Supplementary Materials for

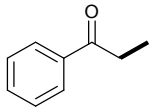
Iridium(I) hydroxides in catalysis: rearrangement of allylic alcohols to ketones

David J. Nelson,[a,b] José A. Fernández-Salas,[a] Byron J. Truscott[a] and Steven P. Nolan[a]*

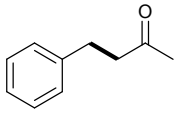
Correspondence to: snolan@st-andrews.ac.uk

This file includes:

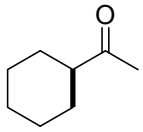
Experimental Details and Characterisation Data



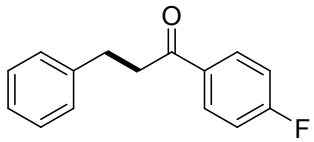
Propiophenone. The general procedure was followed for alcohol isomerisation using microwave irradiation to convert 1-phenyl-2-propen-1-ol (134 mg, 1 mmol) to propiophenone (121 mg, 90%). The ^{1}H NMR spectrum matched the reported data.[1]



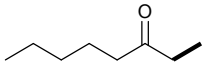
4-Phenylbutan-2-one. The general procedure was followed for alcohol isomerisation using microwave irradiation to convert 1-methyl-3-phenyl-2-propen-1-ol (148.2 mg, 1 mmol) to 4-phenylbutan-2-one (129 mg, 87%). The ^{1}H NMR spectrum matched the reported data.[1]



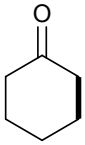
1-Cyclohexylethan-1-one .The general procedure was followed for alcohol isomerisation using microwave irradiation to convert 1-(cyclohex-1-en-1-yl)ethan-1-ol (126 mg, 1 mmol) to 1-cyclohexylethan-1-one (102 mg, 81%) in 2 h. The ^{1}H NMR spectrum matched the reported data.[2]



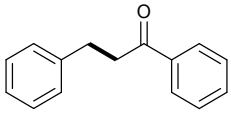
1-(4-Fluorophenyl)-3-phenylpropan-1-one. The general procedure was followed for alcohol isomerisation using microwave irradiation to convert (*E*)-1-(4-fluorophenyl)-3-phenylprop-2-en-1-ol (228 mg, 1 mmol) to 1-(4-fluorophenyl)-3-phenylpropan-1-one (192 mg, 86%). The ^{1}H NMR spectrum matched the reported data.[1]



Octan-3-one. The general procedure was followed for alcohol isomerisation using microwave irradiation to convert oct-1-en-3-ol (128 mg, 1 mmol) to octan-3-one (105 mg, 82%). The ^{1}H NMR spectrum matched the reported data.[1]



Cyclohexanone. The general procedure was followed for alcohol isomerisation using microwave irradiation to convert cyclohex-2-en-1-ol (98 mg, 1 mmol) to cyclohexanone (80 mg, 82%) in 1.5 h using 0.25 mol% of [Ir(COD)(I^{i}Pr)(OH)]. The ^{1}H NMR spectrum matched the reported data.[1]



1,3-Diphenylpropan-1-one. The general procedure was followed for alcohol isomerisation using microwave irradiation to convert (*E*)-1,3-diphenylprop-2-en-1-ol (210 mg, 1 mmol) to 1,3-diphenylpropan-1-one (191 mg, 91%). The ^{1}H NMR spectrum matched the reported data.[1]

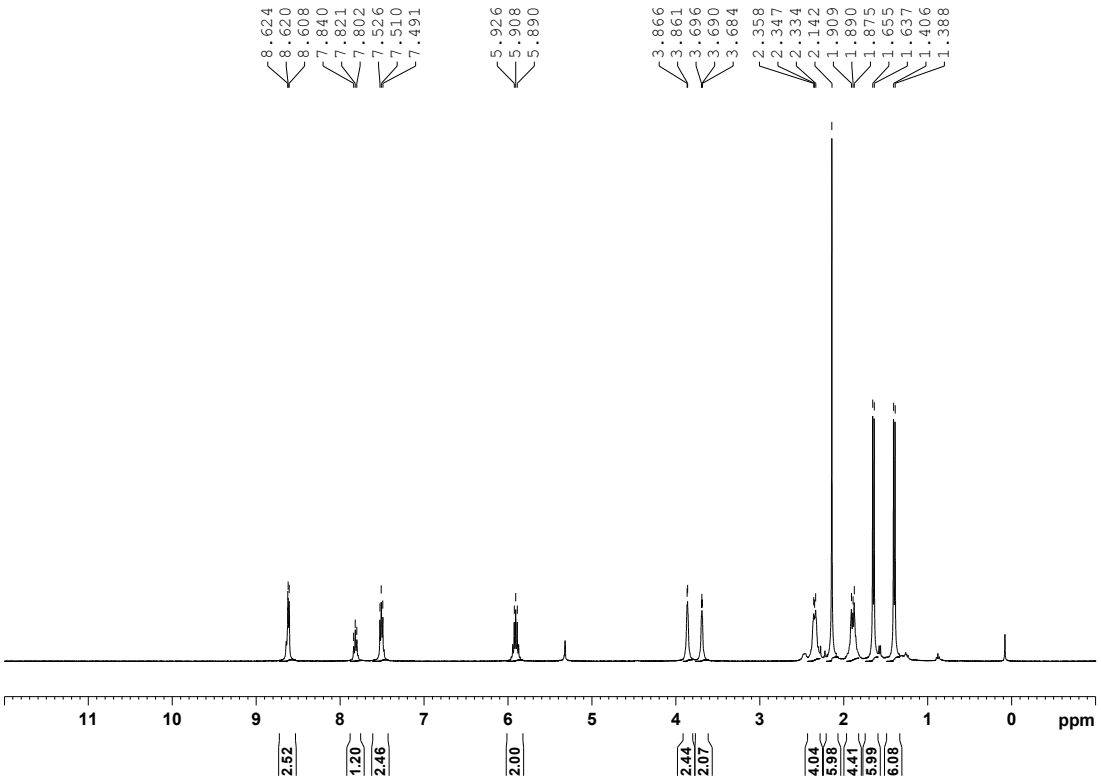


Figure S 1 ^{1}H NMR (400 MHz, CD_2Cl_2) spectrum for [Ir(COD)(I^{i}PrMe)(py)][PF_6]

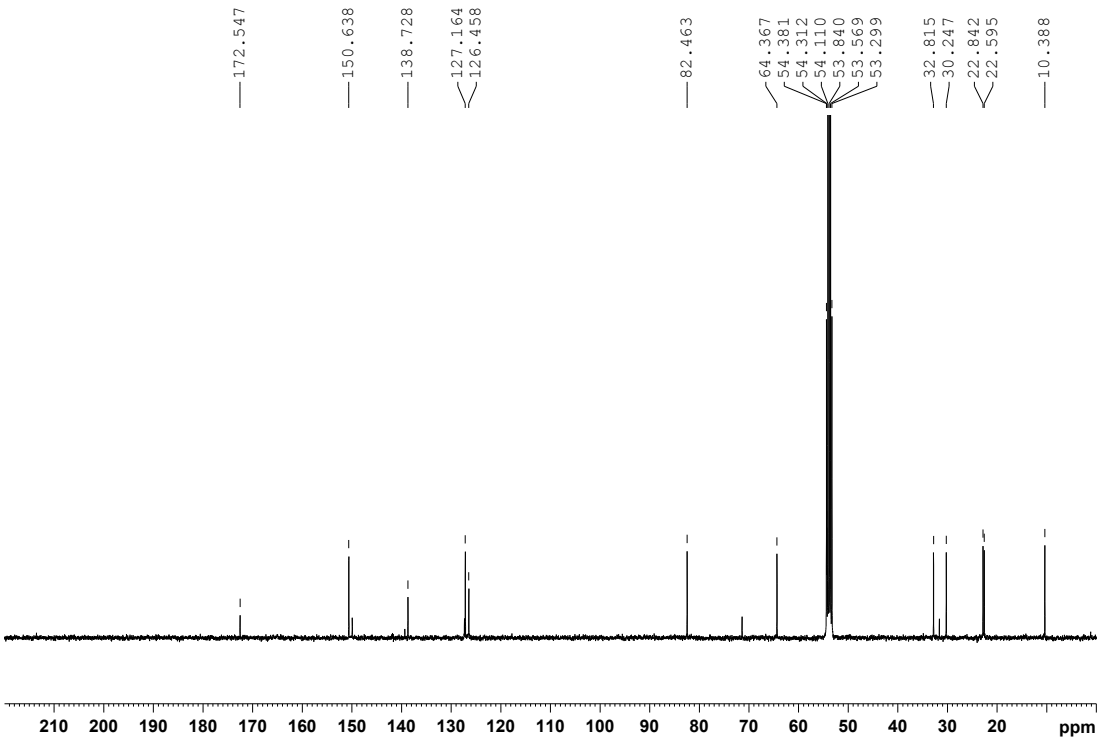


Figure S 2 $^{13}C\{^{1}H\}$ NMR (100 MHz, CD_2Cl_2) spectrum for [Ir(COD)(I^{i}PrMe)(py)][PF_6]

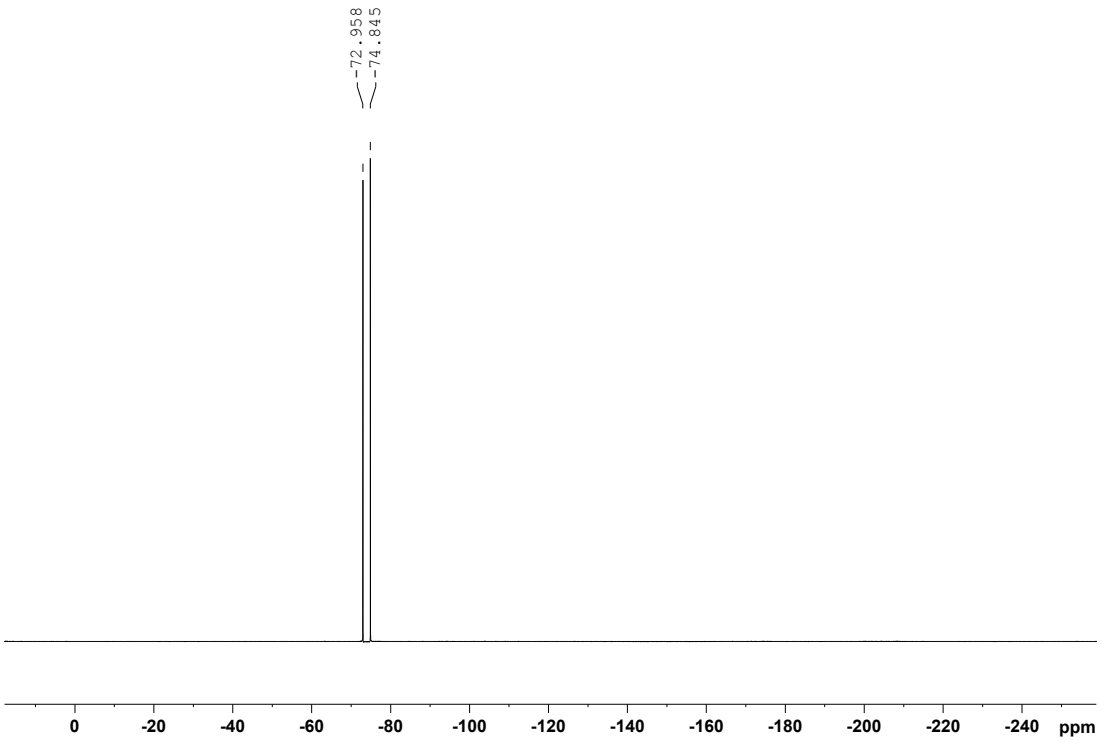


Figure S 3 $^{19}F\{^{1}H\}$ NMR (376 MHz, CD_2Cl_2) spectrum for **Ir(COD)(I*i*PrMe)(py)][PF$_6$]**

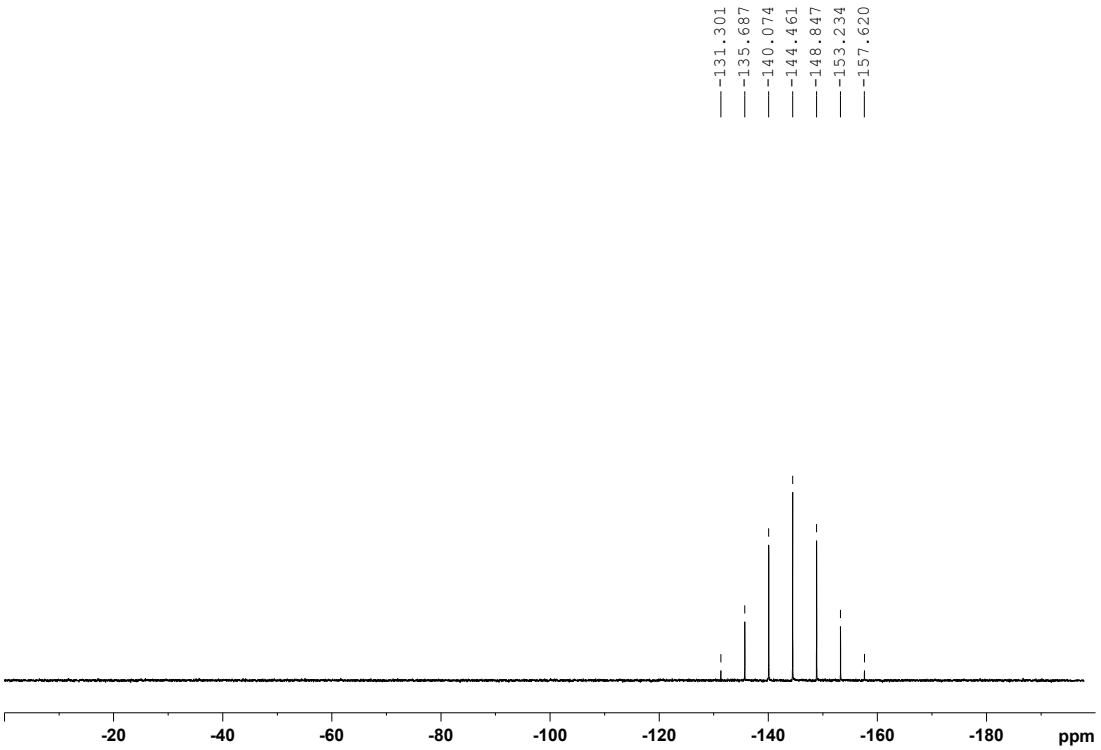


Figure S 4 $^{31}P\{^{1}H\}$ NMR (162 MHz, CD_2Cl_2) spectrum for Ir(COD)(I*i*PrMe)(py)][PF_6]

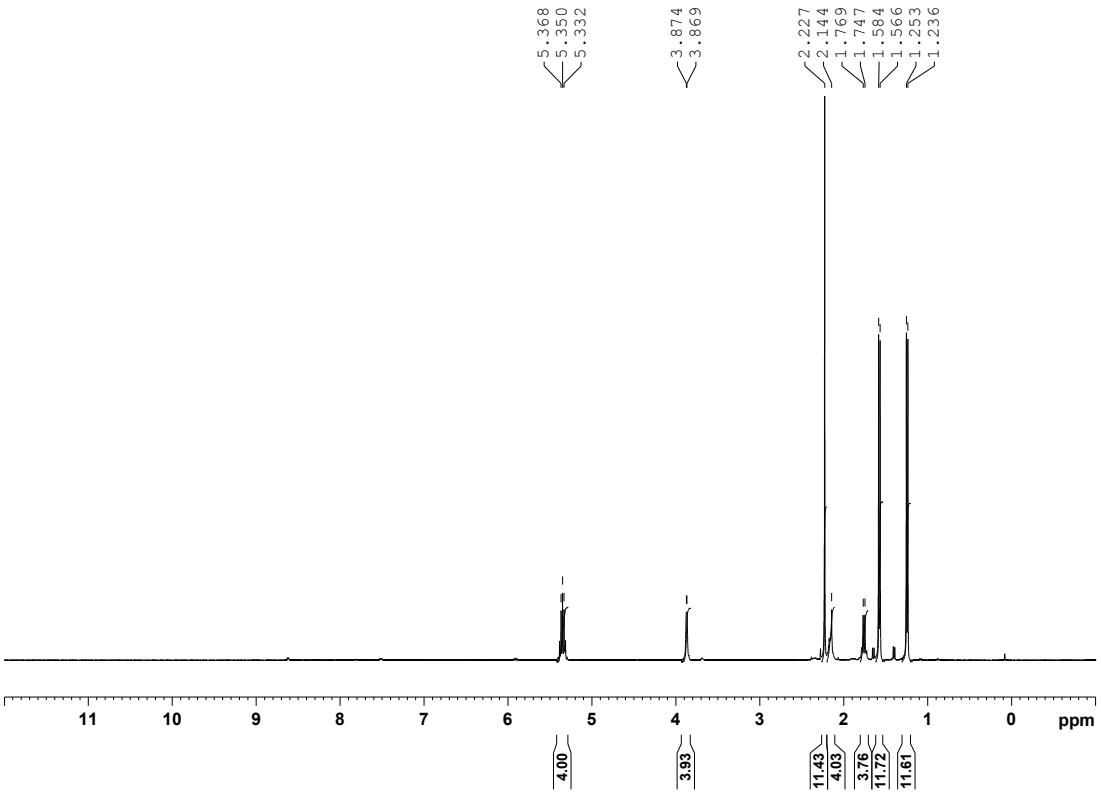


Figure S 5 ^{1}H NMR (300 MHz, CD_2Cl_2) spectrum for [(I^{i}PrMe)$_2$Ir(COD)][PF_6]

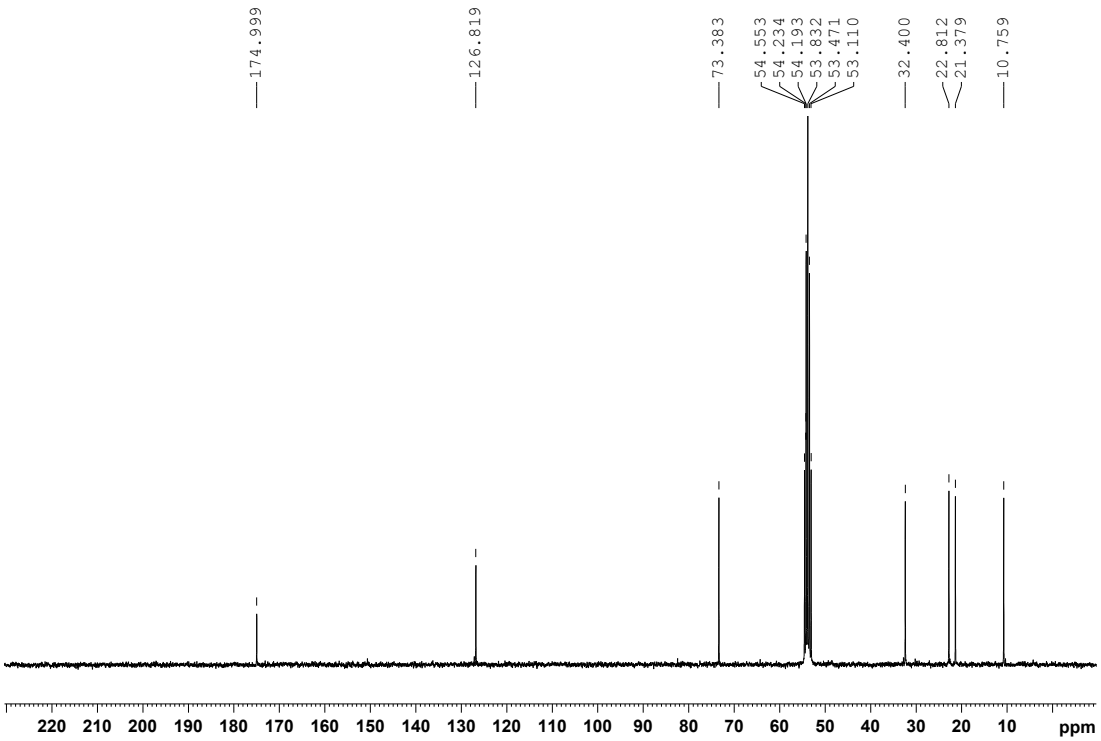


Figure S 6 ^{13}C{^{1}H} NMR (75 MHz, CD_2Cl_2) spectrum for [Ir(COD)(I^{i}PrMe)$_2$][PF_6]

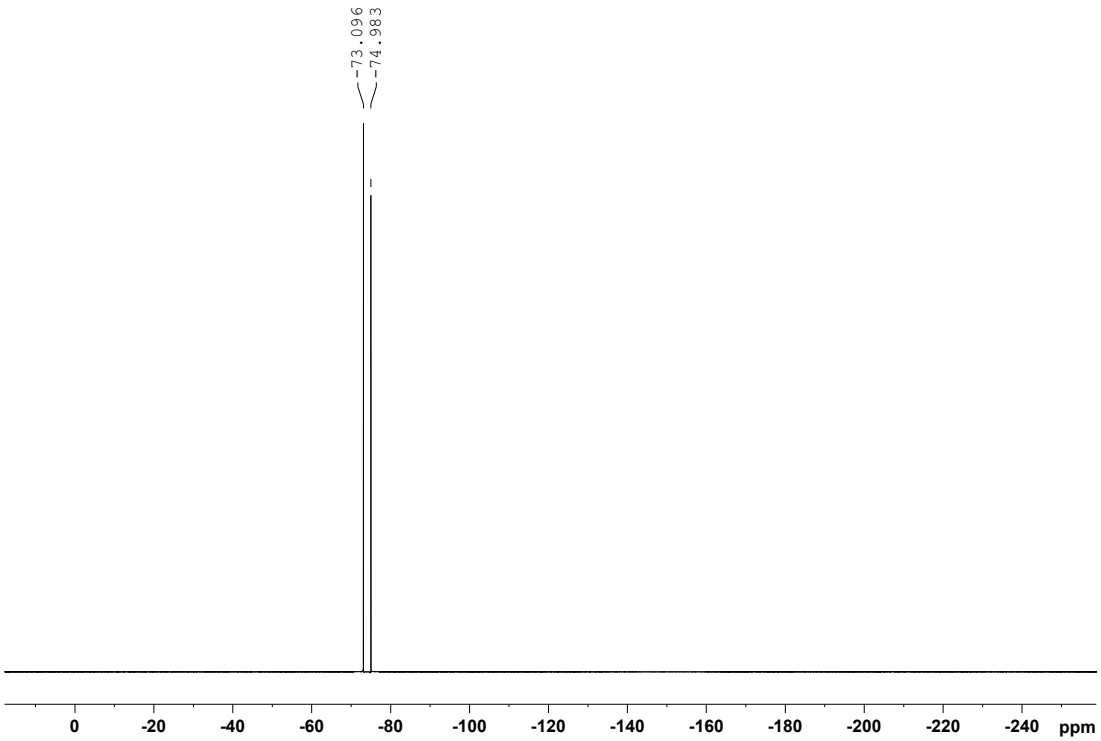


Figure S 7 $^{19}F\{^{1}H\}$ NMR (376 MHz, CD_2Cl_2) spectrum for $[Ir(COD)(I^{i}PrMe)_2][PF_6]$

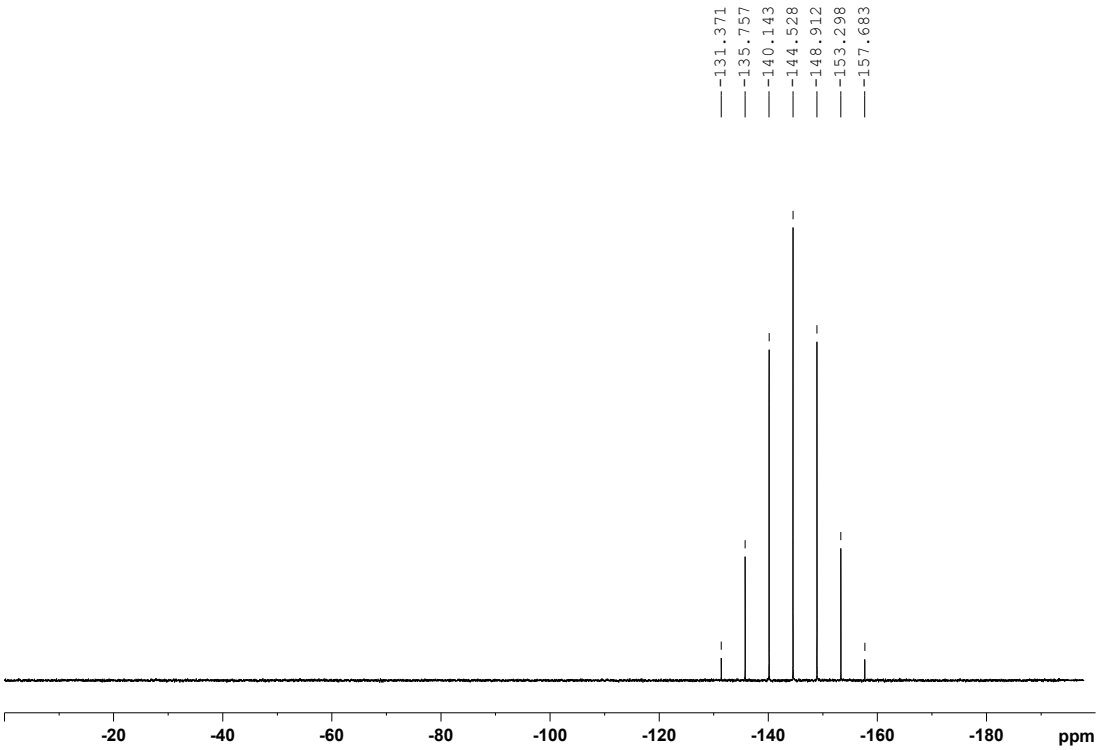


Figure S 8 $^{31}P\{^{1}H\}$ NMR (162 MHz, CD_2Cl_2) spectrum for $[Ir(COD)(I^{i}PrMe)_2][PF_6]$

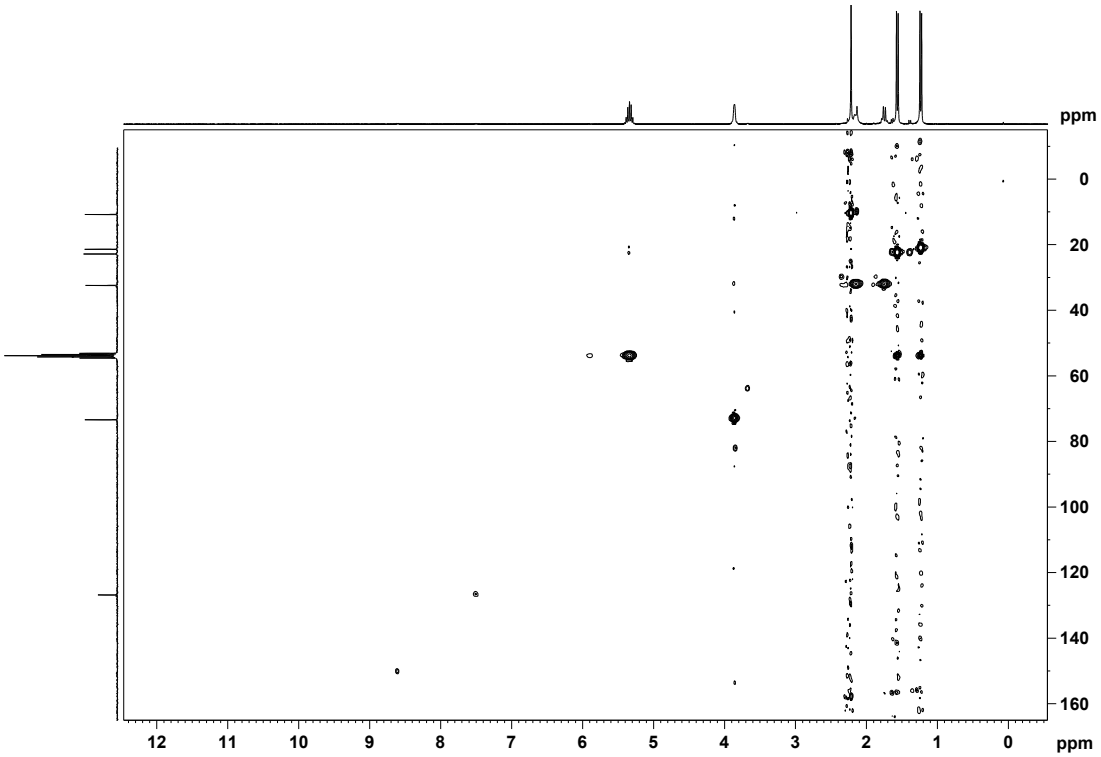


Figure S 9 HSQC NMR (300 MHz, CD_2Cl_2) spectrum for $[Ir(COD)(I^iPrMe)_2][PF_6]$

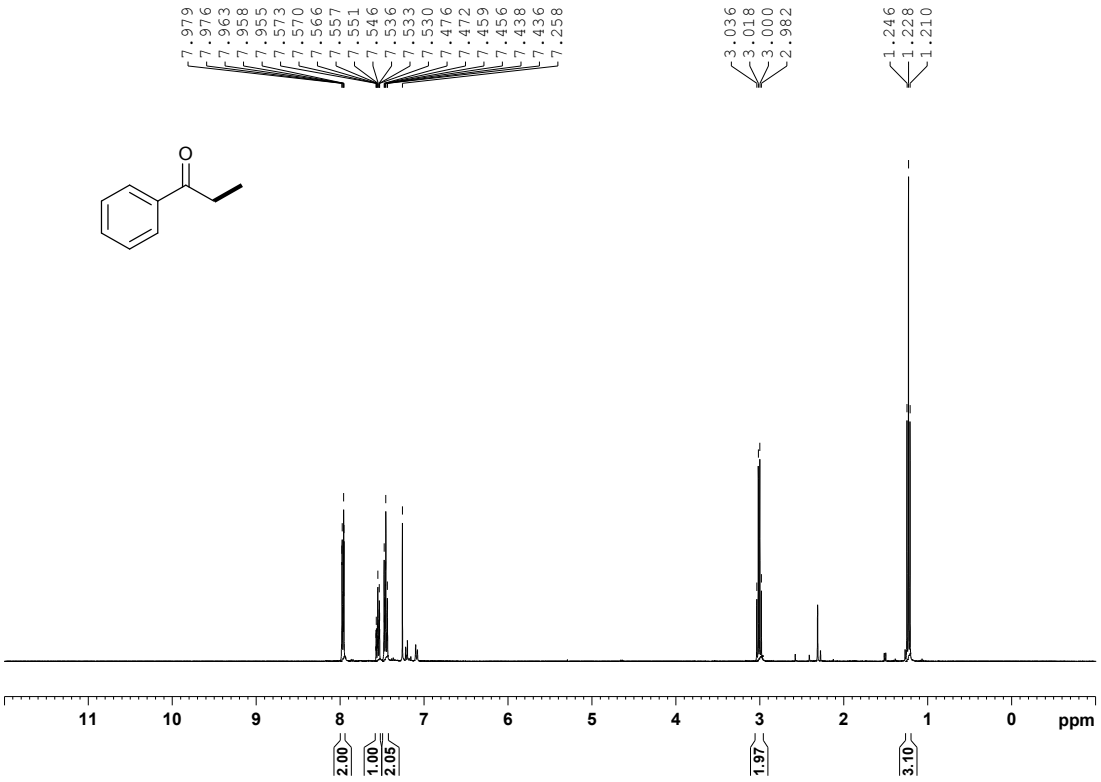


Figure S 10 ^1H NMR (500 MHz, $CDCl_3$) spectrum for propiophenone

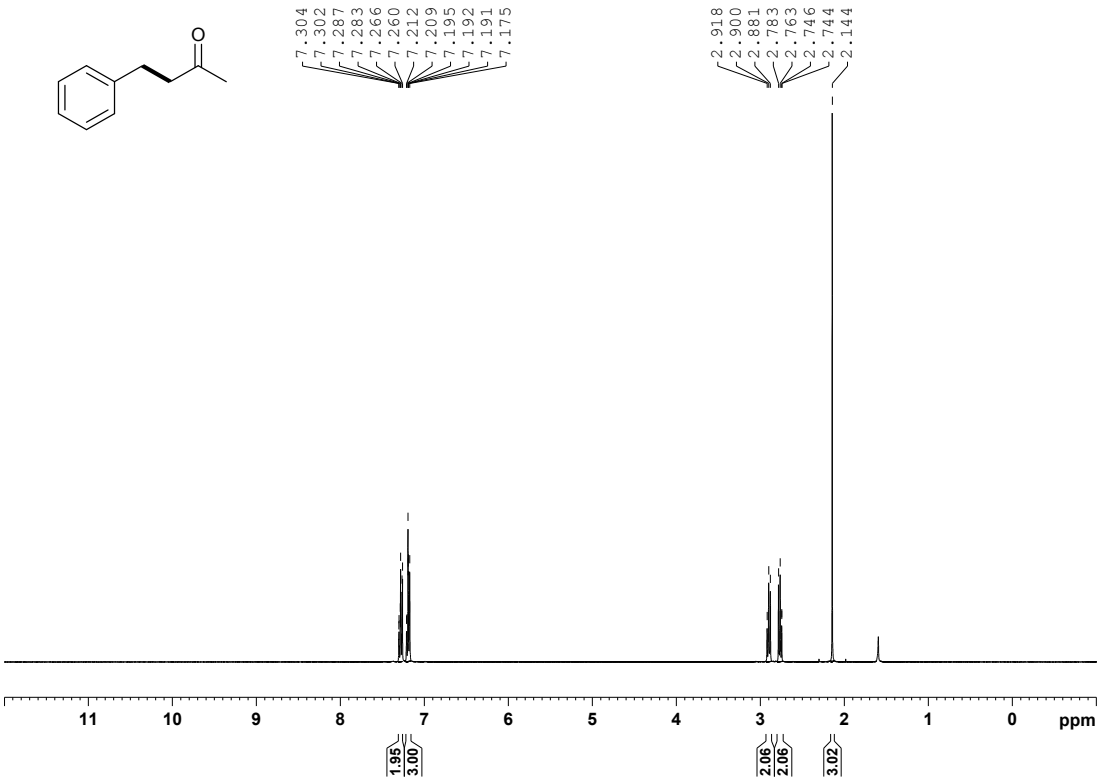


Figure S 11 ^{1}H NMR (400 MHz, $CDCl_3$) spectrum for 4-phenylbutan-2-one

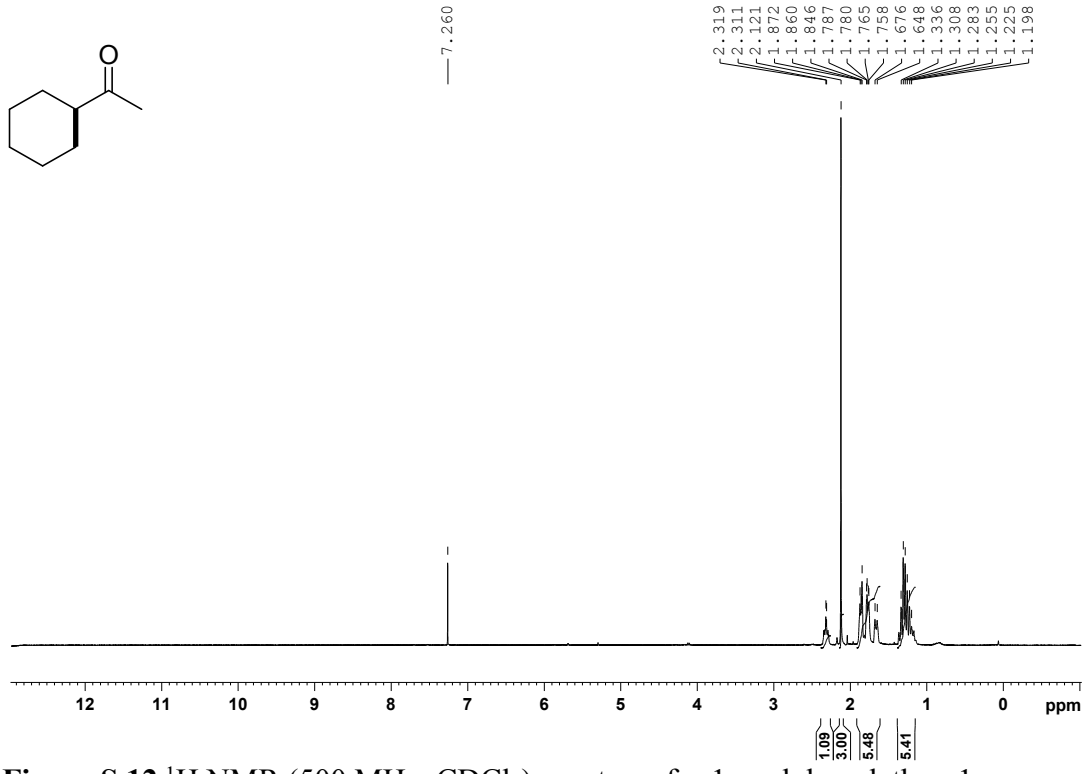


Figure S 12 ^{1}H NMR (500 MHz, $CDCl_3$) spectrum for 1-cyclohexylethan-1-one

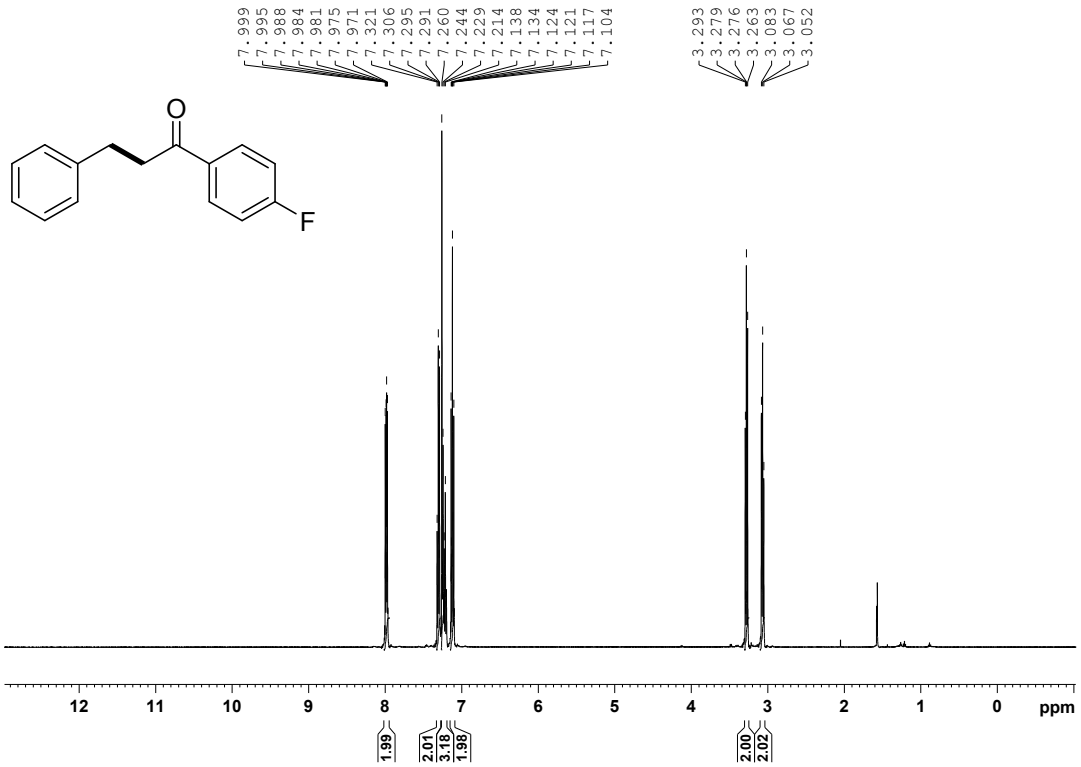


Figure S 13 ^{1}H NMR (500 MHz, $CDCl_3$) spectrum for 1-(4-fluorophenyl)-3-phenylpropan-1-one

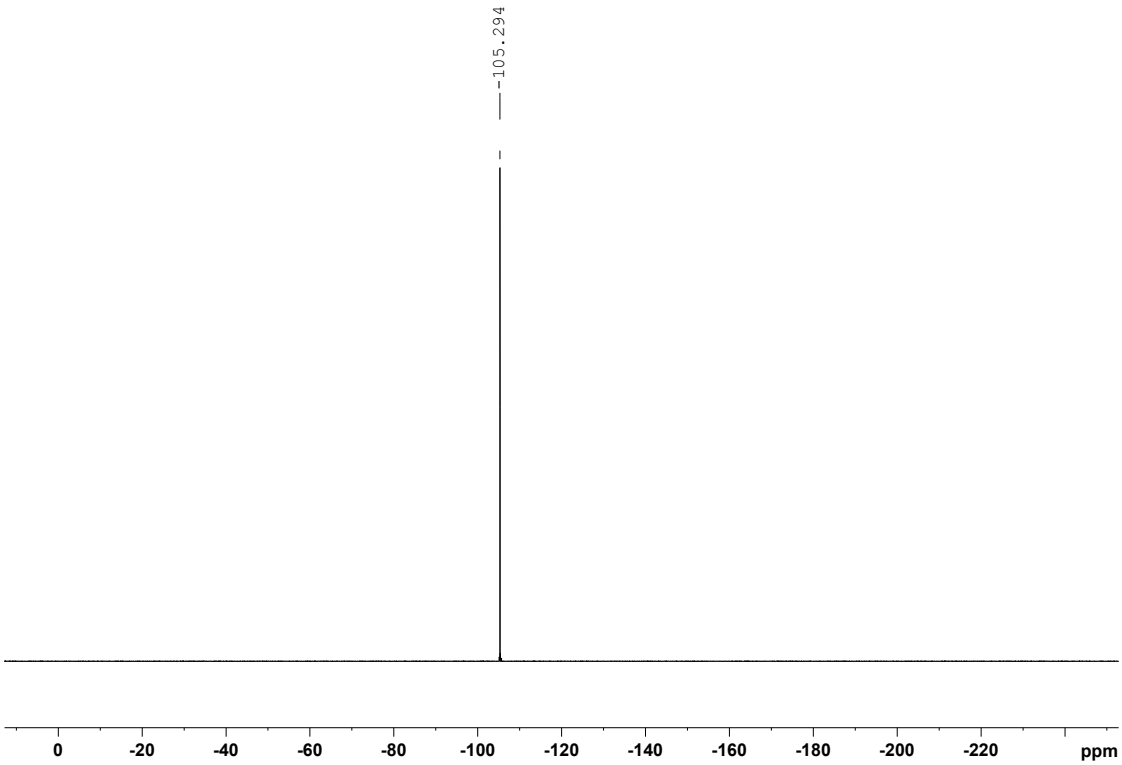


Figure S 14 $^{19}F\{^{1}H\}$ NMR (470 MHz, $CDCl_3$) spectrum for 1-(4-fluorophenyl)-3-phenylpropan-1-one

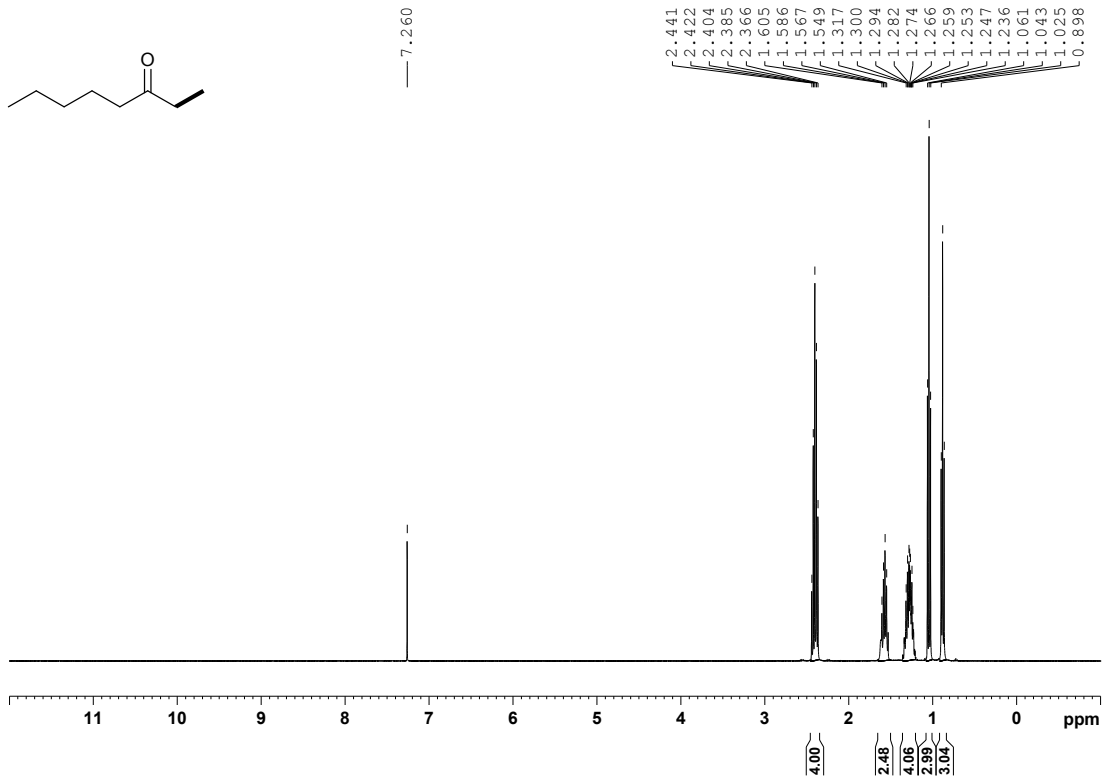


Figure S 15 ^{1}H NMR (400 MHz, $CDCl_3$) spectrum for octan-3-one

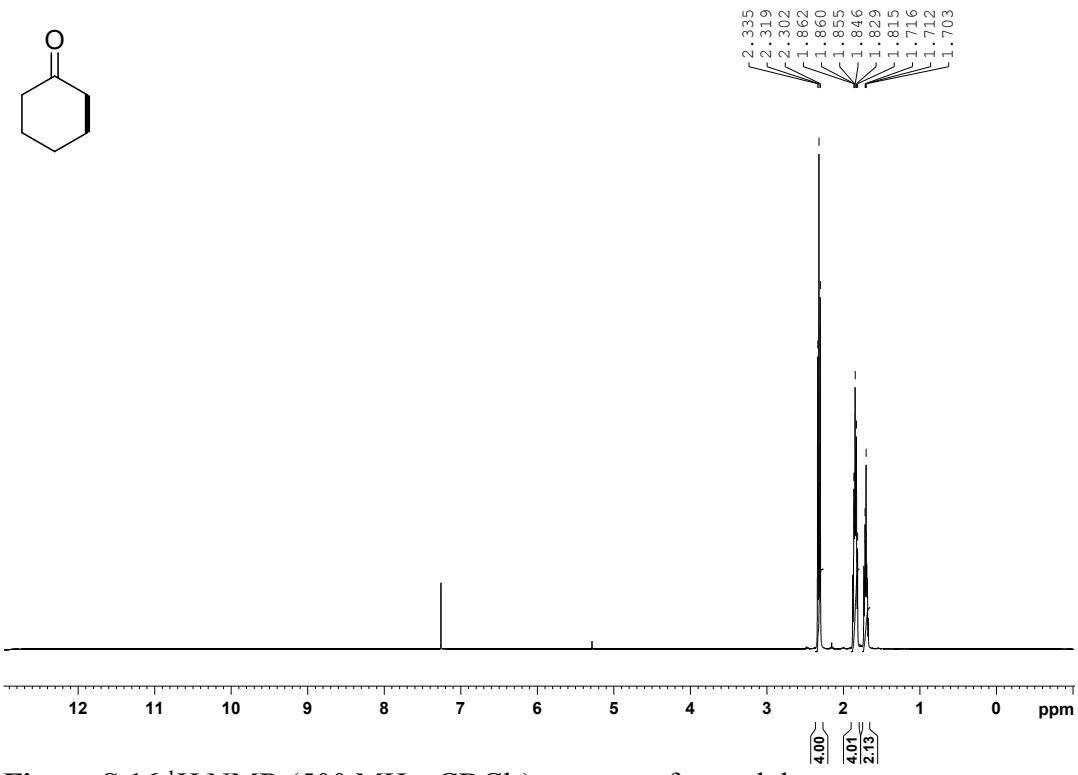


Figure S 16 ^{1}H NMR (500 MHz, $CDCl_3$) spectrum for cyclohexanone

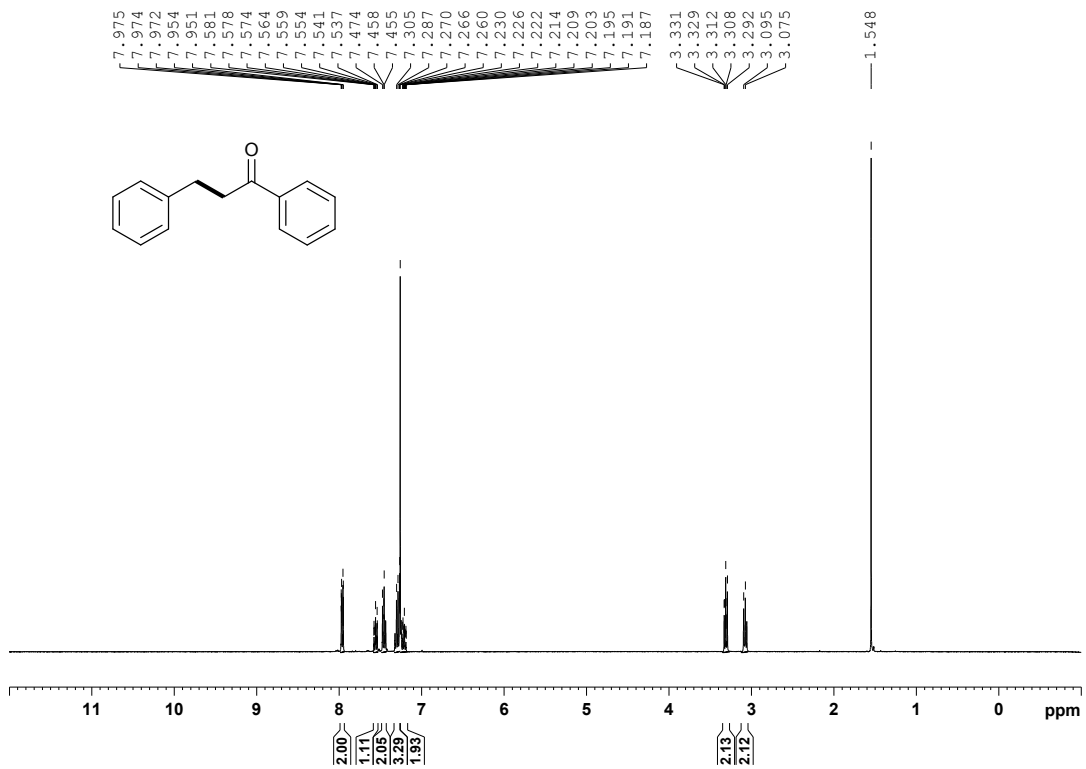


Figure S 17 ^{1}H NMR (500 MHz, $CDCl_3$) spectrum for 1,3-diphenylpropan-1-one

1. S. Manzini, A. Poater, D. J. Nelson, L. Cavallo and S. P. Nolan, *Chem. Sci.*, 2014, **5**, 180-188.
2. Y.-F. Wang, Y.-R. Gao, S. Mao, Y.-L. Zhang, D.-D. Guo, Z.-L. Yan, S.-H. Guo and Y.-Q. Wang, *Org. Lett.*, 2014, **16**, 1610-1613.