	2.3931009748
H	1.7160870952	-2.5488182820	1.5096435500
H	0.0144319048	-2.6798068642	1.9844526129
H	1.0170565430	-2.9371004081	-0.8981588194
H	-0.1970623774	-1.8496530830	-1.5968051375
H	-0.6671466246	-3.0481164567	-0.3670243289
H	1.5995472755	2.2283551431	-2.0067665709
H	2.7436023006	3.0957137301	-0.9594499734
H	1.0608157472	3.6263053624	-1.0566301214
H	3.5372825744	-2.5758464910	-0.3989648417
H	5.0970678224	-2.0951302807	0.3306932036
H	4.8246835492	-1.8770545392	-1.4254436157
H	2.5170326274	2.8528189340	1.5166175477
H	1.2164629348	1.8252293570	2.1544601555
H	0.8381776204	3.3912820488	1.4067746992
H	-5.2759226987	0.1114129361	1.2746867085
H	-0.8101008865	-0.8395932848	0.6908480962

POST-LITHIATION COMPLEXES
58
ENERGY=   -975.6875121
MAXIMUM GRADIENT = 0.0000074   RMS GRADIENT = 0.0000029
ZERO-POINT ENERGY = 0.367077

C	4.7580810418	0.9493548339	-0.8439846507
P	3.2031166849	0.4689526217	0.0240100782
O	2.4631207990	1.7652229570	0.4264950044
C	3.8002921202	-0.4458873728	1.5018968452
C	2.1153054891	-0.5877082194	-0.8570142716
Li	-1.8585060613	-0.2032913323	-0.0615242004
N	-1.1759407968	1.5983228385	-0.0674039941
C	-4.5018852548	-1.7379313386	0.2850733679
N	-0.6714191300	-1.8824108549	-0.2030665257
Li	0.7638532604	1.1636925858	-0.0551560772
O	-3.7830270491	-0.5279499804	0.0875827698
C	-4.6256091287	0.6254048696	0.0618468668
C	-1.4425665151	2.4396412778	1.0905717916
C	-1.4004640773	2.3790630585	-1.2756779264
C	-0.9142779071	-2.7550348323	-1.3589514842
C	-0.4981105007	-2.6537391822	1.0342994907
H	5.3487766479	0.0689052640	-1.1186006619
H	5.3621255565	1.6116582218	-0.2139889782
H	4.4925167455	1.4938227393	-1.7560744555
H	2.9388446920	-0.8408489076	2.0494996514
H	4.3461270421	0.2374445536	2.1598309957
H	4.4558285142	-1.2781522406	1.2241687380
H	2.4025328750	-1.6424268527	-0.7709854453
H	2.0785887536	-0.3141878541	-1.9205522427
H	-3.7733900106	-2.5507790550	0.2911343119
H	-5.0386431311	-1.7205540841	1.2437045069
H	-5.2237420344	-1.9008041319	-0.5270454993
H	-3.9719528648	1.4861239477	-0.0790326710
H	-5.1719957508	0.7229530115	1.0095179481
H	-5.3440171528	0.5568465001	-0.7661662497
H	-1.2852341564	1.8777454234	2.0237642540
H	-2.4837635849	2.8336497500	1.1250089188
H	-0.7904971073	3.3366007812	1.1448709490
H	-2.4409541589	2.7655256358	-1.3713073897
H	-1.2050250293	1.7726726605	-2.1737901264
H	-0.7528227474	3.2794790004	-1.3495386744
H	-0.9391331872	-2.1523766084	-2.2726575513
H	-1.8808369885	-3.2642583154	-1.2570779292
H	-0.1379874843	-3.5281099164	-1.4780700543
H	-1.4385107242	-3.1451441020	1.3139114261
H	-0.2100220500	-1.9791332694	1.8474068509
H	0.2753737199	-3.4335944454	0.9441819712
H	0.2252195264	-1.3736633889	-0.3779731637

59
ENERGY=   -1298.6483242
MAXIMUM GRADIENT = 0.0000094   RMS GRADIENT = 0.0000031
ZERO-POINT ENERGY = 0.365475

C	4.8342689838	0.4296021398	-1.1211900342
P	3.2041067245	0.2842648821	-0.2537815097
S	2.7117633423	2.0820087956	0.5479822020
C	3.5668655063	-0.9650010234	1.0495824144
C	1.8645436303	-0.3558608063	-1.2070525893
Li	-2.0505338797	-0.1706176186	-0.1247094907
N	-1.3358706761	1.6161046261	-0.1547081240
C	-4.6640845891	-1.7102281214	0.3534041212
N	-0.8543744870	-1.8376257759	-0.3595865371
Li	0.5954880359	1.1770045604	-0.2166564441
O	-3.9612455417	-0.5003541634	0.1024826716
C	-4.8098219719	0.6495290715	0.1011154397
C	-1.5787892295	2.4610034643	1.0070060061
C	-1.5992076568	2.3909810775	-1.3599925091
C	-1.1503366652	-2.6926330784	-1.5169567063
C	-0.5979694437	-2.6279574919	0.8517787411
H	5.1356069606	-0.5420289514	-1.5295203511
H	5.6047259254	0.7950439299	-0.4343303405
H	4.7311130587	1.1457246672	-1.9413852544
H	2.6660788035	-1.1290473668	1.6468717172
H	4.3605989786	-0.5964533701	1.7051890189
H	3.8792225708	-1.9137567394	0.5978946377
H	2.0306797178	-1.4160564417	-1.4409604144
H	1.7900630819	0.2012921224	-2.1525266761
H	-3.9328493020	-2.5205432534	0.3333106968
H	-5.1508818195	-1.6812403955	1.3379466982
H	-5.4256087377	-1.8867801936	-0.4184423674
H	-4.1687858540	1.5114263714	-0.0842951946
H	-5.3091439012	0.7591627452	1.0729224585
H	-5.5672116506	0.5651517450	-0.6896907393
H	-1.3946113278	1.9040709758	1.9378340486
H	-2.6212781297	2.8485006515	1.0638072456
H	-0.9305746220	3.3608659218	1.0413715472
H	-2.6444223294	2.7702765825	-1.4266504163
H	-1.4257915956	1.7823696412	-2.2611429183
H	-0.9598261433	3.2947488303	-1.4550259274
H	-1.2379962900	-2.0737801049	-2.4156351317
H	-2.1018824916	-3.2172073071	-1.3667026126
H	-0.3717139914	-3.4517200107	-1.6950077408
H	-1.5118739456	-3.1467815307	1.1664216858
H	-0.2861447105	-1.9628243322	1.6637070736
H	0.1866562620	-3.3879075283	0.7065057131
H	0.0123091823	-1.3056852221	-0.5757082195

60
ENERGY=   -927.0858327
MAXIMUM GRADIENT = 0.0000096   RMS GRADIENT = 0.0000031
ZERO-POINT ENERGY = 0.394052

P	-3.3365596674	0.3581792750	-0.0731184289
B	-2.7296475526	1.9548876472	-1.0069089754
C	-3.6205147176	-1.0390284242	-1.2386467987
C	-2.0430907440	-0.1485193739	1.0325711971
C	-5.0148204089	0.5787796498	0.6909892443
H	-2.2862199542	2.6887562168	-0.1304138648
H	-3.6041350559	2.4822190266	-1.6499281070
H	-1.8157187714	1.5624794241	-1.7265487859
H	-2.6910704934	-1.2543755117	-1.7732593233
H	-4.3888565611	-0.7706198858	-1.9701804611
H	-3.9387345413	-1.9399237922	-0.7024513938
H	-2.2335644362	-1.1409172181	1.4623843537
H	-1.9927270308	0.5714778184	1.8652106153
H	-5.7564563521	0.8407909429	-0.0720716939
H	-4.9664622554	1.3954878644	1.4182733613
H	-5.3322575729	-0.3332136495	1.2086425389
Li	1.8851208396	-0.1463699304	0.0693948892
N	1.2179240354	1.6584398139	-0.0592495492
C	4.6735094108	0.5767793776	-0.1897420837
N	0.6517517771	-1.7594479622	0.4448478012
C	0.8947023004	-2.4727869644	1.7059605957
C	0.4238770205	-2.6864944748	-0.6711393733
C	1.5247238147	2.4418977006	-1.2482619252
Li	-0.7132087103	1.2345007405	-0.0536784671
O	3.7909209655	-0.5427892204	-0.0931857913
C	4.4618004288	-1.7911711669	-0.2042853723
C	1.4664478851	2.4789300072	1.1188999981
H	4.0561892187	1.4708988362	-0.1026418466
H	5.4154457264	0.5501969386	0.6195350913
H	5.1913968441	0.5751131980	-1.1581086661
H	0.9585462053	-1.7514156449	2.5268549137
H	1.8433639610	-3.0213044873	1.6553976444
H	0.0989887735	-3.1967330911	1.9444050669
H	1.3378570522	-3.2539517702	-0.8861790559
H	0.1546675259	-2.1202138838	-1.5688481949
H	-0.3807003671	-3.4107613744	-0.4655094704
H	1.3517525122	1.8498806543	-2.1589333229
H	2.5803105162	2.7944466985	-1.2876625382
H	0.9075956646	3.3591758208	-1.3424182827
H	3.7063398029	-2.5742968435	-0.1177751463
H	5.2031141700	-1.9088183962	0.5979053586
H	4.9676704578	-1.8766748377	-1.1758248691
H	2.5207731166	2.8274468897	1.2047533838
H	1.2421907080	1.9180316963	2.0395747592
H	0.8546554339	3.4060328511	1.1515484797
H	-0.2154279829	-1.1955879740	0.5674086548

BIS-ETHER LITHIUM AMIDE COMPLEX
61
ENERGY= -594.3649135
MAXIMUM GRADIENT = 0.0000077 RMS GRADIENT = 0.0000030
ZERO-POINT ENERGY = 0.327360

Li	1.1950639204	0.1064318895	0.0922810813
N	0.1348292449	-1.5652951317	0.0418740907
O	3.1223338867	0.2252787640	0.1784798400
N	-0.0945499053	1.6010353052	-0.0571412352
C	-0.0366482616	2.4266321410	-1.2461404334
C	-0.2703077720	2.4556648330	1.0997602181
C	0.3100799665	-2.4231414115	-1.1125851449
Li	-1.1543290593	-0.0702609920	-0.1110388883
C	0.0745074531	-2.3876028756	1.2330586862
O	-3.0794932517	-0.2002420682	-0.2191712478
C	3.9542114454	-0.9281613077	0.2368603101
C	3.8419329253	1.4512915688	0.1177643055
C	-3.7863754035	-1.4347350256	-0.1848302938
C	-3.9228746571	0.9444816955	-0.2813862455
H	0.0993339202	1.8072623644	-2.1466544560
H	0.7973330748	3.1660066308	-1.2383880351
H	-0.9543818955	3.0362094950	-1.4143360086
H	0.5522552876	3.1938970777	1.2411086756
H	-0.3193773951	1.8582390816	2.0239033581
H	-1.2003412583	3.0690986737	1.0672353535
H	1.2387673469	-3.0385213860	-1.0776177438
H	0.3613004479	-1.8281940090	-2.0382100835
H	-0.5138105966	-3.1601934111	-1.2529954013
H	-0.0613508950	-1.7655624660	2.1317267081
H	0.9911021279	-2.9981987877	1.4038206009
H	-0.7606353404	-3.1256874035	1.2265797631
H	3.2897405555	-1.7932302739	0.2709878464
H	4.5845740077	-0.9071839445	1.1365849955
H	4.5965994356	-0.9888226246	-0.6525769748
H	4.4667639575	1.5800634169	1.0124123500
H	3.1003686564	2.2505823267	0.0681737045
H	4.4807001240	1.4826616624	-0.7758178498
H	-3.0368215973	-2.2262100071	-0.1306439785
H	-4.3935442816	-1.5602406631	-1.0920176320
H	-4.4406494388	-1.4831121663	0.6966753312
H	-4.5371935559	0.9252464912	-1.1921870693
H	-3.2677086440	1.8171913099	-0.2960374598
H	-4.5813713584	0.9896616583	0.5971178672

DIMETHYL ETHER
62
ENERGY=   -155.0250468
MAXIMUM GRADIENT = 0.0000062   RMS GRADIENT = 0.0000028
ZERO-POINT ENERGY = 0.080304

C	-1.1709020872	-0.2485792085	0.0003780602
O	0.0000009119	0.5366977781	-0.0000002114
C	1.1708994039	-0.2485815058	-0.0003780256
H	-1.2313105519	-0.8939689275	0.8926803123
H	-1.2331248228	-0.8920013885	-0.8932292067
H	-2.0218312745	0.4379299095	0.0020035960
H	1.2313112089	-0.8939683182	-0.8926795262
H	1.2331250858	-0.8920002697	0.8932287850
H	2.0218330289	0.4379319499	-0.0020035990

LITHIATED PHOSPHINE OXIDE DIMER COMPLEX
63
ENERGY= -1706.8247958
MAXIMUM GRADIENT = 0.0000943 RMS GRADIENT = 0.0000324
ZERO-POINT ENERGY = 0.542697

O	8.0	0.5574576524	2.0027324267	-0.0703097305
O	8.0	-0.5574576524	-2.0027324267	-0.0703097305
LI	3.0	1.1604301249	-1.6156051675	0.5744186474
LI	3.0	-1.1604301249	1.6156051675	0.5744186474
P	15.0	2.0063119912	1.4813681605	-0.0033222470
P	15.0	-2.0063119912	-1.4813681605	-0.0033222470
C	6.0	2.2868478876	0.1739319737	1.1144545991
C	6.0	-2.2868478876	-0.1739319737	1.1144545991
C	6.0	2.5555374143	0.8967759801	-1.6606023419
C	6.0	-2.5555374143	-0.8967759801	-1.6606023419
H	1.0	3.3466138122	-0.1192396222	1.1072713499
H	1.0	-3.3466138122	0.1192396222	1.1072713499
H	1.0	2.0086799404	0.4929296080	2.1280895001
H	1.0	-2.0086799404	-0.4929296080	2.1280895001
H	1.0	1.9419835616	0.0396399681	-1.9516250466
H	1.0	-1.9419835616	-0.0396399681	-1.9516250466
H	1.0	3.6064274954	0.5866923298	-1.6407911725
H	1.0	-3.6064274954	-0.5866923298	-1.6407911725
H	1.0	2.4361170649	1.6915232120	-2.4043474261
H	1.0	-2.4361170649	-1.6915232120	-2.4043474261
O	8.0	2.2359981374	-2.7412399392	-0.8336215967
O	8.0	-2.2359981374	2.7412399392	-0.8336215967
C	6.0	1.6325127663	-3.1837638031	-2.0406374998
C	6.0	-1.6325127663	3.1837638031	-2.0406374998
C	6.0	3.6487042714	-2.8303834068	-0.8461444936
C	6.0	-3.6487042714	2.8303834068	-0.8461444936
H	1.0	1.8647655959	-4.2431313263	-2.2291297467
H	1.0	-1.8647655959	4.2431313263	-2.2291297467
H	1.0	1.9856735952	-2.5889770856	-2.8967373648
H	1.0	-1.9856735952	2.5889770856	-2.8967373648
H	1.0	0.5593102128	-3.0470476934	-1.9059493028
H	1.0	-0.5593102128	3.0470476934	-1.9059493028
H	1.0	4.0774396183	-2.2262719304	-1.6597960770
H	1.0	-4.0774396183	2.2262719304	-1.6597960770
H	1.0	4.0011278304	-2.4482113540	0.1133429484
H	1.0	-4.0011278304	2.4482113540	0.1133429484
H	1.0	3.9779747529	-3.8731398201	-0.9709931109
H	1.0	-3.9779747529	3.8731398201	-0.9709931109
O	8.0	1.4830624775	-2.9704417397	2.1530508175
O	8.0	-1.4830624775	2.9704417397	2.1530508175
C	6.0	1.3268615931	-2.4855365119	3.4773164780
C	6.0	-1.3268615931	2.4855365119	3.4773164780
C	6.0	0.8793855279	-4.2417567833	1.9626498417
C	6.0	-0.8793855279	4.2417567833	1.9626498417
H	1.0	1.8046736944	-3.1627923167	4.2012092248
H	1.0	-1.8046736944	3.1627923167	4.2012092248

H	1.0	0.2632360887	-2.3794951036	3.7378697581
H	1.0	-0.2632360887	2.3794951036	3.7378697581
H	1.0	1.8085018031	-1.5075904911	3.5144460004
H	1.0	-1.8085018031	1.5075904911	3.5144460004
H	1.0	1.3393978614	-4.9920908539	2.6232278565
H	1.0	-1.3393978614	4.9920908539	2.6232278565
H	1.0	-0.2007916805	-4.1999296651	2.1581099641
H	1.0	0.2007916805	4.1999296651	2.1581099641
H	1.0	1.0453230447	-4.5146980367	0.9202505851
H	1.0	-1.0453230447	4.5146980367	0.9202505851
C	6.0	3.0802610083	2.9750785393	0.2426674553
C	6.0	-3.0802610083	-2.9750785393	0.2426674553
H	1.0	4.1419577609	2.7041156371	0.2378729517
H	1.0	-4.1419577609	-2.7041156371	0.2378729517
H	1.0	2.8428535745	3.4183742881	1.2158717421
H	1.0	-2.8428535745	-3.4183742881	1.2158717421
H	1.0	2.8978131260	3.7275266947	-0.5335805633
H	1.0	-2.8978131260	-3.7275266947	-0.5335805633

LITHIATED PHOSPHINE SULFIDE DIMER COMPLEX
64
ENERGY= -2352.7302176
MAXIMUM GRADIENT = 0.0000831 RMS GRADIENT = 0.0000312
ZERO-POINT ENERGY = 0.539858

S	16.0	0.7756624665	2.6488593059	-0.1067157896
S	16.0	-0.7756624665	-2.6488593059	-0.1067157896
LI	3.0	1.4451175667	-1.7350214348	0.5768517569
LI	3.0	-1.4451175667	1.7350214348	0.5768517569
P	15.0	2.4087015750	1.4365118159	-0.0865765725
P	15.0	-2.4087015750	-1.4365118159	-0.0865765725
C	6.0	2.3940616810	0.1251750175	1.0825473913
C	6.0	-2.3940616810	-0.1251750175	1.0825473913
C	6.0	2.6724168891	0.7131340523	-1.7615637679
C	6.0	-2.6724168891	-0.7131340523	-1.7615637679
C	6.0	3.8845155916	2.5530096155	0.0565502117
C	6.0	-3.8845155916	-2.5530096155	0.0565502117
H	1.0	3.4311139008	-0.2089129181	1.2501562706
H	1.0	-3.4311139008	0.2089129181	1.2501562706
H	1.0	1.9912440031	0.5100935537	2.0267811435
H	1.0	-1.9912440031	-0.5100935537	2.0267811435
H	1.0	1.8052882353	0.0990816523	-2.0178592921
H	1.0	-1.8052882353	-0.0990816523	-2.0178592921
H	1.0	3.5683471312	0.0809124023	-1.7597498261
H	1.0	-3.5683471312	-0.0809124023	-1.7597498261
H	1.0	2.7888901062	1.5051235233	-2.5072891105
H	1.0	-2.7888901062	-1.5051235233	-2.5072891105
H	1.0	4.8076919403	1.9629295719	0.0078626693
H	1.0	-4.8076919403	-1.9629295719	0.0078626693
H	1.0	3.8431834149	3.0643109789	1.0224871352
H	1.0	-3.8431834149	-3.0643109789	1.0224871352
H	1.0	3.8892398911	3.3036071754	-0.7402284583
H	1.0	-3.8892398911	-3.3036071754	-0.7402284583
O	8.0	2.6220676058	-2.8469795596	-0.7441177761
O	8.0	-2.6220676058	2.8469795596	-0.7441177761
C	6.0	2.2428937700	-3.2727203164	-2.0483153170
C	6.0	-2.2428937700	3.2727203164	-2.0483153170
C	6.0	4.0186598316	-2.9485706681	-0.5146315327
C	6.0	-4.0186598316	2.9485706681	-0.5146315327
H	1.0	2.5270328032	-4.3228162776	-2.2092597559
H	1.0	-2.5270328032	4.3228162776	-2.2092597559
H	1.0	2.7248545195	-2.6515624694	-2.8172187849
H	1.0	-2.7248545195	2.6515624694	-2.8172187849
H	1.0	1.1584050413	-3.1692379647	-2.1085303913
H	1.0	-1.1584050413	3.1692379647	-2.1085303913
H	1.0	4.5825669831	-2.3136621993	-1.2136592245
H	1.0	-4.5825669831	2.3136621993	-1.2136592245
H	1.0	4.2004522497	-2.6167199265	0.5087687637
H	1.0	-4.2004522497	2.6167199265	0.5087687637
H	1.0	4.3588547376	-3.9883021659	-0.6304933066
H	1.0	-4.3588547376	3.9883021659	-0.6304933066

O	8.0	1.8190725289	-3.0053254292	2.1832605904
O	8.0	-1.8190725289	3.0053254292	2.1832605904
C	6.0	1.2892064135	-2.5090280777	3.4069742504
C	6.0	-1.2892064135	2.5090280777	3.4069742504
C	6.0	1.5350607960	-4.3898031310	2.0014393037
C	6.0	-1.5350607960	4.3898031310	2.0014393037
H	1.0	1.7343198198	-3.0369449070	4.2629853655
H	1.0	-1.7343198198	3.0369449070	4.2629853655
H	1.0	0.1972844369	-2.6266041237	3.4340652929
H	1.0	-0.1972844369	2.6266041237	3.4340652929
H	1.0	1.5442066562	-1.4492621549	3.4563832607
H	1.0	-1.5442066562	1.4492621549	3.4563832607
H	1.0	1.9954073534	-4.9843865209	2.8039096036
H	1.0	-1.9954073534	4.9843865209	2.8039096036
H	1.0	0.4522647579	-4.5651611418	1.9804806833
H	1.0	-0.4522647579	4.5651611418	1.9804806833
H	1.0	1.9624078576	-4.6746489692	1.0392552133
H	1.0	-1.9624078576	4.6746489692	1.0392552133

LITHIATED PHOSPHINE BORANE DIMER COMPLEX
65
ENERGY= -1609.6098800
MAXIMUM GRADIENT = 0.0000834 RMS GRADIENT = 0.0000329
ZERO-POINT ENERGY = 0.598015

B	5.0	0.7273471965	2.2336109244	-0.2288237721
B	5.0	-0.7273471965	-2.2336109244	-0.2288237721
LI	3.0	1.6042067336	-1.7990410241	0.5913152041
LI	3.0	-1.6042067336	1.7990410241	0.5913152041
P	15.0	2.4648379692	1.3742664844	-0.0745844486
P	15.0	-2.4648379692	-1.3742664844	-0.0745844486
C	6.0	2.5762789877	0.0484680589	1.0852122729
C	6.0	-2.5762789877	-0.0484680589	1.0852122729
C	6.0	3.0019504600	0.7294873343	-1.7190354171
C	6.0	-3.0019504600	-0.7294873343	-1.7190354171
C	6.0	3.7281639379	2.7128190116	0.2071003514
C	6.0	-3.7281639379	-2.7128190116	0.2071003514
H	1.0	0.3992107966	2.5645200362	0.8984985588
H	1.0	-0.3992107966	-2.5645200362	0.8984985588
H	1.0	-0.0501292171	1.4275697533	-0.7096424548
H	1.0	0.0501292171	-1.4275697533	-0.7096424548
H	1.0	0.8606656996	3.2060782168	-0.9482022643
H	1.0	-0.8606656996	-3.2060782168	-0.9482022643
H	1.0	3.6299293905	-0.2023588373	1.2846468859
H	1.0	-3.6299293905	0.2023588373	1.2846468859
H	1.0	2.1147887396	0.3874531889	2.0232810436
H	1.0	-2.1147887396	-0.3874531889	2.0232810436
H	1.0	2.2831904617	-0.0228367681	-2.0556400943
H	1.0	-2.2831904617	0.0228367681	-2.0556400943
H	1.0	3.9931063835	0.2668635158	-1.6474098149
H	1.0	-3.9931063835	-0.2668635158	-1.6474098149
H	1.0	3.0403275276	1.5371671945	-2.4572336134
H	1.0	-3.0403275276	-1.5371671945	-2.4572336134
H	1.0	4.7389577125	2.2907052384	0.2484432492
H	1.0	-4.7389577125	-2.2907052384	0.2484432492
H	1.0	3.5174128807	3.1992399013	1.1650426619
H	1.0	-3.5174128807	-3.1992399013	1.1650426619
H	1.0	3.6856038848	3.4714251502	-0.5825607240
H	1.0	-3.6856038848	-3.4714251502	-0.5825607240
O	8.0	2.6648377769	-3.0387521947	-0.6692913260
O	8.0	-2.6648377769	3.0387521947	-0.6692913260
C	6.0	2.2870915789	-3.4059346053	-1.9916067187
C	6.0	-2.2870915789	3.4059346053	-1.9916067187
C	6.0	4.0698000327	-3.0869008978	-0.4644870523
C	6.0	-4.0698000327	3.0869008978	-0.4644870523
H	1.0	2.6064971063	-4.4351119202	-2.2112317192
H	1.0	-2.6064971063	4.4351119202	-2.2112317192
H	1.0	2.7400142396	-2.7281857705	-2.7294558407
H	1.0	-2.7400142396	2.7281857705	-2.7294558407
H	1.0	1.2003905585	-3.3353117531	-2.0403057613
H	1.0	-1.2003905585	3.3353117531	-2.0403057613

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H           1.0   4.5907138592  -2.3975837249  -1.1441340020
H           1.0  -4.5907138592   2.3975837249  -1.1441340020
H           1.0   4.2523985702  -2.7875523120   0.5684910096
H           1.0  -4.2523985702   2.7875523120   0.5684910096
H           1.0   4.4508303396  -4.1055377501  -0.6284903831
H           1.0  -4.4508303396   4.1055377501  -0.6284903831
O           8.0   1.9070514085  -3.0365822967   2.2477456297
O           8.0  -1.9070514085   3.0365822967   2.2477456297
C           6.0   1.5983397159  -2.4702495525   3.5147953719
C           6.0  -1.5983397159   2.4702495525   3.5147953719
C           6.0   1.5021689961  -4.3970647157   2.1514909587
C           6.0  -1.5021689961   4.3970647157   2.1514909587
H           1.0   2.1120344982  -3.0165893168   4.3192129892
H           1.0  -2.1120344982   3.0165893168   4.3192129892
H           1.0   0.5150436546  -2.4927392161   3.7004439113
H           1.0  -0.5150436546   2.4927392161   3.7004439113
H           1.0   1.9434737475  -1.4360615867   3.4926768322
H           1.0  -1.9434737475   1.4360615867   3.4926768322
H           1.0   2.0251575020  -5.0082275688   2.9014649206
H           1.0  -2.0251575020   5.0082275688   2.9014649206
H           1.0   0.4175685071  -4.4948313720   2.2920071467
H           1.0  -0.4175685071   4.4948313720   2.2920071467
H           1.0   1.7667537518  -4.7329171944   1.1484514093
H           1.0  -1.7667537518   4.7329171944   1.1484514093
```

DIMETHYLAMINE
ENERGY=   -135.1628450
MAXIMUM GRADIENT = 0.0000050   RMS GRADIENT = 0.0000021
ZERO-POINT ENERGY = 0.092955

N	7.0	0.8921764912	0.0357231687	-0.4842555909
C	6.0	0.5876914725	-1.3892017610	-0.4978993806
C	6.0	0.0045869611	0.7936006080	0.3881528598
H	1.0	0.8192340475	0.4007523462	-1.4316238370
H	1.0	-0.4613135468	-1.6309896750	-0.7578279023
H	1.0	0.7844814217	-1.8107945167	0.4955005257
H	1.0	1.2441415535	-1.8990285753	-1.2111033631
H	1.0	0.2392985963	1.8608330609	0.3145634448
H	1.0	0.1713188072	0.4871991140	1.4281722603
H	1.0	-1.0734138042	0.6597542302	0.1727279833

METHANE
ENERGY=   -40.5183819
MAXIMUM GRADIENT = 0.0000073   RMS GRADIENT = 0.0000030
ZERO-POINT ENERGY = 0.045205

C	6.0	0.2643021966	-0.3740580478	0.0000000000
H	1.0	0.2640006668	0.7191908773	0.0000000000
H	1.0	-0.7663446708	-0.7387024489	0.0000000000
H	1.0	0.7797629037	-0.7383431903	0.8926490790
H	1.0	0.7797629037	-0.7383431903	-0.8926490790

METHYL LITHIUM COMPLEXES
PRE-LITHIATION COMPLEXES
66
ENERGY=   -738.8522679
MAXIMUM GRADIENT = 0.0000082   RMS GRADIENT = 0.0000024
ZERO-POINT ENERGY = 0.235665

O	0.2929377780	0.7154281681	-0.2596801518
P	1.6907312941	0.1096563323	-0.2122868902
C	2.1614716779	-0.4765566699	1.4490008043
C	2.9588160666	1.3370199045	-0.6948513175
C	1.9001770349	-1.3090103072	-1.3371737556
Li	-1.1251777014	-0.5014772152	0.1564356043
C	-0.9431090229	-2.5085520446	0.5730869779
O	-2.7766405104	0.5279094115	0.0403515372
C	-2.8415879529	1.8981675474	-0.3280516504
C	-4.0450586625	-0.0644718504	0.2856940799
H	1.4398746662	-1.2454845414	1.7424025682
H	2.1053161458	0.3560856332	2.1573950110
H	3.1745491791	-0.8926585830	1.4592836787
H	3.9645024788	0.9046579532	-0.6692019750
H	2.9181139546	2.1903044166	-0.0109538110
H	2.7494205621	1.6954907862	-1.7073628347
H	2.9103278662	-1.7279435289	-1.2753837002
H	1.7043129723	-0.9883088974	-2.3654191636
H	-1.7768458721	-2.8413684796	1.2225579077
H	-0.0404260922	-2.9019032179	1.0819224901
H	-1.0412096143	-3.1336452724	-0.3374555047
H	-3.3002846064	2.4959492647	0.4727762253
H	-3.4275959038	2.0265761954	-1.2495765249
H	-1.8140273341	2.2256626454	-0.4931296820
H	-4.6766180286	-0.0194230599	-0.6131014081
H	-4.5598743584	0.4459413450	1.1122583452
H	-3.8565265287	-1.1055274623	0.5532272869
H	1.1601212779	-2.0642439954	-1.0521040801

67

```
ENERGY=   -1061.8076360
MAXIMUM GRADIENT =  0.0000068    RMS GRADIENT = 0.0000027
ZERO-POINT ENERGY = 0.234119
 S           -0.3737410632  -1.3330958150  -0.4738009579
 P           -1.8826232571  -0.0176395158  -0.5712868801
 C           -2.1858912106   0.8730189709   0.9978547834
 C           -3.4659813985  -0.8469663771  -0.9891558782
 C           -1.6494334252   1.2813346496  -1.8382762960
 Li           1.3082917350   0.4496238358   0.0371848583
 C            1.0814213902   2.4752692068   0.2196932485
 O            3.0721040375  -0.3712941475   0.1606897591
 C            3.4452008914  -1.7357123498   0.0272196848
 C            4.1823665397   0.5037171412   0.3443895644
 H           -1.2822607573   1.4475552553   1.2261967876
 H           -2.3760066474   0.1493684948   1.7953959408
 H           -3.0426920543   1.5490152850   0.9001322383
 H           -4.2827561623  -0.1189202798  -1.0399274051
 H           -3.6937973796  -1.5973040967  -0.2270331715
 H           -3.3664137809  -1.3498936750  -1.9549939482
 H           -2.5162545784   1.9509366496  -1.8712600303
 H           -1.5088458081   0.8123446626  -2.8162449681
 H            1.6418047451   2.8057187790   1.1175455980
 H            0.1112596619   2.9997921471   0.3080526740
 H            1.5875879496   2.9846640129  -0.6252957868
 H            3.9664586893  -2.0864783538   0.9289640068
 H            4.1001668212  -1.8772621882  -0.8439486442
 H            2.5271945751  -2.3096693161  -0.1103139521
 H            4.8642873751   0.4471164236  -0.5155691968
 H            4.7322005722   0.2417786116   1.2591067964
 H            3.7740986274   1.5116099935   0.4302091531
 H           -0.7506696408   1.8451304517  -1.5653699711
```

68

```
ENERGY=    -690.2475652
MAXIMUM GRADIENT =  0.0000094    RMS GRADIENT = 0.0000031
ZERO-POINT ENERGY = 0.263103
 B            0.4185295604  -1.3030274862  -0.1288410812
 P            1.9869674957  -0.1765450075   0.2096339837
 C            2.3955953675   0.9424673899  -1.1836633865
 C            3.5091175472  -1.1691160839   0.4964327725
 C            1.8365642650   0.9096236629   1.6767946950
 H            0.7989000302  -2.4439065845  -0.2474699820
 H           -0.0813803710  -0.8963180936  -1.1615483148
 H           -0.3205837691  -1.1690302677   0.8286825135
 H            1.5428847184   1.6131180653  -1.3264247152
 H            2.5437291062   0.3549777928  -2.0950313224
 H            3.2973773148   1.5282330972  -0.9780365835
 H            4.3757039761  -0.5283610579   0.6886117156
 H            3.7083504762  -1.7916613010  -0.3810154480
 H            3.3543084116  -1.8304769634   1.3544385353
 H            2.7343757315   1.5210519858   1.8145829069
 H            1.6757503853   0.2954225487   2.5684210959
 H            0.9621059446   1.5501379380   1.5216558746
 Li          -1.2975518254   0.4030991763  -0.1915421199
 C           -0.9618628345   2.4036098097   0.0500384264
 O           -3.0597325020  -0.3907975936  -0.4259289934
 C           -3.3826048111  -1.7655589039  -0.5869165809
 C           -4.2009653776   0.4609724303  -0.3929357888
 H           -1.7377334214   2.9476524483  -0.5257747833
 H           -0.0180354577   2.8864798943  -0.2682513913
 H           -1.1097893750   2.7454560617   1.0940654247
 H           -3.9161058336  -1.9308778525  -1.5334686238
 H           -4.0093902843  -2.1177895549   0.2443839837
 H           -2.4414244112  -2.3176101255  -0.5946903494
 H           -4.8575319639   0.1946330508   0.4471528991
 H           -4.7670235702   0.3846185853  -1.3317874649
 H           -3.8279010185   1.4782124034  -0.2656617656
```

LITHIATION TRANSITION STRUCTURE COMPLEXES
69
ENERGY=   -738.8304020
MAXIMUM GRADIENT = 0.0000195   RMS GRADIENT = 0.0000067
ZERO-POINT ENERGY = 0.231299
IMAGINARY FREQUENCY = 1277.37
REDUCED MASS = 1.06583

O	-0.3686059391	-0.7746773472	0.1556490168
P	-1.7674416256	-0.1437405673	-0.0358318630
C	-2.6392856198	-0.0086582776	1.5703782593
C	-2.7924430557	-1.3025689443	-1.0260323380
C	-1.6290212520	1.4788219373	-0.7186463012
Li	0.9640164459	0.4954645212	0.0350841242
C	0.9790511318	2.5965777791	-0.0216854443
H	-2.1095296507	0.7117231699	2.2017705774
H	-2.6399384225	-0.9799741936	2.0749443306
H	-3.6716802830	0.3310318984	1.4383035946
H	-3.8116302662	-0.9221847177	-1.1484130580
H	-2.8261443436	-2.2872968700	-0.5467681412
H	-2.3380109765	-1.4153582874	-2.0155460164
H	-2.4184126594	2.1589656767	-0.3840882386
H	-1.5964343414	1.4536281959	-1.8141569166
H	1.5452213844	2.4808010582	0.9253812798
H	0.5638883884	3.6121214698	0.0174666918
H	1.7168705790	2.6064771936	-0.8463539667
H	-0.3696587635	1.9560248649	-0.3248493797
O	2.6901926909	-0.3678330744	0.0204945273
C	2.7366375565	-1.7926009316	0.0739496207
C	3.9725294734	0.2444920219	-0.0350629179
H	3.2782244285	-2.1257779903	0.9699668398
H	3.2356862385	-2.1939570888	-0.8188968509
H	1.7012648488	-2.1337798468	0.1122222735
H	4.5166096851	-0.0754165998	-0.9345212831
H	4.5645010622	-0.0135166233	0.8539065692
H	3.8109130195	1.3234797489	-0.0675310690

70

ENERGY= -1061.7872102

MAXIMUM GRADIENT = 0.0000180 RMS GRADIENT = 0.0000060

ZERO-POINT ENERGY = 0.230074

IMAGINARY FREQUENCY = 1239.11

REDUCED MASS = 1.07203

S	0.5931087839	-1.2049289209	-0.9106638555
P	1.8016735873	-0.0150810411	0.2023416543
C	2.8594557990	1.0536664213	-0.8505602641
C	3.0066210910	-1.0447644951	1.1435168537
C	0.8327057501	1.0930926400	1.2057765508
Li	-1.1000841328	0.4724289316	-0.3890851679
C	-1.0456841291	2.5980513681	-0.4408853800
O	-2.8207868365	-0.2714327094	0.0798477313
C	-3.0744332571	-1.6704392678	0.1969653838
C	-3.9666771800	0.5318535828	0.3516225545
H	2.2134392302	1.7067457372	-1.4434539524
H	3.4577654675	0.4356160521	-1.5255198634
H	3.5215687143	1.6680079548	-0.2302991710
H	3.6777959853	-0.4047522246	1.7265468262
H	3.5930325470	-1.6633050727	0.4562866553
H	2.4558828903	-1.7010736942	1.8226956958
H	1.4503079373	1.8686657390	1.6738515898
H	0.2953090842	0.5334527920	1.9814021978
H	-1.6715611325	2.4072237465	-1.3371535759
H	-0.3142469412	3.3520942188	-0.7673892643
H	-1.6993123188	3.0957164518	0.2944644150
H	-3.8352423398	-1.9855160727	-0.5297687107
H	-3.4202207709	-1.9130212864	1.2109395554
H	-2.1316162614	-2.1813063857	-0.0043764689
H	-4.3216309741	0.3603888722	1.3768498516
H	-4.7757467111	0.3006761363	-0.3542237187
H	-3.6621173400	1.5729057893	0.2366726655
H	-0.0674068966	1.7560697764	0.3974305691

71

ENERGY= -690.2245893

MAXIMUM GRADIENT = 0.0000064 RMS GRADIENT = 0.0000033

ZERO-POINT ENERGY = 0.258953

IMAGINARY FREQUENCY = 1266.21

REDUCED MASS = 1.06462

B	0.6592957552	-1.2410849359	-1.0433176060
P	1.8965257624	-0.2181519184	0.0542087976
C	2.9009071095	0.9661609572	-0.9296094996
C	3.1600845524	-1.2864952626	0.8759146074
C	0.9356978604	0.7759551879	1.1930316364
H	1.2320434284	-2.0377368775	-1.7451087604
H	0.0641613755	-0.4169274395	-1.7310054229
H	-0.0931832642	-1.7777285943	-0.2440443571
H	2.2292837608	1.6674526179	-1.4329196070
H	3.4813947549	0.4302870887	-1.6866863540
H	3.5839639205	1.5305685068	-0.2861248543
H	3.8244075142	-0.6885910443	1.5083291080
H	3.7542520573	-1.8158129248	0.1226632422
H	2.6520238782	-2.0283001523	1.4995141393
H	1.5413235997	1.4909399301	1.7610907757
H	0.4012371818	0.1228881978	1.8966326610
H	0.0339057856	1.5586355889	0.4796718068
Li	-1.0007243748	0.3522775277	-0.3082590030
C	-0.9293525484	2.4888936773	-0.2590471121
O	-2.7719410871	-0.3574841749	0.0169138147
C	-3.2153844499	-1.6678503939	-0.3304106368
C	-3.8201288056	0.4716015304	0.5160561229
H	-1.6067317215	2.3636729676	-1.1277027318
H	-0.1790482857	3.2229791629	-0.5889454793
H	-1.5211989473	2.9829575742	0.5287556723
H	-3.9758742721	-1.6186647327	-1.1212494422
H	-3.6381215365	-2.1744585622	0.5475640237
H	-2.3432608785	-2.2167936139	-0.6871433540
H	-4.2457932737	0.0402075044	1.4319912587
H	-4.6139107492	0.5832411980	-0.2345653799
H	-3.3809209536	1.4459978195	0.7326045049

POST-LITHIATION COMPLEXES
72
ENERGY=   -698.3554385
MAXIMUM GRADIENT = 0.0000084   RMS GRADIENT = 0.0000030
ZERO-POINT ENERGY = 0.189565

O	-0.3924204330	0.8435953087	0.1814528099
P	-1.6056535073	-0.1038814879	-0.0415532916
Li	0.7793973304	-0.6042424435	-0.0099118708
C	-1.0216363653	-1.7155111659	-0.3851707142
C	-2.6572098487	0.6014455277	-1.3758789470
C	-2.6724906900	-0.0943480077	1.4539670872
O	2.6372030243	-0.1877638930	0.1627054302
C	3.8104358733	-0.9849387617	0.0807046143
C	2.8973428048	1.1991710541	0.3968626486
H	-1.1529717971	-2.0196592641	-1.4272957262
H	-1.3891427886	-2.4825517688	0.2999861941
H	-3.5858936243	0.0329719649	-1.4898746567
H	-2.1024783559	0.5604541709	-2.3192470054
H	-2.8926505491	1.6494793193	-1.1627716821
H	-3.6137745067	-0.6237906469	1.2745121313
H	-2.8850461034	0.9355983671	1.7582211872
H	-2.1396717993	-0.5911962540	2.2715544573
H	3.4912719737	-2.0140155411	-0.0977141260
H	4.3802884295	-0.9357957803	1.0186329603
H	4.4506637885	-0.6514593412	-0.7474713002
H	3.4310446794	1.3313061213	1.3475271536
H	1.9243378736	1.6916277101	0.4377691417
H	3.5005663263	1.6169616108	-0.4203186889

73

ENERGY= -1021.3184366

MAXIMUM GRADIENT = 0.0000066 RMS GRADIENT = 0.0000026

ZERO-POINT ENERGY = 0.187735

S	-0.6464562215	1.4956075274	0.7261491706
P	-1.7102413650	-0.1803741507	0.2267112578
Li	0.9312052277	-0.2131542434	0.1728280364
C	-0.6543960119	-1.5844312296	0.2255131347
C	-2.4135320301	-0.0256271368	-1.4662401870
C	-3.2184596256	-0.2505940548	1.2972677669
O	2.8201201878	-0.0316550530	0.0196800646
C	3.7345206023	-1.0824725276	-0.2771585823
C	3.4536523741	1.2245496931	0.2619984703
H	-0.9852604004	-2.3578349504	-0.4734023492
H	-0.5455212432	-1.9954802577	1.2370085287
H	-3.0692209464	-0.8751710509	-1.6876207072
H	-1.5952744173	-0.0058208518	-2.1913415912
H	-2.9798413117	0.9058730730	-1.5493802832
H	-3.8395726819	-1.1077533657	1.0138162377
H	-3.7987243536	0.6734998138	1.2079767261
H	-2.9044859823	-0.3652752875	2.3386601498
H	3.1430494044	-1.9850969333	-0.4422857214
H	4.4250990232	-1.2428819339	0.5615676454
H	4.3109987949	-0.8484289871	-1.1820534116
H	4.1327696303	1.1525277505	1.1217085197
H	2.6602718416	1.9427540118	0.4761639529
H	4.0178998045	1.5463248512	-0.6231706878

74

ENERGY= -649.7541289

MAXIMUM GRADIENT = 0.0000170 RMS GRADIENT = 0.0000065

ZERO-POINT ENERGY = 0.216541

B	-0.6568120918	1.6038177884	0.1396965795
P	-1.7564913444	-0.0086131696	0.0462014013
C	-0.7113022111	-1.3706513686	0.4857380435
C	-2.3315194565	-0.3049761108	-1.6773108501
C	-3.3555718720	0.1708217533	0.9762552050
H	0.1316517476	1.4863995357	-0.8025523915
H	-0.0415342718	1.5132691789	1.1982778273
H	-1.2786071207	2.6333481854	0.0506972885
H	-1.0730982023	-2.3367577141	0.1205735440
H	-0.6015513453	-1.4096567009	1.5797065590
H	-2.9473151648	-1.2089263679	-1.7332722986
H	-1.4612375704	-0.4315248320	-2.3278695085
H	-2.9149414144	0.5489054258	-2.0349301762
H	-3.9571861543	-0.7405307904	0.8900111663
H	-3.9296169818	1.0247388446	0.5989258701
H	-3.1341301377	0.3451402654	2.0340033504
Li	0.8975011283	-0.1041869953	0.0941933517
O	2.7992764651	-0.0294819327	-0.0035195278
C	3.6402030062	-1.1774691612	0.0758843897
C	3.5185717797	1.1982958353	-0.1082487306
H	2.9857073288	-2.0474595846	0.1557590168
H	4.2888195082	-1.1202607584	0.9601093098
H	4.2610162439	-1.2632430541	-0.8258068928
H	4.1583115075	1.3452968380	0.7718507577
H	2.7778678450	1.9978305863	-0.1631194087
H	4.1382957469	1.2036403498	-1.0145340482

ETHER METHYL LITHIUM TETRAMER COMPLEX
75
ENERGY= -809.9998004
MAXIMUM GRADIENT = 0.0000062 RMS GRADIENT = 0.0000018
ZERO-POINT ENERGY = 0.470195

C	6.0	0.9194915953	-1.5716270423	1.2994350015
C	6.0	-1.5716270423	-0.9194915953	-1.2994350015
C	6.0	1.5716270423	0.9194915953	-1.2994350015
C	6.0	-0.9194915953	1.5716270423	1.2994350015
LI	3.0	0.5887810463	-1.0948094133	-0.8609954481
LI	3.0	-1.0948094133	-0.5887810463	0.8609954481
LI	3.0	1.0948094133	0.5887810463	0.8609954481
LI	3.0	-0.5887810463	1.0948094133	-0.8609954481
O	8.0	1.5175714954	-2.4510077208	-2.0021297576
O	8.0	-2.4510077208	-1.5175714954	2.0021297576
O	8.0	2.4510077208	1.5175714954	2.0021297576
O	8.0	-1.5175714954	2.4510077208	-2.0021297576
C	6.0	1.2227758073	-2.4829899726	-3.3932162133
C	6.0	-2.4829899726	-1.2227758073	3.3932162133
C	6.0	2.4829899726	1.2227758073	3.3932162133
C	6.0	-1.2227758073	2.4829899726	-3.3932162133
C	6.0	2.8988614510	-2.6576699680	-1.7239813068
C	6.0	-2.6576699680	-2.8988614510	1.7239813068
C	6.0	2.6576699680	2.8988614510	1.7239813068
C	6.0	-2.8988614510	2.6576699680	-1.7239813068
H	1.0	2.0049409049	-1.4721792290	1.5043556134
H	1.0	-1.4721792290	-2.0049409049	-1.5043556134
H	1.0	1.4721792290	2.0049409049	-1.5043556134
H	1.0	-2.0049409049	1.4721792290	1.5043556134
H	1.0	0.8198799286	-2.6028275669	0.9070828125
H	1.0	-2.6028275669	-0.8198799286	-0.9070828125
H	1.0	2.6028275669	0.8198799286	-0.9070828125
H	1.0	-0.8198799286	2.6028275669	0.9070828125
H	1.0	0.4672119448	-1.6318105972	2.3095138020
H	1.0	-1.6318105972	-0.4672119448	-2.3095138020
H	1.0	1.6318105972	0.4672119448	-2.3095138020
H	1.0	-0.4672119448	1.6318105972	2.3095138020
H	1.0	0.1491716838	-2.3140815658	-3.4954311435
H	1.0	-2.3140815658	-0.1491716838	3.4954311435
H	1.0	2.3140815658	0.1491716838	3.4954311435
H	1.0	-0.1491716838	2.3140815658	-3.4954311435
H	1.0	1.4834068533	-3.4617443264	-3.8197621207
H	1.0	-3.4617443264	-1.4834068533	3.8197621207
H	1.0	3.4617443264	1.4834068533	3.8197621207
H	1.0	-1.4834068533	3.4617443264	-3.8197621207
H	1.0	1.7722056656	-1.6965574525	-3.9299744702
H	1.0	-1.6965574525	-1.7722056656	3.9299744702
H	1.0	1.6965574525	1.7722056656	3.9299744702
H	1.0	-1.7722056656	1.6965574525	-3.9299744702
H	1.0	3.2237638282	-3.6385512735	-2.0980664498

```
H           1.0  -3.6385512735  -3.2237638282   2.0980664498
H           1.0   3.6385512735   3.2237638282   2.0980664498
H           1.0  -3.2237638282   3.6385512735  -2.0980664498
H           1.0   3.0123874484  -2.6246329583  -0.6391093208
H           1.0  -2.6246329583  -3.0123874484   0.6391093208
H           1.0   2.6246329583   3.0123874484   0.6391093208
H           1.0  -3.0123874484   2.6246329583  -0.6391093208
H           1.0   3.5122599396  -1.8702110650  -2.1830414474
H           1.0  -1.8702110650  -3.5122599396   2.1830414474
H           1.0   1.8702110650   3.5122599396   2.1830414474
H           1.0  -3.5122599396   1.8702110650  -2.1830414474
```

LITHIATED PHOSPHINE OXIDE TETRAMER COMPLEX
76
ENERGY= -2173.4091965
MAXIMUM GRADIENT = 0.0000750 RMS GRADIENT = 0.0000281
ZERO-POINT ENERGY = 0.434600

LI	3.0	-0.8587815577	-1.1578970893	-0.9530000300
LI	3.0	-1.1578970893	0.8587815577	0.9530000300
LI	3.0	1.1578970893	-0.8587815577	0.9530000300
LI	3.0	0.8587815577	1.1578970893	-0.9530000300
O	8.0	-1.0612916128	1.3047223055	-0.9169640459
O	8.0	1.3047223055	1.0612916128	0.9169640459
O	8.0	-1.3047223055	-1.0612916128	0.9169640459
O	8.0	1.0612916128	-1.3047223055	-0.9169640459
P	15.0	-2.1238092225	1.0374951541	-2.0463939969
P	15.0	1.0374951541	2.1238092225	2.0463939969
P	15.0	-1.0374951541	-2.1238092225	2.0463939969
P	15.0	2.1238092225	-1.0374951541	-2.0463939969
C	6.0	-3.7943167718	1.2562617491	-1.3251676298
C	6.0	1.2562617491	3.7943167718	1.3251676298
C	6.0	-1.2562617491	-3.7943167718	1.3251676298
C	6.0	3.7943167718	-1.2562617491	-1.3251676298
C	6.0	-2.0041844024	-0.5679899660	-2.6856206944
C	6.0	-0.5679899660	2.0041844024	2.6856206944
C	6.0	0.5679899660	-2.0041844024	2.6856206944
C	6.0	2.0041844024	0.5679899660	-2.6856206944
C	6.0	-1.9325722392	2.4360988856	-3.2277037155
C	6.0	2.4360988856	1.9325722392	3.2277037155
C	6.0	-2.4360988856	-1.9325722392	3.2277037155
C	6.0	1.9325722392	-2.4360988856	-3.2277037155
H	1.0	-3.8363676628	2.1947014900	-0.7631105603
H	1.0	2.1947014900	3.8363676628	0.7631105603
H	1.0	-2.1947014900	-3.8363676628	0.7631105603
H	1.0	3.8363676628	-2.1947014900	-0.7631105603
H	1.0	-3.9980582409	0.4263504826	-0.6410736157
H	1.0	0.4263504826	3.9980582409	0.6410736157
H	1.0	-0.4263504826	-3.9980582409	0.6410736157
H	1.0	3.9980582409	-0.4263504826	-0.6410736157
H	1.0	-4.5632765364	1.2681846268	-2.1038096607
H	1.0	1.2681846268	4.5632765364	2.1038096607
H	1.0	-1.2681846268	-4.5632765364	2.1038096607
H	1.0	4.5632765364	-1.2681846268	-2.1038096607
H	1.0	-1.3096199626	-0.6485082612	-3.5276985647
H	1.0	-0.6485082612	1.3096199626	3.5276985647
H	1.0	0.6485082612	-1.3096199626	3.5276985647
H	1.0	1.3096199626	0.6485082612	-3.5276985647
H	1.0	-2.9738270802	-1.0116779023	-2.9223486819
H	1.0	-1.0116779023	2.9738270802	2.9223486819
H	1.0	1.0116779023	-2.9738270802	2.9223486819
H	1.0	2.9738270802	1.0116779023	-2.9223486819
H	1.0	-0.9386534788	2.3721305274	-3.6831536171

```
H           1.0   2.3721305274   0.9386534788   3.6831536171
H           1.0  -2.3721305274  -0.9386534788   3.6831536171
H           1.0   0.9386534788  -2.3721305274  -3.6831536171
H           1.0  -2.0138043159   3.3980921249  -2.7097504336
H           1.0   3.3980921249   2.0138043159   2.7097504336
H           1.0  -3.3980921249  -2.0138043159   2.7097504336
H           1.0   2.0138043159  -3.3980921249  -2.7097504336
H           1.0  -2.6865859266   2.3807766116  -4.0193549893
H           1.0   2.3807766116   2.6865859266   4.0193549893
H           1.0  -2.3807766116  -2.6865859266   4.0193549893
H           1.0   2.6865859266  -2.3807766116  -4.0193549893
```

LITHIATED PHOSPHINE SULFIDE TETRAMER COMPLEX
77
ENERGY= -3465.1931933
MAXIMUM GRADIENT = 0.0000833 RMS GRADIENT = 0.0000311
ZERO-POINT ENERGY = 0.427066

LI	3.0	-1.1845011454	-1.2176277750	-1.2254925183
LI	3.0	-1.2176277750	1.1845011454	1.2254925183
LI	3.0	1.2176277750	-1.1845011454	1.2254925183
LI	3.0	1.1845011454	1.2176277750	-1.2254925183
S	16.0	-1.0067958845	2.2956756889	-0.9556253765
S	16.0	2.2956756889	1.0067958845	0.9556253765
S	16.0	-2.2956756889	-1.0067958845	0.9556253765
S	16.0	1.0067958845	-2.2956756889	-0.9556253765
P	15.0	-2.3525710791	1.4896229867	-2.3068645461
P	15.0	1.4896229867	2.3525710791	2.3068645461
P	15.0	-1.4896229867	-2.3525710791	2.3068645461
P	15.0	2.3525710791	-1.4896229867	-2.3068645461
C	6.0	-4.0111292771	1.4388892931	-1.5237713410
C	6.0	1.4388892931	4.0111292771	1.5237713410
C	6.0	-1.4388892931	-4.0111292771	1.5237713410
C	6.0	4.0111292771	-1.4388892931	-1.5237713410
C	6.0	-1.9673724153	-0.1258168134	-2.8470450385
C	6.0	-0.1258168134	1.9673724153	2.8470450385
C	6.0	0.1258168134	-1.9673724153	2.8470450385
C	6.0	1.9673724153	0.1258168134	-2.8470450385
C	6.0	-2.5449758349	2.7831059010	-3.6148840896
C	6.0	2.7831059010	2.5449758349	3.6148840896
C	6.0	-2.7831059010	-2.5449758349	3.6148840896
C	6.0	2.5449758349	-2.7831059010	-3.6148840896
H	1.0	-4.2637525237	2.4249994061	-1.1246496658
H	1.0	2.4249994061	4.2637525237	1.1246496658
H	1.0	-2.4249994061	-4.2637525237	1.1246496658
H	1.0	4.2637525237	-2.4249994061	-1.1246496658
H	1.0	-4.0097953808	0.7080982327	-0.7105385578
H	1.0	0.7080982327	4.0097953808	0.7105385578
H	1.0	-0.7080982327	-4.0097953808	0.7105385578
H	1.0	4.0097953808	-0.7080982327	-0.7105385578
H	1.0	-4.7608911204	1.1440893567	-2.2663894223
H	1.0	1.1440893567	4.7608911204	2.2663894223
H	1.0	-1.1440893567	-4.7608911204	2.2663894223
H	1.0	4.7608911204	-1.1440893567	-2.2663894223
H	1.0	-1.1363298859	-0.1119359054	-3.5602885662
H	1.0	-0.1119359054	1.1363298859	3.5602885662
H	1.0	0.1119359054	-1.1363298859	3.5602885662
H	1.0	1.1363298859	0.1119359054	-3.5602885662
H	1.0	-2.8531176592	-0.5836592699	-3.3053596328
H	1.0	-0.5836592699	2.8531176592	3.3053596328
H	1.0	0.5836592699	-2.8531176592	3.3053596328
H	1.0	2.8531176592	0.5836592699	-3.3053596328
H	1.0	-1.5876030057	2.9138820374	-4.1278032020

```
H           1.0   2.9138820374   1.5876030057   4.1278032020
H           1.0  -2.9138820374  -1.5876030057   4.1278032020
H           1.0   1.5876030057  -2.9138820374  -4.1278032020
H           1.0  -2.8437664711   3.7414406530  -3.1788562463
H           1.0   3.7414406530   2.8437664711   3.1788562463
H           1.0  -3.7414406530  -2.8437664711   3.1788562463
H           1.0   2.8437664711  -3.7414406530  -3.1788562463
H           1.0  -3.2957493782   2.4559442435  -4.3428563124
H           1.0   2.4559442435   3.2957493782   4.3428563124
H           1.0  -2.4559442435  -3.2957493782   4.3428563124
H           1.0   3.2957493782  -2.4559442435  -4.3428563124
```

LITHIATED PHOSPHINE BORANE TETRAMER COMPLEX
78
ENERGY= -1978.9250179
MAXIMUM GRADIENT = 0.0000080 RMS GRADIENT = 0.0000031
ZERO-POINT ENERGY = 0.544640

LI	3.0	1.1200233175	0.7656801018	-0.8559296907
LI	3.0	0.7656801018	-1.1200233175	0.8559296907
LI	3.0	-0.7656801018	1.1200233175	0.8559296907
LI	3.0	-1.1200233175	-0.7656801018	-0.8559296907
C	6.0	1.0246154964	-1.5152624313	-1.3523102423
C	6.0	-1.5152624313	-1.0246154964	1.3523102423
C	6.0	1.5152624313	1.0246154964	1.3523102423
C	6.0	-1.0246154964	1.5152624313	-1.3523102423
P	15.0	2.6686936727	-1.2186273589	-2.0224073935
P	15.0	-1.2186273589	-2.6686936727	2.0224073935
P	15.0	1.2186273589	2.6686936727	2.0224073935
P	15.0	-2.6686936727	1.2186273589	-2.0224073935
C	6.0	3.8820753587	-1.8087661291	-0.7723138868
C	6.0	-1.8087661291	-3.8820753587	0.7723138868
C	6.0	1.8087661291	3.8820753587	0.7723138868
C	6.0	-3.8820753587	1.8087661291	-0.7723138868
B	5.0	2.8783380692	0.6717949896	-2.4421713902
B	5.0	0.6717949896	-2.8783380692	2.4421713902
B	5.0	-0.6717949896	2.8783380692	2.4421713902
B	5.0	-2.8783380692	-0.6717949896	-2.4421713902
C	6.0	3.0201950422	-2.2825206603	-3.4894762703
C	6.0	-2.2825206603	-3.0201950422	3.4894762703
C	6.0	2.2825206603	3.0201950422	3.4894762703
C	6.0	-3.0201950422	2.2825206603	-3.4894762703
H	1.0	0.9610163922	-2.5716833990	-1.0462442162
H	1.0	-2.5716833990	-0.9610163922	1.0462442162
H	1.0	2.5716833990	0.9610163922	1.0462442162
H	1.0	-0.9610163922	2.5716833990	-1.0462442162
H	1.0	0.3593955647	-1.4168351759	-2.2287321299
H	1.0	-1.4168351759	-0.3593955647	2.2287321299
H	1.0	1.4168351759	0.3593955647	2.2287321299
H	1.0	-0.3593955647	1.4168351759	-2.2287321299
H	1.0	3.7169066440	-2.8644419036	-0.5332273581
H	1.0	-2.8644419036	-3.7169066440	0.5332273581
H	1.0	2.8644419036	3.7169066440	0.5332273581
H	1.0	-3.7169066440	2.8644419036	-0.5332273581
H	1.0	3.7870012115	-1.2224976824	0.1466826642
H	1.0	-1.2224976824	-3.7870012115	-0.1466826642
H	1.0	1.2224976824	3.7870012115	-0.1466826642
H	1.0	-3.7870012115	1.2224976824	0.1466826642
H	1.0	4.8988659415	-1.6817910763	-1.1565508921
H	1.0	-1.6817910763	-4.8988659415	1.1565508921
H	1.0	1.6817910763	4.8988659415	1.1565508921
H	1.0	-4.8988659415	1.6817910763	-1.1565508921
H	1.0	2.9180993724	1.2668134757	-1.3724824432

```
H           1.0   1.2668134757  -2.9180993724   1.3724824432
H           1.0  -1.2668134757   2.9180993724   1.3724824432
H           1.0  -2.9180993724  -1.2668134757  -1.3724824432
H           1.0   1.8770147014   0.9742567851  -3.0704412111
H           1.0   0.9742567851  -1.8770147014   3.0704412111
H           1.0  -0.9742567851   1.8770147014   3.0704412111
H           1.0  -1.8770147014  -0.9742567851  -3.0704412111
H           1.0   3.8949961306   0.8611083665  -3.0624790755
H           1.0   0.8611083665  -3.8949961306   3.0624790755
H           1.0  -0.8611083665   3.8949961306   3.0624790755
H           1.0  -3.8949961306  -0.8611083665  -3.0624790755
H           1.0   2.3274143692  -2.0184664804  -4.2944304136
H           1.0  -2.0184664804  -2.3274143692   4.2944304136
H           1.0   2.0184664804   2.3274143692   4.2944304136
H           1.0  -2.3274143692   2.0184664804  -4.2944304136
H           1.0   2.8880628223  -3.3411683022  -3.2423590839
H           1.0  -3.3411683022  -2.8880628223   3.2423590839
H           1.0   3.3411683022   2.8880628223   3.2423590839
H           1.0  -2.8880628223   3.3411683022  -3.2423590839
H           1.0   4.0427096834  -2.1151008529  -3.8439809583
H           1.0  -2.1151008529  -4.0427096834   3.8439809583
H           1.0   2.1151008529   4.0427096834   3.8439809583
H           1.0  -4.0427096834   2.1151008529  -3.8439809583
```

UNSOLVATED LITHIATED PHOSPHINE DERIVATIVES

79

ENERGY= -543.2519297

MAXIMUM GRADIENT = 0.0000081 RMS GRADIENT = 0.0000035

ZERO-POINT ENERGY = 0.106366

C	-0.1986515887	-1.4457237763	-1.0365065821
P	-0.2674784324	-0.0000289194	0.1157159296
C	-0.1912638865	1.4496401554	-1.0311466699
C	1.3028592219	-0.0057726913	0.9786951062
O	-1.5504896902	0.0020226852	0.9101378275
Li	2.9656178034	-0.0011113535	-0.1052881863
H	-0.1068761028	-2.3652487464	-0.4483316297
H	0.6388736366	-1.3943577547	-1.7437738965
H	-1.1333241493	-1.5009875289	-1.6034647064
H	-0.0922717272	2.3663782245	-0.4397841043
H	-1.1266204120	1.5131911365	-1.5961311564
H	0.6445011773	1.3953048455	-1.7403142171
H	1.3000502806	0.8698397370	1.6472474702
H	1.2984362997	-0.8875169200	1.6390920487

80

ENERGY= -866.2230826

MAXIMUM GRADIENT = 0.0000142 RMS GRADIENT = 0.0000044

ZERO-POINT ENERGY = 0.105002

C	0.5189639622	-1.1321994087	1.4451498876
P	0.0856126554	-0.0613990889	-0.0000120191
C	0.5189880740	-1.1318531816	-1.4454177745
C	1.3052049760	1.2619094021	0.0000690657
S	-1.8543081070	0.3946170664	0.0000601985
Li	3.2432215132	0.8027132449	0.0002311443
H	0.3962521778	-0.5501825182	2.3635660380
H	1.5517291419	-1.5002315223	1.3863831560
H	-0.1656163931	-1.9836861221	1.4856518946
H	0.3964891160	-0.5495482797	-2.3636806741
H	-0.1656992076	-1.9832356786	-1.4862701072
H	1.5516958865	-1.5000302600	-1.3866065999
H	1.0762889409	1.8887977562	-0.8754337798
H	1.0761778151	1.8888860483	0.8754783311

81

ENERGY= -494.6642058
MAXIMUM GRADIENT = 0.0000078 RMS GRADIENT = 0.0000030
ZERO-POINT ENERGY = 0.133242

C	-0.0734634928	-1.4475748985	-1.0178049104
P	-0.2327159800	0.0011576705	0.1170228399
C	-0.0732053217	1.4388411684	-1.0317898027
C	1.2845092661	0.0058633371	1.1051155537
B	-1.9654989609	0.0058376412	0.9986593852
Li	3.0430424171	0.0031920727	0.1659946414
H	-0.0596502325	-2.3657732892	-0.4218194220
H	0.8439187631	-1.4006792629	-1.6193369421
H	-0.9381537865	-1.4919080859	-1.6868892191
H	-0.0578176058	2.3626337667	-0.4445432083
H	-0.9385263532	1.4777587628	-1.7003996503
H	0.8435389762	1.3852585480	-1.6337419698
H	1.2133019003	0.8822976614	1.7689350778
H	1.2144789677	-0.8656158875	1.7755457632
H	-1.9924558837	1.0218350568	1.6654157404
H	-1.9931862436	-1.0035638632	1.6753025118
H	-2.7892033109	0.0017921392	0.1022559950

82

ENERGY= -543.2989606
MAXIMUM GRADIENT = 0.0000273 RMS GRADIENT = 0.0000132
ZERO-POINT ENERGY = 0.107458

C	1.2083432548	1.4715285565	0.0057687032
P	0.1101240404	0.0016620823	-0.0311151909
C	1.2378223202	-1.4463760926	-0.0399945926
C	-0.9851577315	0.0149918775	-1.4023162938
O	-0.7446358839	-0.0285272806	1.2731386805
Li	-2.2694404927	-0.0193500957	0.2775843603
H	0.5939616225	2.3751169528	-0.0644878193
H	1.9137855420	1.4593429165	-0.8311727182
H	1.7610438472	1.5053131313	0.9500662704
H	0.6411576133	-2.3594862939	-0.1353115262
H	1.7938159488	-1.4971463181	0.9016320146
H	1.9404083317	-1.3957975408	-0.8779022255
H	-0.9277490772	0.9227822250	-2.0076445333
H	-0.9214747155	-0.8776600344	-2.0292647680

83

ENERGY= -866.2618331
MAXIMUM GRADIENT = 0.0000090 RMS GRADIENT = 0.0000033
ZERO-POINT ENERGY = 0.105639

C	-1.3803842121	0.0839125547	-1.4547457371
P	-0.1749851998	0.2206624386	-0.0630303159
C	-1.2215241806	0.0565226027	1.4386225595
C	0.7192821879	1.7368455275	0.0611691424
S	1.1465753287	-1.3470483883	-0.1912460624
Li	2.3581902059	0.5389380978	0.4228212226
H	-0.8421807381	0.1954160241	-2.4002490925
H	-2.1343389815	0.8746833191	-1.3750053361
H	-1.8671468808	-0.8963860113	-1.4445549706
H	-0.5932672760	0.1718049691	2.3262220827
H	-1.6837457357	-0.9339659231	1.4628144519
H	-1.9999509343	0.8272368602	1.4463545981
H	0.9088131887	2.1638214105	-0.9312342044
H	0.2159871493	2.4646483114	0.7027562489

84

ENERGY= -494.6977213
MAXIMUM GRADIENT = 0.0000129 RMS GRADIENT = 0.0000061
ZERO-POINT ENERGY = 0.134699

C	0.8848991142	1.0491633900	1.2775769068
P	0.1584290483	-0.0157050697	-0.0341183222
C	1.6425804565	-0.8056343363	-0.8150600926
C	-0.8366429387	1.0263926436	-1.0800859473
B	-1.0565287968	-1.3396082835	0.7453704137
Li	-2.4292979190	0.1719554776	-0.1125101813
H	0.0813506297	1.5843845129	1.7918726701
H	1.5750823282	1.7805231015	0.8445990444
H	1.4209370887	0.4375292159	2.0094737243
H	1.3120703606	-1.4567439112	-1.6304637873
H	2.1830892260	-1.4165210305	-0.0836370455
H	2.3145531519	-0.0443108415	-1.2248673357
H	-0.4389155163	2.0389553120	-1.1888583564
H	-0.9350587815	0.5657128545	-2.0737796190
H	-1.7846506133	-0.6765410209	1.4950474069
H	-0.5203139824	-2.2328552624	1.3464730978
H	-1.7308276803	-1.7492053265	-0.2008591660