Phenolic 3° Phosphine Oxides as a Class of Metal-Free Catalysts for the Activation of C–O Bonds in Aliphatic Alcohols: Direct Synthesis of Catalyst Candidates, and Kinetic Studies.

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Supporting Information

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Materials

Solvents and reagents were used as received, including: diphenylphosphine (Alfa Aesar), diethylphosphine (98%, Sigma Aldrich), salicylaldehyde (99%, Acros), 5-methylsalicylaldehyde (>98%, TCI America), 5-nitrosalicylaldehyde (>97%, TCI America), 5-methoxysalicylaldehyde (>96%, TCI America), trifluoroacetic acid (99%, Alfa Aesar), deuterochloroform (99.8% D, Cambridge Isotopes), (±)-2-octanol (97%, Sigma Aldrich), 2,4-dinitrobenzoic acid (98% Alfa Aesar), and xylenes (Alfa Aesar).

Instrumentation

^{1}H, ^{13}C, ^{19}F, and ^{31}P NMR were obtained using a 400 MHz Bruker AVANCE^{TM} Spectrometer with a 5 mm multinuclear broad band (BBO) probe. ^{1}H and ^{13}C chemical shifts were referenced to a tetramethylsilane internal standard, and ^{31}P chemical shifts were referenced to an 85 % phosphoric acid external standard.

Fourier-Transform infrared spectroscopy was obtained using a Nexus 470 spectrometer with an attenuated total reflectance (ATR) attachment.

Mass Spectroscopy was performed using an Agilent Technologies 6530 Accurate-Mass Q-TOF LC/MS in the positive ion mode, and was tuned with standard (3200) 4 GHz, HiRes.

Synthetic Procedures

General procedure for the small-scale ARC reactions:

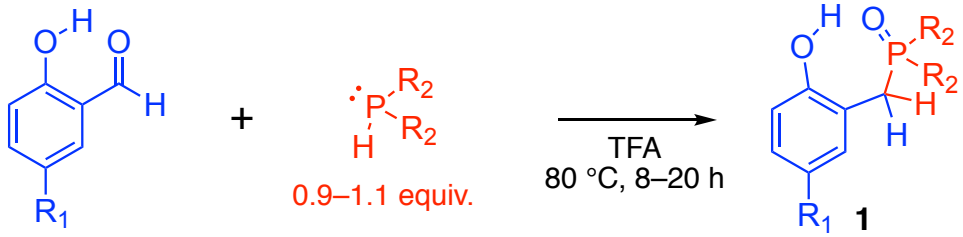
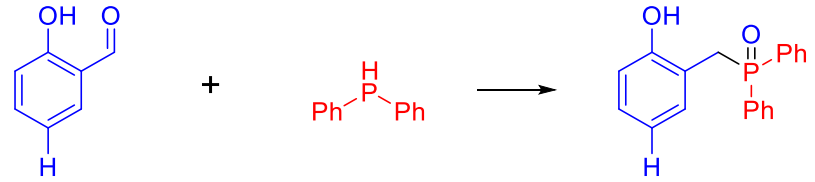


Figure S1. General ARC reaction scheme.

A Teflon-coated stir bar and 35 mL heavy-walled borosilicate pressure tube (Ace Glass Inc., “Tube C”, Product #864807) were oven-dried overnight and then allowed to cool to ambient temperature in air. The tube was then charged with the aldehyde, and then flushed gently with dry nitrogen gas. Then, while maintaining the gentle nitrogen flush, trifluoroacetic acid was added in a single portion, followed quickly by the phosphine, which was also added swiftly in one portion by syringe. The tube was then sealed with a threaded Teflon cap fitted with an o-ring. The sealed tube was then heated in an 80 °C oil bath behind a blast shield for 8–20 hours. The reaction vessel was then removed from the oil bath and allowed to cool for five minutes. Then the reaction tube was opened, and the contents were transferred into a 250 mL separatory funnel that had already been charged with 50 mL of half-saturated sodium bicarbonate (50 mL saturated sodium bicarbonate and 50 mL water). The reaction flask was rinsed with two 25 mL portions of dichloromethane, which were both transferred to the separatory funnel. After agitation, the layers were allowed to separate, and the organic layer was collected. The remaining aqueous phase was extracted with two more portions of dichloromethane (each 50 mL), and the organic phases were all combined, dried over sodium sulfate, and concentrated under vacuum to afford the crude product. Glassware that had contacted phosphines was rinsed in bleach (5 % sodium hypochlorite/water) to quench any residual phosphine, followed by water, and then methanol.

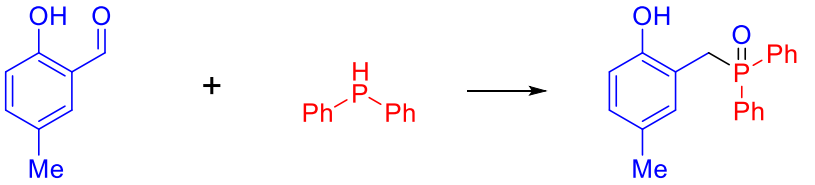


1.80 g
14.7 mmols

2.50 g
13.4 mmols

1a
3.69 g, 11.9 mmols
89.0% yield, 85.9% AE

(2-Hydroxybenzyl)diphenylphosphine oxide (**1a**) (Table **S1** reaction # 1): Prepared from diphenylphosphine (2.5 g, 13.4 mmol, 1 equiv.) and 2-hydroxybenzaldehyde (1.80 g, 14.7 mmol, 1.10 equiv.) concentrated *in vacuo* for a lightly-colored powder (3.69 g 89.3%). Product was then characterized and found to be in agreement with previously reported literature. **^{31}P{ ^{1}H} NMR** (162 MHz) δ_P 37.86; **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H 3.67 (d, J = 13.2 Hz, 2H), 6.61 (dd, J = 18.3, 10.7 Hz, 1H), 6.61 (dd, J = 18.3, 10.7 Hz, 1H), 6.80 (t, J = 8.7 Hz, 1H), 6.99 (t, J = 7.7 Hz, 1H), 7.40 (dd, J = 9.8, 4.8 Hz, 4H), 7.47 (t, J = 7.4 Hz, 2H), 7.67 – 7.58 (m, 4H), 9.26 (s, 1H). **MS** (ESI) $C_{19}H_{17}O_2P$ $[M+H]^+$ calc: 309.1000, found: 309.1336; **TLC** R_f = 0.53 1:3 (EtOAc/Hexane).

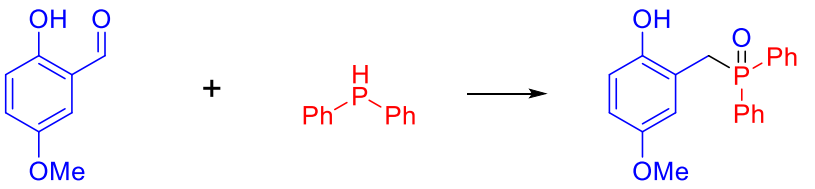


1.98 g
14.5 mmols

2.50 g
13.4 mmols

1b
3.82 g, 11.8 mmols
87.9% yield, 73.4% AE

(2-Hydroxy-5-methylbenzyl)diphenylphosphine oxide (**1b**): Prepared from diphenylphosphine (2.5 g, 13.4 mmol, 1 equiv.) and 2-hydroxy-5-methylbenzaldehyde (1.98 g, 14.5 mmol, 1.8 equiv.) concentrated *in vacuo* to give **1b** as a pale white powder (3.82 g, 88.2%.) **^{31}P{^{1}H} NMR** (162 MHz, $CDCl_3$) δ_P 38.12; **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H 2.13 (s, 2H), 3.69 (d, J = 12.9 Hz, 1H), 6.59 (dd, J = 2.0, 1.1 Hz, 1H), 6.92 (d, J = 1.1 Hz, 1H), 7.50 (m, J = 9.8, 4.3, 2.5, 1.0 Hz, 4H), 7.53 – 7.60 (m, 2H), 7.70 – 7.79 (m, 4H), 10.7 (s, 1H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ_C 20.34 (s), 35.26 (d, J = 67.5 Hz), 119.01 (d, J = 8.6 Hz), 119.29 (d, J = 2.6 Hz), 128.77 (d, J = 11.9 Hz), 129.48 (d, J = 2.9 Hz), 129.69 (d, J = 2.1 Hz), 130.6 (d, J = 98.9 Hz), 130.99 (d, J = 9.5 Hz), 132.09 (d, J = 6.5 Hz), 132.39 (d, J = 2.9 Hz), 154.21 (d, J = 4.1 Hz). **FTIR** (neat, cm^{-1}): 3037, 2731, 1513, 1434, 1280, 1168, 1134, 1099; **MS** (ESI) $C_{20}H_{19}O_2P$ $[M+H]^+$ calc: 323.1156, found: 323.1525; **TLC** R_f = 0.89 1:3 (Hexanes/EtOAc)



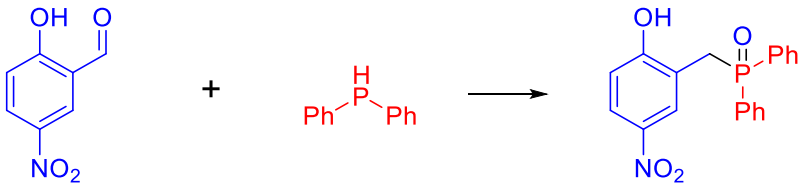
3.35 g
15.8 mmols

2.50 g
13.4 mmols

1c
3.35g, 9.8 mmols
73.6% yield, 68.9% AE

(2-Hydroxy-5-methoxybenzyl)diphenylphosphine oxide (**1c**): Prepared from 2 diphenylphosphine (2.5 g, 13.4 mmol, 1 equiv.) and 2-hydroxy-5-methoxybenzaldehyde (2.41 g, 15.8 mmol, 1.18 equiv.) concentrated *in vacuo* to give 1c as a pale-yellow powder (3.35 g, 73.8%.) **^{31}P{^{1}H} NMR** (162 MHz, $CDCl_3$) δ_P 37.97; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 3.63

(s, 3H), 3.69 (d, J = 12.9 Hz, 2H), 6.32 (t, 1H), 6.29 (dq, J = 8.9, 1.6 Hz, 1H), 6.97 (d, J = 8.75 Hz, 1H), 7.47 – 7.53 (m, 4H), 7.55 – 7.60 (m, 2H), 7.71 – 7.77 (m, 4H), 10.7 (s, 1H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ_C 35.04 (d, J = 67.6 Hz), 55.69 (s), 113.7 (d, J = 3.74 Hz), 117.1 (d, J = 6.29 Hz), 120.1 (d, J = 2.94 Hz), 128.8 (d, J = 12.0 Hz), 130.5 (d, J = 100.7 Hz), 132.5 (d, J = 2.87), 150.4 (s). **FTIR** (neat, cm^{-1}): 3004, 2906, 1658, 1508, 1433, 1271, 1215, and 1164. **MS** (ESI) $C_{20}H_{19}O_3P$ $[M+H]^+$ calc: 339.1105, found: 339.1505; **TLC** R_f = 0.4 2:3 (Hexane/EtOAc)

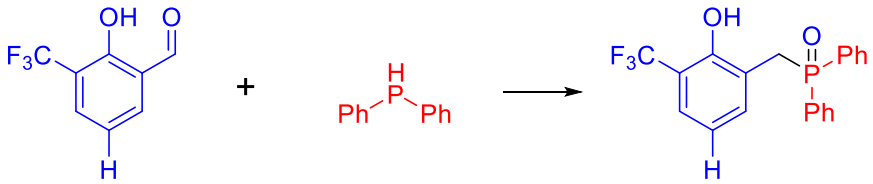


2.47 g
14.8 mmols

2.50 g
13.4 mmols

1d
3.66 g, 10.3 mmols
76.9% yield, 73.6% AE

(2-Hydroxy-5-nitrobenzyl)diphenylphosphine oxide (**1d**): Prepared from diphenylphosphine (2.5 g, 13.4 mmol, 1 equiv.) and 2-hydroxy-5-nitrobenzaldehyde (2.47 g, 14.8 mmol, 1.10 equiv.) concentrated *in vacuo* to afford **1d** as a pale orange powder (3.66 g, 77.1%) Product was then characterized by **^{31}P{^{1}H} NMR** (162 MHz, $CDCl_3$) δ_P 36.37; **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H 3.76 (d, J = 13.0 Hz, 2H), 7.02 (d, J = 8.99 Hz, 1H), 7.52 (m, 4H), 7.60 (m, 2H), 7.75 (m, 4H), 9.44 (s, 1H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ_C 35.5 (d, J = 70.4 Hz), 119.44 (s), 119.86 (d, J = 7.65 Hz), 125.25 (s), 127.56 (d, J = 7.88), 129.13 (d, J = 12.2 Hz), 129.3 (d, J = 101.9 Hz), 130.9 (d, J = 10.0 Hz), 133.01 (d, J = 2.8 Hz), 163.2 (d, J = 3.22 Hz). **FTIR** (neat, cm^{-1}): 3419, 3080, 2590, 1677, 1434, 1335, 1296, 1135, 1118. **MS** (ESI) $C_{19}H_{16}NO_4P$ $[M+H]^+$ calc: 354.0850, found: 355.0884; **TLC** R_f = 0.53 1:3 (Hexane/ EtOAc)

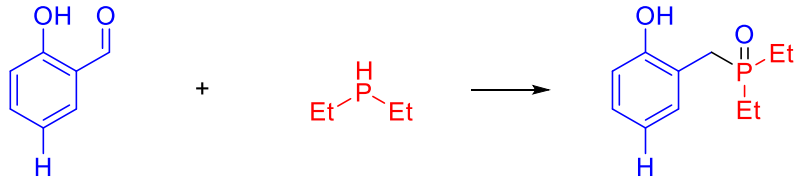


1.08 g
5.68 mmols

1.97 g
8.95 mmols

1e
823 mg, 2.19 mmols
38.5% yield, 26.9% AE

(3-Trifluoromethyl-2-hydroxybenzyl)diphenylphosphine oxide (**1e**): Prepared from diphenylphosphine (1.97 g, 8.95 mmol, 1 equiv.) and 3-trifluoromethyl-2-hydroxybenzaldehyde (1.08 g, 5.68 mmol, 0.635 equiv.) crystallized in ethanol and hexanes to afford opaque white crystals (823.3 mg, 38.5% yield.) Product was then characterized via: **^{31}P{^{1}H} NMR** (162 MHz, $CDCl_3$) δ_P 38.62; **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H 3.76 (d, J = 13.0 Hz, 2H), 6.68 (td, J = 7.9, 0.9 Hz, 1H), 6.77 (dt, J = 7.7, 1.8 Hz, 1H), 7.08 (dp, J = 7.8, 1.5 Hz, 1H), 7.53 – 7.44 (m, 4H), 7.62 – 7.53 (m, 2H), 7.78 – 7.68 (m, 4H), 10.22 (s, 1H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ_C 35.23 (d, J = 66.8 Hz), 120.0 (d, J = 2.2 Hz), 122.26 – 122.17 (m), 122.30 (d), 128.88 (d, J = 12.1 Hz), 130.00 (d, J = 100.3 Hz), 130.95 (d, J = 9.9 Hz), 132.64 (d, J = 2.9 Hz), 139.54 (dq, J = 3.4, 1.7 Hz), 149.5 (d, J = 4.0 Hz); **MS** (ESI) $C_{20}H_{16}F_3O_2P$ $[M+H_3O]^+$ calc: 395.0970, found: 394.8967; **FTIR** (neat, cm^{-1}): 2911.5, 1606.9, 1485.5, 1470.0, 1436.0, 1398.0, 1333.9, 1271.8, 1237.7, 1230.8, 1206.7, 1162.1, 1144.6, 1120.2, 1100.6, 1070.1, 1028.1.

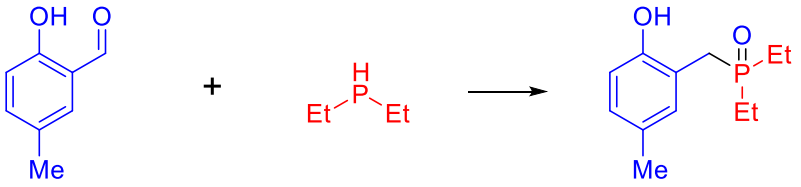


338 mg
2.77 mmols

250 mg
2.77 mmols

2a
396 mg, 1.86 mmols
67.0% yield, 67.3% AE

(2-Hydroxybenzyl)diethylphosphine oxide (**2a**): Prepared from diethylphosphine (250 mg, 2.77 mmol, 1 equiv.) and 2-hydroxybenzaldehyde (338 mg, 2.77 mmol, 1.00 equiv.) which was crystalized by layering DCM and Hexanes to afford clear, colorless crystals (396 mg, 67%). Product was then characterized and found to be in agreement with previously reported literature. **$^{31}P\{^{1}H\}$ NMR** (162 MHz, $CDCl_3$) δ_P 58.49; **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H1.16 (dt, J = 16.1, 7.7 Hz, 6H), 1.77 (dqd, J = 11.9, 7.6, 4.6 Hz, 4H), 3.17 (d, J = 12.9 Hz, 2H), 6.82 (t, J = 7.4 Hz, 1H), 6.98 (d, J = 8.0 Hz, 1H), 7.02 (d, J = 7.5 Hz, 1H), 7.14 (t, J = 7.8 Hz, 1H), 9.90 (s, 1H). ; **^{13}C NMR** (101 MHz, $CDCl_3$) δ_C 5.65 (d, J = 4.9 Hz), 19.52 (d, J = 65.6 Hz), 31.27 (d, J = 61.2 Hz), 118.65 (d, J = 2.3 Hz), 119.38 (d, J =7.9 Hz), 120.42 (d, J = 1.8 Hz), 128.82 (d, J = 2.7 Hz), 131.08 (d, J = 5.7 Hz), 156.12 (d, J = 4.0 Hz). **FTIR** (neat, cm^{-1}): 3040, 2975, 2711, 2596, 1594, 1455, 1246, 1107. **MS** (ESI) $C_{11}H_{17}O_2P$ $[M+H]^+$ calc: 213.1000, found: 213.1277; **TLC** R_f = 0.73 4:1 (MeOH/DCM)

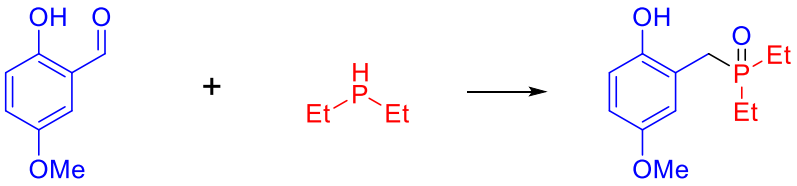


508 mg
3.73 mmols

332 mg
3.69 mmols

2b
144.6 mg, 0.639 mmols
17.3% yield, 17.2% AE

(2-Hydroxy-5-methylbenzyl)diethylphosphine oxide (**2b**): Prepared from diethylphosphine (332 mg, 3.69 mmol, 1 equiv.) and 2-hydroxy-5-methylbenzaldehyde (508 mg, 3.73 mmol, 1.01 equiv.) was crystallized by layering ethanol and hexanes to afford translucent white crystals (144.6 mg 17.3%.) **$^{31}P\{^{1}H\}$ NMR** (162 MHz, $CDCl_3$) δ_P 58.03; **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H 1.16 (dt, *J* = 16.9, 7.7 Hz, 6H), 1.76 (dqd, *J* = 11.7, 7.6, 3.0 Hz, 4H), 2.23 (s, 3H), 3.11 (d, *J* = 12.6 Hz, 2H), 6.81 (d, 1H), 6.86 (d, *J* = 8.2 Hz, 1H), 6.94 (d, *J* = 8.2, 2.6, 1.9, 0.8 Hz, 1H), 9.51 (s, 1H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ_C 5.67 (d, *J* = 4.8 Hz), 19.55 (d, *J* = 65.7 Hz), 20.44 (s), 31.45 (d, *J* = 61.2 Hz), 118.61 (d, *J* = 2.4 Hz), 119.19 (d, *J* = 8.1 Hz), 129.32 (d), 129.56 (d, *J* = 1.9 Hz), 131.49 (d, *J* = 5.9 Hz), 153.77 (d); **MS** (ESI) $C_{12}H_{19}O_2P$ $[M+H]^+$ calc: 227.1156, found: 227.4686 ; **FTIR** (neat, cm^{-1}): 2976, 2940, 2910, 2881, 2721, 1684, 1607, 1513, 1455, 1431, 1400, 1371, 1268, 1243, 1211, 1226, 1146, 1111, 1096, 1942, 1019.

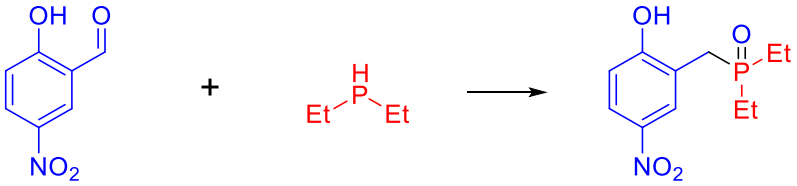


528 mg
2.17 mmols

250 mg
2.77 mmols

2c
403 mg, 1.66 mmols
76.3% yield, 51.8% AE

(2-Hydroxy-5-methoxybenzyl)diethylphosphine oxide (**2c**): Prepared from diethylphosphine (250 mg, 3.47 mmol, 1 equiv.) and 2-hydroxy-5-methoxybenzaldehyde (528 mg, 2.17 mmol, 1.25 equiv.) was crystallized by layering DCM and hexanes to afford opaque golden crystals (403 mg, 76.3%.) **$^{31}P\{^{1}H\}$ NMR** (162 MHz, $CDCl_3$) δ_P 58.56; **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H 1.13 – 1.25 (m, 6H), 1.75 – 1.87 (m, 4H), 3.13 (d, J = 11.9 Hz, 2H), 3.78 (d, J = 1.3 Hz, 3H), 6.56 (s, 1H), 6.74 – 6.79 (m, 1H), 6.97 (d, J = 8.8 Hz, 1H), 9.28 (s, 1H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ_C 5.73 (d, J = 4.7 Hz), 19.62 (d, J = 65.7 Hz), 32.20 (d, J = 60.8 Hz), 55.72, 113.22 (d, J = 2.7 Hz), 116.80 (d, J = 6.0 Hz), 120.33 (d, J = 2.4 Hz), 120.90 (d, J = 8.5 Hz), 150.15 (d, J = 3.8 Hz), 153.50 (d, J = 1.7 Hz). **FTIR** (neat, cm^{-1}): 2947, 2584, 2068, 1863, 1510, 1432, 1213, 1113, 1034. **MS** (ESI) $C_{12}H_{19}O_3P$ $[M+H]^+$ calc: 243.1105, found: 243.1412; **TLC** R_f = 0.59 4:1 (MeOH/DCM)

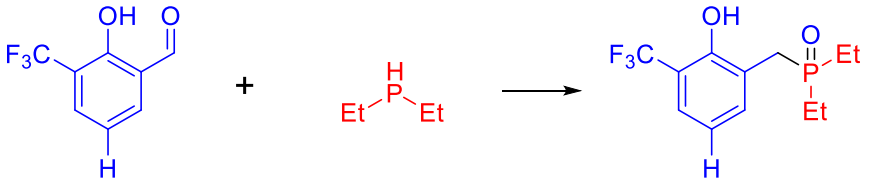


398 mg
2.38 mmols

250 mg
2.77 mmols

2d
564 mg, 2.18 mmols
91.7% yield, 87.1% AE

(2-Hydroxy-5-nitrobenzyl)diethylphosphine oxide (**2d**): Prepared from diethylphosphine (250 mg, 2.77 mmol, 1.16 equiv.) and 2-hydroxy-5-nitrobenzaldehyde (398 mg, 2.38 mmol, 1 equiv.) was crystallized by layering DCM and hexanes to afford a pale yellow powder (564 mg, 91.7%) **$^{31}P\{^{1}H\}$ NMR** (162 MHz, $CDCl_3$) δ_P 61.63; **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H 1.21 (dt, J = 17.6, 7.7 Hz, 6H), 1.91 (dq, J = 12.1, 7.7 Hz, 4H), 3.28 (d, J = 12.3 Hz, 2H), 7.02 (d, J = 8.9 Hz, 1H), 8.00 (t, J = 2.3 Hz, 1H), 8.07 (d, J =8.7 Hz, 1H), 10.00 (s, 1H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ_C 9.84, 19.45 (d, J = 65.5 Hz), 27.15, 125.45, 127.14, 118.80, 119.49, 141.10, 158.61. **FTIR** (neat, cm^{-1}): 2947, 2737, 2584, 1863, 1746, 1510, 1432, 1213, 1157, 1092. **MS** (ESI) $C_{11}H_{16}NO_4P$ $[M+H]^+$ calc: 258.0850, found: 258.1181; **TLC** R_f = 0.76 1:3 (Hexane/EtOAc)



875 mg
4.60 mmols

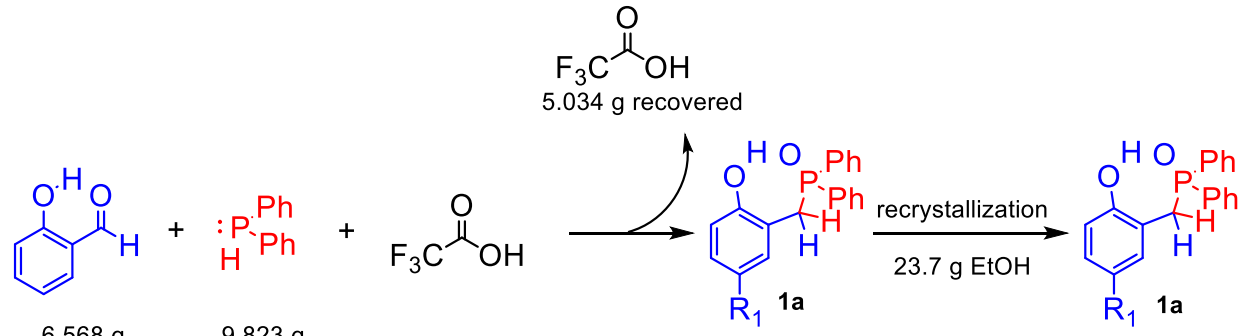
332 mg
3.69 mmols

2e
383 mg, 1.37 mmols
36.9% yield, 31.7% AE

(3-Trifluoromethyl-2-hydroxybenzyl)diethylphosphine oxide (**2d**): Prepared from diethylphosphine (332 mg, 3.69 mmol, 1.00 equiv.) and 3-trifluoromethyl-2-hydroxybenzaldehyde (875 mg, 4.60 mmol, 1.25 equiv.) was purified by flash column chromatography (100% EtOAc) and concentrated *in vacuo* to afford a golden transparent wax-like substrate (383 mg, 36.9%.) **^{31}P{^{1}H} NMR** (162 MHz, $CDCl_3$) δ_P 58.76; **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H 1.11 (dt, J = 17.0, 7.7 Hz, 6H), 1.74 (dq, J = 12.0, 7.7 Hz, 4H), 3.17 (d, J = 12.5 Hz, 2H), 6.78 (t, J = 7.9 Hz, 1H), 6.96 (dt, J = 7.7, 1.7 Hz, 1H), 7.09 (dq, J = 8.3, 1.6 Hz, 1H), 10.15 (s, 1H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ_C 5.40 (d, *J* = 5.0 Hz), 19.55 (d, *J* = 66.0 Hz), 31.47 (d, *J* = 60.3 Hz), 120.03 (d, *J* = 1.9 Hz), 120.74 (d, *J* = 256.8 Hz), 121.98 (dd, *J* = 2.4, 1.1 Hz), 122.68 (d, *J* = 8.3 Hz), 129.60 (d), 139.27 (dd, *J* = 2.8, 1.7 Hz), 149.13 (d, *J* = 3.7 Hz); **MS** (ESI) $C_{12}H_{16}F_3O_2P$ $[M+H_3O]^+$ calc: 299.0979, found: 299.15408; **FTIR** (neat, cm^{-1}): 2976.0, 1606.5, 1489.5, 1473.7, 1408.0, 1265.6, 1209.8, 1168.5, 1118.4, 1043.3.

Large Scale Preparation of (2-hydroxybenzyl)diphenylphosphine oxide (1a):

Run #1 (Table **S1** reaction # 2): Diphenylphosphine (9.82 g, 52.8 mmol, 1 equiv.), salicylaldehyde (6.57 g, 53.8 mmol, 1.02 equiv.), and trifluoroacetic acid (14.2 g) were combined in a nitrogen-flushed, heavy-walled 100 mL borosilicate spherical flask equipped with a Teflon valve and Teflon-coated stir bar. The mixture was stirred in an 80 °C oil bath for 24 h, then, without removing from heat, roughly half of the trifluoroacetic acid was distilled into a liquid nitrogen-cooled receiving flask under reduced pressure (5.03 g recovered and subjected to purity analysis and reuse as solvent for synthesis of **1a**, see Run #3). At this point, ethanol (23.7 g) was added, and the resulting powdery solid was isolated (16.4 g) and was found to be 80.1% **1a** by mass (42.6 mmol, 80.8 % yield), with the remainder comprised primarily of trifluoroacetic acid, salicylaldehyde, and diphenylphosphine oxide.



6.568 g
53.78 mmoles

9.823 g
52.81 mmoles

14.187 g

5.034 g recovered

19.78 g mass
61.5% purity
mmoles

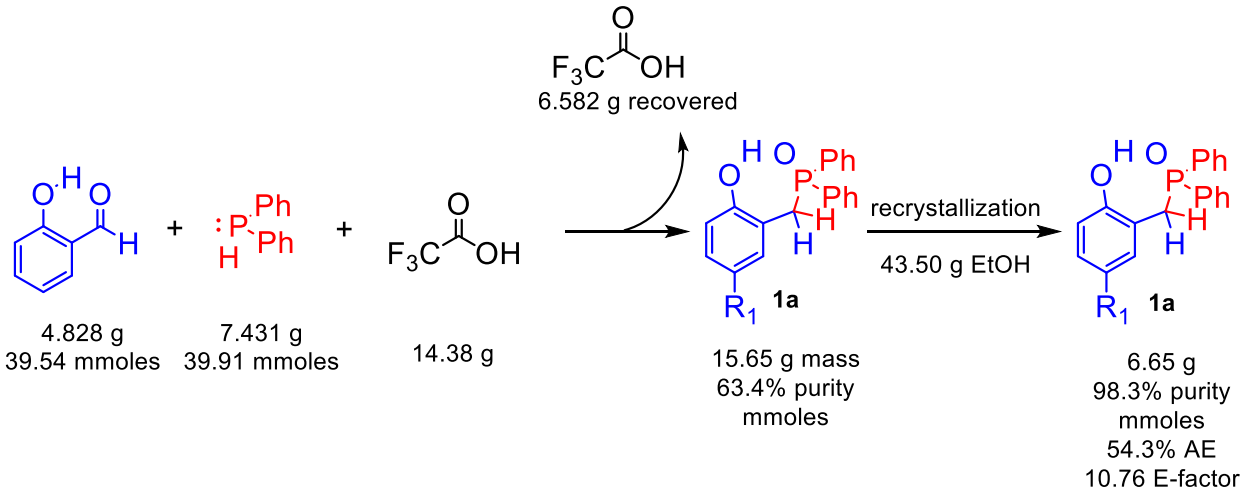
recrystallization

23.7 g EtOH

16.42 g
80.2% purity
mmoles
80.2% AE
2.99 E-factor

Run #2 (Table **S1** reaction # 3): Diphenylphosphine (7.431 g, 39.91 mmol, 1.009 equiv.), salicylaldehyde (4.828 g, 39.54, 1 equiv.), and trifluoroacetic acid (15.166 g) were combined in a nitrogen-flushed, heavy-walled 100 mL borosilicate spherical flask equipped with a Teflon valve and Teflon-coated stir bar. The mixture was stirred in an 80 °C oil bath for 24 h, then, without removing from heat, roughly half of the trifluoroacetic acid was distilled into a liquid nitrogen-cooled receiving flask under reduced pressure (6.582 g recovered and subjected to purity analysis and reused as solvent for synthesis of **1a**, see below). At this point, toluene (7.98 g) was added, and the combined volatiles were distilled under reduced pressure (still at 80 °C). The resulting waxy solid (15.65 g) was found to be 63.4

% **1a** by mass (33.66 mmol, 85.1 % yield, 84.6 % AE), with the remainder comprised primarily of toluene, salicylaldehyde, and diphenylphosphine oxide. The solid was dissolved in refluxing ethanol (36.5 g), and allowed to cool slowly to 20 °C, after which it was cooled to 8 °C overnight. The supernatant mother liquor was then removed, and the crystalline solid was rinsed once with cold ethanol (7.00 g), and dried under reduced pressure, yielding **1a** (6.65 g) in 98.3% purity.



Run #3 (Table **S1** reaction # 4): Reclaimed TFA was used to prepare "Beddoe's Catalyst" (**1a**) consisted of 1.00 equivalents of diphenylphosphine (1.73 g, 9.32 mmol) and 1.02 equivalents of 2-hydroxybenzaldehyde (1.16 g, 9.5 mmol). Product was worked up with sodium bicarbonate and DCM and crystallized from EtOH to afford pale white crystals for 2.81 g with 85.6% purity.

Figure S1. Photographs of 50 mmol reaction setup and distillation setup. A = crude reaction mixture; B = mineral oil hot bath; C = short path distillation head with 10 °C water circulating; D = TFA receiving flask, cooled with liquid nitrogen; E = bump trap; F = corrosive-resistant diaphragm pump.

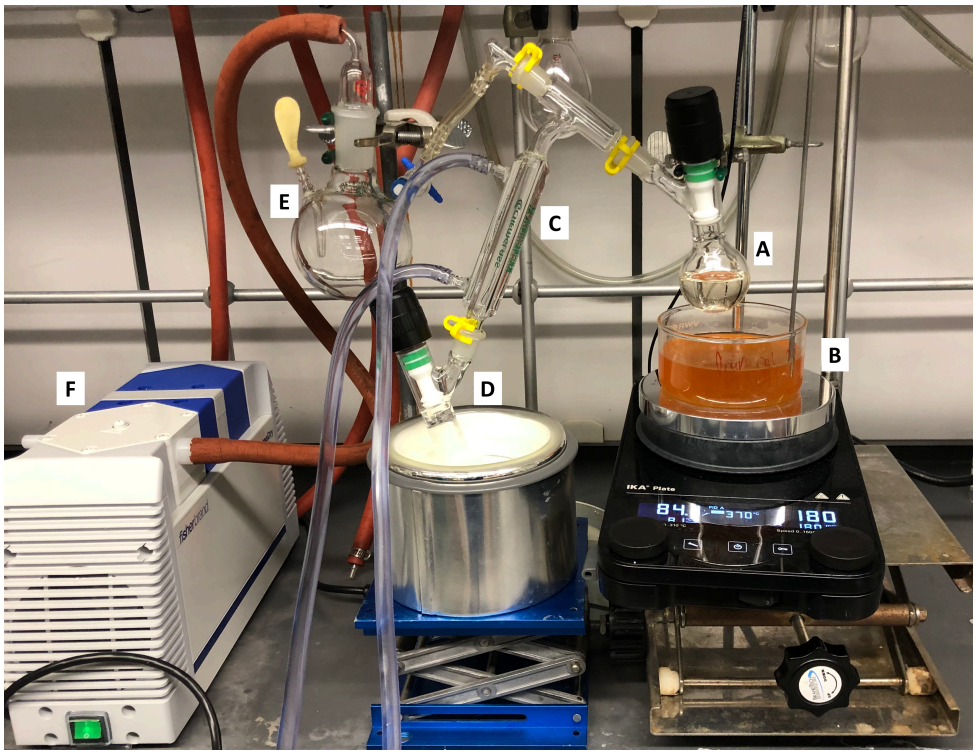


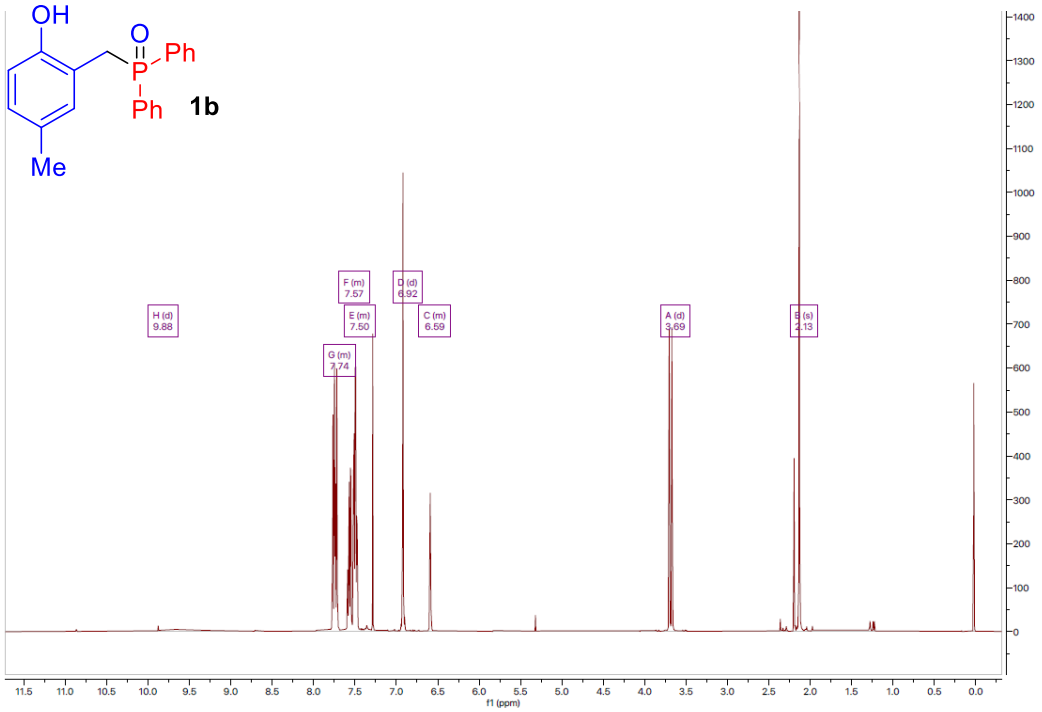
Table S1. Summary of multiple syntheses of **1a**.

Reaction #	1	2	3	4
Yield (mmol)	11.9	42.6	33.7	7.8
% Yield	89.0 %	80.8 %	85.1 %	83.4 %
Atom Economy[1]	85.9 %	80.1 %	84.6 %	83.2 %
E-factor[2]	N/A	N/A	10.8	N/A
Purity[2,3]	N/A	N/A	98.3 %	N/A

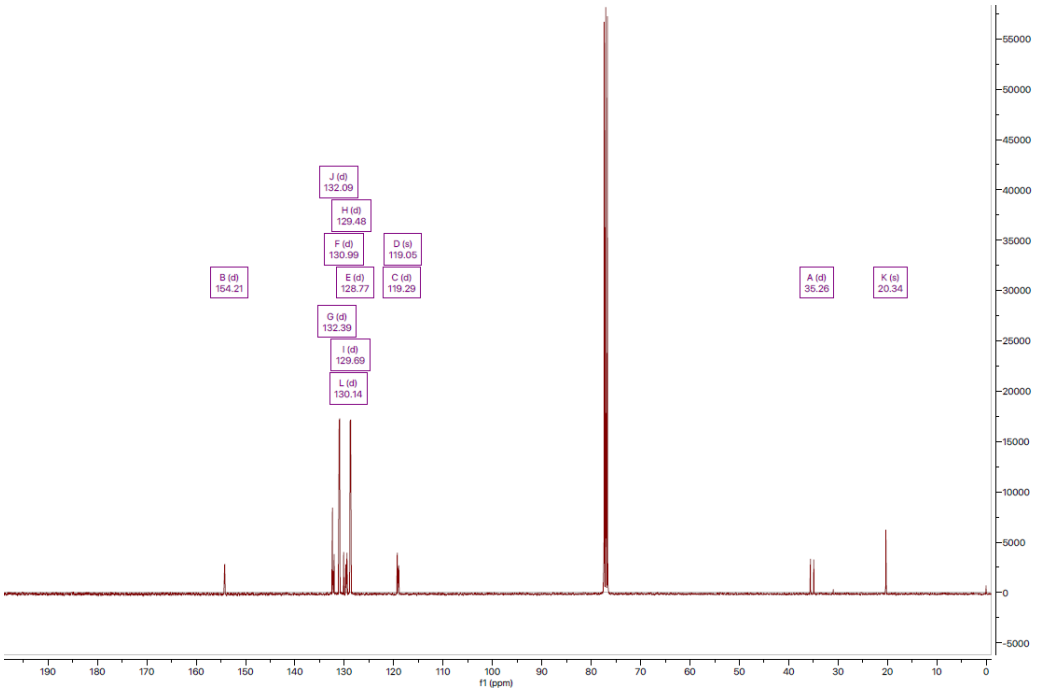
[1] Based on crude yield. [2] After recrystallization from ethanol. [3] Based on ^{1}H NMR integration compared to internal standard.

Spectral Gallery

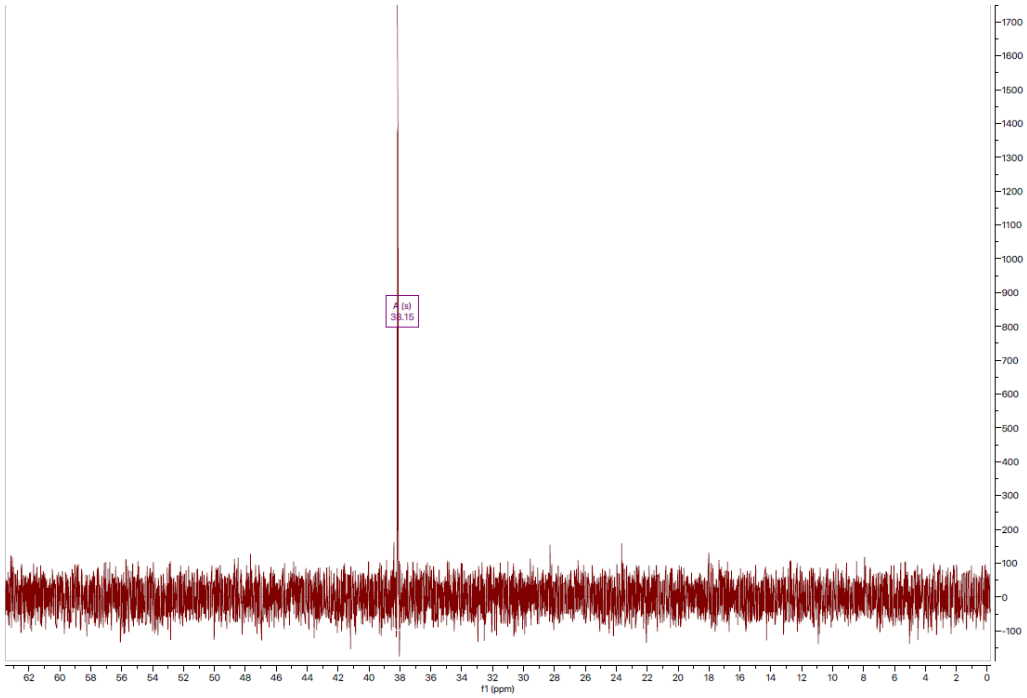
^{1}H NMR spectrum of **1b**



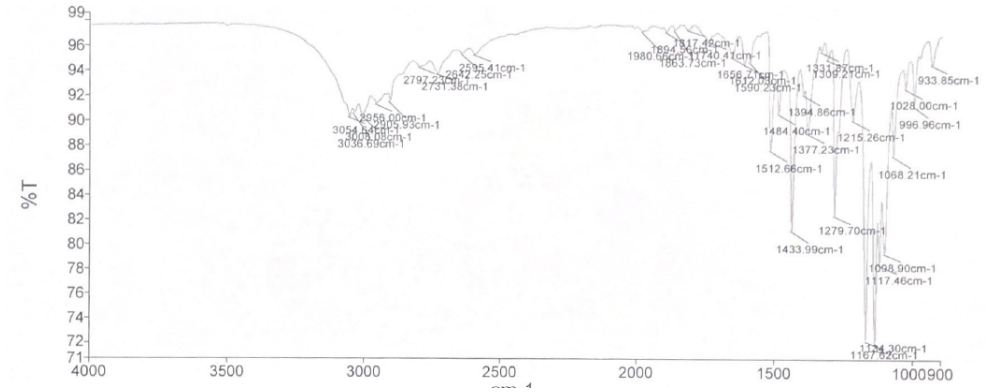
^{13}C NMR spectrum of **1b**



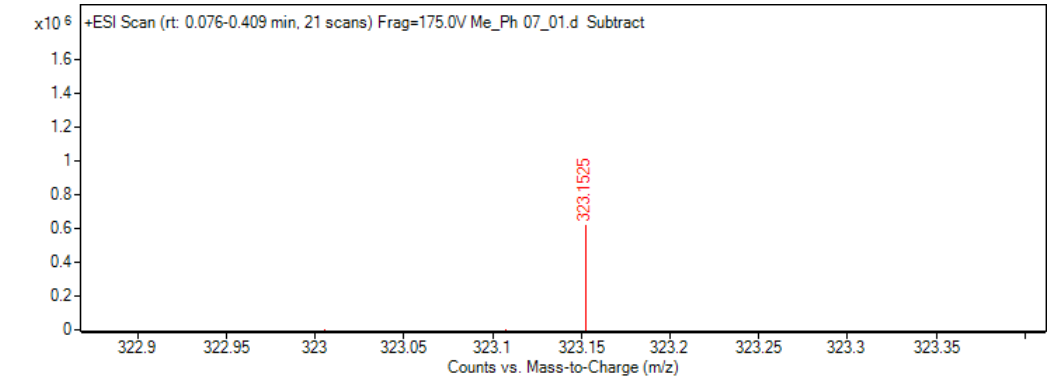
$^{31}P\{^{1}H\}$ NMR spectrum of **1b**



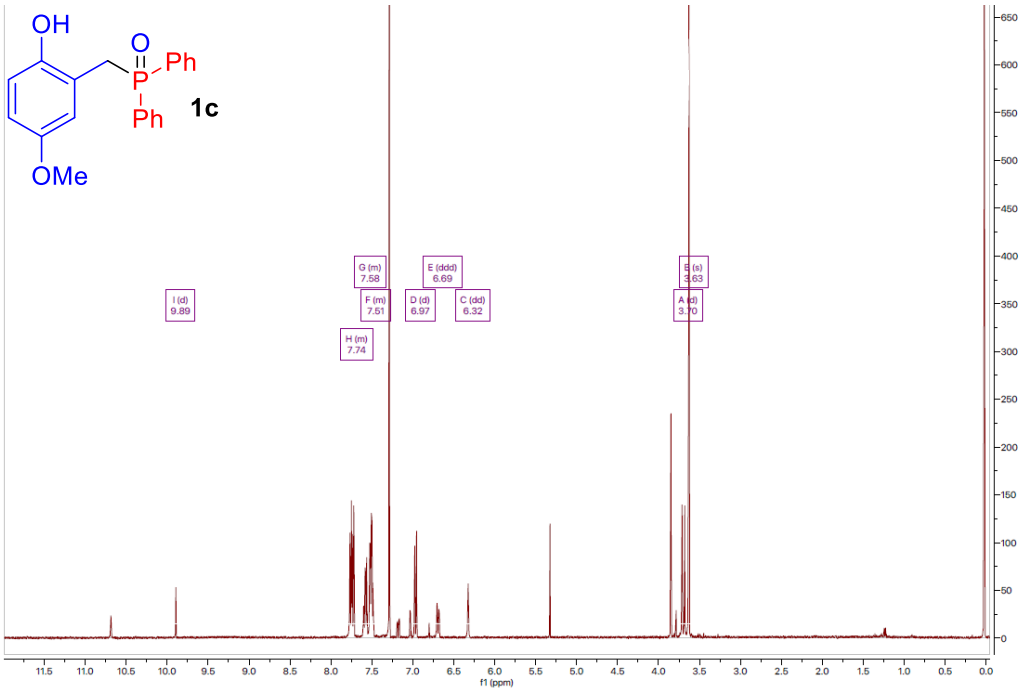
IR spectrum of **1b**



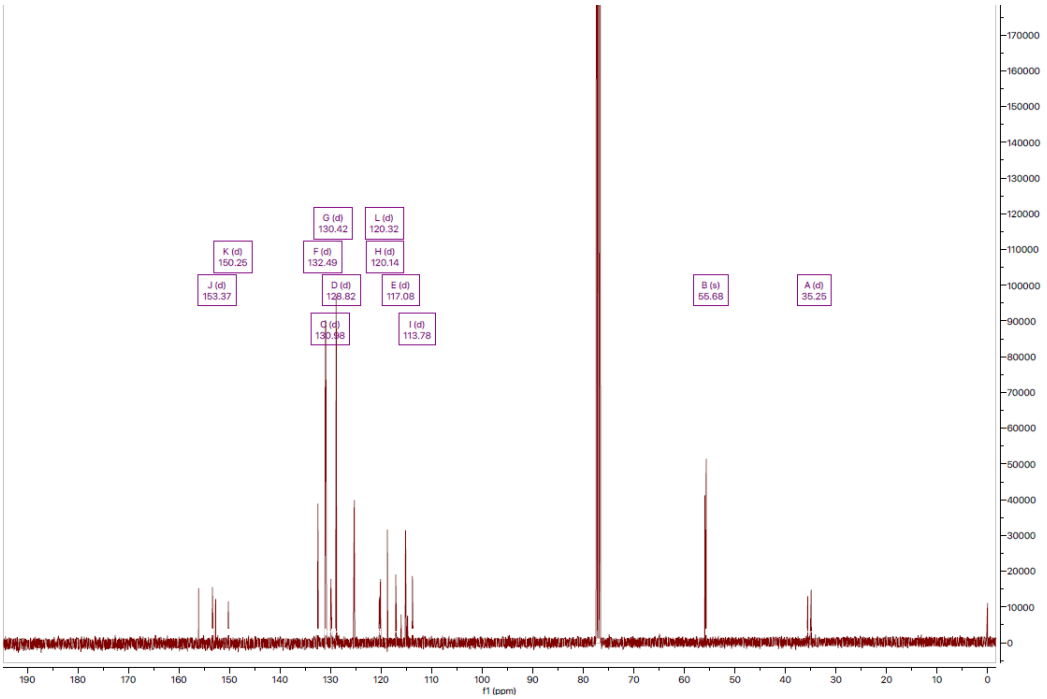
MS of **1b**



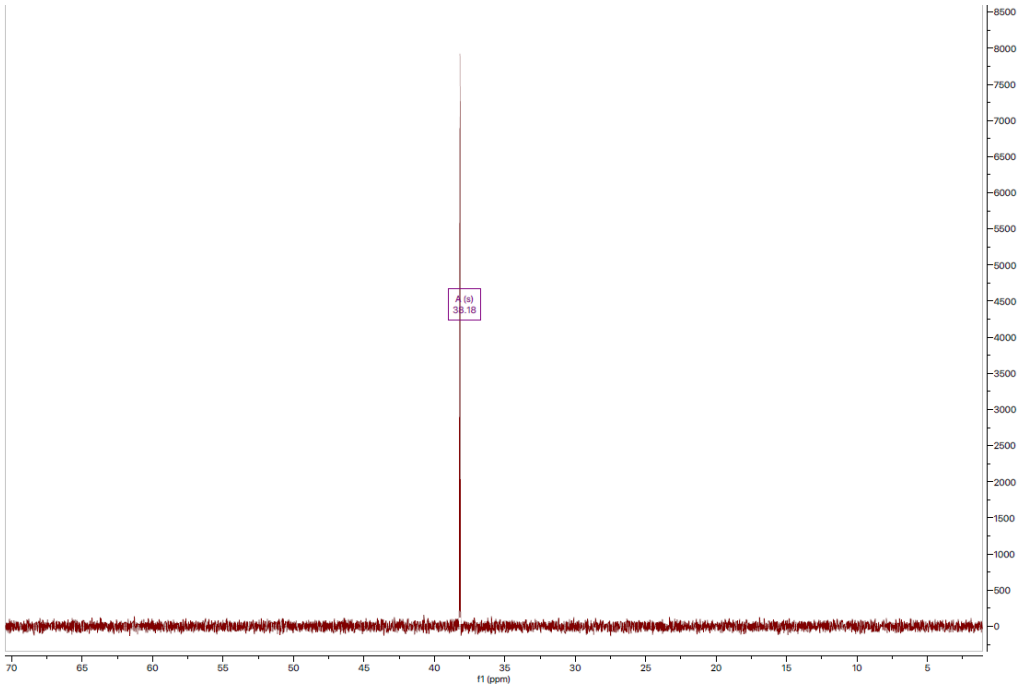
^{1}H NMR spectrum of **1c**



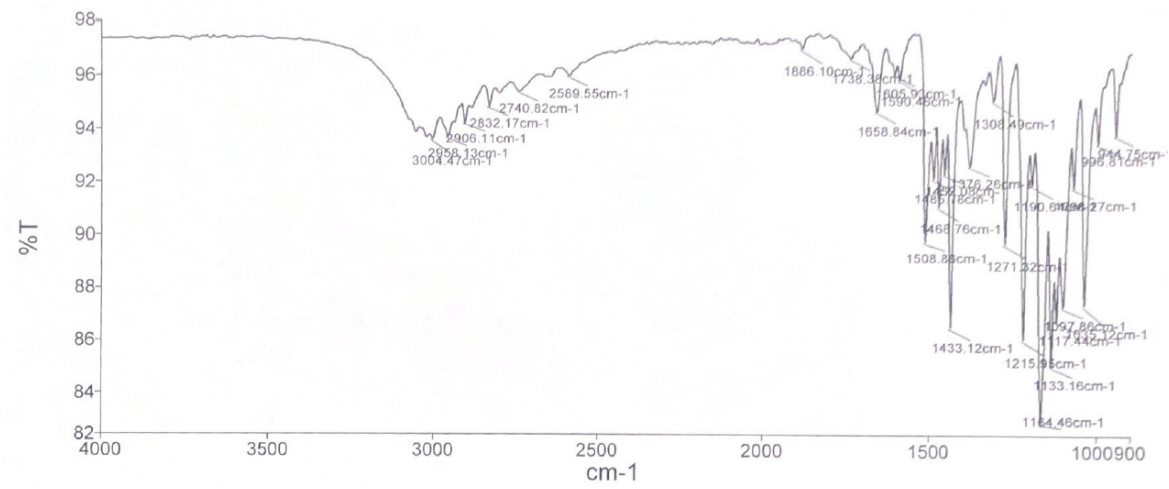
^{13}C NMR spectrum of **1c**



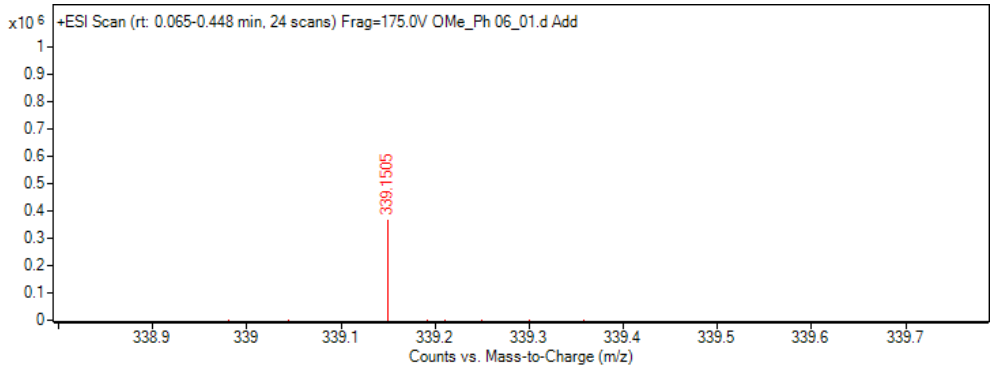
$^{31}P\{^{1}H\}$ NMR spectrum of **1c**



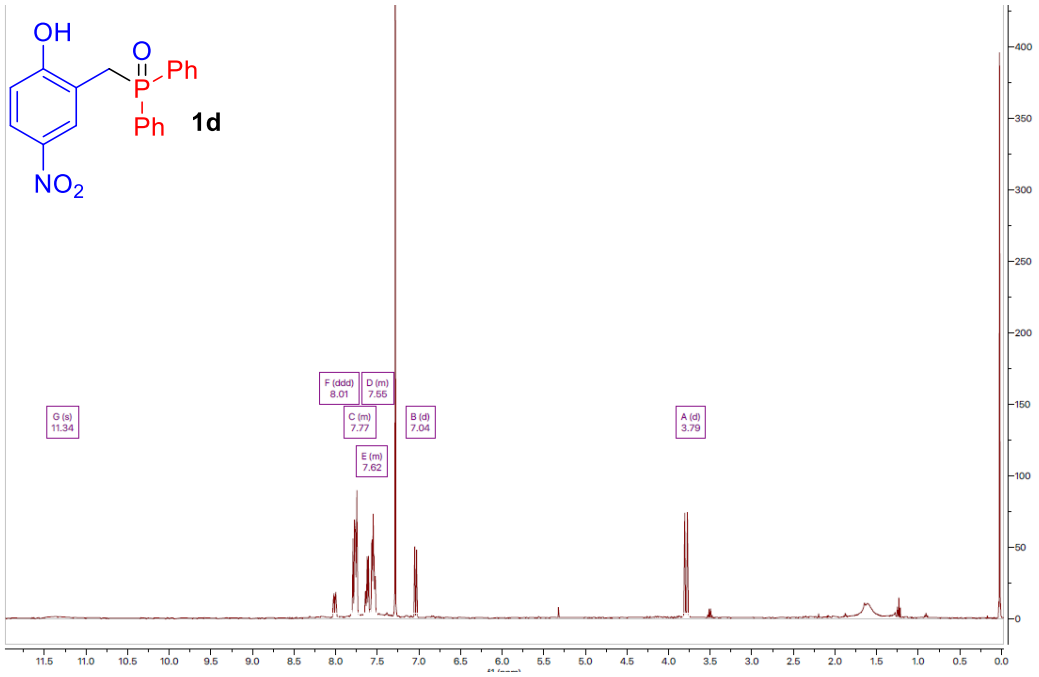
IR spectrum of **1c**



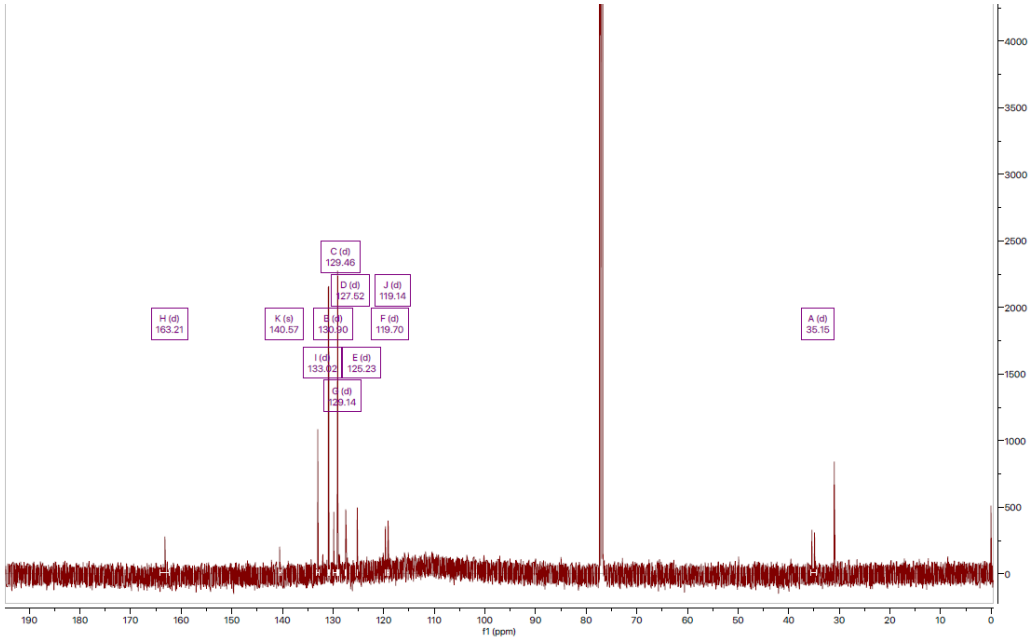
MS of **1c**



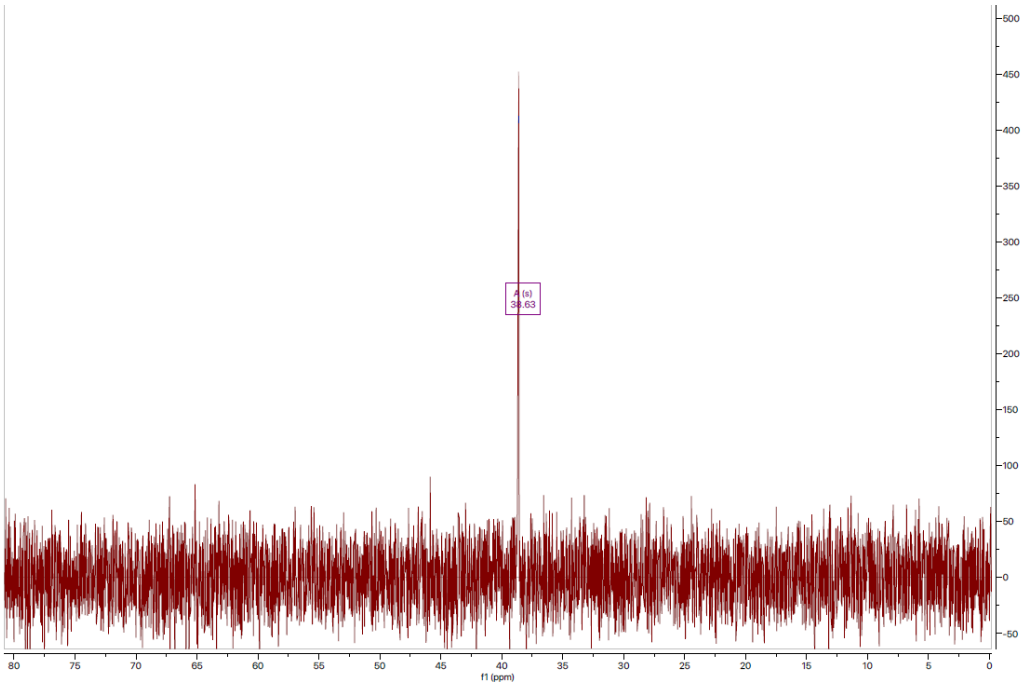
^{1}H NMR spectrum of **1d**



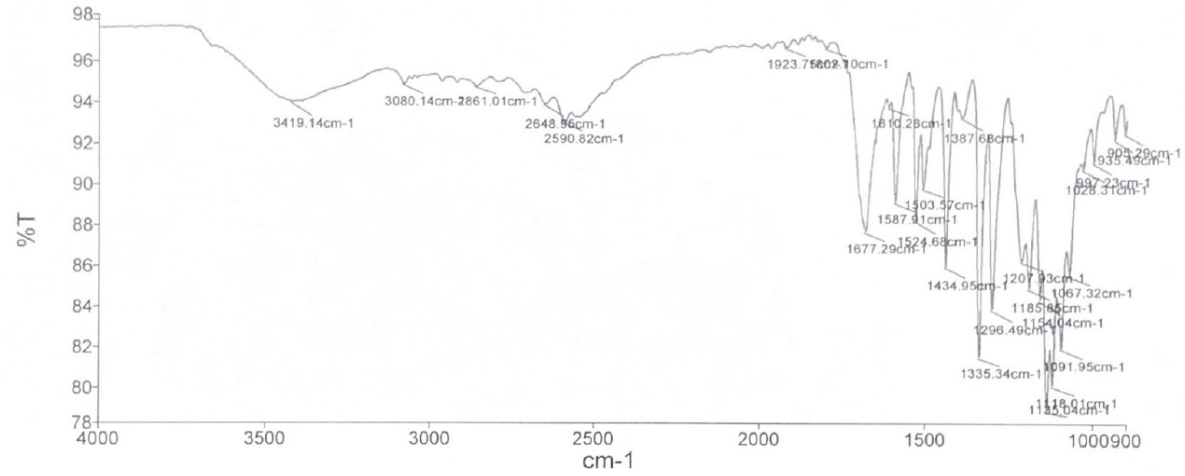
^{13}C NMR spectrum of **1d**



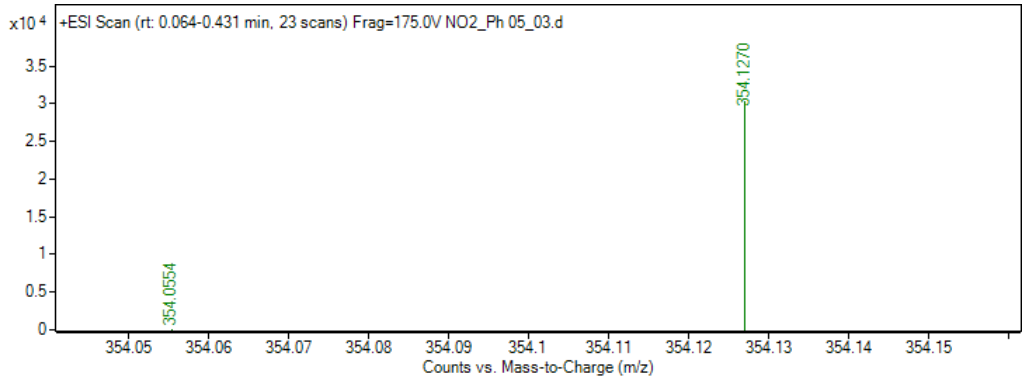
$^{31}P\{^{1}H\}$ NMR spectrum of **1d**



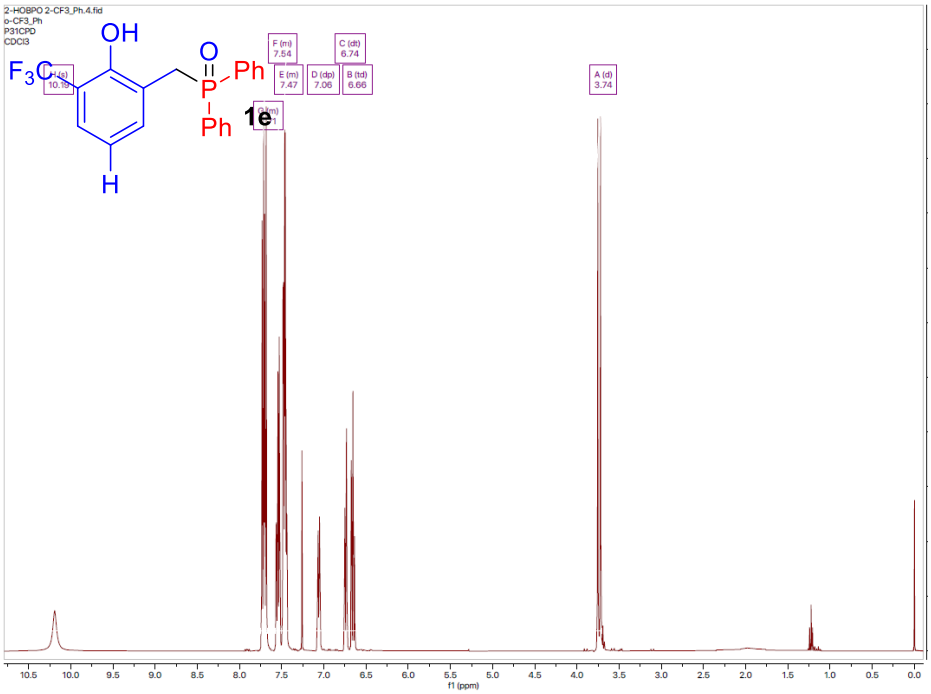
IR spectrum of **1d**



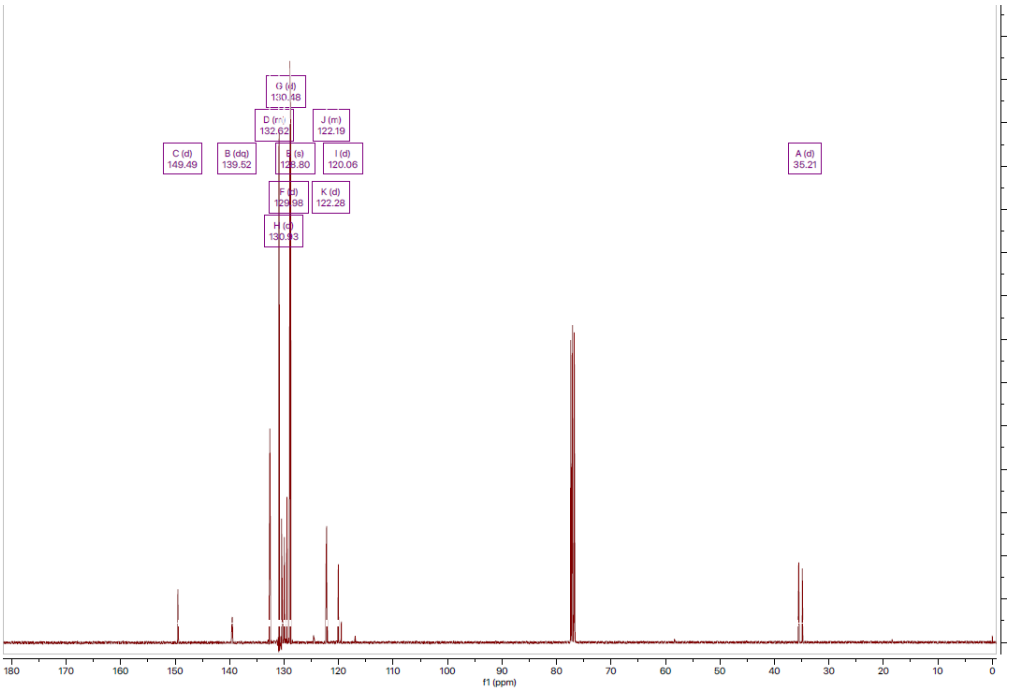
MS of **1d**



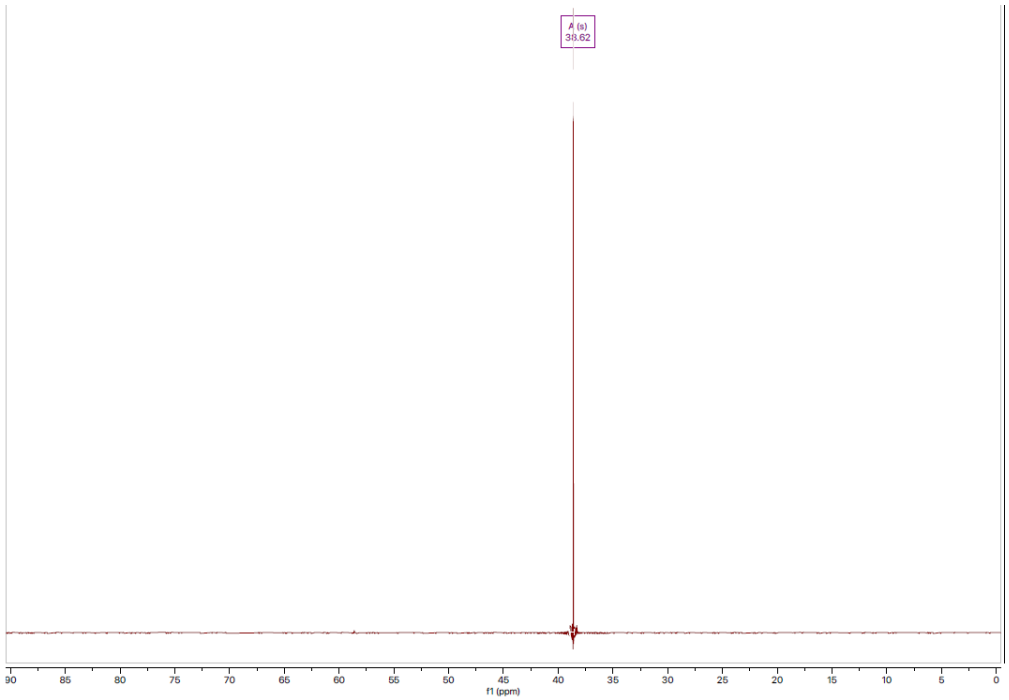
^{1}H NMR Spectrum of **1e**



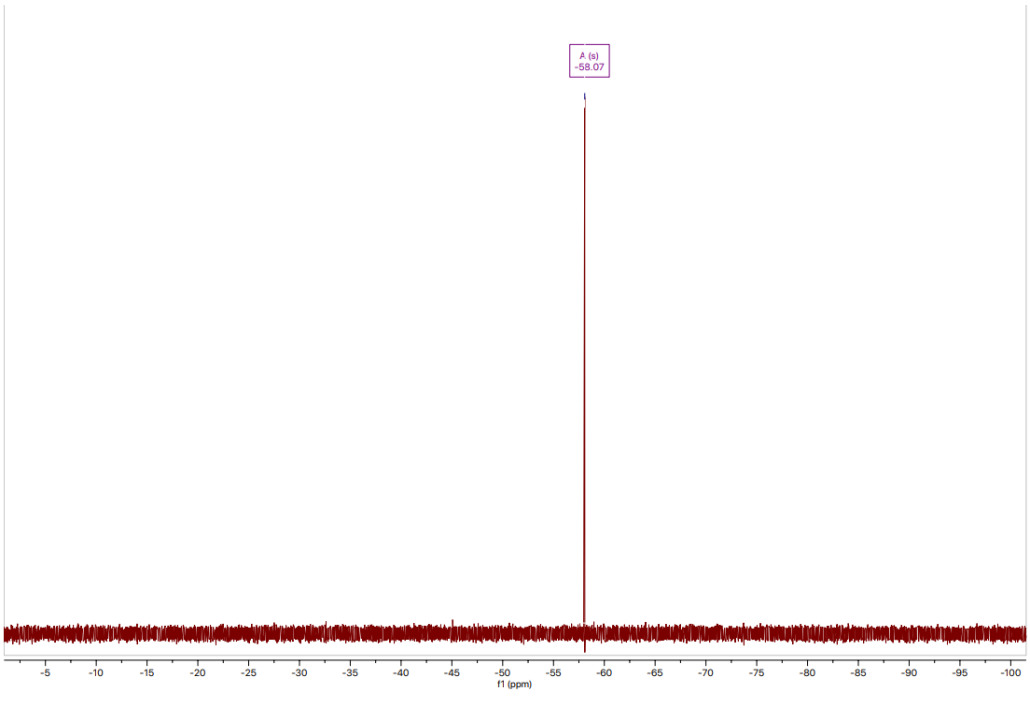
^{13}C CPD NMR Spectrum of **1e**



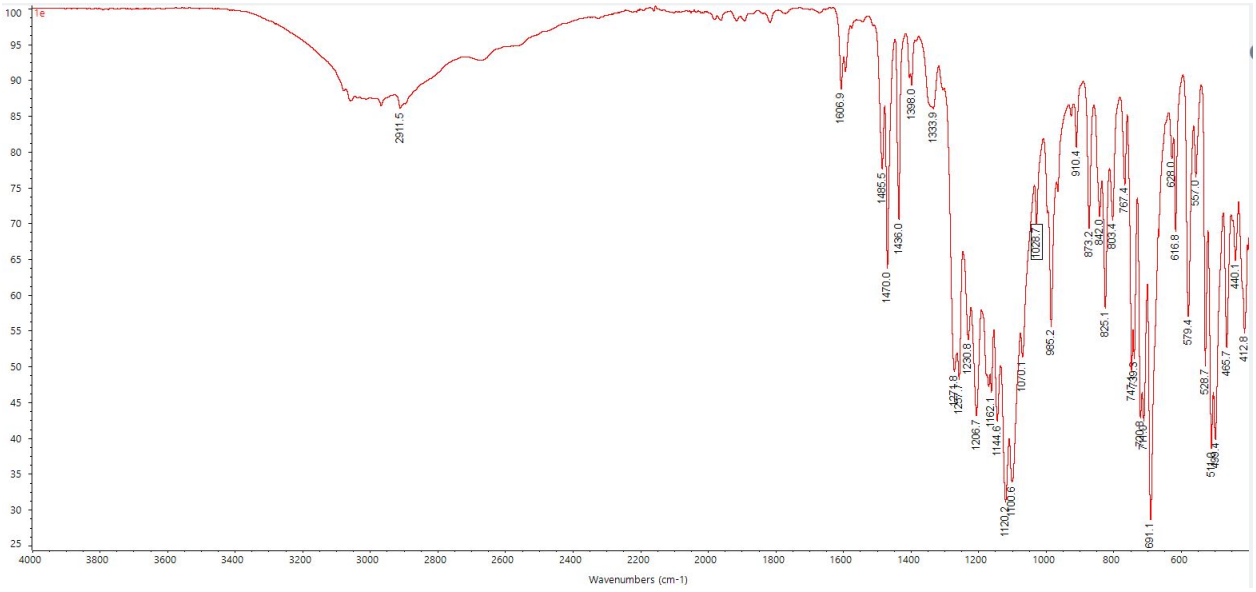
$^{31}P\{^{1}H\}$ NMR Spectrum of **1e**



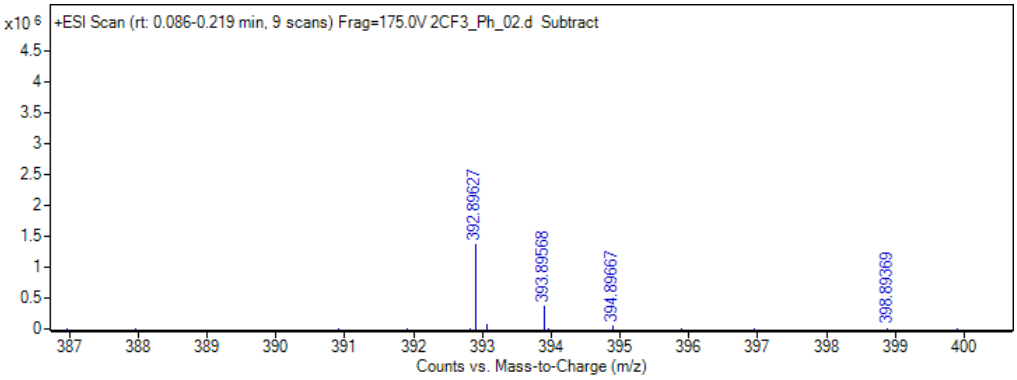
$^{19}F\{^{1}H\}$ NMR Spectrum of **1e**



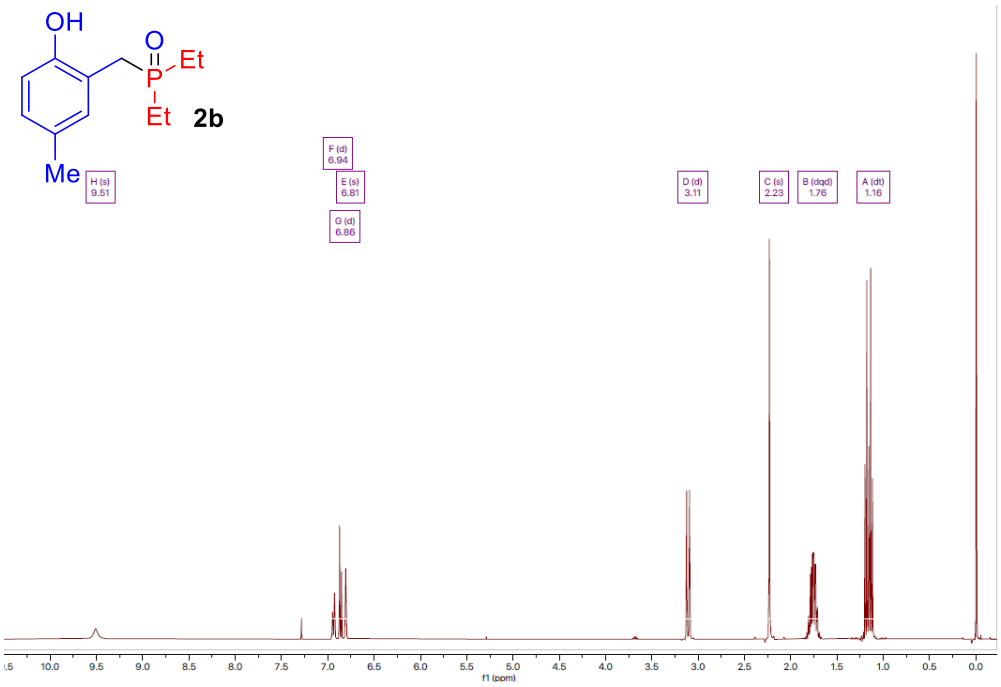
IR Spectrum of **1e**



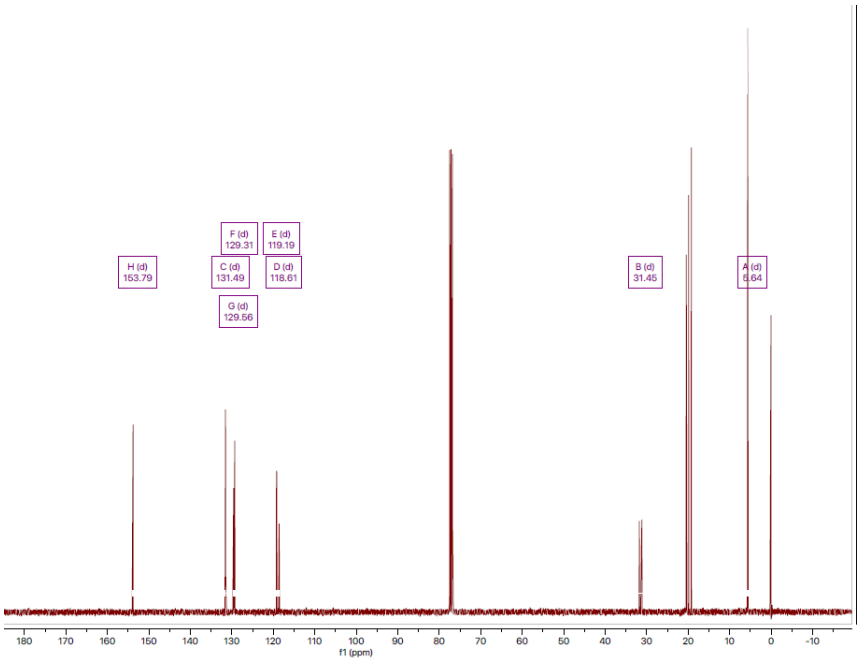
MS of **1e**



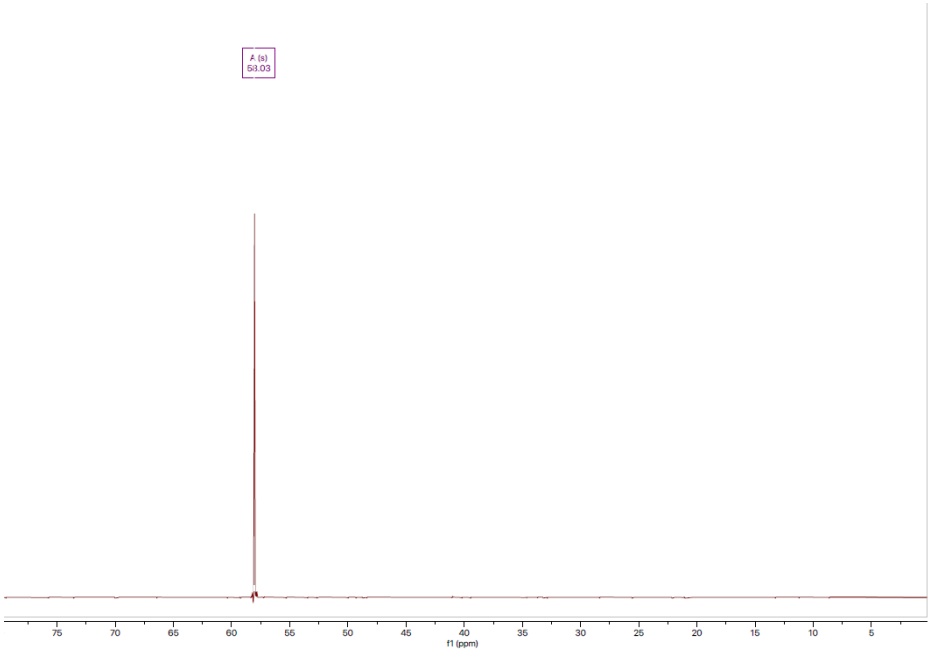
^{1}H Spectrum of **2b**



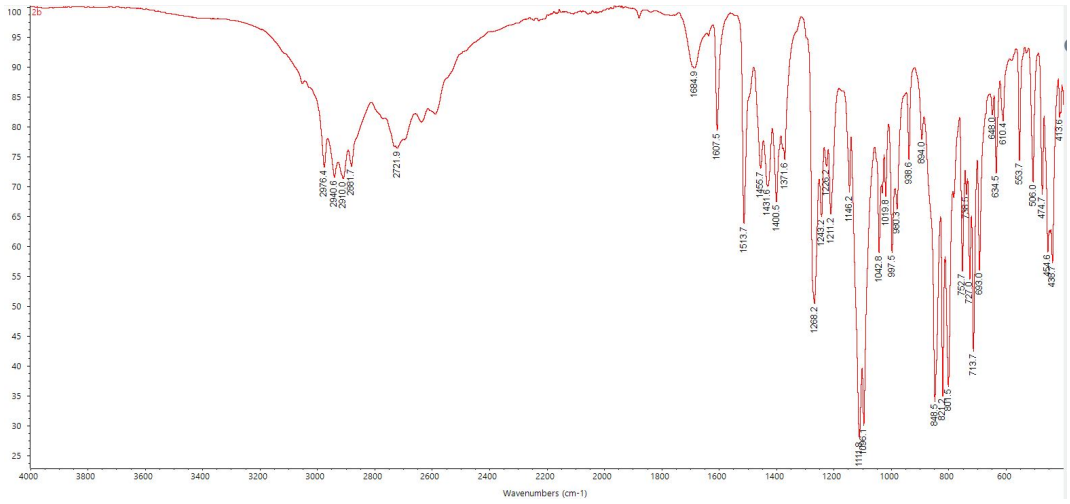
^{13}C NMR Spectrum of **2b**



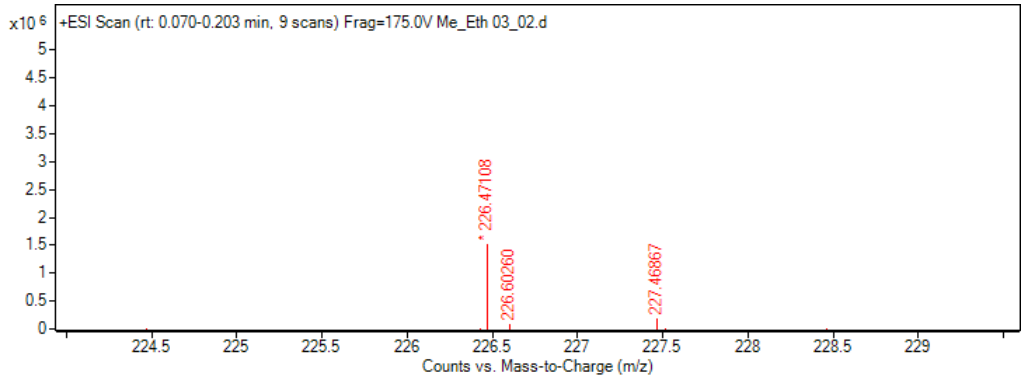
$^{31}P\{^{1}H\}$ Spectrum of **2b**



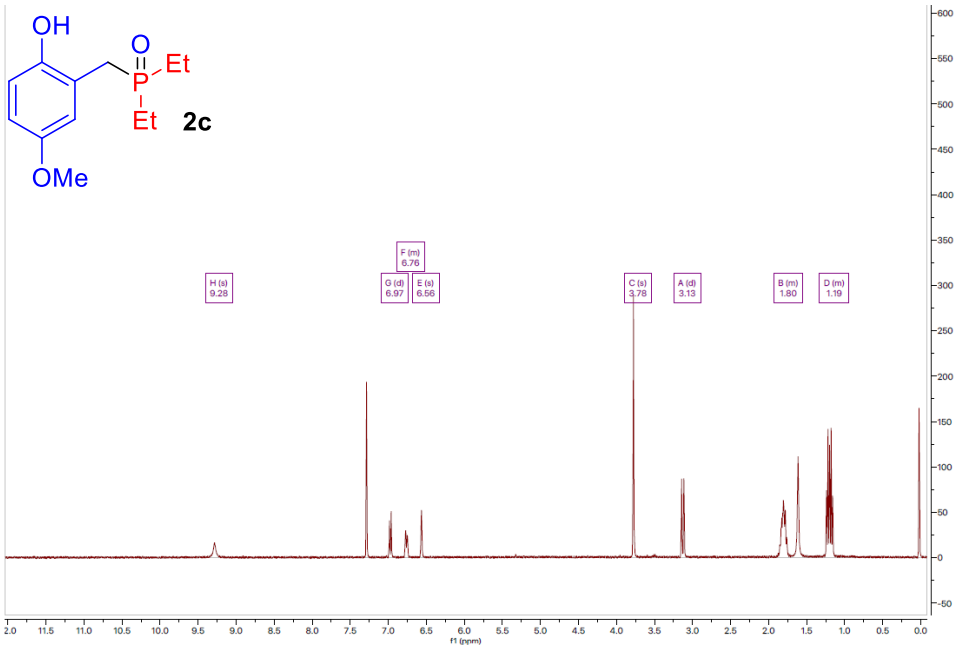
IR Spectrum of **2b**



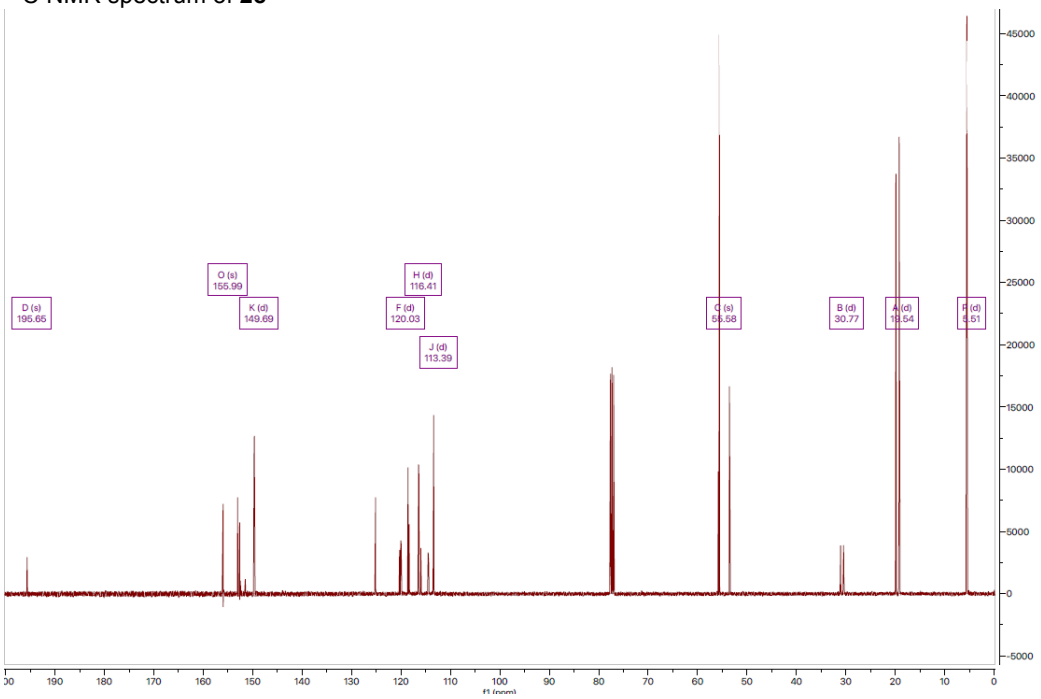
MS of **2b**



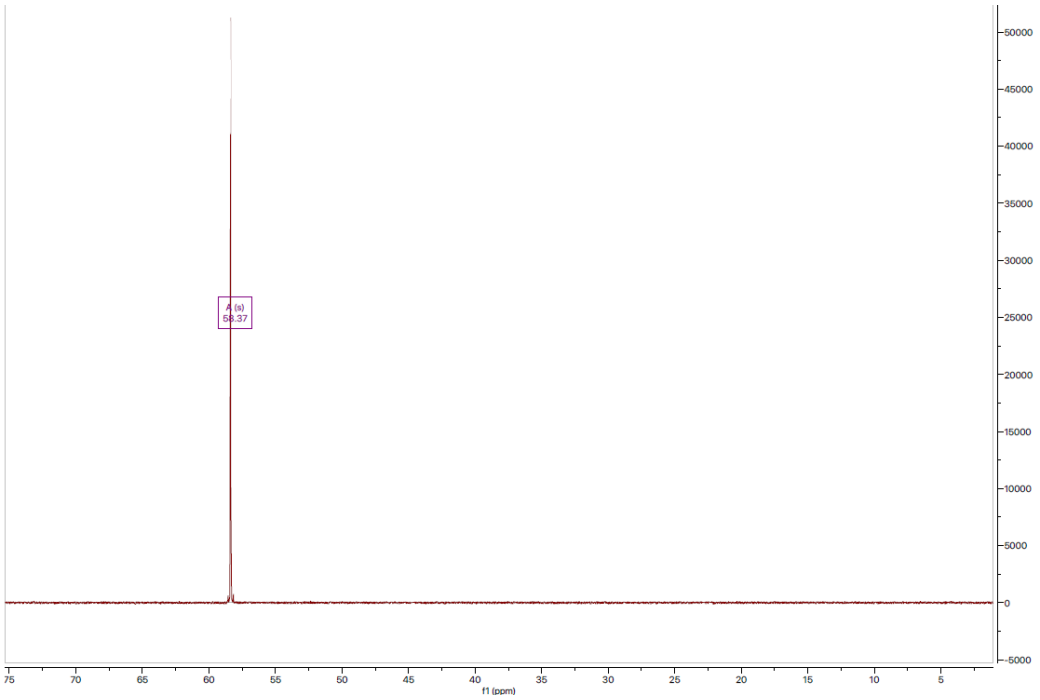
^{1}H NMR spectrum of **2c**



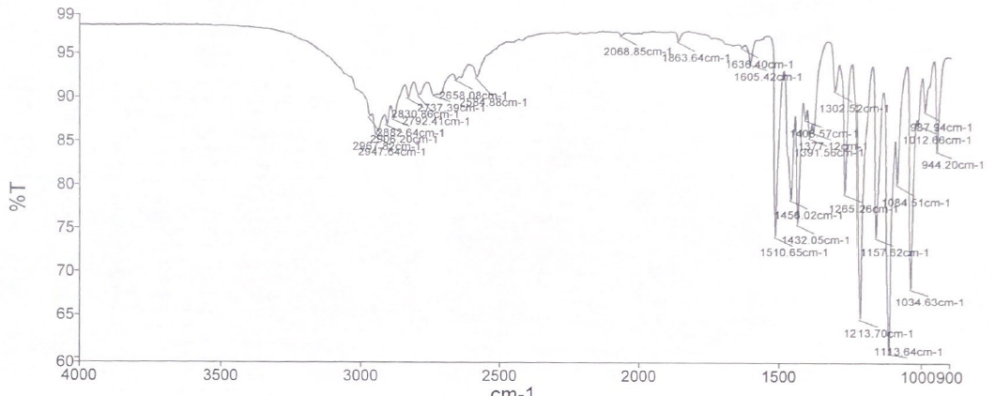
^{13}C NMR spectrum of **2c**



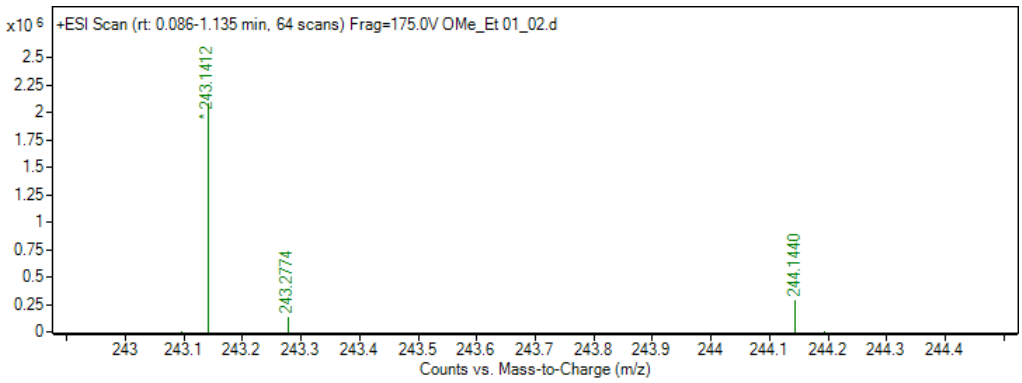
$^{31}P\{^{1}H\}$ NMR spectrum of **2c**



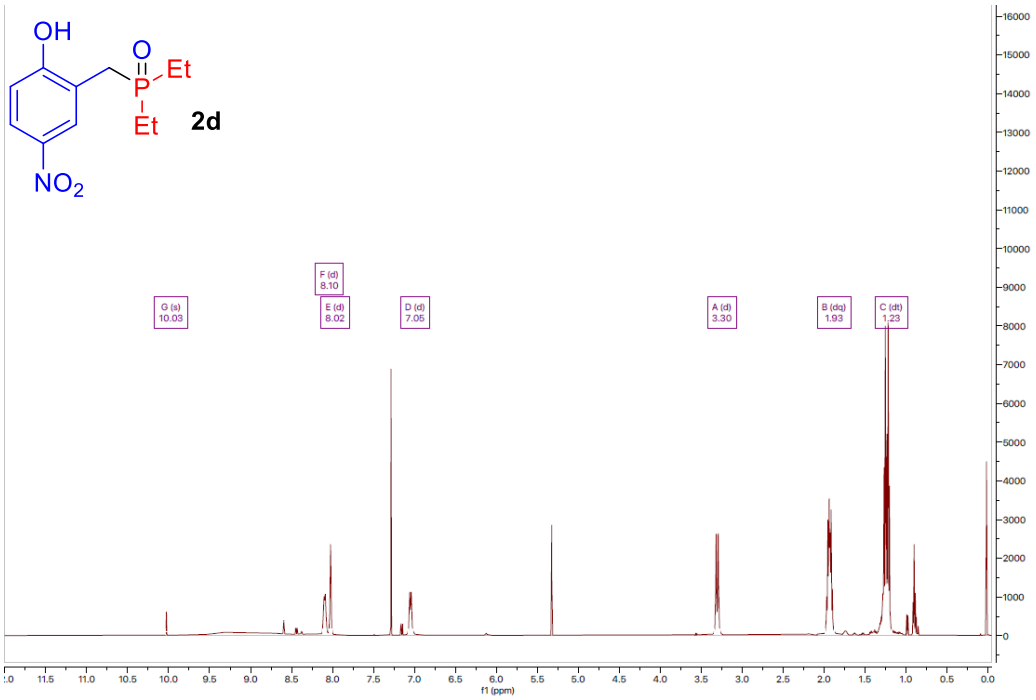
IR spectrum of **2c**



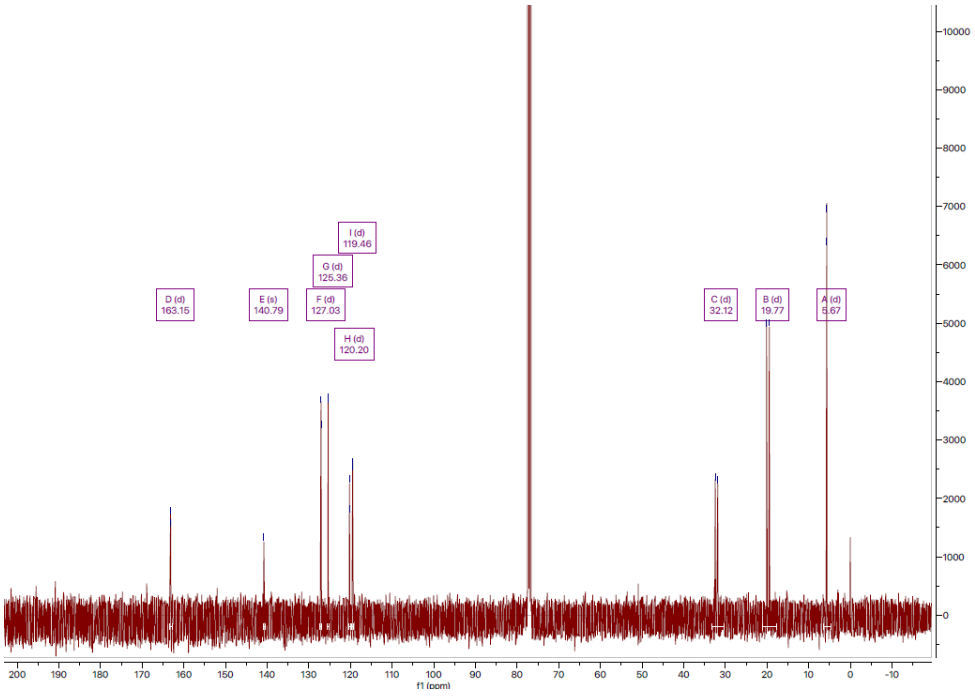
MS of **2c**



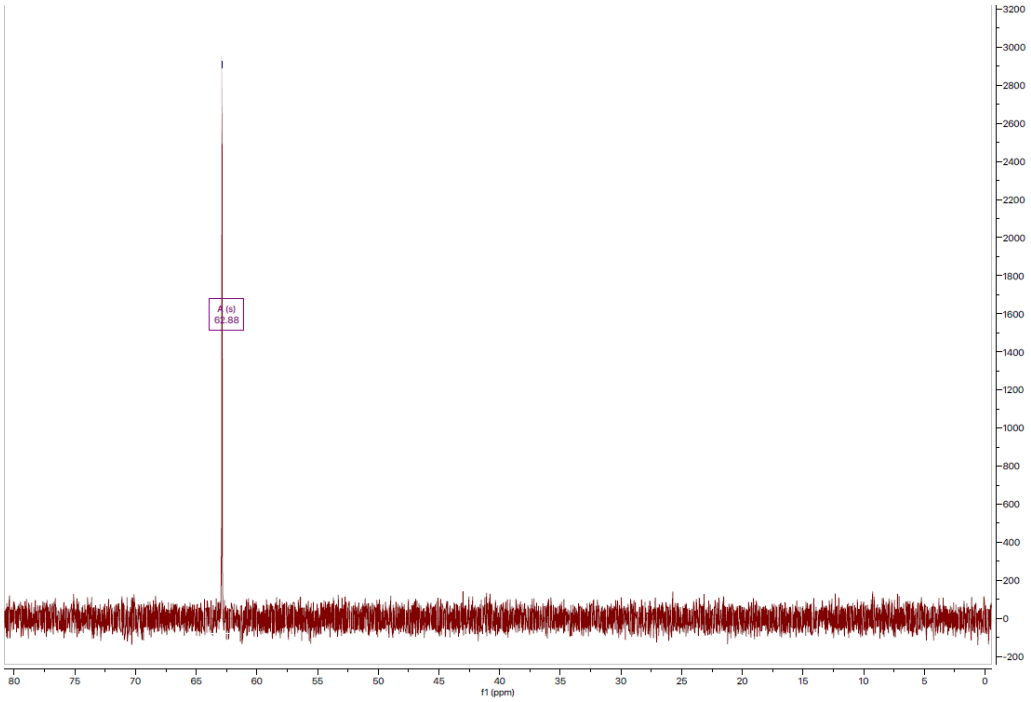
^{1}H NMR spectrum of **2d**



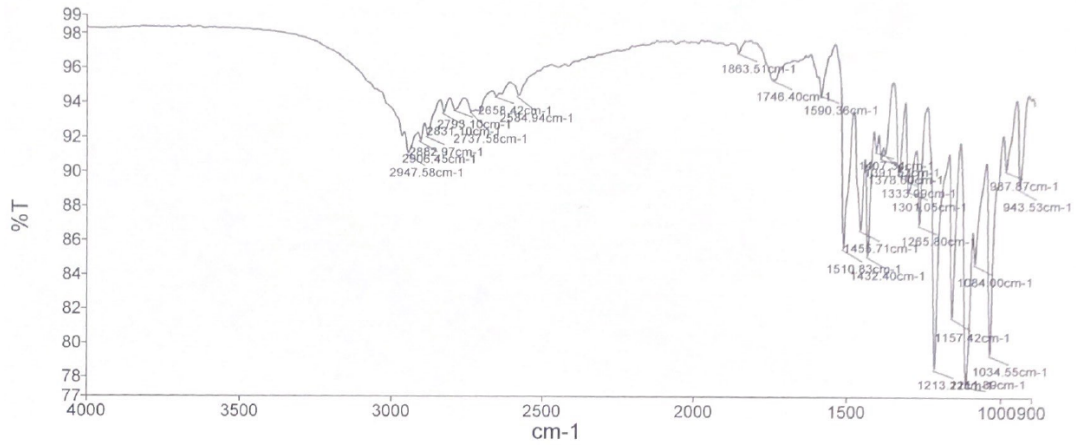
^{13}C NMR spectrum of **2d**



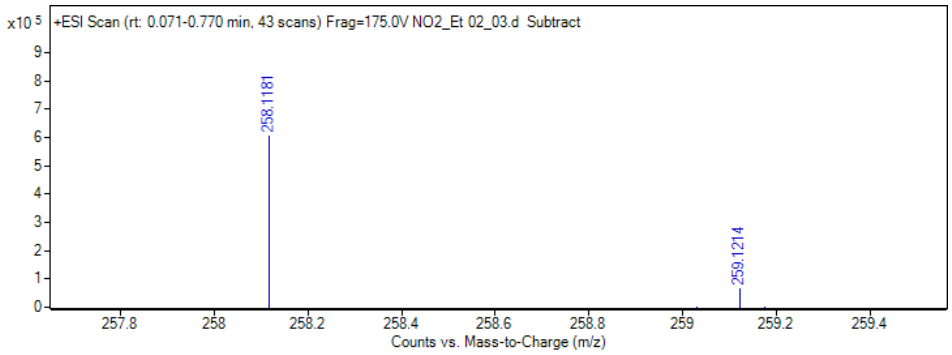
$^{31}P\{^{1}H\}$ NMR spectrum of **2d**



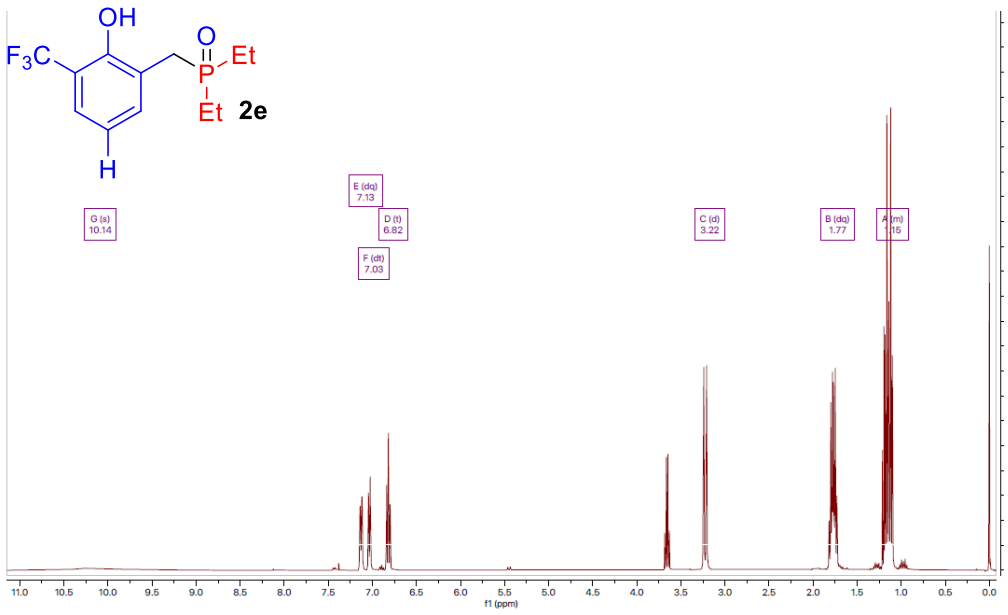
IR spectrum of **2d**



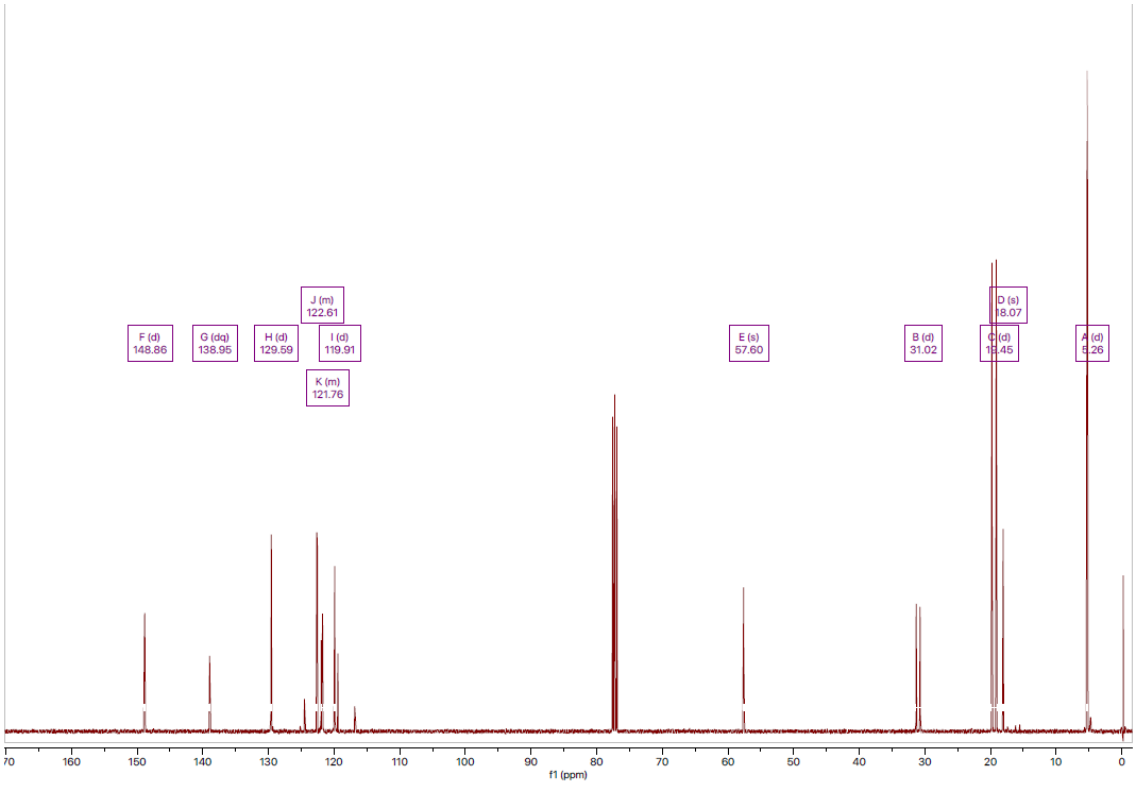
MS of **2d**



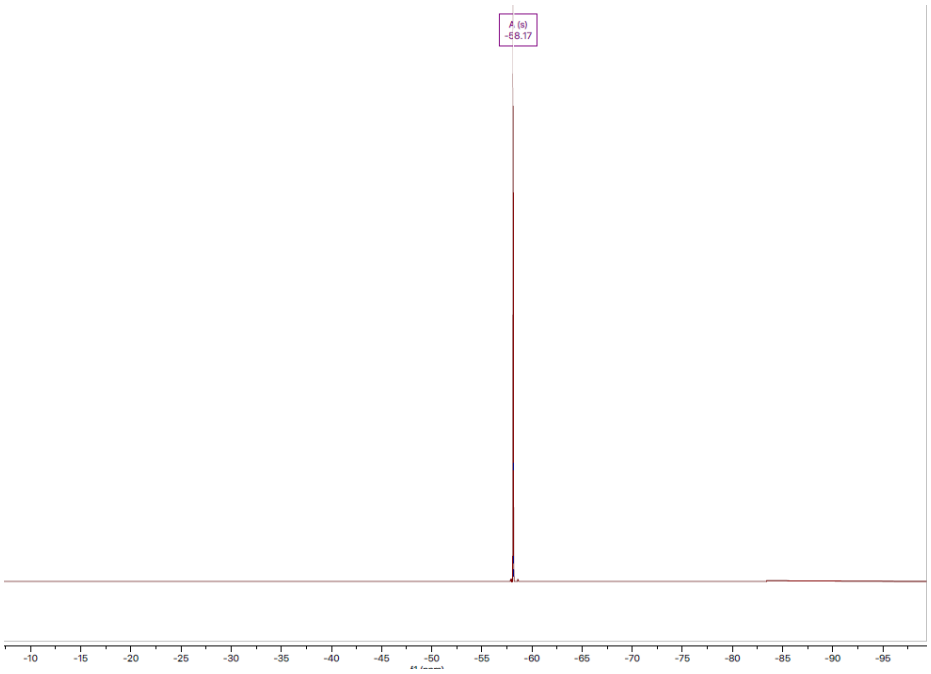
^{1}H NMR Spectrum of **2e**



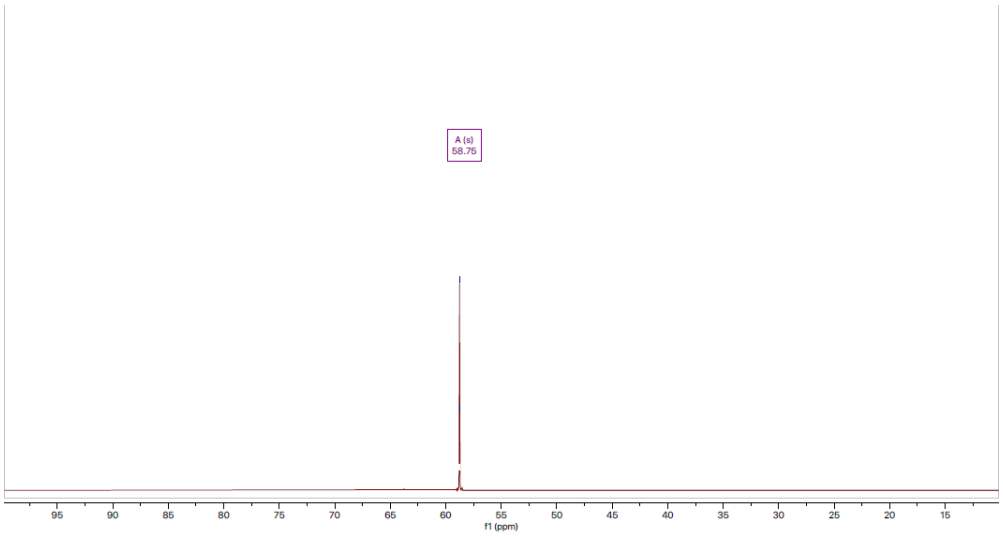
^{13}C NMR of **2e**



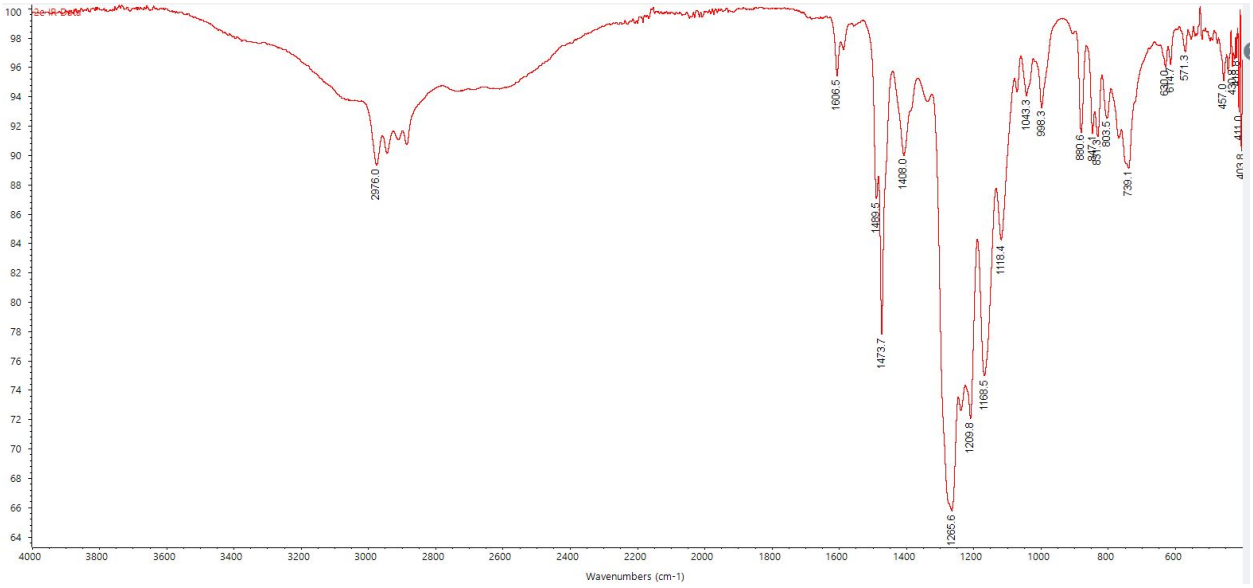
$^{19}F\{^{1}H\}$ NMR of **2e**



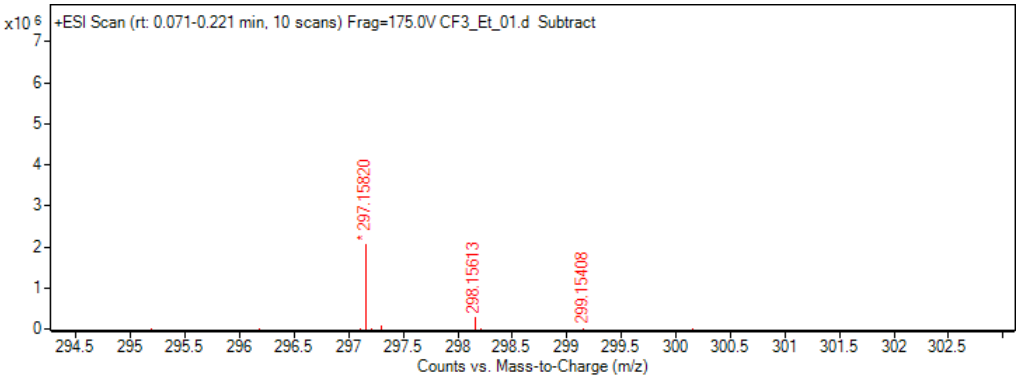
$^{31}P\{^{1}H\}$ NMR Spectrum of **2e**



IR Spectrum of **2e**



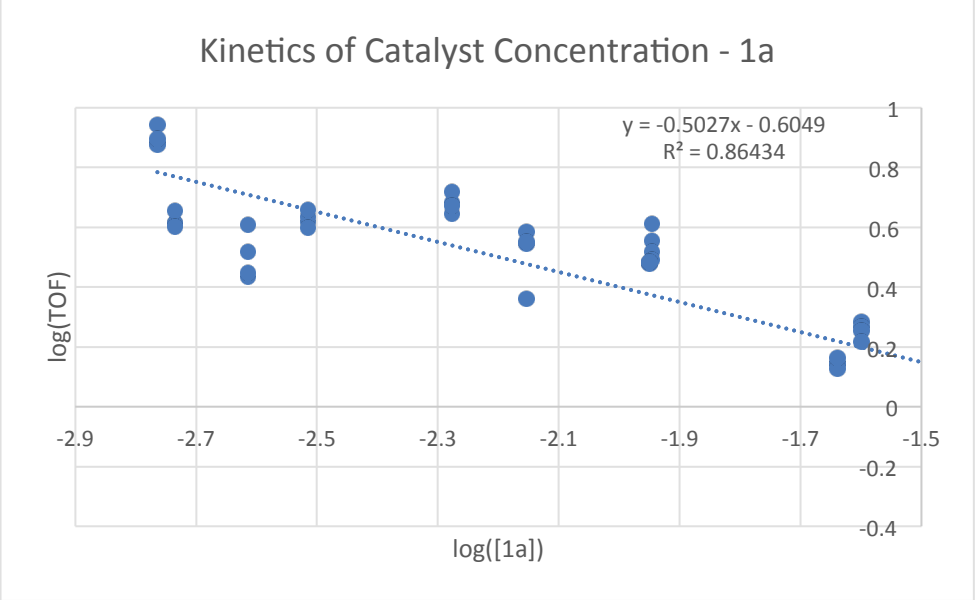
MS of **2e**

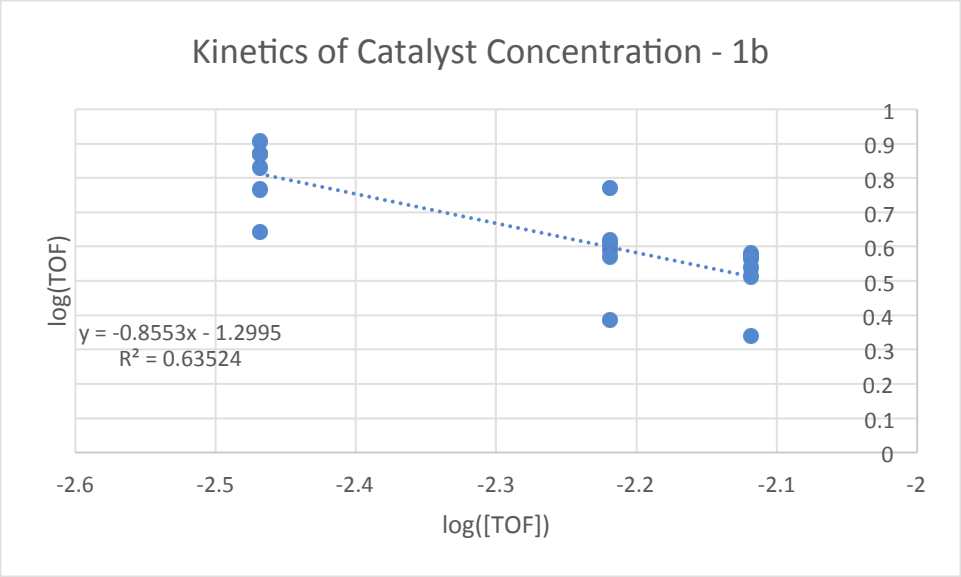


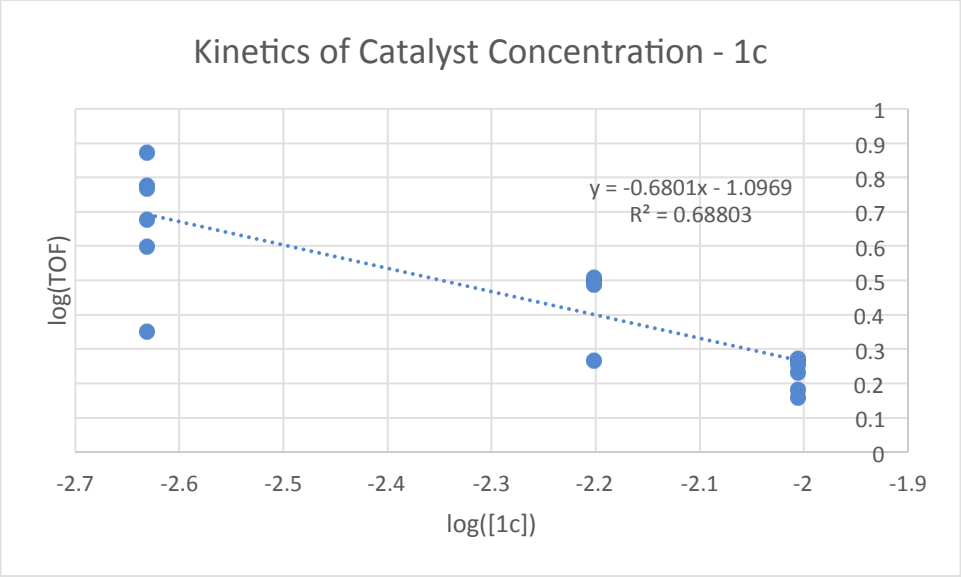
Materials and Methods for Kinetic Studies

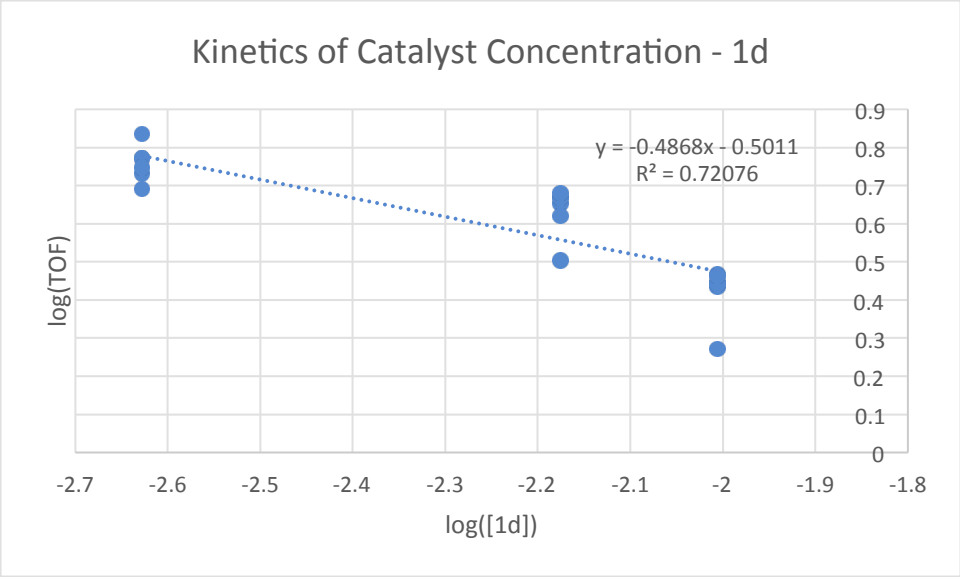
A Teflon-coated stir bar and 35 mL heavy-walled borosilicate pressure tube (Ace Glass Inc., “Tube C”, Product #864807) were oven-dried overnight and then allowed to cool to ambient temperature in air. The tube was then charged with the aldehyde, and then flushed gently with dry nitrogen gas. Then, while maintaining the gentle nitrogen flush, trifluoroacetic acid was added in a single portion, followed quickly by the phosphine, which was also added swiftly in one portion by syringe. The tube was then sealed with a threaded Teflon cap fitted with a Viton o-ring. The sealed tube was then heated in an 80 °C aluminum-pebble bath behind a blast shield for 8–20 hours. The reaction vessel was then removed from the aluminum-pebble bath and allowed to cool to room temperature. Then the reaction tube was opened, and the contents were transferred into a 250 mL separatory funnel that had already been charged with 50 mL of half-saturated sodium bicarbonate (25 mL saturated sodium bicarbonate and 25 mL water). The reaction flask was rinsed with two 25 mL portions of dichloromethane, which were both transferred to the separatory funnel. After agitation, the layers were allowed to separate, and the organic layer was collected. The remaining aqueous phase was extracted with two more portions of dichloromethane (each 50 mL), and the organic phases were all combined, dried over sodium sulfate, and concentrated under vacuum to afford the crude product. All glassware, gloves, and other objects or surfaces which came into contact with phosphines was rinsed immediately in bleach (5 % sodium hypo-chlorite/water) to quench any residual phosphine, followed by water, and finally methanol.

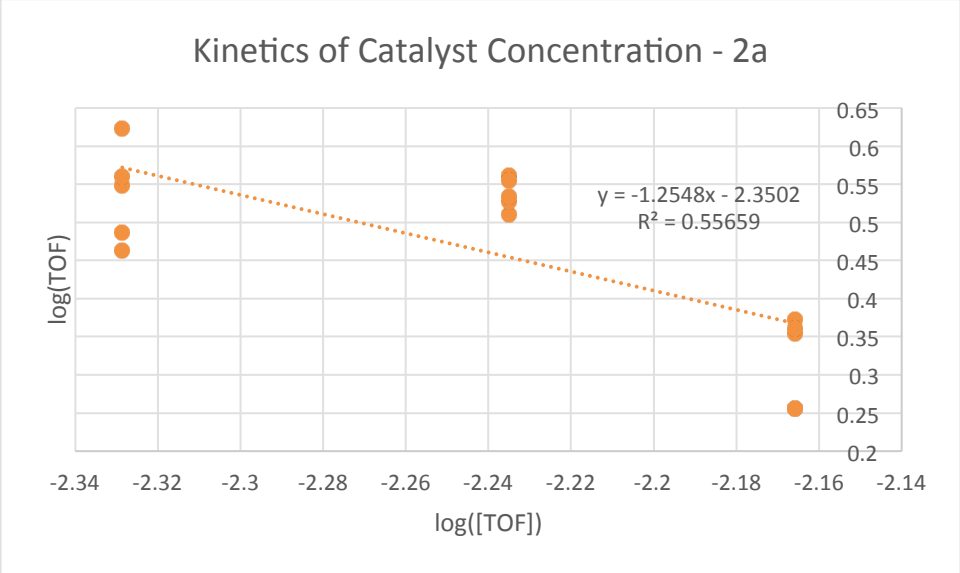
Kinetics of Catalyst Concentration

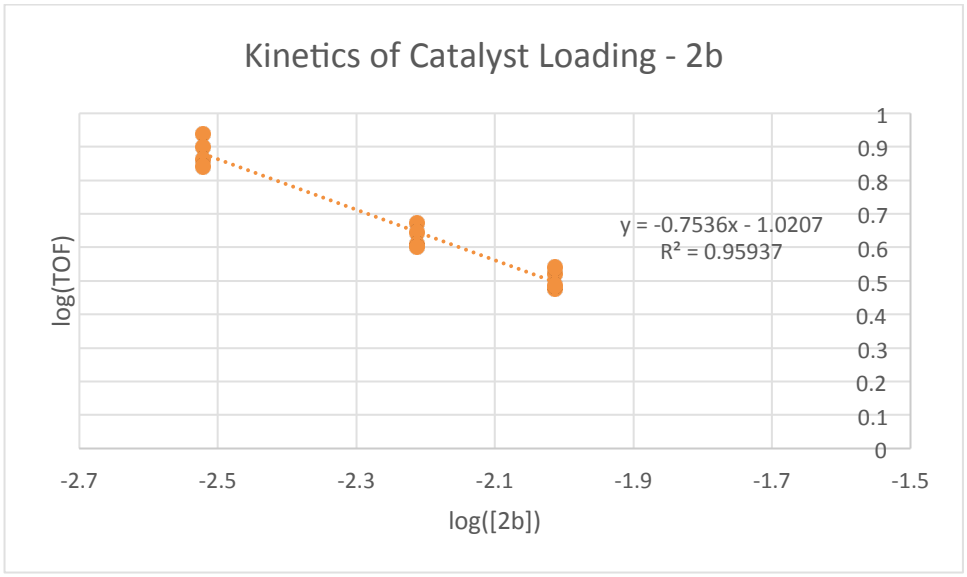


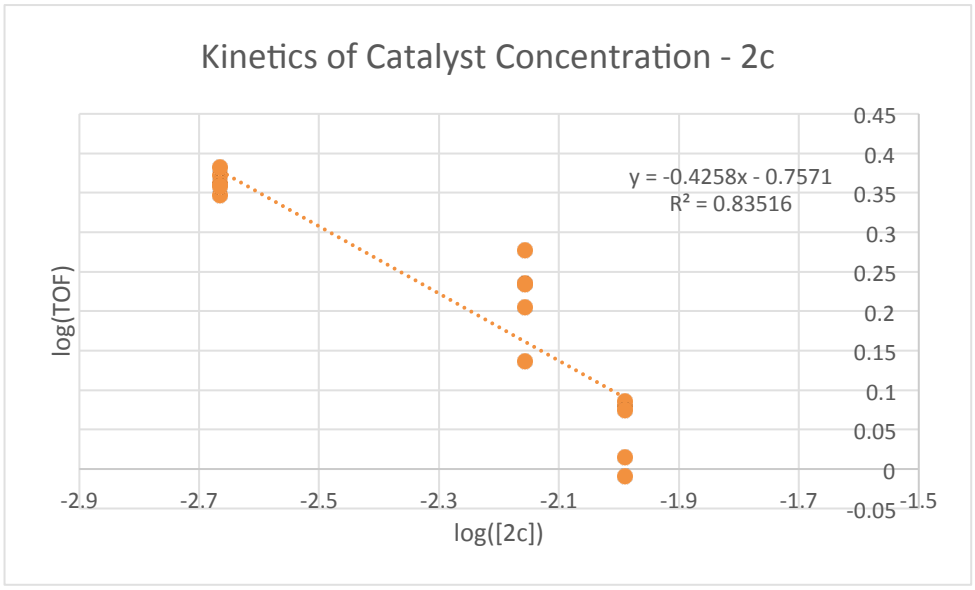

Kinetics of Catalyst Concentration - 1b
log(TOF)
y = -0.8553x - 1.2995
R² = 0.63524
log([TOF])
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
-2.6
-2.5
-2.4
-2.3
-2.2
-2.1
-2

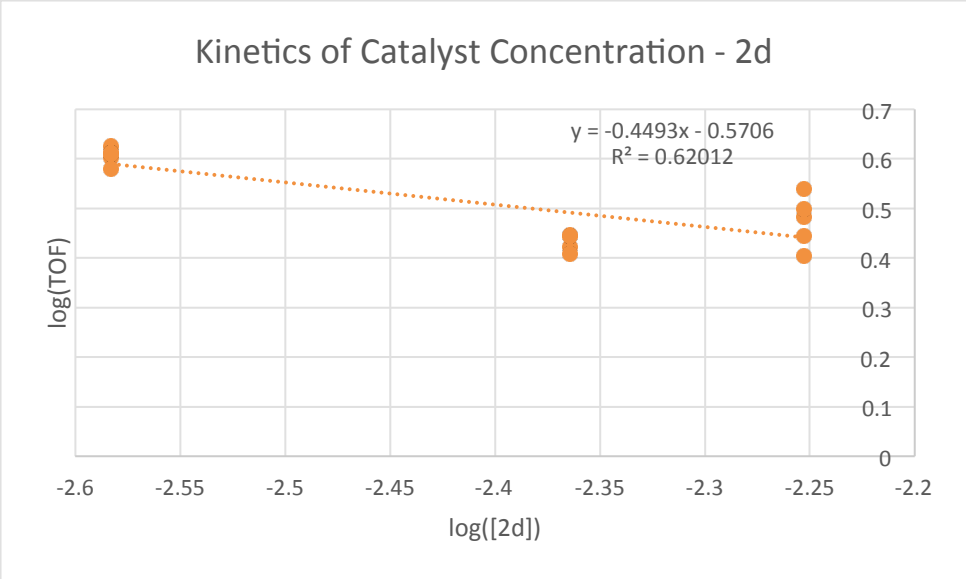

Kinetics of Catalyst Concentration - 1c
log(TOF)
y = -0.6801x - 1.0969
R² = 0.68803
log([1c])
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
-2.7
-2.6
-2.5
-2.4
-2.3
-2.2
-2.1
-2
-1.9


Kinetics of Catalyst Concentration - 1d
y = -0.4868x - 0.5011
R² = 0.72076
log(TOF)
log([1d])
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
-2.7
-2.6
-2.5
-2.4
-2.3
-2.2
-2.1
-2
-1.9
-1.8


Kinetics of Catalyst Concentration - 2a
y = -1.2548x - 2.3502
R² = 0.55659
log(TOF)
log([TOF])
0.65
0.6
0.55
0.5
0.45
0.4
0.35
0.3
0.25
0.2
-2.34
-2.32
-2.3
-2.28
-2.26
-2.24
-2.22
-2.2
-2.18
-2.16
-2.14


Kinetics of Catalyst Loading - 2b
y = -0.7536x - 1.0207
R² = 0.95937
log(TOF)
log([2b])
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
-2.7
-2.5
-2.3
-2.1
-1.9
-1.7
-1.5


Kinetics of Catalyst Concentration - 2c
y = -0.4258x - 0.7571
R² = 0.83516
log(TOF)
log([2c])
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
-0.05
-2.9
-2.7
-2.5
-2.3
-2.1
-1.9
-1.7
-1.5

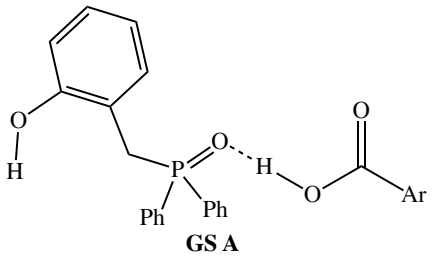

Kinetics of Catalyst Concentration - 2d
y = -0.4493x - 0.5706
R² = 0.62012
log(TOF)
log([2d])
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
-2.6
-2.55
-2.5
-2.45
-2.4
-2.35
-2.3
-2.25
-2.2

Coordinates for computed optimized structures

All structures below were optimized using Gaussian 09, with the xB97X-D functional and 6-311G(d,p) basis set and the preset PCM for toluene (structures optimized with other basis sets and functionals were essentially identical). Energies discussed in the manuscript were thermally corrected to 413.15 K.

In All cases Ar = 2,4-dinitrophenyl.

1. Structures from Table 1.

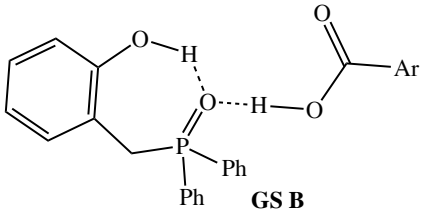


GS A

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.936622	-1.388691	-1.307549
2	6	0	4.634722	-0.954952	-1.501577
3	6	0	3.597068	-1.367311	-0.666762
4	6	0	3.894061	-2.207994	0.417524
5	6	0	5.200566	-2.660629	0.598028
6	6	0	6.212590	-2.257780	-0.257659
7	1	0	6.725137	-1.059684	-1.973455
8	1	0	4.407854	-0.285161	-2.325349
9	1	0	5.395428	-3.322068	1.433542
10	1	0	7.223460	-2.615368	-0.096940
11	6	0	2.184211	-0.908876	-0.936621
12	1	0	1.461162	-1.721335	-0.810484
13	1	0	2.100771	-0.516466	-1.952584
14	8	0	2.954147	-2.637513	1.291378
15	1	0	2.333567	-1.916706	1.490560
16	15	0	1.700239	0.382484	0.250283

17	8	0	1.614786	-0.212602	1.648998
18	6	0	0.155042	1.154671	-0.303043
19	6	0	-0.606954	0.633458	-1.347843
20	6	0	-0.307901	2.269686	0.401779
21	6	0	-1.818443	1.224779	-1.687531
22	1	0	-0.290690	-0.257107	-1.876691
23	6	0	-1.518035	2.854819	0.061165
24	1	0	0.279440	2.676154	1.218431
25	6	0	-2.272707	2.332806	-0.985281
26	1	0	-2.410161	0.796707	-2.487141
27	1	0	-1.873550	3.718224	0.611314
28	1	0	-3.220020	2.789667	-1.248808
29	6	0	2.973157	1.657709	0.158459
30	6	0	4.030156	1.603091	1.065450
31	6	0	2.974213	2.605030	-0.865135
32	6	0	5.084514	2.498206	0.947531
33	1	0	4.019044	0.859462	1.853929
34	6	0	4.031435	3.497147	-0.977991
35	1	0	2.147855	2.653554	-1.567005
36	6	0	5.085840	3.441354	-0.073125
37	1	0	5.908107	2.455255	1.650225
38	1	0	4.031881	4.237150	-1.769728
39	1	0	5.911727	4.137694	-0.164100
40	6	0	-1.351343	-1.208675	1.225678
41	8	0	-0.724674	-1.883964	0.445912
42	8	0	-0.864042	-0.663722	2.320231
43	1	0	0.129721	-0.633584	2.238201
44	6	0	-2.775676	-0.810926	0.965277
45	6	0	-3.468549	-1.300592	-0.138942
46	6	0	-3.379573	0.183681	1.730115
47	6	0	-4.706728	-0.814866	-0.506699
48	6	0	-4.631971	0.678119	1.402798
49	1	0	-2.836110	0.582094	2.575536
50	6	0	-5.268302	0.172057	0.283992

51	1	0	-5.227590	-1.184602	-1.379276
52	1	0	-5.108295	1.453360	1.986354
53	7	0	-2.915028	-2.365481	-1.001227
54	8	0	-2.930540	-3.486771	-0.560197
55	8	0	-2.556334	-2.028518	-2.111060
56	7	0	-6.589486	0.714431	-0.100549
57	8	0	-7.127741	0.231051	-1.073378
58	8	0	-7.041705	1.609655	0.580544

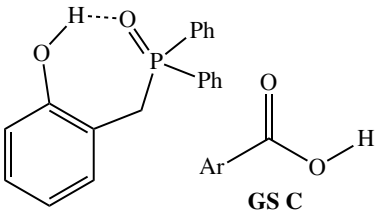


GS B

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-4.240013	-3.801914	-1.881784
2	6	0	-4.504051	-2.883561	-1.365641
3	6	0	-5.187563	-0.564923	-0.023146
4	6	0	-5.543869	-2.092342	-1.834819
5	6	0	-3.804455	-2.510706	-0.221710
6	6	0	-4.124045	-1.327302	0.452545
7	6	0	-5.897910	-0.933556	-1.157435
8	1	0	-6.082361	-2.392494	-2.726214
9	1	0	-6.715711	-0.317788	-1.510628
10	1	0	-5.442554	0.351972	0.497724
11	8	0	-2.807292	-3.273112	0.298607
12	6	0	-3.323657	-0.881275	1.641863
13	1	0	-2.943803	-1.729507	2.215237
14	1	0	-3.933810	-0.277678	2.318908
15	15	0	-1.873423	0.191279	1.304068

16	6	0	-0.631713	-0.788295	0.402708
17	6	0	1.432420	-2.244967	-0.777563
18	6	0	-0.160187	-1.959177	1.002949
19	6	0	-0.043739	-0.343182	-0.780488
20	6	0	0.981501	-1.074444	-1.370726
21	6	0	0.864194	-2.684382	0.414827
22	1	0	-0.592109	-2.305511	1.934786
23	1	0	-0.349270	0.594375	-1.227157
24	1	0	1.440676	-0.702190	-2.278272
25	1	0	1.224657	-3.590193	0.888976
26	1	0	2.238024	-2.809665	-1.233972
27	6	0	-2.410398	1.526805	0.209419
28	6	0	-3.221924	3.669917	-1.362928
29	6	0	-2.338644	2.825268	0.709626
30	6	0	-2.879621	1.304428	-1.088206
31	6	0	-3.285304	2.376062	-1.869500
32	6	0	-2.746896	3.894104	-0.077473
33	1	0	-1.942475	2.986304	1.704805
34	1	0	-2.924372	0.300460	-1.493996
35	1	0	-3.646932	2.200687	-2.875882
36	1	0	-2.681426	4.903561	0.310799
37	1	0	-3.534485	4.506284	-1.977960
38	1	0	-2.593524	-3.985595	-0.305131
39	8	0	-1.348702	0.708471	2.624590
40	6	0	3.332429	1.088434	-0.238383
41	6	0	4.428941	-1.099594	1.047749
42	6	0	4.364170	0.406680	-0.851091
43	6	0	2.807361	0.695989	0.989888
44	6	0	3.375608	-0.406689	1.622282
45	6	0	4.898157	-0.681932	-0.184529
46	1	0	4.748250	0.703894	-1.817209
47	1	0	2.955444	-0.727823	2.565204
48	1	0	4.873647	-1.960286	1.527174
49	7	0	5.995736	-1.432830	-0.829391

50	8	0	6.403146	-1.020768	-1.894700
51	8	0	6.412272	-2.414754	-0.252104
52	7	0	2.811212	2.256654	-0.978465
53	8	0	3.106337	3.346188	-0.554453
54	8	0	2.194614	2.019444	-1.996270
55	6	0	1.556038	1.326362	1.537196
56	8	0	0.917166	2.124532	0.897431
57	8	0	1.216236	0.839965	2.710597
58	1	0	0.223594	0.951088	2.824512



GS C (**1a** and DNBA optimized separately)

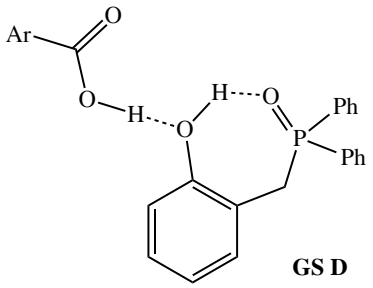
1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.039070	-0.171094	-1.489718
2	6	0	2.659083	-0.263842	-1.587463
3	6	0	1.912452	-1.030840	-0.694639
4	6	0	2.580345	-1.700220	0.345861
5	6	0	3.970356	-1.621530	0.428313
6	6	0	4.694156	-0.866257	-0.479814
7	1	0	4.596866	0.427674	-2.199687
8	1	0	2.143883	0.255880	-2.389619
9	1	0	4.458261	-2.159575	1.232104
10	1	0	5.773594	-0.812791	-0.392374

11	6	0	0.423209	-1.180221	-0.881675
12	1	0	0.128560	-2.234872	-0.834327
13	1	0	0.109243	-0.801002	-1.857426
14	8	0	1.938662	-2.470935	1.251809
15	1	0	1.111543	-2.035806	1.547131
16	15	0	-0.552402	-0.373778	0.432144
17	8	0	-0.265338	-0.991723	1.773520
18	6	0	-2.293518	-0.579848	-0.040622
19	6	0	-3.038374	-1.523647	0.665350
20	6	0	-2.885573	0.133068	-1.083735
21	6	0	-4.364570	-1.757304	0.323195
22	1	0	-2.572638	-2.056734	1.486563
23	6	0	-4.209814	-0.105025	-1.423084
24	1	0	-2.324352	0.888616	-1.622659
25	6	0	-4.948483	-1.051714	-0.721074
26	1	0	-4.942465	-2.488852	0.875924
27	1	0	-4.668732	0.452970	-2.231003
28	1	0	-5.983754	-1.234012	-0.986140
29	6	0	-0.166817	1.395446	0.378321
30	6	0	-0.067654	2.066839	1.595594
31	6	0	0.041367	2.089039	-0.814524
32	6	0	0.219403	3.425574	1.616702
33	1	0	-0.201033	1.512541	2.517737
34	6	0	0.328031	3.446445	-0.789440
35	1	0	-0.002210	1.573908	-1.768076
36	6	0	0.413650	4.115143	0.426536
37	1	0	0.298573	3.944394	2.564870
38	1	0	0.494386	3.980787	-1.717526
39	1	0	0.641803	5.174731	0.445202

DNBA

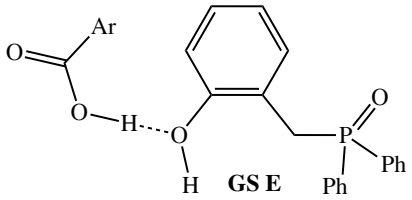
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.937322	-0.751576	0.001502
2	6	0	0.437481	0.548058	-0.029661
3	6	0	-0.917527	0.815153	-0.015299
4	6	0	-1.782881	-0.263261	0.004859
5	6	0	-1.335243	-1.572518	0.006131
6	6	0	0.031401	-1.807228	0.004030
7	6	0	2.397097	-1.101452	0.068760
8	8	0	2.895122	-1.969153	-0.588017
9	8	0	3.032613	-0.397524	1.007555
10	1	0	3.965383	-0.641650	0.974917
11	7	0	1.343648	1.705556	-0.165418
12	8	0	1.014985	2.731185	0.387717
13	8	0	2.328315	1.550985	-0.854797
14	1	0	-1.287767	1.830710	-0.028215
15	7	0	-3.239216	-0.000551	0.011895
16	8	0	-3.593864	1.157538	-0.013907
17	8	0	-3.974273	-0.963559	0.044390
18	1	0	-2.051169	-2.382801	0.011916
19	1	0	0.413442	-2.820126	0.010585



GS D

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.555816	3.861511	1.763495
2	6	0	-2.533781	3.036319	1.232373
3	6	0	-2.353249	2.366489	0.022391
4	6	0	-1.125718	2.515407	-0.639798
5	6	0	-0.152479	3.368003	-0.125567
6	6	0	-0.365361	4.035416	1.069035
7	1	0	-1.725019	4.368496	2.705672
8	1	0	-3.471647	2.906084	1.762988
9	1	0	0.776570	3.481587	-0.672059
10	1	0	0.409260	4.683663	1.461758
11	6	0	-3.475458	1.519907	-0.528960
12	1	0	-3.702249	1.781014	-1.568717
13	1	0	-4.382093	1.679427	0.058118
14	8	0	-0.823782	1.863307	-1.804028
15	1	0	-1.295602	0.991348	-1.860231
16	15	0	-3.054393	-0.258308	-0.559989
17	8	0	-1.954497	-0.480136	-1.568949
18	6	0	-4.565136	-1.162372	-0.982677
19	6	0	-4.447246	-2.206424	-1.899581
20	6	0	-5.814329	-0.850537	-0.442400
21	6	0	-5.569280	-2.940514	-2.261524
22	1	0	-3.476150	-2.424938	-2.329394
23	6	0	-6.932900	-1.586494	-0.808355
24	1	0	-5.924278	-0.033502	0.262879

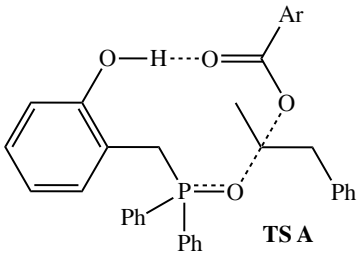
25	6	0	-6.809297	-2.632801	-1.715688
26	1	0	-5.474995	-3.751199	-2.974456
27	1	0	-7.901506	-1.341041	-0.388815
28	1	0	-7.684111	-3.205632	-2.001371
29	6	0	-2.558985	-0.694671	1.123066
30	6	0	-1.216629	-0.502232	1.456931
31	6	0	-3.457908	-1.147882	2.088751
32	6	0	-0.781247	-0.752305	2.750139
33	1	0	-0.508704	-0.164457	0.708730
34	6	0	-3.016670	-1.396063	3.381531
35	1	0	-4.496139	-1.328720	1.834561
36	6	0	-1.681147	-1.195522	3.711444
37	1	0	0.264650	-0.609182	2.988763
38	1	0	-3.714631	-1.755387	4.128956
39	1	0	-1.338953	-1.393734	4.720957
40	6	0	2.639468	1.370952	-1.361375
41	8	0	2.756143	2.537818	-1.625047
42	8	0	1.548788	0.643859	-1.478668
43	1	0	0.765849	1.203189	-1.710427
44	6	0	3.819310	0.537171	-0.928123
45	6	0	4.988767	0.645042	-1.673806
46	6	0	3.803204	-0.356128	0.140124
47	6	0	6.096896	-0.135123	-1.381678
48	1	0	5.015277	1.350101	-2.494877
49	6	0	4.885703	-1.156136	0.452033
50	6	0	6.020849	-1.028102	-0.326614
51	1	0	7.009617	-0.064063	-1.957065
52	1	0	4.850385	-1.851668	1.278632
53	7	0	2.642888	-0.429618	1.047114
54	8	0	2.387805	-1.509305	1.535623
55	8	0	2.052669	0.605234	1.274051
56	7	0	7.194685	-1.867721	-0.006625
57	8	0	8.170857	-1.749149	-0.715612
58	8	0	7.100513	-2.616985	0.941484



GS E

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-3.212496	1.140341	0.089673
2	8	0	-4.659448	1.367548	0.372916
3	6	0	-2.945847	0.223089	-1.488544
4	6	0	-3.526157	-1.159826	-1.394928
5	6	0	-2.742122	-2.256156	-1.033035
6	8	0	-1.398354	-2.056886	-0.850277
7	6	0	-3.299154	-3.516311	-0.861381
8	6	0	-4.664222	-3.694957	-1.034340
9	6	0	-5.465601	-2.617966	-1.389372
10	6	0	-4.893834	-1.365895	-1.566177
11	1	0	-3.463521	0.810767	-2.251081
12	1	0	-1.885843	0.214689	-1.745251
13	1	0	-0.995315	-2.740825	-0.302624
14	1	0	-2.662555	-4.351142	-0.586454
15	1	0	-5.097339	-4.678150	-0.892028
16	1	0	-6.532617	-2.749034	-1.521214
17	1	0	-5.516964	-0.513521	-1.811348
18	6	0	-2.392684	0.100967	1.338059
19	6	0	-3.147017	-0.947355	1.868791
20	6	0	-2.555243	-1.864064	2.727477
21	6	0	-1.214062	-1.733295	3.070224
22	6	0	-0.469749	-0.671584	2.570180
23	6	0	-1.056429	0.244892	1.707238
24	1	0	-4.193358	-1.041819	1.600338

25	1	0	-3.143724	-2.680639	3.130050
26	1	0	-0.751663	-2.452422	3.737017
27	1	0	0.570899	-0.551357	2.848806
28	1	0	-0.463953	1.070426	1.334396
29	6	0	-2.258560	2.675045	-0.084532
30	6	0	-2.893004	3.855606	0.302041
31	6	0	-2.221715	5.067705	0.207242
32	6	0	-0.916493	5.105703	-0.268416
33	6	0	-0.280172	3.933071	-0.658837
34	6	0	-0.952011	2.721472	-0.575375
35	1	0	-3.912517	3.807902	0.668266
36	1	0	-2.718497	5.983266	0.507233
37	1	0	-0.391767	6.052208	-0.335307
38	1	0	0.741773	3.949073	-1.016922
39	1	0	-0.437339	1.817454	-0.883364
40	1	0	-0.103685	-0.957892	-0.907132
41	8	0	0.821500	-0.620299	-0.865714
42	6	0	1.552660	-1.508628	-0.219506
43	8	0	1.147483	-2.562903	0.205496
44	6	0	3.002007	-1.123778	-0.132645
45	6	0	3.484213	0.182101	-0.193758
46	6	0	4.833819	0.469698	-0.234185
47	6	0	5.716338	-0.593867	-0.170265
48	6	0	5.290351	-1.906605	-0.078269
49	6	0	3.927636	-2.160849	-0.066327
50	7	0	2.573272	1.340464	-0.144355
51	8	0	1.853019	1.419720	0.825136
52	8	0	2.652466	2.141483	-1.048812
53	7	0	7.168449	-0.306778	-0.198180
54	8	0	7.501643	0.856361	-0.262500
55	8	0	7.920114	-1.255792	-0.154731
56	1	0	5.195587	1.486683	-0.298973
57	1	0	6.018487	-2.704182	-0.027816
58	1	0	3.554205	-3.175520	-0.014219

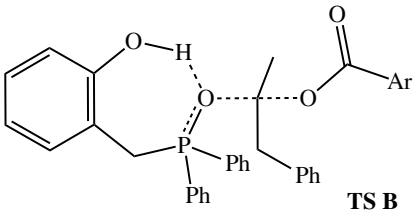


TS A

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.601286	3.696082	-0.216511
2	6	0	-0.476501	3.773338	-0.307225
3	6	0	-3.244928	3.909013	-0.519040
4	6	0	-1.168894	4.847961	0.235229
5	6	0	-1.177834	2.768256	-0.964363
6	6	0	-2.574468	2.816507	-1.053307
7	6	0	-2.551136	4.929409	0.120968
8	1	0	-0.619642	5.627984	0.750139
9	1	0	-3.086826	5.774253	0.536726
10	1	0	-4.328041	3.951154	-0.587007
11	6	0	-3.296549	1.638180	-1.648020
12	1	0	-2.947270	1.422023	-2.661972
13	1	0	-4.368875	1.838440	-1.688607
14	15	0	-3.029139	0.047919	-0.728902
15	6	0	-2.357274	0.504753	0.889532
16	6	0	-1.308425	1.480115	3.274319
17	6	0	-3.117634	1.355851	1.697418
18	6	0	-1.078862	0.136624	1.294669
19	6	0	-0.552989	0.626633	2.483677
20	6	0	-2.595939	1.838198	2.885980
21	1	0	-4.115320	1.654266	1.392580
22	1	0	-0.475933	-0.532088	0.699469
23	1	0	0.456448	0.351020	2.763218
24	1	0	-3.187195	2.505860	3.501469

25	1	0	-0.893051	1.872759	4.195501
26	6	0	-4.673427	-0.650677	-0.389129
27	6	0	-7.109982	-1.931606	0.043399
28	6	0	-4.899897	-1.347625	0.798602
29	6	0	-5.671322	-0.613968	-1.364063
30	6	0	-6.886346	-1.248879	-1.146452
31	6	0	-6.115932	-1.983053	1.012831
32	1	0	-4.124843	-1.390631	1.555708
33	1	0	-5.503051	-0.097272	-2.303208
34	1	0	-7.657889	-1.212440	-1.906671
35	1	0	-6.286992	-2.518291	1.939640
36	1	0	-8.059522	-2.426050	0.213555
37	1	0	-2.488988	-3.367636	-0.230527
38	6	0	-1.612610	-3.295940	0.404099
39	6	0	0.621493	-3.041237	2.030533
40	6	0	-0.377789	-2.995462	-0.168382
41	6	0	-1.730111	-3.464217	1.777167
42	6	0	-0.613955	-3.330112	2.595220
43	6	0	0.739906	-2.881980	0.655159
44	1	0	-2.697745	-3.694259	2.210236
45	1	0	-0.707915	-3.447305	3.668815
46	1	0	1.496204	-2.921806	2.658569
47	6	0	-0.243683	-1.266418	-1.993523
48	1	0	1.700034	-2.631842	0.219131
49	6	0	-0.341441	-0.846659	-3.415059
50	1	0	0.497087	-1.276993	-3.965205
51	1	0	-0.325095	0.237520	-3.498686
52	1	0	-1.270223	-1.238394	-3.833163
53	6	0	-0.266863	-2.719570	-1.645952
54	1	0	0.657114	-3.139806	-2.053846
55	1	0	-1.096526	-3.172934	-2.193813
56	1	0	-0.099969	-0.529517	-1.232201
57	8	0	-2.247646	-0.975811	-1.536091
58	8	0	-0.593532	1.693831	-1.522500

59	6	0	4.327113	0.186160	0.410538
60	6	0	6.143364	-0.520560	-1.538507
61	6	0	5.673093	0.274289	0.703016
62	6	0	3.849342	-0.215912	-0.833303
63	6	0	4.782355	-0.581126	-1.798171
64	6	0	6.564483	-0.087289	-0.292442
65	1	0	6.024539	0.603262	1.671088
66	1	0	4.420179	-0.909722	-2.763921
67	1	0	6.878135	-0.796189	-2.282429
68	7	0	8.009954	-0.012894	-0.005442
69	8	0	8.341069	0.347495	1.104615
70	8	0	8.772335	-0.317097	-0.898683
71	7	0	3.389892	0.467418	1.512221
72	8	0	2.544695	-0.376357	1.733549
73	8	0	3.561115	1.479745	2.151725
74	6	0	2.373799	-0.151033	-1.196715
75	8	0	1.942325	-1.101239	-1.890695
76	8	0	1.771147	0.857626	-0.789360
77	1	0	0.335052	1.530778	-1.224682



TS B

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-1.998693	-0.824334	-0.418609
2	8	0	-1.898640	0.701844	-0.262295

3	6	0	-1.297239	-1.644240	1.055029
4	6	0	-2.197431	-1.609648	2.267820
5	6	0	-2.680092	-2.809310	2.791020
6	6	0	-3.458302	-2.846955	3.937178
7	6	0	-3.766010	-1.657634	4.586949
8	6	0	-3.314749	-0.452004	4.076983
9	6	0	-2.544796	-0.415595	2.916798
10	8	0	-2.144568	0.807504	2.483887
11	1	0	-2.031673	0.818214	1.517682
12	1	0	-3.552864	0.489498	4.556977
13	1	0	-4.367080	-1.666683	5.488987
14	1	0	-3.811579	-3.795018	4.323973
15	1	0	-2.420017	-3.737122	2.291087
16	1	0	-0.327602	-1.160825	1.237536
17	1	0	-1.081620	-2.680306	0.784547
18	6	0	-3.743996	-1.261799	-0.513816
19	6	0	-4.693994	-0.244846	-0.471429
20	6	0	-6.045379	-0.569097	-0.491130
21	6	0	-6.441304	-1.898701	-0.546832
22	6	0	-5.490328	-2.914260	-0.586975
23	6	0	-4.141090	-2.598390	-0.570684
24	1	0	-4.366721	0.788203	-0.425244
25	1	0	-6.788272	0.219094	-0.459548
26	1	0	-7.496084	-2.148420	-0.557525
27	1	0	-5.802437	-3.950989	-0.628422
28	1	0	-3.399863	-3.390285	-0.605825
29	6	0	-1.165902	-1.502768	-1.864080
30	6	0	-1.884152	-1.724582	-3.041931
31	6	0	-1.234840	-2.227407	-4.159852
32	6	0	0.125424	-2.509842	-4.103915
33	6	0	0.844446	-2.281598	-2.936988
34	6	0	0.205103	-1.773279	-1.813617
35	1	0	-2.946478	-1.511720	-3.083229
36	1	0	-1.791395	-2.400205	-5.073539

37	1	0	0.630550	-2.905564	-4.977728
38	1	0	1.909137	-2.472951	-2.896985
39	1	0	0.786907	-1.560466	-0.920010
40	6	0	-0.104639	1.722568	-0.216146
41	6	0	0.141645	1.806488	-1.676365
42	1	0	-0.783780	2.068277	-2.192047
43	1	0	0.550342	0.877515	-2.067941
44	1	0	0.866693	2.605157	-1.847346
45	1	0	0.239913	0.864487	0.328441
46	6	0	-0.560440	2.922783	0.554520
47	6	0	-1.693615	3.705651	-0.067280
48	1	0	-0.799265	2.630164	1.577112
49	1	0	0.340784	3.541707	0.611184
50	6	0	-1.457475	4.634915	-1.078143
51	6	0	-2.507926	5.336060	-1.658305
52	6	0	-3.809997	5.123617	-1.224285
53	6	0	-4.053123	4.212117	-0.203177
54	6	0	-3.002382	3.508522	0.370457
55	1	0	-0.441067	4.816158	-1.412762
56	1	0	-2.306521	6.055352	-2.444075
57	1	0	-4.630108	5.673401	-1.671913
58	1	0	-5.064929	4.052408	0.153145
59	1	0	-3.195192	2.801382	1.169826
60	8	0	2.125917	1.915489	0.292747
61	6	0	2.527573	0.738799	0.432754
62	8	0	1.858432	-0.302174	0.563942
63	6	0	4.039284	0.556921	0.501342
64	6	0	4.710531	-0.388787	-0.266854
65	6	0	6.054770	-0.666911	-0.117595
66	6	0	6.749994	0.062956	0.830209
67	6	0	6.137828	1.035461	1.605615
68	6	0	4.783622	1.275605	1.432201
69	7	0	3.992997	-1.094950	-1.338991
70	8	0	3.246964	-0.433173	-2.029730

71	8	0	4.221859	-2.277958	-1.489439
72	1	0	6.550080	-1.417081	-0.717923
73	7	0	8.189200	-0.201710	1.008059
74	8	0	8.695890	-1.042820	0.294835
75	8	0	8.774733	0.438475	1.856560
76	1	0	6.724059	1.584031	2.330048
77	1	0	4.280251	2.027864	2.026260

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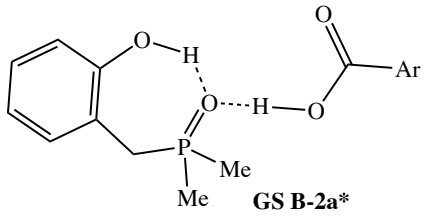
2. GS B Structures for analogs (needed to calculate values for Table 2)

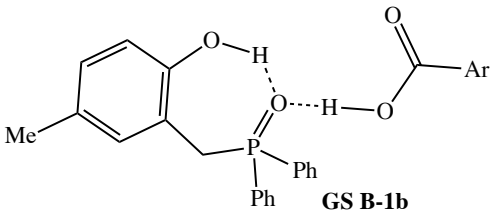
For **1a** (see section 1, above)



GS B-2a*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.394651	0.143982	-1.407232
2	6	0	-4.168708	0.414158	-0.799356
3	6	0	-3.984902	1.661782	-0.179437
4	6	0	-5.004429	2.611555	-0.228867
5	6	0	-6.207360	2.327617	-0.854458
6	1	0	-5.538900	-0.819615	-1.887058
7	1	0	-4.826303	3.568867	0.245829
8	1	0	-6.989163	3.078308	-0.878015
9	6	0	-3.055971	-0.604205	-0.855612
10	1	0	-2.107140	-0.151691	-1.161608
11	1	0	-3.297636	-1.394087	-1.571818
12	8	0	-2.832749	2.012599	0.438110

13	1	0	-2.464578	1.253150	0.923654
14	15	0	-2.702315	-1.368122	0.755423
15	8	0	-2.095432	-0.339850	1.703627
16	6	0	0.880346	-0.005362	0.533411
17	8	0	0.216431	-0.266553	-0.442578
18	8	0	0.438337	0.154554	1.753617
19	1	0	-0.553216	-0.018434	1.776291
20	6	0	2.362329	0.231789	0.419800
21	6	0	3.185213	-0.608803	-0.324670
22	6	0	2.918511	1.383998	0.965191
23	6	0	4.513877	-0.321289	-0.563615
24	6	0	4.253786	1.696542	0.754837
25	1	0	2.290187	2.042079	1.551380
26	6	0	5.024770	0.839526	-0.010679
27	1	0	5.135259	-0.979745	-1.154270
28	1	0	4.699826	2.590145	1.169208
29	7	0	2.676429	-1.895887	-0.836641
30	8	0	3.072185	-2.253965	-1.922756
31	8	0	1.932152	-2.521411	-0.110422
32	7	0	6.448168	1.164539	-0.243250
33	8	0	7.097379	0.378911	-0.899312
34	8	0	6.867590	2.194898	0.238353
35	6	0	-4.264494	-2.003346	1.398382
36	1	0	-4.085402	-2.501999	2.352176
37	1	0	-4.712186	-2.707554	0.693743
38	1	0	-4.947851	-1.166706	1.550945
39	6	0	-1.631129	-2.791115	0.464310
40	1	0	-1.350364	-3.229796	1.423743
41	1	0	-0.729209	-2.464920	-0.055467
42	1	0	-2.150012	-3.541469	-0.135983
43	6	0	-6.414507	1.083155	-1.438435
44	1	0	-7.354005	0.851370	-1.925394

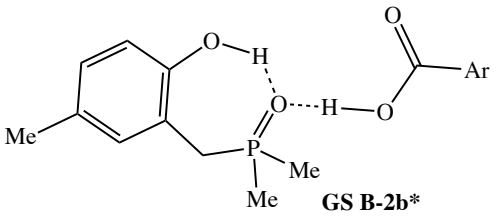


GS B-1b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.471498	-0.865379	-1.263758
2	6	0	3.412175	-1.314419	-0.477648
3	6	0	3.684440	-2.140462	0.621665
4	6	0	4.996996	-2.542037	0.857570
5	6	0	6.029562	-2.098663	0.047723
6	1	0	4.253828	-0.203223	-2.097903
7	1	0	5.183837	-3.198723	1.698772
8	1	0	7.044693	-2.420997	0.257755
9	6	0	2.001436	-0.887662	-0.801954
10	1	0	1.287178	-1.708812	-0.684200
11	1	0	1.942851	-0.509655	-1.825044
12	8	0	2.717184	-2.601781	1.452280
13	1	0	2.083179	-1.890868	1.640333
14	15	0	1.473432	0.413313	0.356255
15	8	0	1.347790	-0.165297	1.758512
16	6	0	-0.056381	1.174281	-0.252377
17	6	0	-0.788196	0.632575	-1.308283
18	6	0	-0.542320	2.298688	0.421329
19	6	0	-1.993000	1.212260	-1.689257
20	1	0	-0.454313	-0.265321	-1.813447
21	6	0	-1.745483	2.872490	0.039268
22	1	0	0.021251	2.720890	1.246713
23	6	0	-2.470348	2.329481	-1.017569
24	1	0	-2.561695	0.767620	-2.496569
25	1	0	-2.119105	3.743153	0.565473

26	1	0	-3.412705	2.777047	-1.312938
27	6	0	2.749782	1.687087	0.286326
28	6	0	3.784900	1.633595	1.218311
29	6	0	2.786569	2.618122	-0.751184
30	6	0	4.853729	2.512573	1.110779
31	1	0	3.747303	0.900692	2.015952
32	6	0	3.858176	3.494415	-0.853840
33	1	0	1.977829	2.664871	-1.473454
34	6	0	4.891438	3.438736	0.075168
35	1	0	5.660336	2.469897	1.832992
36	1	0	3.886606	4.221634	-1.656842
37	1	0	5.728698	4.122406	-0.008139
38	6	0	-1.595474	-1.184715	1.259811
39	8	0	-0.940432	-1.868806	0.511583
40	8	0	-1.146111	-0.616797	2.358664
41	1	0	-0.149916	-0.581104	2.306331
42	6	0	-3.014322	-0.804128	0.948623
43	6	0	-3.666020	-1.316825	-0.170062
44	6	0	-3.653114	0.194315	1.679440
45	6	0	-4.897291	-0.850923	-0.583803
46	6	0	-4.899754	0.669721	1.305174
47	1	0	-3.141670	0.610866	2.536024
48	6	0	-5.494663	0.140447	0.174342
49	1	0	-5.385742	-1.239018	-1.467101
50	1	0	-5.403283	1.447656	1.861704
51	7	0	-3.072919	-2.385297	-1.001143
52	8	0	-3.097918	-3.502913	-0.551451
53	8	0	-2.675157	-2.055134	-2.099658
54	7	0	-6.809027	0.661962	-0.259145
55	8	0	-7.309462	0.161238	-1.243345
56	8	0	-7.294038	1.558897	0.396675
57	6	0	6.913933	-0.698028	-1.865442
58	1	0	7.758759	-1.389960	-1.888180
59	1	0	7.277418	0.256216	-1.470288

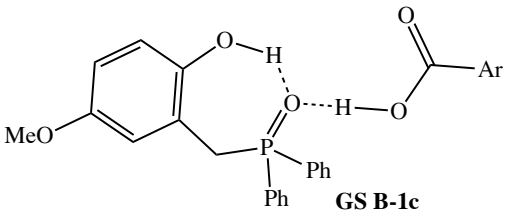
60	1	0	6.591558	-0.526168	-2.895098
61	6	0	5.788462	-1.235660	-1.020475



GS B-2b*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.147039	-0.103274	1.131714
2	6	0	-3.897642	-0.366358	0.566874
3	6	0	-3.698637	-1.587730	-0.091534
4	6	0	-4.734425	-2.520569	-0.119458
5	6	0	-5.956430	-2.241203	0.465656
6	1	0	-5.295372	0.845833	1.640958
7	1	0	-4.553000	-3.464127	-0.620026
8	1	0	-6.746834	-2.984466	0.426807
9	6	0	-2.780204	0.638363	0.707636
10	1	0	-1.847288	0.164590	1.029686
11	1	0	-3.042005	1.401906	1.445024
12	8	0	-2.522805	-1.932235	-0.671282
13	1	0	-2.136568	-1.162931	-1.125199
14	15	0	-2.362690	1.460311	-0.858759
15	8	0	-1.731269	0.465147	-1.825956
16	6	0	1.197362	0.047854	-0.565741
17	8	0	0.506913	0.293986	0.395642
18	8	0	0.793228	-0.068356	-1.803712
19	1	0	-0.194138	0.123800	-1.853928
20	6	0	2.670242	-0.221533	-0.411111

21	6	0	3.484477	0.582549	0.381611
22	6	0	3.221751	-1.369820	-0.969503
23	6	0	4.799116	0.262554	0.654591
24	6	0	4.543340	-1.714254	-0.725412
25	1	0	2.600208	-1.999602	-1.592823
26	6	0	5.305425	-0.893115	0.086934
27	1	0	5.413538	0.892765	1.282159
28	1	0	4.985772	-2.605257	-1.149207
29	7	0	2.984120	1.865412	0.912358
30	8	0	3.353011	2.186955	2.019266
31	8	0	2.274230	2.524170	0.181275
32	7	0	6.714098	-1.252371	0.355422
33	8	0	7.356756	-0.497705	1.053004
34	8	0	7.129206	-2.277584	-0.140760
35	6	0	-3.896157	2.135111	-1.530339
36	1	0	-3.679589	2.668464	-2.457197
37	1	0	-4.362314	2.815768	-0.814615
38	1	0	-4.580514	1.311413	-1.738565
39	6	0	-1.291144	2.861478	-0.476120
40	1	0	-0.977054	3.336553	-1.407469
41	1	0	-0.408639	2.506189	0.057706
42	1	0	-1.823364	3.590970	0.138067
43	6	0	-7.531404	-0.709375	1.711692
44	1	0	-7.831865	-1.491838	2.413792
45	1	0	-8.311491	-0.637753	0.947706
46	1	0	-7.510132	0.237283	2.255635
47	6	0	-6.192079	-1.017433	1.093939

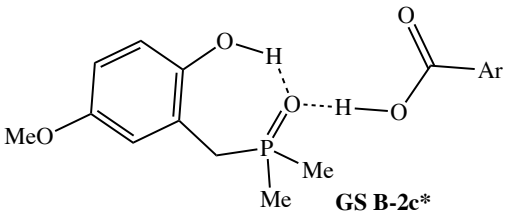


GS B-1c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.606811	-1.125077	-0.832151
2	6	0	4.290821	-0.776370	-1.121795
3	6	0	3.235505	-1.218715	-0.336047
4	6	0	3.502190	-2.002243	0.799104
5	6	0	4.814849	-2.359188	1.073418
6	6	0	5.866786	-1.935247	0.269035
7	1	0	4.107237	-0.150135	-1.987853
8	1	0	5.002151	-2.976582	1.943619
9	1	0	6.875000	-2.236465	0.521294
10	6	0	1.821964	-0.834477	-0.697164
11	1	0	1.128607	-1.671606	-0.567437
12	1	0	1.773220	-0.486570	-1.731192
13	8	0	2.520636	-2.462711	1.619070
14	1	0	1.890301	-1.747127	1.801368
15	15	0	1.233890	0.483397	0.412696
16	8	0	1.091071	-0.055131	1.829140
17	6	0	-0.301520	1.179099	-0.257745
18	6	0	-0.987692	0.584203	-1.315685
19	6	0	-0.837260	2.310008	0.365410
20	6	0	-2.196020	1.117447	-1.749215
21	1	0	-0.614771	-0.318872	-1.782670
22	6	0	-2.044095	2.837337	-0.068801
23	1	0	-0.309145	2.774196	1.191695
24	6	0	-2.722812	2.241430	-1.127739
25	1	0	-2.728842	0.631795	-2.557299

26	1	0	-2.456321	3.713362	0.418241
27	1	0	-3.667676	2.653321	-1.464137
28	6	0	2.470731	1.794266	0.335629
29	6	0	3.472268	1.814852	1.304743
30	6	0	2.508919	2.689042	-0.733217
31	6	0	4.508542	2.732665	1.203050
32	1	0	3.433264	1.109865	2.127118
33	6	0	3.548112	3.603818	-0.829810
34	1	0	1.725979	2.677936	-1.484737
35	6	0	4.547519	3.622914	0.136718
36	1	0	5.289357	2.748277	1.954153
37	1	0	3.578382	4.301879	-1.658126
38	1	0	5.360366	4.335777	0.057455
39	6	0	-1.820230	-1.160746	1.296859
40	8	0	-1.138444	-1.851383	0.579513
41	8	0	-1.403185	-0.556306	2.389222
42	1	0	-0.407358	-0.500319	2.354713
43	6	0	-3.238868	-0.812288	0.948291
44	6	0	-3.862965	-1.369130	-0.165061
45	6	0	-3.903438	0.200976	1.634298
46	6	0	-5.091301	-0.931816	-0.616982
47	6	0	-5.148365	0.648295	1.221698
48	1	0	-3.412860	0.651020	2.486125
49	6	0	-5.714920	0.075805	0.097448
50	1	0	-5.557765	-1.353983	-1.496513
51	1	0	-5.672096	1.437412	1.742804
52	7	0	-3.242405	-2.458479	-0.947368
53	8	0	-3.251606	-3.557588	-0.453389
54	8	0	-2.839325	-2.165199	-2.054321
55	7	0	-7.026594	0.567090	-0.376988
56	8	0	-7.502959	0.028662	-1.353209
57	8	0	-7.533928	1.479137	0.240058
58	6	0	7.895360	-0.970987	-1.430266
59	1	0	8.056563	-2.054453	-1.481905

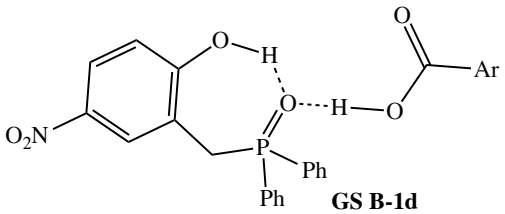
60	1	0	8.229352	-0.603549	-0.452300
61	1	0	8.478571	-0.486256	-2.211542
62	8	0	6.551213	-0.633903	-1.679454



GS B-2c*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.862603	0.036781	-0.958865
2	6	0	3.604600	-0.229906	-0.434217
3	6	0	3.400960	-1.419005	0.287664
4	6	0	4.452263	-2.315306	0.415976
5	6	0	5.703736	-2.053564	-0.130649
6	1	0	5.043275	0.947046	-1.520540
7	1	0	4.273326	-3.232431	0.964033
8	1	0	6.494420	-2.781477	-0.005574
9	6	0	2.472976	0.740779	-0.664012
10	1	0	1.557649	0.226313	-0.972793
11	1	0	2.736559	1.463417	-1.440583
12	8	0	2.197411	-1.752755	0.826031
13	1	0	1.814607	-0.977442	1.270997
14	15	0	2.009496	1.645552	0.843706
15	8	0	1.385876	0.699123	1.862979
16	6	0	-1.503141	0.116476	0.573374
17	8	0	-0.803879	0.336149	-0.387923
18	8	0	-1.119393	0.082304	1.822708
19	1	0	-0.140565	0.312604	1.879793

20	6	0	-2.961975	-0.216151	0.408192
21	6	0	-3.791889	0.518745	-0.433755
22	6	0	-3.479738	-1.357616	1.011125
23	6	0	-5.089002	0.137125	-0.711415
24	6	0	-4.783270	-1.762684	0.763255
25	1	0	-2.845908	-1.934018	1.672585
26	6	0	-5.561644	-1.009345	-0.097988
27	1	0	-5.715024	0.714459	-1.377152
28	1	0	-5.199735	-2.649191	1.221391
29	7	0	-3.329850	1.793277	-1.016606
30	8	0	-3.696496	2.051966	-2.140666
31	8	0	-2.651420	2.508274	-0.308920
32	7	0	-6.951310	-1.433890	-0.370020
33	8	0	-7.610090	-0.737820	-1.112084
34	8	0	-7.336207	-2.449730	0.168124
35	6	0	5.917876	-0.861147	-0.814727
36	6	0	3.515140	2.399217	1.493844
37	1	0	3.269455	2.986528	2.379942
38	1	0	3.978652	3.042515	0.742773
39	1	0	4.214673	1.607937	1.767065
40	6	0	0.912542	2.993268	0.355499
41	1	0	0.575167	3.521222	1.249480
42	1	0	0.045834	2.582983	-0.164556
43	1	0	1.437236	3.692638	-0.298880
44	6	0	8.184738	-1.375680	-1.282480
45	1	0	8.467061	-1.555044	-0.238152
46	1	0	9.014316	-0.895769	-1.798911
47	1	0	7.965923	-2.334662	-1.766947
48	8	0	7.096461	-0.486081	-1.380014

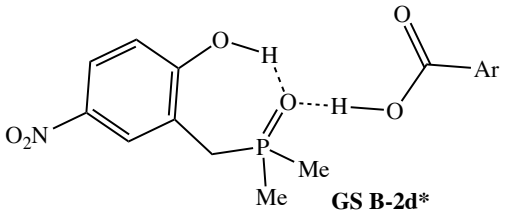


GS B-1d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.158681	-0.793004	-0.976279
2	6	0	3.081658	-1.219256	-0.212447
3	6	0	3.326336	-2.015422	0.923395
4	6	0	4.629599	-2.433800	1.209461
5	6	0	5.692655	-2.022737	0.431536
6	1	0	4.010068	-0.153066	-1.836623
7	1	0	4.780545	-3.066129	2.075040
8	1	0	6.707408	-2.322275	0.654571
9	6	0	1.682363	-0.811422	-0.600934
10	1	0	0.972953	-1.639005	-0.498755
11	1	0	1.666293	-0.459455	-1.634273
12	8	0	2.351788	-2.424850	1.749905
13	1	0	1.668861	-1.734796	1.839113
14	15	0	1.088312	0.508844	0.505572
15	8	0	0.920326	-0.060169	1.908027
16	6	0	-0.423620	1.223036	-0.189451
17	6	0	-1.103010	0.628787	-1.252475
18	6	0	-0.951036	2.366135	0.418460
19	6	0	-2.298262	1.174559	-1.705328
20	1	0	-0.736849	-0.282060	-1.709709
21	6	0	-2.146030	2.904411	-0.034473
22	1	0	-0.426666	2.831399	1.246535
23	6	0	-2.818776	2.308948	-1.097532
24	1	0	-2.825210	0.691296	-2.518675
25	1	0	-2.552831	3.789564	0.440205

26	1	0	-3.753809	2.730423	-1.448967
27	6	0	2.356063	1.787723	0.461414
28	6	0	3.310120	1.808892	1.477225
29	6	0	2.480448	2.635409	-0.639532
30	6	0	4.388602	2.678697	1.388593
31	1	0	3.201788	1.141644	2.324681
32	6	0	3.562554	3.499786	-0.723509
33	1	0	1.733964	2.623730	-1.427514
34	6	0	4.516877	3.517327	0.288083
35	1	0	5.133642	2.695381	2.175065
36	1	0	3.664321	4.157131	-1.578682
37	1	0	5.365470	4.187650	0.215943
38	6	0	-1.977147	-1.144844	1.319489
39	8	0	-1.267646	-1.833895	0.626835
40	8	0	-1.596256	-0.536492	2.423367
41	1	0	-0.601904	-0.484759	2.420933
42	6	0	-3.385683	-0.805916	0.928743
43	6	0	-3.971717	-1.363463	-0.204736
44	6	0	-4.079727	0.196630	1.601321
45	6	0	-5.192303	-0.937872	-0.687767
46	6	0	-5.317275	0.632864	1.156092
47	1	0	-3.618333	0.646698	2.469340
48	6	0	-5.846156	0.059307	0.014180
49	1	0	-5.631147	-1.360408	-1.581362
50	1	0	-5.863730	1.413363	1.666699
51	7	0	-3.313380	-2.437418	-0.977272
52	8	0	-3.334789	-3.543841	-0.500818
53	8	0	-2.865715	-2.123789	-2.061431
54	7	0	-7.150457	0.537704	-0.494208
55	8	0	-7.593553	-0.003700	-1.484096
56	8	0	-7.683653	1.442269	0.111440
57	6	0	5.444160	-1.185973	-0.647844
58	7	0	6.563042	-0.704583	-1.462111
59	8	0	7.681468	-1.070283	-1.157586

60	8	0	6.309259	0.037034	-2.392659



GS B-2d*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.672761	0.008041	-0.817724
2	6	0	-3.428576	0.257889	-0.255240
3	6	0	-3.239473	1.458668	0.461352
4	6	0	-4.276857	2.393586	0.535160
5	6	0	-5.504384	2.142049	-0.042841
6	1	0	-4.857523	-0.902644	-1.373455
7	1	0	-4.091238	3.312681	1.076132
8	1	0	-6.316612	2.853095	0.019301
9	6	0	-2.299615	-0.719607	-0.474320
10	1	0	-1.392028	-0.213539	-0.819923
11	1	0	-2.580211	-1.457170	-1.230242
12	8	0	-2.084395	1.780755	1.060434
13	1	0	-1.629479	0.985001	1.402057
14	15	0	-1.786644	-1.592340	1.036826
15	8	0	-1.151897	-0.601437	2.007031
16	6	0	1.705365	-0.048377	0.642878
17	8	0	0.948226	-0.205166	-0.286486
18	8	0	1.383230	-0.043844	1.911587
19	1	0	0.404079	-0.240850	2.005101
20	6	0	3.166112	0.230257	0.415717
21	6	0	3.921297	-0.509338	-0.490288

22	6	0	3.760663	1.328525	1.027471
23	6	0	5.217532	-0.171066	-0.822377
24	6	0	5.066206	1.688712	0.725529
25	1	0	3.186425	1.907818	1.738938
26	6	0	5.767638	0.934533	-0.198440
27	1	0	5.785337	-0.750421	-1.536961
28	1	0	5.541791	2.541662	1.189802
29	7	0	3.377062	-1.744510	-1.086139
30	8	0	3.675702	-1.983850	-2.233573
31	8	0	2.703255	-2.452034	-0.365293
32	7	0	7.158761	1.312064	-0.529119
33	8	0	7.748660	0.614480	-1.325324
34	8	0	7.611508	2.293455	0.019429
35	6	0	-5.693911	0.936397	-0.702831
36	7	0	-6.995311	0.638965	-1.307833
37	8	0	-7.862950	1.485201	-1.224462
38	8	0	-7.131628	-0.439347	-1.854934
39	6	0	-3.261835	-2.351764	1.744650
40	1	0	-2.982677	-2.922361	2.631769
41	1	0	-3.740741	-3.013199	1.019406
42	1	0	-3.962446	-1.565987	2.030999
43	6	0	-0.679779	-2.926492	0.542340
44	1	0	-0.292369	-3.418587	1.436508
45	1	0	0.155193	-2.515634	-0.027019
46	1	0	-1.214842	-3.658172	-0.066650

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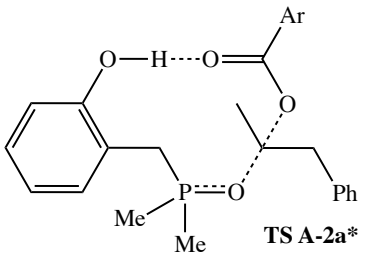
3. TS A Structures for analogs (needed to calculate values for Table 2)

For **1a** (see section 1, above)

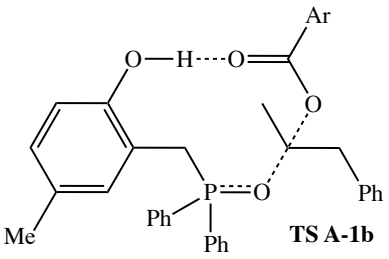


TS A-2a*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.074748	3.336268	0.540027
2	6	0	0.936281	3.390503	0.152986
3	6	0	3.525130	3.463123	-0.854880
4	6	0	1.271189	4.288927	-0.850569
5	6	0	1.905319	2.525719	0.652882
6	6	0	3.208170	2.545208	0.139382
7	1	0	0.507707	4.949171	-1.245092
8	1	0	4.535797	3.485603	-1.252434
9	6	0	4.183791	1.507116	0.623825
10	1	0	4.197949	1.449435	1.715264
11	1	0	5.194773	1.741209	0.280463
12	15	0	3.774648	-0.200997	0.057130
13	1	0	3.194943	-3.999436	-0.206983
14	6	0	2.359832	-3.642943	-0.801225
15	6	0	0.238693	-2.699377	-2.317816
16	6	0	1.282544	-3.030400	-0.164916
17	6	0	2.378611	-3.785719	-2.184022
18	6	0	1.318040	-3.309620	-2.946956
19	6	0	0.217784	-2.566723	-0.935625
20	1	0	3.221879	-4.268181	-2.666087
21	1	0	1.332220	-3.415175	-4.025777
22	1	0	-0.590178	-2.320589	-2.904597
23	6	0	1.313137	-1.427994	1.789455
24	1	0	-0.617634	-2.081151	-0.445590

25	6	0	1.569834	-1.131248	3.221966
26	1	0	1.480853	-0.068301	3.427870
27	1	0	2.579813	-1.466126	3.463538
28	1	0	0.858426	-1.690478	3.831674
29	6	0	1.280587	-2.848704	1.330536
30	1	0	0.376377	-3.282557	1.767722
31	1	0	2.133899	-3.357931	1.784118
32	1	0	1.123667	-0.629738	1.098308
33	8	0	3.308925	-1.132658	1.167867
34	8	0	1.659870	1.611792	1.610045
35	6	0	-2.997763	0.590514	-0.125161
36	6	0	-5.047044	-0.795094	1.086942
37	6	0	-4.265956	0.691963	-0.661463
38	6	0	-2.716319	-0.159654	1.012907
39	6	0	-3.761615	-0.862703	1.602552
40	6	0	-5.276981	-0.015290	-0.035170
41	1	0	-4.465135	1.292832	-1.537778
42	1	0	-3.554167	-1.462849	2.479414
43	1	0	-5.870190	-1.331512	1.538733
44	7	0	-6.641316	0.062088	-0.591736
45	8	0	-6.799287	0.730237	-1.591855
46	8	0	-7.515115	-0.548346	-0.012615
47	7	0	-1.908111	1.273168	-0.846466
48	8	0	-0.880902	0.645832	-1.013740
49	8	0	-2.124982	2.390466	-1.258705
50	6	0	-1.333424	-0.150301	1.641982
51	8	0	-0.844930	-1.278913	1.889450
52	8	0	-0.848900	0.973803	1.841203
53	1	0	0.693376	1.478883	1.767286
54	6	0	5.299879	-0.854753	-0.669713
55	1	0	5.097099	-1.853035	-1.061440
56	1	0	6.069987	-0.922965	0.100579
57	1	0	5.649115	-0.209845	-1.478975
58	6	0	2.627327	-0.040976	-1.328465

59	1	0	2.508559	-1.013672	-1.807219
60	1	0	3.025913	0.680699	-2.044863
61	1	0	1.651316	0.318657	-0.999677
62	6	0	2.566344	4.339060	-1.351533
63	1	0	2.826909	5.047445	-2.128637

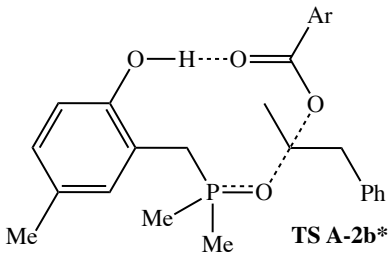


TS A-1b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.496466	3.560873	-0.377581
2	6	0	-0.582465	3.575430	-0.485600
3	6	0	-3.342752	3.562493	-0.717022
4	6	0	-1.337300	4.624627	0.020335
5	6	0	-1.218638	2.514477	-1.118216
6	6	0	-2.613338	2.490243	-1.213947
7	6	0	-2.725261	4.647652	-0.098758
8	1	0	-0.830856	5.443880	0.520912
9	1	0	-4.427439	3.538765	-0.789927
10	6	0	-3.273399	1.252336	-1.757177
11	1	0	-2.902595	1.002810	-2.755565
12	1	0	-4.353707	1.397463	-1.816502
13	15	0	-2.937622	-0.273939	-0.755134
14	6	0	-2.293117	0.297159	0.838116
15	6	0	-1.292011	1.448085	3.164581
16	6	0	-3.091934	1.156255	1.599155

17	6	0	-1.000739	0.008311	1.262400
18	6	0	-0.498896	0.585546	2.422292
19	6	0	-2.593562	1.726762	2.758225
20	1	0	-4.101371	1.392825	1.279431
21	1	0	-0.368100	-0.664975	0.704533
22	1	0	0.520822	0.369442	2.716502
23	1	0	-3.214857	2.400444	3.336554
24	1	0	-0.895567	1.909321	4.062021
25	6	0	-4.548913	-1.029184	-0.380723
26	6	0	-6.924646	-2.396970	0.117840
27	6	0	-4.745957	-1.672793	0.841854
28	6	0	-5.544909	-1.089235	-1.356380
29	6	0	-6.729823	-1.767565	-1.106048
30	6	0	-5.931898	-2.351660	1.088937
31	1	0	-3.971344	-1.639948	1.599961
32	1	0	-5.398122	-0.614618	-2.321010
33	1	0	-7.500290	-1.806805	-1.867227
34	1	0	-6.080498	-2.845101	2.042427
35	1	0	-7.850744	-2.925353	0.313365
36	1	0	-2.235023	-3.632243	-0.087887
37	6	0	-1.366152	-3.487340	0.544511
38	6	0	0.845562	-3.045787	2.161606
39	6	0	-0.144713	-3.155216	-0.039163
40	6	0	-1.481576	-3.594486	1.923873
41	6	0	-0.376955	-3.366892	2.736911
42	6	0	0.962340	-2.947661	0.780372
43	1	0	-2.438954	-3.849963	2.365435
44	1	0	-0.470018	-3.436394	3.814733
45	1	0	1.710510	-2.853159	2.784914
46	6	0	-0.086671	-1.511999	-1.946001
47	1	0	1.911114	-2.671895	0.334954
48	6	0	-0.199002	-1.166832	-3.386388
49	1	0	0.664733	-1.577151	-3.912340
50	1	0	-0.240151	-0.088452	-3.521318

51	1	0	-1.102856	-1.627705	-3.788349
52	6	0	-0.040730	-2.946021	-1.528159
53	1	0	0.904373	-3.339901	-1.913273
54	1	0	-0.844969	-3.465323	-2.054959
55	1	0	0.018935	-0.731914	-1.221972
56	8	0	-2.105654	-1.300656	-1.506290
57	8	0	-0.572760	1.451751	-1.633981
58	6	0	4.399684	0.264124	0.403022
59	6	0	6.255964	-0.447686	-1.505855
60	6	0	5.738682	0.428963	0.694400
61	6	0	3.946855	-0.218137	-0.821416
62	6	0	4.900492	-0.584081	-1.765608
63	6	0	6.650690	0.062942	-0.280583
64	1	0	6.069616	0.819184	1.646799
65	1	0	4.558347	-0.974342	-2.715581
66	1	0	7.006096	-0.723392	-2.234247
67	7	0	8.089764	0.218235	0.006149
68	8	0	8.398684	0.645694	1.098688
69	8	0	8.869689	-0.091878	-0.869767
70	7	0	3.445468	0.552517	1.488161
71	8	0	2.644424	-0.321617	1.751676
72	8	0	3.562002	1.603623	2.075243
73	6	0	2.471336	-0.240175	-1.190790
74	8	0	2.089919	-1.238212	-1.846082
75	8	0	1.818114	0.753264	-0.826924
76	1	0	0.355530	1.344935	-1.313659
77	6	0	-3.532227	5.812101	0.414871
78	1	0	-4.546207	5.505960	0.683671
79	1	0	-3.615753	6.599556	-0.341149
80	1	0	-3.068890	6.254528	1.299880

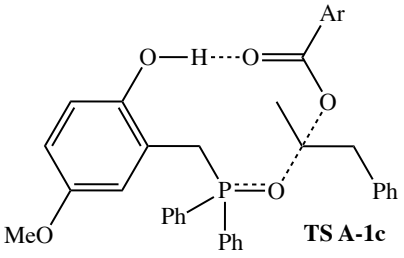


TS A-2b*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.032982	3.062440	-1.006423
2	6	0	-1.056622	3.090278	-0.650744
3	6	0	-3.656296	3.106338	0.302817
4	6	0	-1.471173	4.064209	0.245316
5	6	0	-1.953853	2.115111	-1.073598
6	6	0	-3.262669	2.108795	-0.582172
7	1	0	-0.754253	4.806354	0.581011
8	1	0	-4.675742	3.099696	0.681794
9	6	0	-4.160377	0.958284	-0.949117
10	1	0	-4.141352	0.762116	-2.024136
11	1	0	-5.192743	1.166960	-0.656718
12	15	0	-3.657987	-0.631689	-0.158524
13	1	0	-2.825925	-4.314299	0.612661
14	6	0	-2.035540	-3.824784	1.172394
15	6	0	-0.031231	-2.542579	2.596306
16	6	0	-0.984701	-3.222857	0.483900
17	6	0	-2.085812	-3.789431	2.561297
18	6	0	-1.084040	-3.143455	3.277323
19	6	0	0.021896	-2.587829	1.209346
20	1	0	-2.907750	-4.265698	3.084619
21	1	0	-1.123115	-3.109997	4.360179
22	1	0	0.751483	-2.032154	3.145546
23	6	0	-1.066525	-1.892269	-1.664018
24	1	0	0.835821	-2.109804	0.677555

25	6	0	-1.300732	-1.803691	-3.128114
26	1	0	-1.279230	-0.772998	-3.470571
27	1	0	-2.277763	-2.239018	-3.343651
28	1	0	-0.534883	-2.384935	-3.644063
29	6	0	-0.951305	-3.235752	-1.022041
30	1	0	-0.007464	-3.657188	-1.380417
31	1	0	-1.754707	-3.858436	-1.422025
32	1	0	-0.950820	-0.999325	-1.080559
33	8	0	-3.094222	-1.661942	-1.127850
34	8	0	-1.626772	1.118652	-1.920241
35	6	0	3.044977	0.658380	0.047231
36	6	0	5.216636	-0.719501	-0.939902
37	6	0	4.289139	0.921895	0.584606
38	6	0	2.845719	-0.252420	-0.986150
39	6	0	3.952381	-0.948013	-1.461522
40	6	0	5.362977	0.215263	0.072493
41	1	0	4.423650	1.645129	1.376744
42	1	0	3.809678	-1.671100	-2.254547
43	1	0	6.086492	-1.248599	-1.304312
44	7	0	6.704285	0.465494	0.633964
45	8	0	6.789903	1.269104	1.538713
46	8	0	7.633290	-0.149460	0.153998
47	7	0	1.891875	1.346933	0.655456
48	8	0	0.907198	0.673343	0.885699
49	8	0	2.019270	2.520909	0.922526
50	6	0	1.482508	-0.424554	-1.634559
51	8	0	1.079183	-1.607845	-1.739358
52	8	0	0.928254	0.626318	-1.989302
53	1	0	-0.649892	1.028664	-2.031278
54	6	0	-5.158797	-1.293663	0.610709
55	1	0	-4.903281	-2.217904	1.131857
56	1	0	-5.898008	-1.511832	-0.161980
57	1	0	-5.575252	-0.577409	1.322283
58	6	0	-2.568814	-0.215116	1.220540

59	1	0	-2.403684	-1.105881	1.827582
60	1	0	-3.035260	0.566608	1.824058
61	1	0	-1.608255	0.164254	0.868804
62	6	0	-3.229856	5.191193	1.665620
63	1	0	-4.092806	4.876244	2.257232
64	1	0	-3.519265	6.091195	1.113572
65	1	0	-2.432373	5.472753	2.357365
66	6	0	-2.778298	4.101150	0.728085

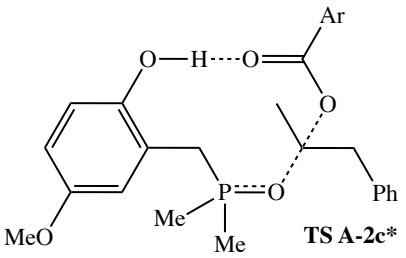


TS A-1c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.477587	2.242162	-2.220253
2	6	0	0.465964	2.454278	-1.895864
3	6	0	-2.116125	2.954845	-1.031645
4	6	0	0.206284	3.552610	-1.101538
5	6	0	-0.557810	1.568022	-2.243797
6	6	0	-1.852791	1.817310	-1.799881
7	6	0	-1.092051	3.813886	-0.662452
8	1	0	1.007531	4.210868	-0.790411
9	1	0	-3.127154	3.113633	-0.676013
10	6	0	-2.935355	0.797039	-2.015049
11	1	0	-2.784439	0.229937	-2.936179
12	1	0	-3.915401	1.276909	-2.068581
13	15	0	-3.009975	-0.468373	-0.679506

14	6	0	-2.542839	0.358043	0.864097
15	6	0	-1.741047	1.752886	3.136241
16	6	0	-3.472166	0.679304	1.851721
17	6	0	-1.203714	0.718899	1.036427
18	6	0	-0.807032	1.417976	2.162518
19	6	0	-3.068783	1.375232	2.985997
20	1	0	-4.509509	0.384224	1.748961
21	1	0	-0.455800	0.484304	0.290348
22	1	0	0.233838	1.698244	2.262239
23	1	0	-3.795810	1.619432	3.752201
24	1	0	-1.430758	2.302897	4.017647
25	6	0	-4.751295	-0.961107	-0.537859
26	6	0	-7.388411	-1.815001	-0.288509
27	6	0	-5.040620	-2.321066	-0.446615
28	6	0	-5.790950	-0.029561	-0.507958
29	6	0	-7.105223	-0.456556	-0.381706
30	6	0	-6.357618	-2.745349	-0.321962
31	1	0	-4.226495	-3.035327	-0.486241
32	1	0	-5.581154	1.033152	-0.572351
33	1	0	-7.908869	0.270078	-0.358771
34	1	0	-6.578504	-3.804183	-0.254312
35	1	0	-8.415739	-2.147283	-0.192931
36	1	0	-2.272916	-2.973534	1.686370
37	6	0	-1.347690	-2.569159	2.084154
38	6	0	1.005318	-1.499118	3.081083
39	6	0	-0.195234	-2.606099	1.303313
40	6	0	-1.327565	-2.004398	3.352527
41	6	0	-0.148801	-1.468457	3.854351
42	6	0	0.983555	-2.065912	1.814092
43	1	0	-2.235852	-1.971960	3.943416
44	1	0	-0.131971	-1.020927	4.841731
45	1	0	1.927803	-1.077033	3.463798
46	6	0	-0.202056	-2.253522	-1.211008
47	1	0	1.878068	-2.084109	1.203173

48	6	0	-0.397720	-2.745752	-2.599608
49	1	0	-0.540638	-1.914536	-3.285363
50	1	0	-1.264976	-3.406646	-2.629424
51	1	0	0.488498	-3.313110	-2.886351
52	6	0	-0.223945	-3.220161	-0.073123
53	1	0	0.644355	-3.868603	-0.221201
54	1	0	-1.111789	-3.843817	-0.199584
55	1	0	0.012475	-1.214397	-1.039923
56	8	0	-2.189096	-1.712842	-0.970599
57	8	0	-0.329664	0.449049	-2.973576
58	6	0	4.181090	0.280331	-0.205968
59	6	0	6.209354	-1.535878	-0.627682
60	6	0	5.442756	0.581110	0.268894
61	6	0	3.896213	-0.887103	-0.908285
62	6	0	4.931976	-1.796889	-1.098565
63	6	0	6.443406	-0.347512	0.045756
64	1	0	5.643699	1.501154	0.799674
65	1	0	4.723044	-2.717054	-1.629437
66	1	0	7.023070	-2.232759	-0.774733
67	7	0	7.798455	-0.060542	0.552883
68	8	0	7.958616	0.975248	1.163891
69	8	0	8.663999	-0.879931	0.326261
70	7	0	3.103420	1.231162	0.120678
71	8	0	2.043891	0.759075	0.480056
72	8	0	3.360296	2.413400	0.056086
73	6	0	2.532904	-1.140300	-1.532473
74	8	0	2.000906	-2.237040	-1.242586
75	8	0	2.113439	-0.238174	-2.271715
76	1	0	0.607835	0.172076	-2.856960
77	6	0	-2.483403	5.042294	0.805339
78	1	0	-3.306318	5.238284	0.106207
79	1	0	-2.374380	5.899717	1.467971
80	1	0	-2.717022	4.149572	1.399800
81	8	0	-1.252045	4.903576	0.137604

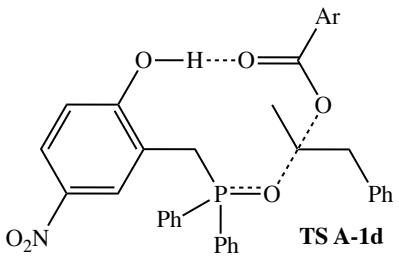


TS A-2c*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.140535	2.781651	-1.350636
2	6	0	-1.162530	2.770291	-0.989916
3	6	0	-3.757354	2.698234	-0.023936
4	6	0	-1.621262	3.793333	-0.164427
5	6	0	-1.993553	1.715177	-1.331958
6	6	0	-3.300940	1.668738	-0.830947
7	6	0	-2.927027	3.767911	0.312819
8	1	0	-0.939660	4.590435	0.099842
9	1	0	-4.766308	2.686586	0.374828
10	6	0	-4.128988	0.442110	-1.101540
11	1	0	-4.086003	0.155883	-2.155176
12	1	0	-5.174054	0.615204	-0.832925
13	15	0	-3.540275	-1.038928	-0.171065
14	1	0	-2.483270	-4.568671	0.934197
15	6	0	-1.730108	-3.982564	1.450757
16	6	0	0.177366	-2.455503	2.761609
17	6	0	-0.712105	-3.379980	0.715069
18	6	0	-1.795647	-3.826413	2.830665
19	6	0	-0.842653	-3.057673	3.489704
20	6	0	0.246297	-2.621116	1.384564
21	1	0	-2.591557	-4.304284	3.391397
22	1	0	-0.894121	-2.930003	4.564998
23	1	0	0.921865	-1.850358	3.265967
24	6	0	-0.856112	-2.257652	-1.547025

25	1	0	1.034408	-2.143254	0.815172
26	6	0	-1.081422	-2.320786	-3.013814
27	1	0	-1.132273	-1.327169	-3.449856
28	1	0	-2.021858	-2.844763	-3.191661
29	1	0	-0.270059	-2.889168	-3.471221
30	6	0	-0.662975	-3.526596	-0.783308
31	1	0	0.308922	-3.918340	-1.097667
32	1	0	-1.421648	-4.232811	-1.128004
33	1	0	-0.804885	-1.308086	-1.049719
34	8	0	-2.901510	-2.111366	-1.042887
35	8	0	-1.608966	0.676727	-2.107110
36	6	0	3.056497	0.693564	-0.032574
37	6	0	5.323757	-0.636534	-0.857706
38	6	0	4.272782	1.079646	0.494470
39	6	0	2.930568	-0.319126	-0.979152
40	6	0	4.085106	-0.987652	-1.372595
41	6	0	5.395769	0.394582	0.065107
42	1	0	4.350021	1.879289	1.217809
43	1	0	3.999738	-1.788085	-2.096557
44	1	0	6.229905	-1.143711	-1.159474
45	7	0	6.709033	0.775798	0.619094
46	8	0	6.730005	1.663561	1.445690
47	8	0	7.681496	0.175887	0.211761
48	7	0	1.854393	1.364893	0.494943
49	8	0	0.910511	0.657145	0.783939
50	8	0	1.905779	2.565518	0.645252
51	6	0	1.592748	-0.633506	-1.627481
52	8	0	1.267584	-1.845348	-1.635266
53	8	0	0.978717	0.344796	-2.077365
54	1	0	-0.627794	0.630562	-2.194386
55	6	0	-5.007777	-1.722991	0.641252
56	1	0	-4.703014	-2.580799	1.243267
57	1	0	-5.721948	-2.052995	-0.115125
58	1	0	-5.476415	-0.974737	1.284088

59	6	0	-2.496260	-0.435382	1.173085
60	1	0	-2.276799	-1.258729	1.853545
61	1	0	-3.021231	0.359757	1.706991
62	1	0	-1.560703	-0.021149	0.794090
63	6	0	-2.671504	5.804910	1.497504
64	1	0	-1.795438	5.475574	2.068947
65	1	0	-3.292950	6.438271	2.128570
66	1	0	-2.336698	6.382090	0.627294
67	8	0	-3.481309	4.716926	1.116957

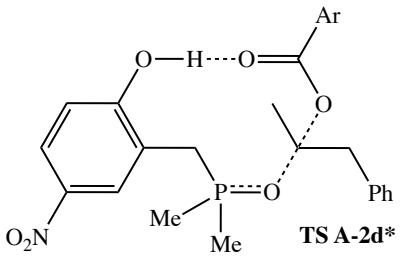


TS A-1d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.427263	2.205597	-2.055101
2	6	0	0.400002	2.406482	-1.778705
3	6	0	-2.244646	2.853877	-1.046418
4	6	0	0.080219	3.523909	-1.032804
5	6	0	-0.594574	1.493404	-2.143315
6	6	0	-1.928891	1.712978	-1.764542
7	6	0	-1.245338	3.742492	-0.685041
8	1	0	0.844837	4.217187	-0.711414
9	1	0	-3.257570	3.042344	-0.713880
10	6	0	-2.959912	0.645418	-1.997267
11	1	0	-2.776961	0.093971	-2.921864
12	1	0	-3.957546	1.085122	-2.055954

13	15	0	-2.993834	-0.634503	-0.665782
14	6	0	-2.512112	0.207351	0.862000
15	6	0	-1.697806	1.687167	3.074753
16	6	0	-3.439301	0.582149	1.832680
17	6	0	-1.168218	0.554751	1.025050
18	6	0	-0.764849	1.296498	2.120883
19	6	0	-3.028908	1.319549	2.937228
20	1	0	-4.481079	0.301057	1.738012
21	1	0	-0.419457	0.268571	0.298504
22	1	0	0.279579	1.565683	2.213837
23	1	0	-3.755467	1.612828	3.685826
24	1	0	-1.384662	2.277205	3.928375
25	6	0	-4.724987	-1.150749	-0.505437
26	6	0	-7.343776	-2.046469	-0.221059
27	6	0	-4.990637	-2.515320	-0.408146
28	6	0	-5.778819	-0.235400	-0.464080
29	6	0	-7.084082	-0.683832	-0.320251
30	6	0	-6.298800	-2.960383	-0.266012
31	1	0	-4.166290	-3.217105	-0.456854
32	1	0	-5.588823	0.830834	-0.531453
33	1	0	-7.898579	0.030052	-0.287430
34	1	0	-6.501718	-4.022430	-0.193451
35	1	0	-8.364245	-2.394964	-0.111346
36	1	0	-2.209016	-3.163086	1.645266
37	6	0	-1.295095	-2.735978	2.045284
38	6	0	1.028499	-1.608638	3.049074
39	6	0	-0.138886	-2.747688	1.269548
40	6	0	-1.293683	-2.165764	3.311449
41	6	0	-0.130059	-1.600576	3.816323
42	6	0	1.025292	-2.179806	1.783863
43	1	0	-2.205004	-2.151957	3.898230
44	1	0	-0.128442	-1.148001	4.801374
45	1	0	1.939105	-1.163948	3.434332
46	6	0	-0.154565	-2.379066	-1.238116

47	1	0	1.923991	-2.178524	1.178520
48	6	0	-0.342435	-2.860538	-2.630544
49	1	0	0.512830	-3.483375	-2.895944
50	1	0	-0.421672	-2.027718	-3.324528
51	1	0	-1.247422	-3.467708	-2.677416
52	6	0	-0.149390	-3.355324	-0.109986
53	1	0	0.738427	-3.976065	-0.263314
54	1	0	-1.017261	-4.005603	-0.242760
55	1	0	0.033228	-1.338392	-1.053238
56	8	0	-2.155883	-1.860393	-0.984067
57	8	0	-0.323326	0.368956	-2.815240
58	6	0	4.213949	0.231119	-0.218008
59	6	0	6.234850	-1.594025	-0.632169
60	6	0	5.475482	0.529496	0.257205
61	6	0	3.926022	-0.936821	-0.918218
62	6	0	4.956927	-1.851654	-1.104992
63	6	0	6.472176	-0.404860	0.037722
64	1	0	5.680739	1.449694	0.786409
65	1	0	4.744396	-2.771669	-1.634600
66	1	0	7.046301	-2.294203	-0.775965
67	7	0	7.828729	-0.121525	0.545613
68	8	0	7.991381	0.915889	1.152511
69	8	0	8.690234	-0.945668	0.322702
70	7	0	3.136346	1.183201	0.102636
71	8	0	2.093824	0.713812	0.513141
72	8	0	3.374114	2.364213	-0.022481
73	6	0	2.561129	-1.181383	-1.538948
74	8	0	2.047303	-2.297618	-1.304168
75	8	0	2.116814	-0.243885	-2.224123
76	1	0	0.637789	0.131931	-2.727349
77	7	0	-1.597469	4.908319	0.126756
78	8	0	-0.697973	5.644511	0.481904
79	8	0	-2.771696	5.073444	0.403928



TS A-2d*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.146170	2.611171	-1.473189
2	6	0	-1.167804	2.555656	-1.117965
3	6	0	-3.784847	2.340076	-0.181838
4	6	0	-1.704230	3.572345	-0.350047
5	6	0	-1.935821	1.429622	-1.418014
6	6	0	-3.251819	1.311093	-0.936309
7	6	0	-3.011099	3.458469	0.100493
8	1	0	-1.121654	4.445687	-0.092360
9	1	0	-4.793769	2.287809	0.207800
10	6	0	-3.999055	0.029250	-1.182259
11	1	0	-3.926260	-0.279856	-2.227850
12	1	0	-5.056079	0.152493	-0.934528
13	15	0	-3.349364	-1.398685	-0.206287
14	1	0	-2.038794	-4.828606	0.996481
15	6	0	-1.344770	-4.169361	1.507723
16	6	0	0.412510	-2.460812	2.805420
17	6	0	-0.365211	-3.506329	0.771968
18	6	0	-1.446318	-3.983077	2.881762
19	6	0	-0.568991	-3.123619	3.533852
20	6	0	0.518333	-2.656119	1.434552
21	1	0	-2.210513	-4.508956	3.443455
22	1	0	-0.648641	-2.973042	4.604363
23	1	0	1.098232	-1.786353	3.305068
24	6	0	-0.555144	-2.458589	-1.520502

25	1	0	1.276653	-2.132342	0.864820
26	6	0	-0.753714	-2.576361	-2.987083
27	1	0	-0.842437	-1.601723	-3.458281
28	1	0	-1.665730	-3.149673	-3.160991
29	1	0	0.089540	-3.120907	-3.414864
30	6	0	-0.277575	-3.687437	-0.720821
31	1	0	0.728391	-4.007040	-1.009695
32	1	0	-0.969405	-4.461756	-1.060332
33	1	0	-0.577678	-1.498537	-1.042589
34	8	0	-2.614963	-2.434420	-1.044296
35	8	0	-1.477326	0.402646	-2.135409
36	6	0	3.070135	0.830364	-0.031038
37	6	0	5.464134	-0.296020	-0.796668
38	6	0	4.235152	1.329416	0.517000
39	6	0	3.055956	-0.197551	-0.969570
40	6	0	4.273593	-0.762458	-1.333359
41	6	0	5.423518	0.744737	0.117084
42	1	0	4.224699	2.138931	1.233562
43	1	0	4.277596	-1.572798	-2.051276
44	1	0	6.418647	-0.721425	-1.074928
45	7	0	6.685995	1.247099	0.694111
46	8	0	6.608673	2.138623	1.512601
47	8	0	7.715942	0.733867	0.311135
48	7	0	1.800985	1.397116	0.458726
49	8	0	0.904512	0.613076	0.704817
50	8	0	1.747586	2.595728	0.617796
51	6	0	1.765284	-0.640923	-1.634695
52	8	0	1.533895	-1.871499	-1.604027
53	8	0	1.086102	0.271331	-2.136473
54	1	0	-0.486962	0.417431	-2.239156
55	6	0	-4.797439	-2.160688	0.566822
56	1	0	-4.459732	-2.991062	1.189359
57	1	0	-5.464408	-2.543869	-0.207324
58	1	0	-5.332600	-1.436640	1.184836

59	6	0	-2.389036	-0.705277	1.156484
60	1	0	-2.129254	-1.503740	1.852542
61	1	0	-2.984195	0.052816	1.670578
62	1	0	-1.472858	-0.231826	0.799590
63	7	0	-3.590242	4.530748	0.912677
64	8	0	-2.903730	5.508092	1.135077
65	8	0	-4.727915	4.380172	1.320359

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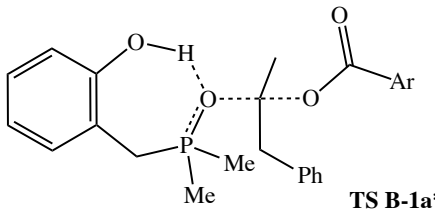
4. TS B Structures for analogs (needed to calculate values for Table 2)

For **1a** (see section 1, above)

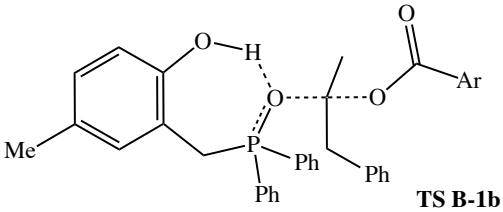


TS B-1a*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-1.985557	-1.690194	1.101384
2	8	0	-2.236112	-0.179481	0.969738
3	6	0	-3.612903	-2.488315	1.260402
4	6	0	-4.495241	-2.245356	0.059578
5	6	0	-4.745062	-3.269695	-0.852183
6	6	0	-5.604630	-3.087553	-1.925530
7	6	0	-6.235491	-1.859987	-2.090578
8	6	0	-5.987604	-0.822886	-1.204977
9	6	0	-5.109123	-0.997689	-0.138952
10	8	0	-4.908541	0.044937	0.705727
11	1	0	-3.958605	0.087806	0.929501

12	1	0	-6.456629	0.146281	-1.324121
13	1	0	-6.917307	-1.705177	-2.918943
14	1	0	-5.789286	-3.899381	-2.618398
15	1	0	-4.269788	-4.234492	-0.702433
16	1	0	-4.069028	-2.076168	2.167076
17	1	0	-3.461535	-3.559117	1.419860
18	6	0	-0.613573	1.146352	0.728256
19	6	0	-0.520159	1.054459	-0.745704
20	1	0	-1.523894	1.083655	-1.174629
21	1	0	0.019008	0.164624	-1.063285
22	1	0	0.010113	1.940013	-1.103161
23	1	0	-0.115233	0.427519	1.353075
24	6	0	-1.199407	2.339357	1.402534
25	6	0	-1.865550	3.339718	0.493251
26	1	0	-1.881909	1.974660	2.173445
27	1	0	-0.352291	2.792495	1.926561
28	6	0	-1.138918	4.416599	-0.010987
29	6	0	-1.729974	5.323123	-0.882152
30	6	0	-3.057352	5.160897	-1.259389
31	6	0	-3.788286	4.088556	-0.762143
32	6	0	-3.196191	3.182509	0.108739
33	1	0	-0.099496	4.538208	0.277781
34	1	0	-1.153205	6.157262	-1.265395
35	1	0	-3.520861	5.868275	-1.937583
36	1	0	-4.824590	3.955108	-1.051272
37	1	0	-3.776082	2.345295	0.481715
38	8	0	1.633106	1.633961	0.849281
39	6	0	2.134915	0.492013	0.977407
40	8	0	1.633119	-0.517533	1.500953
41	6	0	3.543731	0.316875	0.424328
42	6	0	3.938921	-0.852087	-0.218885
43	6	0	5.239710	-1.090613	-0.614187
44	6	0	6.167642	-0.091976	-0.372992
45	6	0	5.824545	1.101853	0.240871

46	6	0	4.509110	1.296015	0.634356
47	7	0	2.940872	-1.879658	-0.563030
48	8	0	3.188482	-3.025747	-0.268090
49	8	0	1.955806	-1.506881	-1.171907
50	1	0	5.529194	-2.012075	-1.099936
51	7	0	7.564335	-0.312107	-0.792279
52	8	0	7.823294	-1.360091	-1.346649
53	8	0	8.364114	0.569058	-0.555699
54	1	0	6.585119	1.853062	0.404019
55	1	0	4.206865	2.216368	1.117786
56	6	0	-1.160485	-2.410604	-0.325149
57	1	0	-0.125506	-2.064296	-0.380052
58	1	0	-1.697276	-2.127521	-1.231855
59	1	0	-1.158734	-3.499472	-0.234502
60	6	0	-0.997993	-2.105691	2.548121
61	1	0	-0.007004	-1.652543	2.434370
62	1	0	-0.890395	-3.189479	2.631426
63	1	0	-1.484655	-1.716688	3.444293



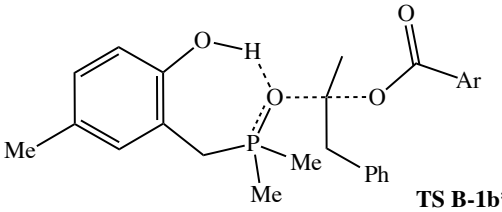
TS B-1b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	1.899097	-0.422257	0.768217
2	8	0	1.754586	0.967366	0.126643
3	6	0	1.286455	-1.703038	-0.380511
4	6	0	2.241667	-2.009082	-1.509840

5	6	0	2.817555	-3.277687	-1.587352
6	6	0	3.663796	-3.656387	-2.621314
7	6	0	3.928855	-2.715544	-3.615988
8	6	0	3.388263	-1.443492	-3.555873
9	6	0	2.556878	-1.073433	-2.502388
10	8	0	2.066172	0.195010	-2.512793
11	1	0	1.933817	0.519854	-1.606043
12	1	0	3.601795	-0.704894	-4.319191
13	1	0	4.576125	-2.979519	-4.446408
14	1	0	2.577716	-4.001305	-0.812830
15	1	0	0.309801	-1.349678	-0.738320
16	1	0	1.097588	-2.607513	0.201958
17	6	0	3.653552	-0.730300	1.042841
18	6	0	4.572029	0.249364	0.675563
19	6	0	5.931861	0.004038	0.825067
20	6	0	6.367934	-1.212847	1.331767
21	6	0	5.448532	-2.191988	1.696971
22	6	0	4.090937	-1.953064	1.553617
23	1	0	4.214075	1.193186	0.278847
24	1	0	6.650032	0.764372	0.541767
25	1	0	7.429359	-1.402731	1.443180
26	1	0	5.791735	-3.141019	2.091411
27	1	0	3.374255	-2.715102	1.842418
28	6	0	1.037136	-0.636089	2.335156
29	6	0	1.714592	-0.417020	3.537489
30	6	0	1.042423	-0.559862	4.742382
31	6	0	-0.300210	-0.921497	4.749425
32	6	0	-0.979117	-1.131102	3.555373
33	6	0	-0.316740	-0.985297	2.343234
34	1	0	2.763568	-0.142697	3.531997
35	1	0	1.567321	-0.390540	5.675265
36	1	0	-0.823229	-1.035295	5.692184
37	1	0	-2.031593	-1.384307	3.554686
38	1	0	-0.869367	-1.110291	1.415334

39	6	0	-0.076882	1.832710	-0.283098
40	6	0	-0.376312	2.367211	1.067698
41	1	0	0.518612	2.828775	1.488385
42	1	0	-0.756407	1.592470	1.730046
43	1	0	-1.141487	3.138937	0.959255
44	1	0	-0.366995	0.829398	-0.529606
45	6	0	0.357111	2.744416	-1.389074
46	6	0	1.444586	3.731288	-1.032258
47	1	0	0.634062	2.152617	-2.261617
48	1	0	-0.563191	3.275069	-1.653353
49	6	0	1.148910	4.921666	-0.371476
50	6	0	2.157964	5.814361	-0.030107
51	6	0	3.477618	5.531118	-0.357424
52	6	0	3.779860	4.354602	-1.033480
53	6	0	2.770448	3.461712	-1.367924
54	1	0	0.118324	5.156026	-0.124842
55	1	0	1.910404	6.736014	0.484340
56	1	0	4.265461	6.228649	-0.096690
57	1	0	4.805650	4.133448	-1.307450
58	1	0	3.009239	2.546904	-1.899293
59	8	0	-2.292865	1.745343	-0.875254
60	6	0	-2.643625	0.567686	-0.639399
61	8	0	-1.930820	-0.426891	-0.413346
62	6	0	-4.143443	0.299487	-0.681232
63	6	0	-4.804552	-0.384168	0.333951
64	6	0	-6.129544	-0.763495	0.250724
65	6	0	-6.817214	-0.410771	-0.896948
66	6	0	-6.216072	0.293402	-1.928727
67	6	0	-4.880352	0.644896	-1.810229
68	7	0	-4.100445	-0.673470	1.592318
69	8	0	-3.413803	0.213350	2.054335
70	8	0	-4.282330	-1.758634	2.106150
71	1	0	-6.616365	-1.306986	1.048277
72	7	0	-8.236255	-0.792153	-1.014279

73	8	0	-8.735268	-1.385947	-0.080844
74	8	0	-8.814197	-0.488156	-2.037127
75	1	0	-6.796157	0.551465	-2.804144
76	1	0	-4.385611	1.192484	-2.602423
77	6	0	4.287686	-5.026980	-2.659838
78	1	0	4.292822	-5.431510	-3.674861
79	1	0	3.746257	-5.728529	-2.021587
80	1	0	5.325524	-4.994958	-2.313020

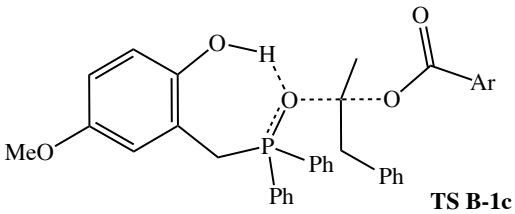


TS B-1b*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-1.881122	-1.314958	1.416543
2	8	0	-2.056420	0.187614	1.144768
3	6	0	-3.543566	-2.013976	1.654484
4	6	0	-4.417564	-1.835095	0.436574
5	6	0	-4.713368	-2.923844	-0.384104
6	6	0	-5.561844	-2.818989	-1.479460
7	6	0	-6.130290	-1.571434	-1.740467
8	6	0	-5.838510	-0.471464	-0.952524
9	6	0	-4.970348	-0.584553	0.130082
10	8	0	-4.724453	0.520064	0.882034
11	1	0	-3.771923	0.543516	1.093900
12	1	0	-6.267880	0.500724	-1.162837
13	1	0	-6.806624	-1.457619	-2.581900
14	1	0	-4.279016	-3.890745	-0.142973

15	1	0	-3.973199	-1.498047	2.519996
16	1	0	-3.444176	-3.072072	1.910438
17	6	0	-0.362101	1.369554	0.718136
18	6	0	-0.341364	1.143287	-0.744357
19	1	0	-1.360752	1.193881	-1.132492
20	1	0	0.130943	0.197755	-1.001894
21	1	0	0.220101	1.960629	-1.202427
22	1	0	0.113022	0.673125	1.384348
23	6	0	-0.836442	2.655178	1.304452
24	6	0	-1.476577	3.615794	0.335432
25	1	0	-1.506142	2.407456	2.131013
26	1	0	0.061190	3.093106	1.751452
27	6	0	-0.711337	4.609209	-0.272100
28	6	0	-1.281471	5.475926	-1.196305
29	6	0	-2.626353	5.356713	-1.523914
30	6	0	-3.395933	4.366906	-0.924128
31	6	0	-2.824793	3.500977	-0.000265
32	1	0	0.341433	4.696852	-0.022130
33	1	0	-0.674425	6.245326	-1.659853
34	1	0	-3.073438	6.033219	-2.243386
35	1	0	-4.446040	4.266913	-1.174298
36	1	0	-3.434850	2.726753	0.452134
37	8	0	1.910091	1.704480	0.712168
38	6	0	2.343550	0.546183	0.920033
39	8	0	1.793558	-0.385867	1.531894
40	6	0	3.726522	0.242684	0.357357
41	6	0	4.038916	-0.993840	-0.199110
42	6	0	5.315127	-1.339193	-0.595968
43	6	0	6.304893	-0.382618	-0.448610
44	6	0	6.045155	0.873259	0.075868
45	6	0	4.751853	1.175385	0.474427
46	7	0	2.975817	-1.983634	-0.445245
47	8	0	1.997644	-1.599580	-1.057486
48	8	0	3.166755	-3.117961	-0.071769

49	1	0	5.539735	-2.311079	-1.012876
50	7	0	7.677195	-0.717970	-0.872207
51	8	0	7.861857	-1.817890	-1.350472
52	8	0	8.532897	0.127703	-0.714990
53	1	0	6.851184	1.588201	0.167898
54	1	0	4.514127	2.146700	0.889298
55	6	0	-5.862295	-4.005221	-2.358275
56	1	0	-6.939639	-4.138495	-2.486904
57	1	0	-5.458744	-4.926993	-1.934442
58	1	0	-5.426300	-3.877433	-3.353597
59	6	0	-1.099193	-2.204996	0.063722
60	1	0	-0.052285	-1.905881	-0.027937
61	1	0	-1.631228	-1.991511	-0.864520
62	1	0	-1.138614	-3.278877	0.261197
63	6	0	-0.900233	-1.640341	2.891483
64	1	0	0.114463	-1.265050	2.720258
65	1	0	-0.856841	-2.714348	3.085694
66	1	0	-1.348378	-1.131866	3.746894



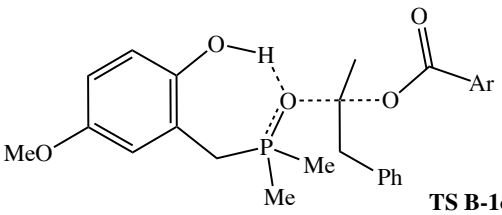
TS B-1c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	1.787048	-0.158947	0.830524
2	8	0	1.602901	1.186727	0.110769
3	6	0	1.253137	-1.523601	-0.260506
4	6	0	2.259408	-1.819141	-1.347165

5	6	0	2.972108	-3.022463	-1.295900
6	6	0	3.889401	-3.355205	-2.282822
7	6	0	4.094111	-2.474958	-3.346252
8	6	0	3.411430	-1.277393	-3.391964
9	6	0	2.504399	-0.928324	-2.391885
10	8	0	1.877466	0.278714	-2.501403
11	1	0	1.764292	0.671337	-1.620184
12	1	0	3.573066	-0.575907	-4.201494
13	1	0	4.804477	-2.746687	-4.117302
14	1	0	2.781730	-3.695330	-0.469366
15	1	0	0.271427	-1.237286	-0.660031
16	1	0	1.097662	-2.407922	0.361221
17	6	0	3.545335	-0.399019	1.147750
18	6	0	4.452929	0.521395	0.631324
19	6	0	5.816243	0.301851	0.787958
20	6	0	6.267173	-0.831306	1.451489
21	6	0	5.358804	-1.749941	1.969293
22	6	0	3.997581	-1.536469	1.818003
23	1	0	4.084084	1.401166	0.115464
24	1	0	6.525763	1.016100	0.387409
25	1	0	7.331275	-1.001834	1.567995
26	1	0	5.713500	-2.631063	2.491002
27	1	0	3.288755	-2.249270	2.227371
28	6	0	0.909829	-0.320107	2.395221
29	6	0	1.543931	0.049691	3.584583
30	6	0	0.861936	-0.048752	4.788050
31	6	0	-0.447779	-0.516181	4.807103
32	6	0	-1.084475	-0.874688	3.625574
33	6	0	-0.412380	-0.773281	2.413994
34	1	0	2.567755	0.406572	3.570165
35	1	0	1.353100	0.237706	5.710622
36	1	0	-0.978600	-0.595164	5.749055
37	1	0	-2.113891	-1.209163	3.631899
38	1	0	-0.936984	-1.009323	1.491892

39	6	0	-0.268553	1.946143	-0.335661
40	6	0	-0.590788	2.535493	0.986679
41	1	0	0.279139	3.067062	1.376144
42	1	0	-0.926307	1.778585	1.692322
43	1	0	-1.397188	3.257625	0.841010
44	1	0	-0.515055	0.919716	-0.530061
45	6	0	0.115825	2.819987	-1.489511
46	6	0	1.166540	3.865683	-1.195825
47	1	0	0.405090	2.198619	-2.337118
48	1	0	-0.828360	3.300219	-1.765911
49	6	0	0.832599	5.071454	-0.582917
50	6	0	1.809223	6.019061	-0.300280
51	6	0	3.133823	5.775592	-0.639475
52	6	0	3.473420	4.583271	-1.268343
53	6	0	2.496568	3.635819	-1.543880
54	1	0	-0.202612	5.274539	-0.328036
55	1	0	1.532176	6.952082	0.177333
56	1	0	3.896201	6.515757	-0.424669
57	1	0	4.502830	4.392113	-1.551029
58	1	0	2.763741	2.708562	-2.039022
59	8	0	-2.481723	1.720373	-0.921414
60	6	0	-2.770934	0.535185	-0.644550
61	8	0	-2.008125	-0.408487	-0.367879
62	6	0	-4.252112	0.180004	-0.700853
63	6	0	-4.889931	-0.507274	0.326660
64	6	0	-6.188597	-0.966934	0.235990
65	6	0	-6.875543	-0.693605	-0.933741
66	6	0	-6.298555	0.010210	-1.979421
67	6	0	-4.987847	0.443602	-1.852351
68	7	0	-4.192016	-0.710683	1.605047
69	8	0	-3.575683	0.234285	2.050258
70	8	0	-4.310207	-1.789802	2.149533
71	1	0	-6.656698	-1.511293	1.044080
72	7	0	-8.267650	-1.161671	-1.060022

73	8	0	-8.746789	-1.754245	-0.115424
74	8	0	-8.845074	-0.924734	-2.100717
75	1	0	-6.877080	0.204464	-2.872146
76	1	0	-4.511927	0.992540	-2.655075
77	6	0	4.469327	-5.399044	-1.231079
78	1	0	4.734066	-4.932232	-0.274083
79	1	0	5.152445	-6.223450	-1.428083
80	1	0	3.445715	-5.788317	-1.172661
81	8	0	4.622589	-4.499127	-2.302911

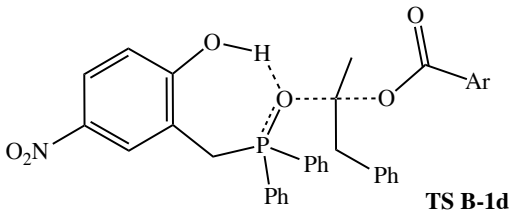


TS B-1c*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-1.779163	-0.968130	1.589581
2	8	0	-1.885473	0.519413	1.221120
3	6	0	-3.469765	-1.577634	1.875258
4	6	0	-4.335632	-1.427017	0.648207
5	6	0	-4.654582	-2.550968	-0.122053
6	6	0	-5.489359	-2.439723	-1.227128
7	6	0	-6.013808	-1.189682	-1.561652
8	6	0	-5.685052	-0.076075	-0.815893
9	6	0	-4.834189	-0.174469	0.284727
10	8	0	-4.552443	0.953364	0.995612
11	1	0	-3.594342	0.965589	1.175965
12	1	0	-6.074073	0.901058	-1.075418
13	1	0	-6.670158	-1.116722	-2.420097

14	1	0	-4.253427	-3.512589	0.174379
15	1	0	-3.873669	-0.990142	2.706543
16	1	0	-3.416954	-2.621633	2.194845
17	6	0	-0.134172	1.571732	0.682529
18	6	0	-0.164584	1.258615	-0.763494
19	1	0	-1.189650	1.343555	-1.130159
20	1	0	0.247644	0.274306	-0.974719
21	1	0	0.428237	2.014649	-1.283330
22	1	0	0.315135	0.887836	1.378600
23	6	0	-0.517411	2.915601	1.200202
24	6	0	-1.138147	3.849215	0.192839
25	1	0	-1.169914	2.757908	2.061839
26	1	0	0.418153	3.328798	1.589490
27	6	0	-0.344737	4.767615	-0.491546
28	6	0	-0.899724	5.606892	-1.449776
29	6	0	-2.257585	5.535019	-1.734648
30	6	0	-3.055534	4.619929	-1.058091
31	6	0	-2.499472	3.781561	-0.100381
32	1	0	0.717731	4.818410	-0.274559
33	1	0	-0.270599	6.317903	-1.973234
34	1	0	-2.692767	6.190222	-2.480636
35	1	0	-4.115961	4.557160	-1.274502
36	1	0	-3.131949	3.065041	0.412137
37	8	0	2.153037	1.761237	0.611994
38	6	0	2.521149	0.593056	0.881175
39	8	0	1.925385	-0.269375	1.550200
40	6	0	3.878224	0.179436	0.325503
41	6	0	4.114989	-1.101761	-0.163158
42	6	0	5.365618	-1.539934	-0.549801
43	6	0	6.408843	-0.634134	-0.464059
44	6	0	6.225429	0.661631	-0.008900
45	6	0	4.955484	1.057773	0.382173
46	7	0	2.996239	-2.042593	-0.346087
47	8	0	2.033403	-1.638546	-0.969245

48	8	0	3.129184	-3.164228	0.086937
49	1	0	5.530917	-2.544603	-0.913278
50	7	0	7.755573	-1.069435	-0.878820
51	8	0	7.873752	-2.203846	-1.293311
52	8	0	8.658326	-0.265022	-0.778577
53	1	0	7.071016	1.334120	0.036425
54	1	0	4.776920	2.062512	0.743676
55	6	0	-1.042942	-1.979270	0.297425
56	1	0	0.013973	-1.727145	0.182880
57	1	0	-1.571682	-1.808994	-0.641570
58	1	0	-1.121048	-3.034779	0.568702
59	6	0	-0.806025	-1.242620	3.080352
60	1	0	0.225851	-0.937342	2.876797
61	1	0	-0.819001	-2.300941	3.350311
62	1	0	-1.218170	-0.651035	3.899592
63	6	0	-5.345803	-4.753103	-1.730897
64	1	0	-4.250220	-4.772453	-1.780515
65	1	0	-5.748315	-5.421769	-2.489536
66	1	0	-5.670176	-5.097009	-0.741282
67	8	0	-5.854673	-3.473730	-2.027505



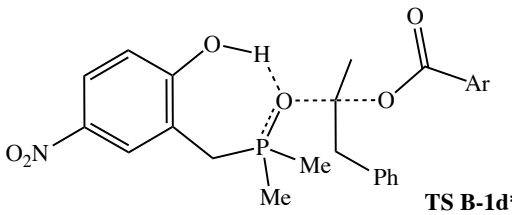
TS B-1d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	1.919039	0.087386	1.082196
2	8	0	1.661517	1.423060	0.094148

3	6	0	1.291198	-1.422521	0.117424
4	6	0	2.165458	-1.866964	-1.033447
5	6	0	2.632774	-3.184711	-1.048150
6	6	0	3.353531	-3.673710	-2.139016
7	6	0	3.621252	-2.869915	-3.253649
8	6	0	3.178898	-1.555934	-3.245835
9	6	0	2.474706	-1.033857	-2.144020
10	8	0	2.118266	0.283176	-2.231537
11	1	0	1.902133	0.754547	-1.361513
12	1	0	3.376071	-0.890450	-4.076750
13	1	0	4.173339	-3.279463	-4.088847
14	1	0	2.425619	-3.854168	-0.222572
15	1	0	0.277051	-1.143282	-0.204267
16	1	0	1.182677	-2.235005	0.840700
17	6	0	3.750140	-0.037692	1.337678
18	6	0	4.569596	0.982674	0.837003
19	6	0	5.956645	0.891649	1.003052
20	6	0	6.515095	-0.211717	1.658312
21	6	0	5.690162	-1.230117	2.154598
22	6	0	4.303529	-1.146559	1.996842
23	1	0	4.118621	1.826678	0.326703
24	1	0	6.596575	1.678659	0.618764
25	1	0	7.590818	-0.281370	1.781254
26	1	0	6.123884	-2.086626	2.659261
27	1	0	3.668763	-1.935731	2.388061
28	6	0	1.081582	0.122891	2.734012
29	6	0	1.810124	0.519799	3.868554
30	6	0	1.180531	0.541961	5.116411
31	6	0	-0.166148	0.173125	5.229592
32	6	0	-0.891365	-0.210862	4.095449
33	6	0	-0.273622	-0.235879	2.838922
34	1	0	2.853368	0.802473	3.782935
35	1	0	1.740125	0.845601	5.994859
36	1	0	-0.650331	0.188970	6.200624

37	1	0	-1.937614	-0.483740	4.163795
38	1	0	-0.861074	-0.504977	1.964646
39	6	0	-0.312768	2.147036	-0.230048
40	6	0	-0.421301	3.039966	0.959546
41	1	0	0.481477	3.649364	1.053662
42	1	0	-0.585310	2.474524	1.876817
43	1	0	-1.269592	3.717903	0.815805
44	1	0	-0.550959	1.102436	-0.143505
45	6	0	-0.111236	2.714260	-1.615397
46	6	0	0.747331	3.962753	-1.728889
47	1	0	0.264662	1.926359	-2.274405
48	1	0	-1.132050	2.935016	-1.956089
49	6	0	0.191497	5.239080	-1.534208
50	6	0	0.980647	6.389177	-1.646636
51	6	0	2.338632	6.279156	-1.966547
52	6	0	2.898882	5.013749	-2.177578
53	6	0	2.109874	3.864150	-2.060322
54	1	0	-0.866251	5.333776	-1.304095
55	1	0	0.533959	7.366928	-1.494972
56	1	0	2.951030	7.170428	-2.060572
57	1	0	3.948121	4.921518	-2.441268
58	1	0	2.545142	2.886718	-2.239416
59	8	0	-2.577420	1.819114	-0.440441
60	6	0	-2.821505	0.575511	-0.192152
61	8	0	-1.963051	-0.332071	0.082257
62	6	0	-4.268330	0.143766	-0.338278
63	6	0	-4.892926	-0.799325	0.496247
64	6	0	-6.164884	-1.301376	0.235336
65	6	0	-6.843894	-0.810195	-0.877326
66	6	0	-6.283482	0.156626	-1.715879
67	6	0	-4.999839	0.623566	-1.436987
68	7	0	-4.254302	-1.256294	1.735412
69	8	0	-3.628348	-0.400050	2.420596
70	8	0	-4.417985	-2.460059	2.074712

71	1	0	-6.618867	-2.040030	0.881432
72	7	0	-8.189161	-1.316056	-1.162800
73	8	0	-8.678506	-2.176143	-0.377078
74	8	0	-8.786063	-0.863456	-2.180692
75	1	0	-6.849319	0.520014	-2.563399
76	1	0	-4.533921	1.367379	-2.070673
77	7	0	3.829181	-5.046432	-2.112539
78	8	0	4.458878	-5.481539	-3.122387
79	8	0	3.596655	-5.743423	-1.078093



TS B-1d*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	1.804769	-0.235241	1.886635
2	8	0	1.904210	1.275932	1.158449
3	6	0	1.858583	-1.533719	0.517044
4	6	0	3.185219	-1.690316	-0.194340
5	6	0	3.776924	-2.957523	-0.232047
6	6	0	4.939637	-3.180097	-0.971105
7	6	0	5.542934	-2.152210	-1.705643
8	6	0	4.977684	-0.886804	-1.664422
9	6	0	3.820290	-0.631022	-0.903164
10	8	0	3.372117	0.659829	-0.913179
11	1	0	2.782939	0.947042	-0.137076
12	1	0	5.416691	-0.056202	-2.202490
13	1	0	6.437641	-2.357206	-2.278068

14	1	0	3.329779	-3.792831	0.292830
15	1	0	1.040545	-1.241765	-0.155788
16	1	0	1.562525	-2.484475	0.971011
17	6	0	0.103462	2.046455	0.256326
18	6	0	-0.388033	2.821317	1.429123
19	1	0	0.443312	3.366198	1.886160
20	1	0	-0.871015	2.181283	2.168094
21	1	0	-1.117022	3.563792	1.086781
22	1	0	-0.102527	0.994261	0.171854
23	6	0	0.679147	2.739207	-0.949302
24	6	0	1.289913	4.110405	-0.725810
25	1	0	1.391148	2.068664	-1.441524
26	1	0	-0.179507	2.816715	-1.631618
27	6	0	0.513431	5.272699	-0.871124
28	6	0	1.073723	6.537954	-0.662472
29	6	0	2.422743	6.657225	-0.309834
30	6	0	3.207204	5.505741	-0.171505
31	6	0	2.645998	4.241105	-0.378610
32	1	0	-0.531492	5.186029	-1.157251
33	1	0	0.460943	7.426014	-0.781740
34	1	0	2.860503	7.637808	-0.151905
35	1	0	4.256839	5.591875	0.091834
36	1	0	3.260466	3.352323	-0.281187
37	8	0	-2.047675	1.634761	-0.531303
38	6	0	-2.265259	0.391447	-0.260928
39	8	0	-1.386920	-0.483811	0.062437
40	6	0	-3.698276	-0.080036	-0.400403
41	6	0	-4.296350	-1.012919	0.464470
42	6	0	-5.560747	-1.545315	0.228195
43	6	0	-6.258162	-1.095745	-0.890772
44	6	0	-5.723376	-0.141568	-1.760097
45	6	0	-4.446701	0.357230	-1.505006
46	7	0	-3.633537	-1.431749	1.705451
47	8	0	-3.028334	-0.551612	2.378893

48	8	0	-3.754815	-2.637688	2.057043
49	1	0	-5.995436	-2.275914	0.896368
50	7	0	-7.596027	-1.634597	-1.151004
51	8	0	-8.061761	-2.482949	-0.338692
52	8	0	-8.209964	-1.220317	-2.174895
53	1	0	-6.303276	0.187964	-2.611928
54	1	0	-3.999982	1.092884	-2.161835
55	6	0	3.272372	-0.454616	3.010277
56	1	0	3.255843	0.332034	3.767332
57	1	0	4.191925	-0.377205	2.427840
58	1	0	3.225974	-1.434788	3.492105
59	6	0	0.255930	-0.502256	2.874964
60	1	0	0.134324	0.309027	3.595265
61	1	0	0.339401	-1.452581	3.409951
62	1	0	-0.602825	-0.539422	2.199019
63	7	0	5.526221	-4.510543	-0.980374
64	8	0	4.971647	-5.415514	-0.285832
65	8	0	6.565796	-4.700448	-1.678542

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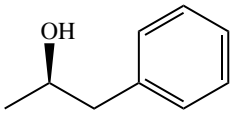
5. Other molecules required for calculating values in Table 2.

H_2O

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.000000	-0.117715	0.000000
2	1	0	0.754910	0.470861	0.000000
3	1	0	-0.754910	0.470860	-0.000000



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.468174	1.902070	0.905975
2	6	0	1.020828	1.042214	0.544331
3	6	0	2.419368	-1.150409	-0.421815
4	6	0	0.377435	-0.190858	0.459037
5	6	0	2.347345	1.179347	0.156494
6	6	0	3.051572	0.083218	-0.327616
7	6	0	1.092882	-1.282908	-0.030428
8	1	0	2.832827	2.146222	0.230797
9	1	0	4.087724	0.189565	-0.628553
10	1	0	2.961062	-2.012261	-0.795796
11	6	0	-2.025941	-0.140548	-0.332366
12	1	0	0.606095	-2.251628	-0.099771
13	6	0	-3.465459	-0.478747	0.035718
14	1	0	-3.562995	-1.527677	0.329244
15	1	0	-4.133385	-0.305023	-0.813439
16	1	0	-3.798534	0.151957	0.864318
17	6	0	-1.072101	-0.338970	0.845269
18	1	0	-1.242650	-1.331969	1.272333
19	1	0	-1.338490	0.395970	1.611795
20	1	0	-1.697147	-0.794260	-1.154377
21	8	0	-1.907754	1.219859	-0.720061
22	1	0	-2.396217	1.344126	-1.533787