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Electronic Supplementary Information

Selective Functionalisation of Aromatic Alcohols with Supramolecularly Regulated Gold(I) Catalysts

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1. General Considerations:

All syntheses were carried out using chemicals as purchased from commercial sources unless otherwise stated. Tetrafluoroborate regulation agents (NH_4BF_4, $LiBF_4$, $NaBF_4$, KBF_4 and $RbBF_4$) were purchased from commercial sources. $CsBF_4$ was prepared reacting Cs_2CO_3 with HBF_4.[1] All regulation agents were azeotropically dried with toluene prior to their use. Air- and moisture-sensitive manipulations or reactions were performed under inert atmosphere, either in a glove box or with standard Schlenk techniques. Glassware was dried *in vacuo* before use with a hot air gun. All solvents were dried and deoxygenated by using a solvent purification system (SPS). Silica gel 60 (230-400 mesh) was used for column chromatography. NMR spectra were recorded at room temperature in 400 MHz or 500 MHz spectrometers in $CDCl_3$ or CD_2Cl_2 unless otherwise cited. ^1H and ^{13}C NMR chemical shifts are quoted in ppm relative to residual solvent peaks. $^{11}B\{^1H\}$ NMR chemical shifts are quoted in ppm relative to $BF_3 \cdot Et_2O$ in $CDCl_3$. $^{19}F\{^1H\}$ NMR chemical shifts are quoted in ppm relative to $CFCl_3$ in $CDCl_3$. $^{31}P\{^1H\}$ NMR chemical shifts are quoted in ppm relative to 85% phosphoric acid in water. HRMS and MS spectra were recorded using ESI ionisation method in positive mode. IR spectra were recorded using Attenuated Total Reflection (ATR) technique.

[1] A round-bottomed flask provided with a stirrer was loaded with Cs_2CO_3 (3.27 g, 9.9 mmol) and 50 mL of MilliQ water. An aqueous HBF_4 solution (50 wt%, 19.9 mmol) was added dropwise to the caesium carbonate-containing solution, observing some bubbling due to the release of CO_2. This solution was stirred for 24 hours at room temperature. Then, water was evaporated, and the solid residue was further dried in a vacuum oven at 120 °C for 24 hours, quantitatively yielding $CsBF_4$ as a white solid. The caesium content was determined by ICP-MS (calcd. for $CsBF_4$ 60.5%, found 60.0±0.5 %).

2. General Structural Comments on X-ray Crystals:

Crystal preparation: Crystals of **3e** and **3f** were grown by solvent diffusion, using CH_2Cl_2 and *n*-pentane at room temperature. The crystals used for structure determination were selected using a Zeiss stereomicroscope using polarised light and prepared under inert conditions immersed in perfluoropolyether as protecting oil for manipulation.

Data collection: Crystal structure determination for samples **3e** and **3f** were carried out using an Apex DUO Kappa 4-axis goniometer equipped with an APEX 2 4K CCD area detector, a Microfocus Source E025 IuS using MoK_α radiation, Quazar MX multilayer Optics as monochromator and an Oxford Cryosystems low temperature device Cryostream 700 plus ($T = -173$ °C). Full-sphere data collection was used with ω and φ scans. *Programs used:* Data collection APEX-2[2], data reduction Bruker Saint[3] V/.60A and absorption correction SADABS[4].

Structure Solution and Refinement: Crystal structure solution was achieved using the computer program SHELXT[5]. Visualisation was performed with the program SHELXle[6]. Missing atoms were subsequently located from difference Fourier synthesis and added to the atom list. Least-squares refinement on F^2 using all measured intensities was carried out using the program SHELXL 2015[7]. All non-hydrogen atoms were refined including anisotropic displacement parameters.

Crystal data have been deposited at the Cambridge Crystallographic Data Centre (CCDC 1992257-1992258).

[2] Data collection with APEX II version v2013.4-1. Bruker (2007). Bruker AXS Inc., Madison, Wisconsin, USA.

[3] Data reduction with Bruker SAINT version V8.30c. Bruker (2007). Bruker AXS Inc., Madison, Wisconsin, USA.

[4] SADABS: V2012/1 Bruker (2001). Bruker AXS Inc., Madison, Wisconsin, USA. R. H. Blessing, An Empirical Correction for Absorption Anisotropy. *Acta Cryst.*, 1995, **A51**, 33-38.

[5] SHELXT; V2014/4 (Sheldrick 2014). G. M. Sheldrick, SHELXT - Integrated Space-Group and Crystal-Structure Determination. *Acta Cryst*., 2015, **A71**, 3-8.

[6] SHELXle; C. B. Hübschle, G. M. Sheldrick and B. Dittrich, ShelXle: A QT Graphical User Interface for SHELXL. *J. Appl. Cryst.*, 2011, **44**, 1281-1284.

[7] SHELXL; SHELXL-2014/7 (Sheldrick 2014). G. M. Sheldrick, Crystal Structure Refinement with SHELXL. *Acta Cryst*., 2015, C**71**, 3-8.

ORTEP figures for 3e and 3f.

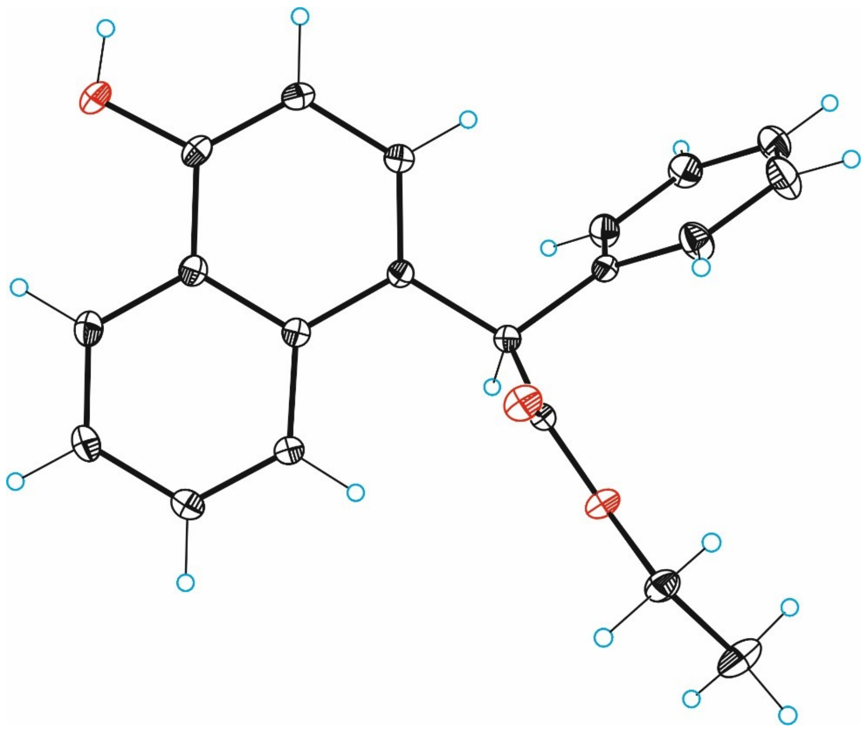


Figure SI 1. ORTEP drawing (thermal ellipsoids drawn at a 50 % probability level) showing the structure of **3e**. Colour scheme: C: black, O: red, H: blue.

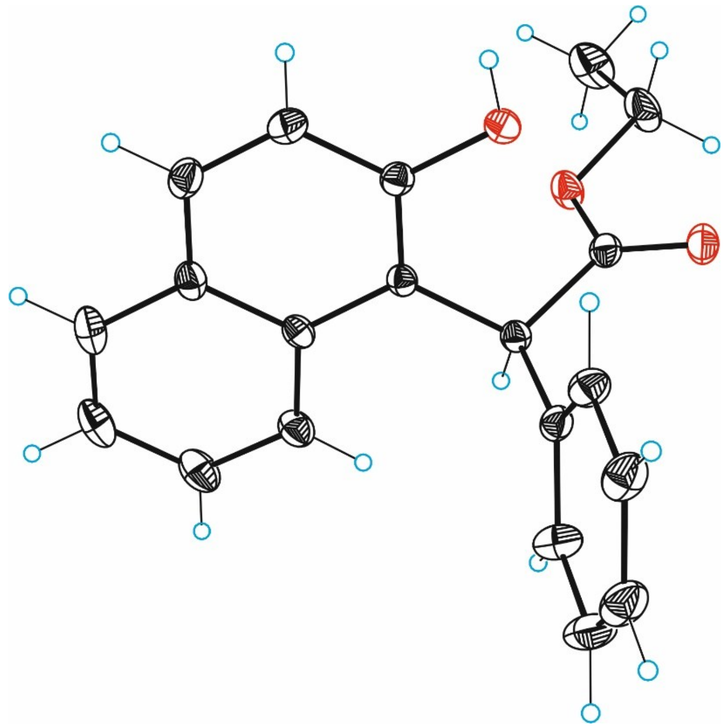
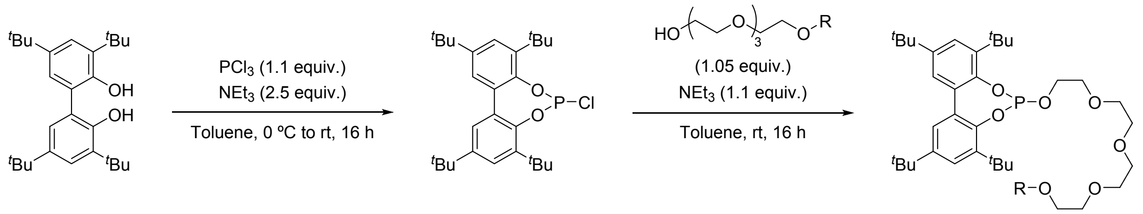


Figure SI 2. ORTEP drawing (thermal ellipsoids drawn at a 50 % probability level) showing the structure of **3f**. Colour scheme: C: black, O: red, H: blue.

3. Syntheses of Ligands L1-L3:

3.1 General procedure for the synthesis of ligands L1-L3.



Scheme SI 1. General synthesis for ligands **L1**-**L3**.

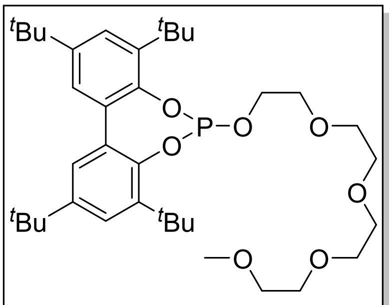
3,3',5,5'-tetra-*tert*-butylbiphenyl-2,2'-diyl chlorophosphite: The preparation of 3,3',5,5'-tetra-*tert*-butylbiphenyl-2,2'-diyl chlorophosphite was performed by slightly varying a reported procedure.[8] Under inert atmosphere, a flame-dried Schlenk flask provided with a stirrer was loaded with PCl_3 (502 µL, 5.73 mmol, 1.2 equiv.), dry toluene (30 mL) and triethylamine (1.74 mL, 12.4 mmol, 2.6 equiv.) and the solution was cooled to 0 °C. In parallel, under inert atmosphere, a flame-dried Schlenk flask provided with a stirrer was loaded with 3,3',5,5'-tetra-*tert*-butyl-2,2'-dihydroxybiphenyl (2 g, 4.77 mmol, 1 equiv.) and was azeotropically dried with toluene (3 x 10 mL), and then anhydrous toluene was added (30 mL). The diol solution was then slowly dropwise added to the PCl_3 and NEt_3 solution. Subsequently, the mixture was allowed to reach room temperature. After stirring for 16 hours, the mixture was filtered under inert atmosphere through Celite® 521, and the precipitate was further washed with toluene (20 mL). Volatiles were evaporated from the combined filtrates under reduced pressure to afford a yellowish solid (quantitative yield). This chlorophosphite was used with no further purification in the following syntheses. The spectroscopic data for this compound is in agreement with the spectroscopic information already reported in the literature.[8] ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.46 (d, J = 2.4 Hz, 2 H), 7.17 (d, J = 2.4 Hz, 2 H), 1.48 (s, 18 H), 1.35 (s, 18 H) ppm. ^{31}P{^{1}H} NMR (162 MHz, $CDCl_3$) δ: 174.6 ppm.

General procedure for ligands synthesis: Under inert atmosphere, in a flame-dried Schlenk flask provided with a stirrer was prepared a solution of 3,3',5,5'-tetra-*tert*-butylbiphenyl-2,2'-diyl chlorophosphite (4.77 mmol, 1.00 equiv.) in 30 mL of

[8] G. J. H. Buisman, P. C. J. Kamer and P. W. N. M. van Leeuwen, Rhodium Catalyzed Asymmetric Hydroformylation with Chiral Diphosphite Ligands. *Tetrahedron: Asymmetry*, 1993, **4**, 1625-1634.

anhydrous toluene and, then, NEt_3 (5.72 mmol, 1.2 equiv.) was added dropwise. In parallel, under inert atmosphere, a flame-dried Schlenk flask provided with a stirrer was loaded with the corresponding mono-functionalised tetraethyleneglycol (TEG) (5.25 mmol, 1.1 equiv.), and was azeotropically dried with toluene (3 x 10 mL) prior to add 30 mL of anhydrous toluene. The monofunctionalised-TEG was solution was slowly dropwise added to the chlorophosphite solution at room temperature. Then, the mixture was stirred for 16 h, and afterwards the reaction mixture was filtered under inert atmosphere through Celite® 521. Volatiles were evaporated to dryness to give the crude product as a yellowish oil. The ligand was purified by means of flash chromatography, using SiO_2 as the stationary phase and a mixture of cyclohexane and ethyl acetate as the eluents.

3.2 Synthesis of ligand L1.

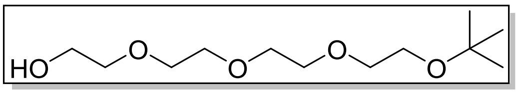


L1

Ligand L1: Ligand **1** was prepared according to the described general procedure, using commercially available tetraethyleneglycol mono-methyl ether and purified by flash chromatography (SiO_2, cyclohexane:AcOEt, 1:0→5:1), yielding to 2.3 g of a colourless thick oil (75.5% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.41 (d, J = 2.4 Hz, 2 H), 7.15 (d, J = 2.4 Hz, 2 H), 3.90 (m, 2 H), 3.70-3.50 (m, 14 H), 3.36 (s, 3 H), 1.48 (s, 18 H), 1.34 (s, 18 H) ppm. $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ: 146.5, 140.0, 132.7, 126.7, 124.4, 72.1, 70.9, 70.8, 70.7, 63.7, 59.2, 35.5, 34.8, 31.7, 31.2 ppm. $^{31}P\{^1H\}$ NMR (162 MHz, $CDCl_3$) δ: 138.8 ppm. IR (neat): 2956, 2905, 2870, 1437, 1395, 1362, 1281, 1229, 1200, 1108, 1090, 1031, 941, 868, 850, 802, 777, 764, 735, 697, 615 cm^{-1}. HRMS ESI-MS (m/z): $[M+H]^+$ calcd. for $C_{37}H_{60}O_7P^+$ 647.4085, found 647.4084.

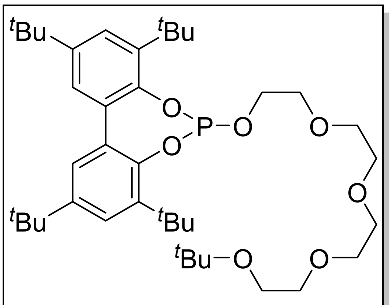
3.3 Synthesis of ligand L2.

Tetraethyleneglycol mono-*tert*-butyl ether: The preparation of tetraethyleneglycol mono-tert-butyl ether was performed by adapting a reported procedure.[9] Tetraethylene glycol (400 mL, 2.32 mol,



[9] A. C. French, A. L. Thompson and B. G. Davis, High-Purity Discrete PEG-Oligomer Crystals Allow Structural Insight. *Angew. Chem., Int. Ed.*, 2009, **48**, 1248-1252.

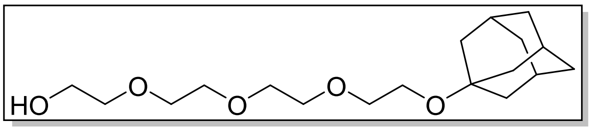
2.69 equiv.), Amberlyst® 15 macroreticular cation exchange resin (17.5 g, H^+ form) and CH_2Cl_2 (1 L) were placed in a 2 L two-necked round bottomed Schlenk flask equipped with a dry ice/acetone condenser. The flask was kept under Ar and with mild stirring. 500 mL of isobutene (8% in CH_2Cl_2, 0.86 mmol, 1 equiv.) were then slowly added *via* cannula. After 6 hours, the reaction mixture was filtered into 200 mL of saturated aqueous $NaHCO_3$, and then extracted with water (2 x 500 mL). The organic layer was dried over anhydrous $MgSO_4$ and evaporated to give a colourless oil (62.3 g, 28.8% yield) consisting only of the mono-entry product. No further purification was performed. The spectroscopic data for this compound is in agreement with the spectroscopic information already reported in the literature.[9] ^{1}H NMR (400 MHz, $CDCl_3$) δ: 3.70 (m, 2 H), 3.65 (m, 8 H), 3.58 (m, 4 H), 3.50 (m, 2 H), 2.27 (br s, 1 H), 1.17 (s, 9 H) ppm. ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ: 73.1, 72.6, 71.3, 70.7, 70.4, 61.8, 61.2, 27.5 ppm.



L2

Ligand L2: Ligand **2** was prepared according to the described general procedure, using tetraethyleneglycol mono-*tert*-butyl ether and purified by flash chromatography (SiO_2, cyclohexane:AcOEt, 1:0→5:1), yielding to 2.9 g of a colourless thick oil (84.4% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.41 (d, J = 2.5 Hz, 2 H), 7.16 (d, J = 2.4 Hz, 2 H), 3.91 (m, 2 H), 3.70-3.53 (m, 12 H), 3.50 (m, 2 H), 1.48 (s, 18 H), 1.34 (s, 18 H), 1.18 (s, 9 H) ppm. ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ: 146.5, 146.3 (d, J_{C-P} = 5.8 Hz), 139.9 (d, J_{C-P} = 1.0 Hz), 132.7 (d, J_{C-P} = 3.6 Hz), 126.6, 124.3, 73.1, 71.3, 70.9, 70.8, 70.7, 63.7 (d, J_{C-P} = 2.1 Hz), 61.3, 35.5, 34.7, 31.6, 31.1 (d, J_{C-P} = 2.6 Hz), 27.6 ppm. ^{31}P{^{1}H} NMR (162 MHz, $CDCl_3$) δ: 138.8 ppm. IR (neat): 2959, 2906, 2869, 1437, 1394, 1362, 1281, 1229, 1198, 1124, 1090, 1036, 941, 869, 851, 777, 764, 736, 697, 615 cm^{-1}. HRMS ESI-MS (m/z): $[M+Na]^+$ calcd. for $C_{40}H_{65}O_7PNa^+$ 711.4360, found 711.4363.

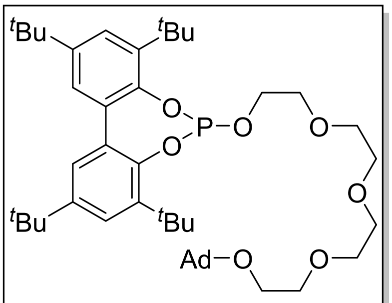
3.4 Synthesis of ligand L3.



Tetraethyleneglycol mono-1-adamantyl ether: The preparation of tetraethyleneglycol mono-1-adamantyl ether was performed as reported in the literature.[10] Tetraethylene glycol (41.5 mL, 0.239

[10] S. S. Agasti, M. Liong, C. Tassa, H. J. Chung, S. Y. Shaw, H. Lee and R. Weissleder, Supramolecular Host-Guest Interaction for Labeling and Detection of Cellular Biomarkers. *Angew. Chem., Int. Ed.*, 2012,

mol, 20 equiv.) was transferred to a round-bottom flask. The flask was heated to 60 °C and triethylamine (5 mL, 0.036 mol, 3 equiv.) was added. After stirring the solution for 5 minutes at 60 °C, 1-bromoadamantane (2.5 g, 0.012 mol, 1 equiv.) was added. A condenser was then attached to the set up, and the reaction mixture was then heated to 180 °C and stirred for 18 hours. After cooling at room temperature, 50 mL of dichloromethane were added to the reaction mixture. The organic layer was then washed with 2 M HCl (4 x 50 mL) and a saturated NaCl solution. The organic layer was subsequently dried over $MgSO_4$, and evaporated to dryness to afford a brown oil (3.69 g, 97% yield). This product was used in without further purification. The spectroscopic data for this compound is in agreement with the spectroscopic information already reported in the literature.[10] ^{1}H NMR (400 MHz, $CDCl_3$) δ: 3.80-3.50 (m, 16 H), 2.56 (br s, 1 H), 2.13 (br s, 3 H), 1.80-1.50 (m, 12 H) ppm. ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ: 72.7, 72.4, 71.4, 70.7, 70.6, 70.4, 61.8, 59.3, 41.5, 36.5, 30.6 ppm.



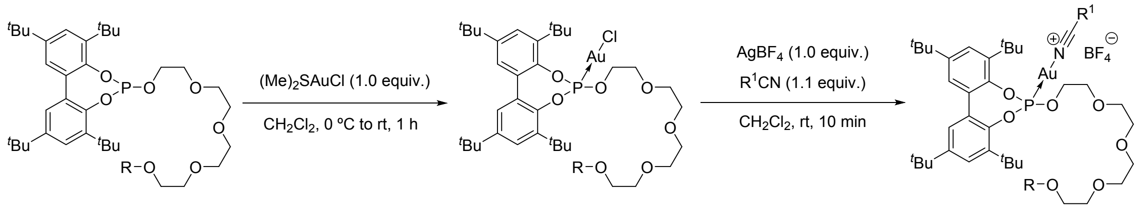
L3

Ligand L3: Ligand **3** was prepared according to the described general procedure, using tetraethyleneglycol mono-1-adamantyl ether and purified by flash chromatography (SiO_2, cyclohexane:AcOEt, 1:0→5:1), yielding to 1.3 g of a colourless thick oil that solidified upon time (72.4% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.46 (m, 2 H), 7.20 (m, 2 H), 3.95 (m, 2 H), 3.75-3.55 (m, 14 H), 2.16 (br s, 3 H), 1.80-1.55 (m, 12 H) 1.53 (s, 18 H), 1.38 (s, 18 H) ppm. ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ: 146.4, 146.2 (d, J_{C-P} = 5.8 Hz), 139.9, 132.7 (d, J_{C-P} = 3.4 Hz), 126.5, 124.2, 72.1, 71.3, 70.9, 70.8, 70.7, 70.6, 63.6, 59.3, 41.6, 36.5, 35.4, 34.7, 31.6, 31.1 (d, J_{C-P} = 2.2 Hz), 30.5 ppm. ^{31}P{^{1}H} NMR (162 MHz, $CDCl_3$) δ: 138.9 ppm. IR (neat): 2954, 2905, 1438, 1395, 1362, 1282, 1229, 1201, 1115, 1090, 1036, 941, 913, 869, 851, 777, 764, 733, 697, 615 cm^{-1}. HRMS ESI-MS (m/z): $[M+Na]^+$ calcd. for $C_{46}H_{71}O_7PNa^+$ 789.4830, found 789.4862.

51, 450-454.

4. Syntheses of Complexes C1-C3:

4.1 General procedure for the synthesis of complexes C1-C3.



Scheme SI 2. General synthesis for complexes **C1-C3**.

General procedure for complexes synthesis: The Au(I) complexes were prepared in two steps adapting reported procedures, first generating the corresponding gold(I) chloride,[11] and then generating the cationic gold(I) complex.[12] In a typical experiment, a solution of the desired ligand (0.3 mmol, 1.0 equiv.) in CH_2Cl_2 (3 mL) was added dropwise to a solution of $(Me)_2SAuCl$ (0.3 mmol, 1.0 equiv.) in CH_2Cl_2 (3 mL) at 0 °C. The resulting solution was allowed to warm to room temperature and stirred for another 30 min. The volatiles were removed under vacuum to quantitatively yield the corresponding Au(I) chloride phosphite complex as a white solid. Subsequently, a solution of the desired gold(I) chlorophosphite (0.3 mmol, 1.0 equiv.) and benzonitrile (0.33 mmol, 1.1 equiv.) in CH_2Cl_2 (6 mL) was added to a solution of $AgBF_4$ (0.3 mmol, 1.0 equiv.) in CH_2Cl_2 (3 mL), observing an immediate the formation of a white precipitate. After stirring for 5 min, the mixture was filtered using a 0.22 μm pore size PTFE syringe filter, and the solvent was evaporated under vacuum. The cationic tetrafluoroborate complex was obtained as a white, foamy solid.

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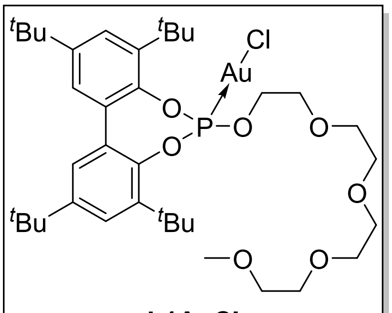
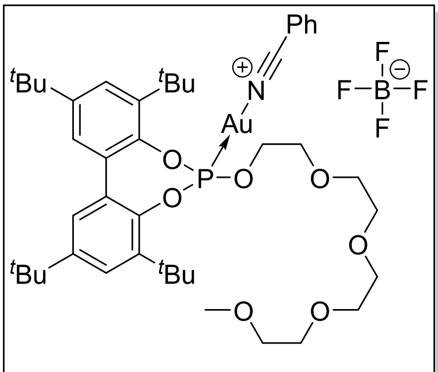
[11] N. Delpont, I. Escofet, P. Pérez-Galan, D. Spiegl, M. Raducan, C. Bour, R. Sinisi and A. M. Echavarren, Modular Chiral Gold(I) Phosphite Complexes. *Catal. Sci. Technol.*, 2013, **3**, 3007-3012.
[12] C. H. M. Amijs, V. López-Carrillo, M. Raducan, P. Pérez-Galan, C. Ferrer and A. M. Echavarren, Gold(I)-Catalyzed Intermolecular Addition of Carbon Nucleophiles to 1,5- and 1,6-Enynes. *J. Org. Chem.*, 2008, **73**, 7721-7730.

4.2 Synthesis of complex C1.



L1AuCl

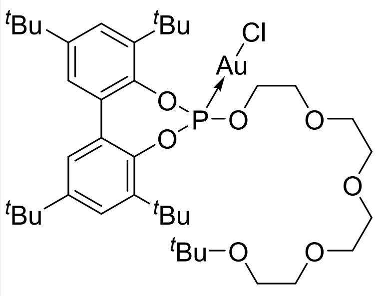
Ligand L1 gold(I) chloride: **L1**AuCl was prepared according to the described general procedure, quantitatively yielding the gold(I) chloride as a white solid. ^{1}H NMR (500 MHz, CD_2Cl_2) δ: 7.54 (d, J = 2.0 Hz, 2 H), 7.22 (d, J = 2.5 Hz, 2 H), 4.35 (m, 2 H), 3.70 (m, 2 H), 3.65-3.54 (m, 10 H), 3.49 (m, 2 H), 3.32 (s, 3 H), 1.53 (s, 18 H), 1.37 (s, 18 H) ppm. ^{13}C{^{1}H} NMR (100 MHz, CD_2Cl_2) δ: 149.1, 144.2 (d, $J_{C–P}$ = 10.5 Hz), 140.4 (d, $J_{C–P}$ = 3.9 Hz), 131.3 (d, $J_{C–P}$ = 2.0 Hz), 127.5, 126.1, 72.3, 71.2, 71.0, 70.9, 70.7, 70.0 (d, $J_{C–P}$ = 6.4 Hz), 69.3, 59.0, 36.0, 35.0, 31.9, 31.5 ppm. ^{31}P{^{1}H} NMR (162 MHz, CD_2Cl_2) δ: 122.9 ppm. IR (neat): 2957, 2870, 1589, 1436, 1396, 1363, 1282, 1221, 1202, 1119, 1084, 1032, 950, 915, 895, 799, 715, 645, 627, 537 cm^{-1}. HRMS ESI-MS (m/z): $[M+Na]^+$ calcd. for $C_{37}H_{59}O_7PAuClNa^+$ 901.3245, found 901.3205.



C1

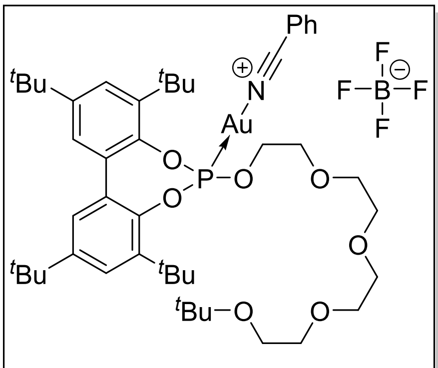
Complex C1: **C1** was prepared according to the described general procedure, obtaining 283 mg (92.0% yield) of the cationic complex as a white solid. ^{1}H NMR (400 MHz, CD_2Cl_2) δ: 7.84 (m, 2 H), 7.79 (tm, J = 7.7 Hz, 1 H), 7.60 (tm, J = 7.9 Hz, 2 H), 7.57 (d, J = 1.9 Hz, 2 H), 7.24 (d, J = 2.4 Hz, 2 H), 4.51 (br d, J = 13.2 Hz, 2 H), 3.78 (br s, 2 H), 3.75-3.60 (m, 10 H), 3.55 (m, 2 H), 3.32 (s, 3 H), 1.54 (s, 18 H), 1.37 (s, 18 H) ppm. ^{11}B{^{1}H} NMR (128 MHz, CD_2Cl_2) δ: −1.2 ppm.^{13}C{^{1}H} NMR (100 MHz, CD_2Cl_2) δ: 149.6, 143.9 (d, $J_{C–P}$ = 10.4 Hz), 140.4 (d, $J_{C–P}$ = 4.1 Hz), 135.9, 133.9, 131.0 (d, $J_{C–P}$ = 2.3 Hz), 130.1, 127.7, 126.3, 120.6, 108.4, 72.1, 70.9, 70.7, 70.3, 70.0 (d, $J_{C–P}$ = 4.7 Hz), 59.1, 36.0, 35.1, 31.8, 31.4 ppm. ^{19}F{^{1}H} NMR (376 MHz, CD_2Cl_2) δ: −152.5 ppm. ^{31}P{^{1}H} NMR (162 MHz, CD_2Cl_2) δ: 112.6 (br s) ppm. IR (neat): 2958, 2283, 1594, 1448, 1397, 1363, 1282, 1221, 1029, 931, 800, 760, 715, 686, 644, 627, 550 cm^{-1}. HRMS ESI-MS (m/z): $[M–PhCN–BF_4]^+$ calcd. for $C_{37}H_{59}O_7PAu^+$ 843.3659, found 843.3634.

4.3 Synthesis of complex C2.



L2AuCl

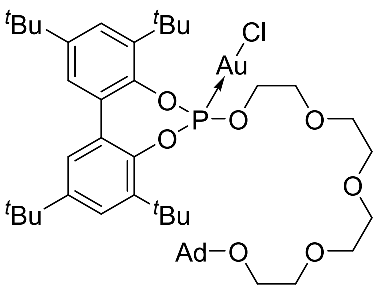
Ligand L2 gold(I) chloride: **L2**AuCl was prepared according to the described general procedure, quantitatively yielding the gold(I) chloride as a white solid. ^{1}H NMR (400 MHz, CD_2Cl_2) δ: 7.57 (d, J = 2.0 Hz, 2 H), 7.24 (d, J = 2.4 Hz, 2 H), 4.38 (m, 2 H), 3.73 (m, 2 H), 3.67-3.57 (m, 8 H), 3.51 (m, 4 H), 1.56 (s, 18 H), 1.39 (s, 18 H), 1.19 (s, 9 H) ppm. 2 H), 3.32 (s, 3 H), 1.53 (s, 18 H), 1.37 (s, 18 H) ppm. ^{13}C{^{1}H} NMR (100 MHz, CD_2Cl_2) δ: 149.2 (d, J_{C-P} = 1.2 Hz), 144.3 (d, J_{C-P} = 10.6 Hz), 140.5 (d, J_{C-P} = 3.8 Hz), 131.4 (d, J_{C-P} = 2.5 Hz), 127.5 (d, J_{C-P} = 0.8 Hz), 126.2, 73.1, 71.7, 71.3, 71.1, 70.9, 70.1 (d, J_{C-P} = 6.4 Hz), 69.3, 61.5, 36.1, 35.1, 32.0, 31.6, 27.7 ppm. ^{31}P{^{1}H} NMR (162 MHz, CD_2Cl_2) δ: 123.0 ppm. IR (neat): 2961, 2869, 1589, 1437, 1396, 1362, 1221, 199, 1120, 1084, 1034, 950, 915, 895, 799, 715, 645, 627, 537 cm^{-1}. HRMS ESI-MS (m/z): $[M+Na]^+$ calcd. for $C_{40}H_{65}O_7PAuClNa^+$ 943.3714, found 943.3754.



C2

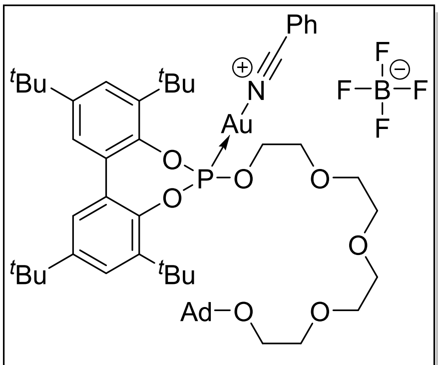
Complex C2: **C2** was prepared according to the described general procedure, obtaining 162 mg (78.1% yield) of the cationic complex as a white solid. ^{1}H NMR (400 MHz, CD_2Cl_2) δ: 7.85-7.65 (m, 3 H), 7.60-7.50 (m, 4 H), 7.23 (d, J = 2.4 Hz, 2 H), 4.52 (br d, J = 14.7 Hz, 2 H), 3.90-3.62 (m, 12 H), 3.58 (m, 2 H), 1.53 (s, 18 H), 1.36 (s, 18 H), 1.22 (s, 9 H) ppm. ^{11}B{^{1}H} NMR (128 MHz, CD_2Cl_2) δ: −1.1 ppm. ^{13}C{^{1}H} NMR (100 MHz, CD_2Cl_2) δ: 149.7, 143.9 (d, J_{C-P} = 10.6 Hz), 140.5 (d, J_{C-P} = 4.0 Hz), 135.0, 133.4, 131.1 (d, J_{C-P} = 2.3 Hz), 130.0, 127.8, 126.4, 120.2, 110.1, 75.0, 71.7, 70.9, 70.8, 70.7, 70.4, 70.3, 61.6, 36.1, 35.2, 31.9, 31.5, 27.8 ppm. ^{19}F{^{1}H} NMR (376 MHz, CD_2Cl_2) δ: −152.6 ppm. ^{31}P{^{1}H} NMR (162 MHz, CD_2Cl_2) δ: 113.8 (br s) ppm. IR (neat): 2961, 2284, 1594, 1448, 1396, 1364, 1282, 1221, 1202, 1032, 932, 800, 760, 687, 644, 627, 550 cm^{-1}. HRMS ESI-MS (m/z): $[M-PhCN-BF_4]^+$ calcd. for $C_{40}H_{65}O_7PAu^+$ 885.4128, found 885.4102.

4.4 Synthesis of complex C3.



L3AuCl

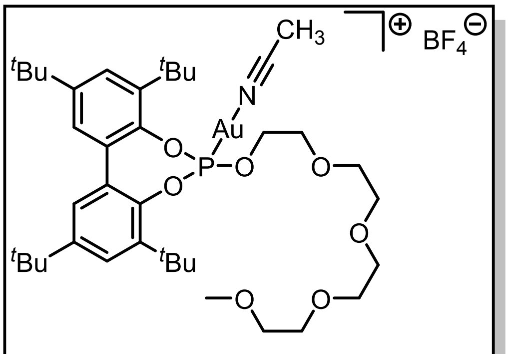
Ligand L3 gold(I) chloride: **L3**AuCl was prepared according to the described general procedure, quantitatively yielding the gold(I) chloride as a white solid. ^{1}H NMR (400 MHz, CD_2Cl_2) δ: 7.56 (d, J = 2.0 Hz, 2 H), 7.23 (d, J = 2.4 Hz, 2 H), 4.36 (m, 2 H), 3.72 (m, 2 H), 3.68-3.50 (m, 12 H), 2.13 (br s, 3 H), 1.80-1.57 (m, 12 H) 1.55 (s, 18 H), 1.38 (s, 18 H) ppm. ^{13}C{^{1}H} NMR (100 MHz, CD_2Cl_2) δ: 149.2, 144.3 (d, J_{C-P} = 10.5 Hz), 140.5 (d, J_{C-P} = 4.0 Hz), 131.4 (d, J_{C-P} = 2.1 Hz), 127.6, 126.2, 72.3, 71.8, 71.3, 71.1, 71.0, 70.1 (d, J_{C-P} = 6.5 Hz), 69.4, 59.7, 42.0, 36.9, 36.1, 35.1, 32.0, 31.6, 31.1 ppm. ^{31}P{^{1}H} NMR (162 MHz, CD_2Cl_2) δ: 122.9 ppm. IR (neat): 2905, 1437, 1396, 1363, 1221, 1116, 1085, 1035, 950, 915, 895, 798, 645, 627 cm^{-1}. HRMS ESI-MS (m/z): [M+Na]$^{+}$ calcd. for $C_{46}H_{71}O_7PAuClNa^{+}$ 1021.4184, found 1021.4180.



C3

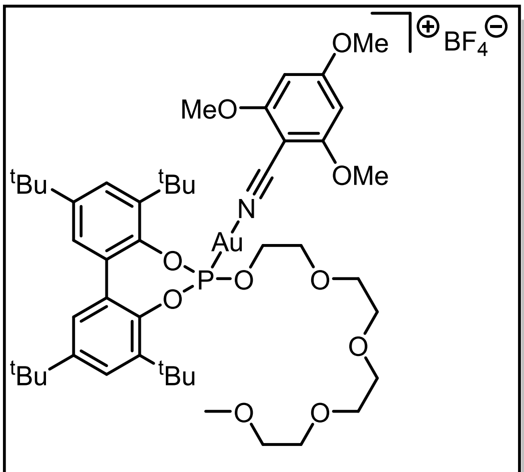
Complex C3: **C3** was prepared according to the described general procedure, obtaining 114 mg (93.1% yield) of the cationic complex as a white solid. ^{1}H NMR (400 MHz, CD_2Cl_2) δ: 7.90-7.69 (m, 3 H), 7.65-7.50 (m, 4 H), 7.24 (d, J = 2.2 Hz, 2 H), 4.52 (br d, J = 14.2 Hz, 2 H), 3.90-3.50 (m, 14 H), 2.14 (br s, 3 H), 1.90-1.57 (m, 12 H) 1.54 (s, 18 H), 1.37 (s, 18 H) ppm. ^{11}B{^{1}H} NMR (128 MHz, CD_2Cl_2) δ: −1.1 ppm. ^{13}C{^{1}H} NMR (100 MHz, CD_2Cl_2) δ: 149.8, 143.9 (d, J_{C-P} = 10.4 Hz), 140.5 (d, J_{C-P} = 3.9 Hz), 135.0, 133.4 131.1 (d, J_{C-P} = 2.0 Hz), 130.0, 127.8, 126.4, 120.2, 110.2, 74.1, 71.9, 71.0, 70.9, 70.4, 70.3, 59.8, 42.2, 36.6, 36.1, 35.2, 32.0, 31.5, 31.2 ppm. ^{19}F{^{1}H} NMR (376 MHz, CD_2Cl_2) δ: −152.5 ppm. ^{31}P{^{1}H} NMR (162 MHz, CD_2Cl_2) δ: 114.3 (br s) ppm. IR (neat): 2097, 2284, 1594, 1449, 1397, 1363, 1282, 1221, 1032, 932, 800, 760, 687, 644, 627, 550 cm^{-1}. HRMS ESI-MS (m/z): [M−PhCN−BF_4]$^{+}$ calcd. for $C_{46}H_{71}O_7PAu^{+}$ 963.4598, found 963.4594.

4.5 Syntheses of complexes $[Au(CH_3CN)(L1)]BF_4$ and $[Au(2,4,6\text{-}(MeO)_3(C_6H_2)CN)(L1)]BF_4$.



$[Au(CH_3CN)(\mathbf{L1})]BF_4$

Complex $[Au(CH_3CN)(\mathbf{L1})]BF_4$: The complex was prepared according to the described general procedure, using **L1**AuCl and acetonitrile instead of benzonitrile. 158 mg (82% yield) of the cationic complex were obtained as a white solid. ^{1}H NMR (400 MHz, CD_2Cl_2) δ: 7.56 (d, J = 2.1 Hz, 2 H), 7.23 (d, J = 2.4 Hz, 2 H), 4.45 (br d, J = 13.9 Hz, 2 H), 3.80-3.50 (m, 14 H), 3.29 (s, 3 H), 2.47 (s, 3 H), 1.52 (s, 18 H), 1.36 (s, 18 H) ppm. ^{11}B{^{1}H} NMR (128 MHz, CD_2Cl_2) δ: −1.2 ppm. ^{13}C{^{1}H} DEPTQ135 NMR (100 MHz, CD_2Cl_2) δ: 149.7, 143.9 (d, J_{C-P} = 12.1 Hz), 140.5 (d, J_{C-P} = 4.2 Hz), 131.1, 127.7, 126.3, 120.6, 108.4, 72.1, 71.2, 70.8, 70.7, 70.4, 70.1, 59.3, 36.0, 35.1, 31.9, 31.5 ppm. ^{19}F{^{1}H} NMR (376 MHz, CD_2Cl_2) δ: −153.0 ppm. ^{31}P{^{1}H} NMR (162 MHz, CD_2Cl_2) δ: 111.2 (br s) ppm. IR (neat): 2958, 2871, 1589, 1438, 1397, 1363, 1282, 1246, 1221, 1203, 1167, 1081, 1029, 931, 916, 897, 880, 853, 800, 760, 715, 685, 645, 628, 537 cm^{-1}. ESI-MS (m/z): $[M-CH_3CN-BF_4]^+$, 843.4.

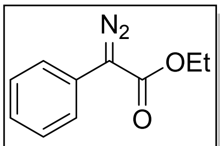


$[Au(2,4,6\text{-}(MeO)_3(C_6H_2)CN)(\mathbf{L1})]BF_4$

Complex $[Au(2,4,6\text{-}(MeO)_3(C_6H_2)CN)(\mathbf{L1})]BF_4$: The complex was prepared according to the described general procedure, but adding stoichiometric amounts of 2,4,6-trimethoxybenzonitrile. The cationic complex was obtained as a white solid (250 mg, 87% yield). ^{1}H NMR (400 MHz, CD_2Cl_2) δ: 7.58 (d, J = 1.8 Hz, 2 H), 7.24 (d, J = 2.4 Hz, 2 H), 6.2 (s, 2 H), 4.37-4.32 (m, 2 H), 3.92 (s, 9 H), 3.75-3.45 (m, 14 H), 3.31 (s, 3 H), 1.55 (s, 18 H), 1.37 (s, 18 H) ppm. ^{11}B{^{1}H} NMR (128 MHz, CD_2Cl_2) δ: −1.2 ppm. ^{13}C{^{1}H} NMR (100 MHz, CD_2Cl_2) δ: 169.4, 166.3, 150.0, 143.9 (d, J_{C-P} = 10.4 Hz), 140.4 (d, J_{C-P} = 4.0 Hz), 131.0 (d, J_{C-P} = 2.1 Hz), 127.9, 126.5, 120.1, 91.6, 72.3, 71.2, 71.0, 70.9, 70.8, 70.7, 70.6, 69.9, 69.8, 59.0, 57.1, 56.9, 36.1, 35.2, 31.9, 31.5 ppm. $^{19}F\{^{1}H\}$ NMR (376 MHz, CD_2Cl_2) δ: −153.5 ppm. $^{31}P\{^{1}H\}$ NMR (162 MHz, CD_2Cl_2) δ: 110.1 (br s) ppm. IR (neat): 2956, 2871, 2249, 1604, 1577, 1461, 1437, 1422, 1397, 1354, 1237, 1210, 1162, 1133, 1081, 1025, 933, 916, 897, 880, 800, 778, 644, 626, 521 cm^{-1}. HRMS ESI-MS (m/z): $[M-(2,4,6\text{-}(MeO)_3(C_6H_2)CN)-BF_4]^+$ calcd. for $C_{37}H_{59}O_7PAu^+$ 843.3658, found 843.3648.

5. Syntheses of Diazo Compounds 2a and 2b:[13]

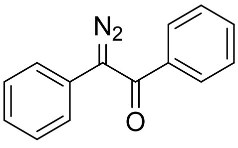
Tosyl azide: The preparation of tosyl azide (TsN_3) was performed adapting a reported procedure.[14] A solution of sodium azide (4.08 g, 62.8 mmol, 1.55 equiv.) in water (20 mL) was added dropwise over 1 h to a solution of *p*-toluenesulfonyl chloride (7.7 g, 40.4 mmol, 1 equiv.) in acetone (30 mL) at 0 ºC. The reaction was warmed at room temperature and stirred for 11 h, then the acetone was removed under vacuum, and the reaction mixture was extracted by AcOEt for three times (3 x 25 mL). The combined organic layers were washed with water (25 mL) and a saturated Na_2CO_3 solution (25 mL) and finally dried over $MgSO_4$, and then the solvent was removed under vacuum. The crude product can be used with no further purification.



2a

Phenyl ethyl diazoacetate (PhEDA), 2a: The preparation of PhEDA was carried as reported in the literature.[15] At room temperature, a solution of 1,8-diazabicyclo-[5.4.0]-undec-7-ene (DBU) (7.56 mL, 50.6 mmol, 1.5 equiv.) in anhydrous CH_3CN (20 mL) was added dropwise to a solution of ethyl phenyl acetate (5.42 mL, 33.7 mmol, 1 equiv.) and *p*-toluenesulfonyl azide (TsN_3, 7.97 g, 40.4 mmol, 1.2 equiv.) in anhydrous CH_3CN (30 mL). Then the reaction mixture was stirred at room temperature for 15 hours. After adding water (20 mL), the resulting mixture was extracted with diethyl ether (3 × 40 mL). The combined organic layers were washed with brine (20 mL) and dried over anhydrous $MgSO_4$. After the removal of the solvent under reduced pressure, the residual was purified by a silica gel column chromatography with cyclohexane/ethyl acetate (30:1) as the eluent to give **2a** as a red oil (3.21 g, 50.1% yield). ^{1}H and ^{13}C{^{1}H} NMR data were in agreement with those previously reported.[15] ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.49 (dm, *J* = 8.6 Hz, 2 H), 7.39 (tm, *J* = 7.8 Hz, 2 H), 7.19 (tm, *J* = 7.4 Hz, 1 H), 4.34 (q, *J* = 7.1 Hz, 2 H), 1.35 (t, *J* = 7.1 Hz, 3 H) ppm. ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ: 165.3, 129.0, 125.8, 125.7, 124.1, 61.1, 14.6 ppm.

[13] Azide and, especially, diazo compounds are potentially explosive and presumed to be toxic (see: A. Ford, H. Miel, A. Ring, C. N. Slattery, A. R. Maguire and M. A. McKervey, Modern Organic Synthesis with α-Diazocarbonyl Compounds. *Chem. Rev.*, 2015, **115**, 9981-10080). For this reason, these compounds should not be heated and contact with metallic accessories should be avoided. One should take all reported steps to handle these compounds safely.
[14] N. Wang, R. Li, L. Li, S. Xu, H. Song and B. Wang, Rhodium(III)-Catalyzed Intermolecular Amidation with Azides via C(sp^3)-H Functionalization. *J. Org. Chem.*, 2014, **79**, 5379-5385.
[15] M. Hu, Z. He, B. Gao, L. Li, C. Ni and J. Hu, Copper-Catalyzed *gem*-Difluoroolefination of Diazo Compounds with $TMSCF_3$ via C-F Bond Cleavage. *J. Am. Chem. Soc.*, 2013, **135**, 17302-17305.

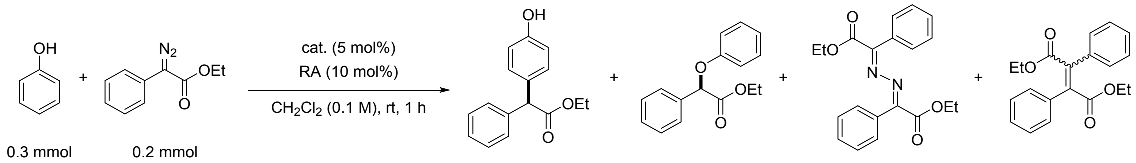


2b

2-diazo-1,2-diphenylethan-1-one, 2b: The preparation of substrate **2b** was performed by a Swern-type oxidation as reported in the literature.[16] To a flame-dried Schlenk flask provided with a stirrer under inert atmosphere were added dry DMSO (0.634 mL, 8.92 mmol, 2 equiv.) and THF (30 mL) and were stirred at −55 °C. Oxalyl chloride (0.64 mL, 6.69 mmol, 1.5 equiv.) was added dropwise to this solution, observing bubbling due to the release of CO_2. The reaction was maintained at −55 ºC until gas evolution ceased (~20 min) at which point the reaction was cooled further to −78 ºC. A solution of benzyl monohydrazone (1 g, 4.46 mmol, 1 equiv.) and Et_3N (1.88 mL, 13.4 mmol, 3 equiv.) in THF (15 mL) was added dropwise to provide a bright yellow solution containing a white precipitate. The reaction mixture was maintained at −78 °C for 1 h and was then vacuum filtered under an atmosphere of nitrogen through a medium porosity sintered glass funnel. The filtrate was diluted with diethyl ether (200 mL) and washed with water (400 mL), sat. aq. $NaHCO_3$ (2 x 200 mL), brine (200 mL), dried over Na_2SO_4, and concentrated *in vacuo* to provide **2b** (0.35 g, 35.6% yield) as a fair orange solid. ^1H and $^{13}C\{^1H\}$ NMR data were in agreement with those previously reported.[17] ^1H NMR (500 MHz, $CDCl_3$) δ: 7.57-7.50 (m, 2H), 7.46-7.36 (m, 3H), 7.36-7.28 (m, 4H), 7.21-7.14 (m, 1H) ppm. $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$) δ: 188.5, 138.1, 131.8, 129.2, 128.6, 127.9, 127.1, 126.2, 126.1 ppm.

[16] M. I. Javed and M. Brewer, Diazo Preparation via Dehydrogenation of Hydrazones with "Activated" DMSO. *Org. Lett.*, 2007, **9**, 1789-1792.
[17] H. Keipour, A. Jalba, L. Delage-Laurin and T. Ollevier, Copper-Catalyzed Carbenoid Insertion Reactions of α-Diazoesters and α-Diazoketones into Si-H and S-H Bonds. *J. Org. Chem.*, 2017, **82**, 3000-3010.

6. General Procedure for Au-mediated Selective Functionalisation of Aromatic Alcohols:



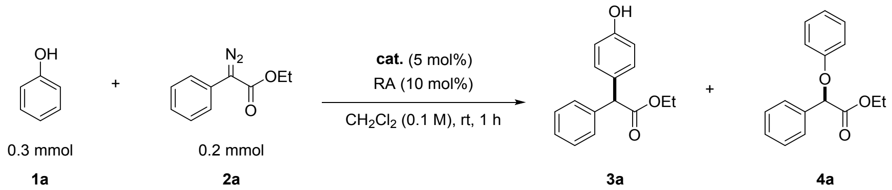
Scheme SI 3. General procedure for gold(I)-catalysed phenol **1a** functionalisation with PhEDA **2a**.

In the glove box, under inert atmosphere, to a dried screw-capped vial (10 mL) provided with a septum and a stirrer were transferred the catalyst (5 mol%) and the regulation agent (RA, 10 mol%), along with 0.5 mL of CH_2Cl_2, and the solution was stirred for 5 minutes. Phenol (**1a**, 0.3 mmol) was subsequently added with 0.5 mL of CH_2Cl_2, and the solution was let stir for 5 minutes. After that time, PhEDA (**2a**, 0.2 mmol) solution in 1 mL of CH_2Cl_2 (final solution concentration 0.1 M) was dropwise added, observing intense bubbling due to the release of N_2. Once the addition was complete, the solution was stirred for 1 hour, to ensure the complete consumption of the diazo compound (checked by TLC analysis, AcOEt:Cy 1:6). This solution was filtrated through nylon filter (0.45 μm), evaporated to dryness and then analysed by quantitative NMR.

NMR yield: The yield towards functionalised aromatic alcohols was calculated using ^1H qNMR, employing 1,3,5-trimethoxybenzene (TMB) as internal standard. The different isomers, **3** (C–H functionalisation product) and **4** (O–H functionalisation product), were quantified by identifying the corresponding characteristic methylene proton signals (δ = 6.0-4.5 ppm).

7. Complete Set of Results for Au-mediated Selective Functionalisation of Aromatic Alcohols:

7.1. Control experiments:



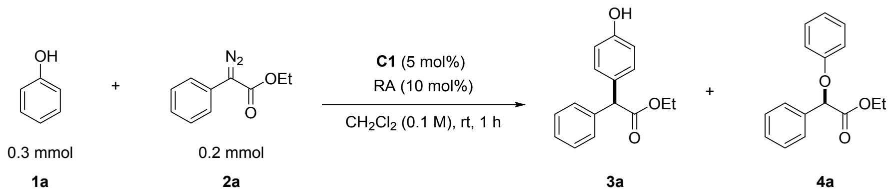
Scheme SI 4. Control experiments for Au-mediated selective functionalisation of **1a** with **2a**.

Table SI 1. Control experiments for Au-mediated selective functionalisation of **1a** with **2a**.[a]

Entry	cat.	RA	3a % yield	4a % yield	3:4 ratio
1	$AgBF_4$	none	6.7	55.6	1:8
2	$(Me_2S)AuCl$	none	<1	<1	-
3	none	$CsBF_4$	n.d.	n.d.	-
4[b]	**C1**	NaBArF	1.4	7.0	1:5
5	**L1**AuCl	none	<1	<1	-
6[c]	[Au(A)(**L1**)]BF_4	none	76.0	1.0	>50 : 1
7[d]	[Au(B)(**L1**)]BF_4	none	66.0	5.7	11:1

[a]Reactions were performed under inert atmosphere for 1 h at 25 °C. Yields determined by ^{1}H NMR using 1,3,5-trimethoxybenzene as internal standard. [b]15 mol% of NaBArF. [c]A = CH_3CN. [d]B = 2,4,6-$(CH_3O)_3(C_6H_2)CN$.

7.2. Catalytic Au-mediated Selective Functionalisation of 1a with 2a using complex C1:



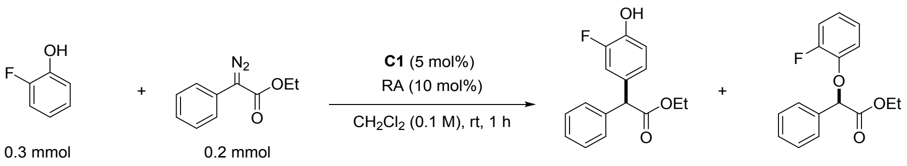
Scheme SI 5. Catalytic Au-mediated selective functionalisation of **1a** with **2a** using complex **C1**.

Table SI 2. Catalytic Au-mediated selective functionalisation of **1a** with **2a** using complex **C1**.[a]

Entry	RA	3a % yield	4a % yield	3:4 ratio	Regulation effects 3/4
1	none	83.0	2.9	28:1	-
2	$LiBF_4$	83.5	2.4	35:1	+0.5/−0.5
3	$NaBF_4$	87.3	3.0	30:1	+4.3/+0.1
4	KBF_4	86.1	2.4	37:1	+3.1/−0.5
5	$RbBF_4$	85.5	2.8	31:1	+2.5/−0.1
6	$CsBF_4$	87.7 (80.0)	1.5	58:1	+4.7/−1.4
7	NH_4BF_4	72.6	3.1	24:1	−10.4/+0.2

[a]Reactions were performed under inert atmosphere and reacted for 1 h at 25 ºC. Yields determined by ^1H NMR using 1,3,5-trimethoxybenzene as internal standard. Isolated yields in parentheses.

7.3. Catalytic Au-mediated Selective Functionalisation of 1b with 2a using complex C1:



1b **2a** **3b** **4b**

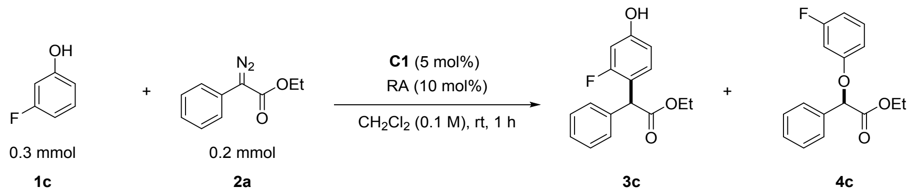
Scheme SI 6. Catalytic Au-mediated selective functionalisation of **1b** with **2a** using complex **C1**.

Table SI 3. Catalytic Au-mediated selective functionalisation of **1b** with **2a** using complex **C1**.[a]

Entry	RA	3b % yield	4b % yield	3:4 ratio	Regulation effects 3/4
1	none	41.0	6.2.	7:1	-
2	$LiBF_4$	46.3	6.7	7:1	+5.3/+0.5
3	$NaBF_4$	46.7	5.3	9:1	+5.7/–0.9
4	KBF_4	50.6	4.2	12:1	+9.6/–2.0
5	$RbBF_4$	60.6 (59.6)	5.6	11:1	+19.6/–0.6
6	$CsBF_4$	40.6	7.8	5:1	–0.4/+1.6

[a]Reactions were performed under inert atmosphere and reacted for 1 h at 25 ºC. Yields determined by ^{1}H NMR using 1,3,5-trimethoxybenzene as internal standard. Isolated yields in parentheses.

7.4. Catalytic Au-mediated Selective Functionalisation of 1c with 2a using complex C1:



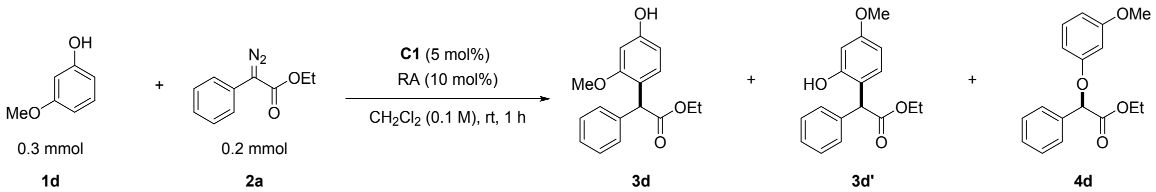
Scheme SI 7. Catalytic Au-mediated selective functionalisation of **1c** with **2a** using complex **C1**.

Table SI 4. Catalytic Au-mediated selective functionalisation of **1c** with **2a** using complex **C1**.[a]

Entry	RA	3c % yield	4c % yield	3:4 ratio	Regulation effects 3/4
1	none	65.0	3.9	17:1	-
2	$LiBF_4$	63.0	3.4.	18:1	−2.0/−0.5
3	$NaBF_4$	63.4	5.3	12:1	−1.6/+1.4
4	KBF_4	61.6	5.4	11:1	−3.4/+1.5
5	$RbBF_4$	66.1	6.5	10:1	+1.1/+2.6
6	$CsBF_4$	68.3 (60.2)	3.9	18:1	+3.3/0

[a]Reactions were performed under inert atmosphere and reacted for 1 h at 25 ºC. Yields determined by ^{1}H NMR using 1,3,5-trimethoxybenzene as internal standard. Isolated yields in parentheses.

7.5. Catalytic Au-mediated Selective Functionalisation of 1d with 2a using complex C1:



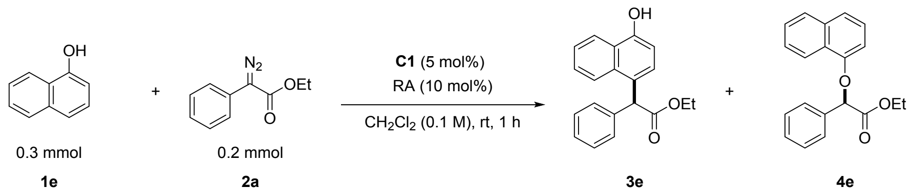
Scheme SI 8. Catalytic Au-mediated selective functionalisation of **1d** with **2a** using complex **C1**.

Table SI 5. Catalytic Au-mediated selective functionalisation of **1d** with **2a** using complex **C1**.[a]

Entry	RA	3d % yield	3d' % yield	4d % yield[b]	3:4 ratio	Regulation effects 3/4
1	None	42.1	44.6	n.d.	-	-
2	$LiBF_4$	40.6	43.0	n.d.	-	−3.1/-
3	$NaBF_4$	38.0	43.4	n.d.	-	−5.3/-
4	KBF_4	43.7	44.8	n.d.	-	+1.8/-
5	$RbBF_4$	39.0	39.3	n.d.	-	−8.4/-
6	$CsBF_4$	44.7 (38.8)	45.9 (38.8)	n.d.	-	+3.9/-

[a]Reactions were performed under inert atmosphere and reacted for 1 h at 25 ºC. Yields determined by ^{1}H NMR using 1,3,5-trimethoxybenzene as internal standard. Isolated yields in parentheses. [b]O–H insertion product could not be isolated.

7.6. Catalytic Au-mediated Selective Functionalisation of 1e with 2a using complex C1:



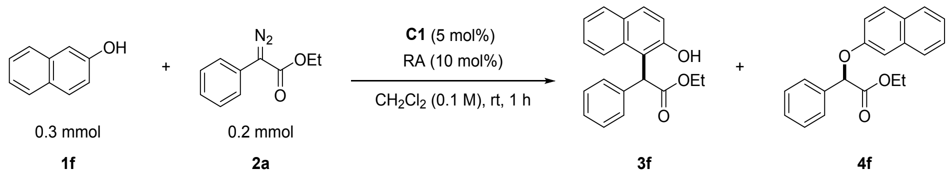
Scheme SI 9. Catalytic Au-mediated selective functionalisation of **1e** with **2a** using complex **C1**.

Table SI 6. Catalytic Au-mediated selective functionalisation of **1e** with **2a** using complex **C1**.[a]

Entry	RA	3e % yield	4e % yield[b]	3:4 ratio	Regulation effects 3/4
1	none	88.9	n.d.	-	-
2	$LiBF_4$	94.3	n.d.	-	+5.4/-
3	$NaBF_4$	92.7	n.d.	-	+3.8/-
4	KBF_4	81.9	n.d.	-	−7.0/-
5	$RbBF_4$	98.5	n.d.	-	+9.6/-
6	$CsBF_4$	98.7 (81.6)	n.d.	-	+9.8/-

[a]Reactions were performed under inert atmosphere and reacted for 1 h at 25 ºC. Yields determined by ^{1}H NMR using 1,3,5-trimethoxybenzene as internal standard. Isolated yields in parentheses. [b]O–H insertion product could not be isolated.

7.7. Catalytic Au-mediated Selective Functionalisation of 1f with 2a using complex C1:



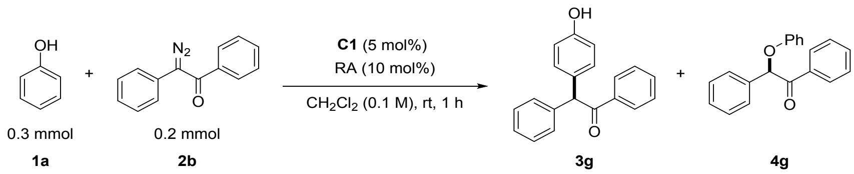
Scheme SI 10. Catalytic Au-mediated selective functionalisation of **1f** with **2a** using complex **C1**.

Table SI 7. Catalytic Au-mediated selective functionalisation of **1f** with **2a** using complex **C1**.[a]

Entry	RA	3f % yield	4f % yield[b]	3:4 ratio	Regulation effects 3/4
1	none	44.1	n.d.	-	-
2	$LiBF_4$	19.3	n.d.	-	–24.8/-
3	$NaBF_4$	36.8	n.d.	-	–7.3/-
4	KBF_4	46.1	n.d.	-	+2.0/-
5	$RbBF_4$	47.9 (50.1)	n.d.	-	+3.8/-
6	$CsBF_4$	43.9	n.d.	-	–0.2/-

[a]Reactions were performed under inert atmosphere and reacted for 1 h at 25 ºC. Yields determined by ^{1}H NMR using 1,3,5-trimethoxybenzene as internal standard. Isolated yields in parentheses. [b]O–H insertion product could not be isolated.

7.8. Catalytic Au-mediated Selective Functionalisation of 1a with 2b using complex C1:



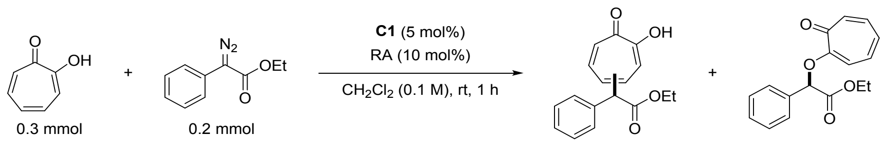
Scheme SI 11. Catalytic Au-mediated selective functionalisation of **1a** with **2b** using complex **C1**.

Table SI 8. Catalytic Au-mediated selective functionalisation of **1a** with **2b** using complex **C1**.[a]

Entry	RA	3g % yield	4g % yield[b]	3:4 ratio	Regulation effects 3/4
1	none	14.9	n.d.	-	-
2	$LiBF_4$	14.4	n.d.	-	–0.5/-
3	$NaBF_4$	14.2	n.d.	-	–0.7/-
4	KBF_4	15.9	n.d.	-	+1.0/-
5	$RbBF_4$	28.4	n.d.	-	+13.5/-
6	$CsBF_4$	34.4 (17.4)	n.d.	-	+19.5/-

[a]Reactions were performed under inert atmosphere and reacted for 1 h at 25 ºC. Yields determined by ^{1}H NMR using 1,3,5-trimethoxybenzene as internal standard. Isolated yields in parentheses. Unidentified by-products were observed ^{1}H NMR. [b]O–H insertion product could not be isolated.

7.9. Catalytic Au-mediated Selective Functionalisation of 1h with 2a using complex C1:



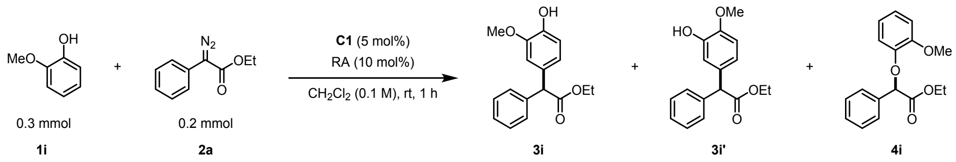
Scheme SI 12. Catalytic Au-mediated selective functionalisation of **1h** with **2a** using complex **C1**.

Table SI 9. Catalytic Au-mediated selective functionalisation of **1h** with **2a** using complex **C1**.[a]

Entry	RA	3h % yield[b]	4h % yield	3:4 ratio	Regulation effects 3/4
1	none	n.d.	16.7	-	-
2	$LiBF_4$	n.d.	11.7	-	-/–5.0
3	$NaBF_4$	n.d.	16.3	-	-/–0.4
4	KBF_4	n.d.	15.5	-	-/–1.2
5	$RbBF_4$	n.d.	17.7 (10.6)	-	-/+1.0
6	$CsBF_4$	n.d.	16.6	-	-/–0.1

[a]Reactions were performed under inert atmosphere and reacted for 1 h at 25 ºC. Yields determined by ^{1}H NMR using 1,3,5-trimethoxybenzene as internal standard. Isolated yields in parentheses. [b]C–H insertion product could not be isolated.

7.10. Catalytic Au-mediated Selective Functionalisation of 1i with 2a using complex C1:



Scheme SI 13. Catalytic Au-mediated selective functionalisation of **1i** with **2a** using complex **C1**.

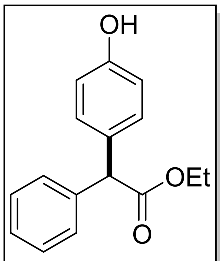
Table SI 10. Catalytic Au-mediated selective functionalisation of **1i** with **2a** using complex **C1**.[a]

Entry	RA	Yield (%) 3i	Yield (%) 3i'	Yield (%) 4i	3:4 Ratio	Regulation effects 3/4
1	None	26.4	60.6	0.5	>50:1	-
2	$LiBF_4$	26.7 (18.5)	65.5(50.0)	1.4	>50:1	□5.2/+0.9
3	$CsBF_4$	25.3	61.7	1.5	>50:1	0/+1.0

[a] Reactions were performed under inert atmosphere for 1 h at 25 °C. Yields determined by ^1H NMR using 1,3,5-trimethoxybenzene as internal standard. Isolated yields in parentheses. Products **3i** and **3i'** were isolated as a mixture.

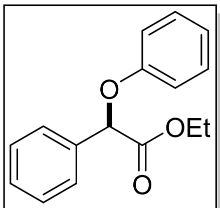
8. Characterisation of Functionalised Products 3, 4, 5 and 6:

Functionalised aromatic alcohols esters were isolated from the crude reactions by column chromatography using SiO_2 and ethyl acetate (AcOEt) and cyclohexane (Cy) mixtures as the eluents. O–H functionalisation isomers **4** were formed in low amounts, which made isolation not possible. Thus, O–H functionalisation isomers were selectively prepared using $AgBF_4$ when possible (**4a**-**4c**), since $AgBF_4$ catalysed their formation (see Table SI 1, entry 1). Aside of functionalised aromatic alcohols, when using phenyl-ethyl-diazoacetate **2a** the corresponding diazo coupling products (**5** and **6**, see Scheme SI 3) were obtained as minor components of the reaction mixture, therefore their characterisation has been also included in this section.



3a

Ethyl 2-(4-hydroxyphenyl)-2-phenylacetate, 3a: The preparation of product **3a** was afforded using the general procedure employing complex **C1** and $CsBF_4$ as the regulation agent. The reaction crude mixture was purified by column chromatography using SiO_2 and Cy and AcOEt as the eluents (30:1→10:1, Cy:AcOEt), to afford **3a** as a colourless solid (41.0 mg, 80.0% yield). ^{1}H and $^{13}C\{^{1}H\}$ NMR data were in agreement with those previously reported.[18] ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.28-7.15 (m, 5 H), 7.11 (dm, J = 8.5 Hz, 2 H), 6.70 (dm, J = 8.6 Hz, 2 H), 4.88 (s, 1 H), 4.64 (br s, 1 H), 4.13 (q, J = 7.1 Hz, 2 H), 1.18 (t, J = 7.1 Hz, 3 H) ppm. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ: 173.3, 155.0, 139.1, 130.9, 130.0, 128.7, 128.6, 127.3, 115.6, 61.4, 56.5, 14.2 ppm.



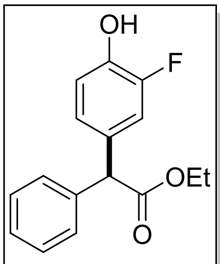
4a

Ethyl 2-phenoxy-2-phenylacetate, 4a: The preparation of product **4a** was afforded using the general procedure employing $AgBF_4$ as the catalyst. The reaction crude mixture was purified by column chromatography using SiO_2 and Cy and AcOEt as the eluents (30:1, Cy:AcOEt), to afford **4a** as a yellow oil (22.0 mg, 42.9% yield). ^{1}H and $^{13}C\{^{1}H\}$ NMR data were in agreement with those previously reported.[19] ^{1}H NMR

[18] Z. Yu, B. Ma, M. Chen, H.-H. Wu, L. Liu and J. Zhang, Highly Site-Selective Direct C-H Bond Functionalization of Phenols with α-Aryl-α-diazoacetates and Diazooxindoles via Gold Catalysis. *J. Am. Chem. Soc.*, 2014, **136**, 6904-6907.

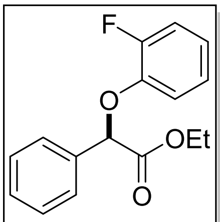
[19] G. Tseberlidis, A. Caselli and R. Vicente, Carbene X-H Bond Insertions Catalyzed by Copper(I) Macrocyclic Pyridine-Containing Ligand (PcL) Complexes. *J. Organomet. Chem.*, 2017, **835**, 1-5.

(400 MHz, $CDCl_3$) δ: 7.52 (dm, J = 7.9 Hz, 2 H), 7.36-7.26 (m, 3 H), 7.24-7.16 (m, 2 H), 6.94-6.86 (m, 3 H), 5.55 (s, 1 H), 4.13 (m, 2 H), 1.13 (t, J = 7.1 Hz, 3 H) ppm. $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ: 170.1, 157.5, 135.7, 129.7, 129.0, 128.9, 127.2, 121.9, 115.6, 78.8, 61.7, 14.1 ppm.



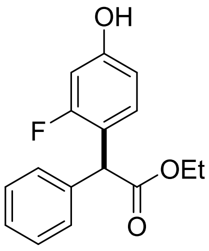
3b

Ethyl 2-(3-fluoro-4-hydroxyphenyl)-2-phenylacetate, 3b: The preparation of product **3b** was afforded using the general procedure employing complex **C1** and $RbBF_4$ as the regulation agent. The reaction crude mixture was purified by column chromatography using SiO_2 and Cy and AcOEt as the eluents (30:1→10:1, Cy:AcOEt), to afford **3b** as a pale yellowish oil (32.7 mg, 59.6% yield). ^1H and $^{13}C\{^1H\}$ NMR data were in agreement with those previously reported.[22] ^1H NMR (400 MHz, $CDCl_3$) δ: 7.37-7.27 (m, 5 H), 7.07 (dd, J = 11.6, 2.0 Hz, 1 H), 7.00-6.90 (m, 2 H), 5.02 (br s, 1 H), 4.92 (s, 1 H), 4.21 (q, J = 7.1 Hz, 2 H), 1.26 (t, J = 7.1 Hz, 3 H) ppm. $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ: 172.6, 151.0 (d, J_{C-F} = 237.9 Hz), 142.9 (d, J_{C-F} = 14.5 Hz), 138.5, 131.7 (d, J_{C-F} = 6.0 Hz), 128.8, 128.5, 127.5, 125.1 (d, J_{C-F} = 3.5 Hz), 117.3 (d, J_{C-F} = 2.1 Hz), 116.0 (d, J_{C-F} = 19.4 Hz), 61.5, 56.2, 14.2 ppm. $^{19}F\{^1H\}$ NMR (376 MHz, $CDCl_3$) δ: −140.5 ppm.



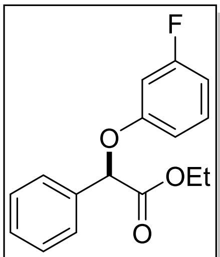
4b

Ethyl 2-(2-fluorophenoxy)-2-phenylacetate, 4b: The preparation of product **4b** was afforded using the general procedure employing $AgBF_4$ as the catalyst. The reaction crude mixture was purified by column chromatography using SiO_2 and Cy and AcOEt as the eluents (30:1, Cy:AcOEt), to afford **4b** as a pale yellow oil (13.9 mg, 25.3% yield). ^1H NMR (400 MHz, $CDCl_3$) δ: 7.62-7.56 (m, 2 H), 7.44-7.34 (m, 3 H), 7.14-7.04 (m, 1 H), 7.03-6.90 (m, 3 H), 5.64 (s, 1 H), 4.20 (m, 2 H), 1.20 (t, J = 7.1 Hz, 3 H) ppm. $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ: 169.7, 153.5 (d, J_{C-F} = 246.8 Hz), 145.3 (d, J_{C-F} = 10.8 Hz), 135.3, 129.2, 128.9, 127.3, 124.4 (d, J_{C-F} = 4.1 Hz), 123.0 (d, J_{C-F} = 7.2 Hz), 117.9 (d, J_{C-F} = 1.3 Hz), 116.8 (d, J_{C-F} = 18.4 Hz), 80.3, 61.8, 14.1 ppm. $^{19}F\{^1H\}$ NMR (376 MHz, $CDCl_3$) δ: −131.8 ppm. IR (neat): 3069, 2989, 2925, 2853, 1734, 1613, 1592, 1506, 1477, 1455, 1367, 1322, 1306, 1278, 1258, 1212, 1178, 1110, 1083, 1055, 1019, 947, 929, 915, 886, 843, 798, 779, 752, 725, 688, 615, 491 cm^{-1}. HRMS ESI-MS (m/z): $[M+Na]^+$ calcd. for $C_{16}H_{15}FO_3Na^+$ 297.0897, found 297.0887.



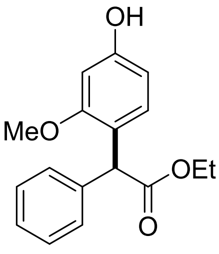
3c

Ethyl 2-(2-fluoro-4-hydroxyphenyl)-2-phenylacetate, 3c: The preparation of product **3c** was afforded using the general procedure employing complex **C1** and $CsBF_4$ as the regulation agent. The reaction crude mixture was purified by column chromatography using SiO_2 and Cy and AcOEt as the eluents (30:1→10:1, Cy:AcOEt), to afford **3c** as a colourless oil that solidified upon standing (33 mg, 60.2% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.39-7.27 (m, 5 H), 6.94 (t, J = 8.6 Hz, 1 H), 6.49 (dd, J = 11.3, 2.5 Hz, 1 H), 6.44 (dd, J = 8.5, 2.5 Hz, 1 H), 6.01 (br s, 1 H), 5.19 (s, 1 H), 4.23 (m, 2 H), 1.26 (t, J = 7.1 Hz, 3 H) ppm. $^{13}C\{^1H\}$ NMR (76 MHz, $CDCl_3$) δ: 173.6, 160.9 (d, J_{C-F} = 245.9 Hz), 156.7 (d, J_{C-F} = 11.6 Hz), 137.1, 130.4 (d, J_{C-F} = 5.3 Hz), 128.9, 128.8, 127.6, 117.7 (d, J_{C-F} = 15.1 Hz), 111.5 (d, J_{C-F} = 2.9 Hz), 103.3 (d, J_{C-F} = 25.2 Hz), 61.9, 49.8 (d, J_{C-F} = 2.6 Hz), 14.1 ppm. $^{19}F\{^1H\}$ NMR (376 MHz, $CDCl_3$) δ: −115.1 ppm. IR (neat): 3400 (OH), 3321 (OH), 3061, 3029, 2983, 2903, 1713, 1624, 1596, 1507, 1493, 1454, 1371, 1340, 1300, 1272, 1238, 1191, 1151, 1109, 1089, 1021, 964, 846, 822, 791, 737, 699, 628, 599, 563, 547, 527 cm^{-1}. HRMS ESI-MS (m/z): $[M+Na]^+$ calcd. for $C_{16}H_{15}FO_3Na^+$ 297.0897, found 297.0894.



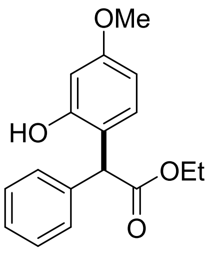
4c

Ethyl 2-(3-fluorophenoxy)-2-phenylacetate, 4c: The preparation of product **4c** was afforded using the general procedure employing $AgBF_4$ as the catalyst. The reaction crude mixture was purified by column chromatography using SiO_2 and Cy and AcOEt as the eluents (30:1, Cy:AcOEt), to afford **4c** as a pale yellow oil (21.2 mg, 38.6% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.60-7.54 (m, 2 H), 7.44-7.34 (m, 3 H), 7.25-7.17 (m, 1 H), 6.77-6.65 (m, 3 H), 5.59 (s, 1 H), 4.21 (m, 2 H), 1.21 (t, J = 7.1 Hz, 3 H) ppm. $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$) δ: 169.6, 163.6 (d, J_{C-F} = 246.0 Hz), 158.7 (d, J_{C-F} = 10.7 Hz), 135.2, 130.5 (d, J_{C-F} = 10.0 Hz), 129.2, 129.0, 127.2, 111.2 (d, J_{C-F} = 2.8 Hz), 108.8 (d, J_{C-F} = 21.3 Hz), 103.6 (d, J_{C-F} = 25.0 Hz), 79.0, 61.9, 14.1 ppm. $^{19}F\{^1H\}$ NMR (376 MHz, $CDCl_3$) δ: −111.3 ppm. IR (neat): 2982, 1751, 1610, 1594, 1488, 1448, 1370, 1261, 1205, 1182, 1165, 1134, 1083, 1055, 1024, 964, 850, 831, 762, 726, 695, 678 cm^{-1}. HRMS ESI-MS (m/z): $[M+Na]^+$ calcd. for $C_{16}H_{15}FO_3Na^+$ 297.0897, found 297.0890.



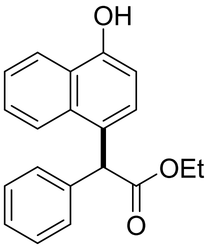
3d

Ethyl 2-(4-hydroxy-2-methoxyphenyl)-2-phenylacetate, 3d: The preparation of product **3d** was afforded using the general procedure employing complex **C1** and $CsBF_4$ as the regulation agent. The reaction crude mixture was purified by column chromatography using SiO_2 and Cy and AcOEt as the eluents (30:1→10:1, Cy:AcOEt), to afford **3d** as a colourless oil (22.2 mg, 38.8% yield). Assignment was done by comparing with reported methyl 2-(4-hydroxy-2-methoxyphenyl)-2-phenylacetate.[22] ^1H NMR (500 MHz, $CDCl_3$) δ: 7.30-7.15 (m, 5 H), 6.65 (d, J = 8.4 Hz, 1 H), 6.25 (d, J = 2.4 Hz, 1 H), 6.14 (dd, J = 8.3, 2.4 Hz, 1 H), 5.68 (br s, 1 H), 5.10 (s, 1 H), 4.12 (m, 2 H), 3.65 (s, 3 H), 1.16 (t, J = 7.1 Hz, 3 H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ: 174.3, 157.8, 156.5, 137.9, 129.8, 129.1, 128.7, 127.2, 119.7, 107.0, 99.1, 61.3, 55.4, 50.8, 14.2 ppm. IR (neat): 3392 (OH), 2980, 2251, 1709, 1615, 1597, 1508, 1467, 1432, 1369, 1296, 1195, 1157, 1111, 1032, 957, 907, 834, 727, 698, 647, 539 cm^{-1}. HRMS ESI-MS (m/z): $[M-H]^-$ calcd. for $C_{17}H_{17}O_4^-$ 285.1132, found 285.1131.



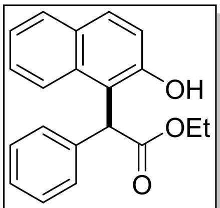
3d'

Ethyl 2-(2-hydroxy-4-methoxyphenyl)-2-phenylacetate, 3d': The preparation of product **3d'** was afforded using the general procedure employing complex **C1** and $CsBF_4$ as the regulation agent. The reaction crude mixture was purified by column chromatography using SiO_2 and Cy and AcOEt as the eluents (30:1→10:1, Cy:AcOEt), to afford **3d'** as a colourless oil (22.2 mg, 38.8% yield). Assignment was done by comparing with reported methyl 2-(2-hydroxy-4-methoxyphenyl)-2-phenylacetate.[22] ^1H NMR (500 MHz, $CDCl_3$) δ: 7.77 (s, 1 H), 7.25-7.10 (m, 5 H), 6.92 (d, J = 8.4 Hz, 1 H), 6.42-6.34 (m, 2 H), 4.96 (s, 1 H), 4.20 (m, 2 H), 3.67 (s, 3 H), 1.23 (t, J = 7.1 Hz, 3 H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ: 175.7, 160.7, 156.1, 137.4, 131.8, 128.7, 127.9, 127.4, 116.4, 106.6, 103.5, 62.2, 55.4, 54.3, 14.2 ppm. IR (neat): 3391 (OH), 2981, 2838, 1705, 1617, 1519, 1445, 1370, 1292, 1199, 1161, 1105, 1025, 960, 908, 831, 728, 698, 636 cm^{-1}. HRMS ESI-MS (m/z): $[M-H]^-$ calcd. for $C_{17}H_{17}O_4^-$ 285.1132, found 285.1133.



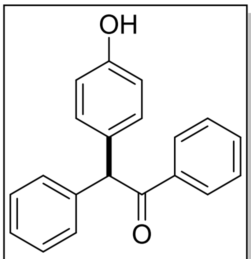
3e

Ethyl 2-(4-hydroxynaphthalen-1-yl)-2-phenylacetate, 3e: The preparation of product **3e** was afforded using the general procedure employing complex **C1** and $CsBF_4$ as the regulation agent. The reaction crude mixture was purified by column chromatography using SiO_2 and Cy and AcOEt as the eluents (30:1→10:1, Cy:AcOEt), to afford **3e** as a pale yellow oil that solidified upon standing (50 mg, 81.6% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.23 (dd, *J* = 6.9, 2.0 Hz, 1 H), 7.95 (dd, *J* = 7.1, 1.8 Hz, 1 H), 7.49 (m, 2 H), 7.36-7.27 (m, 5 H), 7.13 (d, *J* = 7.8 Hz, 1 H), 6.69 (d, *J* = 7.9 Hz, 1 H), 5.68 (s, 1 H), 5.39 (br s, 1 H), 4.24 (m, 2 H), 1.25 (t, *J* = 7.1 Hz, 3 H) ppm. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ: 173.6, 151.4, 138.3, 132.8, 129.1, 128.8, 127.4, 127.1, 127.0, 126.6, 125.1, 123.2, 122.7, 108.1, 61.6, 53.4, 14.3 ppm. IR (neat): 3401 (OH), 3064, 3029, 2981, 2936, 1708, 1626, 1599, 1587, 1518, 1496, 1475, 1453, 1378, 1351, 1309, 1278, 1258, 1178, 1148, 1094, 1061, 1023, 907, 813, 759, 730, 710, 697, 648 cm^{-1}. HRMS ESI-MS (m/z): $[M-H]^-$ calcd. for $C_{20}H_{17}O_3^-$ 305.1183, found 305.1177.



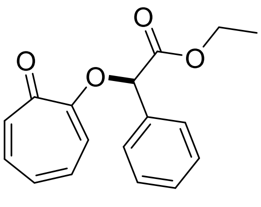
3f

Ethyl 2-(2-hydroxynaphthalen-1-yl)-2-phenylacetate, 3f: The preparation of product **3f** was afforded using the general procedure employing complex **C1** and $RbBF_4$ as the regulation agent. The reaction crude mixture was purified by column chromatography using SiO_2 and Cy and AcOEt as the eluents (30:1→10:1, Cy:AcOEt), to afford **3f** as a colourless solid (30.7 mg, 50.1% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.39 (s, 1 H), 7.95 (d, *J* = 8.7 Hz, 1 H), 7.74 (d, *J* = 7.5 Hz, 1 H), 7.70 (d, *J* = 8.8 Hz, 1 H), 7.43 (t, *J* = 8.4 Hz, 1 H), 7.28 (t, *J* = 7.8 Hz, 1 H), 7.25-7.05 (m, 6 H), 5.93 (s, 1 H), 4.24 (m, 2 H), 1.24 (t, *J* = 7.1 Hz, 3 H) ppm. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ: 176.4, 154.4, 136.7, 133.5, 130.5, 129.6, 129.1, 128.8, 127.6, 127.5, 127.3, 123.4, 121.8, 120.8, 114.6, 62.7, 48.7, 14.2 ppm. IR (neat): 3378 (OH), 3066, 3025, 2978, 2951, 2923, 1709, 1627, 1606, 1581, 1511, 1497, 1474, 1453, 1438, 1390, 1367, 1356, 1342, 1305, 1275, 1256, 1207, 1176, 1111, 1066, 1024, 986, 938, 813, 771, 748, 729, 715, 698, 625, 597 cm^{-1}. HRMS ESI-MS (m/z): $[M-H]^-$ calcd. for $C_{20}H_{17}O_3^-$ 305.1183, found 305.1181.



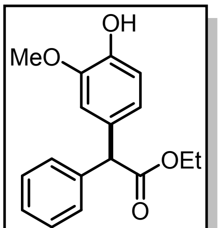
3g

2-(4-hydroxyphenyl)-1,2-diphenylethan-1-one, 3g: The preparation of product **3g** was afforded using the general procedure employing complex **C1** and $CsBF_4$ as the regulation agent. The reaction crude mixture was purified by column chromatography using SiO_2 and Cy and AcOEt as the eluents (10:1→5:1, Cy:AcOEt), to afford **3g** as a yellow oil (10 mg, 17.4% yield). ^{1}H and $^{13}C\{^{1}H\}$ NMR data were in agreement with those previously reported.[20] ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.00 (dm, *J* = 8.6 Hz, 2 H), 7.51 (tm, *J* = 7.4 Hz, 1 H), 7.41 (tm, *J* = 7.6 Hz, 2 H), 7.35-7.20 (m, 5 H), 7.13 (dm, *J* = 8.6 Hz, 2 H), 6.76 (dm, *J* = 8.6 Hz, 2 H), 5.98 (s, 1 H), 5.03 (br s, 1 H) ppm. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ: 198.8, 154.8, 139.5, 136.9, 133.2, 131.3, 130.5, 129.1, 129.1, 128.8, 128.7, 127.2, 115.8, 58.7 ppm.

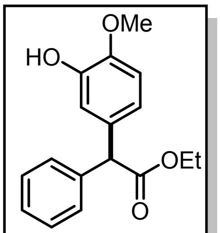


4h

Ethyl 2-((7-oxocyclohepta-1,3,5-trien-1-yl)oxy)-2-phenylacetate, 4h: The preparation of product **4h** was afforded using the general procedure employing complex **C1** and $RbBF_4$ as the regulation agent. The reaction crude mixture was purified by column chromatography using SiO_2 and Cy and AcOEt as the eluents (10:1→2:1, Cy:AcOEt), to afford **4h** as a red oil (6.0 mg, 10.6% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.58 (dd, *J* = 7.8, 1.6 Hz, 2 H), 7.42-7.31 (m, 3 H), 7.22-7.16 (m, 2 H), 7.04-6.84 (m, 3 H), 6.04 (s, 1 H), 4.19 (m, 2 H), 1.19 (t, *J* = 7.1 Hz, 3 H) ppm. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ: 181.0, 169.3, 16.4, 138.8, 136.3, 135.1, 132.5, 130.2, 129.1, 128.7, 127.5, 121.2, 79.1, 61.6, 14.0 ppm. IR (neat): 2979, 2925, 1745, 1627, 1575, 1496, 1469, 1391, 1369, 1260, 1228, 1171, 1086, 1028, 960, 912, 871, 773, 727, 695, 503 cm^{-1}. HRMS ESI-MS (m/z): $[M+Na]^+$ calcd. for $C_{17}H_{16}O_4Na$ 307.0941, found 307.0945.



3i

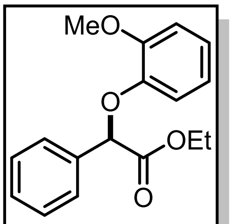


3i'

Ethyl 2-(4-hydroxy-3-methoxyphenyl)-2-phenylacetate, **3i** and ethyl 2-(3-hydroxy-4-methoxyphenyl)-2-phenylacetate, **3i'**: Products **3i/3i'** were prepared following the general procedure employing complex **C1** and $LiBF_4$ as the regulation agent. The reaction crude mixture was purified by column chromatography using SiO_2 and Cy and AcOEt as the eluents (30:1→10:1, Cy:AcOEt), to afford a

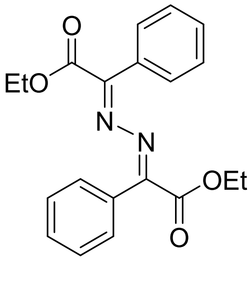
[20] G. Danoun, A. Tlili, F. Monnier and M. Taillefer, Direct Copper-Catalyzed α-Arylation of Benzyl Phenyl Ketones with Aryl Iodides: Route towards Tamoxifen. *Angew. Chem., Int. Ed.*, 2012, **51**, 12815-12819.

colourless oil as mixture of positional isomers **3i**/**3i'** (ratio 1.0:2.5) that could not be separated with standard preparative techniques. Assignments were done by analysing the aromatic region in ^{1}H NMR combined with GOESY (Gradient–enhanced nuclear Overhauser Effect SpectroscopY) analysis (see section 3.5.11). Isomers **3i**+**3i'** (39.2 mg, 69% yield). ^{1}H NMR (400 MHz, acetone-d$_6$) δ: 7.55 (s, 1 H, **3i**), 7.53 (s, 1 H, **3i'**), 7.38-7.20 (m, 8 H, **3i**+**3i'**), 6.98 (d, *J* = 1.9 Hz, 1 H, **3i'**), 6.88 (d, *J* = 8.3 Hz, 1 H, **3i**), 6.86 (d, *J* = 2.2 Hz, 1 H, **3i**), 6.82 (dd, *J* = 8.2, 1.9 Hz, 1 H, **3i'**), 6.80-6.76 (m, 1 H, **3i**+**3i'**), 5.00 (s, 1 H, **3i'**), 4.97 (s, 1 H, **3i**), 4.20-4.13 (m, 2 H, **3i**+**3i'**), 3.81 (s, 3 H, **3i**), 3.79 (s, 3 H, **3i'**), 1.21 (t, *J* = 7.1 Hz, 3 H, **3i**+**3i'**). ^{13}C{^{1}H} NMR (126 MHz, acetone-d$_6$) δ: 172.0, 147.3, 146.6, 146.4, 145.7, 139.8, 139.6, 132.0, 130.3, ,128.3, 128.2, 126.7, 121.1, 119.4, 115.3, 114.7, 112.1, 111.3, 60.4, 56.1, 55.9, 55.2, 13.4 ppm. IR (neat): 3438 (OH), 2962, 2934, 2849, 1728, 1602, 1511, 1452, 1368, 1270, 1144, 1025, 869, 800, 762, 725, 698, 645, 553 cm^{-1}. HRMS ESI-MS (m/z): [M+Na]$^+$ calcd. for $C_{17}H_{18}O_4Na^+$ 309.1097, found 309.1091.



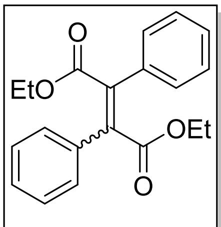
4i

Ethyl 2-(2-methoxyphenoxy)-2-phenylacetate, **4i**: Product **4i** was prepared following the general procedure employing $AgBF_4$ as the catalyst. The reaction crude mixture was purified by column chromatography using SiO_2 and Cy and AcOEt as the eluents (30:1, Cy:AcOEt), to afford **4i** as a yellow oil (14.6 mg, 26% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.65-7.55 (m, 2 H), 7.42-7.31 (m, 3 H), 7.01-6.78 (m, 4 H), 5.63 (s, 1 H), 4.24-4.17 (m, 2 H), 3.87 (s, 3 H), 1.21 (t, J = 7.1 Hz, 3 H) ppm. ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ: 170.3, 150.7, 147.0, 136.0, 129.9, 128.9, 128.8, 128.2, 127.3, 123.3, 120.9, 117.8, 112.8, 80.4, 61.6, 56.2, 14.2 ppm. IR (neat): 3065, 2981, 2837, 1750, 1731, 1593, 1498, 1455, 1369, 1328, 1252, 1205, 1174, 1126, 1112, 1049, 1026, 916, 836, 741, 695, 521 cm^{-1}. HRMS ESI-MS (m/z): [M+Na]$^+$ calcd. for $C_{17}H_{18}O_4Na^+$ 309.1097, found 309.1092.



5

Ethyl benzoylformate azine, 5: Product **5** was prepared reacting PhEDA **2a** (0.26 mmol) with $AgBF_4$ (10 mol%) in 2 mL of CH_2Cl_2 for 1 hour. After evaporation, the reaction crude mixture was purified by column chromatography using SiO_2 and Cy and AcOEt as the eluents (30:1, Cy:AcOEt), to afford **5** as a yellow solid (9.1 mg, 9.9% yield). ^{1}H and $^{13}C\{^{1}H\}$ NMR data were in agreement with those previously reported.[21] ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.85-7.75 (m, 4 H), 7.55-7.35 (m, 6 H), 4.50 (q, J = 7.1 Hz, 4 H), 1.42 (t, J = 7.1 Hz, 6 H) ppm. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ: 165.3, 162.2, 132.0, 131.3, 128.8, 128.0, 61.7, 14.5 ppm.



6

Diethyl 2,3-diphenylbutenoate, 6: Product **6** was prepared reacting PhEDA **2a** (0.26 mmol) with $AgBF_4$ (10 mol%) in 2 mL of CH_2Cl_2 for 1 hour. After evaporation, the reaction crude mixture was purified by column chromatography using SiO_2 and Cy and AcOEt as the eluents (30:1, Cy:AcOEt), to afford **6** as a pale yellow oil (18.3 mg, 21.5% yield). ^{1}H and $^{13}C\{^{1}H\}$ NMR data were in agreement with those previously reported.[22] ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.50-7.30 (m, 10 H), 4.00 (q, J = 7.1 Hz, 4 H), 0.94 (t, J = 7.1 Hz, 6 H) ppm. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ: 168.2, 137.8, 135.7, 128.8, 128.5, 128.3, 61.4, 13.7 ppm.

[21] R. Glaser, G. S. Chen and C. L. Barnes, Conjugation in Azines. Stereochemical Analysis of Benzoylformate Azines in the Solid State, in Solution, and in the Gas Phase. *J. Org. Chem.*, 1993, **58**, 7446-7455.

[22] *E* or *Z* configuration could not be univocally assigned according to previous reports. See: (a) C. Zhou and R. C. Larock, Regio- and Stereoselective Route to Tetrasubstituted Olefins by the Palladium-Catalyzed Three-Component Coupling of Aryl Iodides, Internal Alkynes, and Arylboronic Acids. *J. Org. Chem.*, 2005, **70**, 3765-3777. For NMR spectroscopic data for *E*-diethyl 2,3-diphenylbutenoate see: (b) L. Zhou, W. Zhang and H. Jiang, Carbon Nanotubes-Supported Palladium Nanoparticles for the Suzuki Reaction in Supercritical Carbon Dioxide. A Facile Method for the Synthesis of Tetrasubstituted Olefins. *Sci. China, Ser. B: Chem.*, 2008, **51**, 241-247.

9. Spectroscopic data:

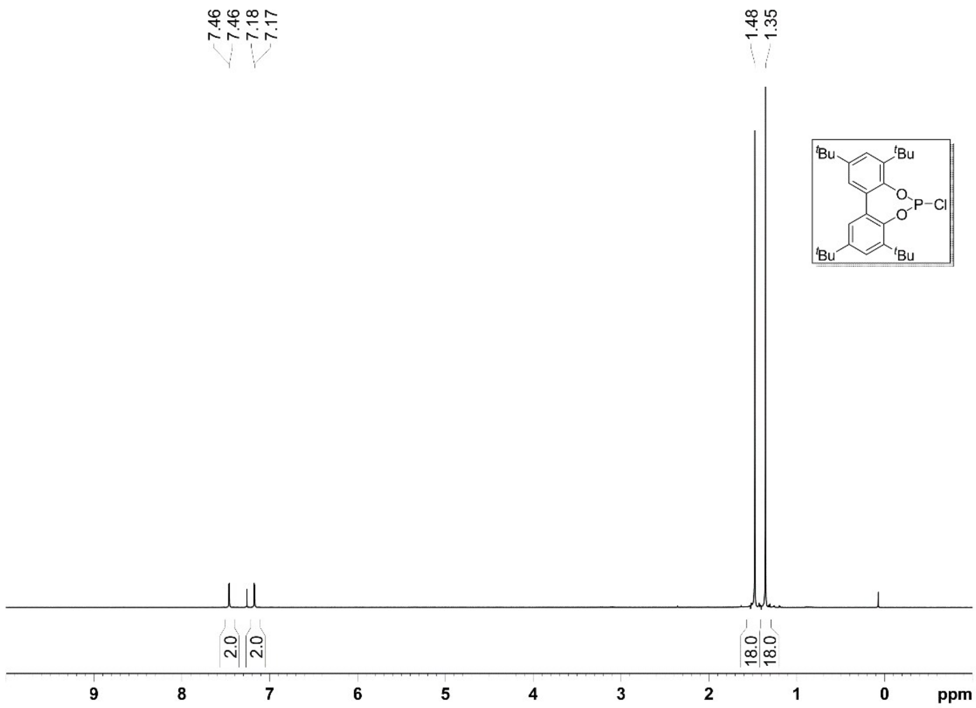


Figure SI 3. ^{1}H NMR (400 MHz, $CDCl_3$) for 3,3',5,5'-tetra-*tert*-butylbiphenyl-2,2'-diyl chlorophosphite.

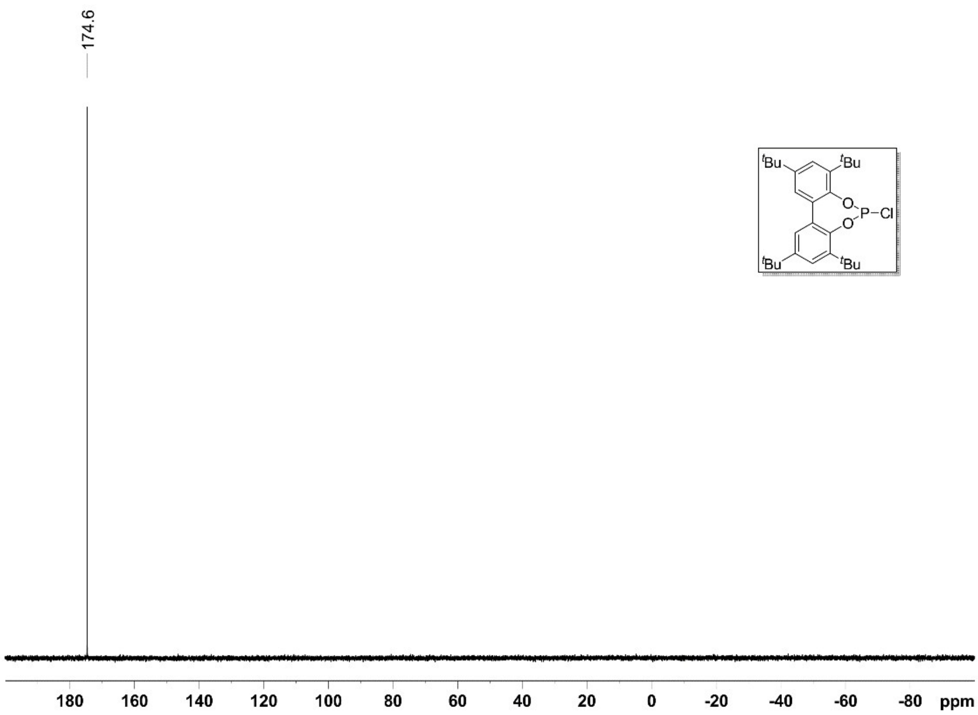


Figure SI 4. ^{31}P{^{1}H} NMR (162 MHz, $CDCl_3$) for 3,3',5,5'-tetra-*tert*-butylbiphenyl-2,2'-diyl chlorophosphite.

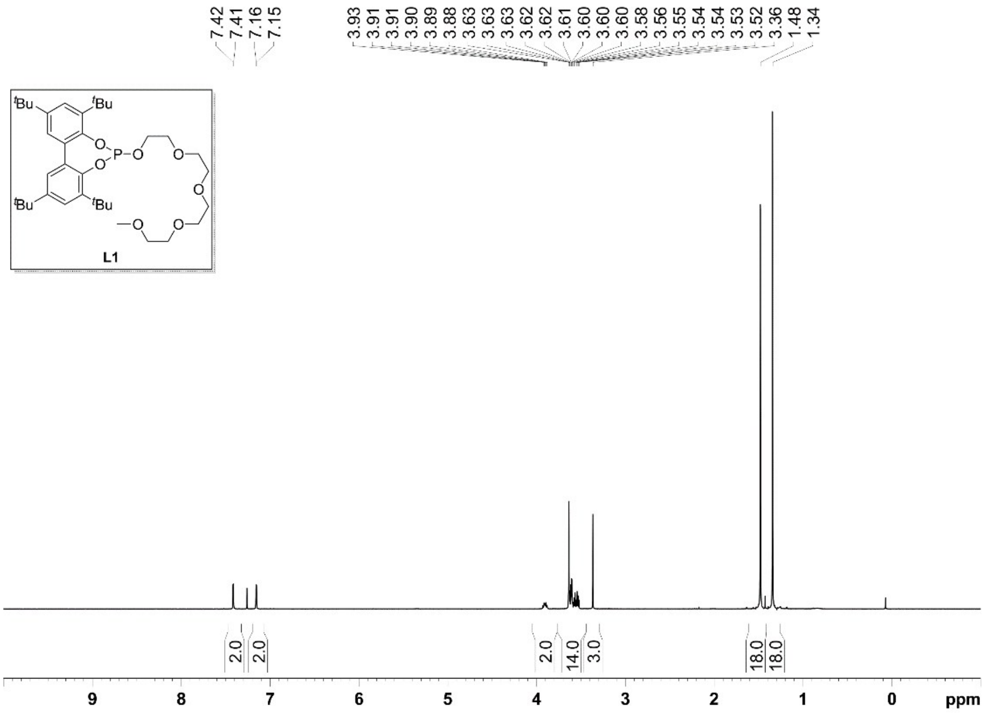


Figure SI 5. ^{1}H NMR (400 MHz, $CDCl_3$) for ligand **L1**.

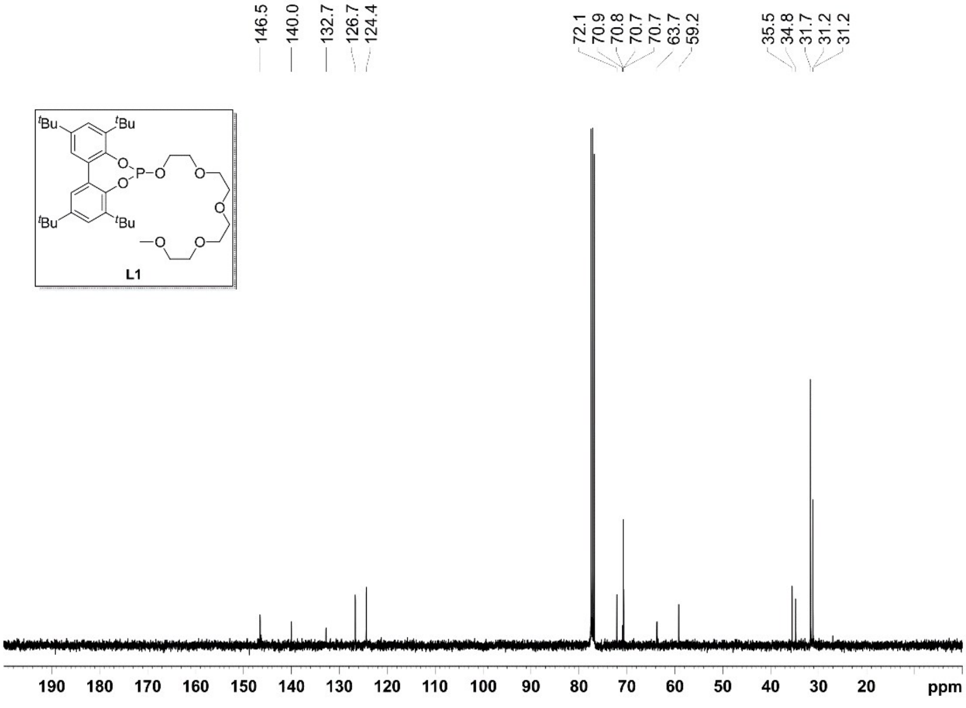


Figure SI 6. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) for ligand **L1**.

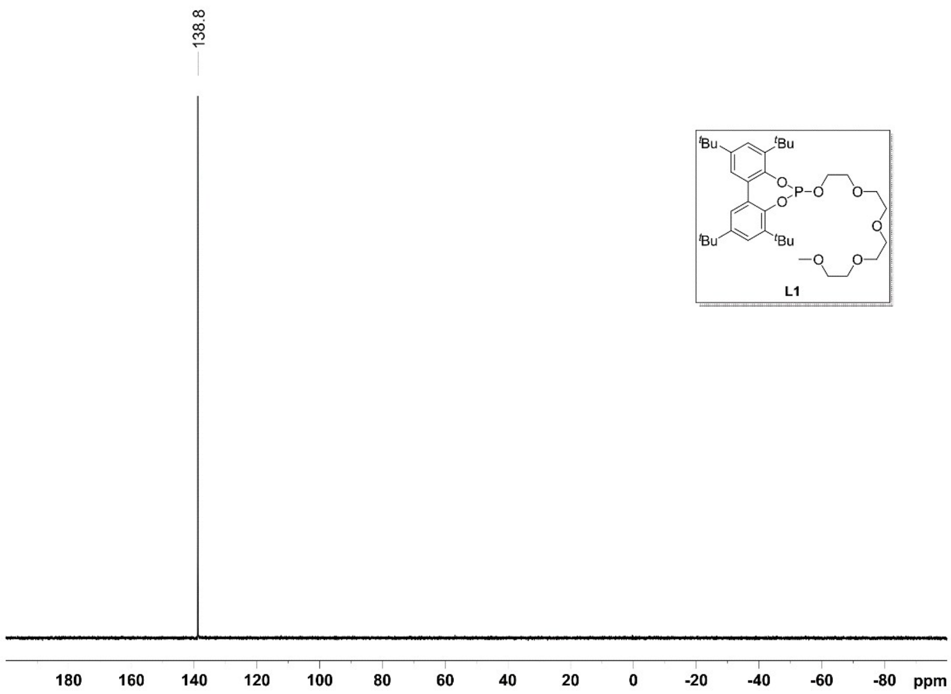


Figure SI 7. $^{31}P\{^{1}H\}$ NMR (162 MHz, $CDCl_3$) for ligand **L1**.

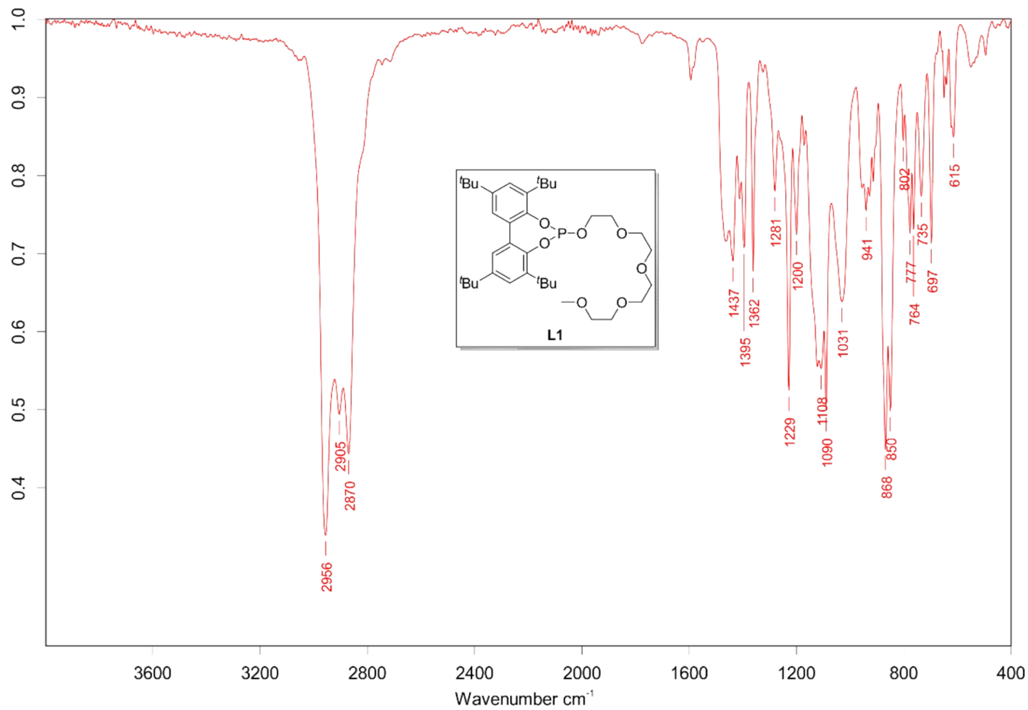


Figure SI 8. IR spectrum for ligand **L1**.

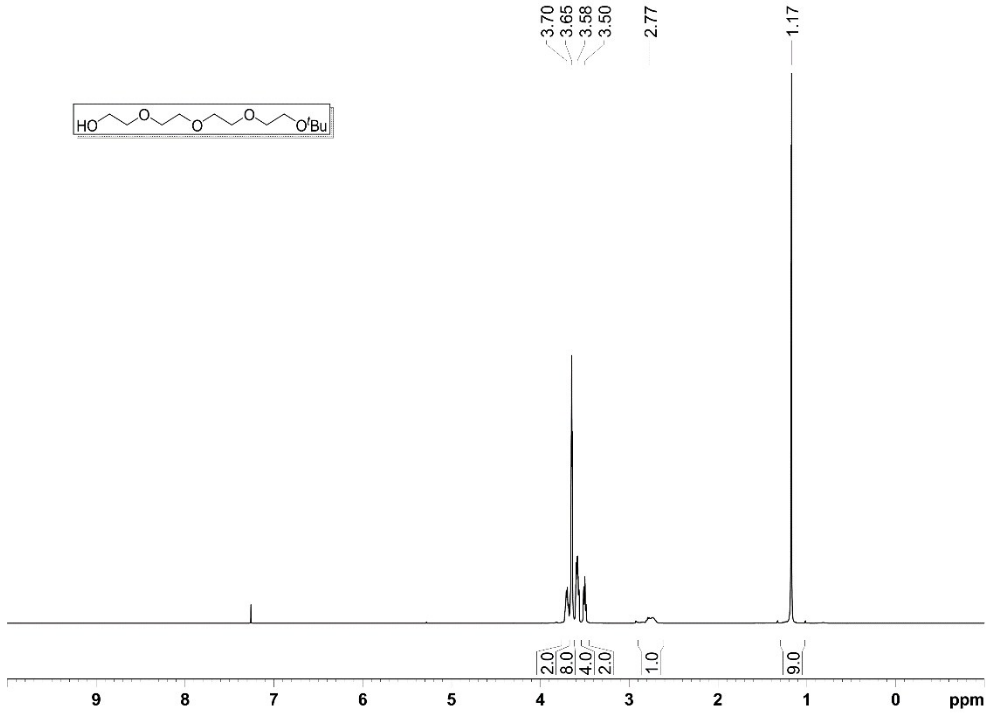


Figure SI 9. ^{1}H NMR (400 MHz, $CDCl_3$) for tetraethyleneglycol mono-*tert*-butyl ether.

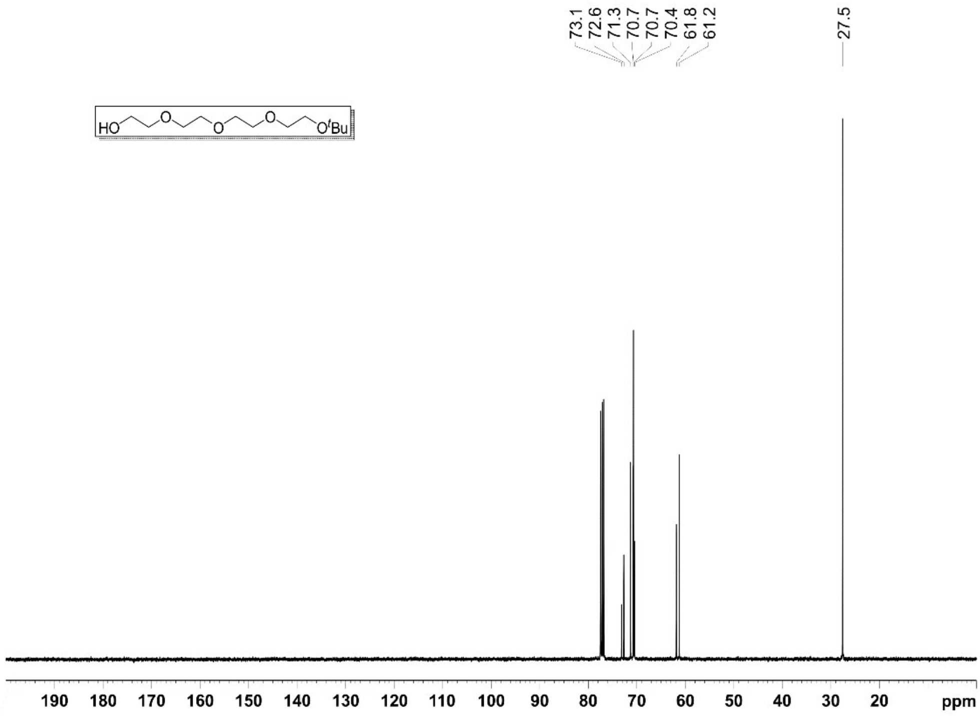


Figure SI 10. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) for tetraethyleneglycol mono-*tert*-butyl ether.

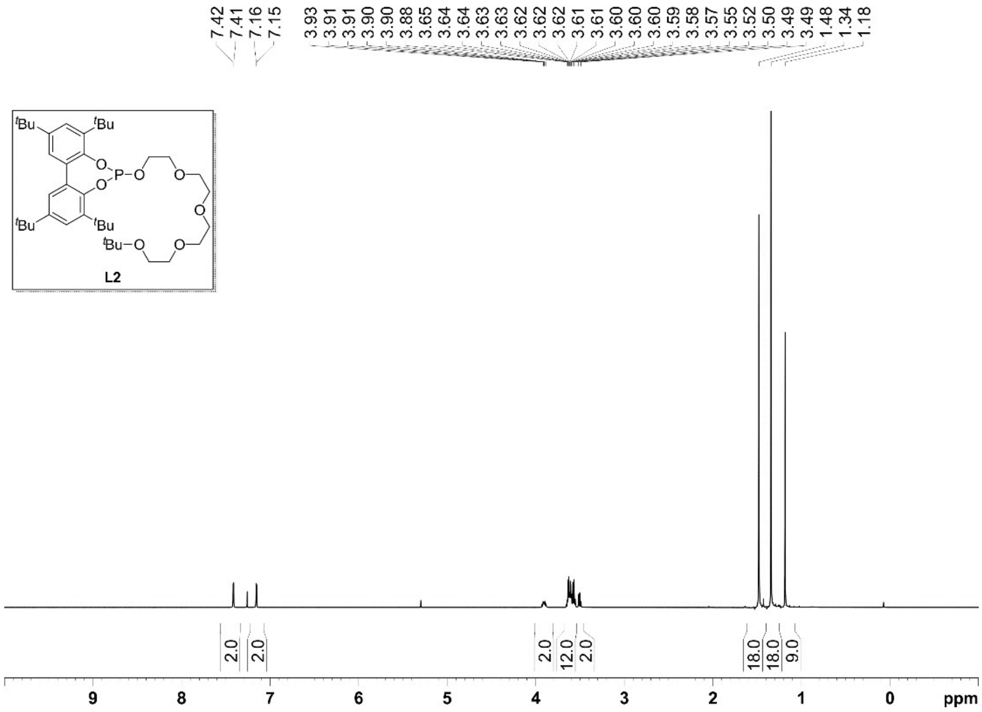


Figure SI 11. ^{1}H NMR (400 MHz, $CDCl_3$) for ligand **L2**.

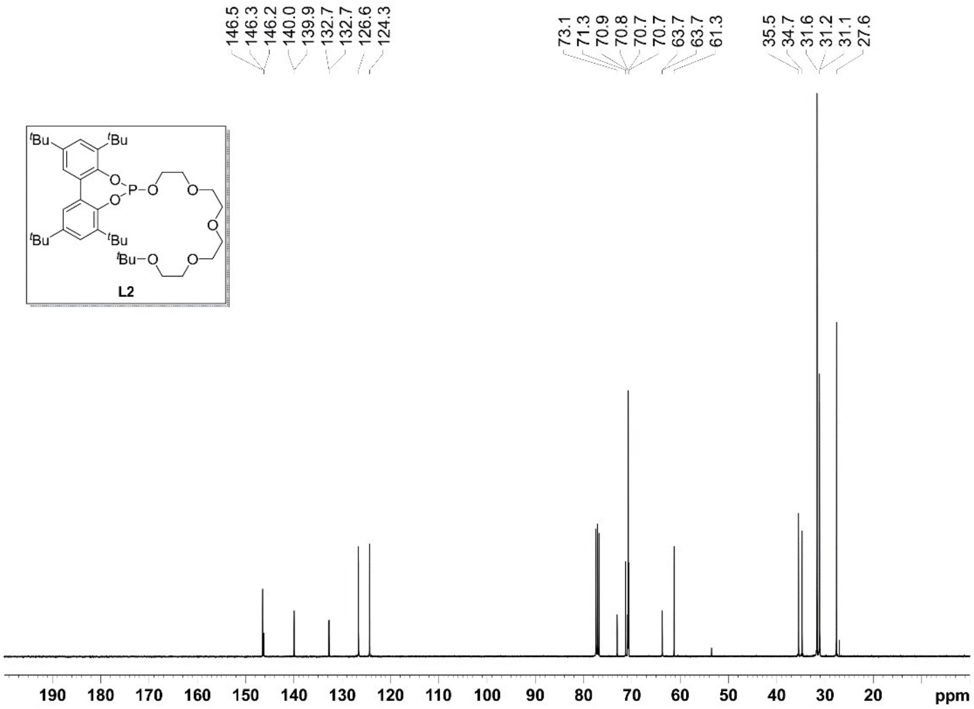


Figure SI 12. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) for ligand **L2**.

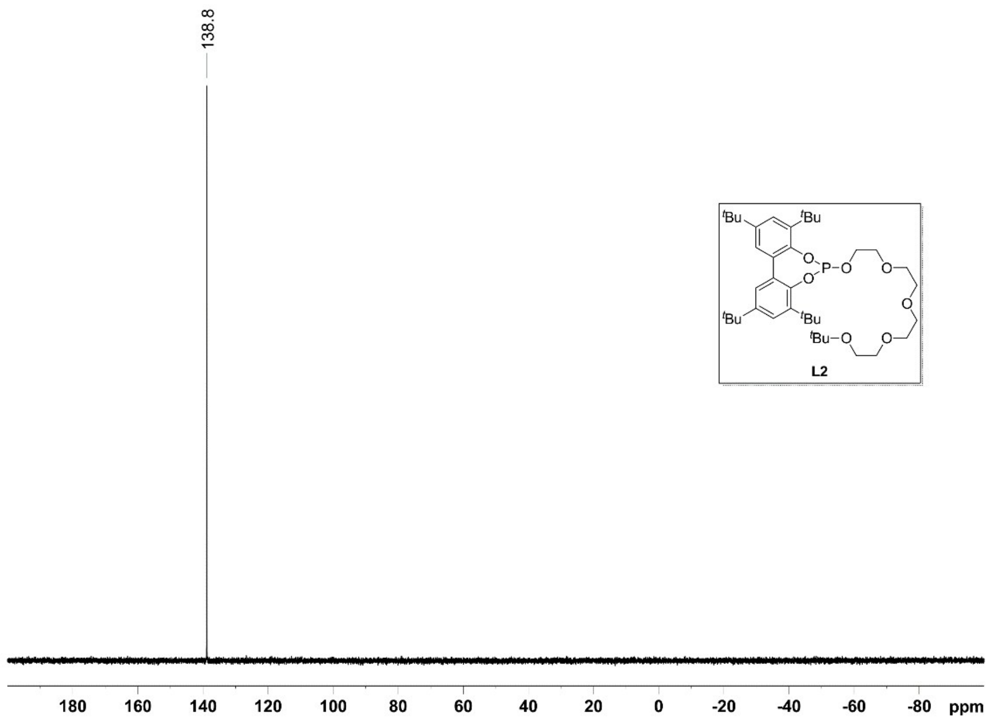


Figure SI 13. $^{31}P\{^1H\}$ NMR (162 MHz, $CDCl_3$) for ligand **L2**.

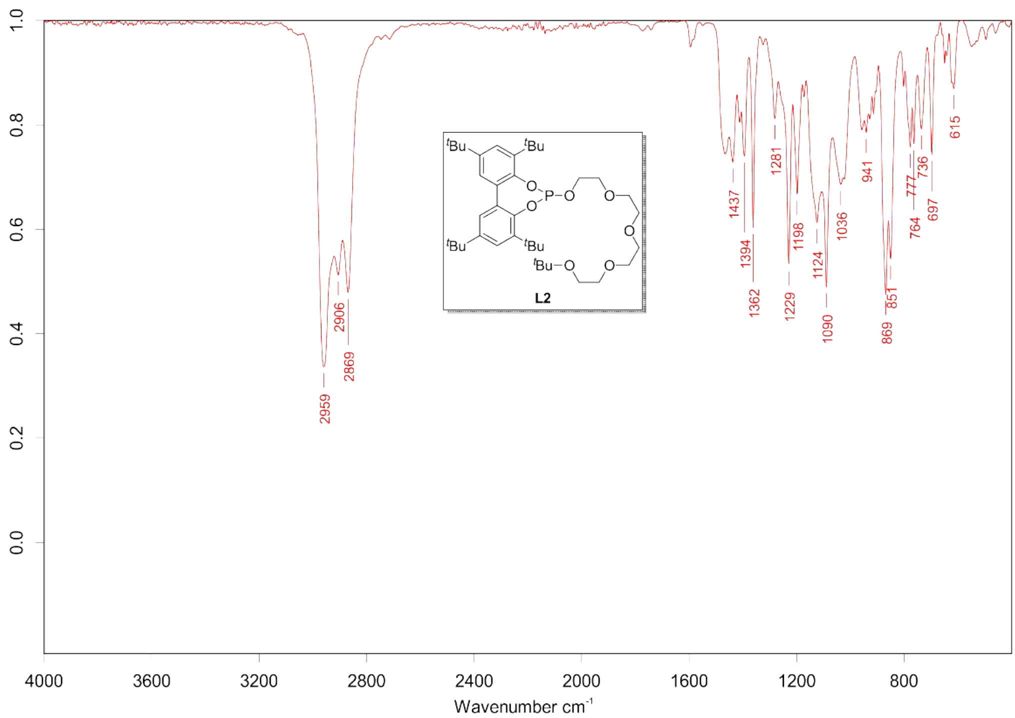


Figure SI 14. IR spectrum for ligand **L2**.

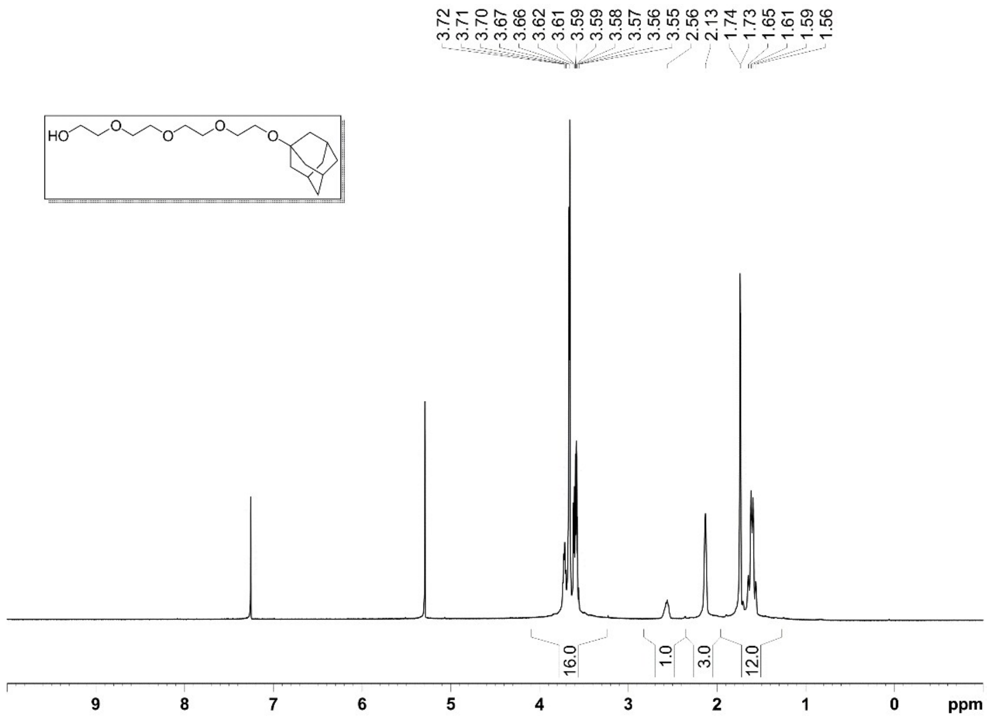


Figure SI 15. ^{1}H NMR (400 MHz, $CDCl_3$) for tetraethyleneglycol mono-1-adamantyl ether.

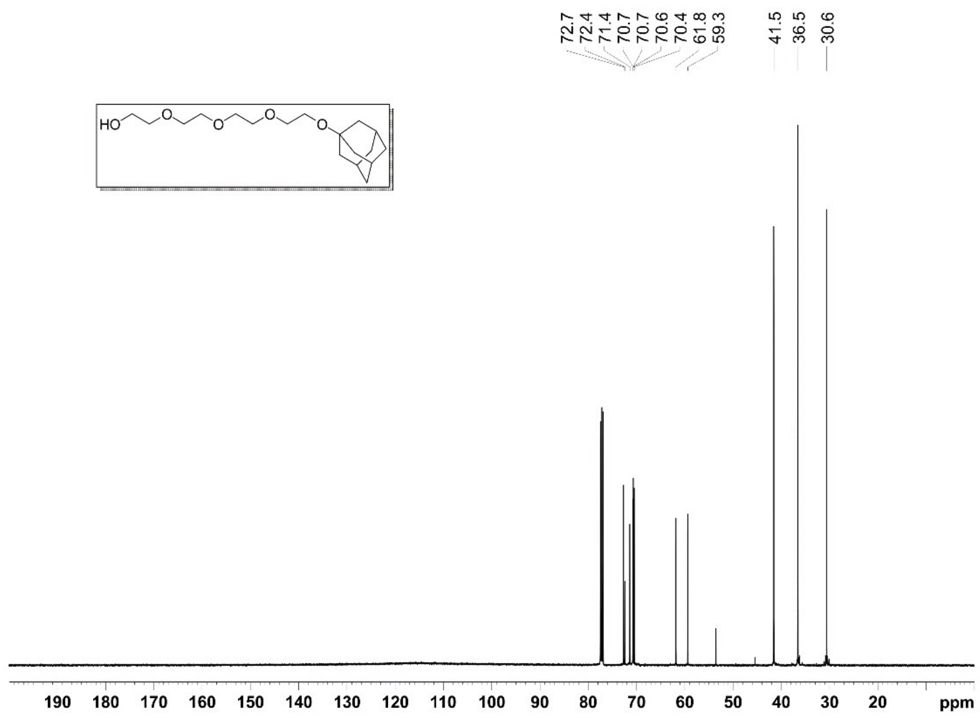


Figure SI 16. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) for tetraethyleneglycol mono-1-adamantyl ether.

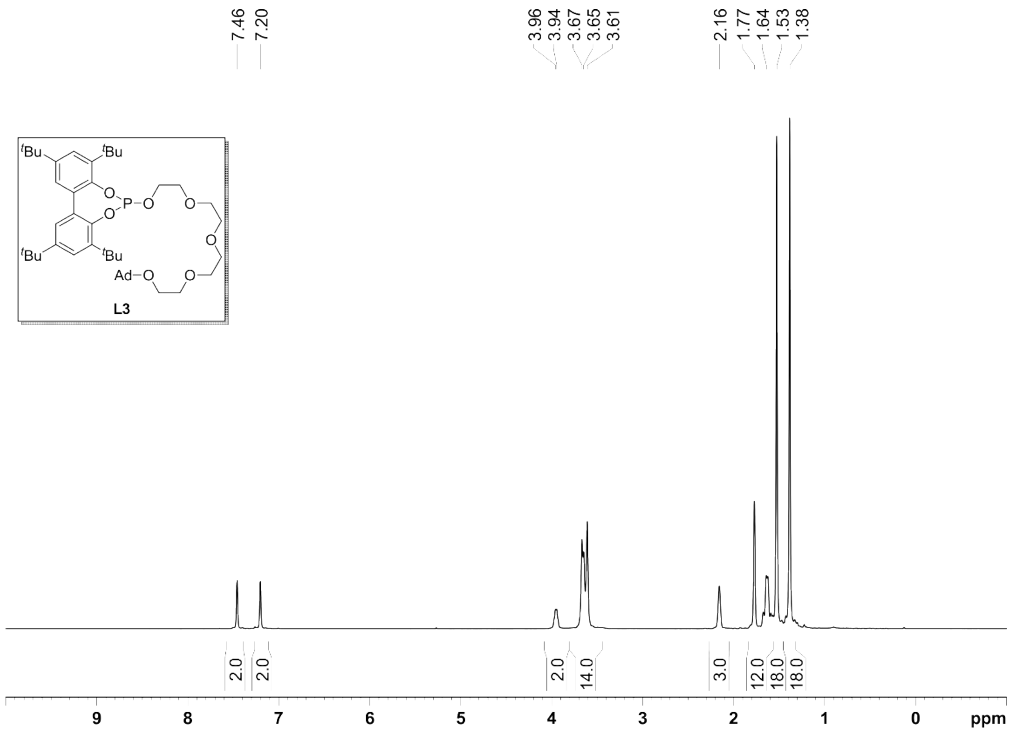


Figure SI 17. ^{1}H NMR (400 MHz, $CDCl_3$) for ligand **L3**.

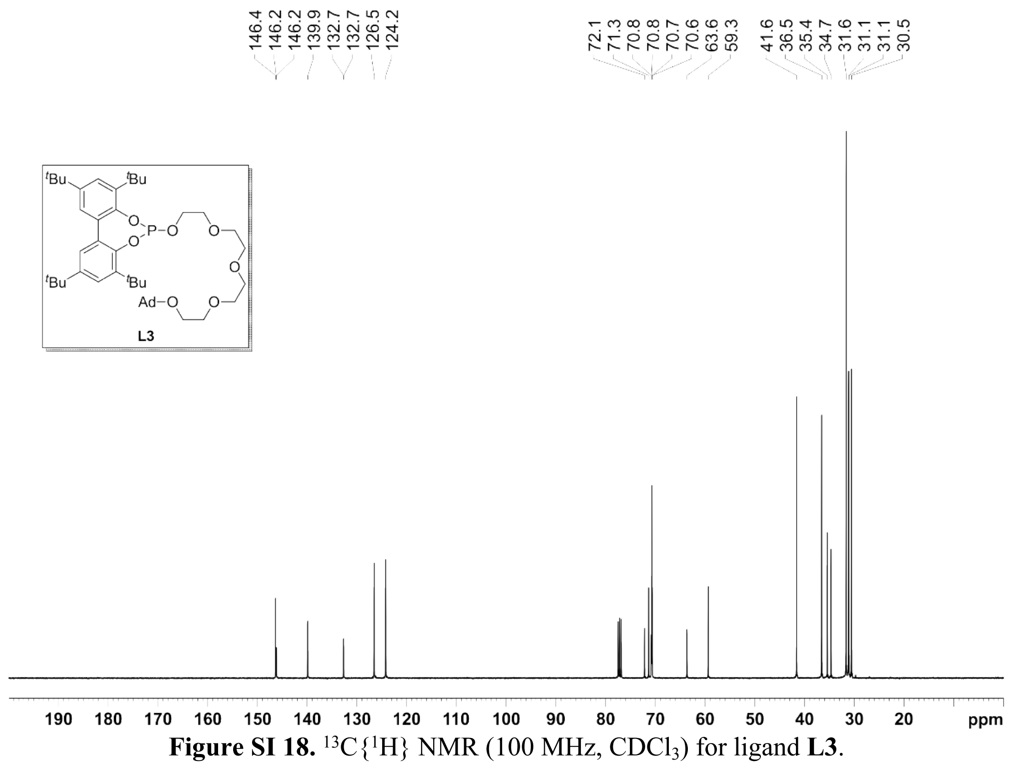


Figure SI 18. $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) for ligand **L3**.

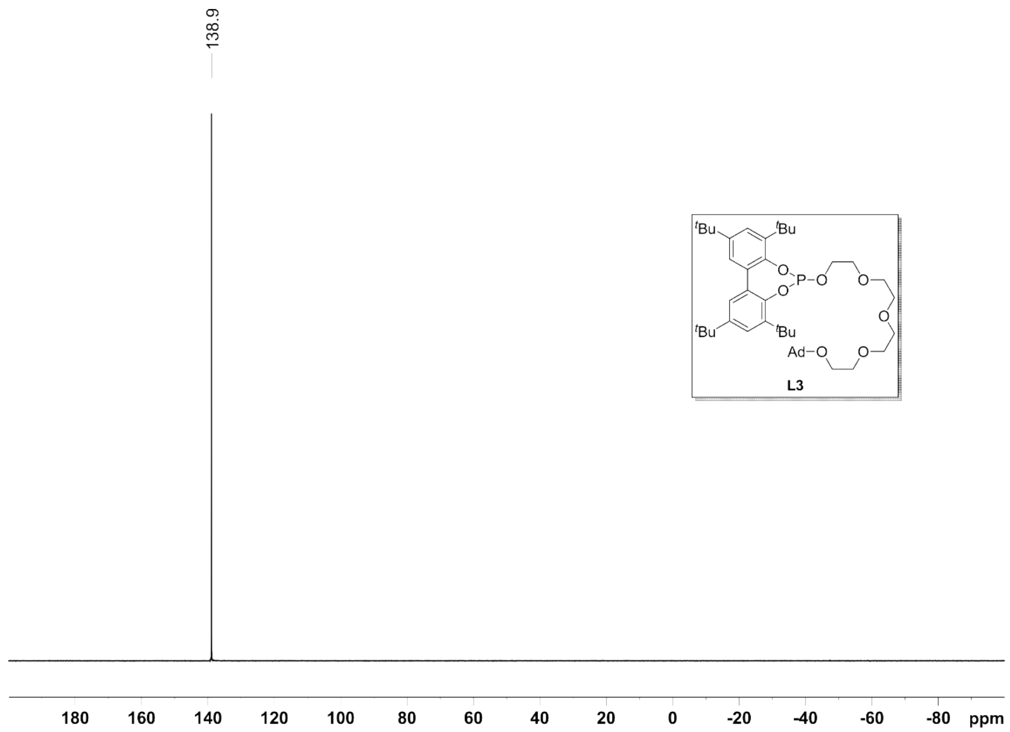


Figure SI 19. $^{31}P\{^{1}H\}$ NMR (162 MHz, $CDCl_3$) for ligand **L3**.

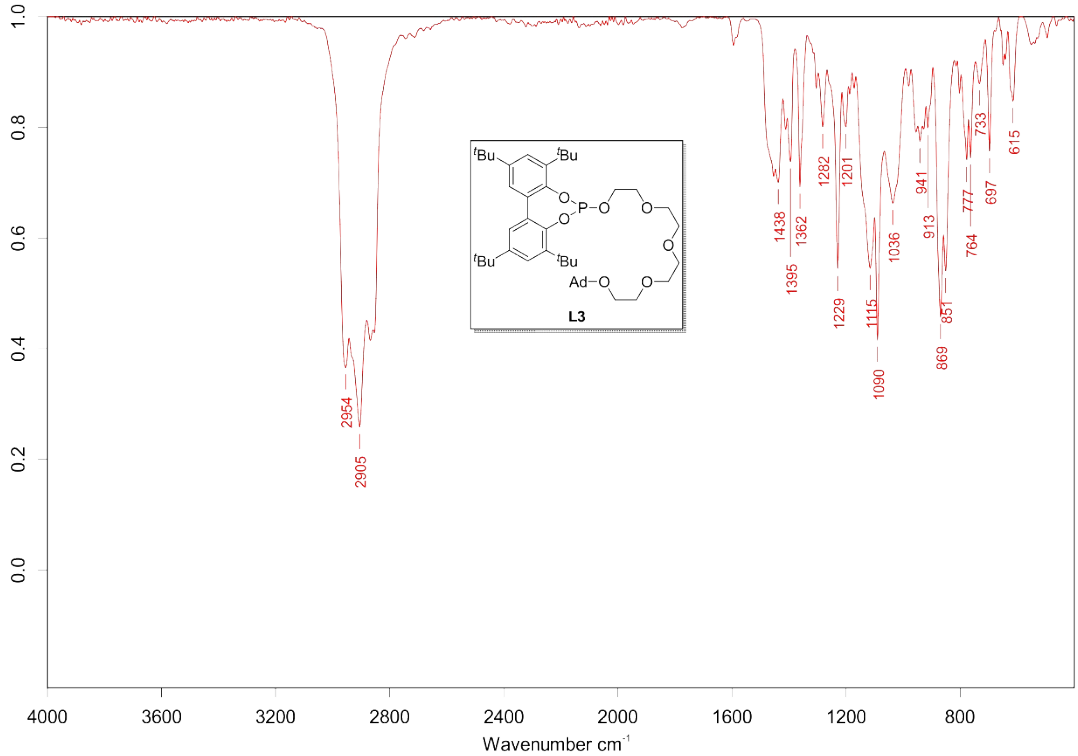


Figure SI 20. IR spectrum for ligand **L3**.

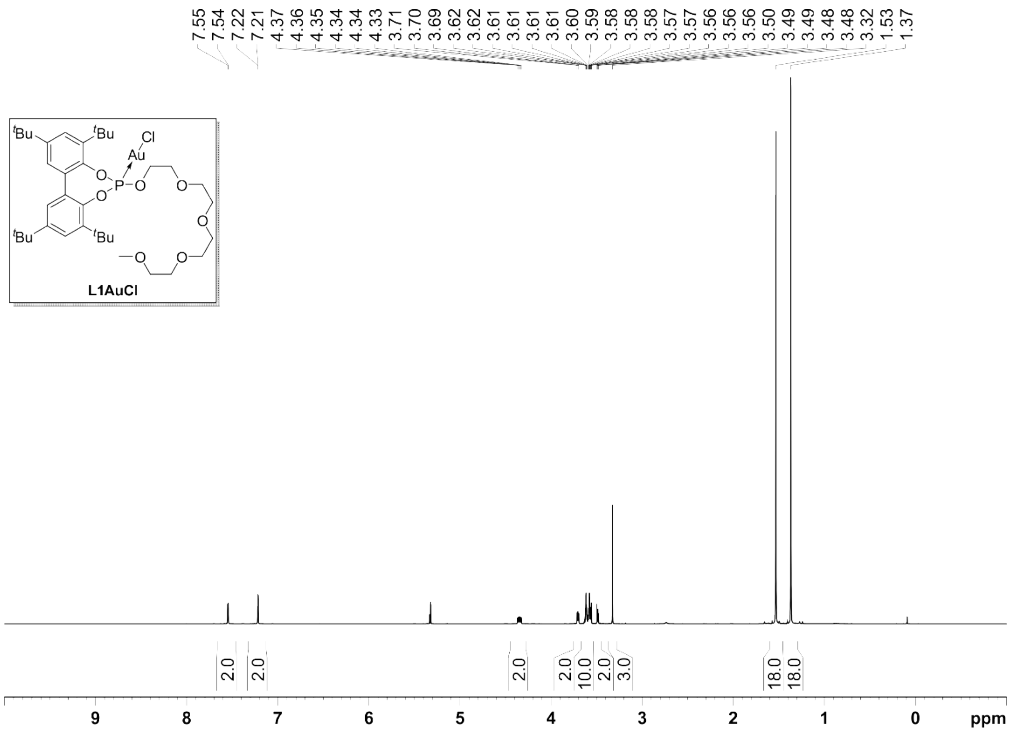


Figure SI 21. ^{1}H NMR (500 MHz, CD_2Cl_2) for complex **L1AuCl**.

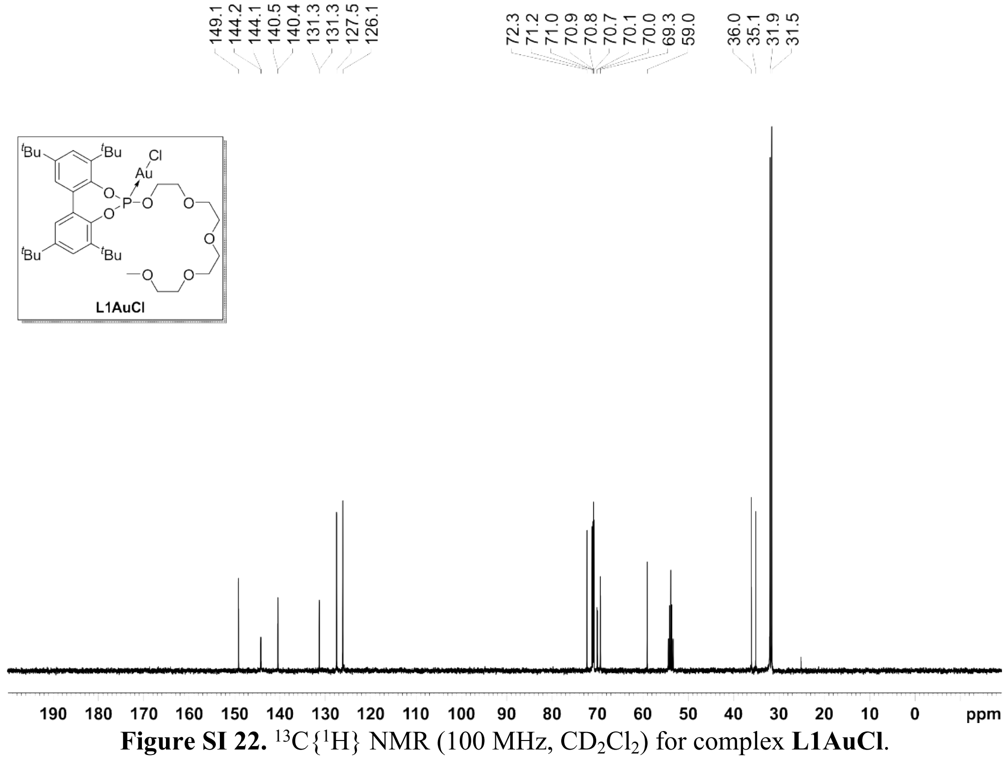


Figure SI 22. $^{13}C\{^{1}H\}$ NMR (100 MHz, CD_2Cl_2) for complex **L1AuCl**.

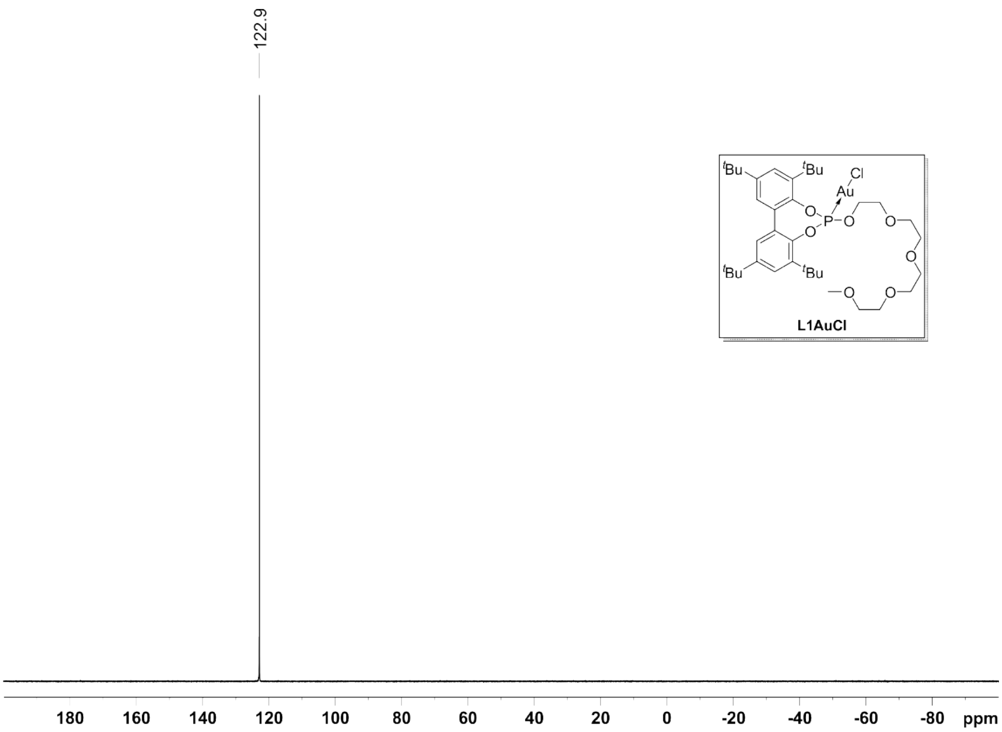


Figure SI 23. $^{31}P\{^{1}H\}$ NMR (202 MHz, CD_2Cl_2) for complex **L1AuCl**.

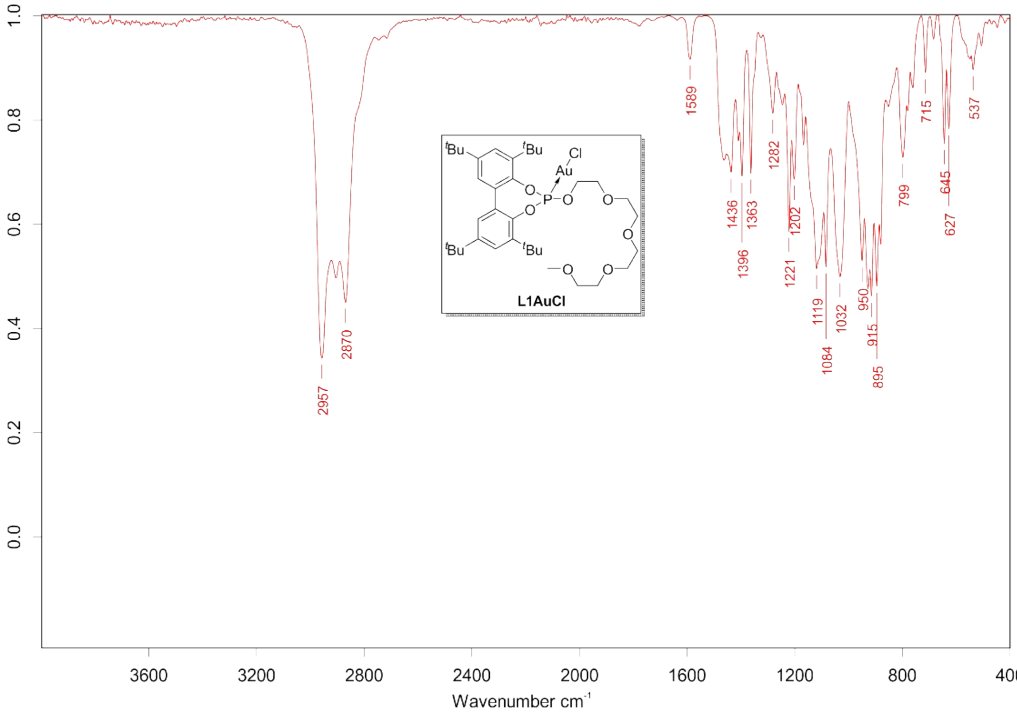


Figure SI 24. IR spectrum for complex **L1AuCl**.

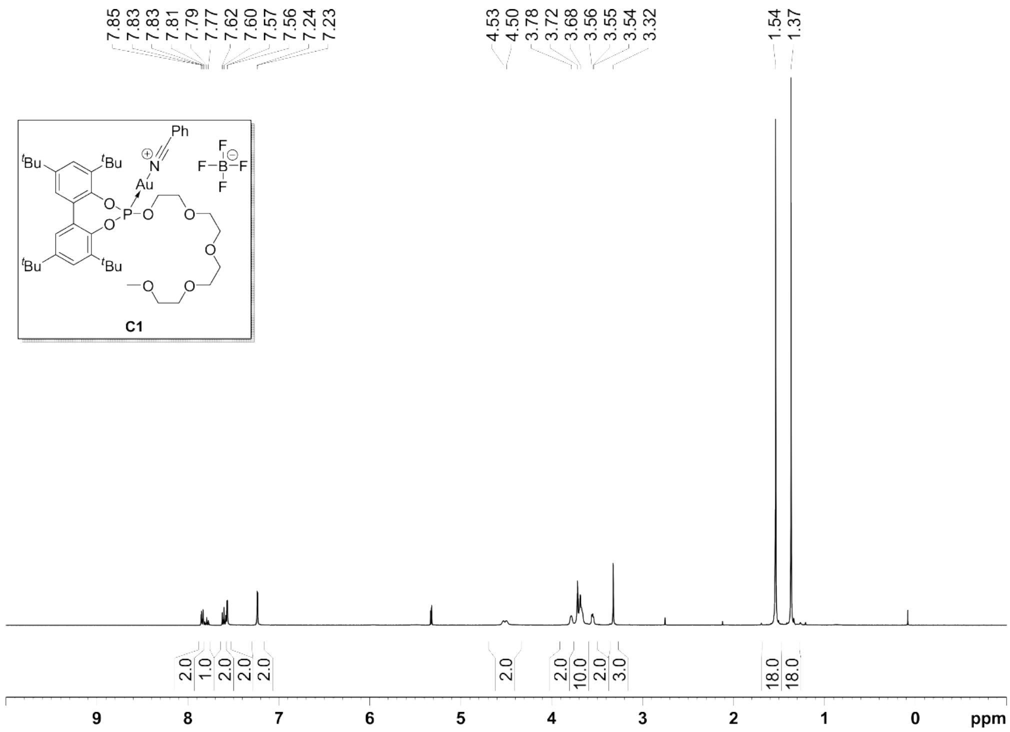


Figure SI 25. ^{1}H NMR (400 MHz, CD_2Cl_2) for complex **C1**.

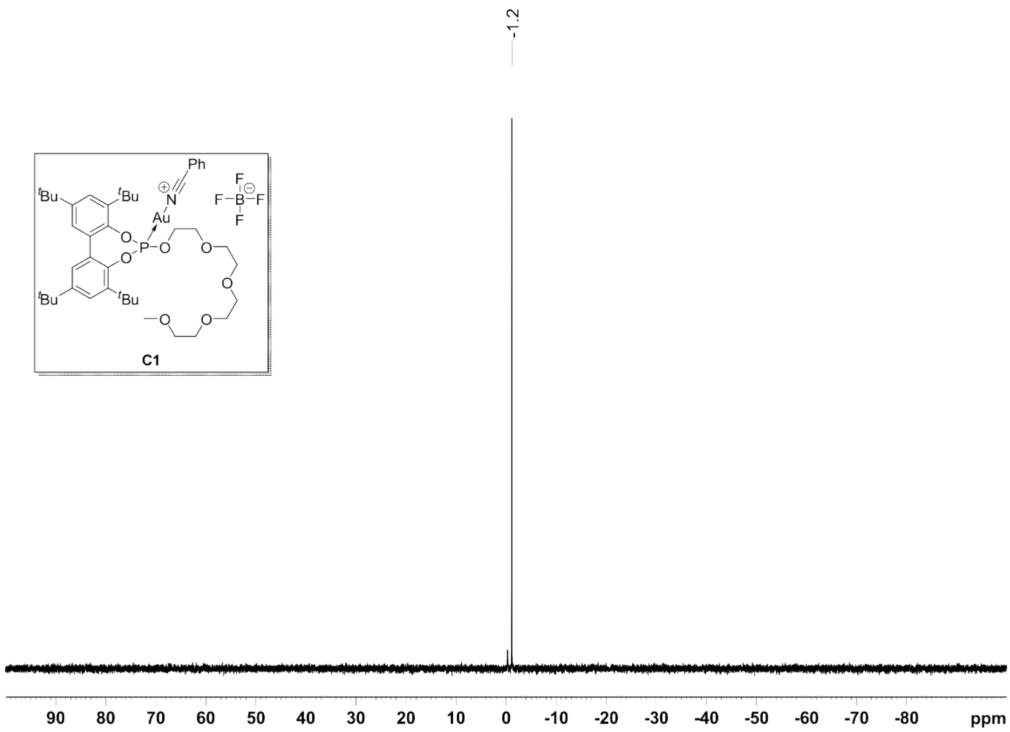


Figure SI 26. $^{11}B\{^{1}H\}$ NMR (128 MHz, CD_2Cl_2) for complex **C1**.

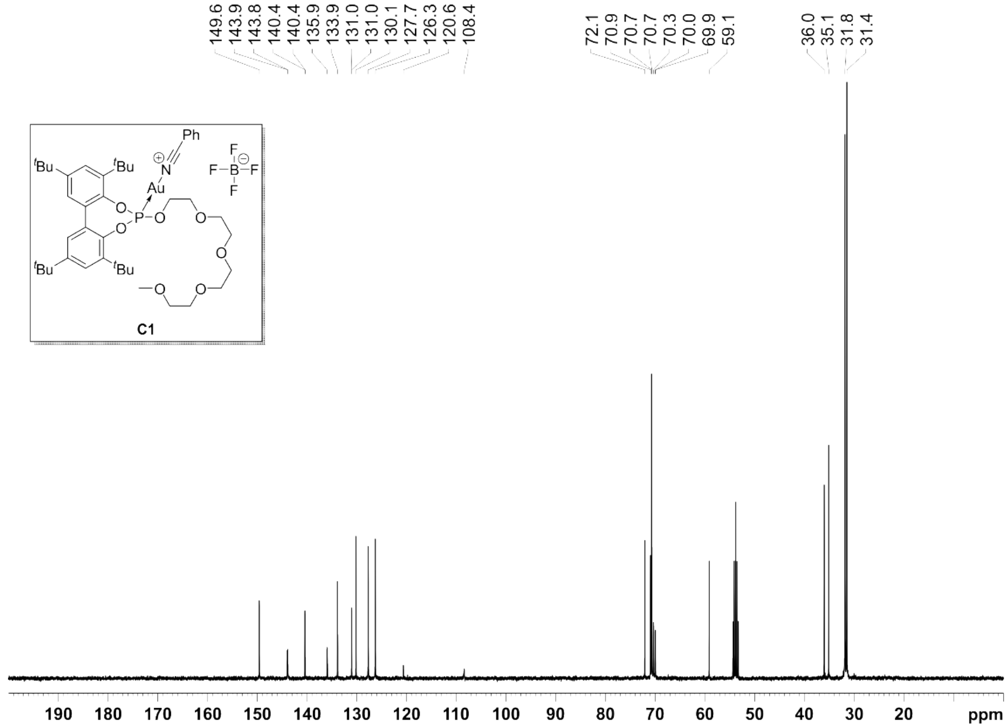


Figure SI 27. $^{13}C\{^1H\}$ NMR (126 MHz, CD_2Cl_2) for complex **C1**.

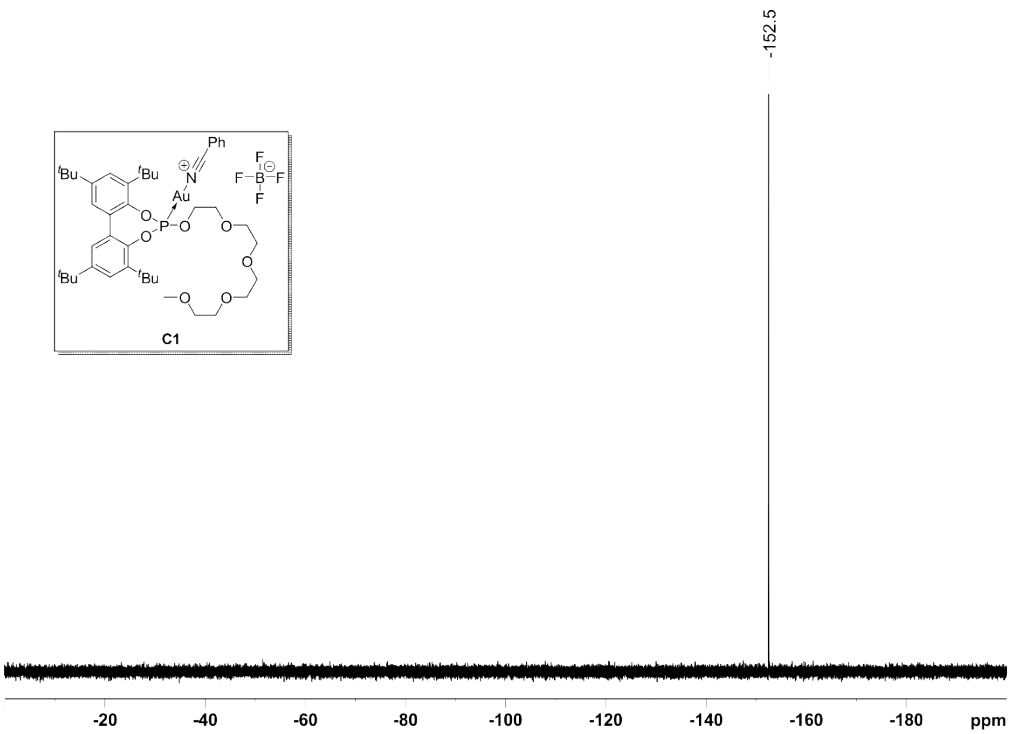


Figure SI 28. $^{19}F\{^1H\}$ NMR (376 MHz, CD_2Cl_2) for complex **C1**.

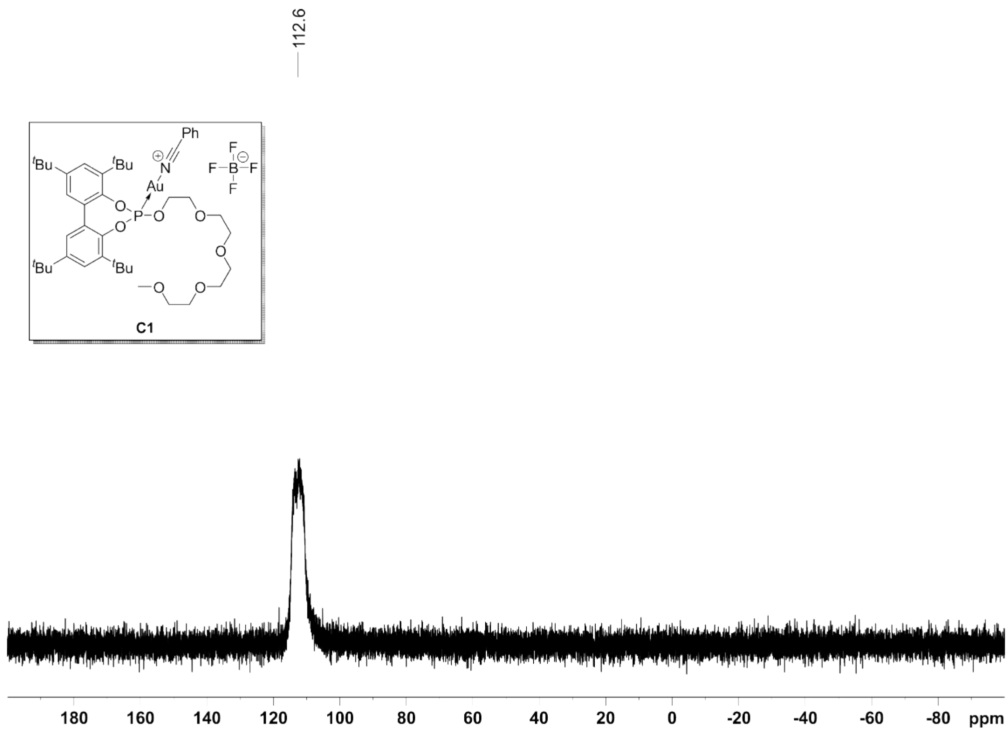


Figure SI 29. $^{31}P\{^1H\}$ NMR (162 MHz, CD_2Cl_2) for complex **C1**.

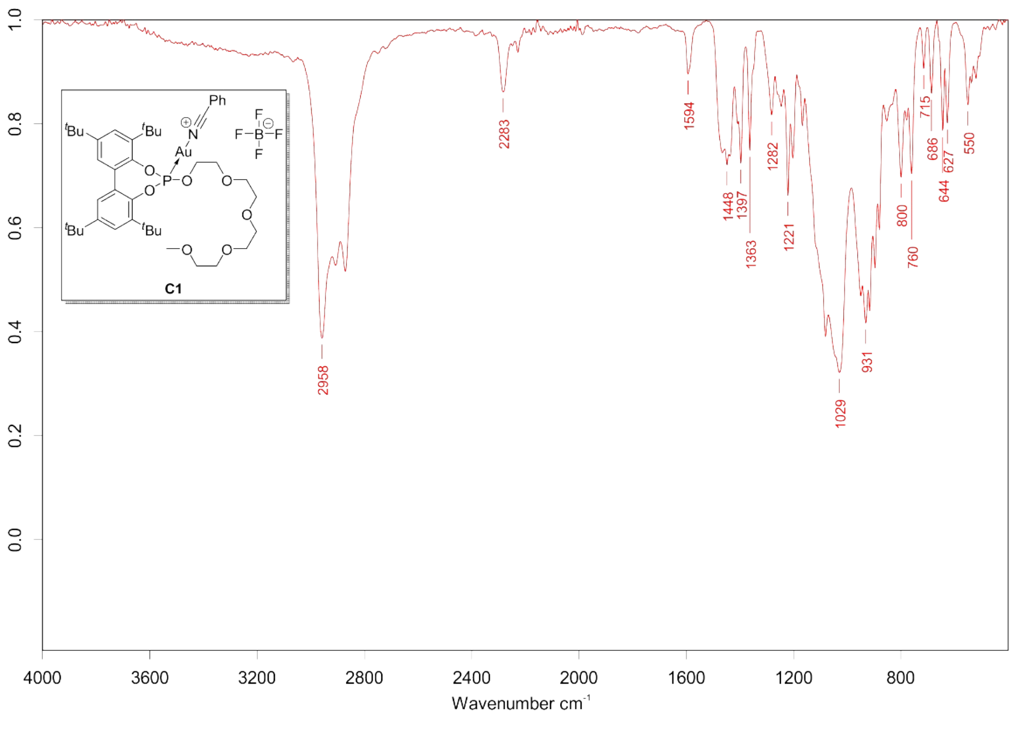


Figure SI 30. IR spectrum for complex **C1**.

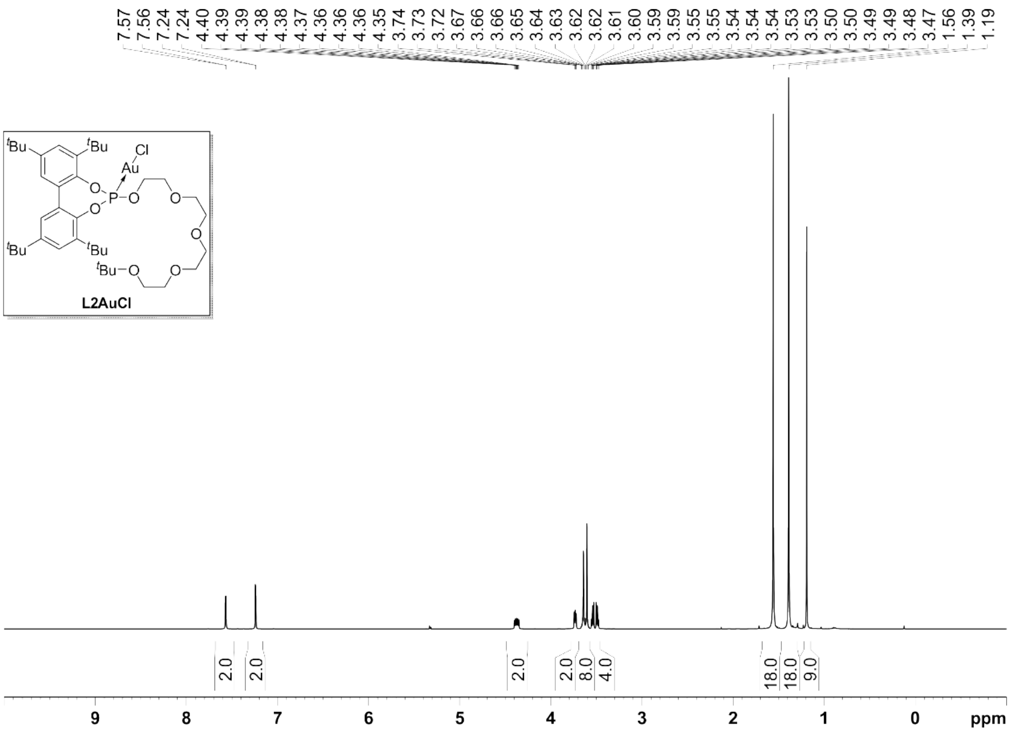


Figure SI 31. ^{1}H NMR (400 MHz, CD_2Cl_2) for complex **L2AuCl**.

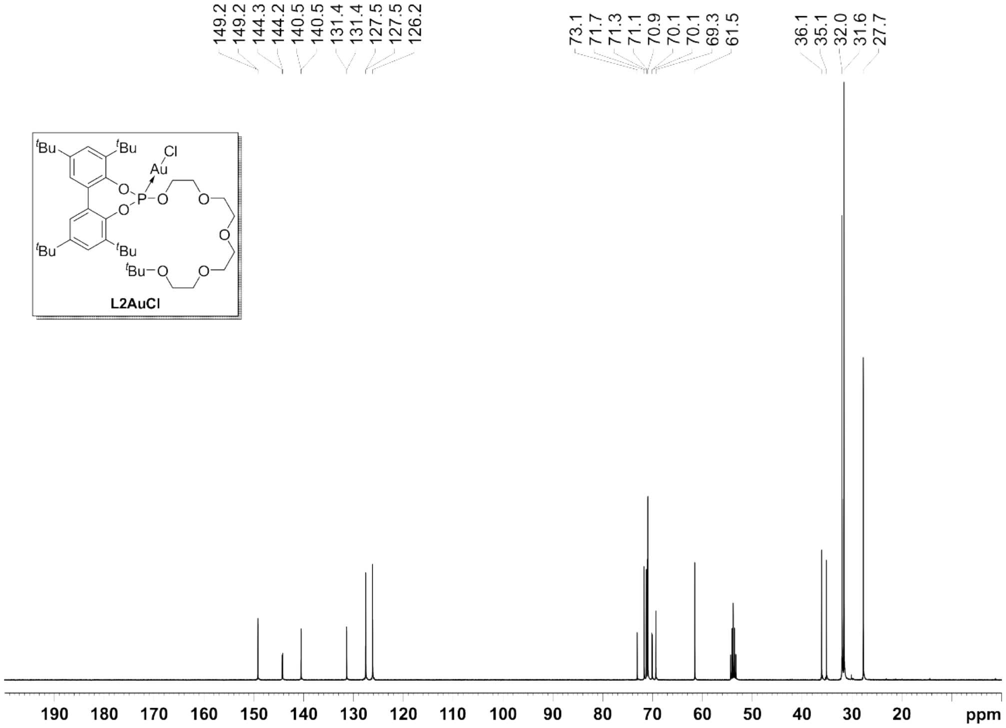


Figure SI 32. $^{13}C\{^{1}H\}$ NMR (100 MHz, CD_2Cl_2) for complex **L2AuCl**.

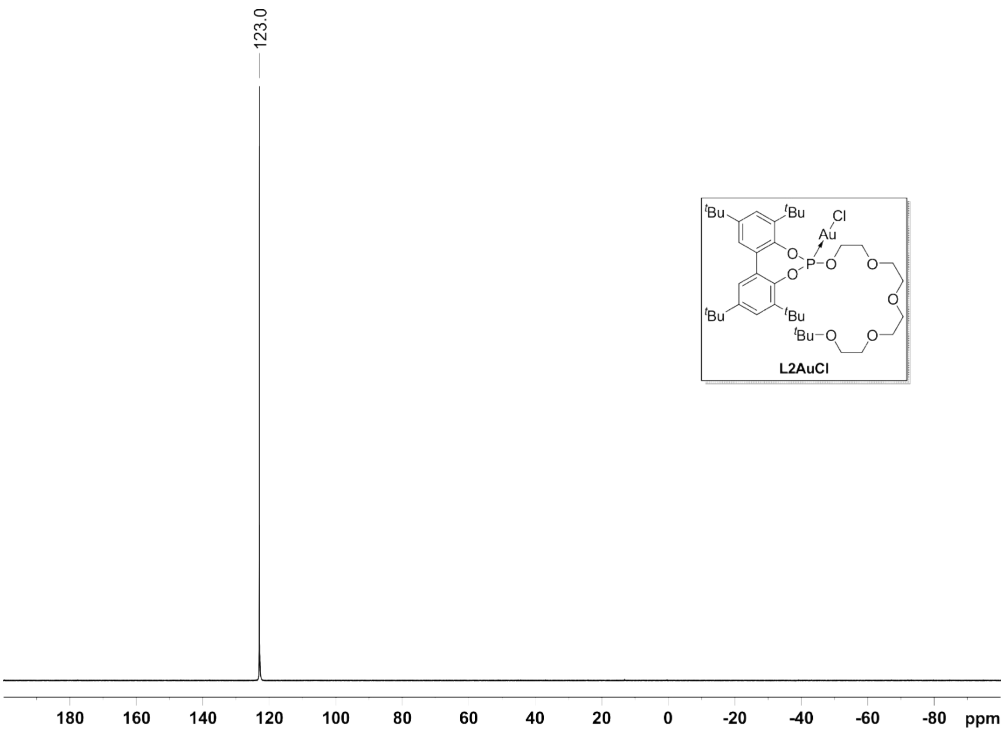


Figure SI 33. $^{31}P\{^{1}H\}$ NMR (162 MHz, CD_2Cl_2) for complex **L2AuCl**.

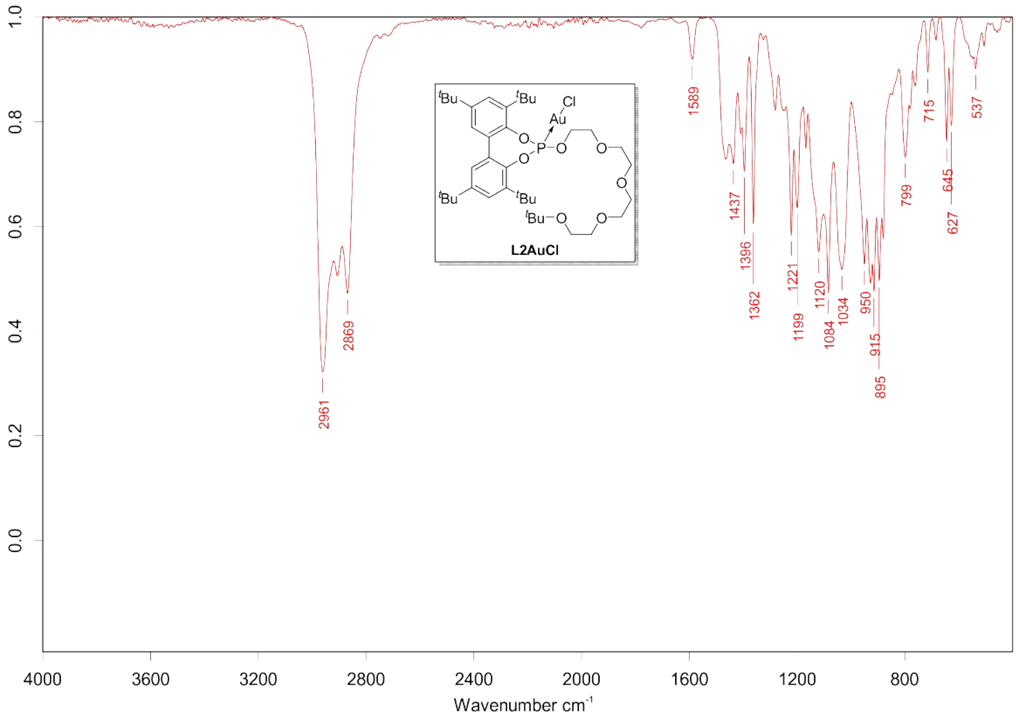


Figure SI 34. IR spectrum for complex **L2AuCl**.

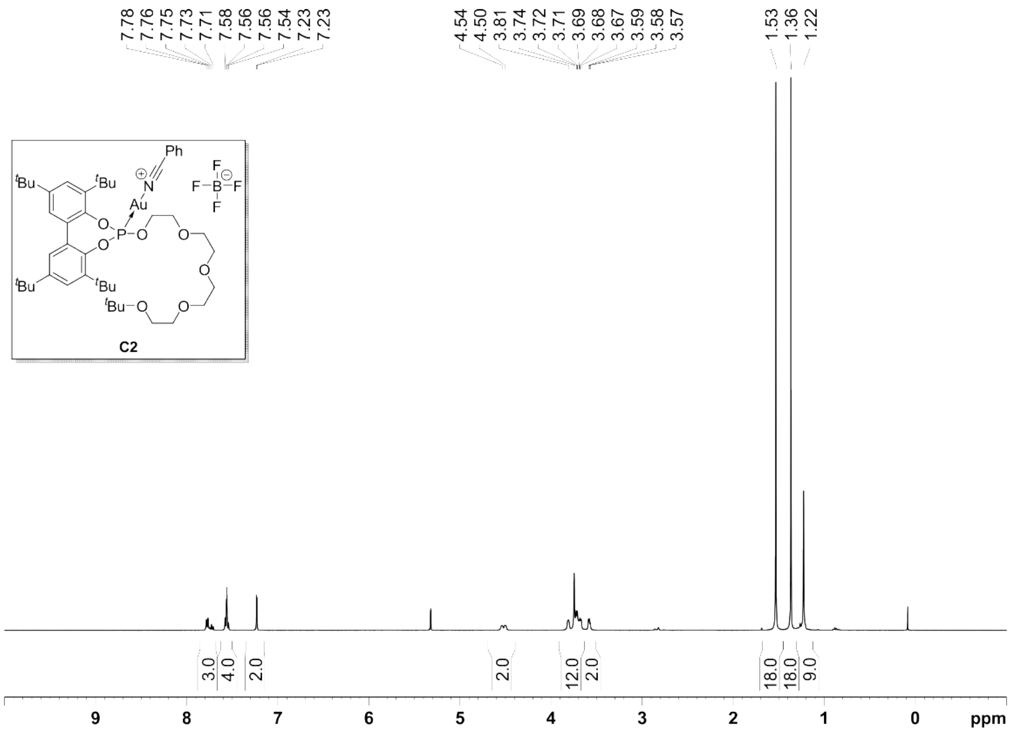


Figure SI 35. ^{1}H NMR (400 MHz, CD_2Cl_2) for complex **C2**.

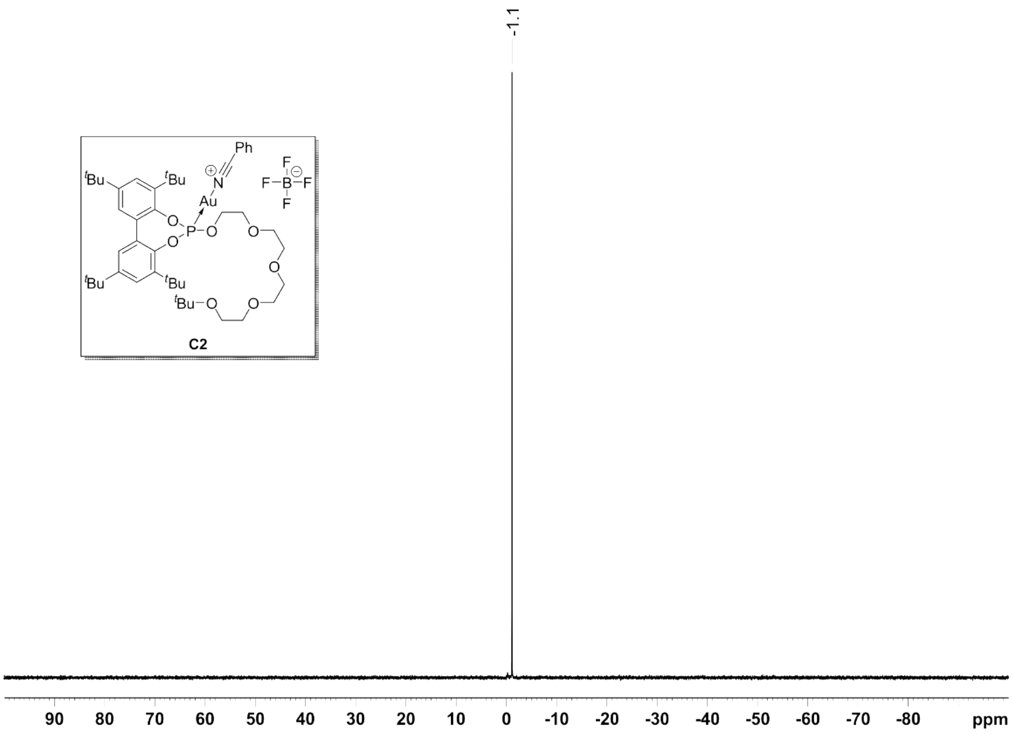


Figure SI 36. $^{11}B\{^{1}H\}$ NMR (128 MHz, CD_2Cl_2) for complex **C2**.

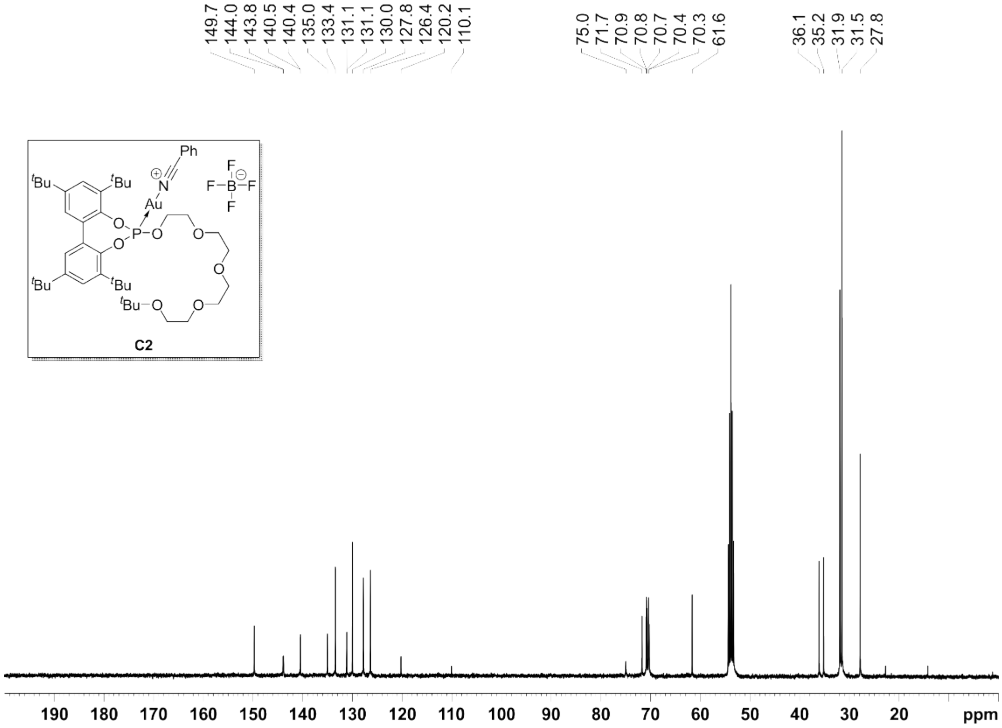


Figure SI 37. $^{13}C\{^1H\}$ NMR (126 MHz, CD_2Cl_2) for complex **C2**.

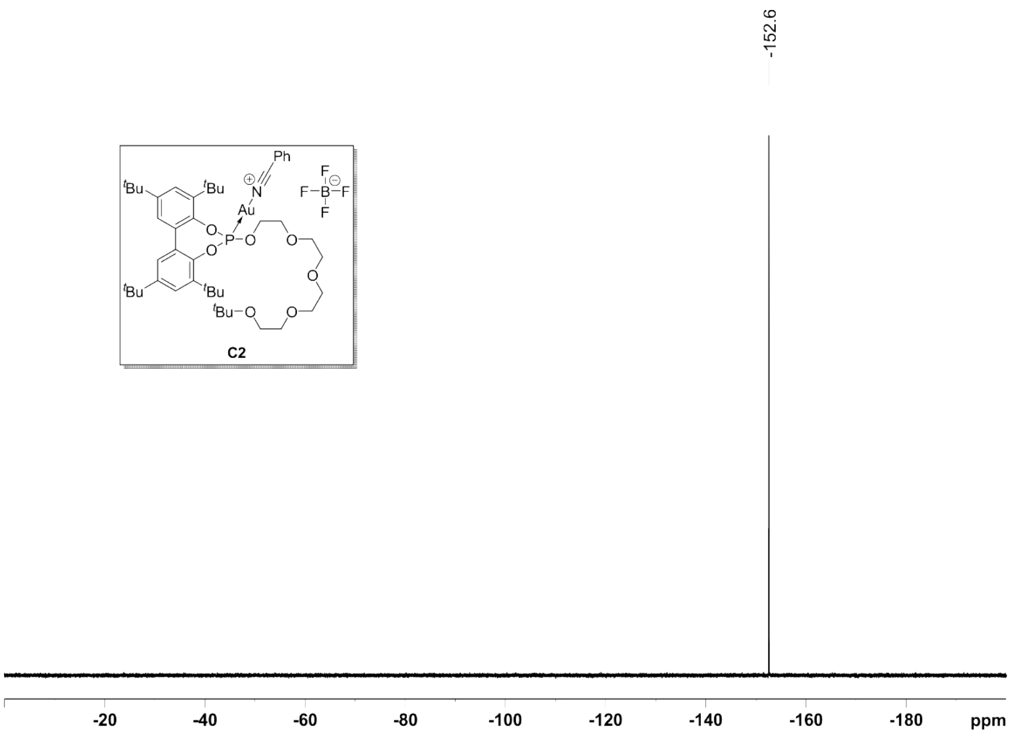


Figure SI 38. $^{19}F\{^1H\}$ NMR (376 MHz, CD_2Cl_2) for complex **C2**.

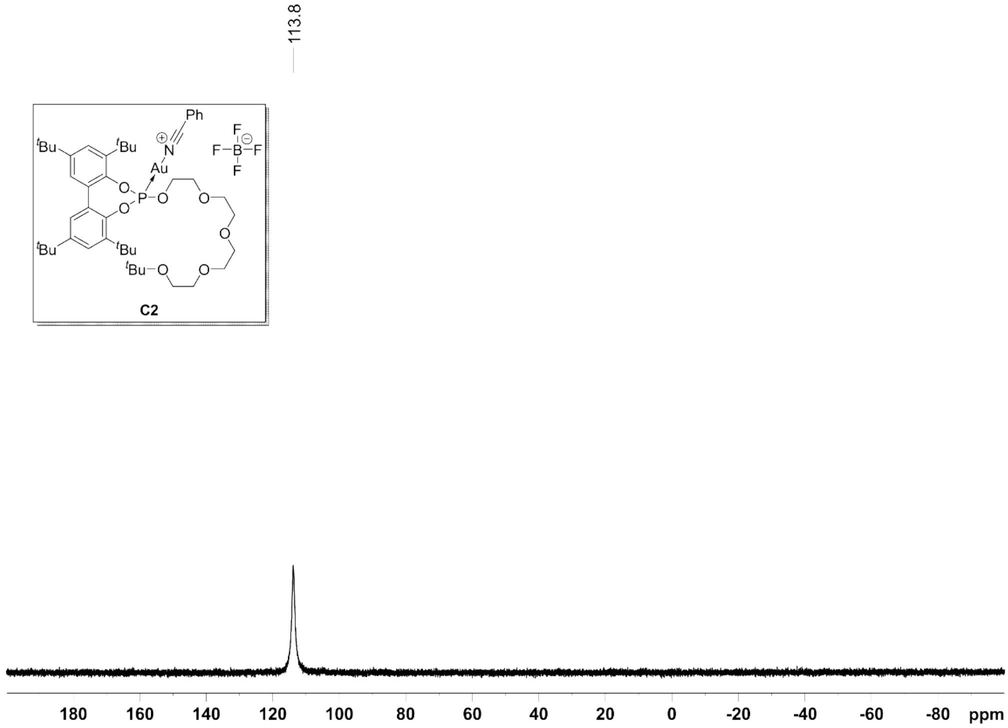


Figure SI 39. $^{31}P\{^1H\}$ NMR (162 MHz, CD_2Cl_2) for complex **C2**.

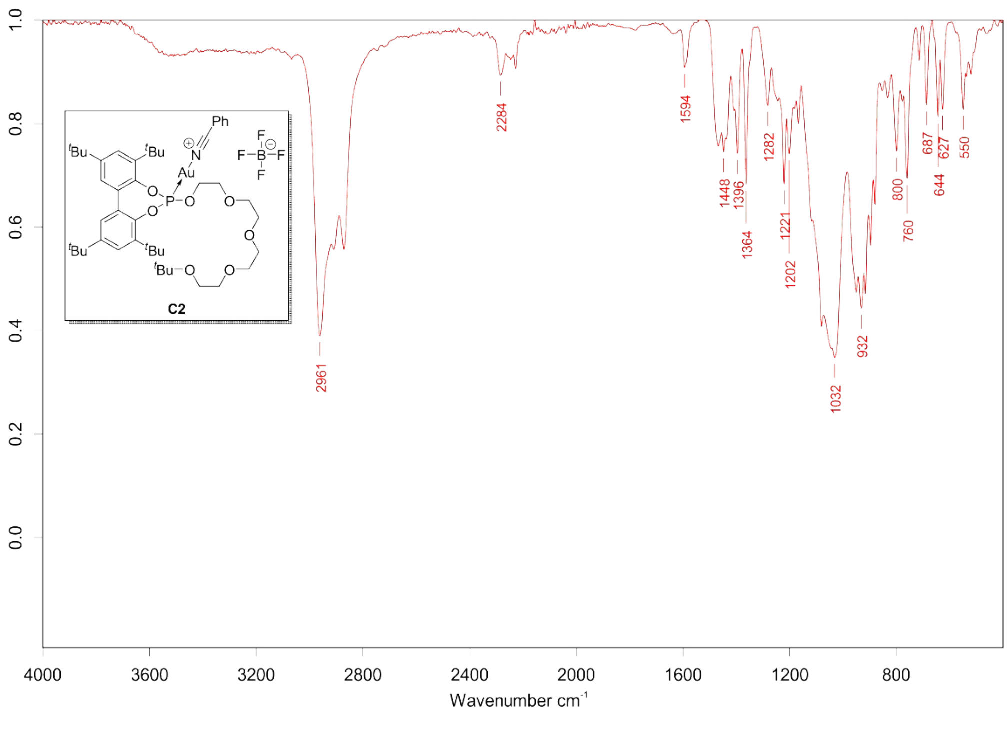


Figure SI 40. IR spectrum for complex **C2**.

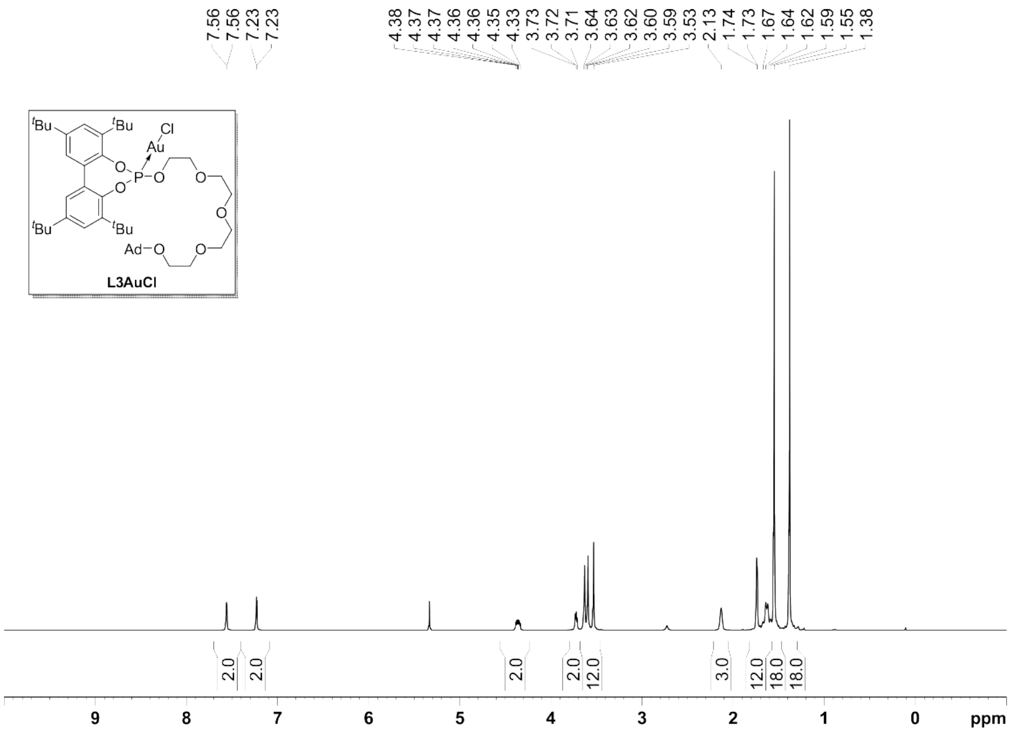


Figure SI 41. ^{1}H NMR (400 MHz, CD_2Cl_2) for complex **L3AuCl**.

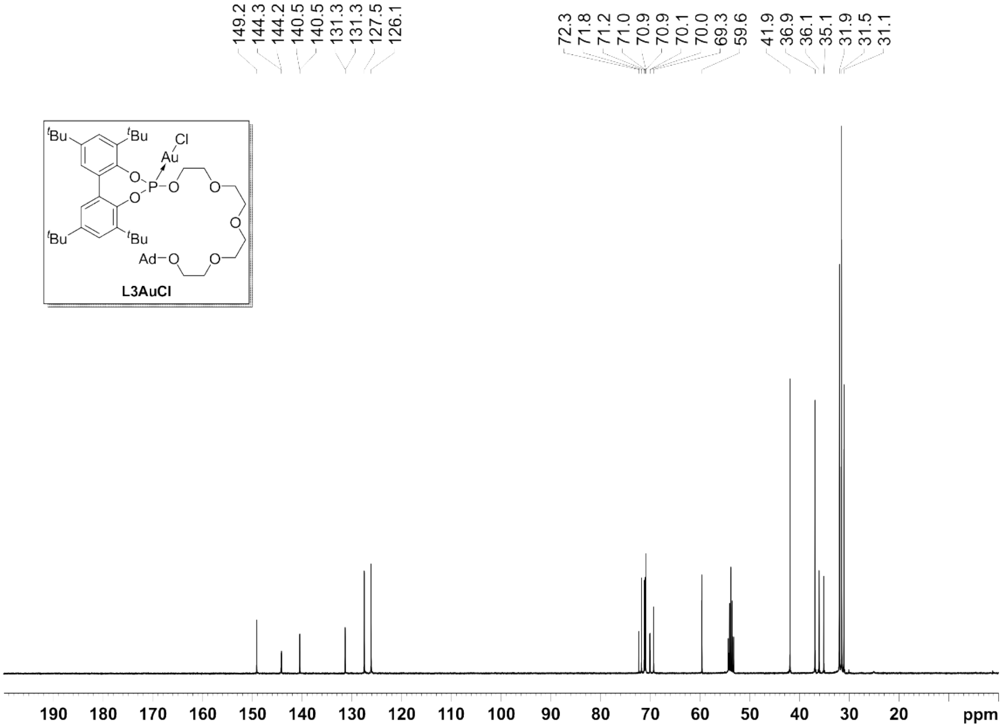


Figure SI 42. $^{13}C\{^{1}H\}$ NMR (100 MHz, CD_2Cl_2) for complex **L3AuCl**.

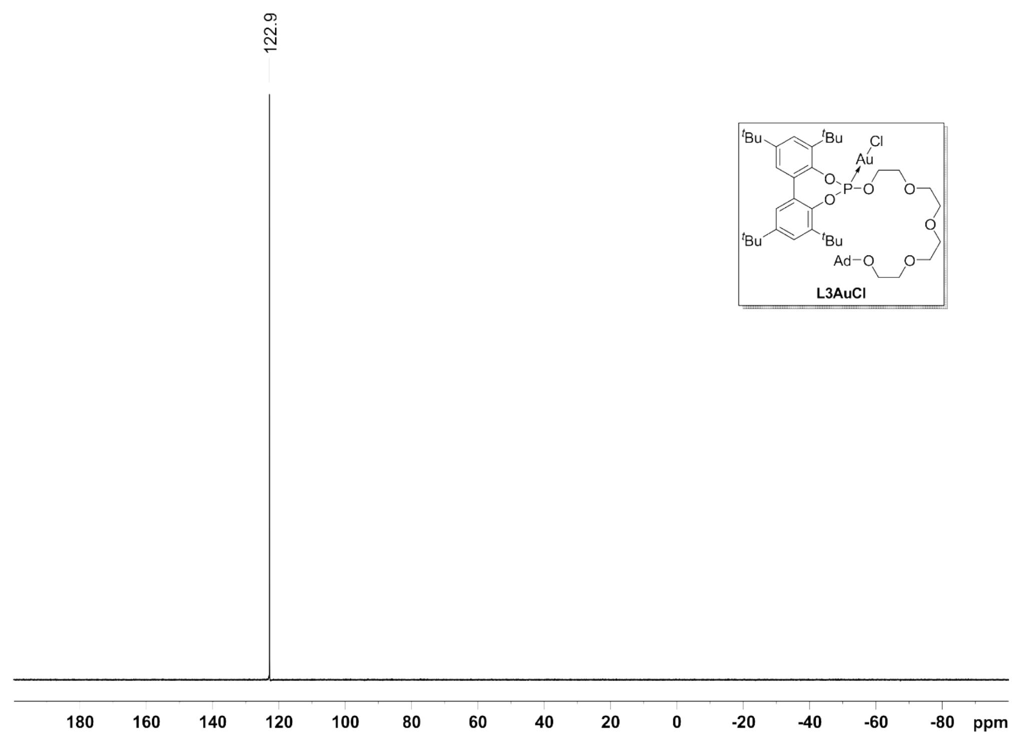


Figure SI 43. $^{31}P\{^{1}H\}$ NMR (162 MHz, CD_2Cl_2) for complex **L3AuCl**.

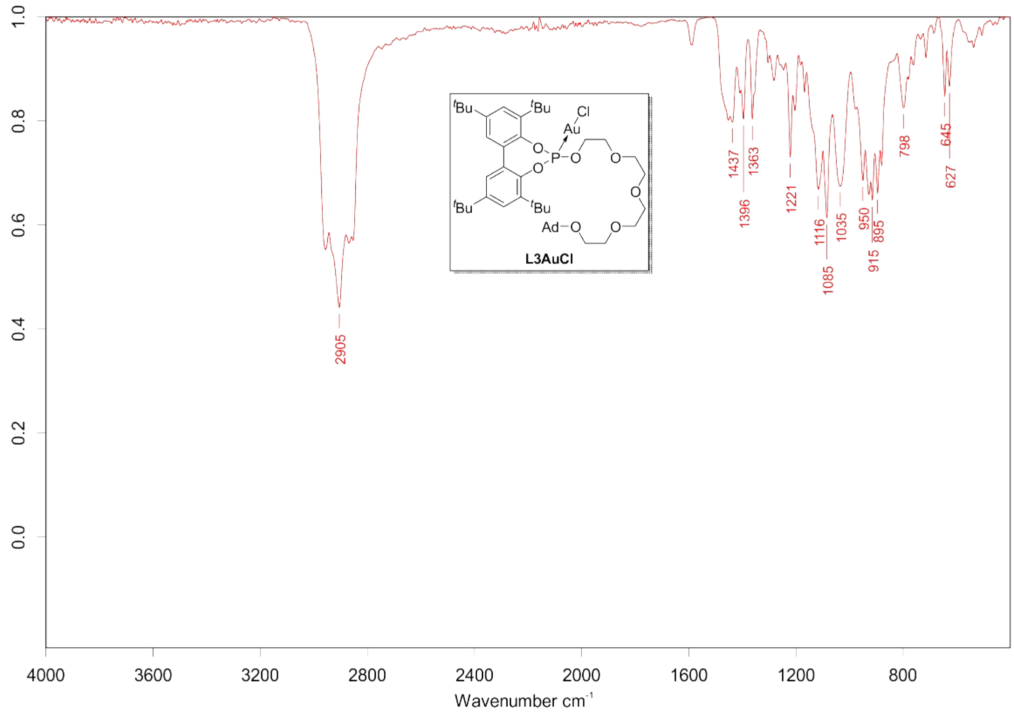


Figure SI 44. IR spectrum for complex **L3AuCl**.

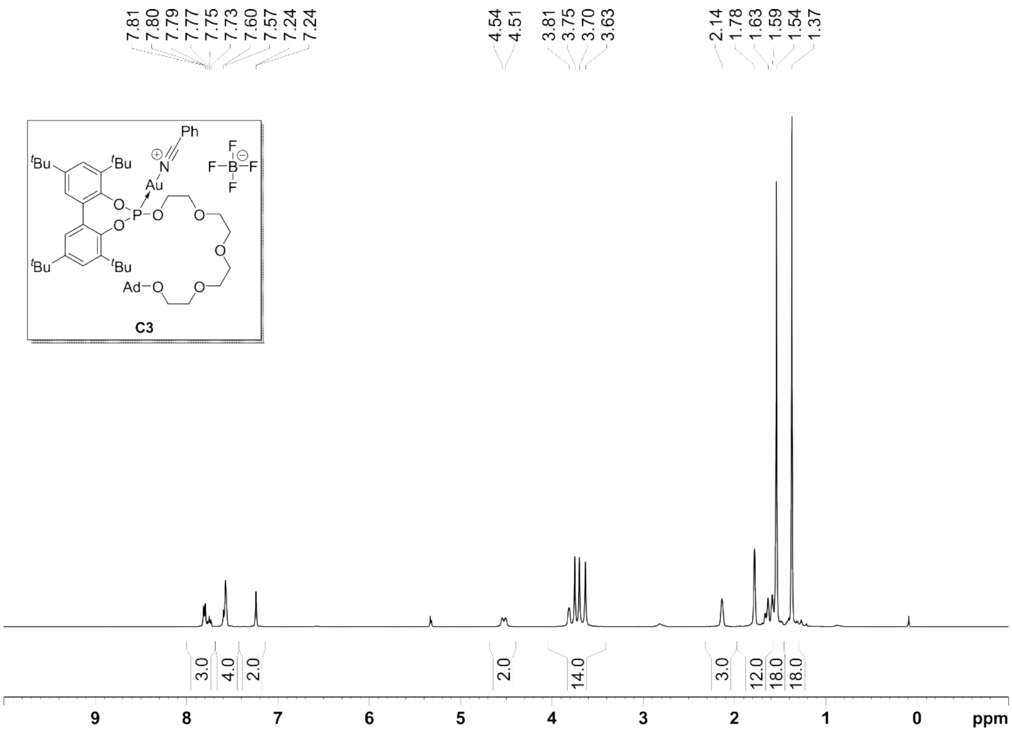


Figure SI 45. ^{1}H NMR (400 MHz, CD_2Cl_2) for complex **C3**.

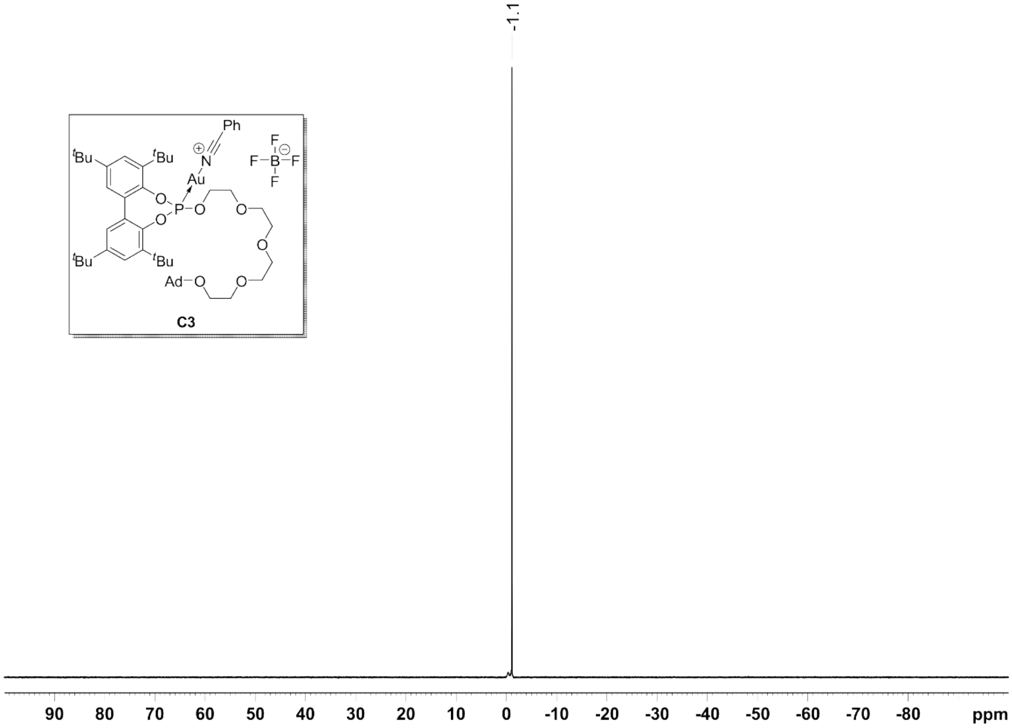


Figure SI 46. $^{11}B\{^1H\}$ NMR (128 MHz, CD_2Cl_2) for complex **C3**.

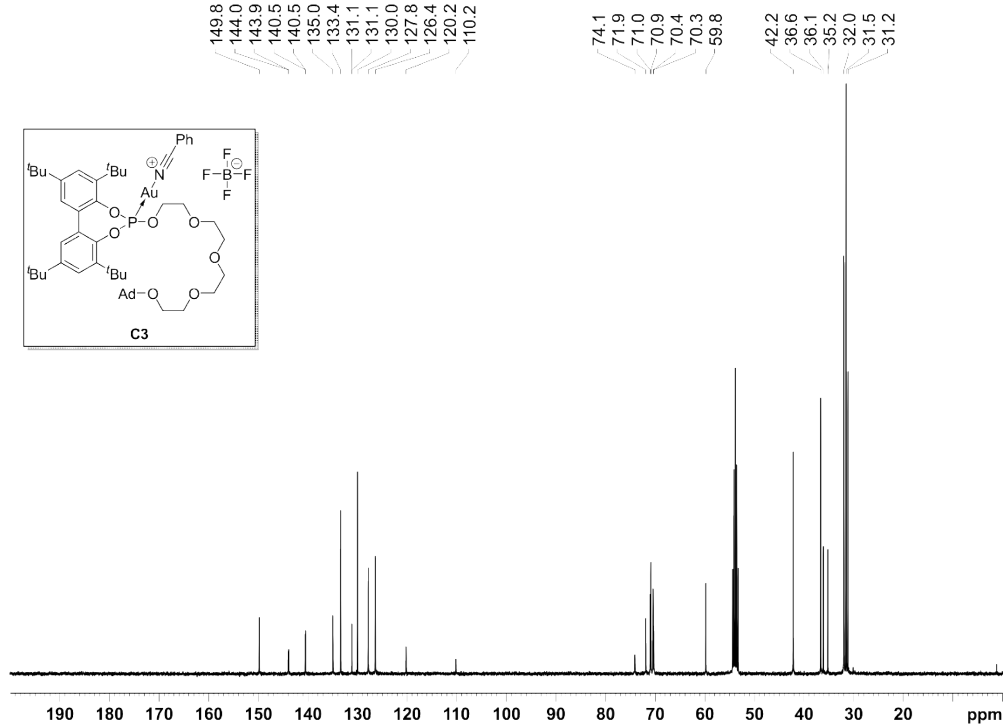


Figure SI 47. $^{13}C\{^1H\}$ NMR (126 MHz, CD_2Cl_2) for complex **C3**.

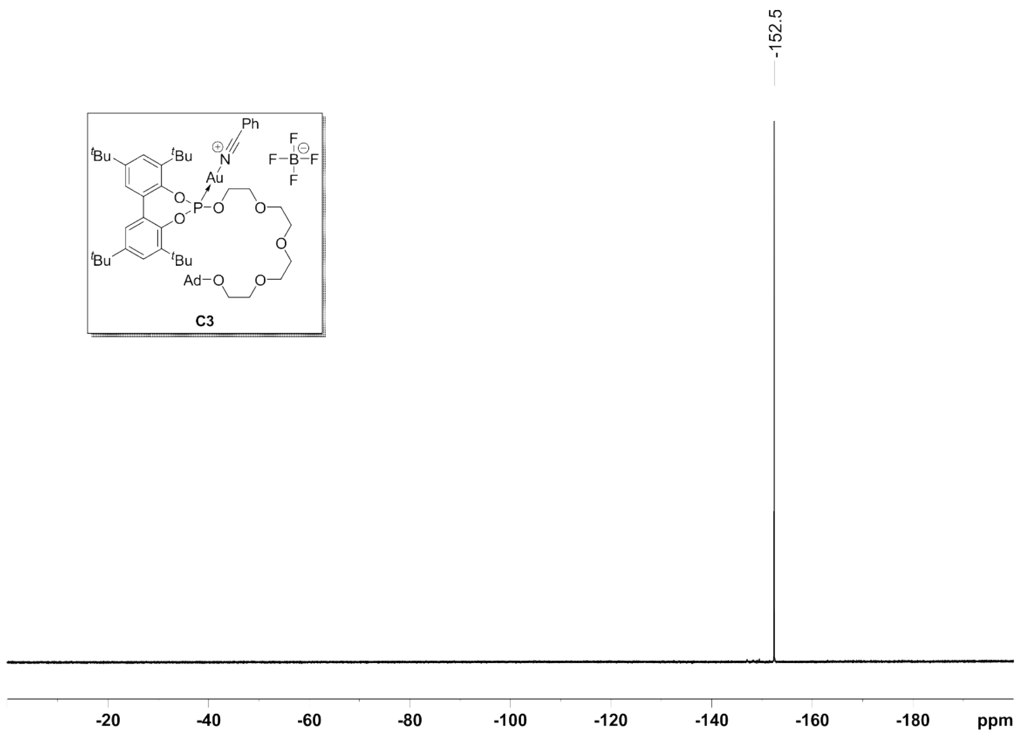


Figure SI 48. $^{19}F\{^1H\}$ NMR (376 MHz, CD_2Cl_2) for complex **C3**.

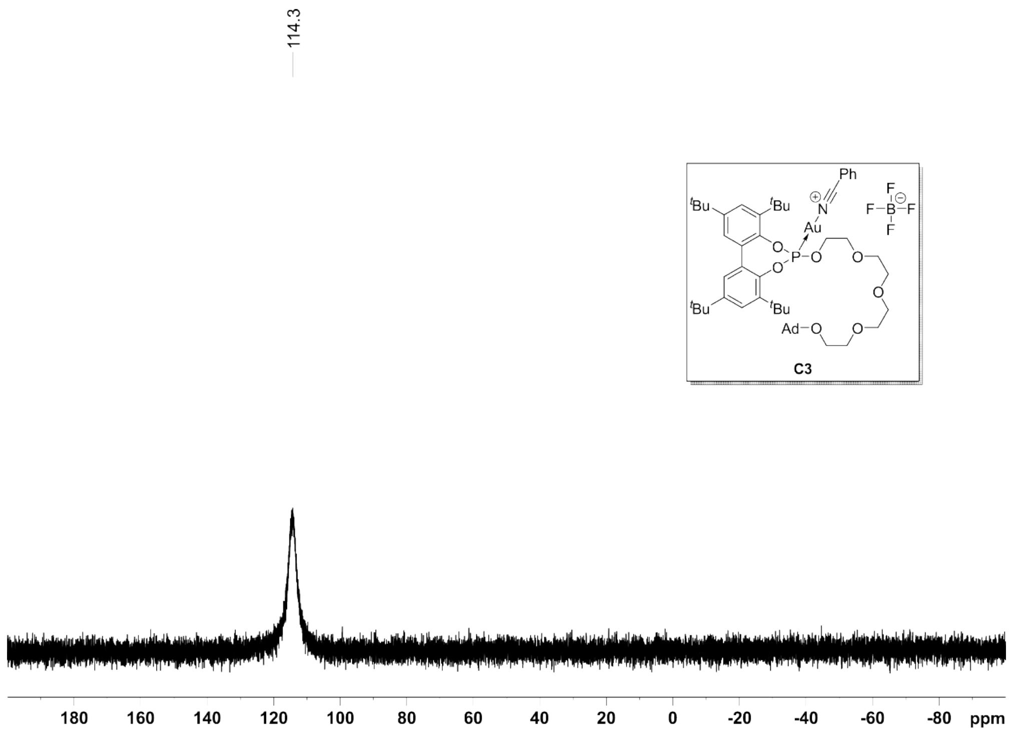


Figure SI 49. $^{31}P\{^{1}H\}$ NMR (162 MHz, CD_2Cl_2) for complex **C3**.

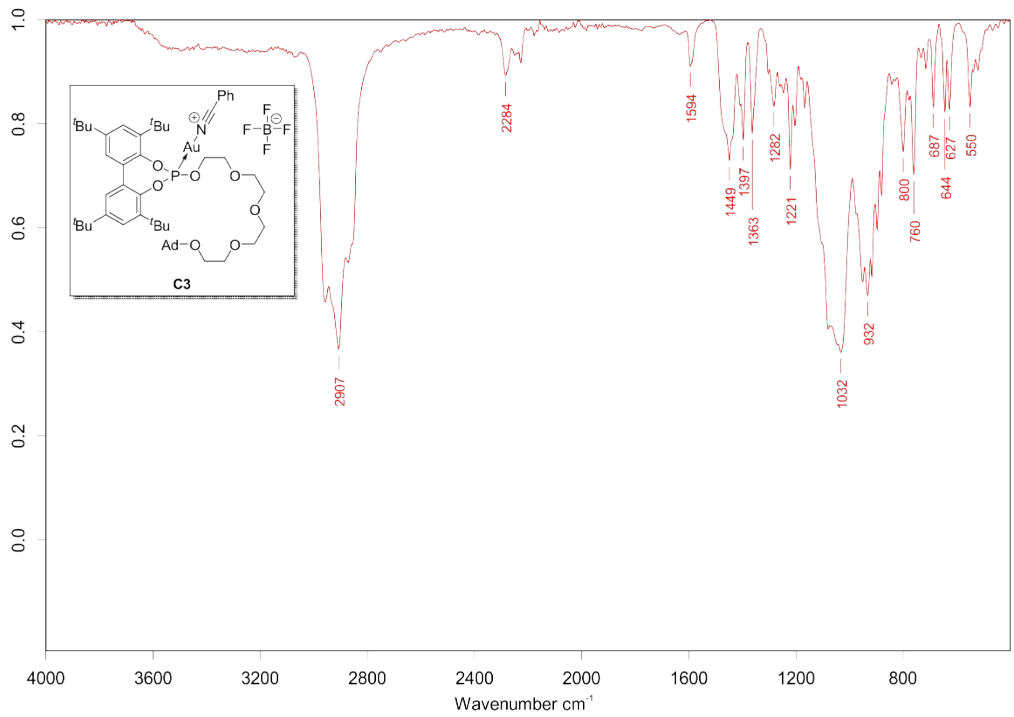


Figure SI 50. IR spectrum for complex **C3**.

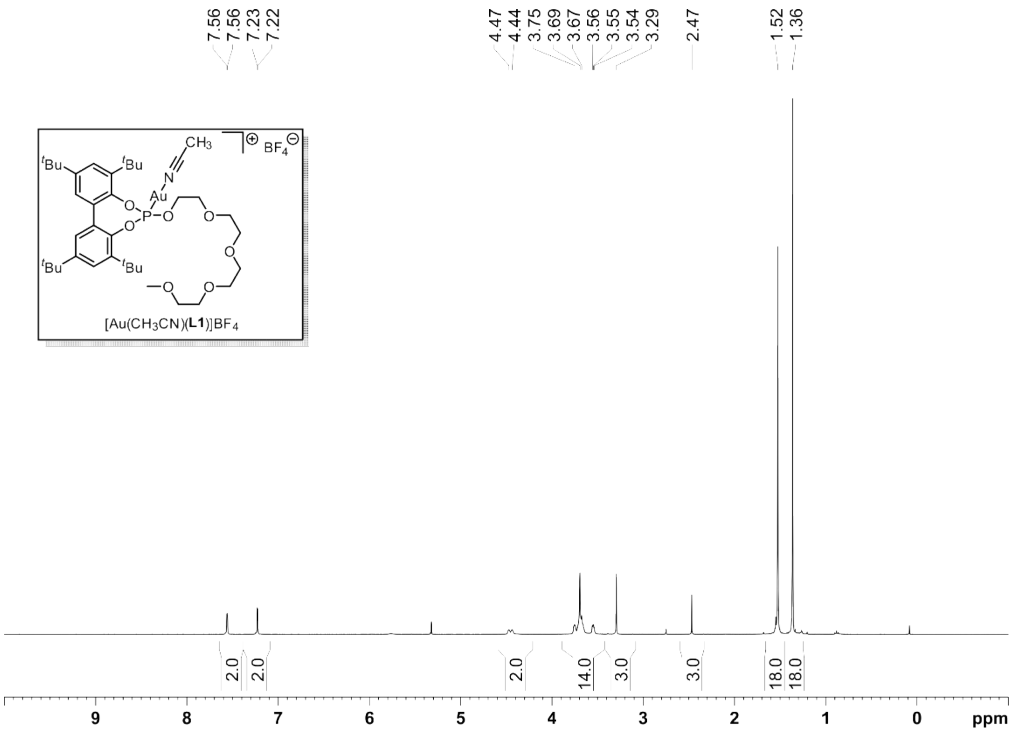


Figure SI 51. ^{1}H NMR spectrum (400 MHz, CD_2Cl_2) for complex [Au(CH_3CN)(**L1**)]BF_4.

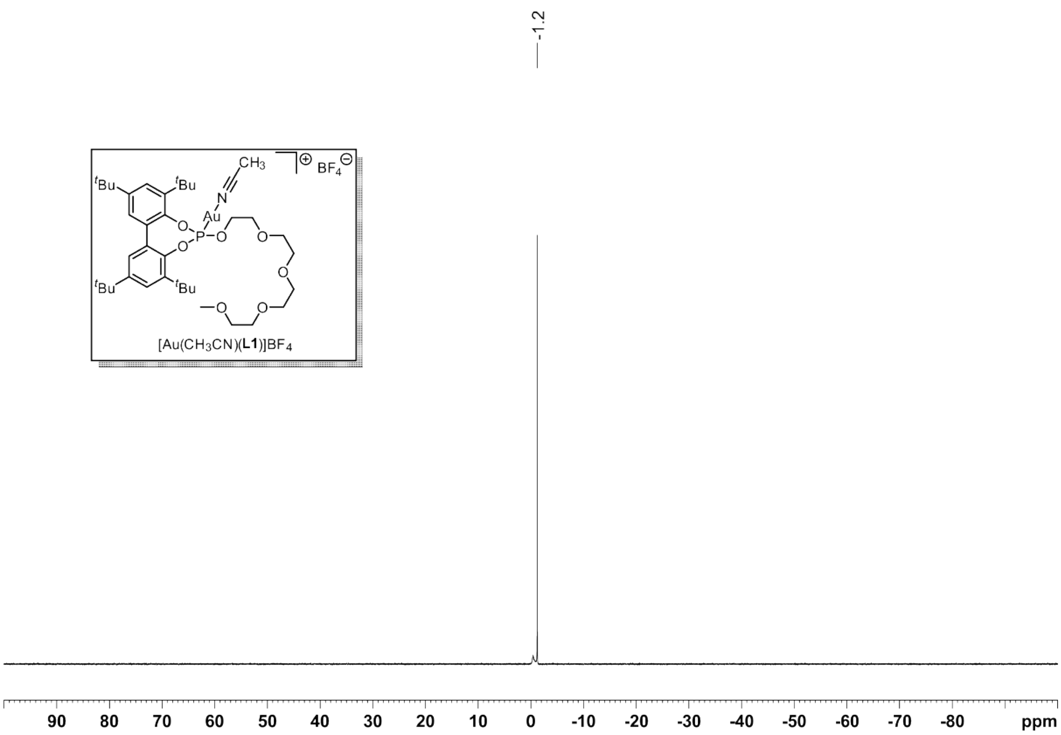


Figure SI 52. $^{11}B\{^{1}H\}$ NMR spectrum (128 MHz, CD_2Cl_2) for complex [Au(CH_3CN)(**L1**)]BF_4.

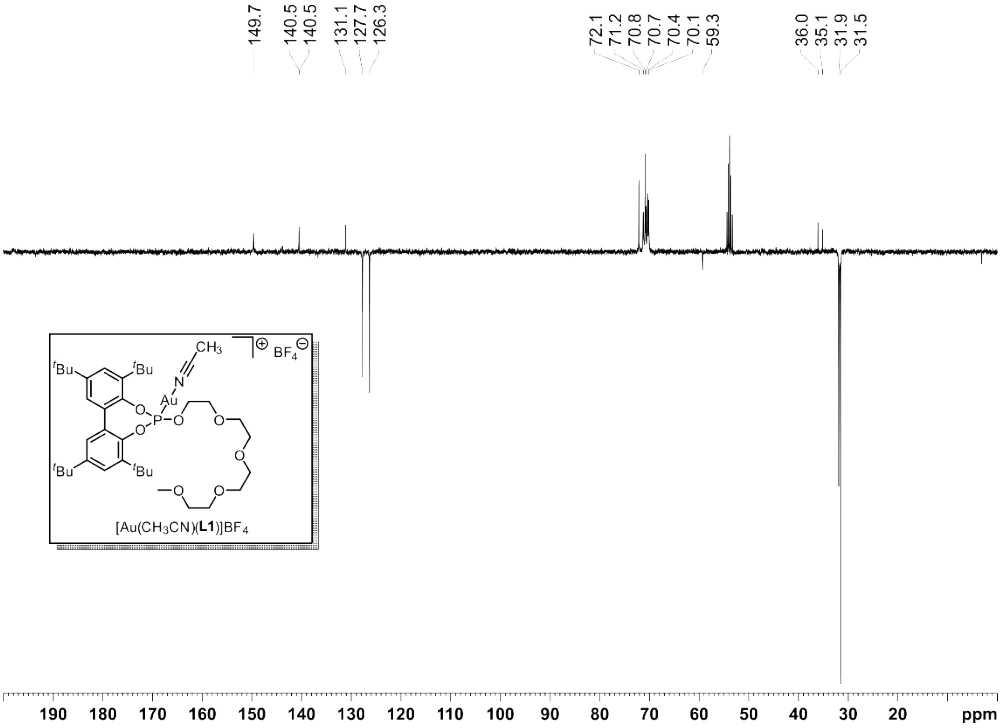


Figure SI 53. $^{13}C\{^{1}H\}$ DEPTQ135 NMR spectrum (126 MHz, CD_2Cl_2) for complex [Au(CH_3CN)(**L1**)]BF_4.

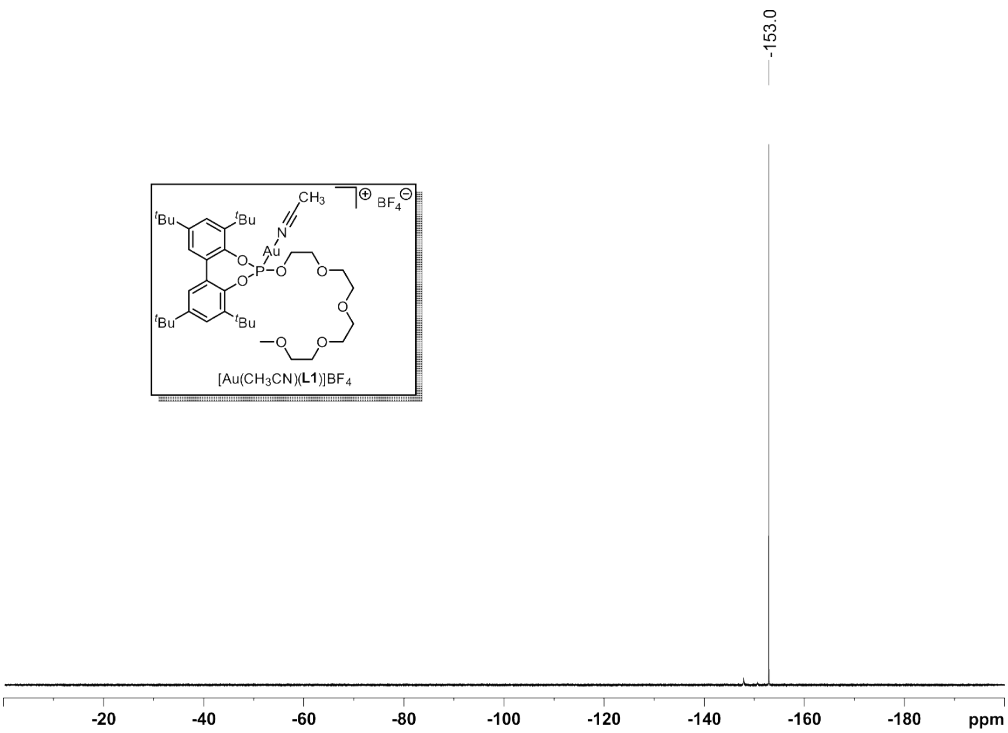


Figure SI 54. $^{19}F\{^{1}H\}$ NMR spectrum (376 MHz, CD_2Cl_2) for complex [Au(CH_3CN)(**L1**)]BF_4.

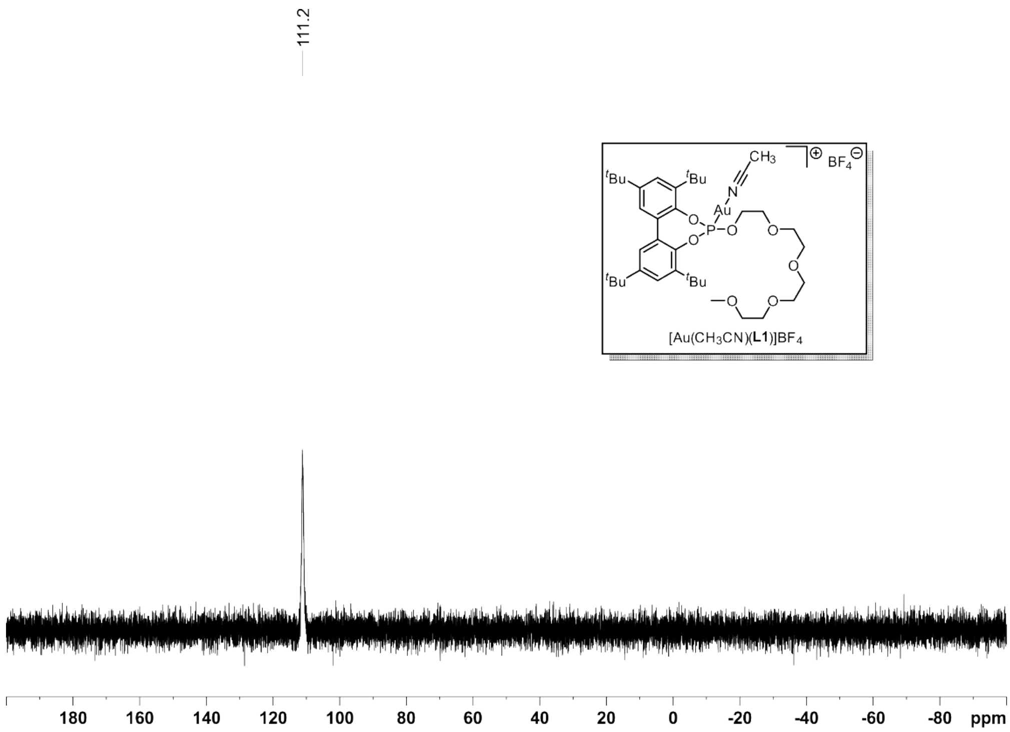


Figure SI 55. $^{31}P\{^{1}H\}$ NMR spectrum (162 MHz, CD_2Cl_2) for complex [Au(CH_3CN)(**L1**)]BF_4.

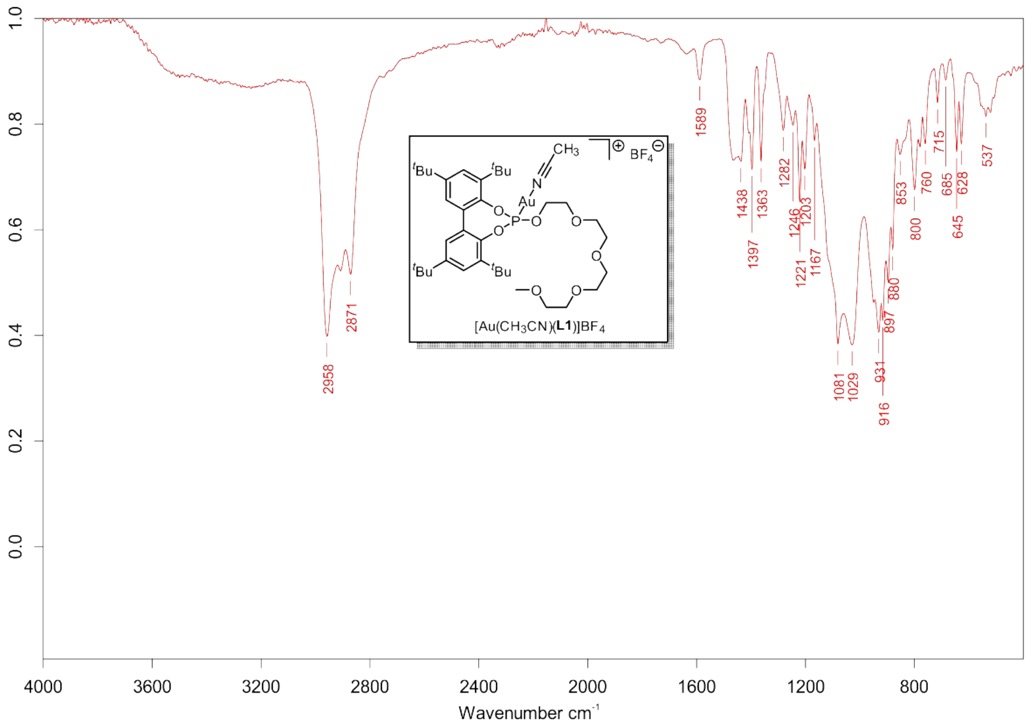


Figure SI 56. IR spectrum for complex [Au(CH_3CN)(**L1**)]BF_4.

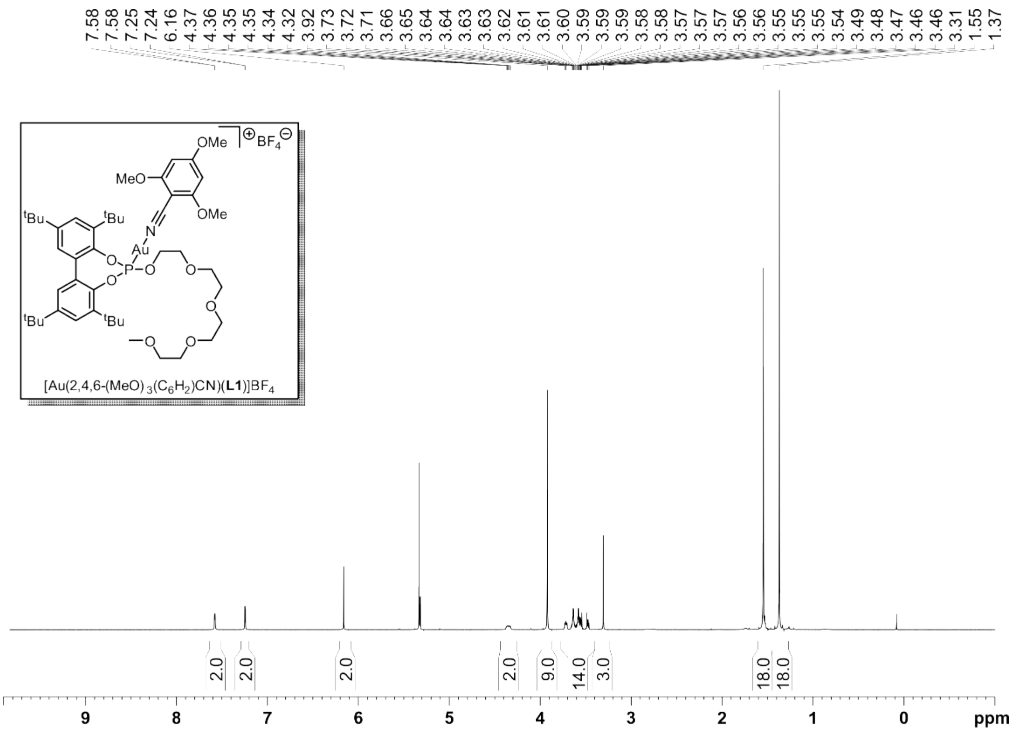


Figure SI 57. ^{1}H NMR spectrum (400 MHz, CD_2Cl_2) for complex [Au(2,4,6-(MeO)$_3$(C_6H_2)CN)(**L1**)]BF_4.

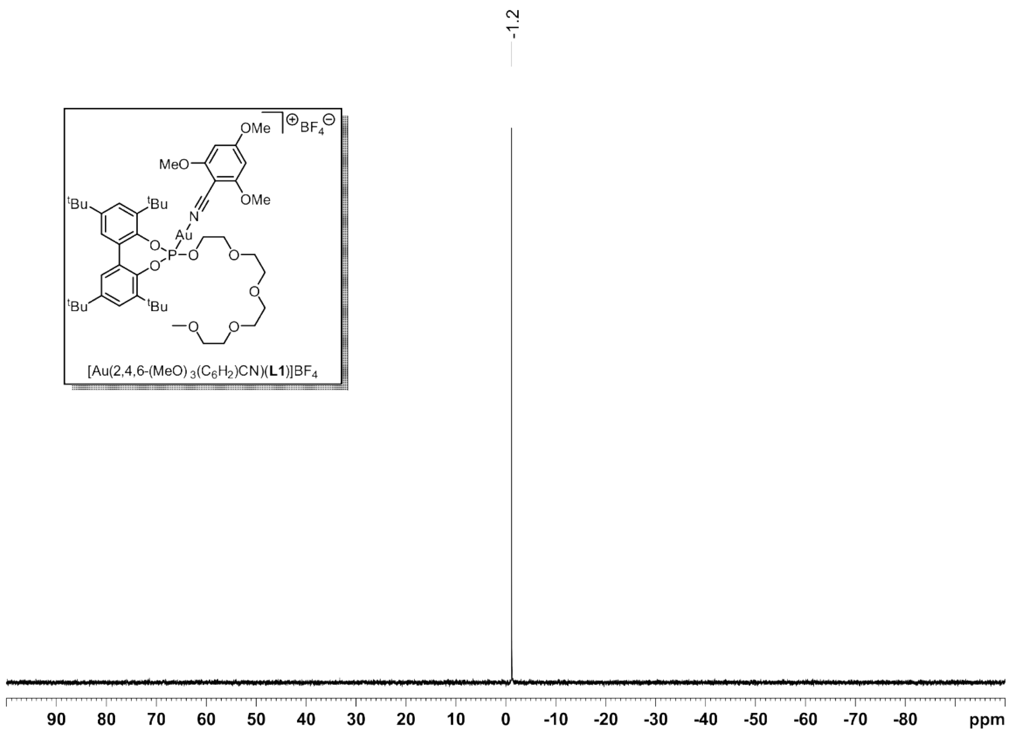


Figure SI 58. $^{11}B\{^{1}H\}$ NMR spectrum (128 MHz, CD_2Cl_2) for complex [Au(2,4,6-(MeO)$_3$(C_6H_2)CN)(**L1**)]BF_4.

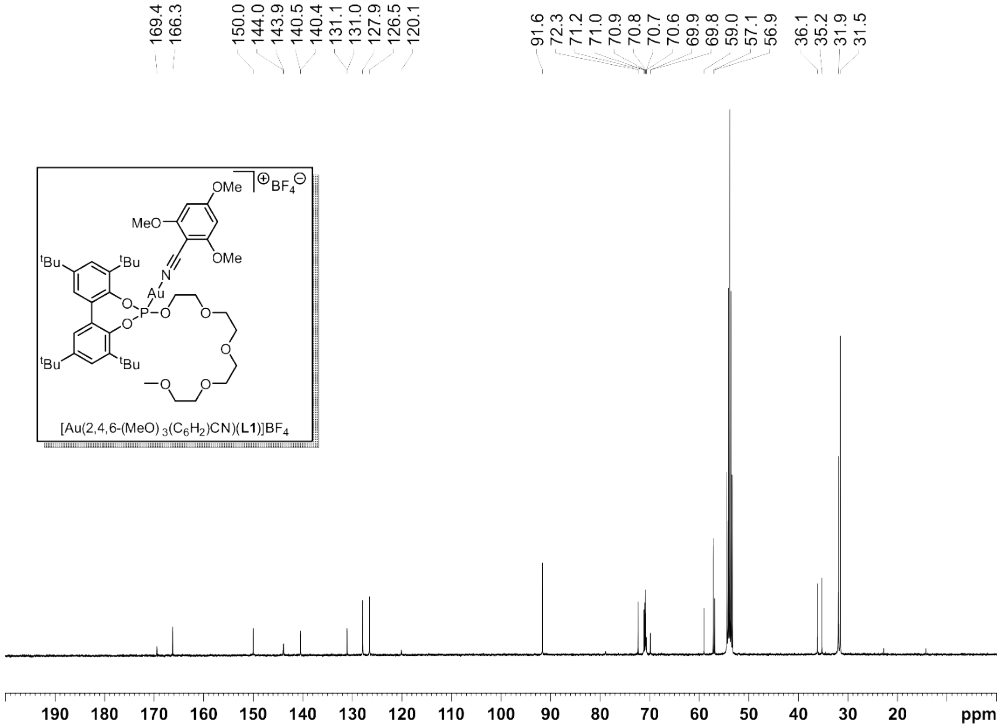


Figure SI 59. $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz, CD_2Cl_2) for complex [Au(2,4,6-(MeO)$_3$(C_6H_2)CN)(**L1**)]BF_4.

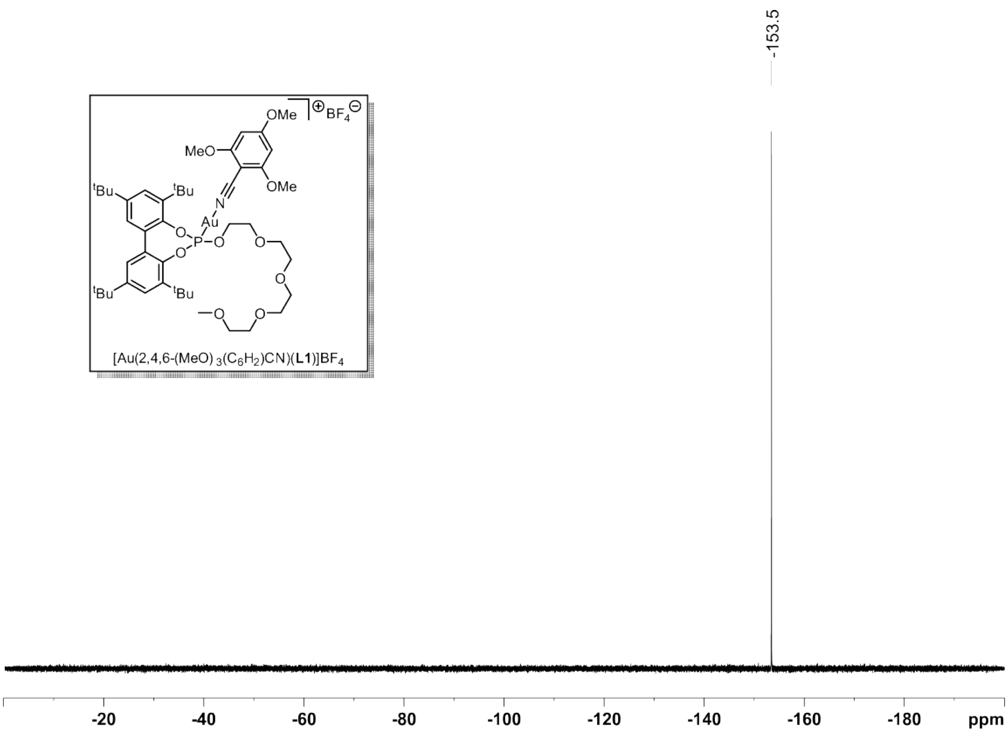


Figure SI 60. $^{19}F\{^{1}H\}$ NMR spectrum (376 MHz, CD_2Cl_2) for complex [Au(2,4,6-(MeO)$_3$(C_6H_2)CN)(**L1**)]BF_4.

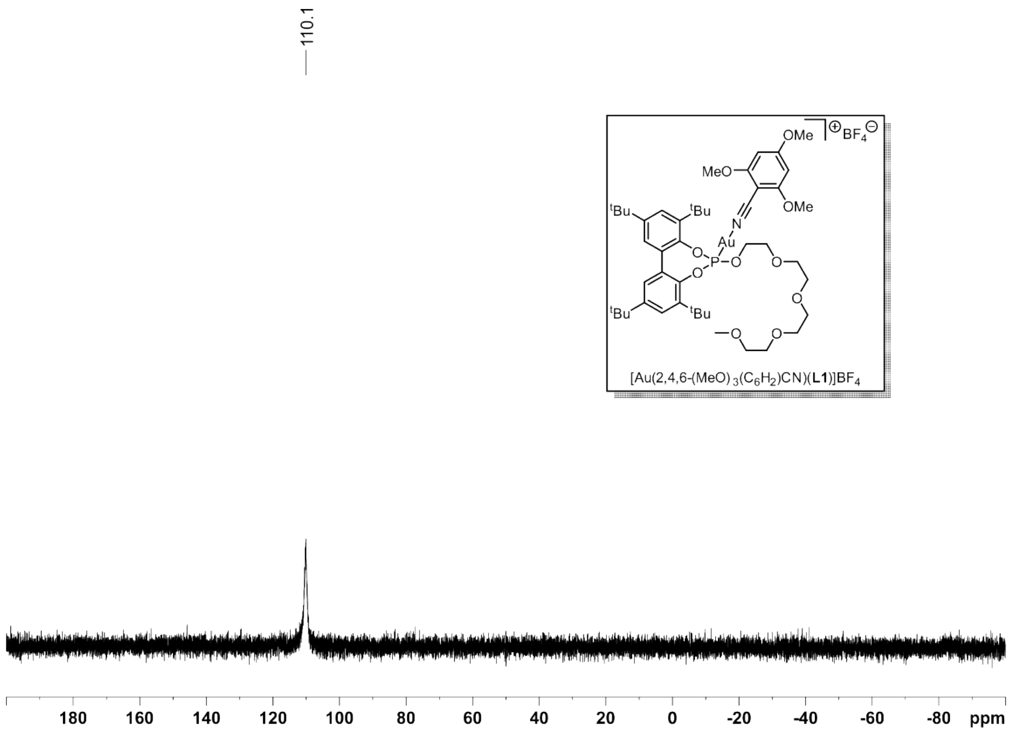


Figure SI 61. $^{31}P\{^1H\}$ NMR spectrum (162 MHz, CD_2Cl_2) for complex $[Au(2,4,6\text{-}(MeO)_3(C_6H_2)CN)(\mathbf{L1})]BF_4$.

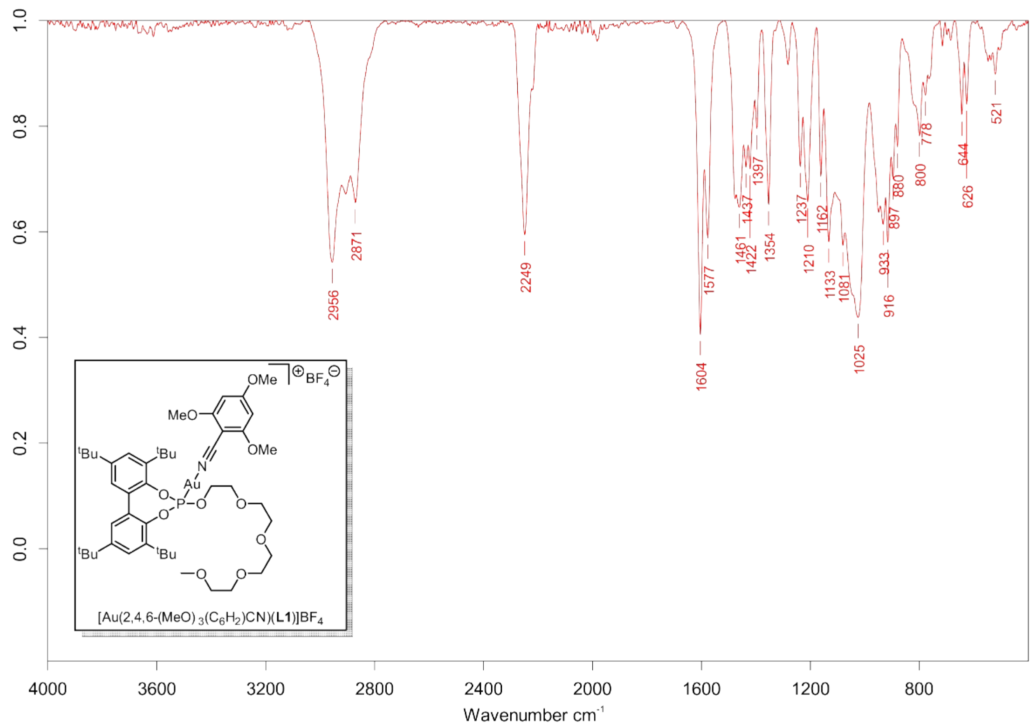


Figure SI 62. IR spectrum for complex $[Au(2,4,6\text{-}(MeO)_3(C_6H_2)CN)(\mathbf{L1})]BF_4$.

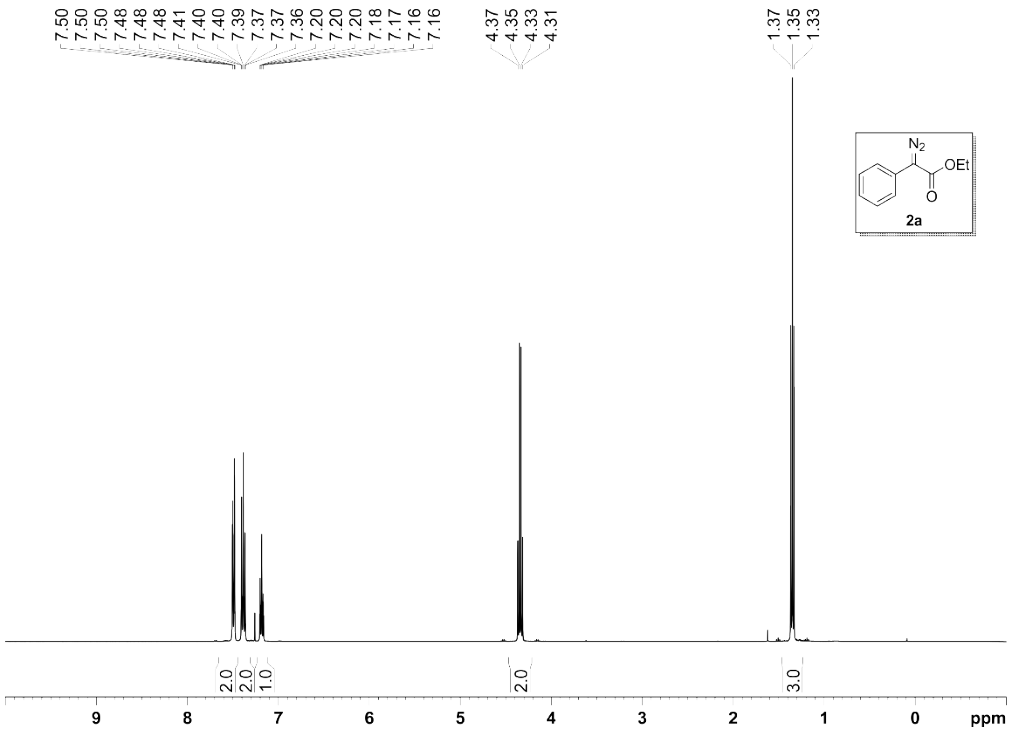


Figure SI 63. ^{1}H NMR (400 MHz, $CDCl_3$) for **2a**.

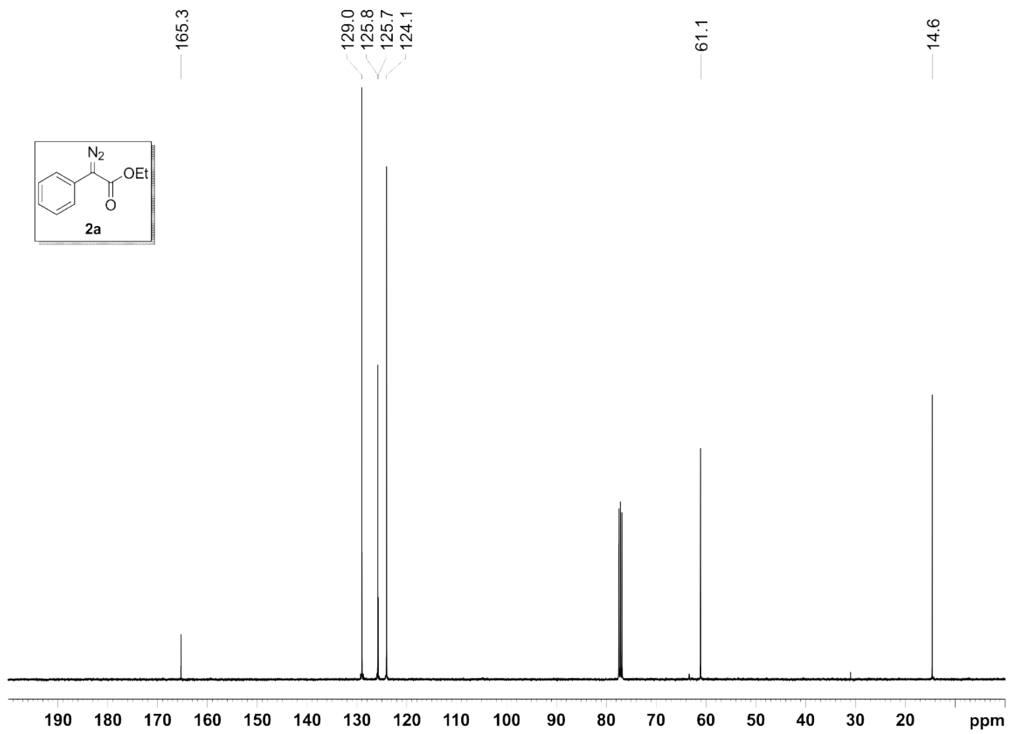


Figure SI 64. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) for **2a**.

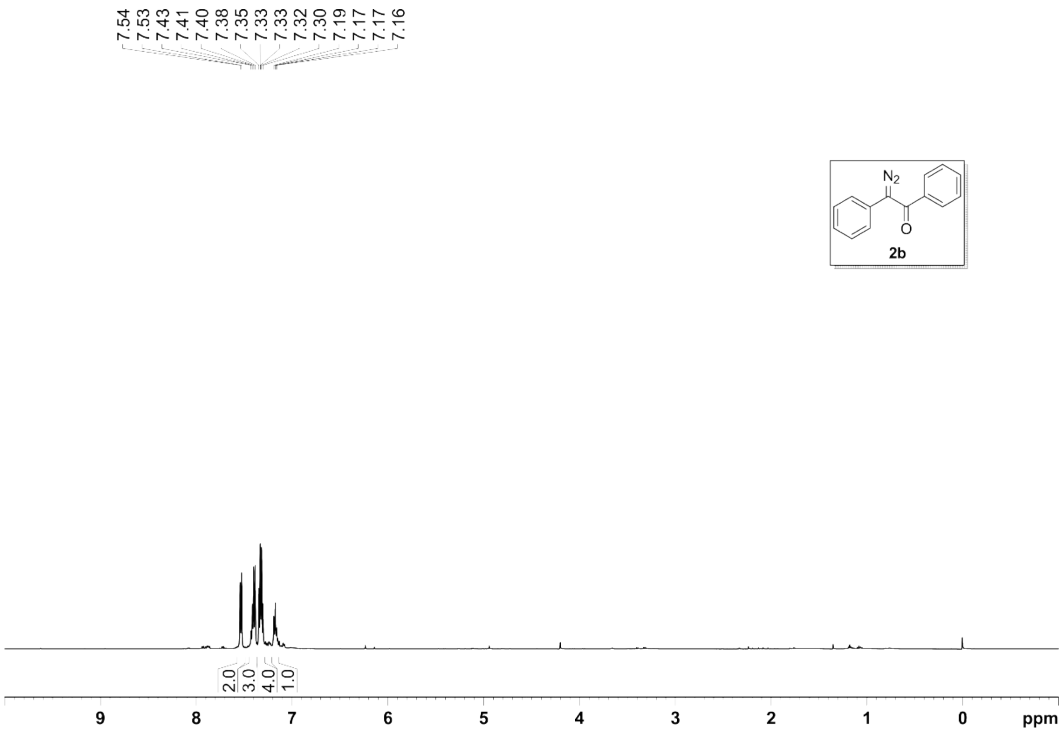


Figure SI 65. ^{1}H NMR (500 MHz, $CDCl_3$) for **2b**.

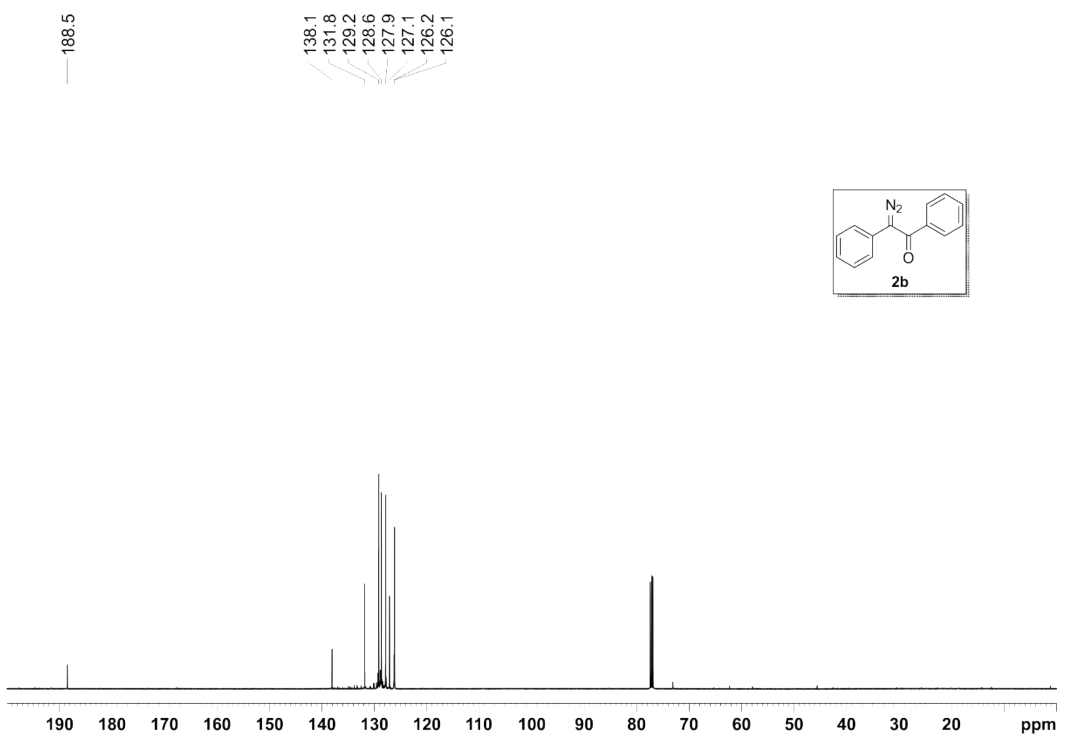


Figure SI 66. $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$) for **2b**.

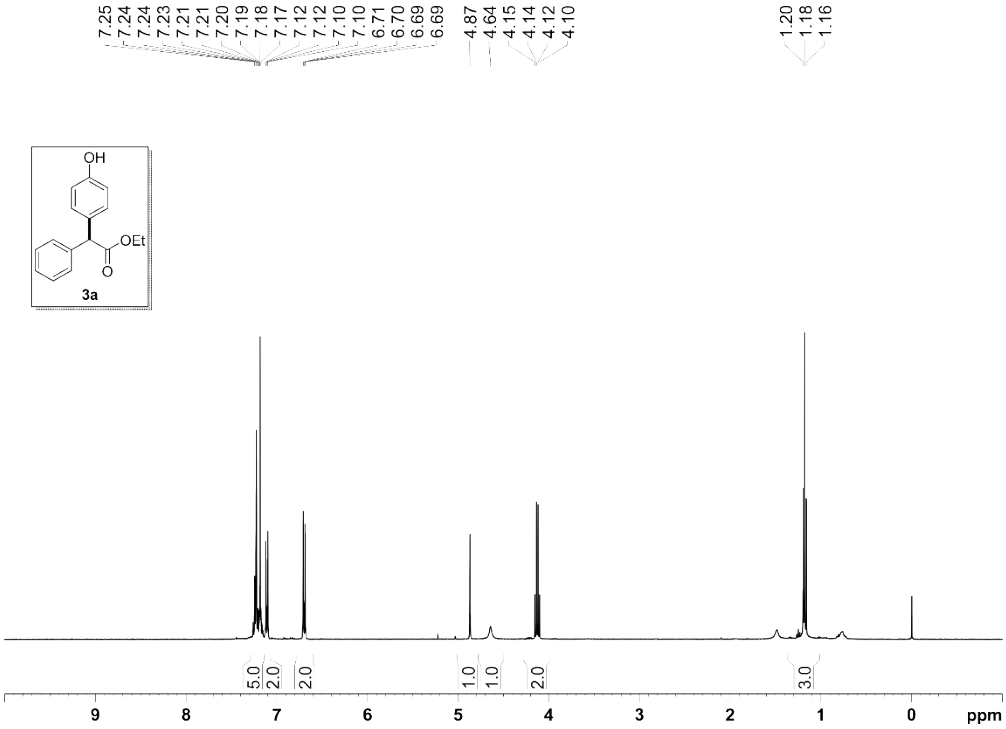


Figure SI 67. ^{1}H NMR (400 MHz, $CDCl_3$) for **3a**.

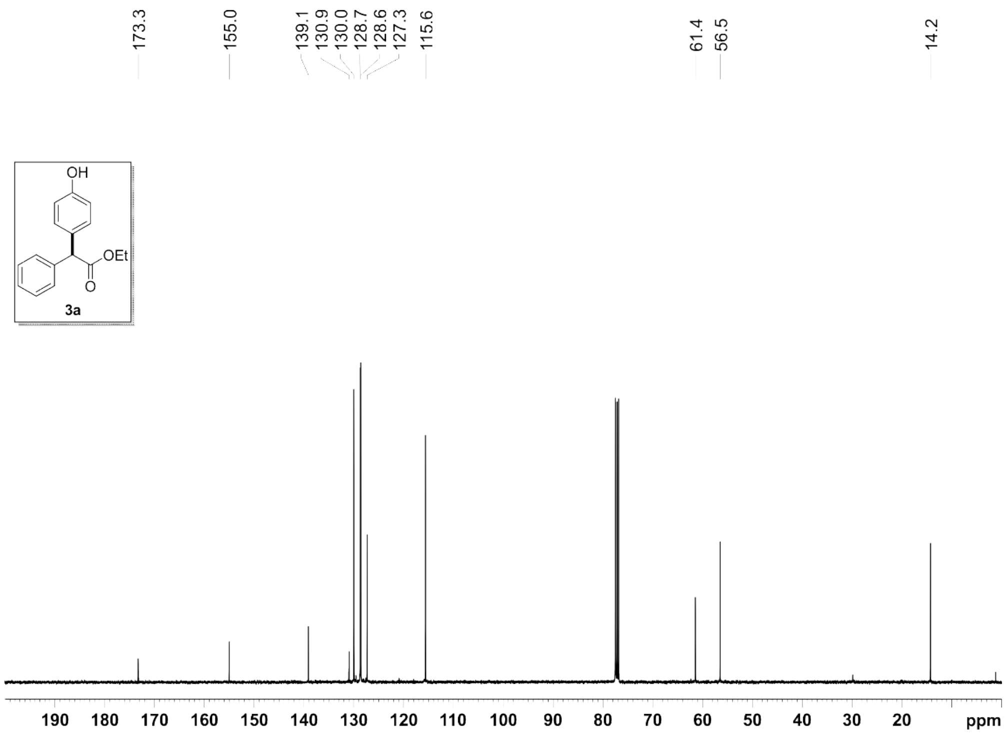


Figure SI 68. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) for **3a**.

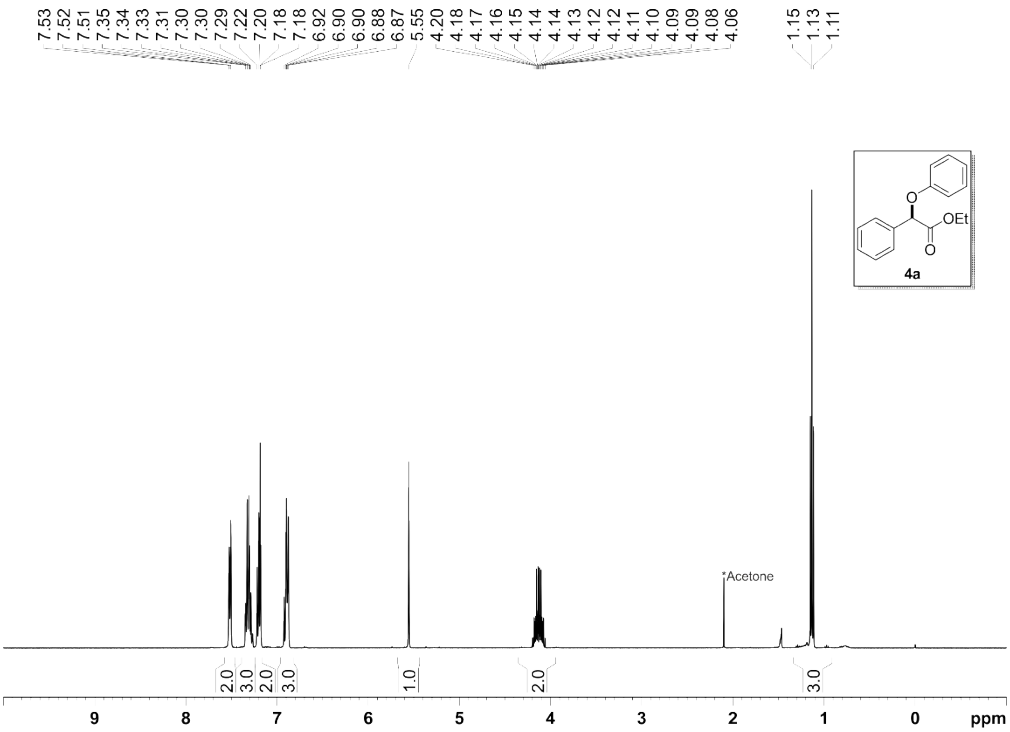


Figure SI 69. ^{1}H NMR (400 MHz, CDCl$_3$) for **4a**.

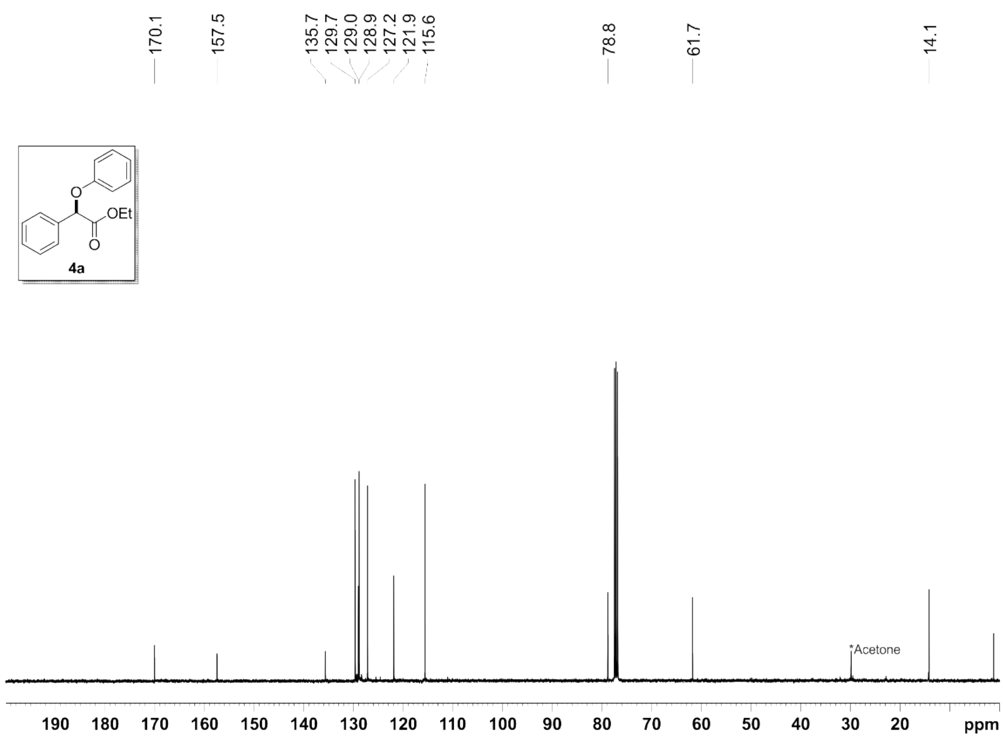


Figure SI 70. ^{13}C{^{1}H} NMR (100 MHz, CDCl$_3$) for **4a**.

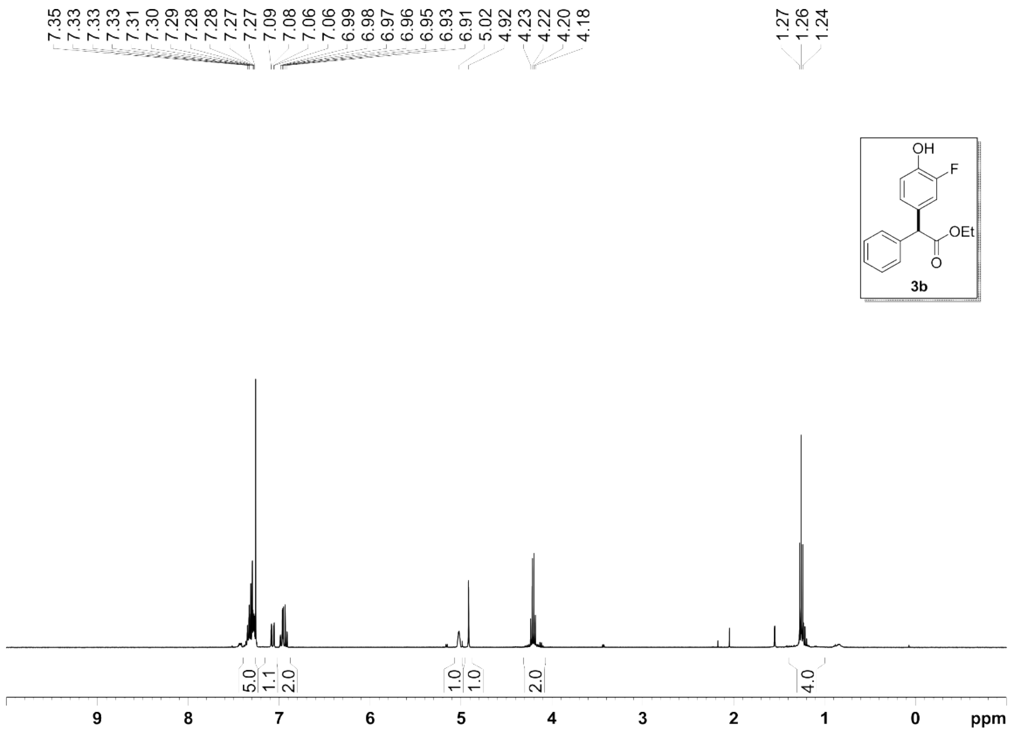


Figure SI 71. ^{1}H NMR (400 MHz, $CDCl_3$) for **3b**.

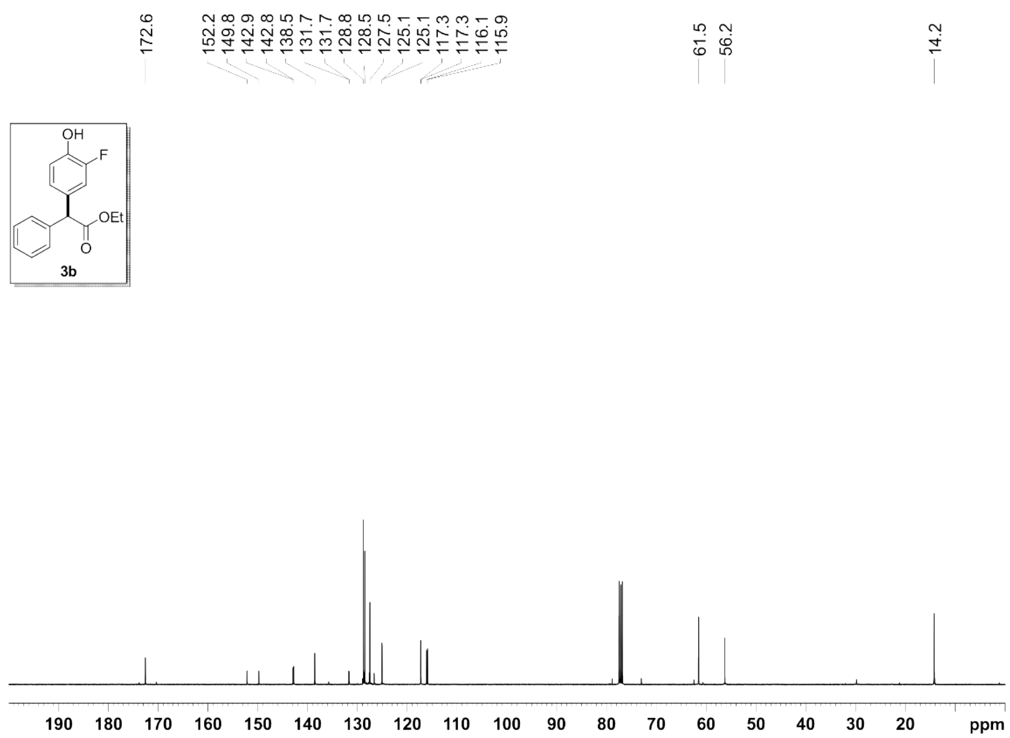


Figure SI 72. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) for **3b**.

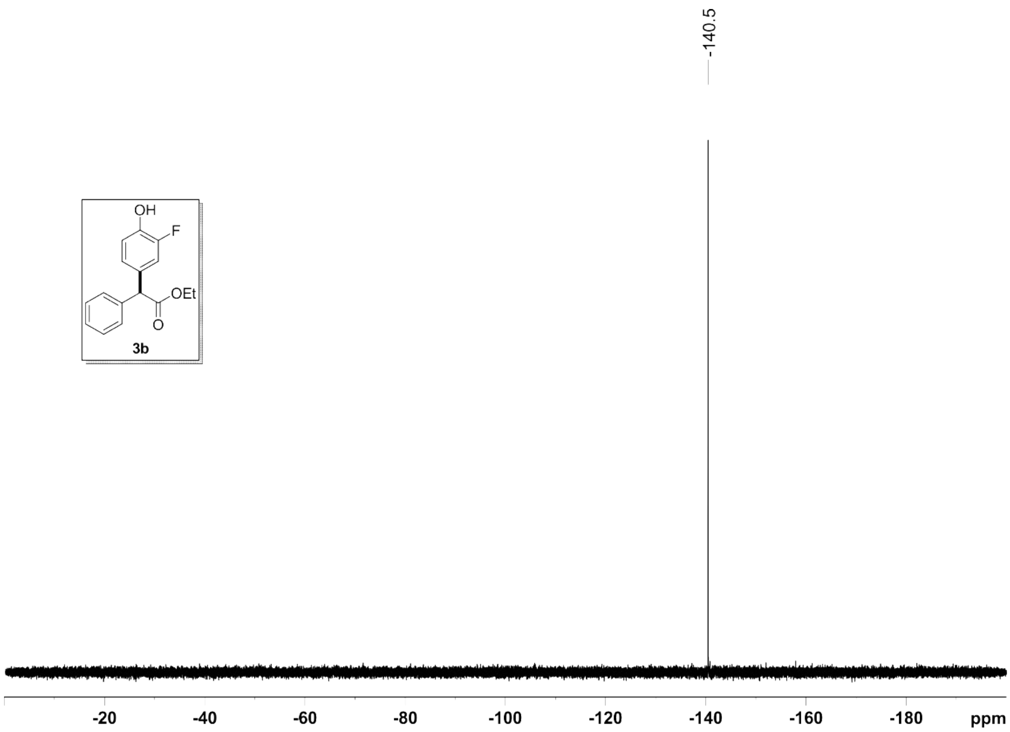


Figure SI 73. $^{19}F\{^{1}H\}$ NMR (376 MHz, $CDCl_3$) for **3b**.

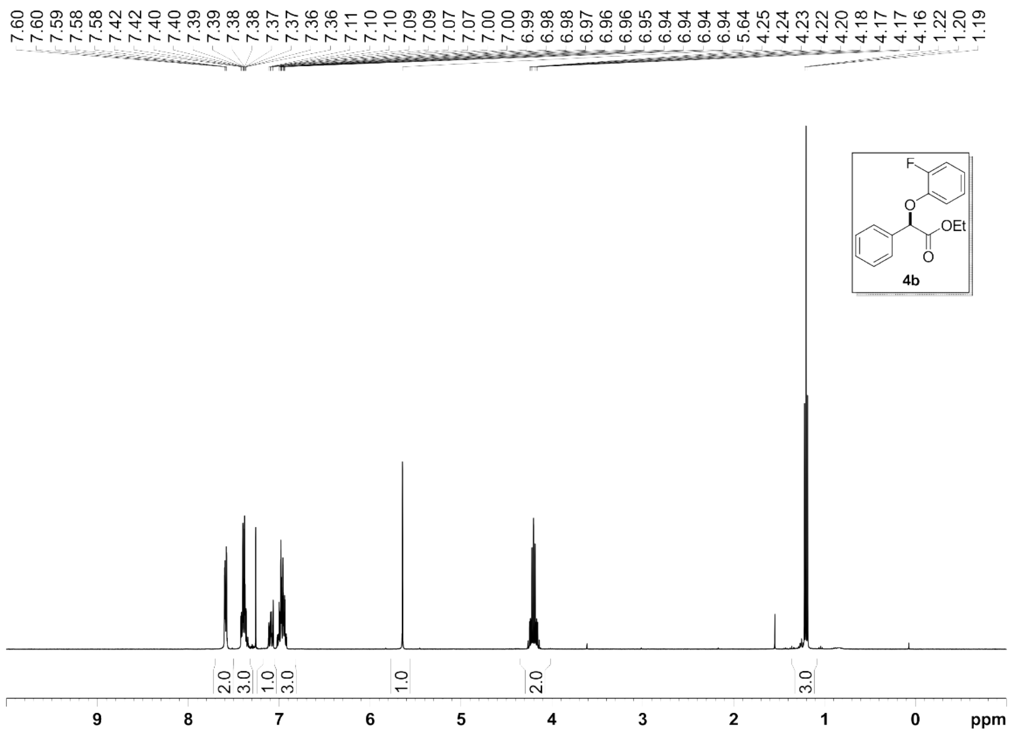


Figure SI 74. ^{1}H NMR (400 MHz, $CDCl_3$) for **4b**.

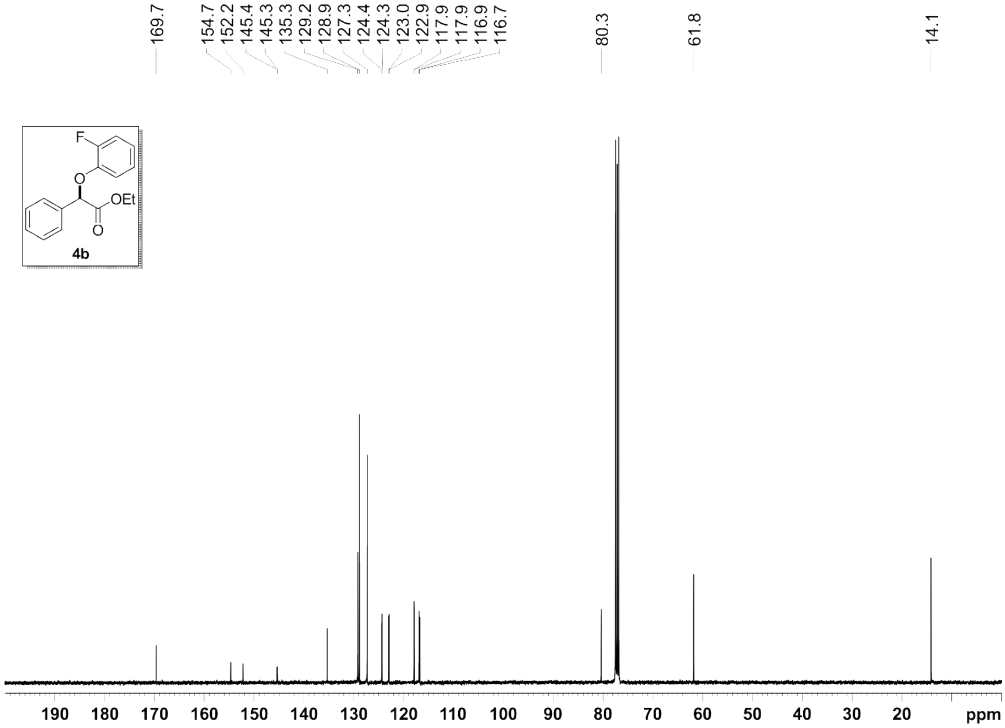


Figure SI 75. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) for **4b**.

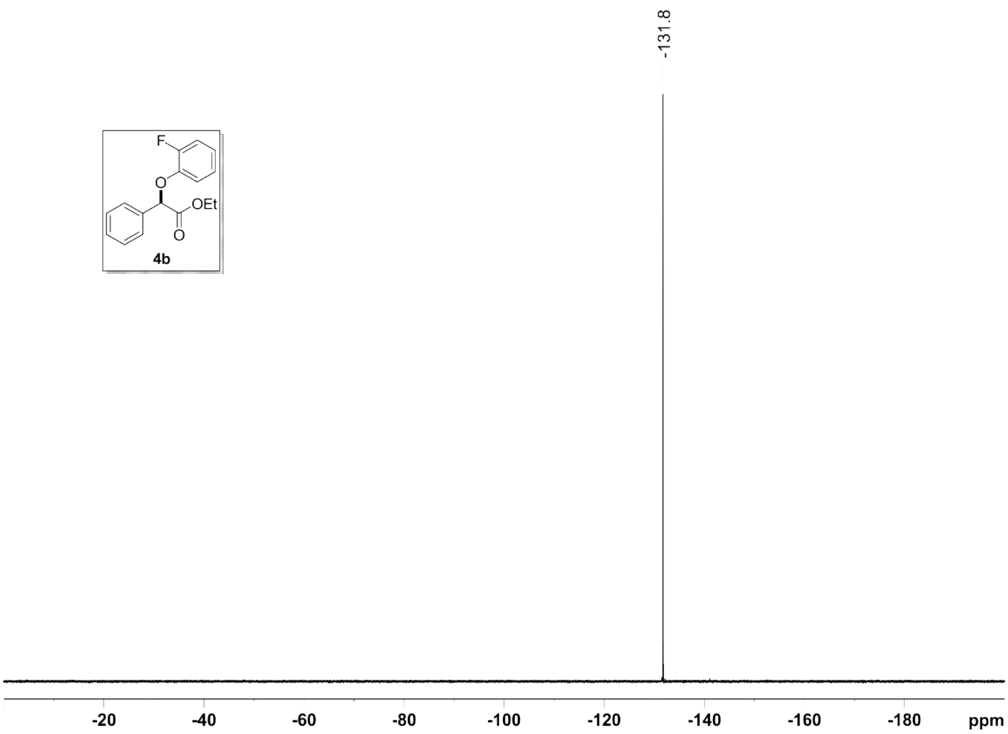


Figure SI 76. $^{19}F\{^{1}H\}$ NMR (376 MHz, $CDCl_3$) for **4b**.

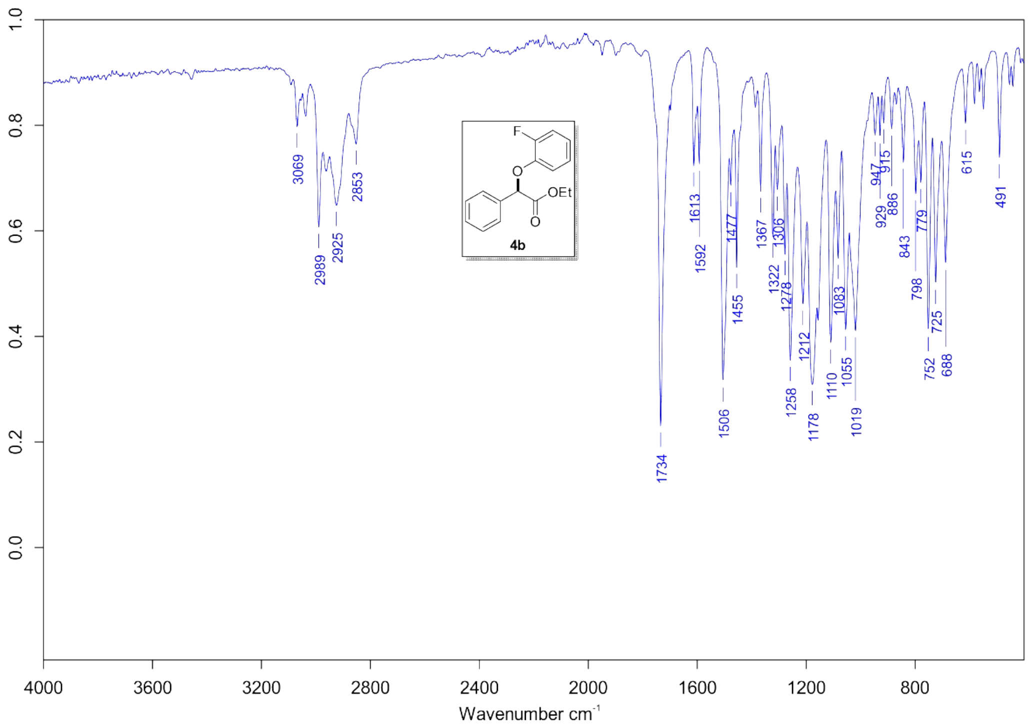


Figure SI 77. IR spectrum for **4b**.

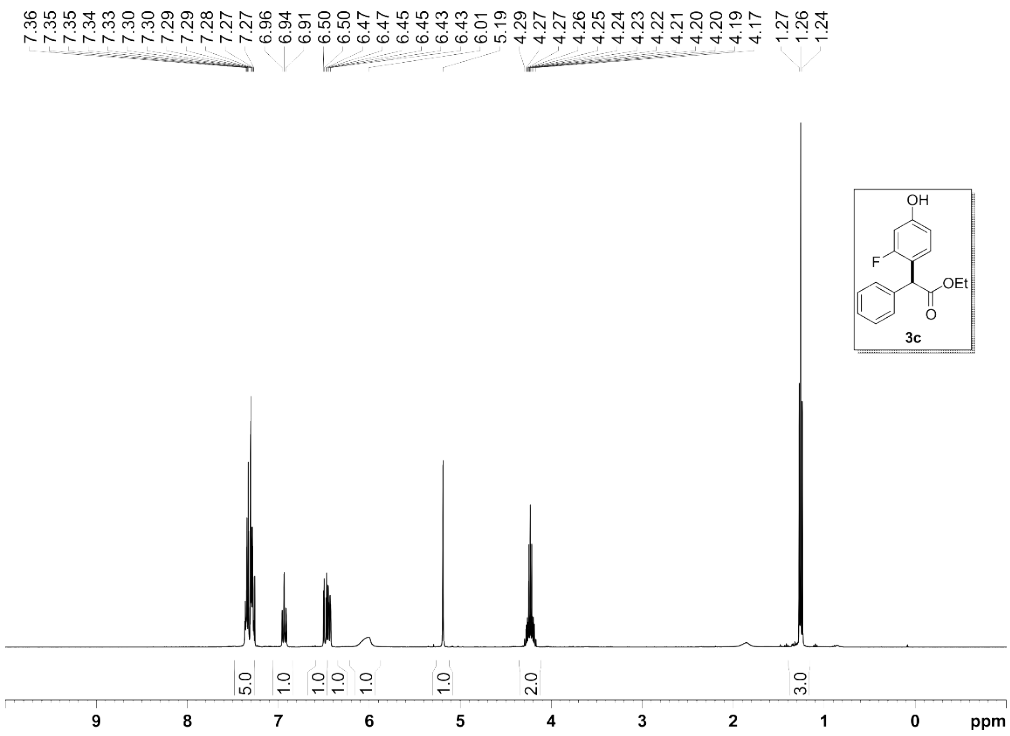


Figure SI 78. ^{1}H NMR (400 MHz, $CDCl_3$) for **3c**.

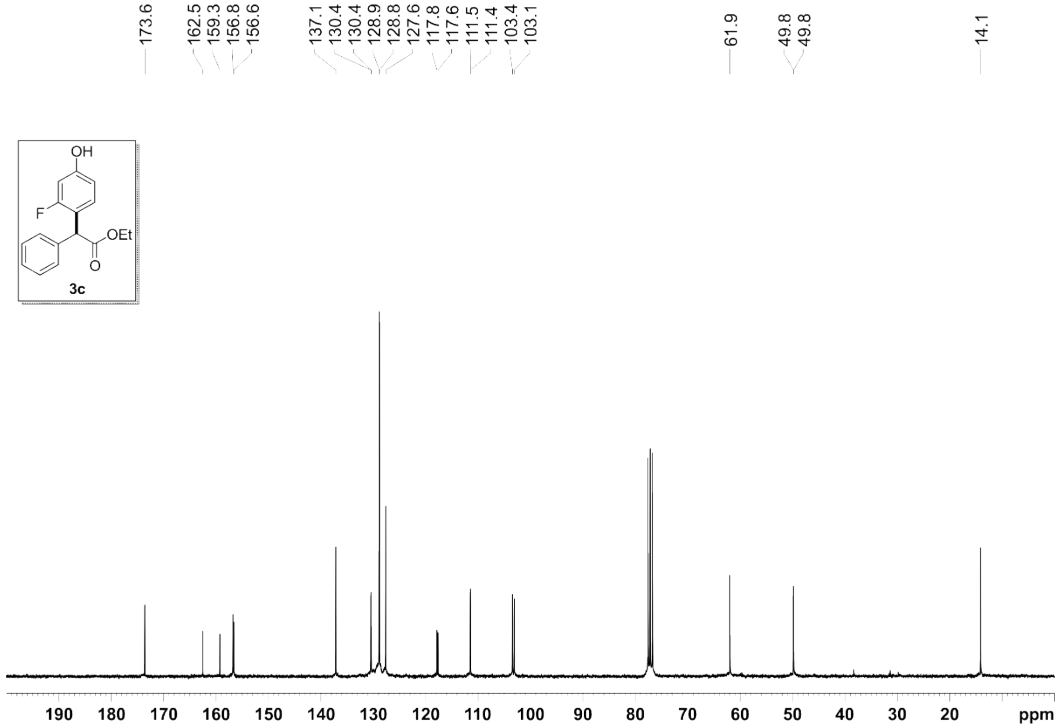


Figure SI 79. $^{13}C\{^{1}H\}$ NMR (76 MHz, $CDCl_3$) for **3c**.

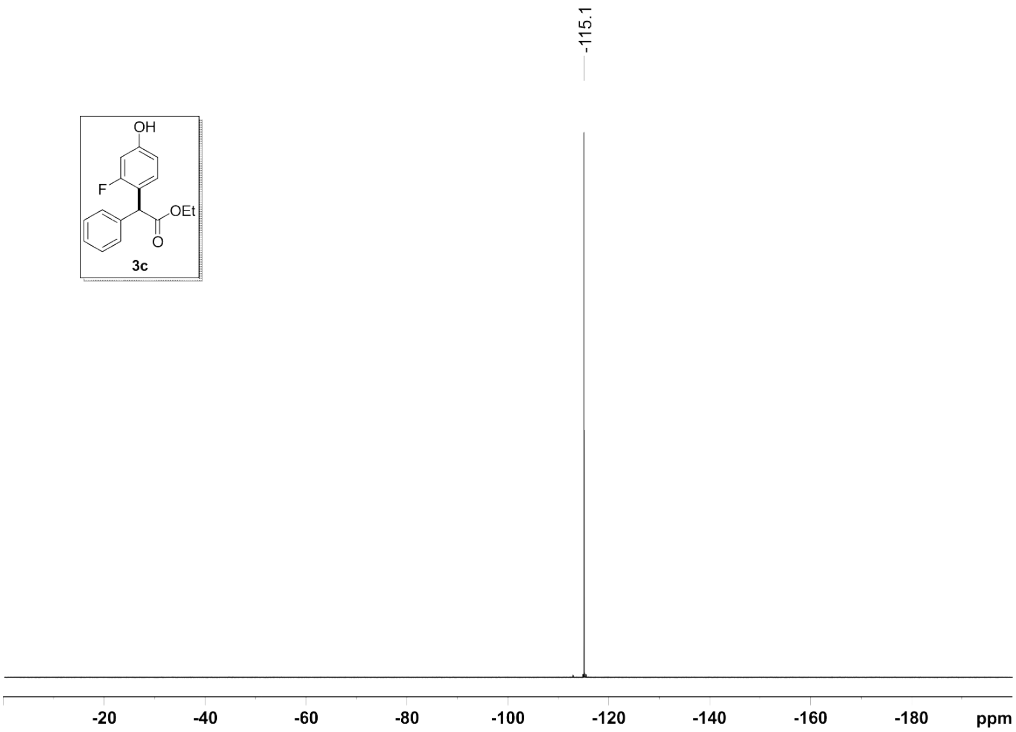


Figure SI 80. $^{19}F\{^{1}H\}$ NMR (376 MHz, $CDCl_3$) for **3c**.

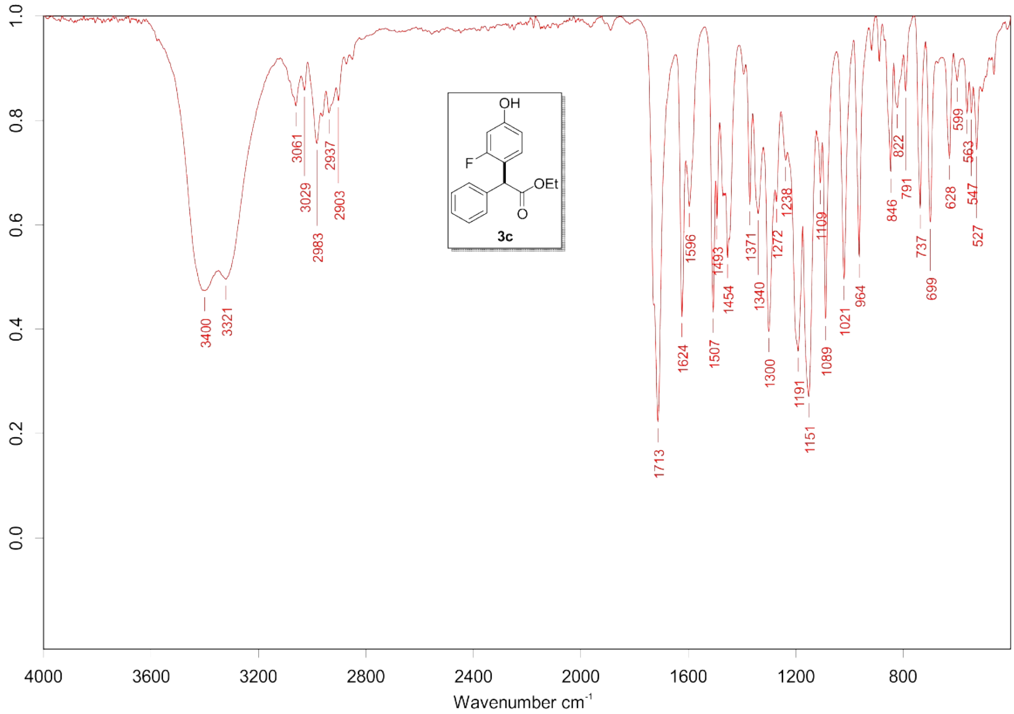


Figure SI 81. IR spectrum for **3c**.

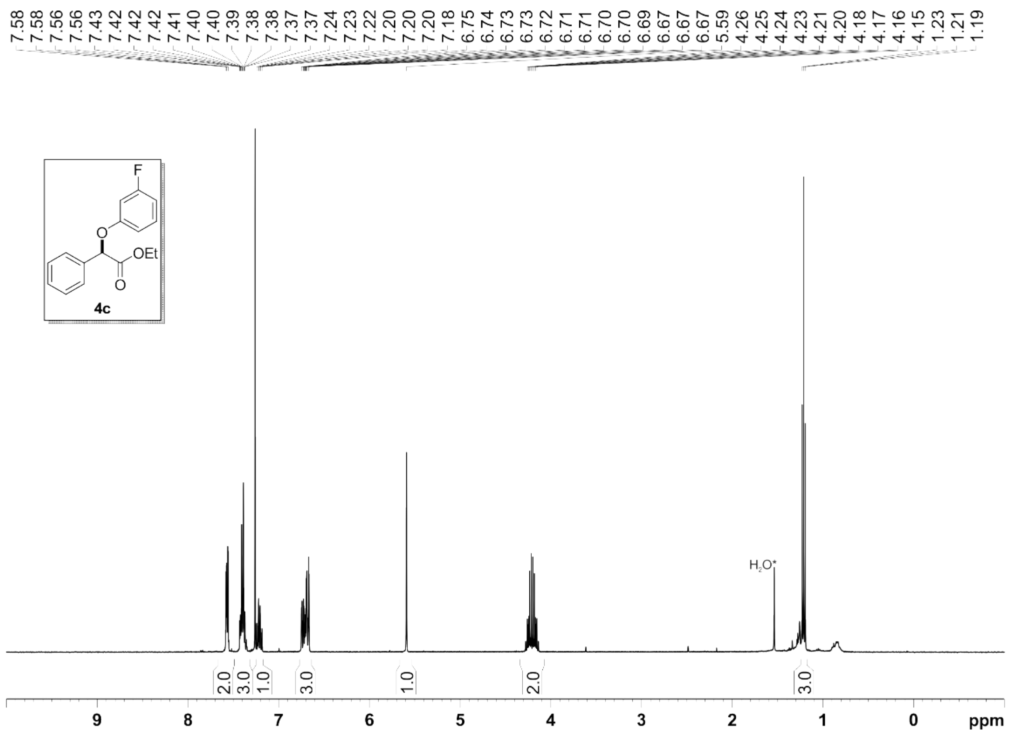


Figure SI 82. ^{1}H NMR (400 MHz, $CDCl_3$) for **4c**.

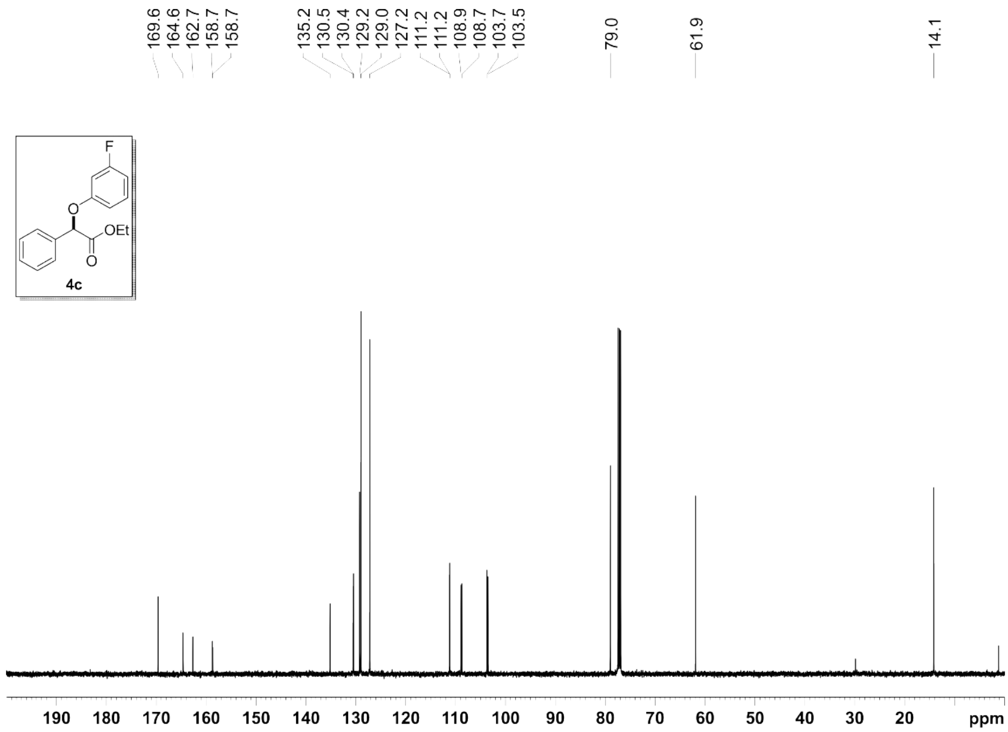


Figure SI 83. $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$) for **4c**.

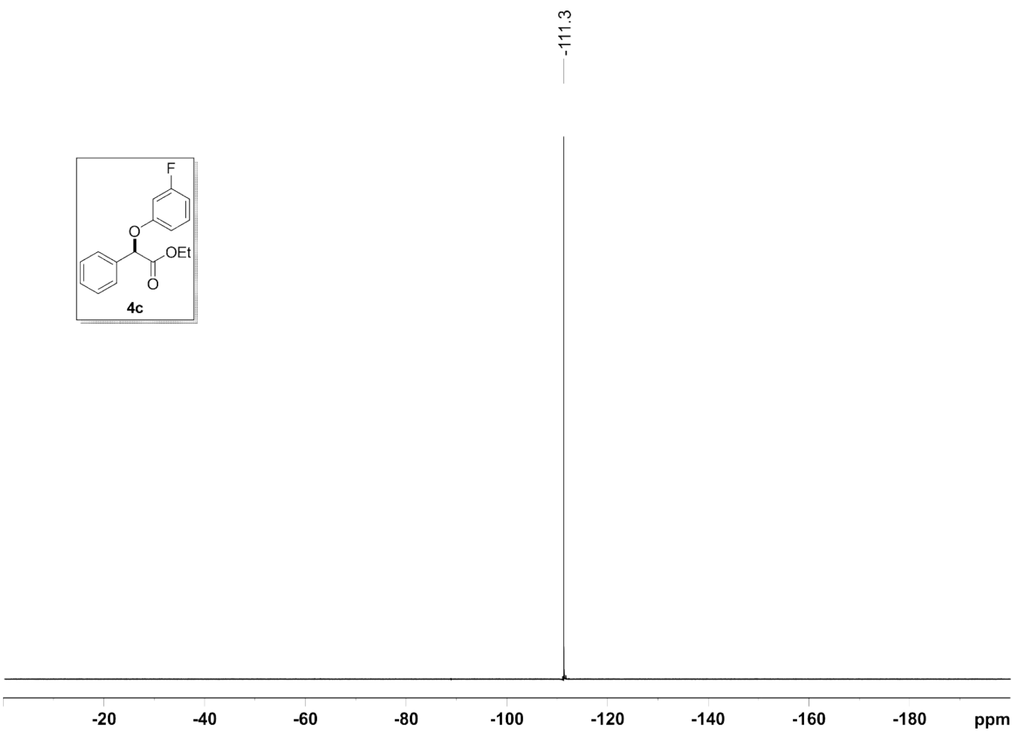


Figure SI 84. $^{19}F\{^{1}H\}$ NMR (376 MHz, $CDCl_3$) for **4c**.

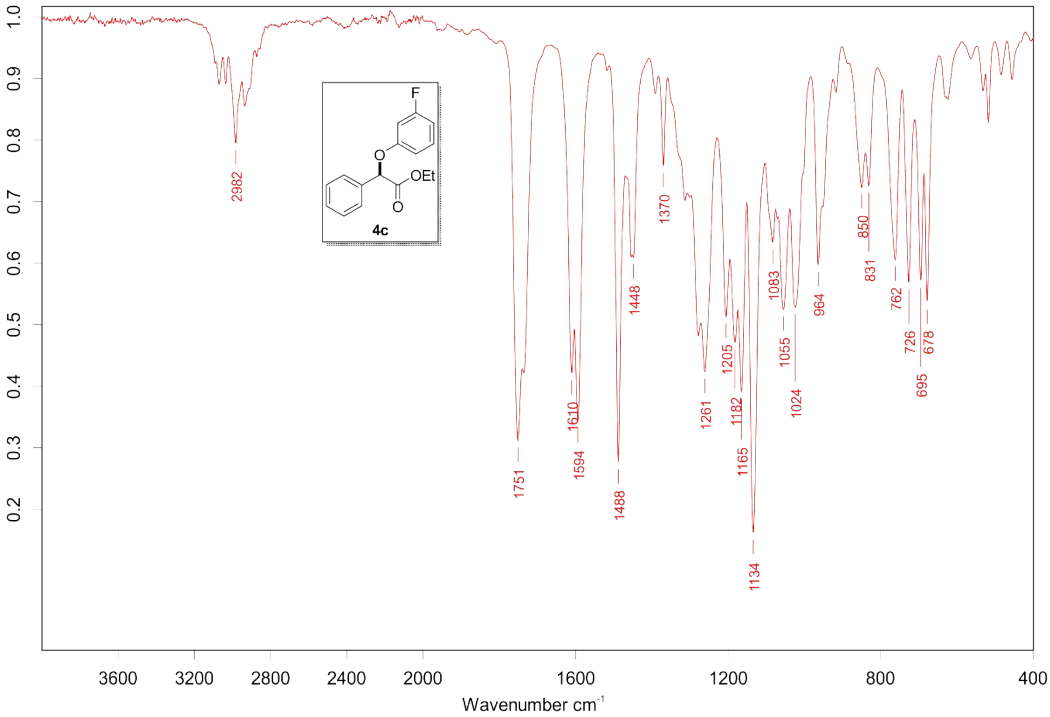


Figure SI 85. IR spectrum for **4c**.

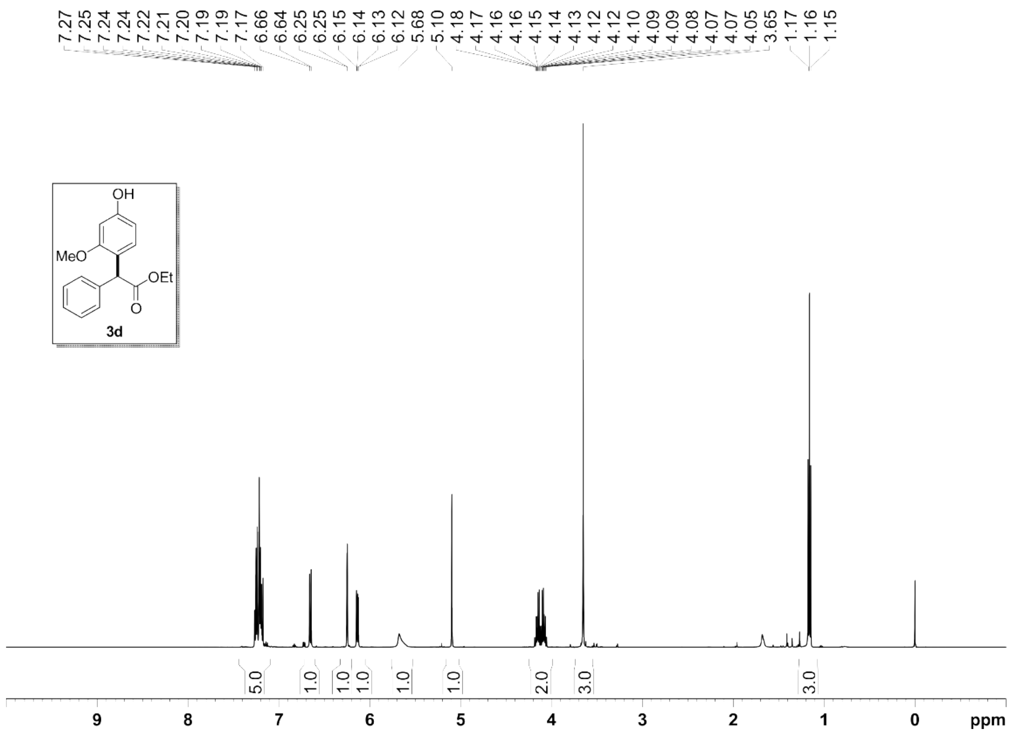


Figure SI 86. ^{1}H NMR (500 MHz, $CDCl_3$) for **3d**.

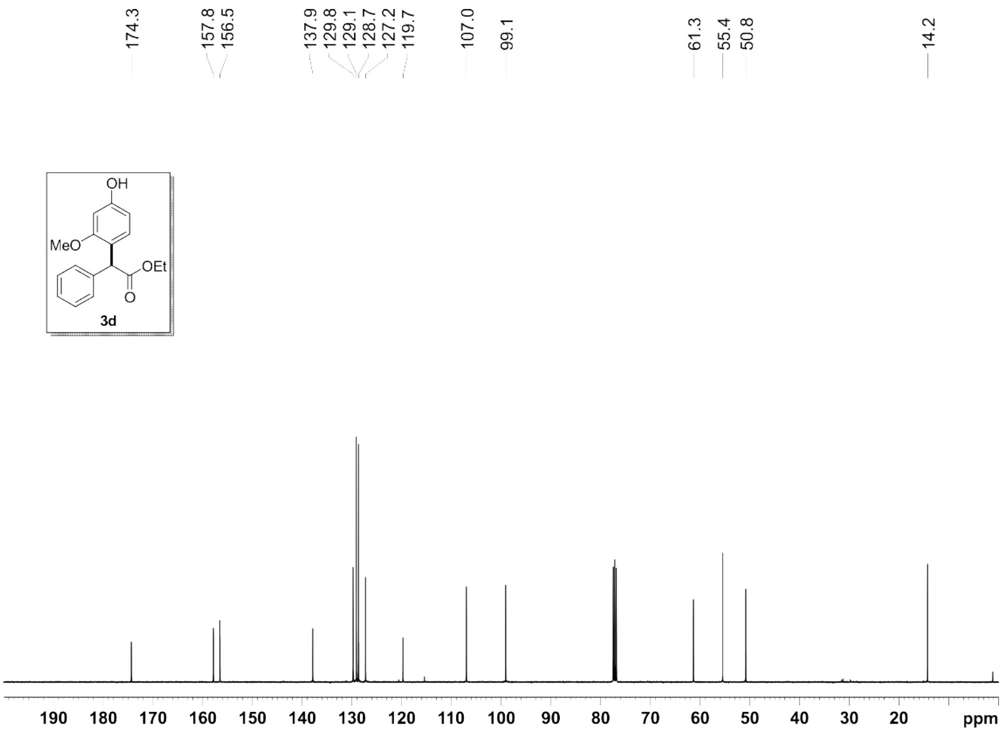


Figure SI 87. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) for **3d**.

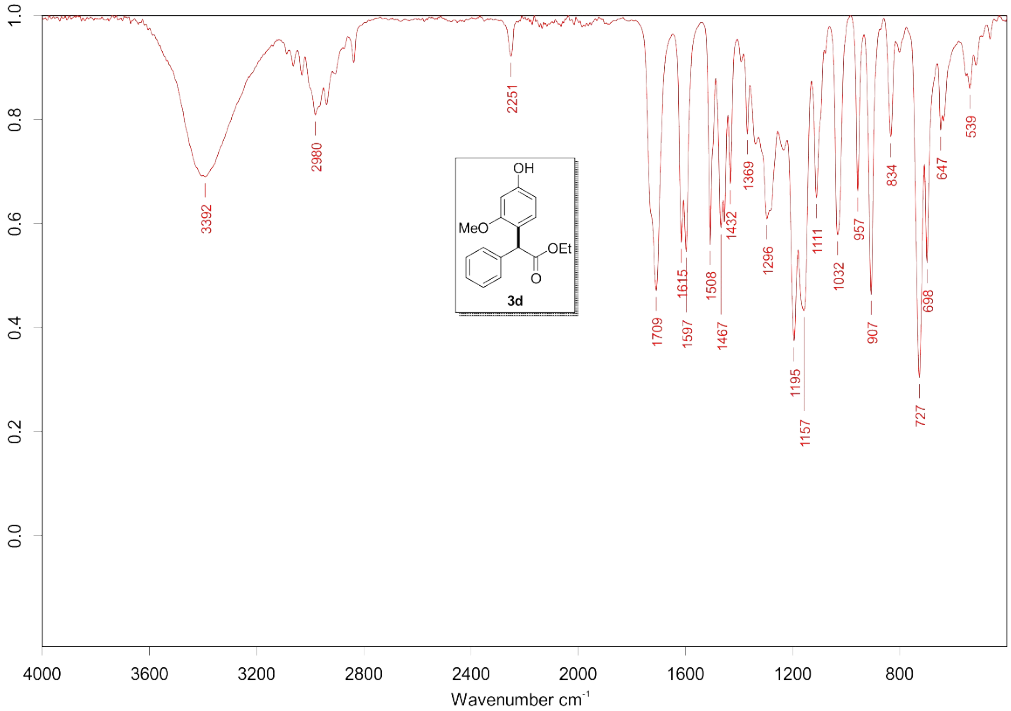


Figure SI 88. IR spectrum for **3d**.

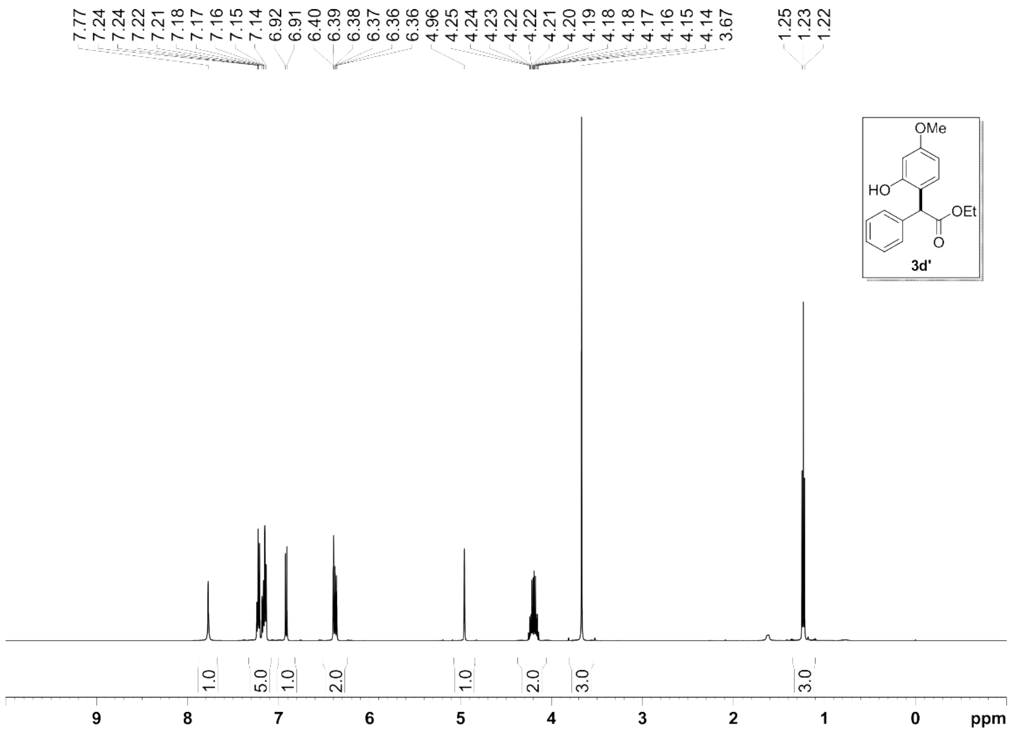


Figure SI 89. ^{1}H NMR (500 MHz, $CDCl_3$) for **3d'**.

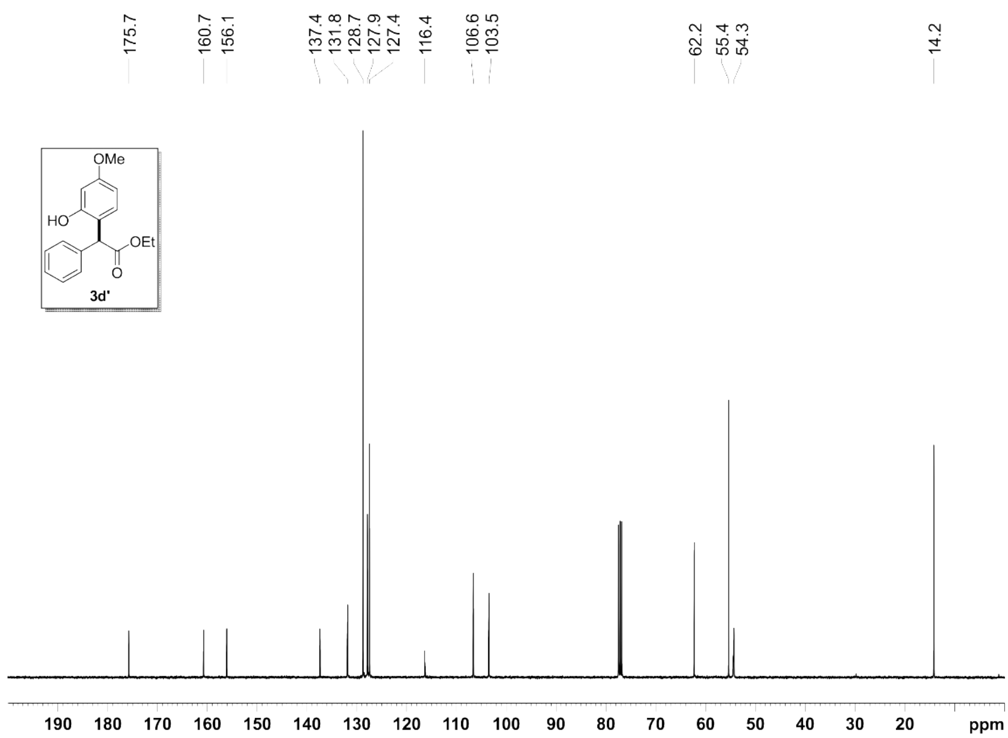


Figure SI 90. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) for **3d'**.

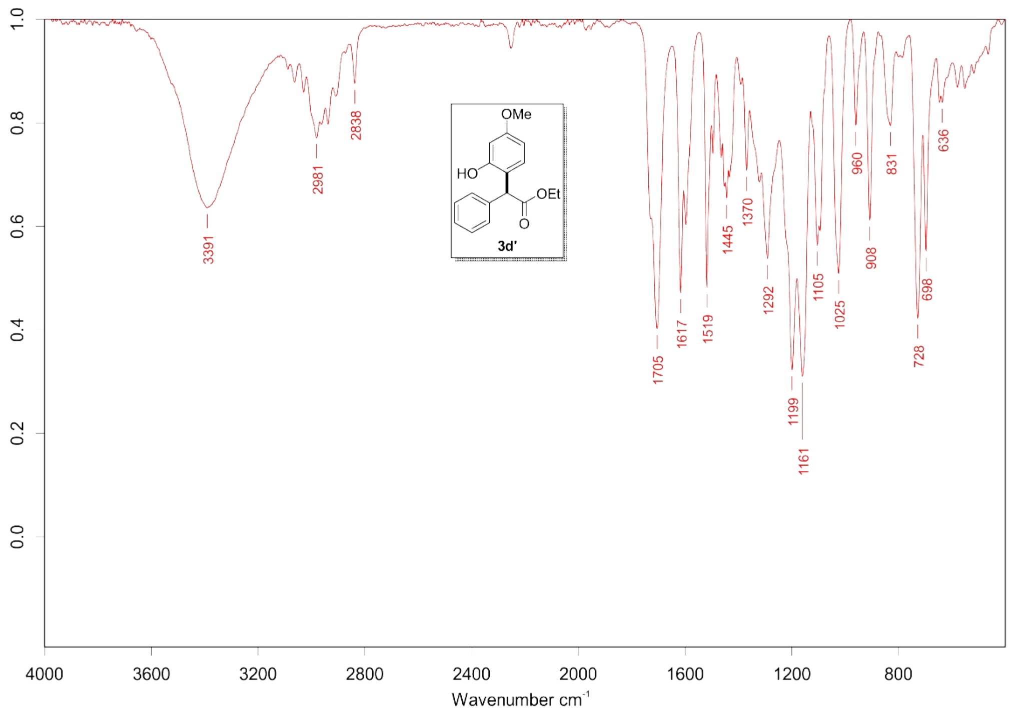


Figure SI 91. IR spectrum for **3d'**.

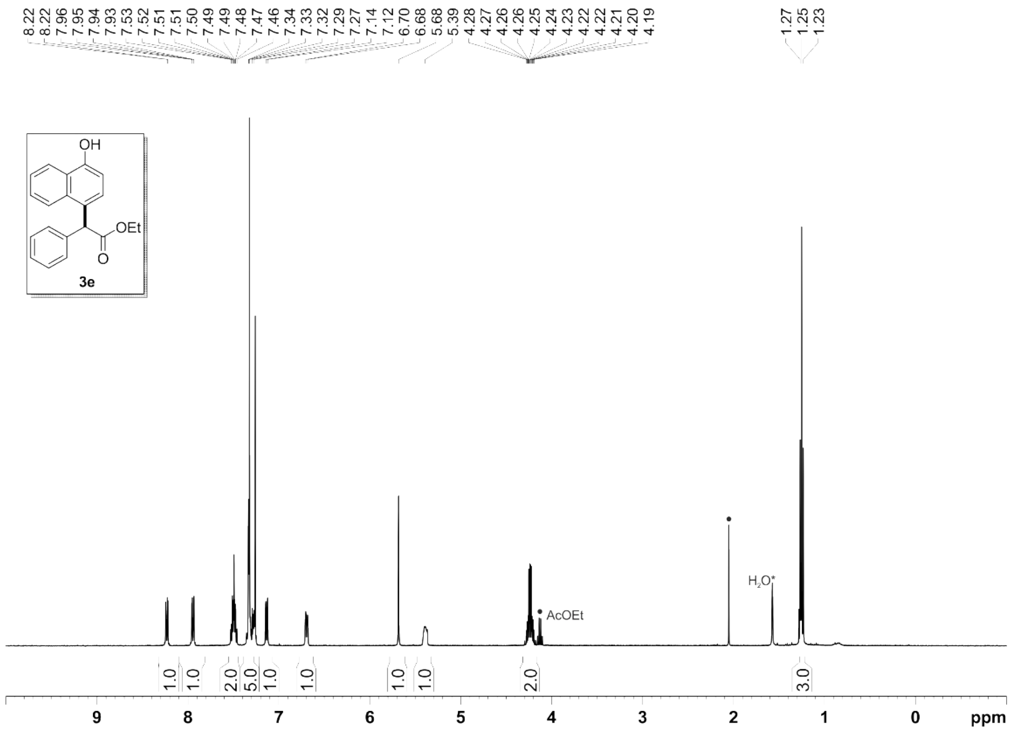


Figure SI 92. ^{1}H NMR (400 MHz, $CDCl_3$) for **3e**.

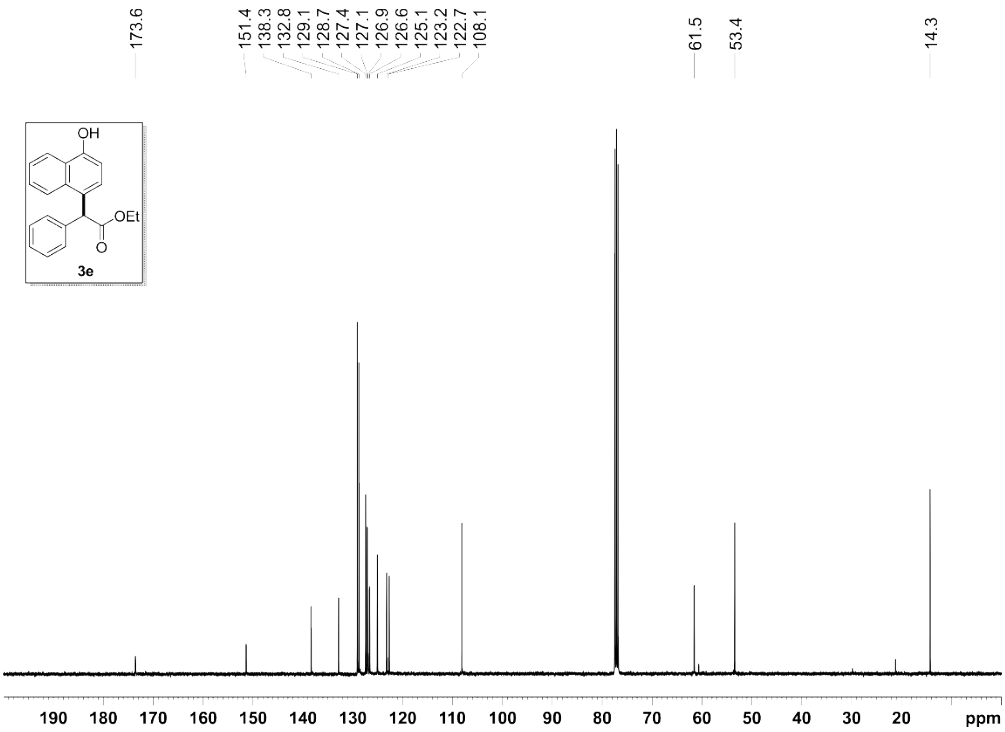


Figure SI 93. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) for **3e**.

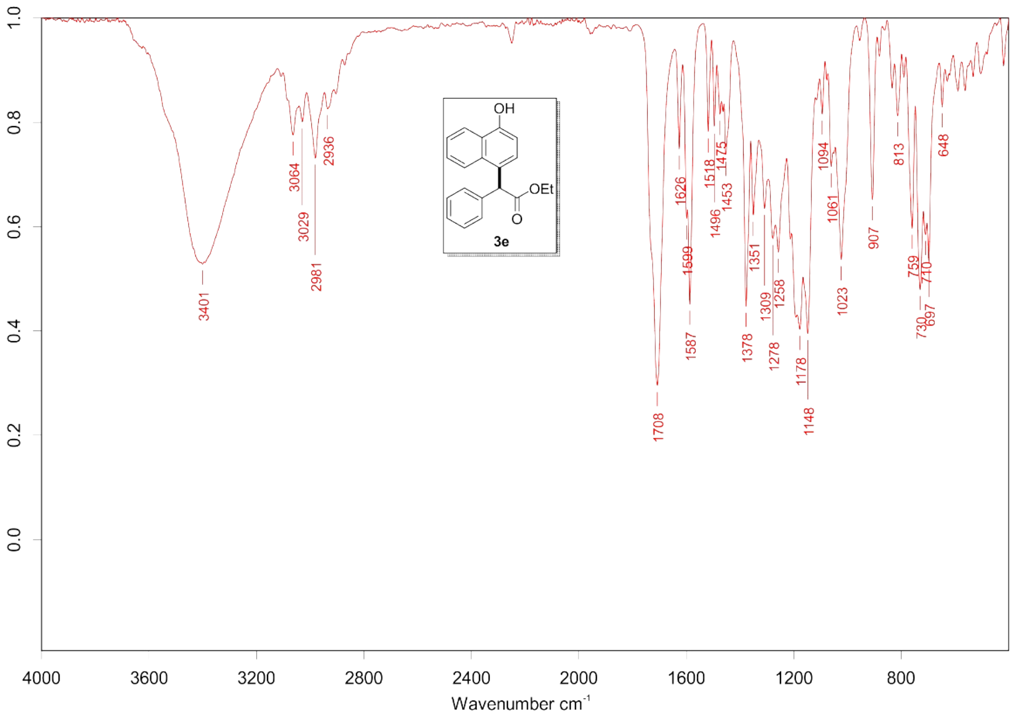


Figure SI 94. IR spectrum for **3e**.

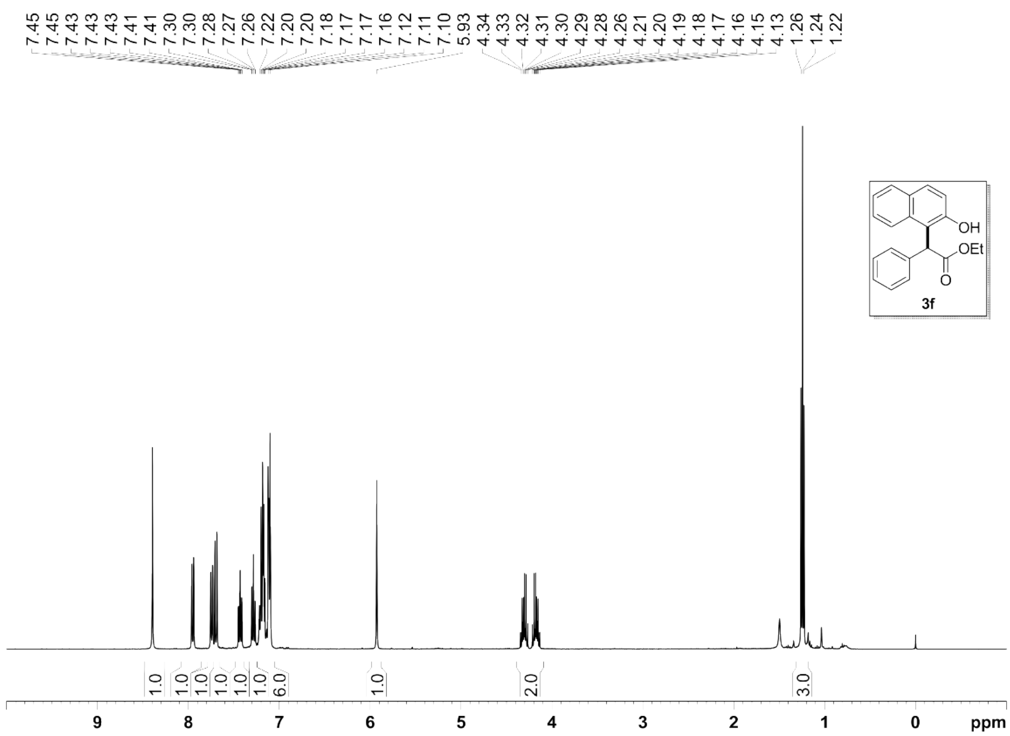


Figure SI 95. ^{1}H NMR (400 MHz, $CDCl_3$) for **3f**.

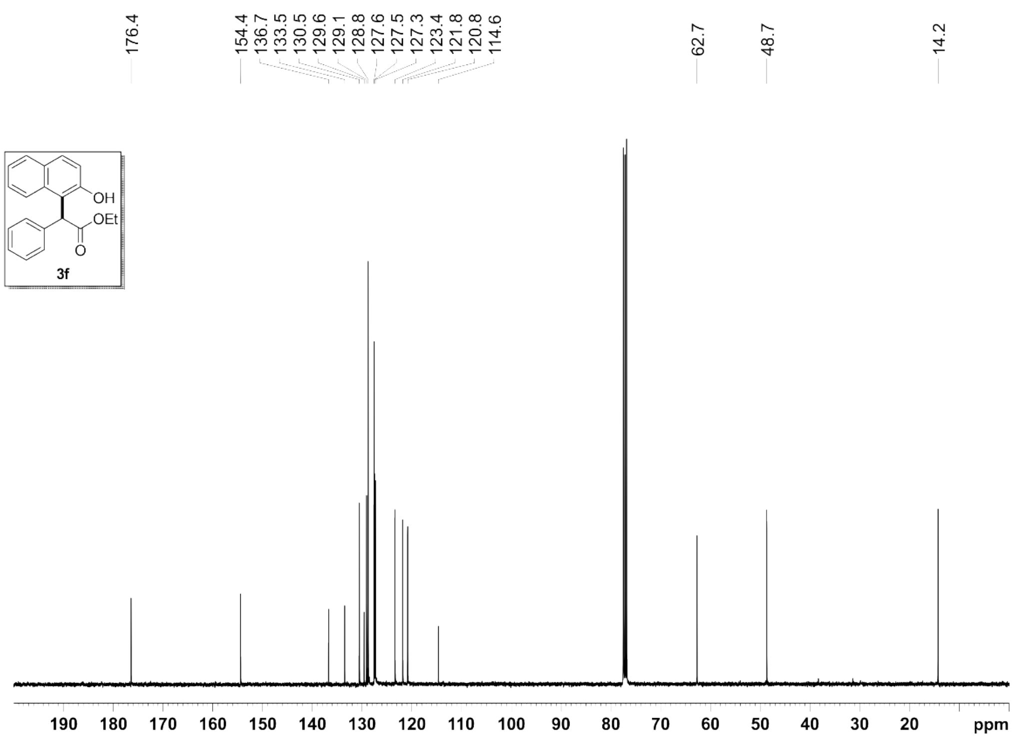


Figure SI 96. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) for **3f**.

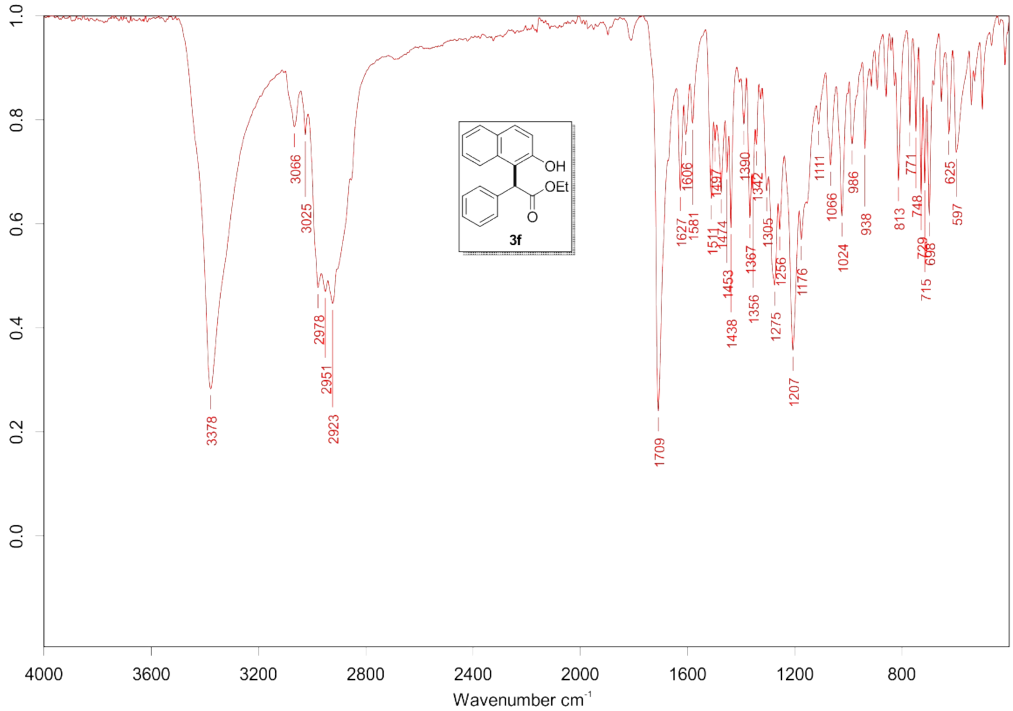


Figure SI 97. IR spectrum for **3f**.

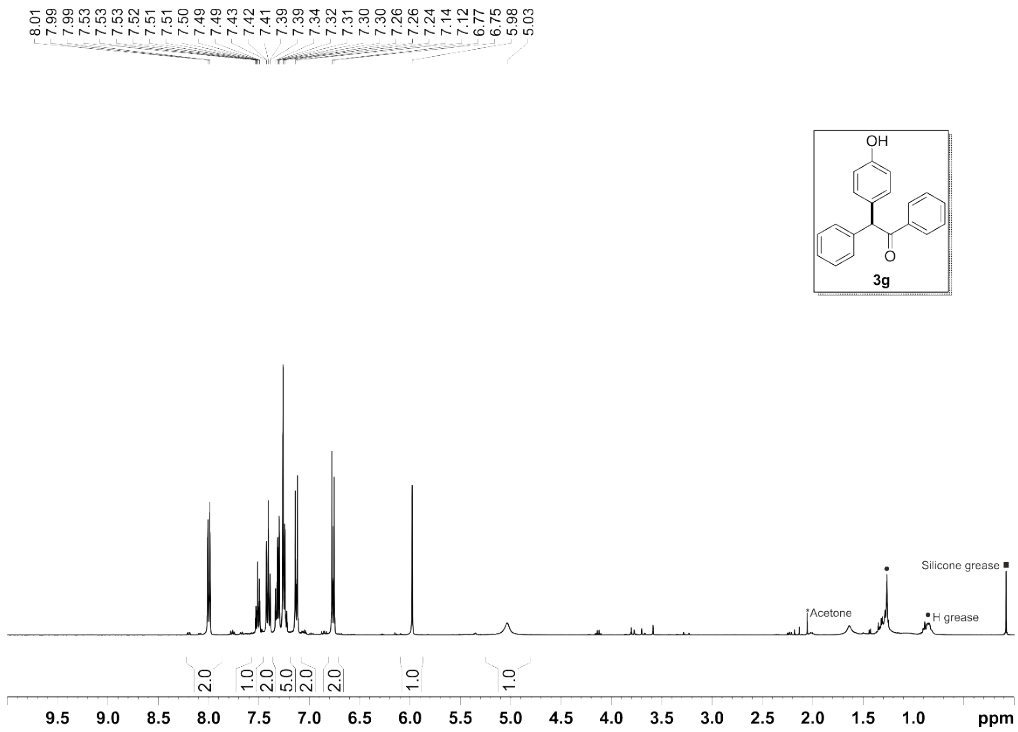


Figure SI 98. ^{1}H NMR (400 MHz, $CDCl_3$) for **3g**.

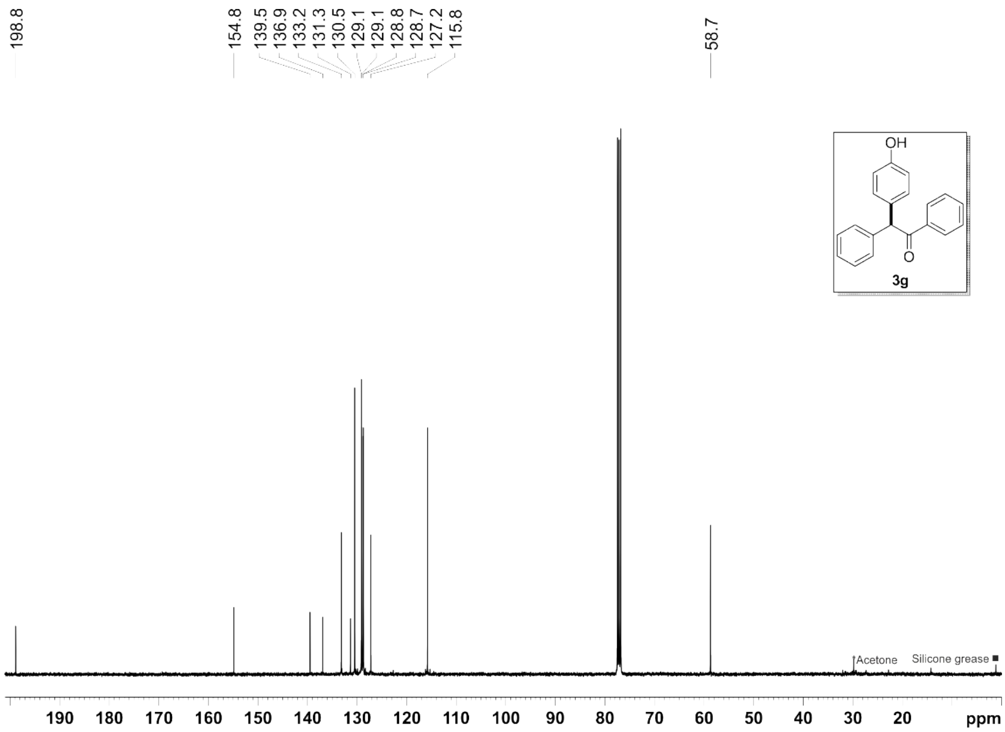


Figure SI 99. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) for **3g**.

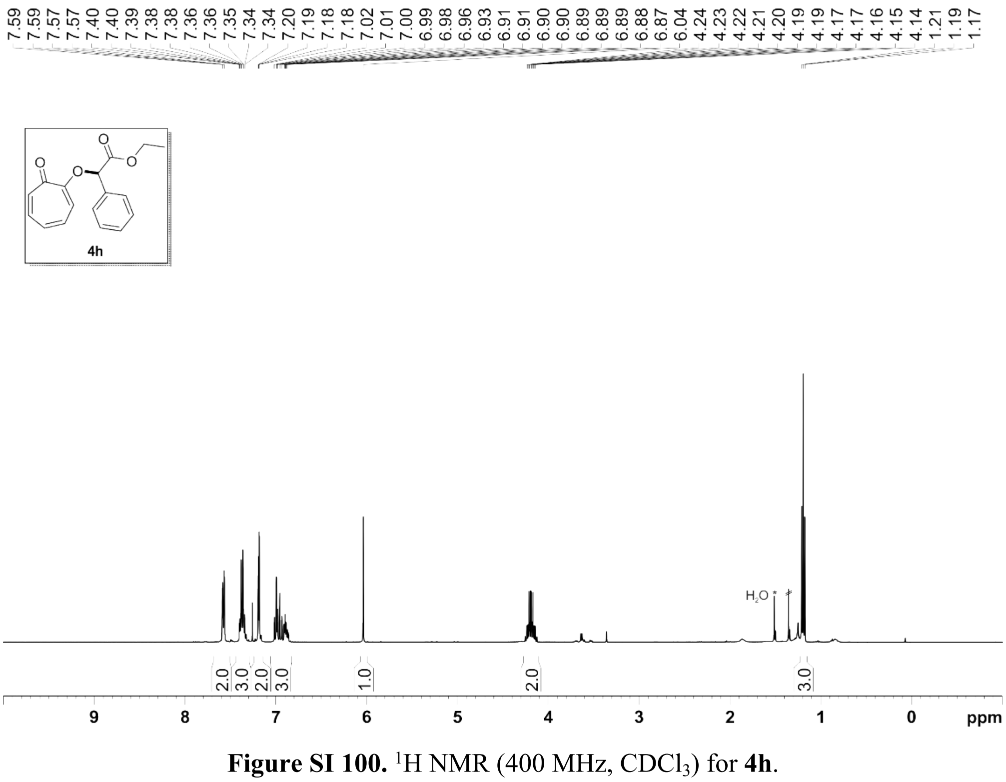


Figure SI 100. ^{1}H NMR (400 MHz, $CDCl_3$) for **4h**.

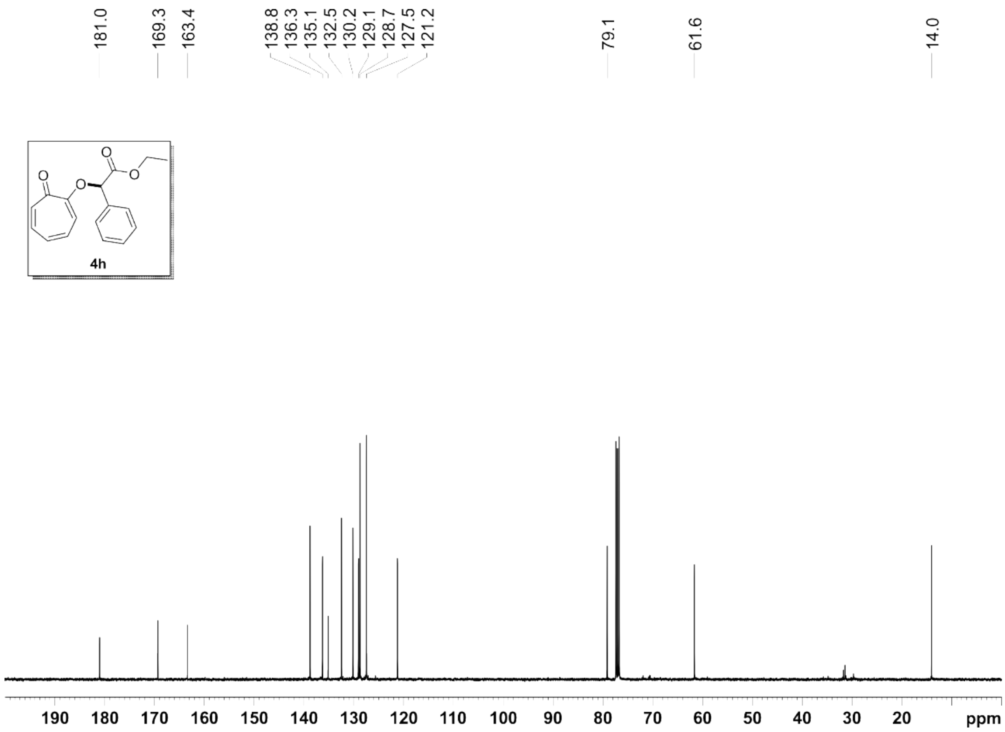


Figure SI 101. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) for **4h**.

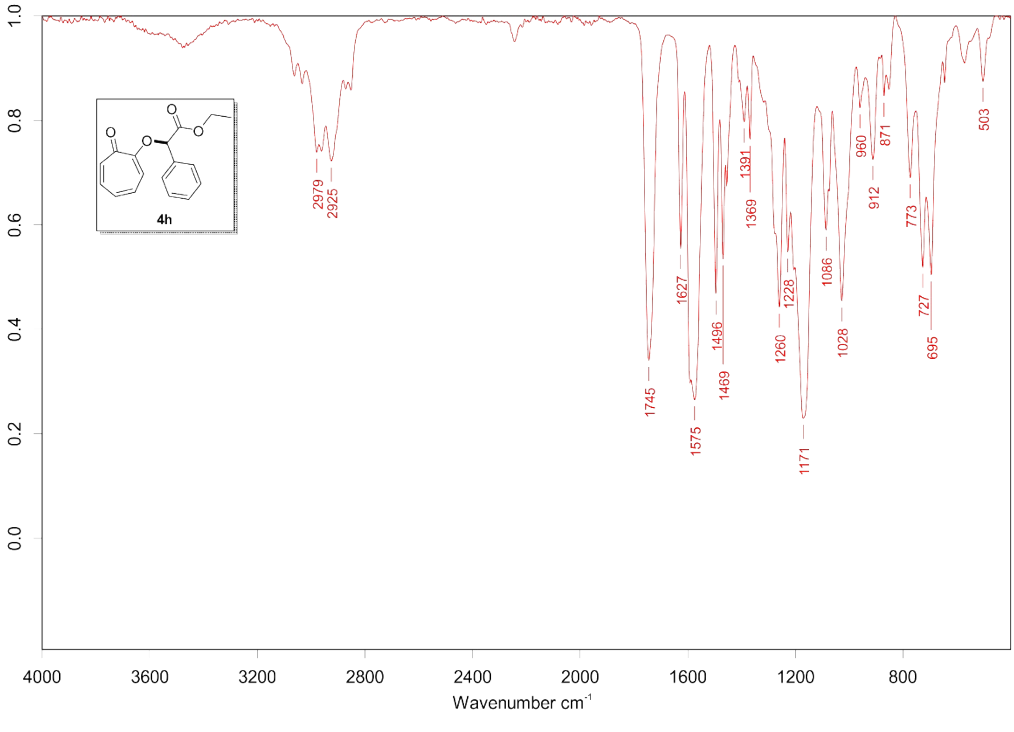


Figure SI 102. IR spectrum for **4h**.

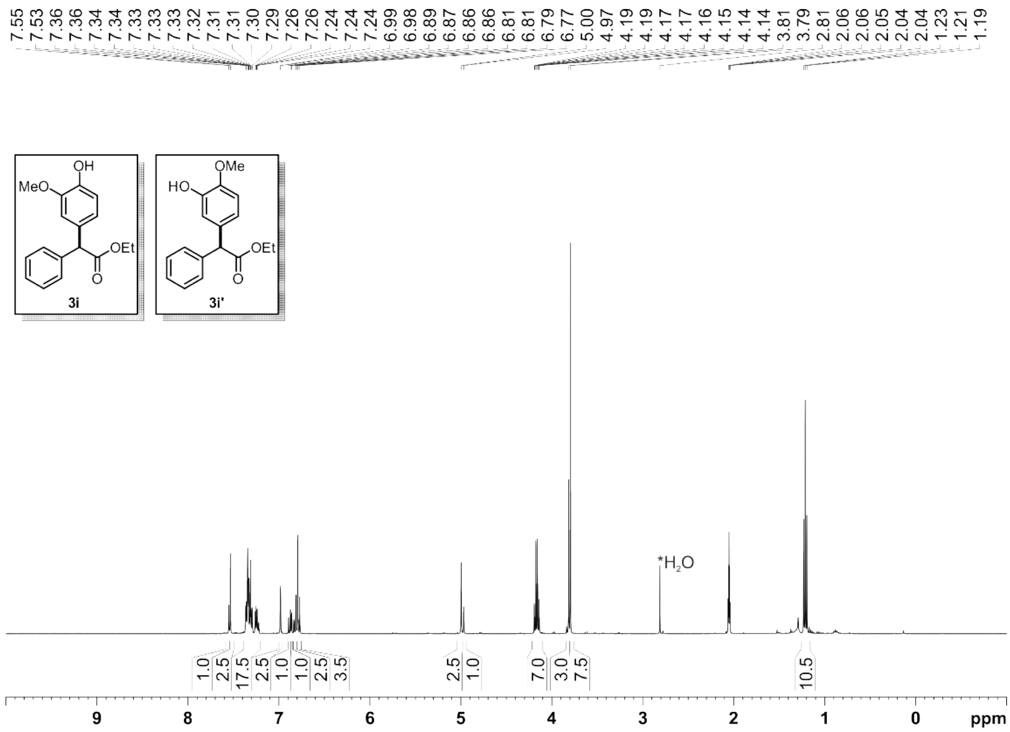


Figure SI 103. ^{1}H NMR spectrum (400 MHz, acetone-d_6) for **3i**+**3i'** isomeric mixture (ratio **3i**:**3i'** 1.0 : 2.5).

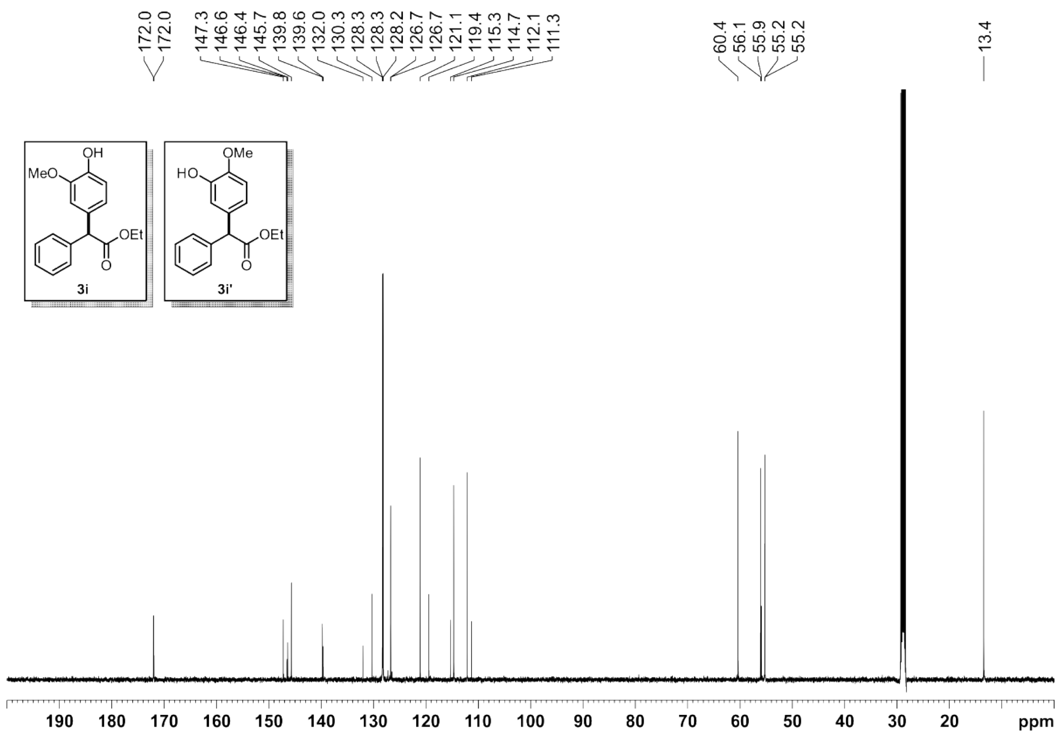


Figure SI 104. $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz, acetone-d_6) for **3i**+**3i'** isomeric mixture.

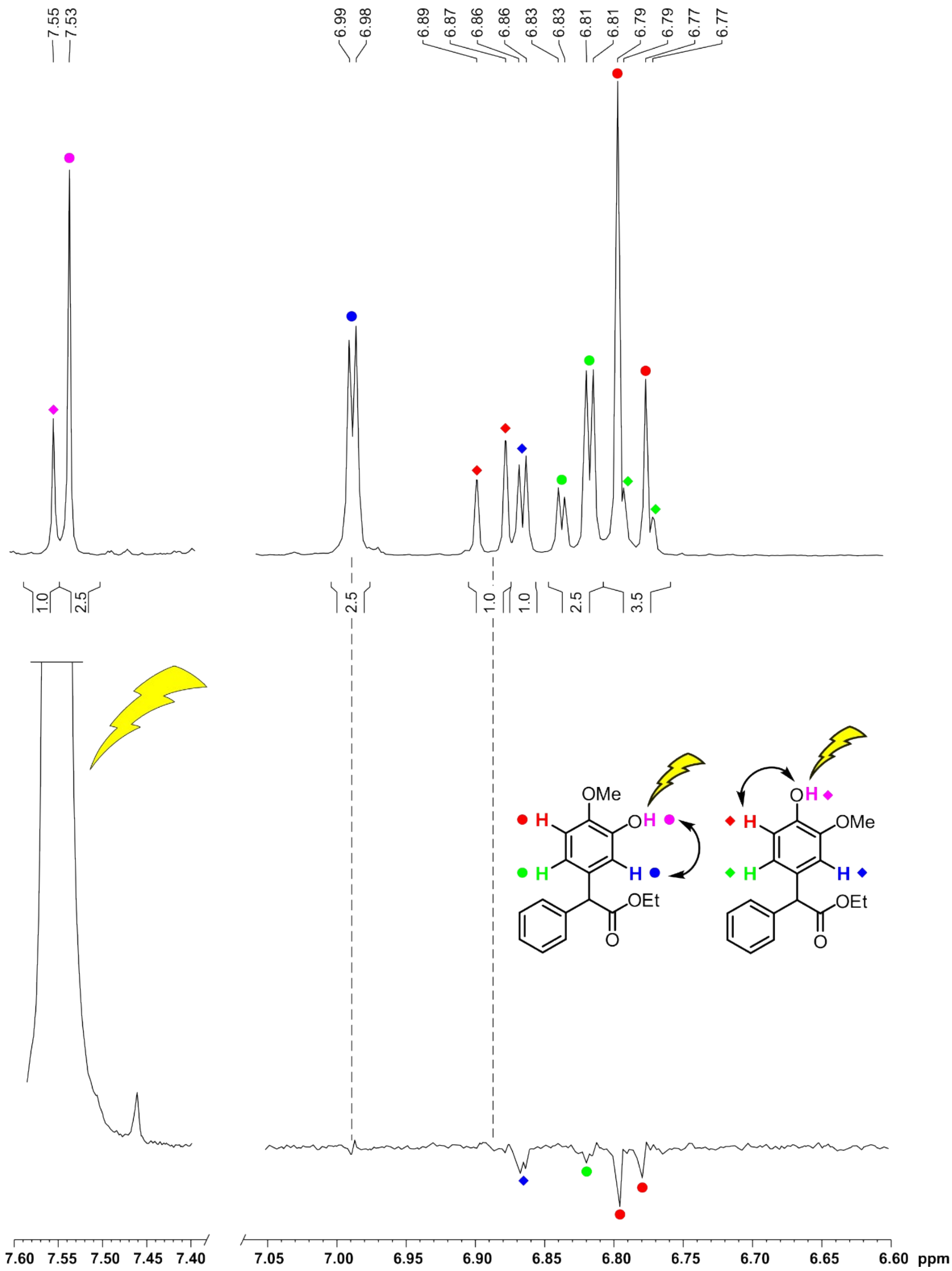


Figure SI 105. *Up*: Detail of the aromatic region of the ^{1}H NMR spectrum (400 MHz, acetone-d$_6$) for the **3i**+**3i'** mixture (ratio **3i**:**3i'** 1.0 : 2.5). *Down*: GOESY spectrum (500 MHz, acetone-d$_6$) upon irradiation of the –OH signals (δ: 7.54 ppm).

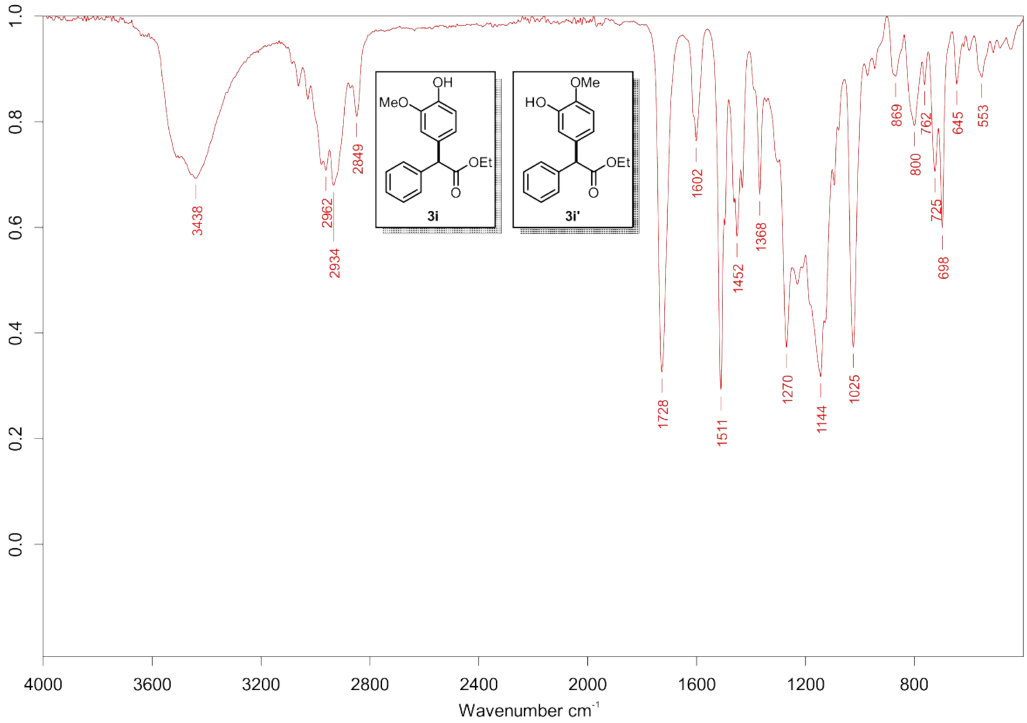


Figure SI 106. IR spectrum for **3i**+**3i'** isomeric mixture.

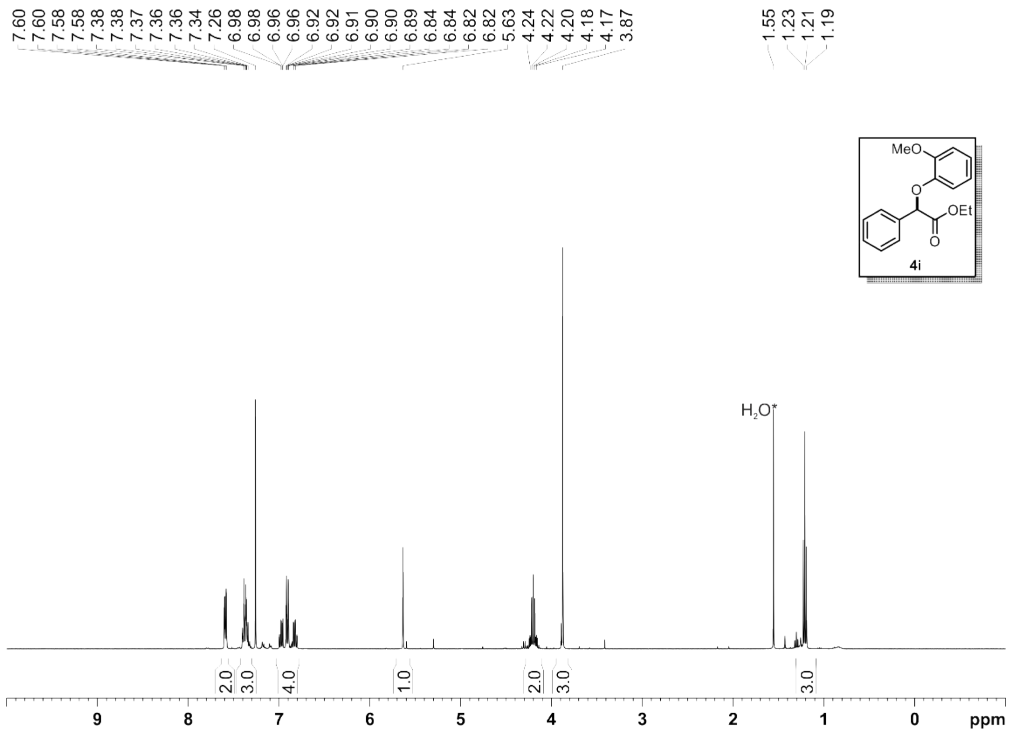


Figure SI 107. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) for **4i**.

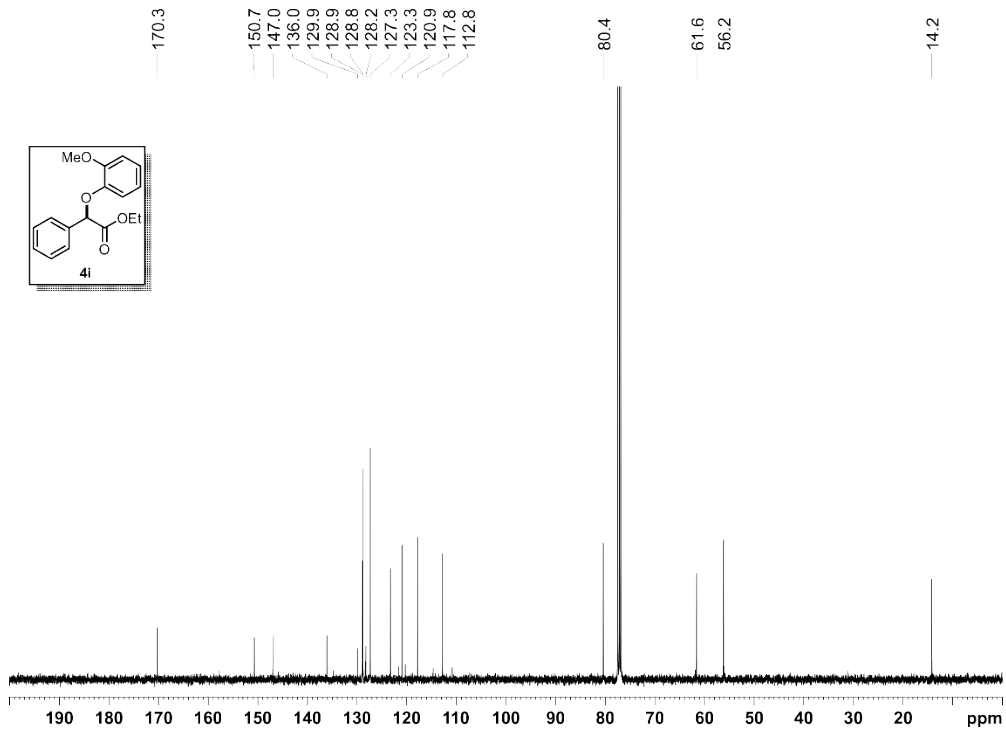


Figure SI 108. $^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) for **4i**.

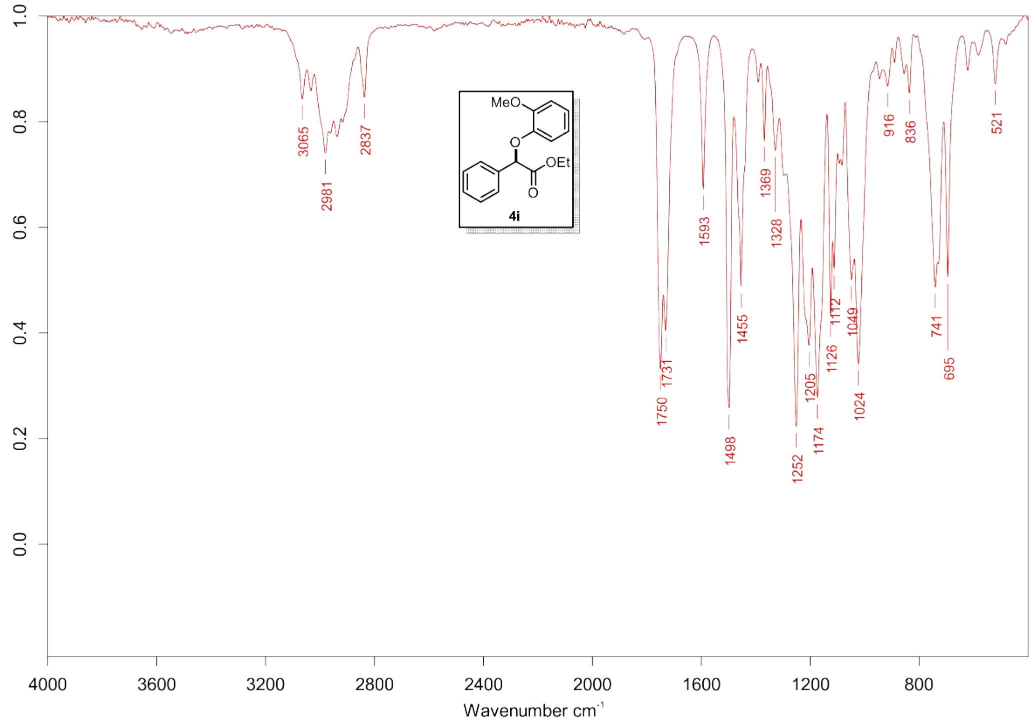


Figure SI 109. IR spectrum for **4i**.

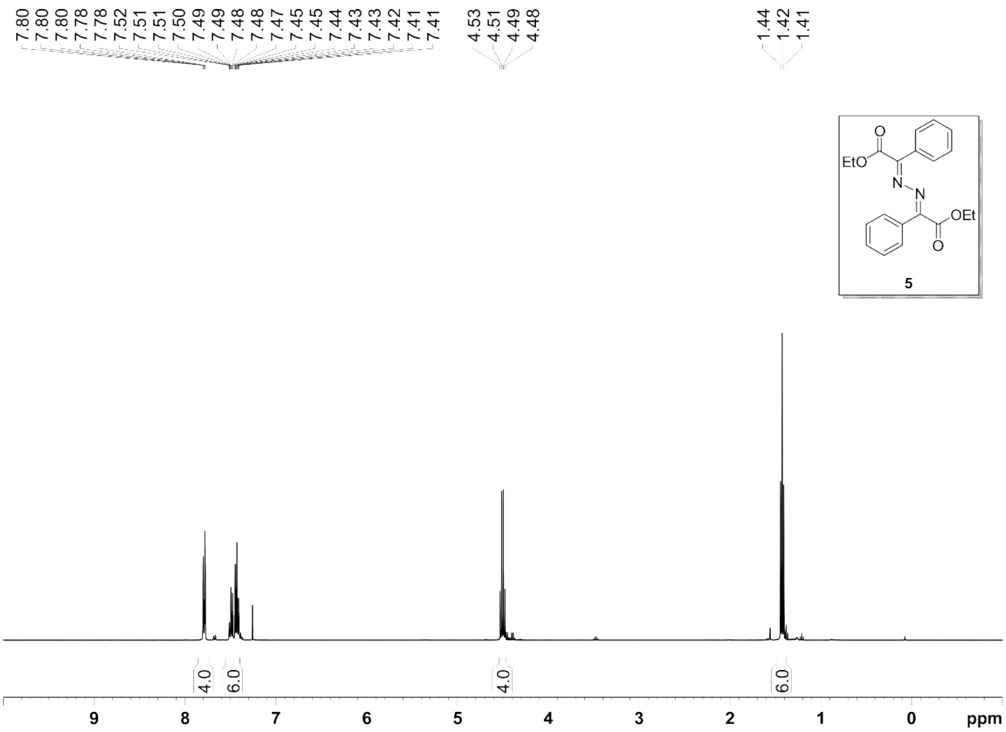


Figure SI 110. ^{1}H NMR (400 MHz, $CDCl_3$) for **5**.

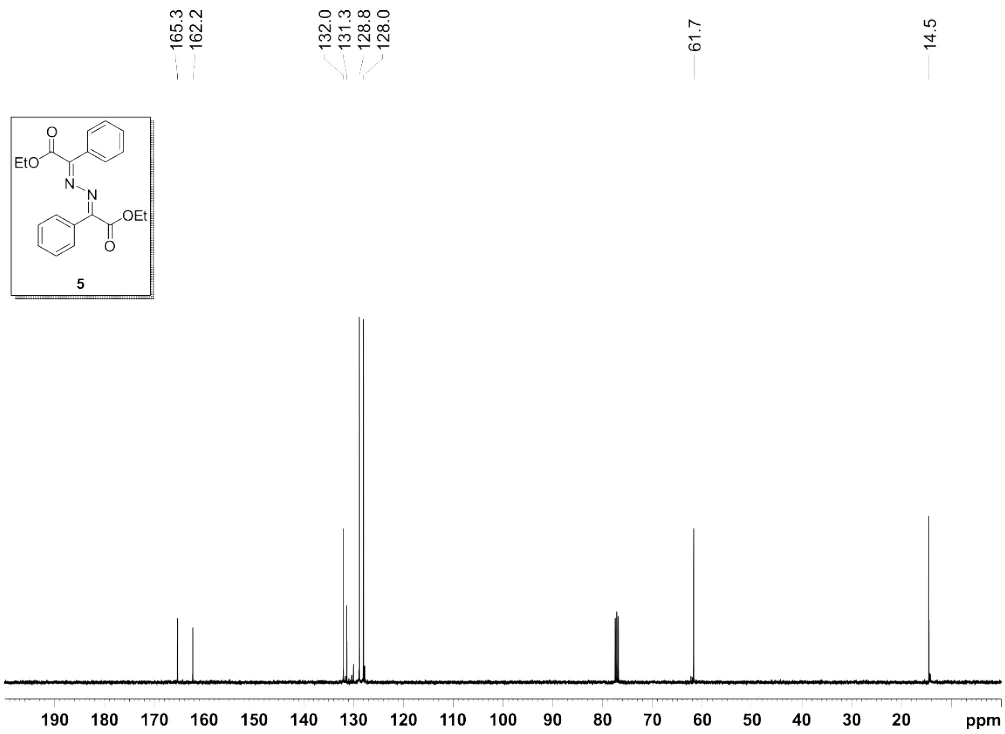


Figure SI 111. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) for **5**.

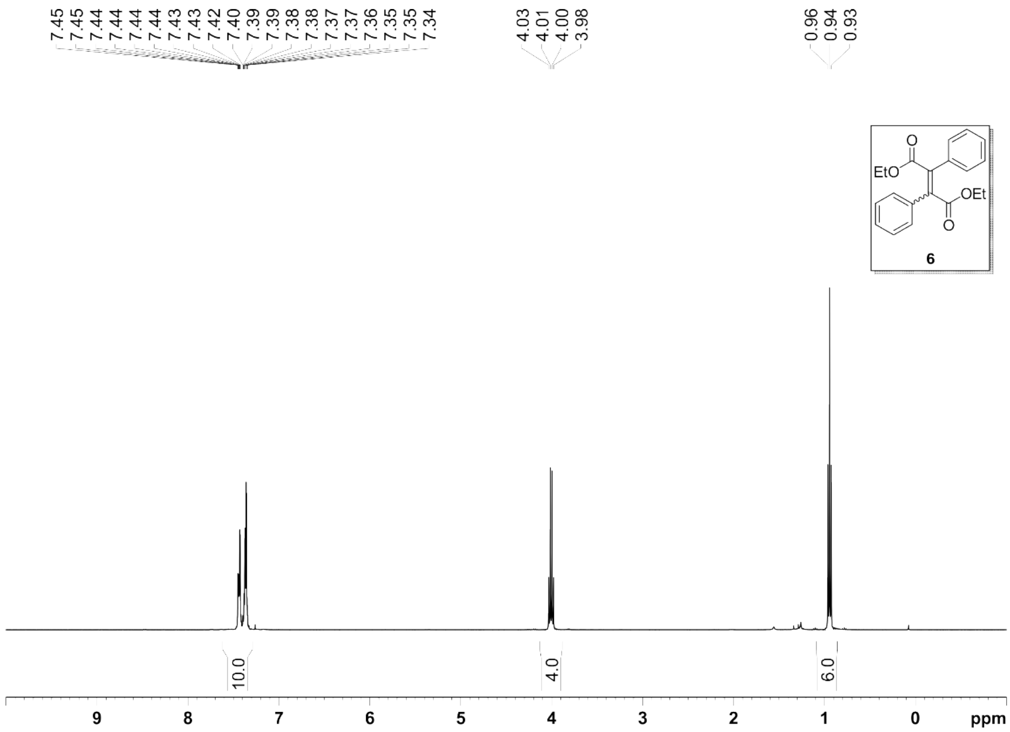


Figure SI 112. ^{1}H NMR (400 MHz, $CDCl_3$) for **6**.

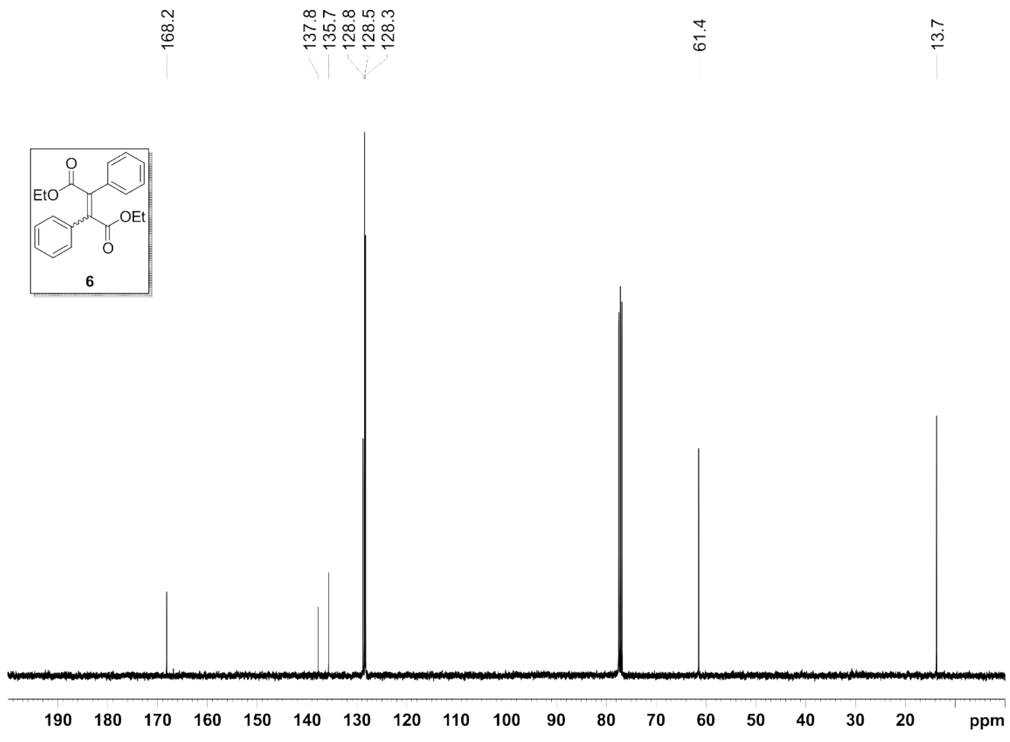


Figure SI 113. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) for **6**.

10. Theoretical Methods

The energies of all compounds included in this study were computed at the BP86[23]-D3/def2-TZVPD[24]//BP86-D3/def2-SVP level of theory. The calculations have been performed by using the program TURBOMOLE version 7.0.[25] For the calculations we have used the DFT-D functional with the latest available correction for dispersion (D3).[26] TS structures were characterised by means of frequency analysis calculations. In order to reproduce solvent effects, we have used the conductor-like screening model COSMO,[27] which is a variant of the dielectric continuum solvation models.[28] CH_2Cl_2 has been used as solvent.

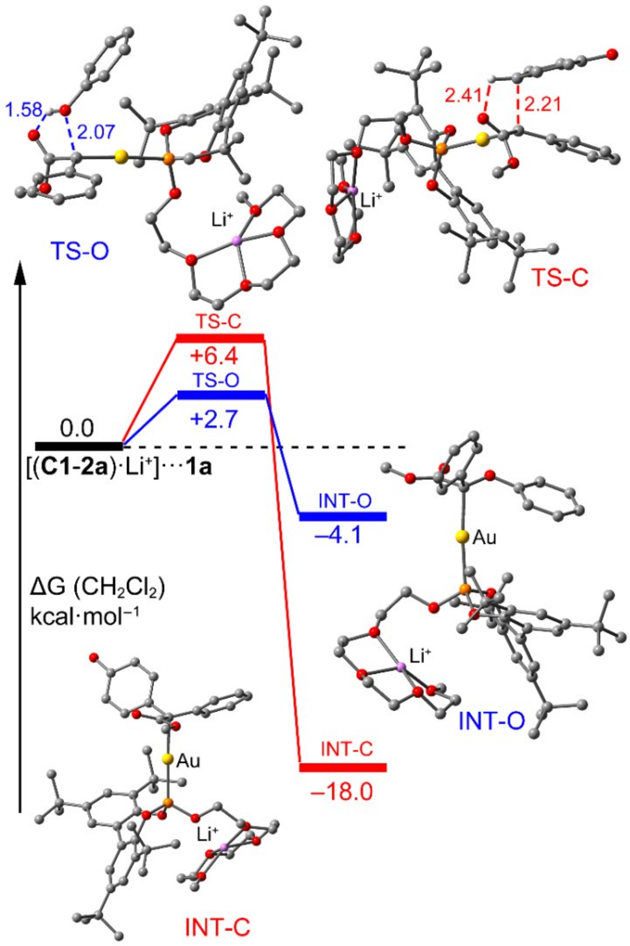


Figure SI 114. Energetic profile obtained for the O–H (in blue) and *para*-C_{sp2}–H (in red) insertion reactions of catalyst **C1** and substrate **2a** into phenol **1a** in the absence of RA. Distances in Å.

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[23] (a) J. P. Perdew, Density-functional Approximation for the Correlation Energy of the Inhomogeneous Electron Gas. *Phys. Rev. B*, 1986, **33**, 8822-8824. (b) A. D. Becke, Density-functional Exchange-energy Approximation with Correct Asymptotic Behaviour. *Phys. Rev. A*, 1988, **38**, 3098-3100.

[24] F. Weigend and R. Ahlrichs, Balanced Basis Sets of Split Valence, Triple Zeta Valence and Quadruple Zeta Valence Quality for H to Rn: Design and Assessment of Accuracy. *Phys. Chem. Chem. Phys.*, 2005, **7**, 3297-3305.

[25] R. Ahlrichs, M. Bär, M. Häser, H. Horn and C. Kölmel, Electronic Structure Calculations on Workstation Computers: The Program System Turbomole. *Chem. Phys. Lett.*, 1989, **162**, 165-169.

[26] S. Grimme, J. Antony, S. Ehrlich and H. Krieg, A Consistent and Accurate Ab Initio Parametrization of Density Functional Dispersion Correction (DFT-D) for the 94 Elements H-Pu. *J. Chem. Phys.*, 2010, **132**, 154104/154101-154104/154119.

[27] A. Klamt and G. Schueuermann, COSMO: A New Approach to Dielectric Screening in Solvents with Explicit Expressions for the Screening Energy and its Gradient. *J. Chem. Soc., Perkin Trans. 2*, 1993, 799-805.

[28] A. Klamt, The COSMO and COSMO-RS Solvation Models. *WIREs Comput. Mol. Sci.*, 2011, **1**, 699-709.

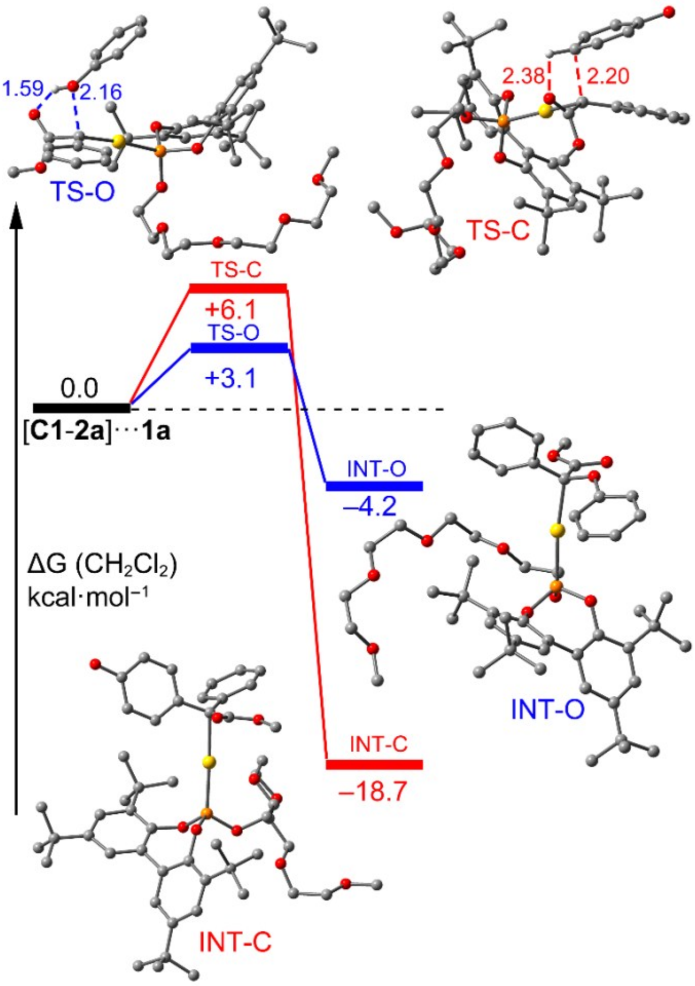

Figure SI 115. Energetic profile obtained for the O–H (in blue) and *para*-C_{sp2}–H (in red) insertion reactions of catalyst **C1** and substrate **2a** into phenol **1a** for Li^+. Distances in Å.

Cartesian Coordinates

[C1-2a]···1a:

Au	-1.2214603	-1.1604627	-0.9590938
P	0.9649100	-0.4430327	-1.4596770
O	2.0452627	0.0984267	-0.3597347
O	0.7454777	0.8085173	-2.4932716
O	1.9484671	-1.5375505	-2.1471928
O	1.4453917	-3.9492906	-0.4544699
O	2.0227213	-4.5835728	2.5623046
O	3.3524657	-3.3299558	4.9061506
O	5.8090968	-1.7329232	4.4853204
C	1.7422974	1.2594213	0.3850692
C	1.5822277	1.1578788	1.7907036
C	1.2791290	2.3610557	2.4579429
H	1.1336356	2.3222103	3.5449490
C	1.1582957	3.6126038	1.8131134
C	1.4100792	3.6549295	0.4336474
H	1.3609414	4.6053276	-0.1129948
C	1.7275611	2.4904485	-0.3050567
C	2.1499900	2.6355251	-1.7310877
C	3.0503977	3.6747795	-2.0476980
H	3.4523443	4.2691534	-1.2144088
C	3.4528367	3.9472232	-3.3663411
C	2.8821618	3.1622333	-4.3864857
H	3.1549968	3.3800712	-5.4238024
C	1.9740658	2.1052233	-4.1538936

C	1.6683056	1.8350342	-2.7964356
C	1.8177381	-0.1595839	2.5693916
C	3.2642408	-0.6598987	2.3146471
H	3.4644053	-1.5748884	2.9066779
H	3.9982244	0.1112031	2.6236131
H	3.4400511	-0.8911892	1.2479132
C	1.6578558	0.0397258	4.0931429
H	1.8816616	-0.9199585	4.5998230
H	0.6295566	0.3455631	4.3761859
H	2.3642197	0.7961732	4.4909813
C	0.8016636	-1.2491001	2.1466476
H	0.9364455	-2.1458754	2.7830536
H	0.9545294	-1.5927676	1.1066096
H	-0.2399958	-0.8814823	2.2621564
C	0.7925984	4.8677860	2.6343055
C	0.6908839	6.1286269	1.7521394
H	1.6538244	6.3713657	1.2581493
H	0.4145694	7.0022703	2.3759831
H	-0.0850006	6.0239637	0.9662485
C	1.8822657	5.1094740	3.7102926
H	1.6373075	6.0084996	4.3124955
H	2.8755466	5.2700818	3.2441466
H	1.9732689	4.2549319	4.4108026
C	-0.5761500	4.6448723	3.3260057
H	-0.8533545	5.5354287	3.9273471
H	-0.5572315	3.7738660	4.0117772
H	-1.3782059	4.4704482	2.5804724
C	4.4715997	5.0731025	-3.6469368
C	3.9037430	6.4195029	-3.1299755
H	4.6251614	7.2405475	-3.3204272
H	3.7074373	6.3964957	-2.0392888
H	2.9527878	6.6761608	-3.6401915
C	5.7960566	4.7521559	-2.9083800
H	6.5435246	5.5515132	-3.0920126
H	6.2281761	3.7934325	-3.2608090
H	5.6528232	4.6745294	-1.8118514
C	4.7772648	5.2203666	-5.1517446
H	5.5145035	6.0336821	-5.3065190
H	3.8726383	5.4818042	-5.7380227
H	5.2137635	4.2953463	-5.5805846
C	1.3337808	1.3459478	-5.3456257
C	-0.2110722	1.4760070	-5.2811667
H	-0.6698499	0.9555483	-6.1477899
H	-0.5171937	2.5409869	-5.3276506
H	-0.6298866	1.0401393	-4.3553796
C	1.7502639	-0.1449312	-5.3277622
H	1.3062500	-0.6741481	-6.1963979
H	1.4166510	-0.6539984	-4.4076073
H	2.8524579	-0.2504435	-5.3918580
C	1.7832503	1.9283352	-6.7050233
H	1.2852314	1.3686508	-7.5222672
H	2.8763248	1.8354736	-6.8645650
H	1.5031763	2.9948439	-6.8194199
C	1.5014819	-2.8397828	-2.5940486
H	1.8675157	-2.9554247	-3.6335769
H	0.3894430	-2.8853224	-2.6016311
C	2.0586682	-3.9519720	-1.7287348
H	1.8560981	-4.9123490	-2.2674159
H	3.1679645	-3.8516947	-1.6463757
C	1.6802028	-5.1683568	0.2458063
H	2.7728102	-5.3789451	0.3273176
H	1.2172310	-6.0143896	-0.3199299
C	1.0975791	-5.1383271	1.6492912
H	0.1307027	-4.5748110	1.6349027
H	0.8536598	-6.1897031	1.9457135
C	1.6373484	-4.7362004	3.9187337
H	1.1725429	-5.7413242	4.0770059
H	0.8756048	-3.9707040	4.2100281
C	2.8403616	-4.6450524	4.8397963
H	2.5215409	-4.9967064	5.8547386
H	3.6234661	-5.3567490	4.4790880
C	4.4736136	-3.2481189	5.7750072
H	5.2364837	-4.0159100	5.4996199
H	4.1628073	-3.4515492	6.8307921
C	5.1240941	-1.8800702	5.7100570
H	4.3509904	-1.0817355	5.8444320
H	5.8305238	-1.7945360	6.5752542

C	6.5384086	-0.5282355	4.4039237
H	7.0483577	-0.5099768	3.4216180
H	7.3113312	-0.4512937	5.2079443
H	5.8801774	0.3717366	4.4800250
C	-5.6541557	-3.4306789	1.5480768
C	-5.1249039	-2.7750010	0.4393328
C	-3.7299430	-2.4207650	0.3920391
C	-2.9103182	-2.7560163	1.5241038
C	-3.4493206	-3.4142559	2.6250844
C	-4.8205287	-3.7533728	2.6401887
H	-6.7216241	-3.6942677	1.5754937
H	-5.7816093	-2.5144555	-0.4031147
H	-1.8455571	-2.4794874	1.4971001
H	-2.8111392	-3.6664074	3.4844184
H	-5.2447924	-4.2718028	3.5138987
C	-3.1549193	-1.7662137	-0.7312027
C	-4.0231606	-1.4414289	-1.9009696
O	-4.8633214	-0.5365487	-1.8733456
O	-3.7651109	-2.1825489	-2.9762375
C	-4.5330797	-1.8930011	-4.1724558
H	-4.2086322	-2.6381478	-4.9177213
H	-5.6169624	-1.9879675	-3.9698182
H	-4.3154623	-0.8662630	-4.5236269
C	-5.2164682	3.7061756	2.3194065
C	-5.6093408	4.5436808	1.2557613
C	-5.7139741	4.0145114	-0.0453666
C	-5.4300743	2.6658608	-0.2895999
C	-5.0383790	1.8249954	0.7830710
C	-4.9308080	2.3563638	2.0923776
H	-5.1374574	4.1136027	3.3387265
H	-6.0227829	4.6625533	-0.8796063
H	-5.5109911	2.2473780	-1.3046564
H	-4.6278804	1.6855211	2.9092624
O	-4.7645089	0.5122075	0.6095487
H	-4.9056368	0.2449887	-0.3433840
H	-5.8363720	5.6038791	1.4412326

[(C1-2a)·Li$^+$]···1a:

Au	-1.8090043	-1.1548254	-0.4553659
P	0.4884510	-0.6617907	-0.3903831
O	1.3184012	-0.1758622	0.9420453
O	0.6800748	0.5269674	-1.4899500
O	1.5268058	-1.8934978	-0.7471145
O	2.9312681	-4.3495740	-0.3399772
O	4.5802308	-4.8062426	1.6773535
O	4.7361775	-2.3460797	2.5743888
O	5.0319481	-1.4777053	0.0875112
Li	4.0926369	-3.0654730	0.7820045
C	1.0883771	1.1167196	1.4888320
C	0.5553613	1.2424346	2.7991799
C	0.3806686	2.5615666	3.2634779
H	-0.0397812	2.7012556	4.2666887
C	0.7142163	3.7153797	2.5199300
C	1.3007070	3.5184491	1.2612512
H	1.5977668	4.3786387	0.6480432
C	1.5182554	2.2259488	0.7274494
C	2.2601299	2.1185200	-0.5670075
C	3.4006592	2.9307368	-0.7508918
H	3.7471500	3.5229984	0.1083922
C	4.0809571	3.0080972	-1.9797710
C	3.5502990	2.2665546	-3.0540111
H	4.0334435	2.3521216	-4.0324780
C	2.4143163	1.4299906	-2.9527788
C	1.8307923	1.3340150	-1.6650707
C	0.2464694	0.0341748	3.7213309
C	1.5392548	-0.7938795	3.9396633
H	1.3309538	-1.6503598	4.6142215
H	2.3220070	-0.1737224	4.4220616
H	1.9497432	-1.1938522	2.9937709
C	-0.2497393	0.4872161	5.1133708
H	-0.4378466	-0.4051702	5.7433523
H	-1.1994024	1.0557906	5.0583375
H	0.4982178	1.1089349	5.6439163
C	-0.8637226	-0.8587724	3.1156731
H	-1.1172463	-1.6787290	3.8191549
H	-0.5534646	-1.3283173	2.1617805

H	-1.7858198	-0.2714444	2.9292394
C	0.4497259	5.1165335	3.1097483
C	0.8638232	6.2408901	2.1383954
H	1.9493122	6.2186897	1.9109798
H	0.6485294	7.2273117	2.5947724
H	0.3048175	6.1927781	1.1817642
C	1.2597094	5.2774020	4.4220717
H	1.0814267	6.2798960	4.8622718
H	2.3485034	5.1774624	4.2369342
H	0.9731077	4.5266167	5.1854106
C	-1.0635592	5.2634316	3.4125706
H	-1.2720212	6.2662303	3.8377673
H	-1.4173783	4.5127127	4.1477332
H	-1.6701345	5.1506096	2.4914591
C	5.3243192	3.9130834	-2.1227326
C	4.9187000	5.3810037	-1.8297950
H	5.7976787	6.0494104	-1.9306389
H	4.5227869	5.5080795	-0.8019404
H	4.1420950	5.7310378	-2.5394329
C	6.4036194	3.4647147	-1.1047933
H	7.3007160	4.1120141	-1.1828394
H	6.7263434	2.4202186	-1.2976172
H	6.0422630	3.5265479	-0.0582765
C	5.9328443	3.8481120	-3.5385580
H	6.8272232	4.4997529	-3.5912441
H	5.2254802	4.2041838	-4.3146040
H	6.2574708	2.8222470	-3.8084887
C	1.8135740	0.7663846	-4.2209908
C	0.3753129	1.3078200	-4.4393386
H	-0.0584850	0.8661970	-5.3601831
H	0.3863992	2.4086334	-4.5689493
H	-0.2954696	1.0689354	-3.5927302
C	1.7858376	-0.7759514	-4.0943798
H	1.3918852	-1.2245711	-5.0292036
H	1.1399612	-1.1073762	-3.2626749
H	2.8060829	-1.1817613	-3.9316024
C	2.6327441	1.1028618	-5.4874107
H	2.1591446	0.6213274	-6.3659488
H	3.6746188	0.7284741	-5.4300751
H	2.6643515	2.1910787	-5.6913321
C	1.0476226	-3.1542227	-1.2736239
H	0.4888254	-2.9991051	-2.2212730
H	0.3719730	-3.6364341	-0.5355657
C	2.2353745	-4.0527977	-1.5572164
H	1.8460994	-4.9902053	-2.0118914
H	2.9210985	-3.5767020	-2.2939449
C	3.5547946	-5.6484499	-0.2787741
H	4.4893865	-5.6565931	-0.8844474
H	2.8730416	-6.4290900	-0.6817230
C	3.8460381	-5.9281806	1.1849432
H	2.8919951	-6.0354150	1.7513081
H	4.4252684	-6.8727828	1.2915706
C	4.6200366	-4.6630682	3.1033563
H	5.1586589	-5.5109557	3.5818510
H	3.5806305	-4.6397237	3.5070746
C	5.3476598	-3.3601174	3.3844202
H	5.2863165	-3.1087919	4.4664984
H	6.4230771	-3.4547274	3.1096029
C	5.5280225	-1.1627221	2.3964672
H	6.5991895	-1.4502334	2.2962051
H	5.4295917	-0.4774208	3.2674528
C	5.0543765	-0.4807829	1.1248707
H	4.0396118	-0.0375686	1.2409631
H	5.7597069	0.3377555	0.8636984
C	5.1290488	-0.9429639	-1.2376342
H	5.1095990	-1.7982496	-1.9385372
H	6.0892686	-0.3993501	-1.3675095
H	4.2863962	-0.2558897	-1.4644512
C	-6.9835474	-2.7877136	0.8457529
C	-6.1065311	-2.2675829	-0.1022591
C	-4.7147648	-2.0620938	0.2155683
C	-4.2721634	-2.4028220	1.5421385
C	-5.1554459	-2.9270640	2.4786987
C	-6.5132868	-3.1209426	2.1342705
H	-8.0432277	-2.9378263	0.5924577
H	-6.4826840	-2.0018597	-1.1004323
H	-3.2142099	-2.2386558	1.7964004

H	-4.8044466	-3.1880413	3.4877481
H	-7.2115111	-3.5333554	2.8788709
C	-3.7946424	-1.5520778	-0.7368297
C	-4.2819148	-1.2396359	-2.1160642
O	-5.0177589	-0.2800895	-2.3640200
O	-3.8109262	-2.0719293	-3.0415433
C	-4.2367833	-1.8388405	-4.4117583
H	-3.7785134	-2.6483046	-5.0036590
H	-5.3402811	-1.8792546	-4.4839527
H	-3.8836944	-0.8484045	-4.7559161
C	-5.8296251	4.2902952	1.3959823
C	-5.8793117	5.0802461	0.2282200
C	-5.7511958	4.4701630	-1.0363870
C	-5.5721223	3.0870505	-1.1417945
C	-5.5248196	2.2943226	0.0350018
C	-5.6531972	2.9069961	1.3081605
H	-5.9397289	4.7634600	2.3833644
H	-5.7976702	5.0826157	-1.9492957
H	-5.4781735	2.6039409	-2.1266857
H	-5.6252549	2.2710656	2.2048322
O	-5.3676518	0.9529904	-0.0051048
H	-5.3412496	0.6239627	-0.9510623
H	-6.0257003	6.1677014	0.3033513

[(C1-2a)·Cs^+]···1a:

Au	-2.0230624	-0.5795618	-0.5344900
P	0.3190984	-0.4327390	-0.5342253
O	1.2105691	0.1246741	0.7392675
O	0.6893491	0.5485367	-1.7826219
O	1.1848204	-1.8260114	-0.6807519
O	2.4611489	-4.3971417	-0.3150778
O	4.9625280	-4.9295471	1.1173702
O	6.2065941	-3.1046383	2.9836220
O	6.0814205	-0.1959242	2.6591476
C	1.1835426	1.5070599	1.0753891
C	0.6571483	1.9208349	2.3278523
C	0.6913015	3.3082342	2.5729963
H	0.2828553	3.6723458	3.5233243
C	1.2187267	4.2613035	1.6734303
C	1.7861432	3.7769675	0.4853711
H	2.2275011	4.4714440	-0.2407872
C	1.7975667	2.3985713	0.1677034
C	2.5207491	1.9669993	-1.0688123
C	3.7818412	2.5404619	-1.3425234
H	4.2202981	3.1962409	-0.5755546
C	4.4647376	2.3117215	-2.5510886
C	3.8174229	1.5119474	-3.5133176
H	4.3106194	1.3639155	-4.4791925
C	2.5548588	0.9061162	-3.3199297
C	1.9641884	1.1084856	-2.0483289
C	0.1317607	0.9420934	3.4120467
C	1.2414828	-0.0787048	3.7796329
H	0.8905022	-0.7473797	4.5922502
H	2.1522500	0.4415375	4.1402215
H	1.5139076	-0.7116449	2.9136725
C	-0.2543875	1.6831247	4.7126539
H	-0.5987764	0.9457769	5.4645506
H	-1.0835080	2.4015041	4.5570569
H	0.6023504	2.2288312	5.1549190
C	-1.1330049	0.1967052	2.9217594
H	-1.5227664	-0.4637435	3.7235016
H	-0.9296981	-0.4420765	2.0398299
H	-1.9376828	0.9095735	2.6513855
C	1.1657996	5.7630269	2.0241080
C	1.8059476	6.6370804	0.9262921
H	2.8802442	6.4027237	0.7794827
H	1.7422934	7.7051933	1.2139525
H	1.2877237	6.5300368	-0.0485606
C	1.9280503	6.0065033	3.3519028
H	1.8995605	7.0828139	3.6172197
H	2.9920889	5.7062483	3.2651256
H	1.4841945	5.4473639	4.2001362
C	-0.3154655	6.1903802	2.1903027
H	-0.3761008	7.2678077	2.4459366
H	-0.8236873	5.6287025	2.9997626
H	-0.8872415	6.0304842	1.2536587

C	5.8363230	2.9728035	-2.8074289
C	5.6617407	4.5138522	-2.8001047
H	6.6346515	5.0126440	-2.9869237
H	5.2794297	4.8851904	-1.8280148
H	4.9553157	4.8395753	-3.5898985
C	6.8243983	2.5620655	-1.6867832
H	7.8143190	3.0336240	-1.8534690
H	6.9739032	1.4622203	-1.6686156
H	6.4723385	2.8841247	-0.6854611
C	6.4406249	2.5557527	-4.1638323
H	7.4296013	3.0373966	-4.2976074
H	5.8090865	2.8725389	-5.0182034
H	6.5958546	1.4595294	-4.2329940
C	1.8497044	0.1754295	-4.4935037
C	0.5232199	0.9114104	-4.8219753
H	0.0223526	0.4188074	-5.6805425
H	0.7180361	1.9653943	-5.1057270
H	-0.1790017	0.9095446	-3.9671997
C	1.5621892	-1.3053358	-4.1490075
H	1.0937112	-1.8114691	-5.0175420
H	0.8731799	-1.4033557	-3.2918796
H	2.5016782	-1.8458954	-3.9103216
C	2.7130563	0.1825138	-5.7754561
H	2.1626048	-0.3337741	-6.5867200
H	3.6760145	-0.3507957	-5.6422816
H	2.9295447	1.2090470	-6.1311585
C	0.5477556	-3.0978121	-0.9858543
H	-0.1840188	-2.9765305	-1.8117558
H	0.0158157	-3.4621347	-0.0819442
C	1.6034640	-4.0986041	-1.4065668
H	1.0708785	-5.0187002	-1.7500460
H	2.1771937	-3.7051175	-2.2793241
C	3.3427683	-5.4891636	-0.5928029
H	4.0859290	-5.2047992	-1.3757248
H	2.7638979	-6.3587725	-0.9842953
C	4.0533456	-5.9306058	0.6692424
H	3.3022961	-6.1629287	1.4618457
H	4.6010363	-6.8768104	0.4430246
C	5.6951157	-5.3543827	2.2687484
H	6.1819036	-6.3392922	2.0736635
H	5.0063014	-5.4882314	3.1371070
C	6.7803432	-4.3565104	2.6165201
H	7.3697384	-4.7798500	3.4638342
H	7.4807732	-4.2291358	1.7557589
C	7.1502052	-2.2152470	3.5812859
H	8.0361513	-2.0813227	2.9143922
H	7.5275709	-2.6366292	4.5437822
C	6.4724530	-0.8794385	3.8513923
H	5.5469977	-1.0524081	4.4408787
H	7.1455246	-0.2421771	4.4685756
C	7.0997297	0.6352635	2.1080447
H	6.6787840	1.1264569	1.2105437
H	8.0036263	0.0597178	1.8030208
H	7.4112923	1.4234768	2.8299374
C	-7.1691486	-2.6114622	0.1083529
C	-6.3498948	-1.6262111	-0.4414299
C	-4.9323567	-1.5996546	-0.1561172
C	-4.4138168	-2.6075838	0.7371920
C	-5.2433974	-3.5721277	1.2896477
C	-6.6246242	-3.5805514	0.9720802
H	-8.2419765	-2.6303794	-0.1325633
H	-6.7804627	-0.8874074	-1.1302216
H	-3.3389568	-2.5848253	0.9740683
H	-4.8354828	-4.3312696	1.9731029
H	-7.2775163	-4.3540044	1.4052414
C	-4.0601323	-0.6448885	-0.7323645
C	-4.6341588	0.4699891	-1.5424258
O	-5.4760770	1.2578939	-1.0971478
O	-4.1061946	0.5706004	-2.7607594
C	-4.5970943	1.6432896	-3.6064245
H	-4.0758652	1.5204033	-4.5700117
H	-5.6923301	1.5577088	-3.7408359
H	-4.3586349	2.6237236	-3.1518472
C	-9.6654672	1.7062131	3.0420624
C	-10.1297903	2.7505056	2.2143946
C	-9.4074458	3.1014587	1.0552801
C	-8.2339805	2.4207426	0.7177784

C	-7.7686217	1.3705581	1.5536105
C	-8.4950790	1.0157869	2.7205993
H	-10.2272464	1.4339618	3.9482195
H	-9.7663999	3.9180252	0.4108834
H	-7.6612939	2.6915382	-0.1824896
H	-8.1132583	0.2007068	3.3524841
O	-6.6402662	0.6811717	1.2837612
H	-6.2162966	1.0101578	0.4387435
H	-11.0514802	3.2915999	2.4739904
Cs	4.0599410	-1.9233141	1.0324041

TS-O (no RA):

Au	-2.1733641	0.5517244	-0.1238980
P	0.0547641	0.6480111	-0.8512496
O	1.1798207	-0.4365925	-0.3854866
O	0.6535761	2.1089407	-0.4077117
O	0.2540721	0.4829621	-2.4517310
O	-1.1079837	-2.0309154	-3.1429418
O	-0.1312345	-4.9093032	-2.7074068
O	2.1908310	-6.2470567	-1.3176405
O	4.5746740	-4.7915685	-0.3738878
C	2.0179837	-0.3288688	0.7390243
C	2.0090083	-1.3732781	1.7002344
C	2.9205626	-1.2357164	2.7655597
H	2.9380812	-2.0222666	3.5303347
C	3.8101650	-0.1491003	2.9104682
C	3.7973692	0.8282820	1.9056343
H	4.4700701	1.6939553	1.9628012
C	2.9216600	0.7548044	0.7969341
C	3.0533703	1.7998289	-0.2633106
C	4.3450487	2.1744749	-0.6883516
H	5.1960848	1.5892935	-0.3105228
C	4.5620815	3.2447145	-1.5742426
C	3.4337932	3.9831367	-1.9808672
H	3.5884577	4.8528284	-2.6271263
C	2.1087933	3.6680587	-1.6031863
C	1.9557916	2.5199874	-0.7898923
C	1.0811421	-2.6099454	1.6004822
C	1.2674865	-3.3440989	0.2475972
H	0.6449883	-4.2605224	0.2372533
H	2.3153197	-3.6712449	0.0960275
H	0.9696186	-2.7322202	-0.6216295
C	1.3796722	-3.6333550	2.7199188
H	0.7081281	-4.5072578	2.6020188
H	1.2079536	-3.2219509	3.7356470
H	2.4198834	-4.0119428	2.6650018
C	-0.3928966	-2.1661544	1.7735934
H	-1.0603549	-3.0527906	1.7346320
H	-0.7139472	-1.4718826	0.9709516
H	-0.5541370	-1.6573981	2.7461868
C	4.7469273	-0.0774667	4.1354466
C	5.6354954	1.1825605	4.1144943
H	6.2977749	1.2107044	3.2252166
H	6.2883722	1.1978050	5.0104924
H	5.0358723	2.1154306	4.1276079
C	5.6683770	-1.3232674	4.1507179
H	6.3447628	-1.2932152	5.0300135
H	6.2973942	-1.3660156	3.2381816
H	5.0911907	-2.2679261	4.2085188
C	3.8943799	-0.0509719	5.4294222
H	4.5497377	-0.0033224	6.3235201
H	3.2604471	-0.9551055	5.5292682
H	3.2269562	0.8349642	5.4488667
C	5.9936906	3.5797580	-2.0458295
C	6.8814716	3.8947286	-0.8153302
H	7.9154038	4.1366073	-1.1373556
H	6.9462621	3.0363346	-0.1165170
H	6.4888883	4.7640171	-0.2490275
C	6.5726100	2.3573691	-2.8030556
H	7.6053139	2.5710157	-3.1481641
H	5.9589828	2.1109047	-3.6936203
H	6.6141512	1.4537233	-2.1625988
C	6.0256876	4.7974860	-2.9917141
H	7.0684297	4.9963249	-3.3108051
H	5.6517311	5.7187252	-2.5001433
H	5.4282175	4.6277018	-3.9106749

C	0.9326616	4.6009429	-1.9968583
C	0.2572159	5.1372570	-0.7064429
H	-0.5771478	5.8201144	-0.9696239
H	0.9817657	5.7111491	-0.0939275
H	-0.1491472	4.3194179	-0.0816075
C	-0.1125407	3.8665612	-2.8719482
H	-0.8861659	4.5847228	-3.2137978
H	-0.6272668	3.0628708	-2.3151025
H	0.3615852	3.4249013	-3.7721423
C	1.4214929	5.8230167	-2.8071240
H	0.5572257	6.4777040	-3.0382237
H	1.8811814	5.5316237	-3.7730144
H	2.1531601	6.4346638	-2.2429308
C	-0.8357704	0.3479768	-3.3926453
H	-0.7068986	1.1479979	-4.1484502
H	-1.8097784	0.4994746	-2.8747488
C	-0.8132927	-1.0065829	-4.0697163
H	-1.5758154	-0.9649615	-4.8888008
H	0.1790318	-1.1749740	-4.5546301
C	-1.4814190	-3.2426107	-3.7929207
H	-0.7884904	-3.4663523	-4.6377834
H	-2.5105118	-3.1390283	-4.2186420
C	-1.4510747	-4.4305612	-2.8471278
H	-1.9001849	-4.1449416	-1.8625433
H	-2.1079548	-5.2248205	-3.2846132
C	-0.0611837	-6.2269264	-2.1890021
H	-0.7519122	-6.8984119	-2.7588655
H	-0.3751061	-6.2644775	-1.1165976
C	1.3484602	-6.7738746	-2.3202703
H	1.3028028	-7.8912307	-2.2484345
H	1.7298025	-6.5285157	-3.3425591
C	3.5333891	-6.6686614	-1.4671229
H	3.9677696	-6.2837373	-2.4228409
H	3.5933289	-7.7864461	-1.5041590
C	4.3837198	-6.1908904	-0.3057800
H	3.8996472	-6.4864796	0.6590233
H	5.3665968	-6.7239014	-0.3560386
C	5.4705646	-4.3152818	0.6060793
H	5.5632735	-3.2203662	0.4735007
H	6.4838504	-4.7754216	0.5033879
H	5.1115205	-4.5191926	1.6448112
C	-7.1730468	-1.7437746	0.6794077
C	-6.4191024	-0.5815695	0.5115547
C	-4.9914741	-0.6353229	0.4885890
C	-4.3583879	-1.9029646	0.6534433
C	-5.1183152	-3.0636583	0.8179010
C	-6.5246499	-2.9866107	0.8307997
H	-8.2716214	-1.6903587	0.6958349
H	-6.9318260	0.3866125	0.4060439
H	-3.2588162	-1.9505855	0.6429546
H	-4.6187302	-4.0362211	0.9386058
H	-7.1223627	-3.9016307	0.9617547
C	-4.1950422	0.5596396	0.3225291
C	-4.8694129	1.8061315	-0.1918756
O	-5.0885280	2.8187272	0.4833944
O	-5.1531193	1.7111306	-1.4895705
C	-5.7157383	2.8894833	-2.1233336
H	-5.9104064	2.5958448	-3.1682503
H	-6.6531303	3.1879908	-1.6170550
H	-4.9943647	3.7277598	-2.0784817
C	-1.7160765	0.6888703	4.8246317
C	-0.9636559	1.8755311	4.7463064
C	-1.3376832	2.8862440	3.8415405
C	-2.4538577	2.7159051	3.0097985
C	-3.2051908	1.5256759	3.1040354
C	-2.8389780	0.5065345	4.0053490
H	-1.4322544	-0.0977683	5.5395984
H	-0.7550783	3.8175382	3.7820037
H	-2.7536804	3.5019611	2.3000447
H	-3.4539153	-0.4027762	4.0628487
O	-4.3275119	1.3216106	2.3362345
H	-4.6362879	2.1756389	1.8705279
H	-0.0869292	2.0153150	5.3952416

TS-O (Li^+):

Au	-2.2354032	-0.1665230	-0.3638127

P	0.0948361	-0.4519489	-0.3774095
O	1.0878783	-0.3402196	0.9267702
O	0.6622397	0.6301667	-1.4560650
O	0.6130948	-1.9596178	-0.8001442
O	1.0003079	-4.7597612	-0.3289589
O	2.3962916	-5.7951697	1.6691843
O	3.5865896	-3.6042274	2.4765529
O	4.0449677	-2.9326120	-0.0486375
Li	2.6051307	-4.0204893	0.7396460
C	1.4445874	0.9181703	1.4814244
C	1.0794078	1.2209763	2.8203593
C	1.5092680	2.4723776	3.3048472
H	1.2383894	2.7475483	4.3310803
C	2.2698493	3.3946223	2.5527951
C	2.6452762	3.0091342	1.2577791
H	3.2459102	3.6820847	0.6328506
C	2.2627460	1.7654523	0.7007948
C	2.8119164	1.4068314	-0.6438887
C	4.1695277	1.6920303	-0.9093770
H	4.7861547	2.0615348	-0.0767621
C	4.7375476	1.5340104	-2.1862231
C	3.8818969	1.1082862	-3.2215172
H	4.2939821	1.0260084	-4.2322331
C	2.5134991	0.8008832	-3.0397274
C	2.0289198	0.9063236	-1.7123505
C	0.3215285	0.2357537	3.7485925
C	1.1485588	-1.0662834	3.9077041
H	0.6166515	-1.7740212	4.5772035
H	2.1344597	-0.8493616	4.3667902
H	1.3250972	-1.5727417	2.9405157
C	0.1121576	0.8244362	5.1624416
H	-0.4158865	0.0817406	5.7934521
H	-0.5069512	1.7435389	5.1497237
H	1.0708302	1.0575377	5.6668462
C	-1.0833559	-0.0880831	3.1836942
H	-1.6393900	-0.7333761	3.8949392
H	-1.0352327	-0.6282646	2.2184672
H	-1.6732190	0.8391785	3.0327742
C	2.6689529	4.7509514	3.1710027
C	3.4790676	5.6197651	2.1875002
H	4.4337824	5.1386192	1.8928797
H	3.7360012	6.5864400	2.6642824
H	2.9070339	5.8500726	1.2655798
C	3.5338949	4.5002017	4.4330971
H	3.8293815	5.4651158	4.8931287
H	4.4614379	3.9468878	4.1808353
H	2.9908166	3.9190398	5.2053660
C	1.3870232	5.5259748	3.5684222
H	1.6540420	6.5058009	4.0139412
H	0.7812737	4.9760759	4.3162845
H	0.7447773	5.7176145	2.6846483
C	6.2255629	1.8752265	-2.4210975
C	6.4526712	3.3778485	-2.1101059
H	7.5151729	3.6476523	-2.2775786
H	6.2076898	3.6284735	-1.0582915
H	5.8315184	4.0207732	-2.7660563
C	7.1074038	1.0164636	-1.4793447
H	8.1787144	1.2652741	-1.6218563
H	6.9846126	-0.0662600	-1.6920082
H	6.8693341	1.1889732	-0.4099177
C	6.6631266	1.6067624	-3.8756293
H	7.7377147	1.8498010	-3.9950159
H	6.1067213	2.2325924	-4.6017584
H	6.5332033	0.5429814	-4.1616489
C	1.6118665	0.4872489	-4.2635575
C	0.5240936	1.5885630	-4.3793143
H	-0.1180362	1.3956075	-5.2628511
H	0.9886542	2.5860190	-4.5132348
H	-0.1237475	1.6295866	-3.4833148
C	0.9430475	-0.9029137	-4.1389016
H	0.3613336	-1.1246912	-5.0568905
H	0.2468656	-0.9473984	-3.2825412
H	1.7014827	-1.7037251	-4.0182884
C	2.4161666	0.4861892	-5.5833504
H	1.7301761	0.2746273	-6.4270405
H	3.2061796	-0.2923249	-5.5991814
H	2.8892378	1.4665649	-5.7891810

C	-0.2964806	-2.9638235	-1.3072984
H	-0.7504339	-2.6324393	-2.2654741
H	-1.1075397	-3.1449812	-0.5707495
C	0.4734548	-4.2455798	-1.5590691
H	-0.2336056	-4.9783290	-2.0070330
H	1.2925700	-4.0736336	-2.2928054
C	1.0438664	-6.1972962	-0.2259838
H	1.8732958	-6.6041064	-0.8485166
H	0.0900673	-6.6439228	-0.5827680
C	1.2477008	-6.5287331	1.2413008
H	0.3554020	-6.2178582	1.8329192
H	1.3914567	-7.6245397	1.3748018
C	2.5609622	-5.6609330	3.0871562
H	2.7270966	-6.6487457	3.5713718
H	1.6444838	-5.2058666	3.5300388
C	3.7723963	-4.7689379	3.2934828
H	3.8773263	-4.5002538	4.3679898
H	4.6983747	-5.3010286	2.9758421
C	4.7843658	-2.8586868	2.2151726
H	5.6291141	-3.5662940	2.0537655
H	5.0419335	-2.1957995	3.0709868
C	4.5487187	-2.0387255	0.9595304
H	3.8188924	-1.2155680	1.1303154
H	5.5094652	-1.5845840	0.6325121
C	4.2418228	-2.4671281	-1.3886565
H	3.8253920	-3.2346360	-2.0673811
H	5.3254520	-2.3525818	-1.6050098
H	3.7283769	-1.4977828	-1.5642449
C	-7.5183673	-1.0802132	1.1200543
C	-6.6196028	-0.6636532	0.1367409
C	-5.2332455	-0.4978752	0.4385932
C	-4.7953121	-0.7568953	1.7702282
C	-5.6976077	-1.1776141	2.7502065
C	-7.0594931	-1.3395624	2.4276861
H	-8.5840904	-1.2018445	0.8764547
H	-6.9908878	-0.4478875	-0.8765939
H	-3.7305307	-0.6205096	2.0134688
H	-5.3481330	-1.3787178	3.7735114
H	-7.7709669	-1.6671217	3.2010643
C	-4.2979767	-0.0416703	-0.5706018
C	-4.7188958	-0.1578516	-2.0198455
O	-4.9983431	0.8046653	-2.7428598
O	-4.7155261	-1.4191891	-2.4386752
C	-5.0813451	-1.6461750	-3.8285314
H	-5.0556481	-2.7400826	-3.9636356
H	-6.0955722	-1.2508753	-4.0258242
H	-4.3583098	-1.1453590	-4.4999593
C	-2.9268347	4.5036671	1.3484481
C	-2.1258380	5.0833125	0.3470951
C	-2.1871869	4.5994597	-0.9725265
C	-3.0419628	3.5361953	-1.2982824
C	-3.8510451	2.9773638	-0.2884279
C	-3.7942850	3.4471081	1.0377436
H	-2.8919562	4.8932340	2.3767423
H	-1.5717964	5.0605761	-1.7593311
H	-3.1066995	3.1595949	-2.3304527
H	-4.4562667	3.0026824	1.7947011
O	-4.7599237	1.9776418	-0.5724606
H	-4.9151874	1.8690190	-1.5795323
H	-1.4617555	5.9250571	0.5924637

TS-O (Cs^+):

Au	-2.9246053	-0.5661496	-0.0645346
P	-0.6024025	-0.3383293	-0.2606948
O	0.3523724	0.4492148	0.8328167
O	-0.2722656	0.3723772	-1.6943206
O	0.2469637	-1.7407884	-0.2113574
O	1.7175913	-4.0654028	0.6758369
O	4.5494305	-4.1237415	1.4622191
O	6.1731906	-1.8247101	2.1917346
O	5.4622124	0.9196615	1.7142500
C	0.6381313	1.8373087	0.7809739
C	0.2818209	2.6692832	1.8750340
C	0.6668285	4.0210411	1.7642946
H	0.3990115	4.6989330	2.5838847
C	1.3738132	4.5597411	0.6658637

C	1.7406169	3.6722691	-0.3576085
H	2.2952628	4.0340621	-1.2328848
C	1.3950563	2.3007216	-0.3187625
C	1.8945859	1.4204062	-1.4205426
C	3.2352285	1.5514310	-1.8455413
H	3.8913364	2.2226682	-1.2720972
C	3.7355665	0.8704167	-2.9719945
C	2.8211633	0.0939702	-3.7122905
H	3.1749016	-0.3917034	-4.6274334
C	1.4637194	-0.0841845	-3.3552372
C	1.0586965	0.5422955	-2.1518087
C	-0.4400016	2.1536981	3.1475772
C	0.4022434	1.0369307	3.8200014
H	-0.0957045	0.6921657	4.7493759
H	1.4049508	1.4176882	4.1023118
H	0.5328457	0.1587403	3.1599945
C	-0.6288864	3.2763373	4.1935008
H	-1.1325299	2.8600239	5.0882739
H	-1.2628231	4.1030237	3.8154410
H	0.3363459	3.7031710	4.5314810
C	-1.8502968	1.6228413	2.7911633
H	-2.3790196	1.3005494	3.7120205
H	-1.8123634	0.7489095	2.1101718
H	-2.4639135	2.4068857	2.3027563
C	1.7130287	6.0651319	0.6287274
C	2.4921369	6.4520124	-0.6448991
H	3.4648595	5.9235633	-0.7159977
H	2.7122385	7.5378362	-0.6343802
H	1.9133826	6.2454480	-1.5683509
C	2.5775684	6.4276242	1.8634896
H	2.8229393	7.5089781	1.8548217
H	3.5328148	5.8643422	1.8638798
H	2.0557932	6.2160270	2.8182347
C	0.3945478	6.8807688	0.6637270
H	0.6164420	7.9667669	0.6393523
H	-0.1942175	6.6832315	1.5818679
H	-0.2450031	6.6438450	-0.2104461
C	5.2228497	1.0081611	-3.3646284
C	5.5933258	2.5071873	-3.4995224
H	6.6555567	2.6121384	-3.7995355
H	5.4661492	3.0624814	-2.5488045
H	4.9729460	3.0050056	-4.2716508
C	6.0895762	0.3605535	-2.2519601
H	7.1678368	0.4740999	-2.4874392
H	5.8815477	-0.7280900	-2.1716286
H	5.9128480	0.8240925	-1.2591822
C	5.5408476	0.3081569	-4.7016664
H	6.6136986	0.4376924	-4.9459146
H	4.9596739	0.7360952	-5.5433699
H	5.3453305	-0.7829360	-4.6631525
C	0.4848971	-0.8171516	-4.3115273
C	-0.6161472	0.1845392	-4.7535571
H	-1.3110430	-0.3074711	-5.4649260
H	-0.1697809	1.0572924	-5.2708815
H	-1.2089706	0.5571622	-3.8971347
C	-0.1658392	-2.0537420	-3.6437249
H	-0.8043312	-2.5821101	-4.3808026
H	-0.8087270	-1.7789617	-2.7874603
H	0.6050315	-2.7720220	-3.2962193
C	1.2017624	-1.3155952	-5.5867835
H	0.4629119	-1.8059466	-6.2509917
H	1.9901533	-2.0630711	-5.3657305
H	1.6579495	-0.4873013	-6.1639548
C	-0.3653358	-3.0391694	0.0226115
H	-1.2399272	-3.1779208	-0.6464415
H	-0.7046085	-3.0960272	1.0778384
C	0.6506178	-4.1267928	-0.2571881
H	0.1149618	-5.1041141	-0.1785990
H	1.0246229	-4.0414509	-1.3060590
C	2.5691957	-5.2124089	0.6012565
H	3.0642697	-5.2675725	-0.3977216
H	1.9667524	-6.1427789	0.7285168
C	3.6170200	-5.1760094	1.6942570
H	3.1264730	-5.0588820	2.6906521
H	4.1401968	-6.1617590	1.6961860
C	5.6636426	-4.1761000	2.3561885
H	6.1477121	-5.1800671	2.3077972

H	5.3282021	-4.0156708	3.4087916
C	6.6951367	-3.1335228	1.9780589
H	7.6009509	-3.2973507	2.6087428
H	7.0034670	-3.2691858	0.9128185
C	7.1430343	-0.7991994	1.9829187
H	7.4203238	-0.7358491	0.9031022
H	8.0760175	-1.0247056	2.5520097
C	6.6097232	0.5330121	2.4676402
H	6.3561007	0.4694953	3.5531457
H	7.4210664	1.2916903	2.3580717
C	5.0185987	2.2311755	2.0442037
H	4.1150239	2.4475119	1.4415213
H	5.7956440	2.9948304	1.8113157
H	4.7579661	2.3177838	3.1242418
C	-7.6525154	-2.3280241	2.2583130
C	-6.9719196	-1.9615449	1.0966428
C	-5.6626505	-1.3920161	1.1670696
C	-5.0783903	-1.1959922	2.4541193
C	-5.7614446	-1.5692482	3.6134750
C	-7.0483362	-2.1355741	3.5177621
H	-8.6601239	-2.7640839	2.1925687
H	-7.4573316	-2.1032007	0.1190580
H	-4.0755339	-0.7461450	2.5168251
H	-5.2989820	-1.4201947	4.6002630
H	-7.5873695	-2.4274026	4.4320313
C	-4.9540828	-0.9971728	-0.0302990
C	-5.4286076	-1.5542637	-1.3546473
O	-5.9774981	-0.8845359	-2.2356137
O	-5.1402982	-2.8459288	-1.4779040
C	-5.5090805	-3.4824621	-2.7334672
H	-5.2133494	-4.5389017	-2.6239022
H	-6.5993328	-3.3949829	-2.8989003
H	-4.9725880	-3.0045056	-3.5749782
C	-4.6839444	4.0920449	0.6527848
C	-4.0752417	4.5602435	-0.5266124
C	-4.0711027	3.7581522	-1.6828808
C	-4.6662174	2.4881535	-1.6669482
C	-5.2834270	2.0367239	-0.4820781
C	-5.2903771	2.8280677	0.6832181
H	-4.7073921	4.7267819	1.5511369
H	-3.6104792	4.1291392	-2.6107114
H	-4.6812224	1.8613052	-2.5717597
H	-5.8008146	2.4542801	1.5822023
O	-5.9319626	0.8218836	-0.4296495
H	-6.0986448	0.4290587	-1.3600861
H	-3.6163005	5.5594872	-0.5498429
Cs	3.4457369	-1.2843262	0.7846025

TS-C (no RA):

Au	-1.9261899	-0.3609763	-0.5796413
P	0.3705417	-0.4587520	-0.9734754
O	1.4277768	-0.5087700	0.2714507
O	0.7938272	0.8871200	-1.8132347
O	0.9083767	-1.7410788	-1.8049634
O	0.5566132	-4.3388224	-0.5179577
O	2.4833431	-4.7706006	1.6447740
O	3.9050770	-2.6039690	2.9767478
O	6.2849829	-2.8882199	1.0814204
C	1.4527568	0.6038540	1.1398526
C	0.9333188	0.5157859	2.4544657
C	1.0628045	1.6866413	3.2361233
H	0.6667690	1.6532821	4.2611494
C	1.6649141	2.8814186	2.7951008
C	2.1825270	2.8935599	1.4886829
H	2.6605422	3.7957216	1.0858349
C	2.0943831	1.7656985	0.6442224
C	2.7377374	1.8266816	-0.7028320
C	4.0302123	2.3953341	-0.7982179
H	4.5312682	2.6691082	0.1393011
C	4.6673816	2.5979350	-2.0300398
C	3.9463741	2.2467777	-3.1920287
H	4.4168708	2.4335764	-4.1649850
C	2.6586585	1.6745067	-3.1826726
C	2.0972702	1.4299176	-1.9000089
C	0.2639335	-0.7143803	3.1297924
C	1.0764646	-1.0846605	4.4001827

H	0.5611666	-1.9045063	4.9427460
H	1.1792653	-0.2368696	5.1062989
H	2.0884954	-1.4443943	4.1250806
C	-1.1814817	-0.3200638	3.5314227
H	-1.6831612	-1.1731613	4.0326359
H	-1.7849695	-0.0519616	2.6382922
H	-1.2105205	0.5407950	4.2286164
C	0.1807034	-1.9938493	2.2696150
H	-0.2759710	-2.7930539	2.8903043
H	1.1664890	-2.3539319	1.9230187
H	-0.4790729	-1.8726283	1.3856230
C	1.7414353	4.1031768	3.7372000
C	2.4425152	5.3054703	3.0719755
H	3.4892989	5.0720293	2.7898523
H	2.4760757	6.1584974	3.7791633
H	1.9086213	5.6511323	2.1631557
C	2.5366964	3.7183262	5.0104815
H	2.6032825	4.5839175	5.7020108
H	3.5700748	3.4048954	4.7576768
H	2.0583706	2.8861552	5.5648706
C	0.3068258	4.5340072	4.1351599
H	0.3411309	5.4077782	4.8183463
H	-0.2408441	3.7239011	4.6574609
H	-0.2844280	4.8235562	3.2420895
C	6.0863446	3.1940961	-2.1534167
C	6.7013020	3.5162044	-0.7763842
H	7.7195547	3.9345837	-0.9076597
H	6.7963792	2.6114226	-0.1420184
H	6.1062387	4.2687642	-0.2199876
C	7.0061124	2.1747032	-2.8726400
H	8.0308317	2.5867829	-2.9785393
H	6.6398239	1.9285234	-3.8896340
H	7.0754284	1.2271734	-2.3007232
C	6.0224951	4.5055548	-2.9781377
H	7.0355519	4.9466624	-3.0781379
H	5.3702031	5.2559182	-2.4865042
H	5.6318550	4.3372030	-4.0018881
C	1.9096135	1.4043615	-4.5145326
C	0.5706524	2.1892606	-4.5292977
H	0.0445748	2.0202217	-5.4917884
H	0.7537963	3.2786380	-4.4314533
H	-0.1012801	1.8789954	-3.7078657
C	1.6473674	-0.1101753	-4.6990519
H	1.1275182	-0.2900977	-5.6629635
H	1.0247656	-0.5248862	-3.8881450
H	2.5999693	-0.6770587	-4.7152986
C	2.7266587	1.8774716	-5.7382578
H	2.1428690	1.6851438	-6.6607533
H	3.6867009	1.3330300	-5.8402986
H	2.9429380	2.9643262	-5.7064819
C	0.0495551	-2.8089491	-2.2845572
H	-0.0098246	-2.7192298	-3.3885693
H	-0.9718524	-2.6980418	-1.8577918
C	0.6296993	-4.1565825	-1.9099728
H	0.0441530	-4.9335096	-2.4671923
H	1.6847131	-4.2236108	-2.2747192
C	1.0769397	-5.5929113	-0.0954350
H	2.0330710	-5.8172884	-0.6261712
H	0.3583605	-6.4160318	-0.3333318
C	1.3550497	-5.5780494	1.3957667
H	0.4537590	-5.2094742	1.9473559
H	1.5322156	-6.6329205	1.7280238
C	2.9276129	-4.8001463	2.9901279
H	3.1415151	-5.8507290	3.3120902
H	2.1459675	-4.3966137	3.6803110
C	4.2032511	-3.9903764	3.1145333
H	4.6636283	-4.1938174	4.1137964
H	4.9222989	-4.3160786	2.3330616
C	5.0380965	-1.7631639	2.8192719
H	5.8603737	-2.0585641	3.5148064
H	4.7058083	-0.7430165	3.1050170
C	5.5809063	-1.7003315	1.3950270
H	4.7290475	-1.5406232	0.6883189
H	6.2558900	-0.8087597	1.3068984
C	6.7589292	-2.9186313	-0.2471733
H	7.2918023	-3.8779537	-0.3934984
H	7.4708375	-2.0825742	-0.4553759

H	5.9284626	-2.8525497	-0.9917677
C	-6.4704803	1.4561807	2.0002015
C	-5.9143810	0.4825904	1.1641853
C	-4.6304242	0.6692968	0.5711039
C	-3.9617221	1.9040362	0.8165830
C	-4.5218140	2.8793944	1.6479281
C	-5.7765099	2.6559280	2.2457000
H	-7.4518254	1.2822940	2.4663321
H	-6.4625919	-0.4535647	0.9871878
H	-2.9710881	2.0653199	0.3625653
H	-3.9750205	3.8141221	1.8426276
H	-6.2153718	3.4189679	2.9066989
C	-3.9913117	-0.3639913	-0.2388732
C	-4.4101617	-1.8136610	-0.0942252
O	-4.5936272	-2.6183881	-0.9941240
O	-4.4356086	-2.1412705	1.2203747
C	-4.5989701	-3.5457603	1.5154798
H	-4.6241701	-3.6170966	2.6163314
H	-5.5385957	-3.9305077	1.0742447
H	-3.7484938	-4.1272540	1.1086247
C	-6.1081377	-0.2262003	-2.1004550
C	-4.7015435	-0.0515651	-2.2991569
C	-4.2085675	1.2679888	-2.5567992
C	-5.0344851	2.3696519	-2.4125457
C	-6.4081347	2.1782641	-2.0781227
C	-6.9464522	0.8672470	-1.9546579
H	-6.5031633	-1.2492703	-2.0209461
H	-3.1499048	1.4073476	-2.8243693
H	-4.6493349	3.3899337	-2.5701287
H	-8.0231890	0.7593133	-1.7612428
O	-7.2517393	3.2008367	-1.8998272
H	-6.7888080	4.0544225	-2.0240934
H	-4.1167347	-0.9284623	-2.6082318

TS-C (Li^+):

Au	-1.8775878	-0.3350533	-0.2917048
P	0.4367566	-0.3446396	-0.5561857
O	1.4563773	-0.3314966	0.7305615
O	0.8553401	0.9708583	-1.4225972
O	1.1117081	-1.6721808	-1.2622060
O	1.5690399	-4.4467525	-0.9570845
O	2.8039663	-5.5097404	1.1236330
O	3.7546502	-3.3267632	2.2181094
O	4.4424332	-2.4260057	-0.1856678
Li	2.9750819	-3.6463544	0.3461447
C	1.5165173	0.8583701	1.5053211
C	0.9854026	0.8998886	2.8169025
C	1.1390343	2.1323256	3.4918192
H	0.7249460	2.2072330	4.5070874
C	1.7858137	3.2640386	2.9567451
C	2.3236065	3.1418919	1.6638460
H	2.8373869	3.9906725	1.1939637
C	2.2051245	1.9493476	0.9185024
C	2.8600178	1.8722522	-0.4235486
C	4.1800431	2.3548201	-0.5605451
H	4.6937663	2.6978705	0.3473595
C	4.8308852	2.3994035	-1.8059817
C	4.0945036	1.9664450	-2.9265141
H	4.5786620	2.0175913	-3.9120382
C	2.7649170	1.4863897	-2.8794659
C	2.1910700	1.4141266	-1.5867091
C	0.2625368	-0.2423175	3.5863930
C	0.9520508	-0.4364041	4.9641248
H	0.4402612	-1.2394535	5.5324498
H	0.9227658	0.4747732	5.5907001
H	2.0154511	-0.7273366	4.8426789
C	-1.2154990	0.1737225	3.8037479
H	-1.7569899	-0.6072694	4.3761434
H	-1.7377710	0.3066102	2.8329297
H	-1.3025600	1.1230938	4.3674495
C	0.2680775	-1.6250982	2.8947447
H	-0.2056453	-2.3578373	3.5799682
H	1.2932800	-1.9794825	2.6715801
H	-0.3223579	-1.6329600	1.9570185
C	1.8871159	4.5620742	3.7860261
C	2.6400101	5.6749568	3.0285783

H	3.6836386	5.3847577	2.7902739
H	2.6901378	6.5865306	3.6562510
H	2.1325876	5.9561174	2.0830904
C	2.6462741	4.2663187	5.1048141
H	2.7314874	5.1898427	5.7128075
H	3.6725958	3.8962502	4.9047182
H	2.1274645	3.5091982	5.7266671
C	0.4593977	5.0702471	4.1127148
H	0.5117835	6.0000553	4.7148951
H	-0.1243301	4.3305294	4.6970851
H	-0.1065437	5.2973031	3.1860830
C	6.2727717	2.9233863	-1.9813811
C	6.9098295	3.3285915	-0.6366276
H	7.9432629	3.6909801	-0.8051973
H	6.9739030	2.4755855	0.0704454
H	6.3534236	4.1497617	-0.1411300
C	7.1487409	1.8187577	-2.6251074
H	8.1857010	2.1847513	-2.7680538
H	6.7696422	1.5079051	-3.6193226
H	7.1956840	0.9170452	-1.9799888
C	6.2489097	4.1676788	-2.9071466
H	7.2759737	4.5624429	-3.0447478
H	5.6276049	4.9777368	-2.4744835
H	5.8472919	3.9330075	-3.9134698
C	2.0986848	1.1232170	-4.2387661
C	0.5923491	0.7839539	-4.1760564
H	0.2238103	0.6193397	-5.2088877
H	-0.0036766	1.6024114	-3.7290981
H	0.3926821	-0.1410875	-3.6029605
C	2.8380049	-0.0999249	-4.8406754
H	2.4083194	-0.3652981	-5.8285223
H	2.7441597	-0.9853318	-4.1774548
H	3.9184174	0.0958578	-4.9900743
C	2.2354498	2.3337699	-5.2023605
H	1.7658647	2.0940606	-6.1781186
H	3.2888135	2.6045347	-5.4065183
H	1.7298868	3.2306023	-4.7910985
C	0.3124403	-2.6501385	-1.9693863
H	-0.0116440	-2.2441022	-2.9515490
H	-0.5898443	-2.9087126	-1.3747436
C	1.1582690	-3.8851989	-2.2095336
H	0.5369919	-4.6152401	-2.7741363
H	2.0459129	-3.6412875	-2.8362968
C	1.7211389	-5.8793388	-0.9422434
H	2.6488772	-6.1752357	-1.4836282
H	0.8564807	-6.3702766	-1.4400645
C	1.7805627	-6.2987538	0.5150485
H	0.8021406	-6.1021838	1.0118004
H	2.0028403	-7.3865317	0.5972258
C	2.7989120	-5.4793142	2.5561494
H	2.9758494	-6.4911391	2.9842271
H	1.8103307	-5.1151134	2.9215523
C	3.9188214	-4.5398340	2.9665551
H	3.8850387	-4.3501238	4.0622617
H	4.9065554	-4.9936706	2.7221931
C	4.9317386	-2.5085875	2.1450760
H	5.8240509	-3.1635220	2.0223794
H	5.0637560	-1.9081762	3.0725989
C	4.7867264	-1.5989536	0.9392887
H	3.9997137	-0.8273807	1.0916490
H	5.7531916	-1.0787569	0.7583405
C	4.7283725	-1.8210948	-1.4517647
H	4.4361141	-2.5436625	-2.2362013
H	5.8162449	-1.6156910	-1.5474292
H	4.1630183	-0.8746117	-1.5886550
C	-6.6646854	1.5574039	1.7558071
C	-6.0204616	0.5231948	1.0681218
C	-4.6850754	0.6804493	0.5865962
C	-4.0591937	1.9482046	0.7808128
C	-4.7054283	2.9805888	1.4656075
C	-6.0102561	2.7860258	1.9599785
H	-7.6853873	1.4072296	2.1378819
H	-6.5398013	-0.4341848	0.9272151
H	-3.0340569	2.0939498	0.4031791
H	-4.1921111	3.9406887	1.6249086
H	-6.5188740	3.5956401	2.5054536
C	-3.9580670	-0.4001390	-0.0703119

C	-4.3205230	-1.8534652	0.1746786
O	-4.2383934	-2.7599310	-0.6411026
O	-4.6373524	-2.0462600	1.4759818
C	-4.8496329	-3.4181069	1.8787787
H	-5.0823784	-3.3792789	2.9565253
H	-5.6902624	-3.8636084	1.3126045
H	-3.9394750	-4.0220604	1.6960180
C	-5.9474948	-0.6210704	-2.0741062
C	-4.5513886	-0.3219266	-2.1967485
C	-4.1696072	1.0171172	-2.5356815
C	-5.1023088	2.0388895	-2.5356014
C	-6.4733453	1.7372743	-2.2712591
C	-6.8926408	0.3898547	-2.0737645
H	-6.2529214	-1.6690988	-1.9419097
H	-3.1136096	1.2408089	-2.7515227
H	-4.8067907	3.0766603	-2.7582381
H	-7.9662551	0.1904451	-1.9462590
O	-7.4204818	2.6745834	-2.2309209
H	-7.0469487	3.5632528	-2.4051585
H	-3.8677954	-1.1570032	-2.4015098

TS-C (Cs^+):

Au	18.6205325	10.1089021	5.9054331
P	20.7050834	11.0992846	5.6105841
O	21.4312851	11.8740150	6.8758265
O	20.6240315	12.2303103	4.4325910
O	21.9850079	10.1657392	5.1994915
O	24.4722855	8.6930891	5.3280435
O	27.1515721	9.8484730	5.5580176
O	27.6202292	12.2256661	7.1406432
O	25.6001980	14.1007297	7.9881930
C	20.8111603	13.0566914	7.3565493
C	20.1467098	13.0934496	8.6048446
C	19.5935513	14.3482950	8.9516890
H	19.0568029	14.4151965	9.9088447
C	19.6861806	15.5131070	8.1634578
C	20.4082606	15.4181764	6.9598296
H	20.5248944	16.2945800	6.3090902
C	20.9801423	14.1999028	6.5386485
C	21.7979053	14.1741402	5.2863139
C	22.7734320	15.1829499	5.0990074
H	22.9369223	15.8915605	5.9216052
C	23.5142694	15.2924798	3.9113603
C	23.2036570	14.3836005	2.8737264
H	23.7290393	14.4945114	1.9172093
C	22.2390444	13.3580875	2.9755204
C	21.5972334	13.2419435	4.2395921
C	20.0034773	11.9437422	9.6416661
C	20.6846859	12.3966719	10.9619686
H	20.5803208	11.6072493	11.7340058
H	20.2385198	13.3227753	11.3725468
H	21.7678463	12.5816264	10.8100574
C	18.4970071	11.6819124	9.9001355
H	18.3733030	10.8812285	10.6577346
H	17.9843600	11.3528977	8.9722379
H	17.9700522	12.5789000	10.2796794
C	20.6459194	10.5960391	9.2439763
H	20.5157846	9.8834290	10.0832995
H	21.7305066	10.6837916	9.0421605
H	20.1548427	10.1432540	8.3576632
C	19.0123491	16.8209078	8.6321511
C	19.2561493	17.9824119	7.6470754
H	20.3341987	18.2194070	7.5404574
H	18.7558524	18.8987767	8.0179414
H	18.8450780	17.7703018	6.6387838
C	19.5782576	17.2250083	10.0176376
H	19.1022935	18.1636565	10.3668140
H	20.6727510	17.3976002	9.9696906
H	19.3883911	16.4535109	10.7906420
C	17.4835930	16.5862875	8.7446646
H	16.9777079	17.5127012	9.0852354
H	17.2369804	15.7870307	9.4721257
H	17.0498460	16.3024689	7.7638219
C	24.5875600	16.3800509	3.6922745
C	24.8301070	17.2154833	4.9662732
H	25.6244942	17.9641460	4.7772756

H	25.1608362	16.5852259	5.8178012
H	23.9258823	17.7768757	5.2776938
C	25.9259775	15.7131631	3.2854675
H	26.7021188	16.4849808	3.1087839
H	25.8366579	15.1193732	2.3538270
H	26.2994941	15.0422227	4.0880939
C	24.1189450	17.3280374	2.5575496
H	24.8728029	18.1228520	2.3864544
H	23.1591022	17.8189453	2.8167914
H	23.9774736	16.7915563	1.5980398
C	21.8550720	12.5135865	1.7301551
C	20.3453393	12.7158648	1.4303308
H	20.0637675	12.1469411	0.5205522
H	20.1203716	13.7847057	1.2402916
H	19.7049646	12.3709380	2.2634824
C	22.1561729	11.0102424	1.9445475
H	21.9017918	10.4432776	1.0258164
H	21.5789876	10.5782246	2.7801252
H	23.2354337	10.8460665	2.1469463
C	22.6384631	12.9600755	0.4749573
H	22.3137467	12.3498431	-0.3907110
H	23.7325829	12.8141294	0.5821982
H	22.4509388	14.0207245	0.2150837
C	22.0756758	8.7474128	5.5141602
H	21.1498468	8.2269365	5.1889742
H	22.1944149	8.6213049	6.6108326
C	23.2694040	8.1642091	4.7883715
H	23.2345531	7.0544511	4.9145250
H	23.1872192	8.3771210	3.6957526
C	25.6382066	8.1622876	4.6911744
H	25.7443756	8.5799557	3.6614923
H	25.5499373	7.0550000	4.5935077
C	26.8789598	8.4507347	5.5110644
H	26.7522945	8.0435570	6.5430520
H	27.7317538	7.9043047	5.0417654
C	28.3745000	10.1263562	6.2417970
H	29.2326224	9.6551115	5.7060051
H	28.3453212	9.6982561	7.2719803
C	28.6185568	11.6192627	6.3240281
H	29.6319661	11.7783970	6.7626790
H	28.6279218	12.0720060	5.3019397
C	27.9052654	13.5794107	7.4840151
H	27.8672524	14.2349836	6.5794012
H	28.9330667	13.6638081	7.9093400
C	26.9199236	14.0661885	8.5265434
H	26.9580662	13.3988529	9.4208753
H	27.2315112	15.0859947	8.8551954
C	24.6529318	14.6208796	8.9144135
H	23.6598056	14.6074872	8.4248116
H	24.8953035	15.6697525	9.2009382
H	24.6065003	14.0077426	9.8440683
C	13.4674042	10.0355370	7.8918263
C	14.5172148	9.2858948	7.3516373
C	15.6368634	9.9254042	6.7355748
C	15.6099454	11.3496345	6.6352374
C	14.5568196	12.0961747	7.1703899
C	13.4844495	11.4404969	7.8062589
H	12.6271711	9.5247139	8.3849878
H	14.4958697	8.1910087	7.4356047
H	16.4573014	11.8593255	6.1487418
H	14.5702476	13.1941102	7.1023585
H	12.6575690	12.0265409	8.2358279
C	16.7816524	9.1776246	6.2370104
C	17.0740107	7.7714367	6.7301168
O	17.4886439	6.8429263	6.0551388
O	16.9264236	7.7151138	8.0745220
C	17.3320126	6.4767088	8.7033915
H	17.1599116	6.6216143	9.7834490
H	16.7280055	5.6317167	8.3205001
H	18.4007262	6.2696181	8.5003649
C	15.0906163	7.8209366	4.3933464
C	16.2471439	8.6186029	4.1213023
C	16.0622369	9.9172442	3.5493690
C	14.7974004	10.4712754	3.4504228
C	13.6624890	9.7053102	3.8557865
C	13.8188793	8.3605606	4.2986501
H	15.2312421	6.7796907	4.7175224

H	16.9395032	10.4967011	3.2233921
H	14.6524757	11.4842473	3.0419676
H	12.9157076	7.7797802	4.5341436
O	12.4182175	10.1852031	3.8112569
H	12.4058421	11.1011073	3.4645571
H	17.2150697	8.1069456	4.0321368
Cs	24.8060580	11.8962620	5.8859450

INT-O (no RA):

Au	19.6961637	10.0256595	5.1959801
P	21.4362749	11.4649752	4.6311951
O	22.2009537	12.4401797	5.6944934
O	20.7479658	12.4733499	3.5420950
O	22.7839192	10.8208645	3.9944398
O	23.1717757	8.5199077	5.8657060
O	23.7458694	8.3769087	8.9684968
O	24.3809912	10.1466594	11.2586281
O	26.1332646	12.4770415	10.7861941
C	21.5258125	13.5148018	6.3116460
C	21.3713514	13.5123240	7.7220258
C	20.7036842	14.6280565	8.2644946
H	20.5549506	14.6575281	9.3512140
C	20.2272778	15.7136619	7.4955351
C	20.4798750	15.6872008	6.1156452
H	20.1567336	16.5170676	5.4738643
C	21.1475097	14.6037649	5.4967526
C	21.5093013	14.7186758	4.0511677
C	22.0390542	15.9439017	3.5942132
H	22.2452117	16.7205217	4.3450306
C	22.3203616	16.1822558	2.2379890
C	22.0049735	15.1567243	1.3262138
H	22.1778774	15.3378588	0.2606969
C	21.4723726	13.9033102	1.7027498
C	21.2905477	13.7002138	3.0925088
C	21.9774999	12.4163200	8.6323517
C	23.5147980	12.3645667	8.4240989
H	23.9727974	11.6359488	9.1221248
H	23.9653463	13.3572708	8.6266208
H	23.7820277	12.0718357	7.3923448
C	21.7208211	12.7082233	10.1275712
H	22.2015331	11.9120940	10.7294347
H	20.6401194	12.7208340	10.3778005
H	22.1624714	13.6740698	10.4462139
C	21.3550862	11.0320009	8.3319043
H	21.7747127	10.2802342	9.0287899
H	21.5957765	10.6721006	7.3144279
H	20.2526062	11.0501030	8.4574584
C	19.4910878	16.8808829	8.1886908
C	19.0445434	17.9639288	7.1854573
H	19.9058409	18.4254125	6.6619690
H	18.5124304	18.7759757	7.7205923
H	18.3490139	17.5624206	6.4201763
C	20.4371932	17.5370634	9.2269151
H	19.9251209	18.3795200	9.7359851
H	21.3502829	17.9366187	8.7404483
H	20.7573832	16.8202055	10.0091497
C	18.2326130	16.3365945	8.9107543
H	17.6965452	17.1598349	9.4263983
H	18.4866913	15.5743639	9.6739432
H	17.5285961	15.8729705	8.1893535
C	22.9335478	17.5299082	1.8002164
C	21.9804153	18.6829439	2.2065187
H	22.4057678	19.6607498	1.9002952
H	21.8167080	18.7211512	3.3023125
H	20.9900108	18.5743377	1.7192917
C	24.3013811	17.7163579	2.5052974
H	24.7590926	18.6834346	2.2103241
H	25.0075746	16.9068841	2.2296246
H	24.2027602	17.7173597	3.6092734
C	23.1584913	17.6001285	0.2759256
H	23.6040561	18.5790691	0.0080721
H	22.2100407	17.5062592	-0.2907685
H	23.8552659	16.8134942	-0.0785447
C	21.0486196	12.8735995	0.6218126
C	19.5275054	12.5935568	0.7485701
H	19.2090747	11.8728817	-0.0333732

H	18.9437779	13.5252573	0.6056961
H	19.2609452	12.1728049	1.7359938
C	21.8454453	11.5533695	0.7614485
H	21.5723342	10.8590118	-0.0599007
H	21.6329475	11.0442627	1.7173718
H	22.9373656	11.7382399	0.7042192
C	21.3017336	13.4064651	-0.8066163
H	20.9648451	12.6486617	-1.5420258
H	22.3759919	13.5985172	-1.0019556
H	20.7382081	14.3380212	-1.0137738
C	22.9298664	9.4268019	3.6483711
H	23.3786889	9.4049288	2.6355541
H	21.9330431	8.9336835	3.6074125
C	23.8283012	8.6948383	4.6259106
H	24.0794582	7.7059673	4.1631816
H	24.7900950	9.2497066	4.7472326
C	23.8478459	7.5781745	6.6956852
H	24.9126014	7.8721048	6.8506374
H	23.8472877	6.5787117	6.1937573
C	23.1884497	7.4501391	8.0604171
H	22.0824391	7.5803116	7.9468074
H	23.3526094	6.4072508	8.4320925
C	23.3388414	8.1702872	10.3121627
H	23.2479428	7.0765558	10.5241487
H	22.3368066	8.6282940	10.5037818
C	24.3618288	8.7344046	11.2811198
H	24.1082500	8.3579875	12.3054464
H	25.3679890	8.3216271	11.0209106
C	25.3502706	10.6728438	12.1540464
H	26.3483168	10.2079262	11.9644684
H	25.0699414	10.4393273	13.2118891
C	25.4828844	12.1753441	12.0011692
H	24.4734951	12.6561377	12.0541041
H	26.0698228	12.5584895	12.8749364
C	26.3889947	13.8545488	10.6261719
H	26.9099161	13.9897019	9.6586837
H	27.0405033	14.2574585	11.4402117
H	25.4505347	14.4610111	10.6127402
C	15.9481983	8.0994204	8.7615594
C	16.2538598	8.4006639	7.4253268
C	17.5988846	8.5302690	7.0155520
C	18.6267406	8.3548421	7.9646291
C	18.3155699	8.0402711	9.2969804
C	16.9762339	7.9141747	9.7007021
H	14.8955255	8.0058344	9.0684052
H	15.4452578	8.5393731	6.6935566
H	19.6786480	8.4751101	7.6616179
H	19.1278415	7.9073092	10.0273711
H	16.7332890	7.6791941	10.7478833
C	17.9044528	8.8001938	5.5532773
C	18.3265435	7.6426998	4.7643655
O	17.9051040	7.5163411	3.5307573
O	19.0820893	6.7110486	5.2688658
C	19.4895196	5.5944347	4.4322454
H	20.0624059	4.9303462	5.0996582
H	18.5992147	5.0747905	4.0319006
H	20.1238598	5.9566216	3.6010526
C	16.3959539	12.8677483	5.8885647
C	15.5001493	13.3157385	4.9066595
C	15.0564517	12.4238009	3.9141119
C	15.5123063	11.0979650	3.8966521
C	16.4168084	10.6665689	4.8829042
C	16.8577961	11.5381464	5.8924955
H	16.7433301	13.5530437	6.6758578
H	14.3496481	12.7607012	3.1410157
H	15.1709922	10.3910374	3.1257336
H	17.5260366	11.1913682	6.6924343
O	16.8054612	9.3280553	4.7936185
H	15.1421039	14.3554563	4.9159953
H	17.2443805	8.2709523	3.4388743

INT-O (Li^+):

Au	19.1027494	9.8960989	5.4957534
P	21.0521311	11.1753986	5.5660856
O	21.5543788	12.0453429	6.8657710
O	20.8516062	12.2585668	4.3660100

O	22.4992651	10.4079205	5.3652152
O	24.6034759	8.7015670	6.3110090
O	26.1002199	9.1215417	8.4607336
O	25.4188469	11.6038922	8.9307666
O	25.5541361	12.1417299	6.3381811
Li	25.1650183	10.4506062	7.2733700
C	20.8829640	13.2327825	7.2605695
C	20.2659117	13.2931855	8.5384520
C	19.6564508	14.5210596	8.8651424
H	19.1607957	14.6049576	9.8395576
C	19.6500299	15.6526821	8.0191342
C	20.3292600	15.5434558	6.7968291
H	20.3653762	16.3965084	6.1073605
C	20.9733624	14.3480630	6.3972823
C	21.7683380	14.3701118	5.1296425
C	22.5812048	15.4953795	4.8683924
H	22.6719288	16.2544844	5.6594942
C	23.2532537	15.6730905	3.6453652
C	23.0552597	14.6906164	2.6550459
H	23.5306467	14.8332275	1.6794731
C	22.2596084	13.5358228	2.8360307
C	21.6769020	13.3832063	4.1182601
C	20.3110209	12.1354695	9.5702623
C	21.7883722	11.8118248	9.9145226
H	21.8320880	10.9927286	10.6628130
H	22.2899197	12.6958282	10.3574580
H	22.3674725	11.4982967	9.0259294
C	19.6043405	12.5172250	10.8908296
H	19.6752286	11.6696205	11.6015086
H	18.5269750	12.7333153	10.7461640
H	20.0730025	13.3937835	11.3800146
C	19.6006370	10.8708249	9.0298732
H	19.5902198	10.0782740	9.8063632
H	20.1040916	10.4501754	8.1379554
H	18.5465745	11.0864987	8.7623179
C	18.9345270	16.9451345	8.4659722
C	19.0332743	18.0586170	7.4037426
H	20.0832526	18.3555808	7.2060089
H	18.5009679	18.9632399	7.7587952
H	18.5692525	17.7605658	6.4412571
C	19.5835967	17.4577993	9.7780118
H	19.0830805	18.3880353	10.1153093
H	20.6592932	17.6849954	9.6319370
H	19.5002745	16.7212796	10.6025273
C	17.4359009	16.6375691	8.7160420
H	16.9057609	17.5543245	9.0456008
H	17.2907102	15.8717687	9.5044228
H	16.9426042	16.2749929	7.7908564
C	24.1226537	16.9280759	3.4121633
C	23.2252304	18.1887745	3.5137511
H	23.8278357	19.1038944	3.3433584
H	22.7517083	18.2839489	4.5114972
H	22.4167778	18.1677659	2.7549503
C	25.2302687	16.9960617	4.4939856
H	25.8559608	17.8995783	4.3483958
H	25.8997294	16.1124497	4.4362036
H	24.8117764	17.0469747	5.5197440
C	24.7980377	16.9200158	2.0252134
H	25.4220760	17.8279110	1.9072507
H	24.0579732	16.9262643	1.1994394
H	25.4642483	16.0437209	1.8881076
C	21.9777840	12.5829947	1.6431818
C	20.4560217	12.5967336	1.3367115
H	20.2398893	11.9404724	0.4686040
H	20.1174514	13.6194727	1.0757914
H	19.8519756	12.2447262	2.1944052
C	22.4432114	11.1375809	1.9451313
H	22.2886815	10.4981557	1.0522744
H	21.8756595	10.6897190	2.7802651
H	23.5239811	11.1092572	2.1957669
C	22.7145881	13.0357579	0.3622723
H	22.4726358	12.3369712	-0.4627465
H	23.8169313	13.0321841	0.4825114
H	22.4031824	14.0464577	0.0337149
C	22.5814078	9.0106387	5.0098690
H	22.1599034	8.8416557	3.9955613
H	22.0125335	8.3997964	5.7427431

C	24.0382658	8.5883086	4.9984933
H	24.0780576	7.5304863	4.6564874
H	24.6166518	9.2003691	4.2708425
C	25.5886964	7.7022203	6.6439237
H	26.5407535	7.9031565	6.1011393
H	25.2317724	6.6895603	6.3543136
C	25.7938506	7.7626051	8.1467072
H	24.8635647	7.4492637	8.6756454
H	26.6170535	7.0777990	8.4515002
C	25.9917755	9.4856033	9.8435010
H	26.7322887	8.9365773	10.4661968
H	24.9706167	9.2388792	10.2171739
C	26.2569407	10.9792587	9.9131747
H	26.0422977	11.3627416	10.9352751
H	27.3251316	11.1913883	9.6783928
C	25.8051777	12.9377529	8.5704765
H	26.9162601	12.9970449	8.5177608
H	25.4509385	13.6776848	9.3224831
C	25.2047560	13.2335936	7.2077122
H	24.0970983	13.3377845	7.2535917
H	25.6237964	14.1882981	6.8221741
C	25.5237889	12.4769997	4.9460470
H	25.8206382	11.5720063	4.3835222
H	26.2534342	13.2852826	4.7251743
H	24.5106827	12.8001587	4.6250275
C	14.5378506	8.0165056	7.8809930
C	15.1538645	8.4366466	6.6913422
C	16.5615462	8.4415211	6.5847330
C	17.3371999	8.0159281	7.6828332
C	16.7155529	7.5816537	8.8645728
C	15.3145413	7.5838045	8.9685360
H	13.4399277	8.0226329	7.9535299
H	14.5390241	8.7656246	5.8411581
H	18.4365854	8.0258405	7.6141542
H	17.3310132	7.2486554	9.7138105
H	14.8284426	7.2531137	9.8985024
C	17.2047111	8.8412877	5.2617950
C	17.5928719	7.6969792	4.4136126
O	17.3396516	7.7384698	3.1368586
O	18.1510240	6.6400378	4.9159474
C	18.4511490	5.5058853	4.0471755
H	18.8576370	4.7324972	4.7186026
H	17.5234745	5.1532395	3.5597552
H	19.1946597	5.8024028	3.2839893
C	16.0947065	13.0244160	5.7974608
C	15.6139036	13.7097825	4.6719831
C	15.3877454	13.0079343	3.4746356
C	15.6506074	11.6324764	3.3977388
C	16.1371120	10.9619910	4.5327148
C	16.3542621	11.6415623	5.7431020
H	16.2569107	13.5611121	6.7440029
H	15.0024051	13.5332691	2.5880359
H	15.4727118	11.0745371	2.4662635
H	16.6702316	11.1024499	6.6466016
O	16.3450050	9.5872995	4.3820874
H	15.4024363	14.7874534	4.7279696
H	16.8036159	8.5925352	3.0439462

INT-O (Cs^+):

Au	18.5469537	9.7553183	5.5854888
P	20.5807442	10.8841792	5.7297410
O	21.0804139	11.7453982	7.0494651
O	20.5720333	11.9547171	4.5027014
O	21.9675985	10.0263906	5.5496781
O	24.4931187	8.6469130	5.8775225
O	27.1129424	9.9006453	6.2828189
O	27.4400076	12.3444216	7.8008847
O	25.3379076	14.2118978	8.4542847
C	20.5539408	13.0239524	7.3662451
C	19.8647498	13.2240531	8.5911973
C	19.4146821	14.5388507	8.8281427
H	18.8657022	14.7320274	9.7577923
C	19.6269081	15.6232087	7.9475946
C	20.3749499	15.3706823	6.7872752
H	20.5848730	16.1798015	6.0759622
C	20.8659717	14.0798071	6.4801516

C	21.7494487	13.9280246	5.2806243
C	22.7566819	14.8961394	5.0623525
H	22.9094620	15.6589273	5.8394026
C	23.5393830	14.9182387	3.8924791
C	23.2499411	13.9513656	2.9080005
H	23.8061832	13.9865671	1.9660426
C	22.2618584	12.9487683	3.0480574
C	21.5734080	12.9321345	4.2872605
C	19.6595113	12.1130119	9.6541493
C	21.0361189	11.5485555	10.0958103
H	20.8947955	10.7737361	10.8768246
H	21.6676662	12.3492038	10.5321645
H	21.5879261	11.0862219	9.2550834
C	18.9579598	12.6544107	10.9208493
H	18.8503123	11.8339832	11.6580213
H	17.9397590	13.0364561	10.7081577
H	19.5387832	13.4605408	11.4116428
C	18.7709561	10.9756552	9.0951991
H	18.6024410	10.2043812	9.8742559
H	19.2314108	10.4688839	8.2240441
H	17.7786801	11.3588712	8.7830329
C	19.0563327	17.0159717	8.2890969
C	19.4034557	18.0639998	7.2121179
H	20.4981528	18.2084736	7.1066572
H	18.9716070	19.0454737	7.4916784
H	18.9906946	17.7952975	6.2182675
C	19.6410469	17.4913937	9.6441652
H	19.2387880	18.4912385	9.9049498
H	20.7462228	17.5728273	9.5982390
H	19.3839165	16.8057760	10.4760713
C	17.5128974	16.9162012	8.3982121
H	17.0812732	17.9066750	8.6484655
H	17.1954211	16.2077177	9.1892983
H	17.0647744	16.5831263	7.4398788
C	24.6441451	15.9831469	3.7128893
C	24.0606245	17.3950946	3.9725924
H	24.8434369	18.1652562	3.8200522
H	23.6837660	17.5145031	5.0083102
H	23.2268911	17.6181033	3.2768673
C	25.7759213	15.6985589	4.7348999
H	26.5664158	16.4741724	4.6642069
H	26.2569539	14.7180605	4.5286398
H	25.4035007	15.6885526	5.7797647
C	25.2488409	15.9622904	2.2937720
H	26.0229043	16.7502707	2.2050968
H	24.4860594	16.1626722	1.5147532
H	25.7406742	14.9964223	2.0584412
C	21.9040908	12.0272174	1.8506629
C	20.4163670	12.2528296	1.4683752
H	20.1567994	11.6278863	0.5892137
H	20.2369736	13.3109289	1.1905302
H	19.7251770	11.9919877	2.2910999
C	22.1462467	10.5350199	2.1845107
H	21.9228236	9.9131304	1.2937819
H	21.5091510	10.1787339	3.0129402
H	23.2065843	10.3561318	2.4593547
C	22.7566446	12.3570222	0.6044589
H	22.4523484	11.6933114	-0.2287088
H	23.8400955	12.1913109	0.7734893
H	22.6124986	13.3996846	0.2587351
C	22.0886504	8.6165479	5.8724020
H	21.2115292	8.0608928	5.4762909
H	22.1217379	8.4940228	6.9757192
C	23.3573966	8.0749299	5.2471426
H	23.3530288	6.9644474	5.3757278
H	23.3545889	8.2832125	4.1504595
C	25.7229810	8.1514072	5.3392029
H	25.8922569	8.5603111	4.3143280
H	25.6807277	7.0404558	5.2520250
C	26.8873547	8.4947198	6.2451025
H	26.6962166	8.1011192	7.2725907
H	27.7891971	7.9678586	5.8511127
C	28.2864037	10.2279945	7.0310365
H	29.1842327	9.7560178	6.5659254
H	28.2009378	9.8357812	8.0723012
C	28.4969477	11.7274162	7.0708487
H	29.4787626	11.9233894	7.5633878

H	28.5606860	12.1408656	6.0342921
C	27.6782963	13.7210213	8.0895675
H	27.6739844	14.3277438	7.1518532
H	28.6803529	13.8491724	8.5629435
C	26.6319910	14.2392203	9.0547971
H	26.6400979	13.6250415	9.9868929
H	26.9057200	15.2831946	9.3384814
C	24.3442353	14.7902928	9.2943552
H	23.3755806	14.7351113	8.7611861
H	24.5696194	15.8588565	9.5142319
H	24.2566855	14.2467610	10.2634786
C	13.6084076	8.4921786	7.6095444
C	14.3833998	8.7359541	6.4643968
C	15.7890932	8.6186635	6.5214990
C	16.4015913	8.2508759	7.7374883
C	15.6204821	7.9926798	8.8754615
C	14.2222126	8.1158959	8.8157842
H	12.5140292	8.5915237	7.5535562
H	13.8951398	9.0205122	5.5212835
H	17.4984150	8.1654931	7.7972425
H	16.1090264	7.7022050	9.8176942
H	13.6113309	7.9229458	9.7101779
C	16.6044571	8.8205045	5.2490720
C	16.9788100	7.5581511	4.5774341
O	16.8603753	7.4678582	3.2840562
O	17.3930239	6.5326274	5.2512819
C	17.6853260	5.2826479	4.5547058
H	17.9565469	4.5703470	5.3503366
H	16.7856311	4.9403153	4.0108495
H	18.5246479	5.4329004	3.8502445
C	15.7627343	13.0988520	5.2363646
C	15.4537768	13.6900888	4.0023779
C	15.3039857	12.8805072	2.8621048
C	15.4720217	11.4908640	2.9508662
C	15.7882120	10.9146505	4.1932878
C	15.9269219	11.7045780	5.3475280
H	15.8600675	13.7206835	6.1385699
H	15.0524738	13.3318252	1.8907598
H	15.3508934	10.8497661	2.0649881
H	16.1061819	11.2459401	6.3297057
O	15.9115697	9.5219195	4.2013798
H	15.3157665	14.7785142	3.9284199
H	16.4117683	8.3415772	3.0386331
Cs	24.6771208	11.8567820	6.4797141

INT-C (no RA):

Au	19.3175335	10.1982483	5.7677838
P	20.9852510	11.7816384	5.5939483
O	21.2735525	12.8246103	6.8193279
O	20.5695123	12.7391248	4.3222952
O	22.5096126	11.2848215	5.3879982
O	22.1604985	9.0075642	7.1713015
O	24.5158373	8.6024430	8.9808435
O	26.5003733	10.4463479	8.0482536
O	29.0011795	8.9394500	7.1980035
C	20.3864139	13.8833718	7.1006187
C	19.6494035	13.9135877	8.3105272
C	18.8544900	15.0645577	8.5122416
H	18.2742371	15.1206540	9.4445070
C	18.7664488	16.1440028	7.6123812
C	19.5439951	16.0660250	6.4452319
H	19.5206412	16.8763871	5.7051461
C	20.3665827	14.9525847	6.1717657
C	21.2169417	14.9869608	4.9443827
C	21.9299253	16.1718508	4.6487648
H	21.9199868	16.9712225	5.4012150
C	22.6418116	16.3297631	3.4514103
C	22.5664483	15.2768393	2.5127698
H	23.0737340	15.4091462	1.5493936
C	21.8765577	14.0680830	2.7335547
C	21.2622467	13.9322842	4.0062040
C	19.6763845	12.8714429	9.4628849
C	20.3051620	13.5528349	10.7085738
H	20.3204874	12.8458881	11.5638490
H	19.7399649	14.4512679	11.0257862
H	21.3492664	13.8650646	10.5051083

C	18.2241321	12.4356093	9.7907773
H	18.2282326	11.6971848	10.6191251
H	17.7413849	11.9628118	8.9102677
H	17.5821513	13.2794698	10.1103744
C	20.4846216	11.5881692	9.1840286
H	20.4256857	10.9339025	10.0777380
H	21.5510403	11.7877048	8.9755167
H	20.0751851	11.0053914	8.3324730
C	17.8563657	17.3489445	7.9344129
C	17.8991801	18.4198942	6.8254477
H	18.9174982	18.8375671	6.6894599
H	17.2320366	19.2637879	7.0928615
H	17.5539533	18.0233091	5.8489432
C	18.3221613	18.0005098	9.2615927
H	17.6800970	18.8705743	9.5103220
H	19.3687517	18.3592594	9.1858362
H	18.2682023	17.2945448	10.1146735
C	16.3930344	16.8602074	8.0840299
H	15.7234778	17.7122990	8.3226540
H	16.2836382	16.1145001	8.8974445
H	16.0300650	16.3945039	7.1447216
C	23.4651783	17.5938916	3.1266799
C	23.4167207	18.6265473	4.2709681
H	24.0272974	19.5121522	4.0029480
H	23.8249993	18.2185258	5.2177870
H	22.3854388	18.9857905	4.4648257
C	24.9439535	17.1896444	2.8962876
H	25.5555694	18.0840960	2.6570320
H	25.0542437	16.4768577	2.0542669
H	25.3741321	16.7138635	3.8010728
C	22.9040286	18.2589867	1.8439845
H	23.4872715	19.1695845	1.5951266
H	21.8447574	18.5588340	1.9786928
H	22.9555399	17.5836333	0.9664444
C	21.7319771	13.0226086	1.5966347
C	20.2262738	12.8476521	1.2628799
H	20.1014337	12.1150003	0.4381278
H	19.7830040	13.8077544	0.9292956
H	19.6485739	12.4870910	2.1353180
C	22.3454155	11.6579719	1.9929102
H	22.3108289	10.9643413	1.1272099
H	21.7922623	11.1856034	2.8230924
H	23.4057767	11.7687215	2.2974580
C	22.4436728	13.4821735	0.3042556
H	22.2907537	12.7203421	-0.4863739
H	23.5378397	13.5965506	0.4431341
H	22.0394380	14.4393053	-0.0802462
C	22.8820698	9.9102612	5.0946777
H	23.7234252	9.9777613	4.3784400
H	22.0338357	9.3850470	4.6036941
C	23.3056121	9.1722670	6.3446858
H	23.7151715	8.1803793	6.0303738
H	24.1280349	9.7073610	6.8676772
C	22.3014003	8.0753872	8.2418881
H	22.7177413	7.1122647	7.8602121
H	21.2740363	7.8831153	8.6113757
C	23.1660145	8.5689053	9.3947621
H	22.8195133	9.5841336	9.7086013
H	23.0220384	7.8876762	10.2734519
C	25.3834586	9.3243438	9.8400606
H	25.5640547	8.7651867	10.7918843
H	24.9332408	10.3112755	10.1088527
C	26.7067872	9.5527452	9.1369780
H	27.4292502	9.9893368	9.8694033
H	27.1348426	8.5859649	8.7920626
C	27.6817154	10.9439315	7.4426656
H	28.4192704	11.2646509	8.2186214
H	27.3779643	11.8458031	6.8702297
C	28.3718874	9.9820537	6.4807365
H	27.6194702	9.5748292	5.7570702
H	29.1213701	10.5593415	5.8786013
C	29.6759347	8.0191254	6.3666683
H	30.1400380	7.2539872	7.0180985
H	30.4802343	8.5109907	5.7674181
H	28.9833076	7.5080067	5.6537575
C	18.8478405	5.6045173	7.8804633
C	18.5015967	6.4363938	6.8022500

C	18.1175753	7.7791686	7.0207691
C	18.0973882	8.2553841	8.3559316
C	18.4423725	7.4228319	9.4292594
C	18.8204823	6.0888999	9.1973664
H	19.1331300	4.5597883	7.6831937
H	18.5273345	6.0240600	5.7862145
H	17.7884390	9.2930962	8.5536173
H	18.4087268	7.8187477	10.4555910
H	19.0869509	5.4308186	10.0379921
C	17.6476140	8.7286541	5.9315159
C	17.7523575	8.3789996	4.5315165
O	16.9438772	8.8952311	3.6212818
O	18.6331130	7.5136344	4.0760827
C	18.7594327	7.3100423	2.6448157
H	19.5395198	6.5387402	2.5325403
H	17.8008957	6.9602887	2.2184246
H	19.0696362	8.2521714	2.1535616
C	15.2363598	8.6678794	6.7408571
C	16.3163582	9.4256224	6.2154922
C	16.0685554	10.7841866	5.9043037
C	14.8019588	11.3628127	6.0965226
C	13.7446133	10.5928388	6.6226502
C	13.9781117	9.2346384	6.9453748
H	15.3951284	7.6096949	6.9985062
H	16.8909503	11.4175892	5.5298461
H	14.6456878	12.4266686	5.8551059
H	13.1485750	8.6407156	7.3557281
O	12.5031252	11.0820435	6.8452485
H	12.4668064	12.0237995	6.5893915
H	16.2818009	9.4603430	4.1086417

INT-C (Li^+):

Au	19.0352215	10.0771716	5.7164458
P	21.0420381	11.2077778	5.5834410
O	21.5937561	12.1750925	6.7854433
O	20.9366504	12.1746288	4.2741790
O	22.4158632	10.3092616	5.4764195
O	24.1808784	8.5603318	6.8329708
O	25.3645892	9.1433329	9.1242750
O	24.8357714	11.7065494	9.2334098
O	25.3741941	11.9439009	6.6401552
Li	24.7063423	10.3871853	7.6702693
C	20.8340931	13.3353682	7.0916479
C	20.1083762	13.4283743	8.3032405
C	19.4148283	14.6444187	8.4982995
H	18.8337162	14.7528524	9.4255335
C	19.4249296	15.7254408	7.5943582
C	20.2018112	15.5810858	6.4319345
H	20.2505919	16.3917995	5.6935967
C	20.9222795	14.3980309	6.1600309
C	21.7853451	14.3504357	4.9396411
C	22.5940506	15.4755836	4.6479986
H	22.6244684	16.2854819	5.3887042
C	23.3336087	15.5763187	3.4602792
C	23.2097531	14.5173324	2.5327930
H	23.7426818	14.6042693	1.5783503
C	22.4265352	13.3647706	2.7454398
C	21.7667127	13.2926803	4.0011326
C	20.0329438	12.3818143	9.4509277
C	20.5984235	13.0364896	10.7408305
H	20.5342736	12.3245623	11.5892278
H	20.0418830	13.9477669	11.0325980
H	21.6624586	13.3198989	10.6094627
C	18.5512668	11.9869978	9.6801560
H	18.4722122	11.2637514	10.5177536
H	18.1179274	11.5123979	8.7753329
H	17.9162832	12.8568301	9.9374465
C	20.8302654	11.0774104	9.2263332
H	20.7137578	10.4390360	10.1257141
H	21.9113284	11.2654856	9.0795454
H	20.4508671	10.4916207	8.3637564
C	18.6143401	17.0017507	7.9046113
C	18.7637791	18.0662764	6.7989425
H	19.8146797	18.3999468	6.6807376
H	18.1652730	18.9620324	7.0582851
H	18.4008461	17.7029055	5.8160472

C	19.1105059	17.6091892	9.2418874
H	18.5388252	18.5291110	9.4802699
H	20.1836826	17.8824823	9.1852371
H	18.9812905	16.9114480	10.0936285
C	17.1135634	16.6326855	8.0287448
H	16.5143195	17.5375333	8.2575241
H	16.9296635	15.9001156	8.8406808
H	16.7286367	16.2014609	7.0817737
C	24.2193946	16.7946225	3.1250506
C	24.2348665	17.8315875	4.2663036
H	24.8897379	18.6818517	3.9909899
H	24.6288499	17.4072798	5.2126665
H	23.2269945	18.2491138	4.4658573
C	25.6731786	16.3193148	2.8739659
H	26.3218005	17.1825020	2.6209417
H	25.7403540	15.6000714	2.0328973
H	26.0985582	15.8317256	3.7756195
C	23.6725894	17.4810982	1.8463161
H	24.2935245	18.3634339	1.5895192
H	22.6300347	17.8294508	1.9920383
H	23.6845034	16.8029115	0.9696636
C	22.2362431	12.3217342	1.6117533
C	20.7341916	12.2632118	1.2242375
H	20.5875497	11.5463159	0.3901146
H	20.3784101	13.2548547	0.8796136
H	20.0957770	11.9456494	2.0703310
C	22.7298208	10.9202904	2.0456756
H	22.6111584	10.2028152	1.2079934
H	22.1620987	10.5316999	2.9089072
H	23.8048914	10.9434766	2.3181208
C	23.0258726	12.7064179	0.3404330
H	22.8490763	11.9429973	-0.4431434
H	24.1199774	12.7471229	0.5158753
H	22.7027645	13.6805293	-0.0760492
C	22.3859416	8.8796313	5.2485984
H	22.0848695	8.6631908	4.2017958
H	21.6590176	8.4007196	5.9385465
C	23.7780391	8.3248810	5.4787201
H	23.7440378	7.2326245	5.2711560
H	24.5065345	8.7805450	4.7704496
C	25.0329164	7.5517831	7.4109657
H	26.0651432	7.6372575	7.0009070
H	24.6493469	6.5343266	7.1778619
C	25.0201682	7.7731160	8.9125718
H	24.0042204	7.5678563	9.3230460
H	25.7442494	7.0899699	9.4107786
C	25.0801622	9.6642651	10.4284913
H	25.6696996	9.1390543	11.2125057
H	23.9972770	9.5303007	10.6593229
C	25.4590241	11.1341038	10.3923055
H	25.1294999	11.6432267	11.3249623
H	26.5643576	11.2422761	10.3083102
C	25.4071429	12.9502562	8.8016832
H	26.5150016	12.8991036	8.9046621
H	25.0385449	13.8000182	9.4186229
C	25.0301532	13.1496034	7.3450617
H	23.9444178	13.3592365	7.2199900
H	25.5991515	14.0138823	6.9380043
C	25.5310674	12.1306390	5.2290505
H	25.7921817	11.1484486	4.7933294
H	26.3577590	12.8429734	5.0200804
H	24.5961346	12.5081515	4.7617287
C	17.8566692	5.1950197	6.5390867
C	17.4915285	6.3612690	5.8446050
C	17.6001509	7.6298322	6.4569232
C	18.0787326	7.6862798	7.7908733
C	18.4409046	6.5213944	8.4819002
C	18.3340660	5.2667943	7.8569229
H	17.7508571	4.2180904	6.0434634
H	17.1097398	6.2667293	4.8202328
H	18.1364247	8.6605126	8.3013472
H	18.7961444	6.5932459	9.5211033
H	18.6083182	4.3492881	8.3986589
C	17.1494832	8.9350461	5.8087105
C	16.8739604	8.9675397	4.3764089
O	15.9957544	9.7959200	3.8573187
O	17.4805032	8.1734877	3.5288955

C	17.2125933	8.3029575	2.1027369
H	17.8066546	7.5053928	1.6272226
H	16.1346640	8.1610760	1.9023689
H	17.5363971	9.2998238	1.7486549
C	15.0552137	8.9843432	7.2686790
C	16.0676676	9.6982437	6.5759665
C	15.9626374	11.1115925	6.5419309
C	14.8904388	11.7849367	7.1528276
C	13.8934237	11.0552331	7.8348303
C	13.9944730	9.6436902	7.8900414
H	15.1036074	7.8864327	7.3184463
H	16.7515749	11.7103363	6.0535833
H	14.8431318	12.8847963	7.1144840
H	13.2141779	9.0823799	8.4242445
O	12.8382984	11.6249282	8.4528835
H	12.8598425	12.5950910	8.3413982
H	15.5586911	10.2792986	4.6185654

INT-C (Cs^+):

Au	18.3557300	9.9585897	5.7982775
P	20.3917906	11.0365873	5.8559332
O	20.8522522	12.0133138	7.0986371
O	20.5419149	11.9618514	4.5202065
O	21.7164065	10.0739269	5.8590495
O	24.1122114	8.5489032	6.4511470
O	26.8196957	9.6093021	6.7077315
O	27.3332739	12.2090631	7.8675600
O	25.3626501	14.2665466	8.2768236
C	20.2749068	13.3021495	7.2333778
C	19.4080350	13.6135283	8.3073676
C	18.9511545	14.9517766	8.3417312
H	18.2689821	15.2309623	9.1571732
C	19.3129826	15.9488935	7.4140479
C	20.2112832	15.5806909	6.3964123
H	20.5311366	16.3152405	5.6458619
C	20.7095668	14.2652176	6.2900079
C	21.7177404	13.9647376	5.2255110
C	22.7924114	14.8689612	5.0382181
H	22.8883593	15.6989136	5.7499150
C	23.7078700	14.7327281	3.9818897
C	23.4825266	13.6783287	3.0669246
H	24.1479230	13.5977968	2.1991187
C	22.4357531	12.7381372	3.1791336
C	21.6059373	12.8775114	4.3253810
C	18.9471127	12.6797868	9.4620368
C	19.4266132	13.2950647	10.8052944
H	19.0955076	12.6619337	11.6534411
H	19.0220521	14.3118946	10.9746122
H	20.5329453	13.3616417	10.8424007
C	17.3984729	12.5981888	9.4559573
H	17.0478135	11.9634033	10.2951543
H	17.0233019	12.1521555	8.5119129
H	16.9218065	13.5909707	9.5717523
C	19.4869119	11.2339433	9.4112032
H	19.1131076	10.6860503	10.2997820
H	20.5924328	11.1905448	9.4319804
H	19.1298684	10.6821886	8.5163160
C	18.7379616	17.3754546	7.5443700
C	19.2617196	18.3136671	6.4380296
H	20.3643204	18.4288287	6.4752375
H	18.8253952	19.3238853	6.5667397
H	18.9810182	17.9623203	5.4245053
C	19.1426323	17.9647713	8.9200732
H	18.7374816	18.9910546	9.0310861
H	20.2452739	18.0227944	9.0238946
H	18.7529391	17.3636175	9.7660543
C	17.1923984	17.3115076	7.4420673
H	16.7598720	18.3282234	7.5378699
H	16.7468381	16.6862945	8.2419431
H	16.8714808	16.8973109	6.4645245
C	24.8750329	15.7185983	3.7559646
C	25.0466968	16.6873458	4.9446504
H	25.9169308	17.3490559	4.7657099
H	25.2266594	16.1432991	5.8953215
H	24.1654695	17.3463016	5.0803247
C	26.1994673	14.9360419	3.5723352

H	27.0382747	15.6394234	3.3972767
H	26.1689482	14.2449460	2.7065138
H	26.4465536	14.3425313	4.4786251
C	24.5860847	16.5435469	2.4741172
H	25.4075860	17.2647002	2.2875063
H	23.6431076	17.1180818	2.5721511
H	24.4975370	15.8980356	1.5771884
C	22.1658621	11.7188220	2.0389145
C	20.7474549	11.9793490	1.4640948
H	20.5512444	11.2847089	0.6218615
H	20.6637455	13.0128296	1.0718785
H	19.9556341	11.8338060	2.2226137
C	22.2769424	10.2564052	2.5338814
H	22.1252919	9.5620011	1.6822957
H	21.5262948	10.0134709	3.3054269
H	23.2843464	10.0521295	2.9529186
C	23.1738753	11.8836851	0.8790028
H	22.9333085	11.1520376	0.0826729
H	24.2195435	11.6883158	1.1934257
H	23.1286811	12.8907087	0.4191555
C	21.7145260	8.7298036	6.4197270
H	20.7891755	8.1946405	6.1154341
H	21.7384079	8.7998714	7.5270727
C	22.9272074	7.9799281	5.9133677
H	22.8221289	6.9141884	6.2324245
H	22.9422476	7.9928709	4.7975959
C	25.2908951	7.8501193	6.0390175
H	25.5056627	8.0523024	4.9624951
H	25.1419152	6.7503416	6.1487605
C	26.4758150	8.2398158	6.8980104
H	26.2472025	8.0413246	7.9728072
H	27.3310508	7.5810887	6.6138959
C	28.0217582	9.9533842	7.4008669
H	28.8788142	9.3569406	7.0071246
H	27.9195200	9.7214713	8.4872251
C	28.3362038	11.4245163	7.2271088
H	29.3361019	11.6206953	7.6816647
H	28.4122628	11.6817837	6.1419132
C	27.6617555	13.5937712	7.9522123
H	27.6736022	14.0613326	6.9367971
H	28.6806425	13.7254643	8.3871992
C	26.6699966	14.3079097	8.8476387
H	26.6659284	13.8350635	9.8587038
H	27.0067332	15.3645679	8.9717858
C	24.4172988	15.0018997	9.0479431
H	23.4332011	14.9147477	8.5485912
H	24.6916525	16.0795688	9.1096351
H	24.3346069	14.6024203	10.0850046
C	17.2407938	5.0953766	6.7190582
C	16.9025599	6.2153279	5.9400373
C	16.9233394	7.5138499	6.4961103
C	17.2827808	7.6477010	7.8617326
C	17.6190369	6.5287380	8.6366787
C	17.6032184	5.2441063	8.0666890
H	17.2061773	4.0935399	6.2647208
H	16.6127107	6.0600094	4.8928857
H	17.2691293	8.6454706	8.3284862
H	17.8850994	6.6605691	9.6964912
H	17.8604882	4.3630475	8.6732347
C	16.4972676	8.7721506	5.7450598
C	16.3658350	8.7269010	4.2926813
O	15.5131866	9.4911018	3.6480936
O	17.0847986	7.9205502	3.5512812
C	16.9520150	7.9646307	2.1015534
H	17.6251070	7.1749900	1.7293770
H	15.9062299	7.7585412	1.8078252
H	17.2633465	8.9572805	1.7249100
C	14.2849154	8.8181405	7.0183280
C	15.3239048	9.5310824	6.3658002
C	15.1674769	10.9336407	6.2292635
C	14.0216749	11.5961323	6.7032472
C	12.9991787	10.8670195	7.3473613
C	13.1501407	9.4677072	7.5042268
H	14.3717060	7.7289351	7.1449461
H	15.9716768	11.5345345	5.7695960
H	13.9348628	12.6883872	6.5886699
H	12.3495696	8.9070380	8.0083133

O	11.8733956	11.4261974	7.8365207
H	11.8670127	12.3880054	7.6659464
H	14.9826808	9.9898685	4.3373426
Cs	24.5515790	11.7694545	6.5565749