Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting information for:

Iridium complexes of an *ortho*-trifluoromethylphenyl substituted PONOP pincer ligand

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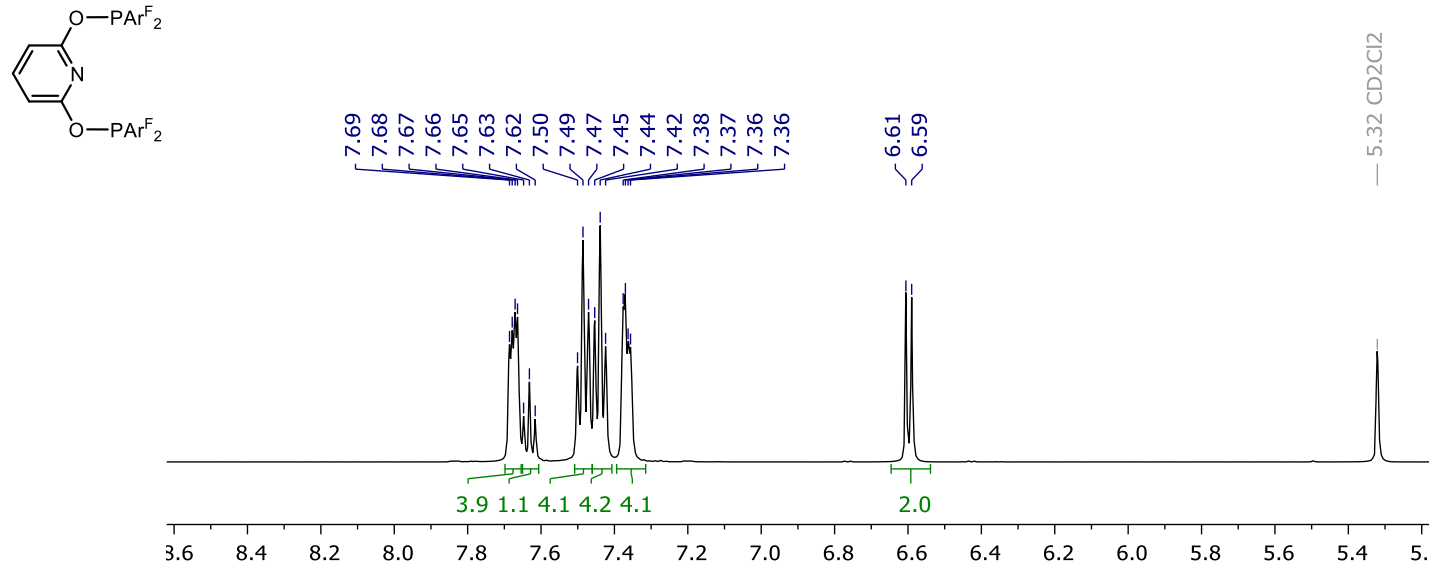
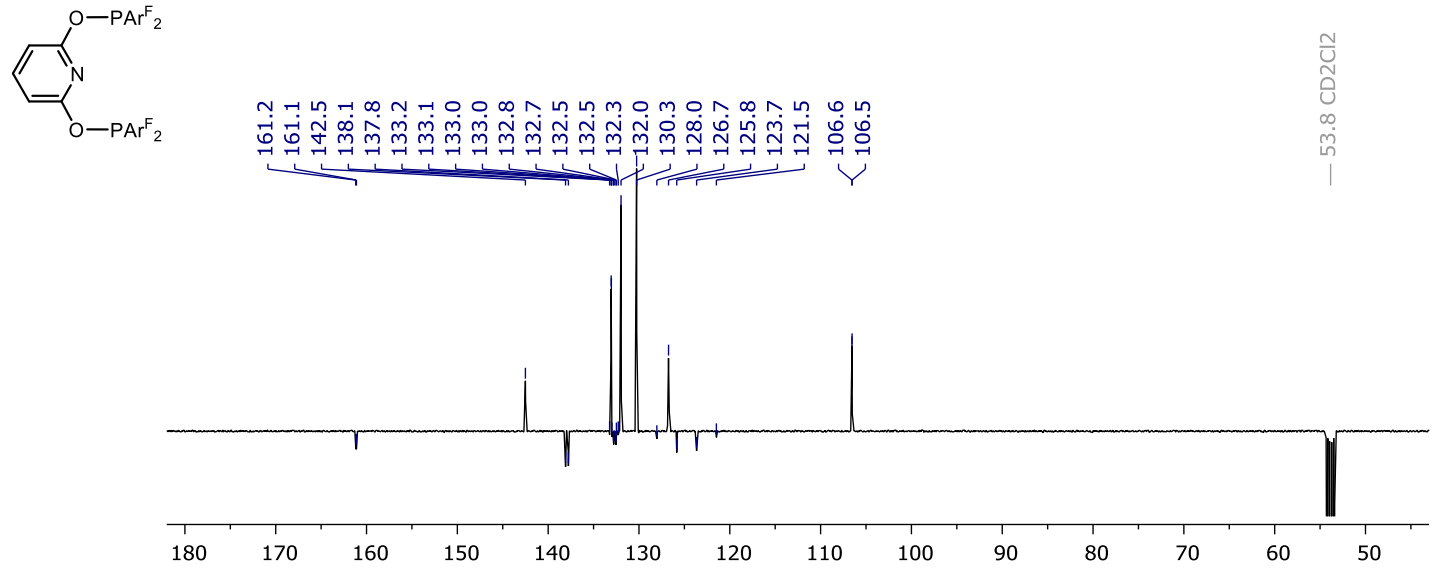
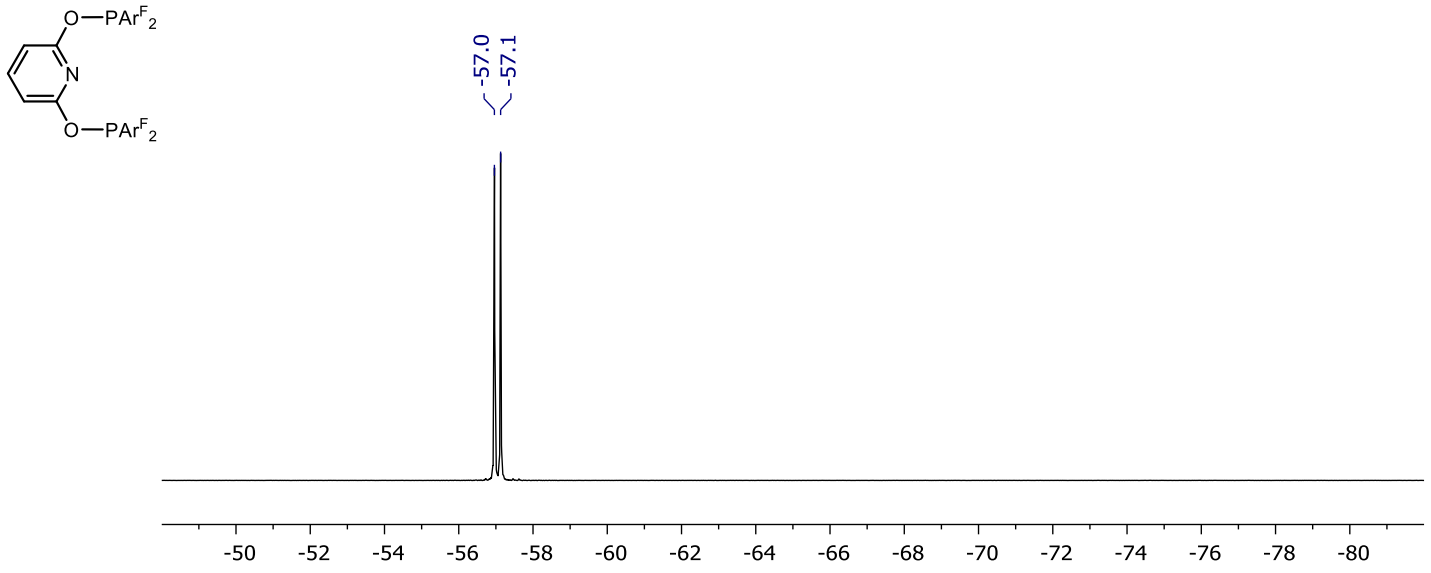
^{1}H NMR spectrum of PONOP-Ar^{F}: CD_2Cl_2, 500 MHz



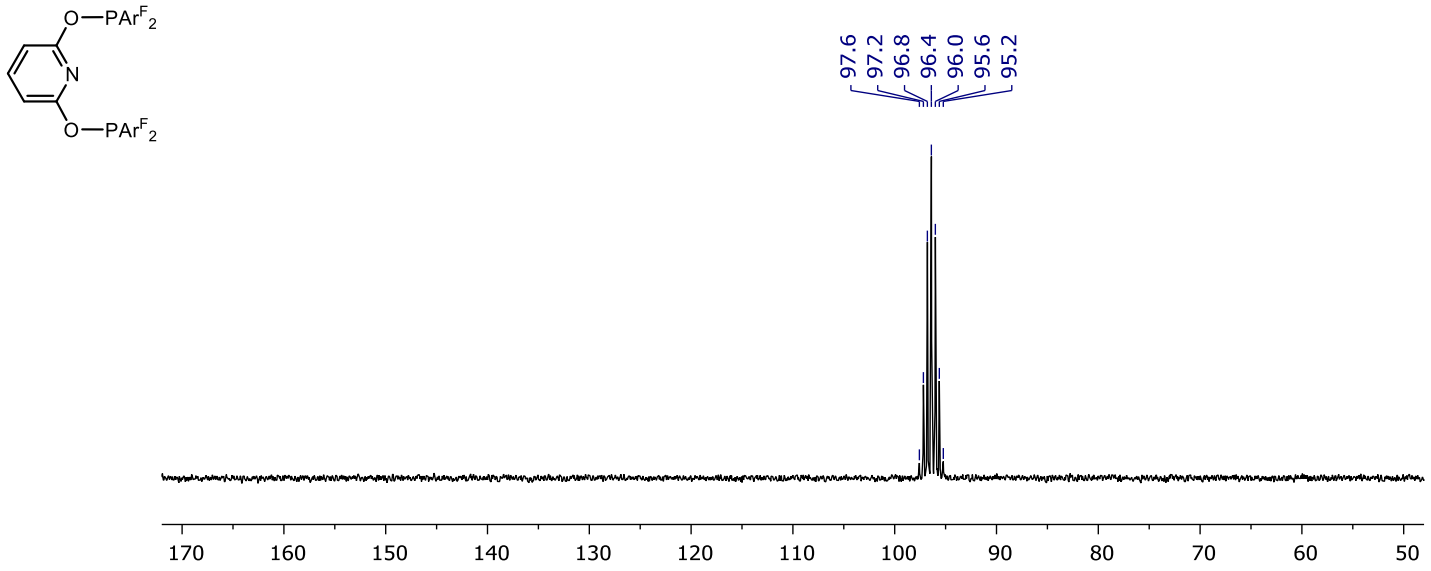
$^{13}C\{^{1}H\}$ APT NMR spectrum of PONOP-Ar^{F}: CD_2Cl_2, 126 MHz



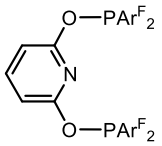
$^{19}F\{^{1}H\}$ NMR spectrum of PONOP-Ar^{F}: CD_2Cl_2, 376 MHz

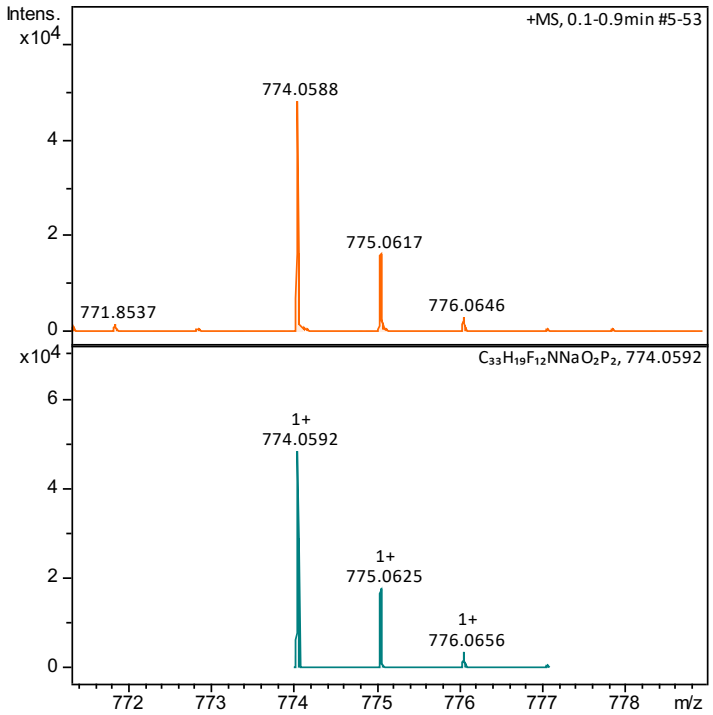


$^{31}P\{^{1}H\}$ NMR spectrum of PONOP-Ar^{F}: CD_2Cl_2, 162 MHz

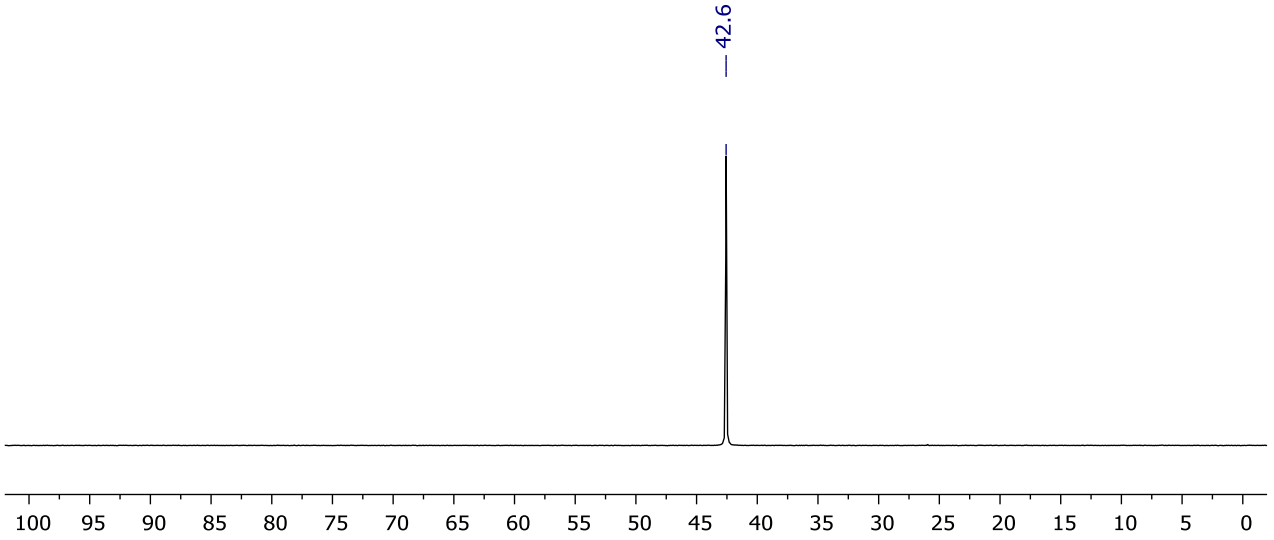


HR ESI-MS (positive ion, 4 kV) of PONOP-Ar^F: 774.0588 ([M+Na]$^+$, calcd 774.0592) *m/z*

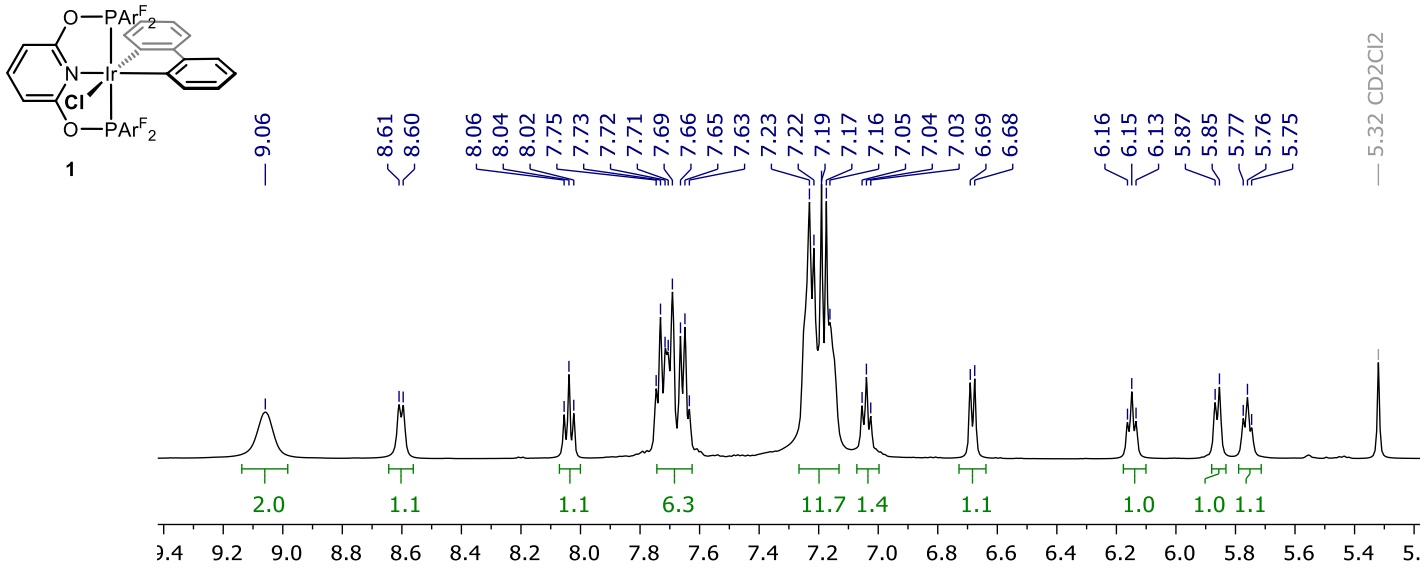




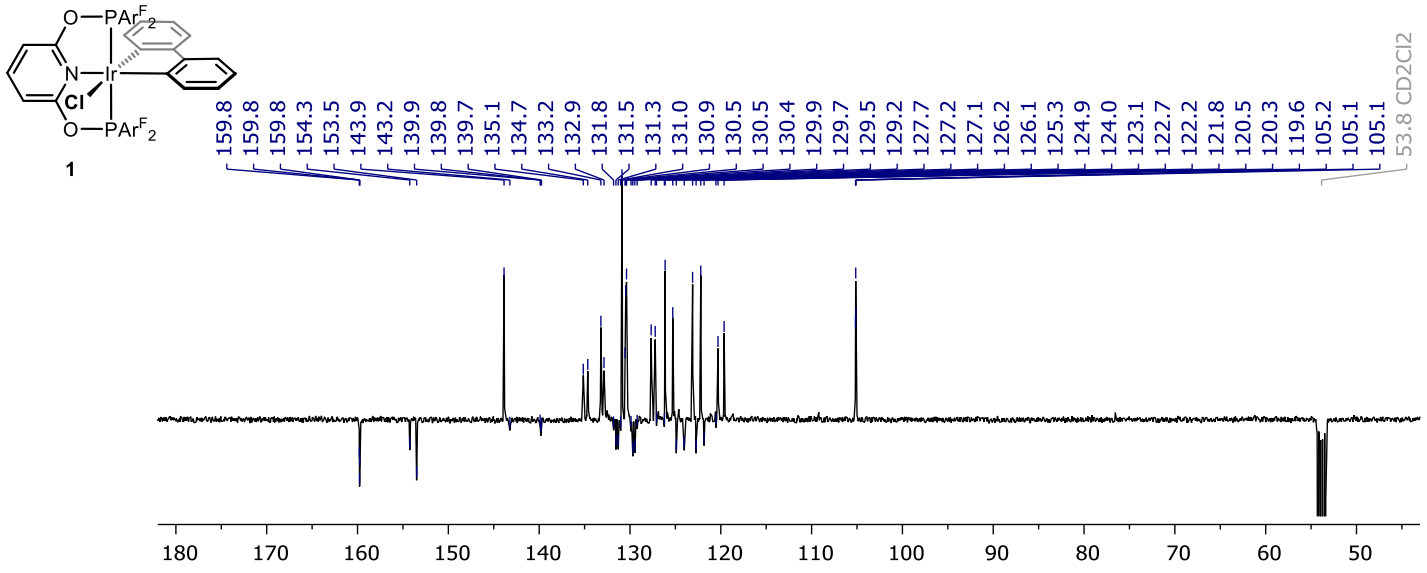
$^{31}P\{^{1}H\}$ NMR spectrum of attempted preparation of PONOP-Ph: CD_2Cl_2, 162 MHz



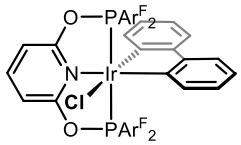
^{1}H NMR spectrum of [Ir(PONOP-Ar^{F})(biph)Cl]: CD_2Cl_2, 500 MHz



$^{13}C\{^{1}H\}$ APT NMR spectrum of [Ir(PONOP-Ar^{F})(biph)Cl]: CD_2Cl_2, 126 MHz



$^{19}F\{^{1}H\}$ NMR spectrum of [Ir(PONOP-Ar^{F})(biph)Cl]: CD_2Cl_2, 282 MHz



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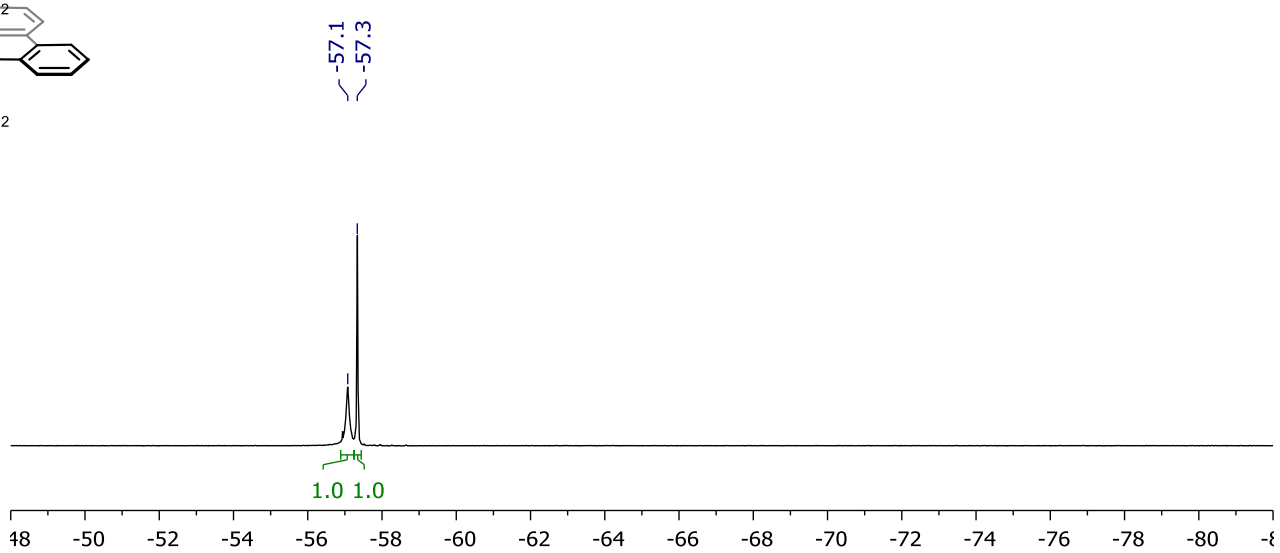
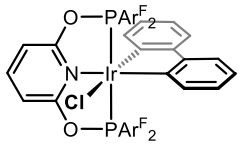


$^{31}P\{^{1}H\}$ NMR spectrum of [Ir(PONOP-Ar^{F})(biph)Cl]: CD_2Cl_2, 121 MHz



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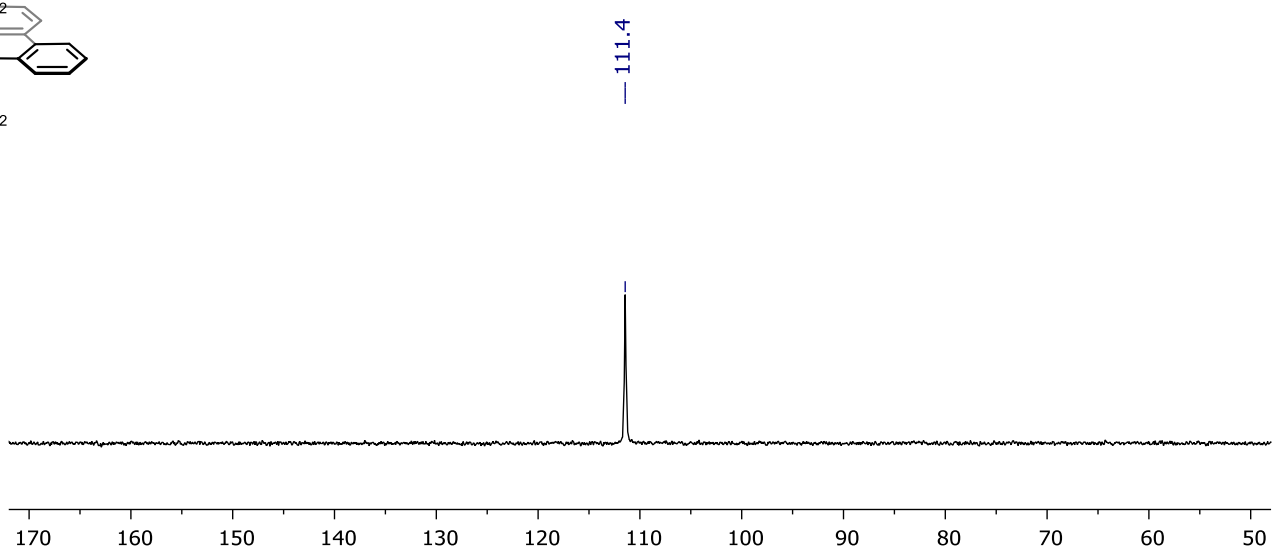
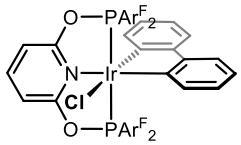


HR ESI-MS (positive ion, 4 kV) of [Ir(PONOP-Ar^F)(biph)Cl]: 1096.0945 ([*M*–Cl]$^+$, calcd 1096.0952) *m/z*



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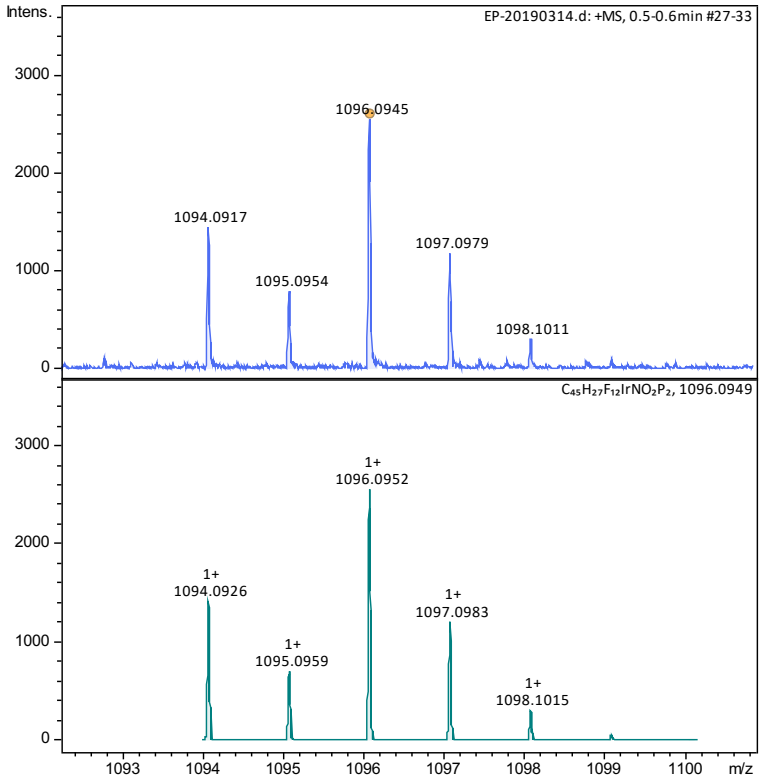
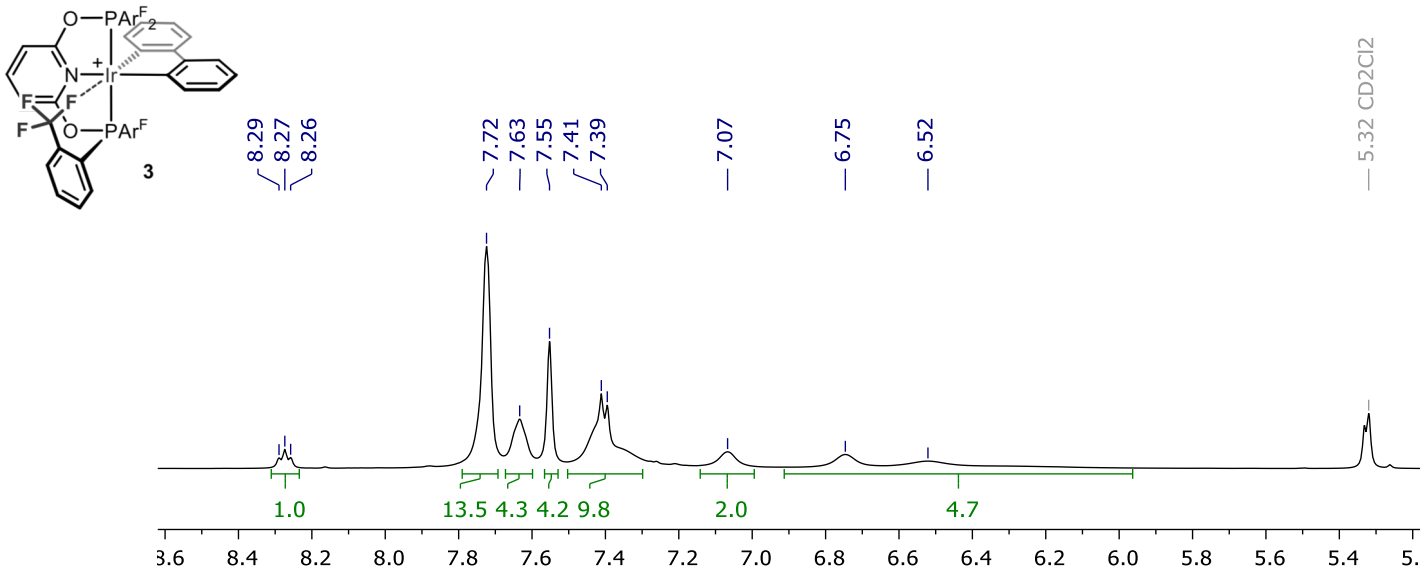
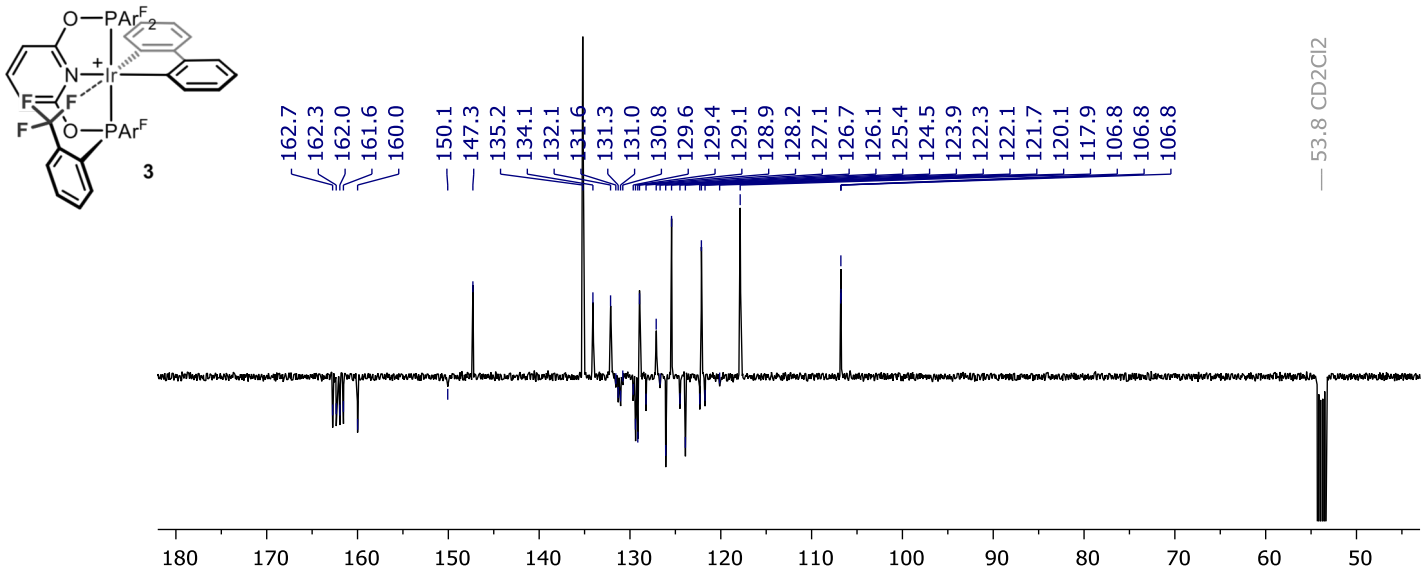


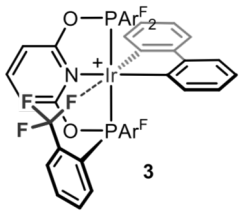
^{1}H NMR spectrum of [Ir(PONOP-Ar^{F})(biph)][BAr$^{f}_{4}$]: CD_2Cl_2, 500 MHz



$^{13}C\{^{1}H\}$ APT NMR spectrum of [Ir(PONOP-Ar^{F})(biph)][BAr$^{f}_{4}$]: CD_2Cl_2, 126 MHz



$^{19}F\{^{1}H\}$ NMR spectrum of [Ir(PONOP-Ar^{F})(biph)][BAr$^{f}_{4}$]: CD_2Cl_2, 376 MHz



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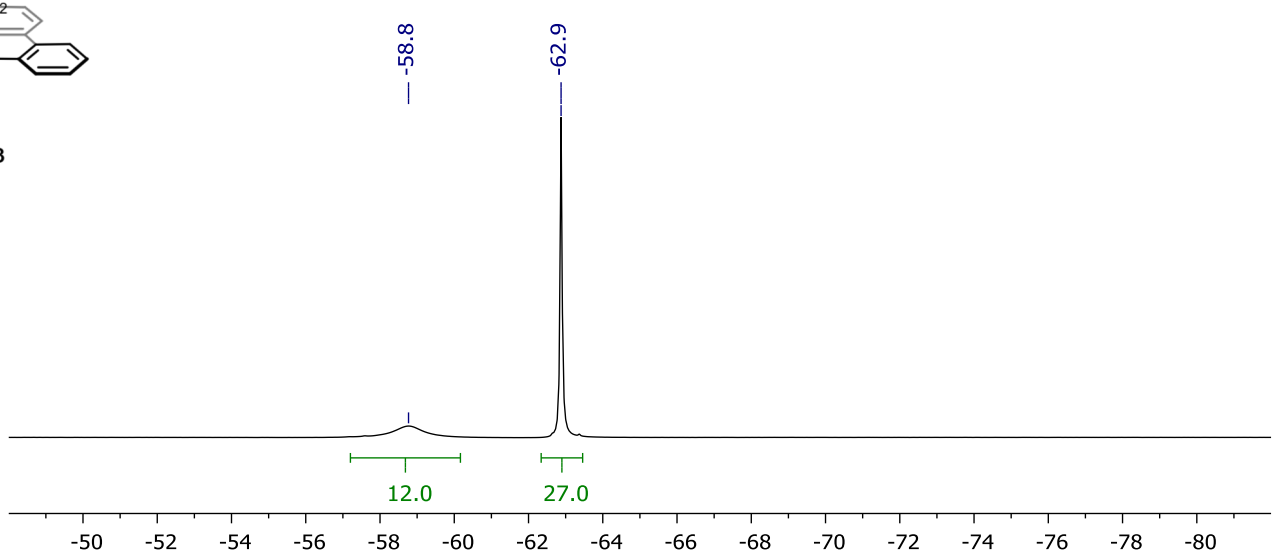
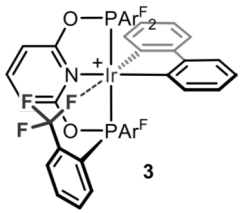


$^{31}P\{^{1}H\}$ NMR spectrum of [Ir(PONOP-Ar^{F})(biph)][BAr$^{f}_{4}$]: CD_2Cl_2, 162 MHz



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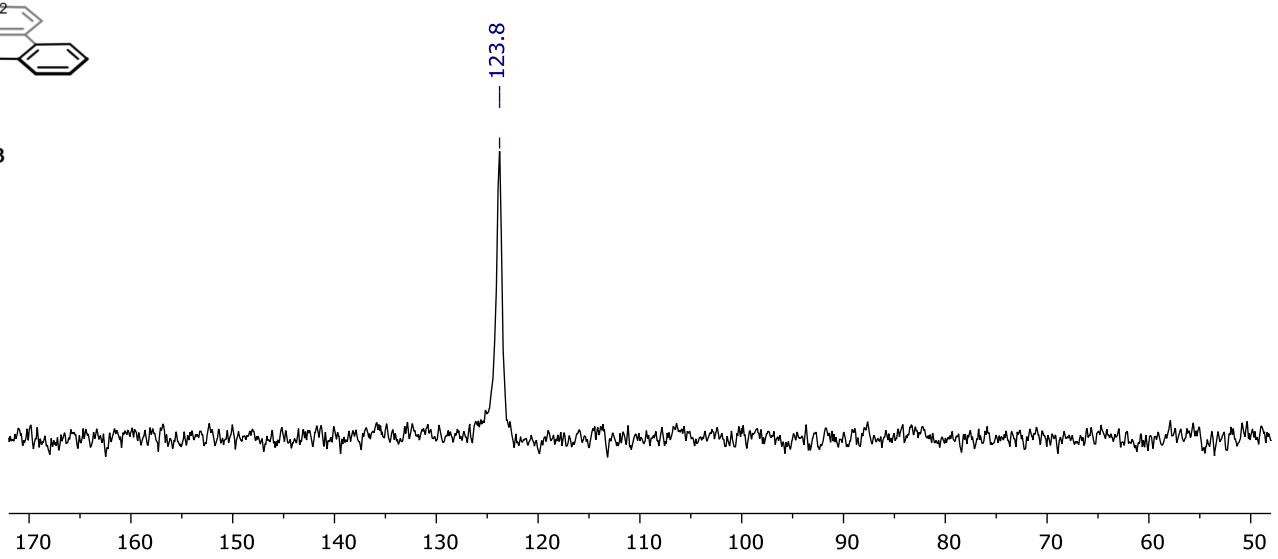
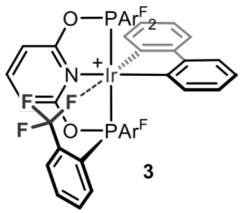


HR ESI-MS (positive ion, 4 kV) of [Ir(PONOP-Ar^F)(biph)][BAr$^f_4$]: 1096.0963 ([*M*]$^+$, calcd 1096.0952) *m/z*



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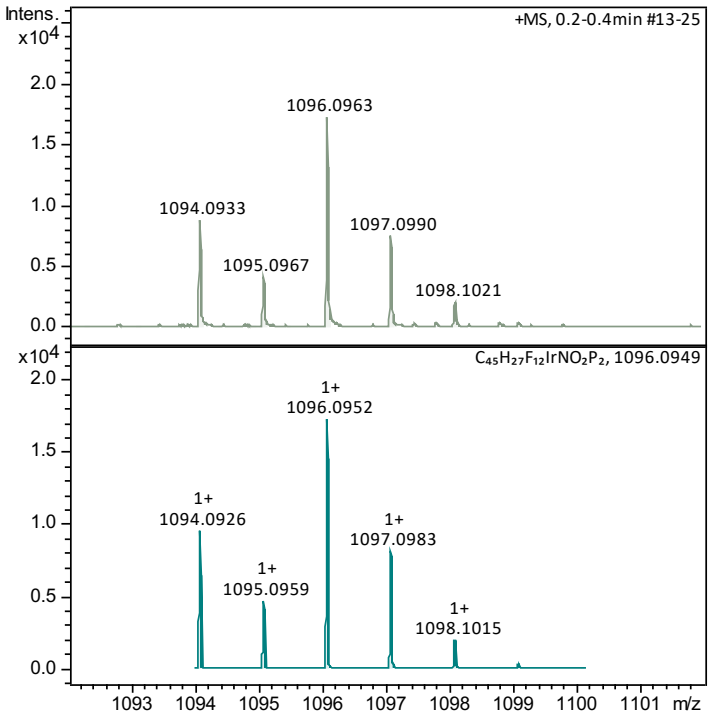
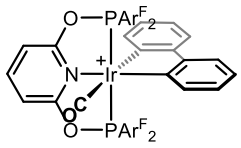


^{1}H NMR spectrum of [Ir(PONOP-Ar^{F})(biph)(CO)][BAr$^{f}_{4}$]: CD_2Cl_2, 500 MHz



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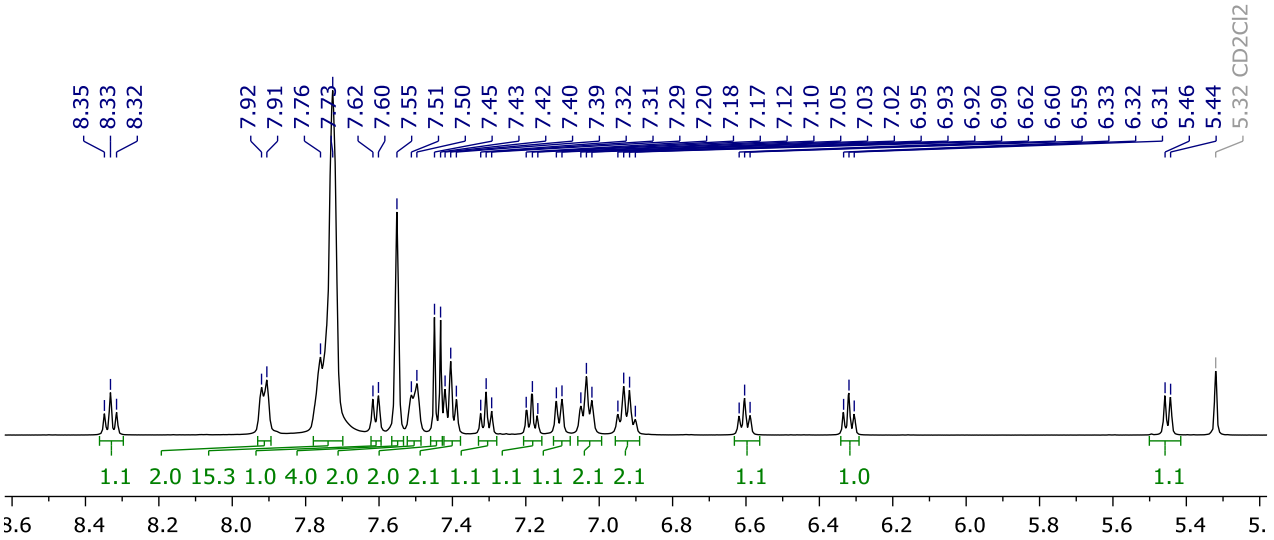
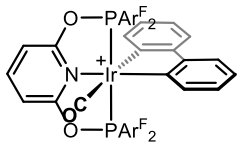


$^{13}C\{^{1}H\}$ APT NMR spectrum of [Ir(PONOP-Ar^{F})(biph)(CO)][BAr$^{f}_{4}$]: CD_2Cl_2, 126 MHz



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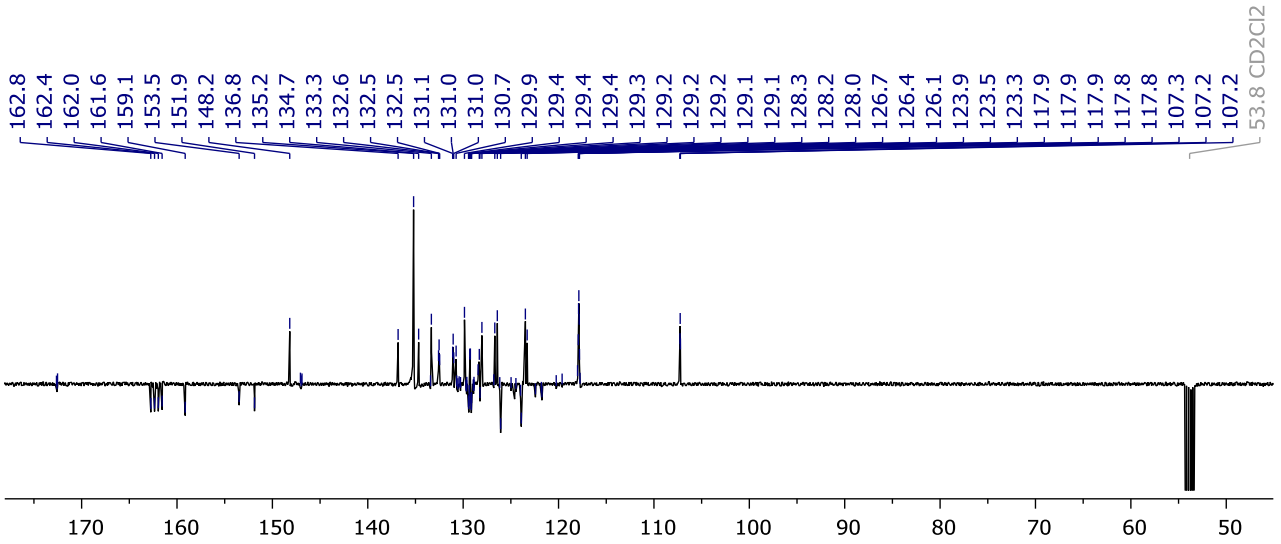
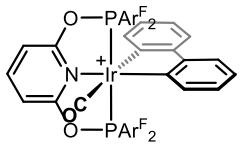


$^{19}F\{^{1}H\}$ NMR spectrum of [Ir(PONOP-Ar^{F})(biph)(CO)][BAr$^{f}_{4}$]: CD_2Cl_2, 376 MHz



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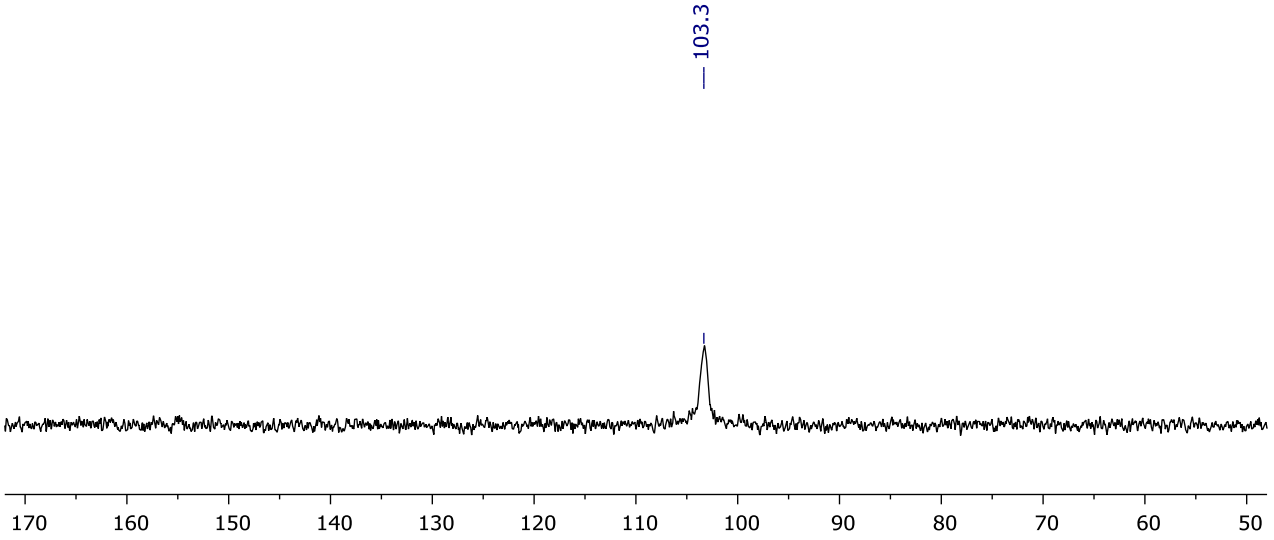
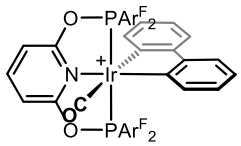


$^{31}P\{^{1}H\}$ NMR spectrum of [Ir(PONOP-Ar^{F})(biph)(CO)][BAr$^{f}_{4}$]: CD_2Cl_2, 162 MHz



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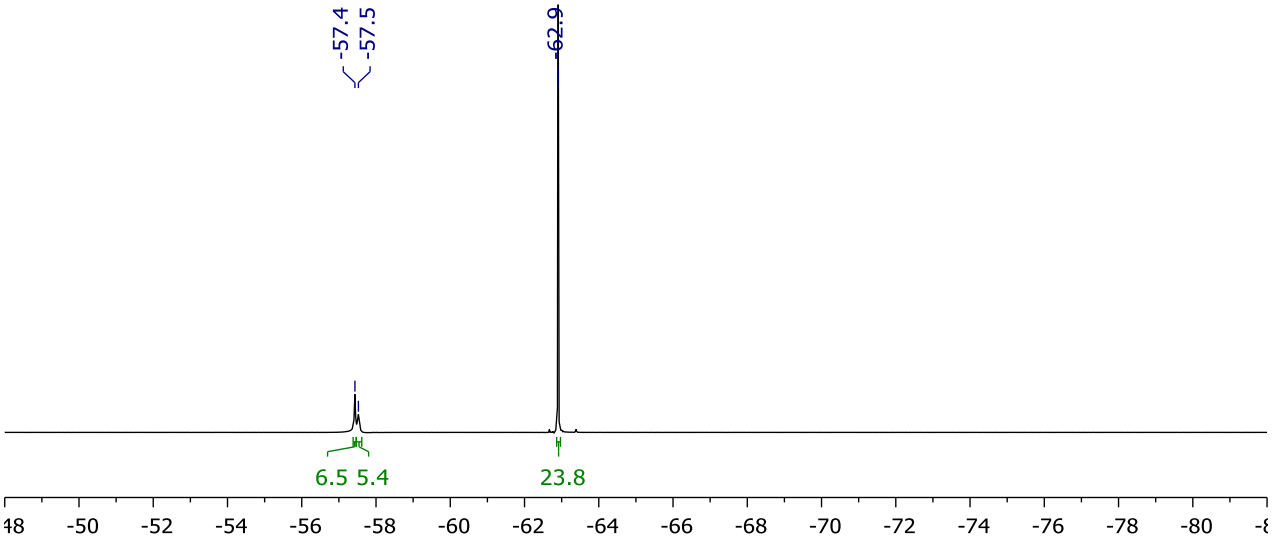
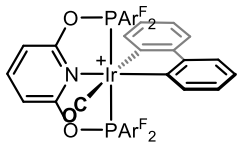


HR ESI-MS (positive ion, 4 kV) of [Ir(PONOP-Ar^F)(biph)(CO)][BAr$^f_4$]: 1124.0902 ([*M*]$^+$, calcd 1124.0901) *m/z*



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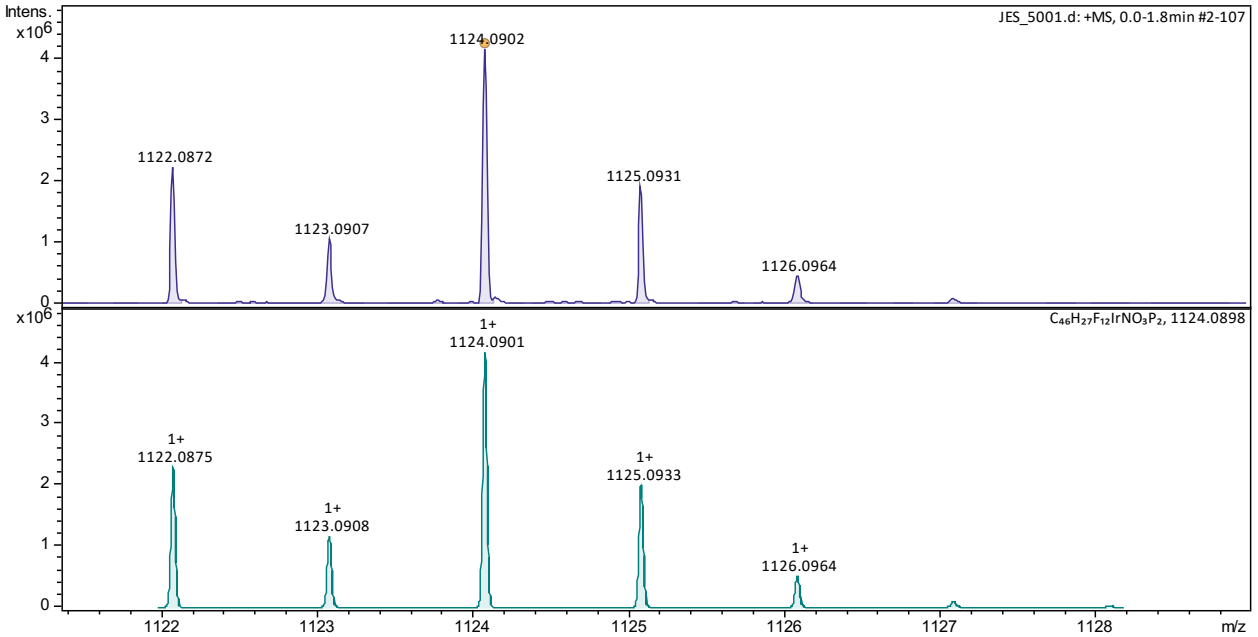
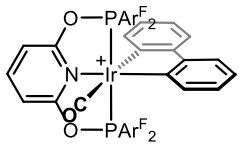


IR spectrum of [Ir(PONOP-Ar^F)(biph)(CO)][BAr$^f_4$]:



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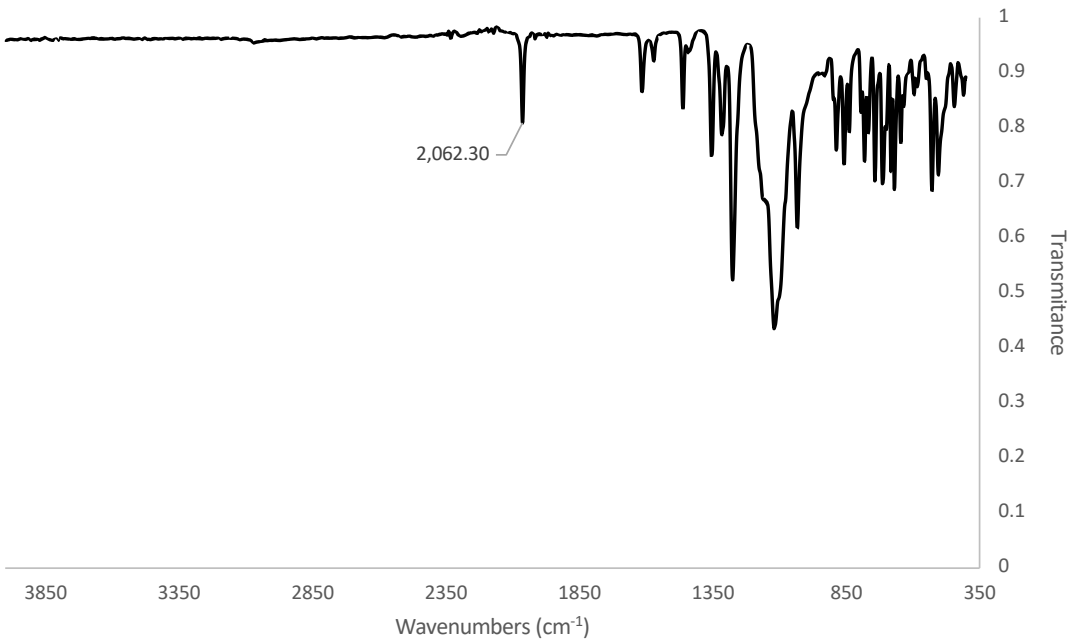
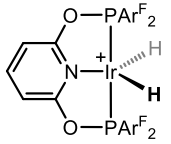


^{1}H NMR spectrum of [Ir(PONOP-Ar^{F})(H)$_2$][BAr$^{f}_4$]: CD_2Cl_2, 500 MHz



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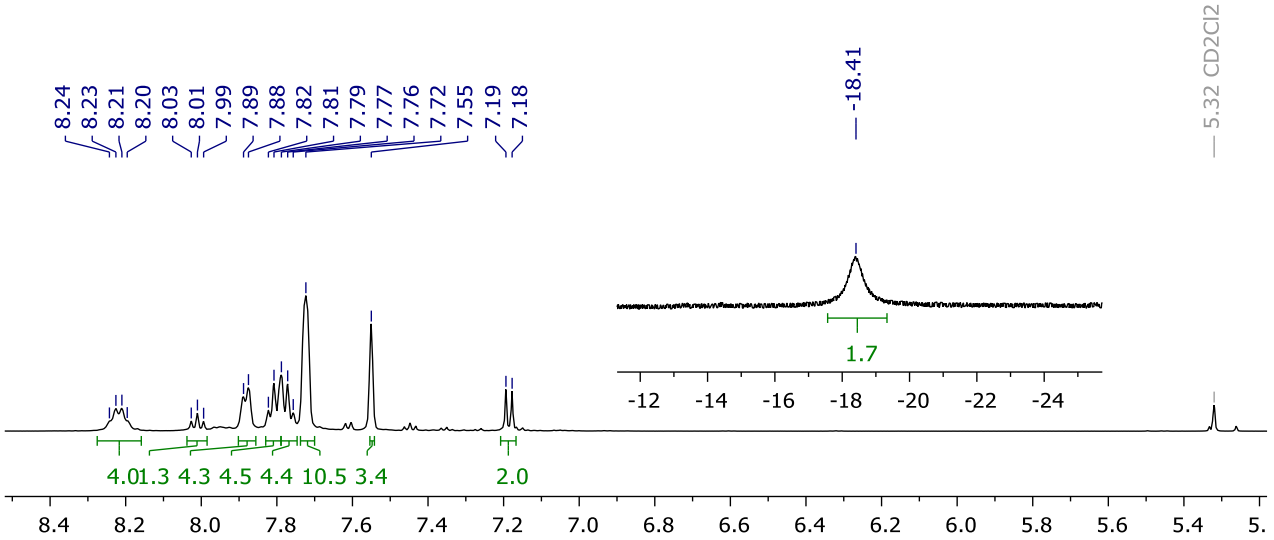
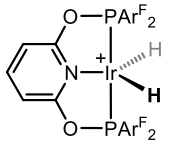


$^{13}C\{^{1}H\}$ APT NMR spectrum of $[Ir(PONOP\text{-}Ar^{F})(H)_2][BAr^{f}_4]$: CD_2Cl_2, 126 MHz



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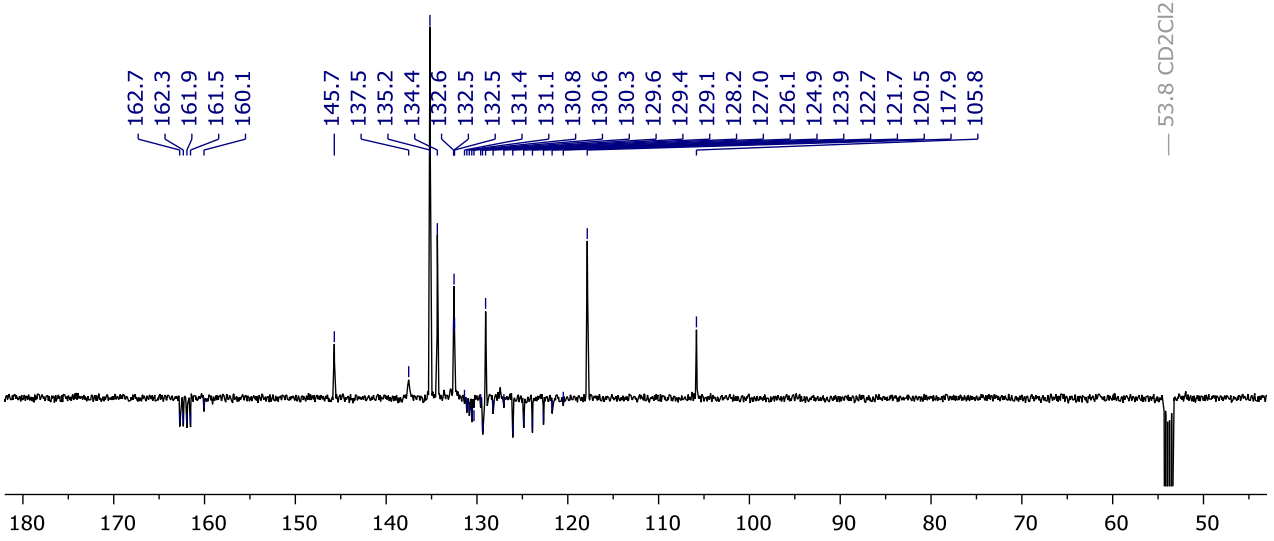
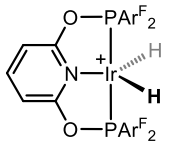


$^{19}F\{^{1}H\}$ NMR spectrum of $[Ir(PONOP\text{-}Ar^{F})(H)_2][BAr^{f}_4]$: CD_2Cl_2, 376 MHz



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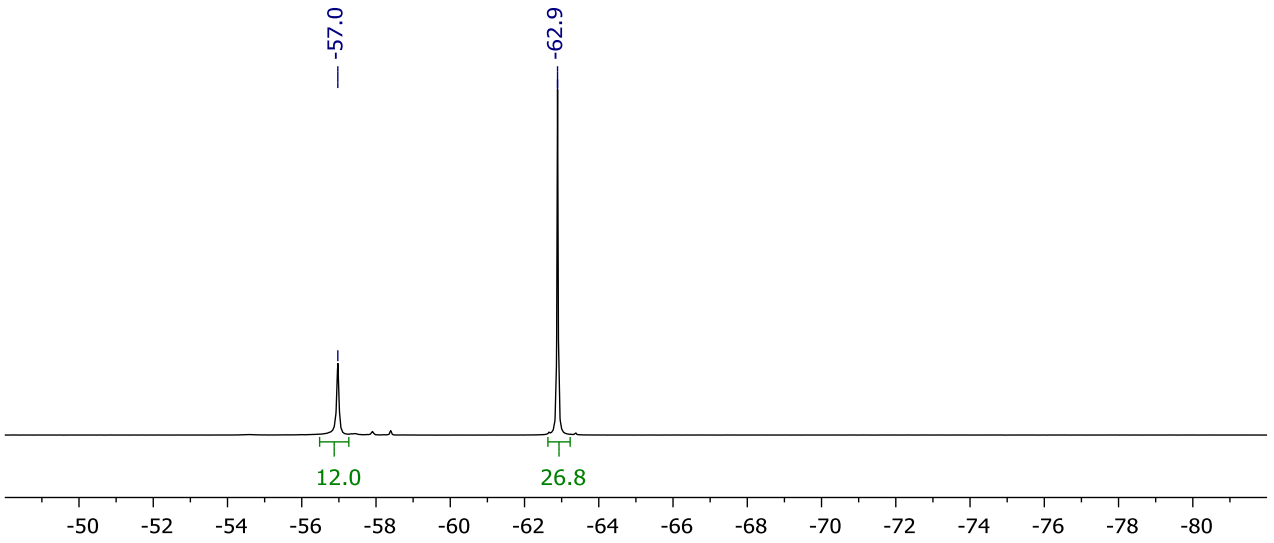
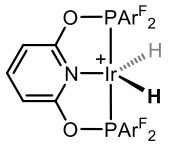


$^{31}P\{^{1}H\}$ NMR spectrum of $[Ir(PONOP\text{-}Ar^{F})(H)_2][BAr^{f}_4]$: CD_2Cl_2, 162 MHz



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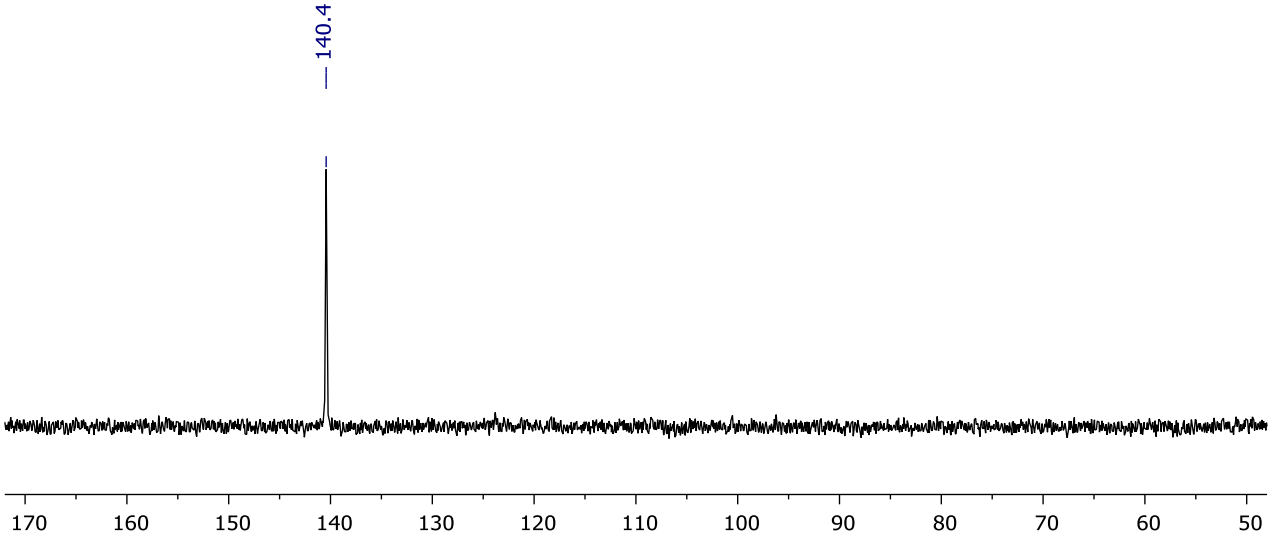
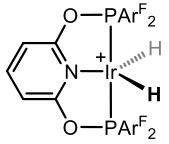
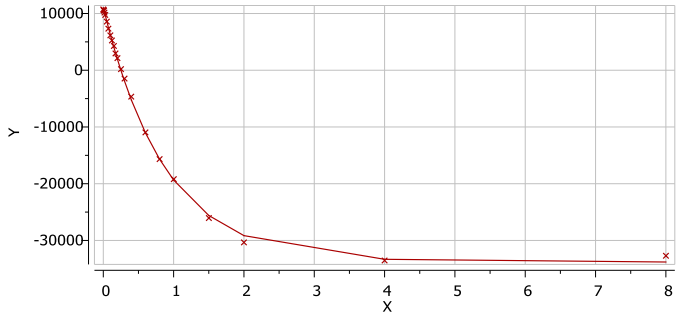


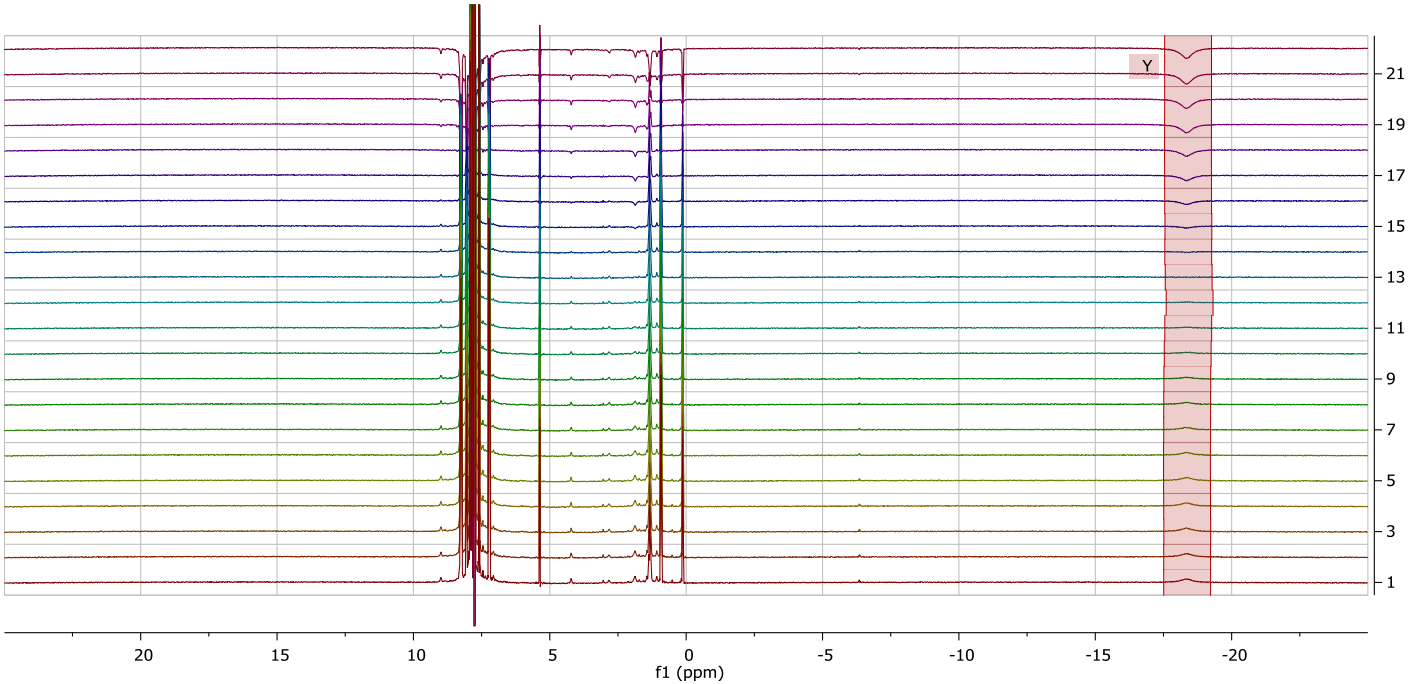
T_1 NMR experiment of [Ir(PONOP-Ar^F)(H)$_2$][BAr$^f_4$]: CD_2Cl_2, 600 MHz, 298 K



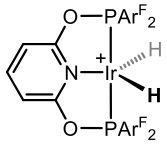
5

B+F*exp(-x*1/T_1)
B= -33803.86
F= 44881.62
T_1 =0.88259 ± 0.01659





HR ESI-MS (positive ion, 4 kV) of [Ir(PONOP-Ar^F)(H)$_2$][BAr$^f_4$]: 946.0487 ([*M*]$^+$, calcd 946.0481) *m/z*



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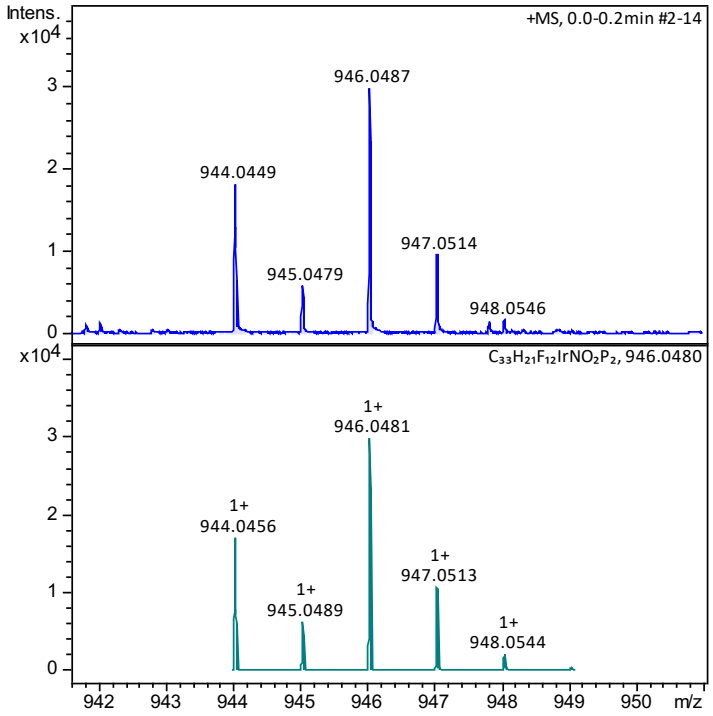
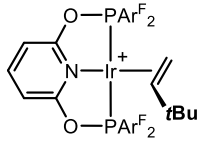


^{1}H NMR spectrum of [Ir(PONOP-Ar^{F})(TBE)][BAr$^{f}_{4}$]: d_{8}-toluene, 400 MHz



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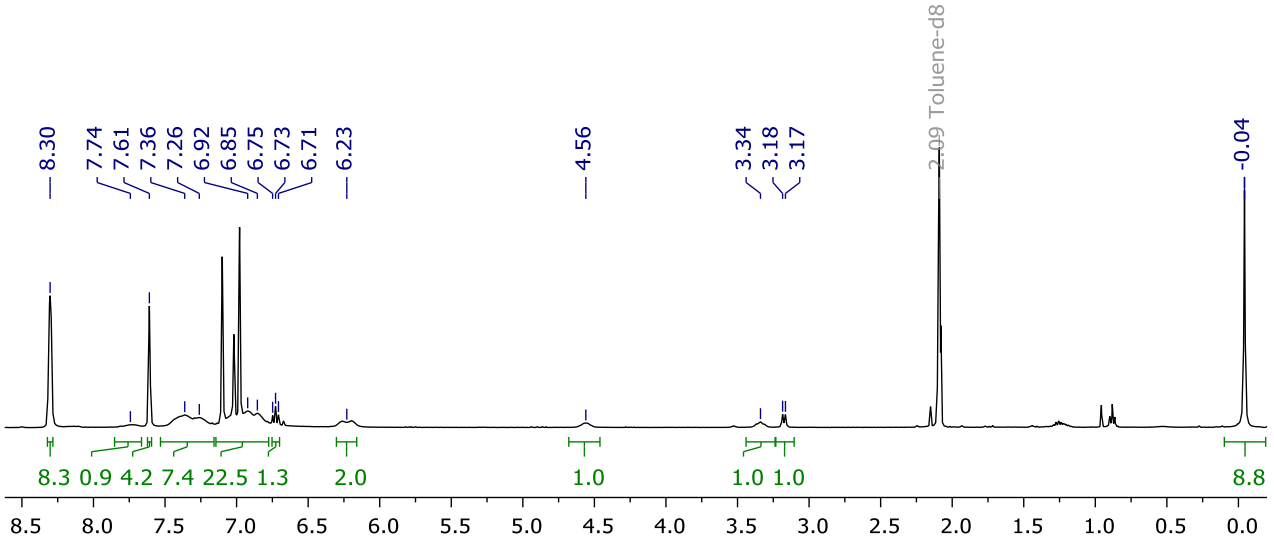
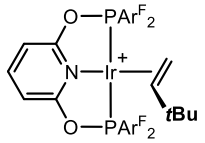


$^{13}C\{^{1}H\}$ APT NMR spectrum of [Ir(PONOP-Ar^{F})(TBE)][BAr$^{f}_{4}$]: d_8-toluene, 126 MHz



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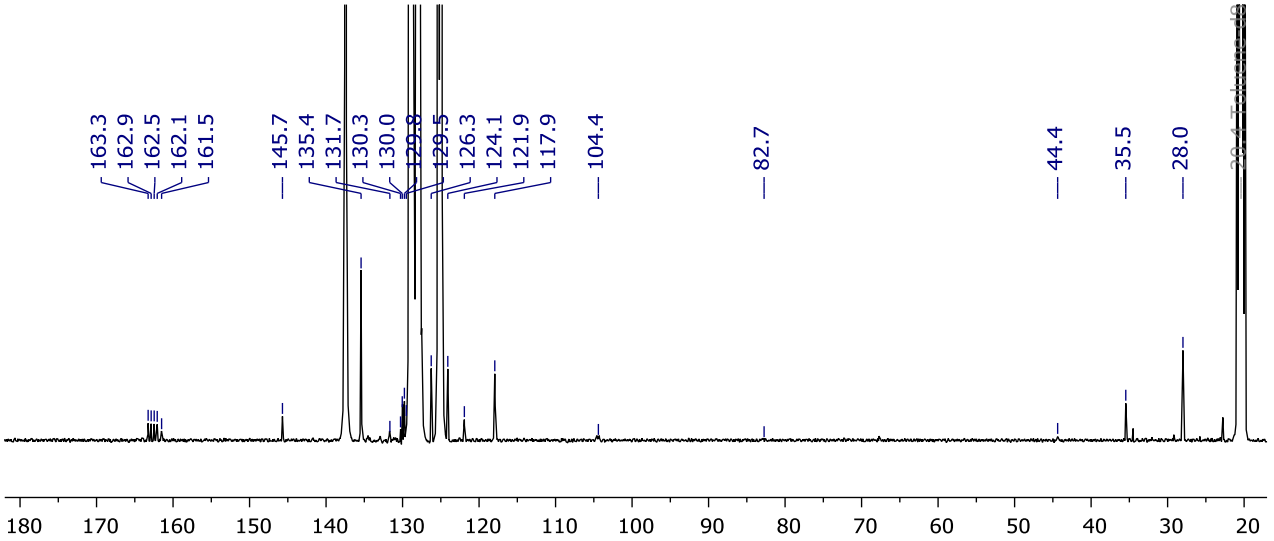
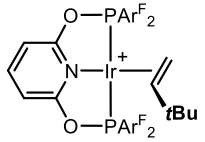


$^{19}F\{^{1}H\}$ NMR spectrum of [Ir(PONOP-Ar^{F})(TBE)][BAr$^{f}_{4}$]: d_8-toluene, 376 MHz



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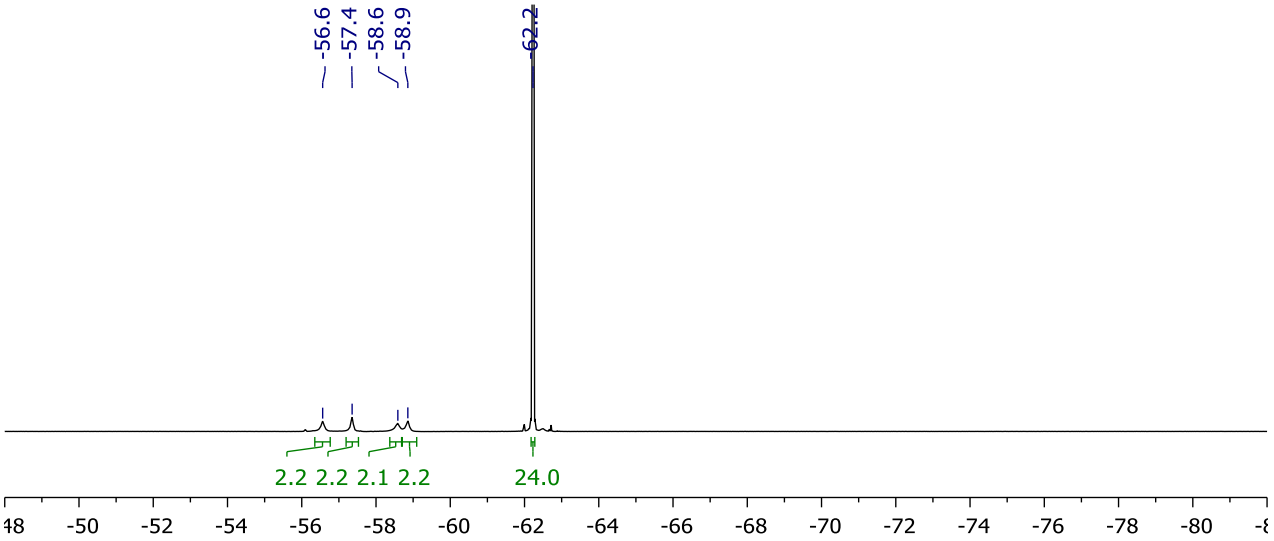
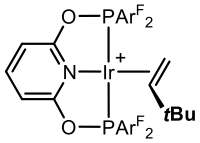


$^{31}P\{^{1}H\}$ NMR spectrum of [Ir(PONOP-Ar^{F})(TBE)][BAr$^{f}_{4}$]: d_8-toluene, 162 MHz



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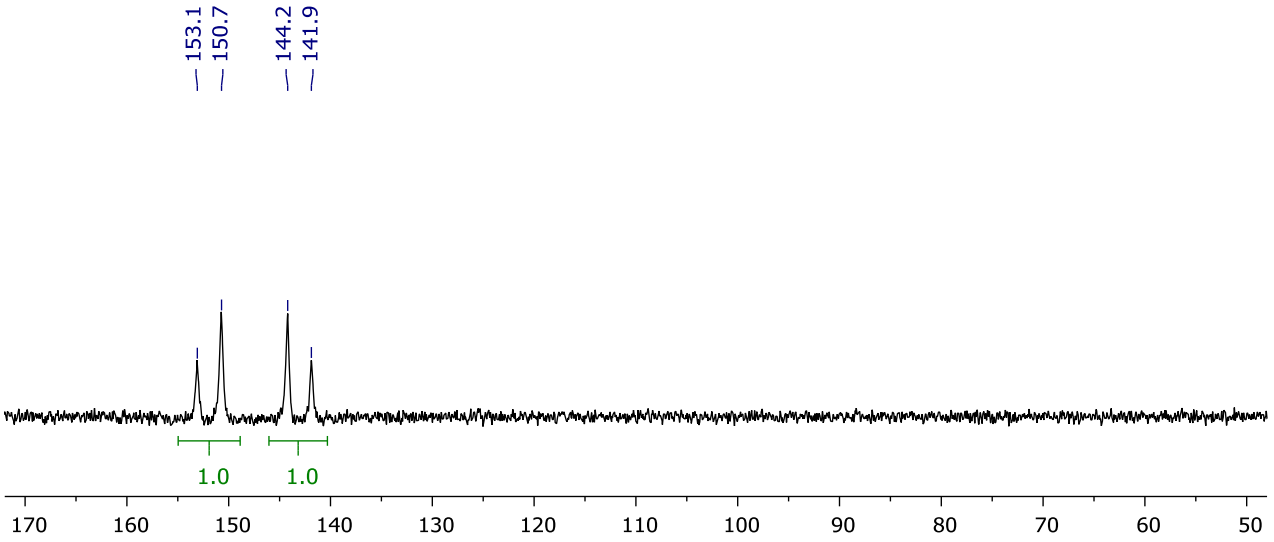
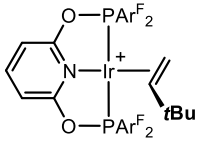


HR ESI-MS (positive ion, 4 kV) of [Ir(PONOP-Ar^F)(TBE)][BAr$^f_4$]: 1028.1251 ([*M*]$^+$, calcd 1028.1264) *m/z*



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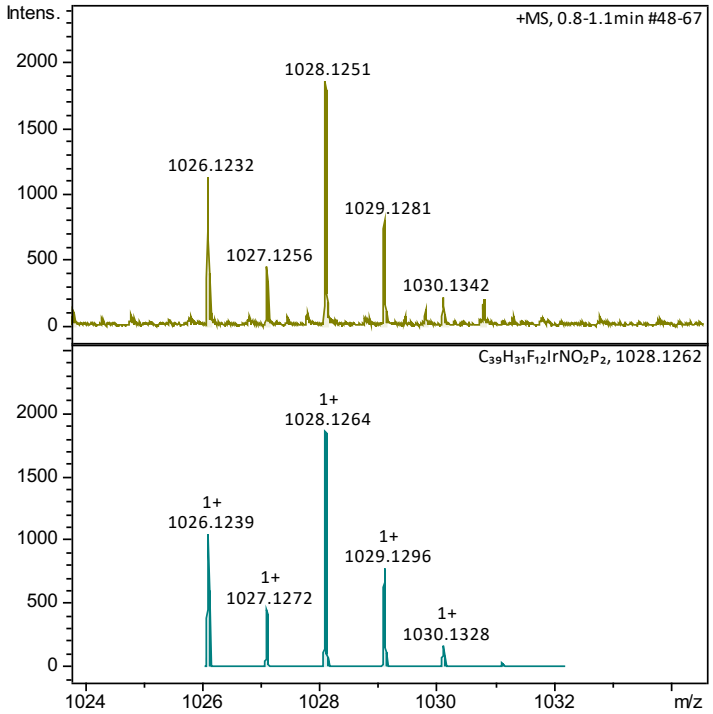
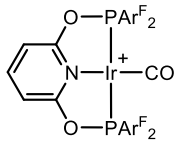


^{1}H NMR spectrum of [Ir(PONOP-Ar^{F})(CO)][BAr$^{f}_{4}$]: CD_2Cl_2, 500 MHz



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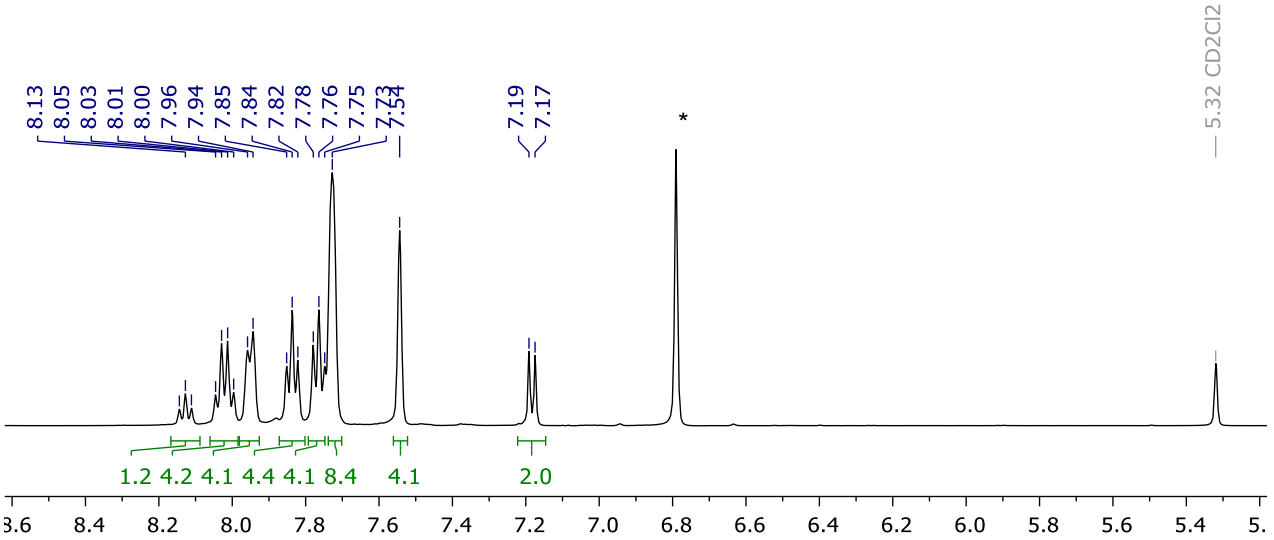
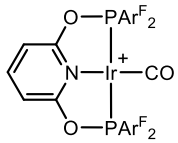


$^{13}C\{^{1}H\}$ APT NMR spectrum of [Ir(PONOP-Ar^{F})(CO)][BAr$^{f}_{4}$]: CD_2Cl_2, 126 MHz



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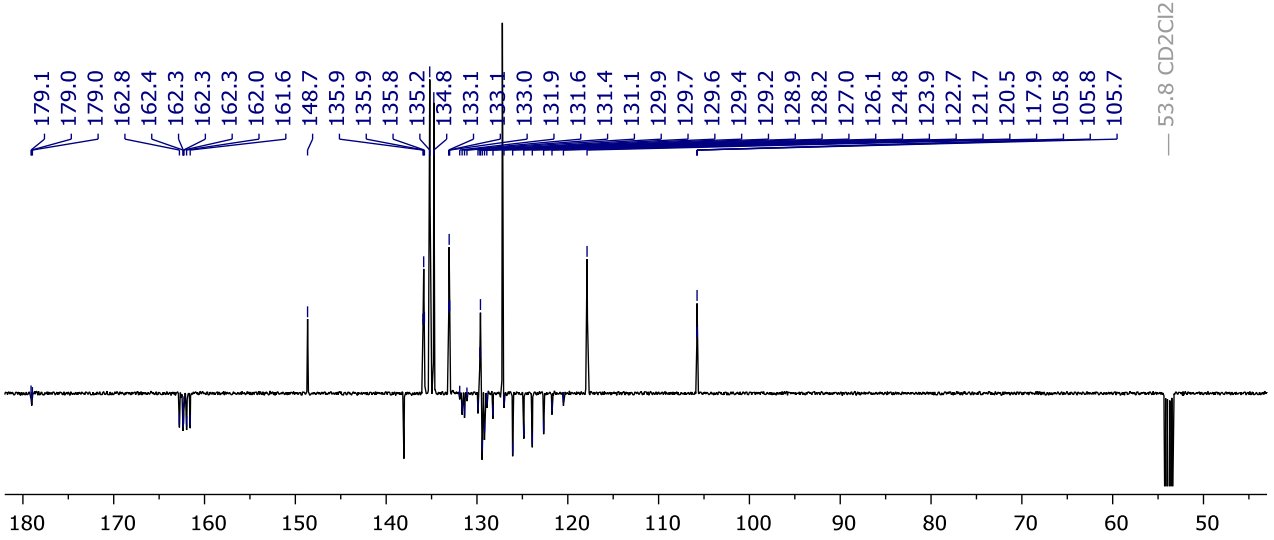
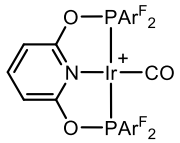


$^{19}F\{^{1}H\}$ NMR spectrum of [Ir(PONOP-Ar^{F})(CO)][BAr$^{f}_{4}$]: CD_2Cl_2, 376 MHz



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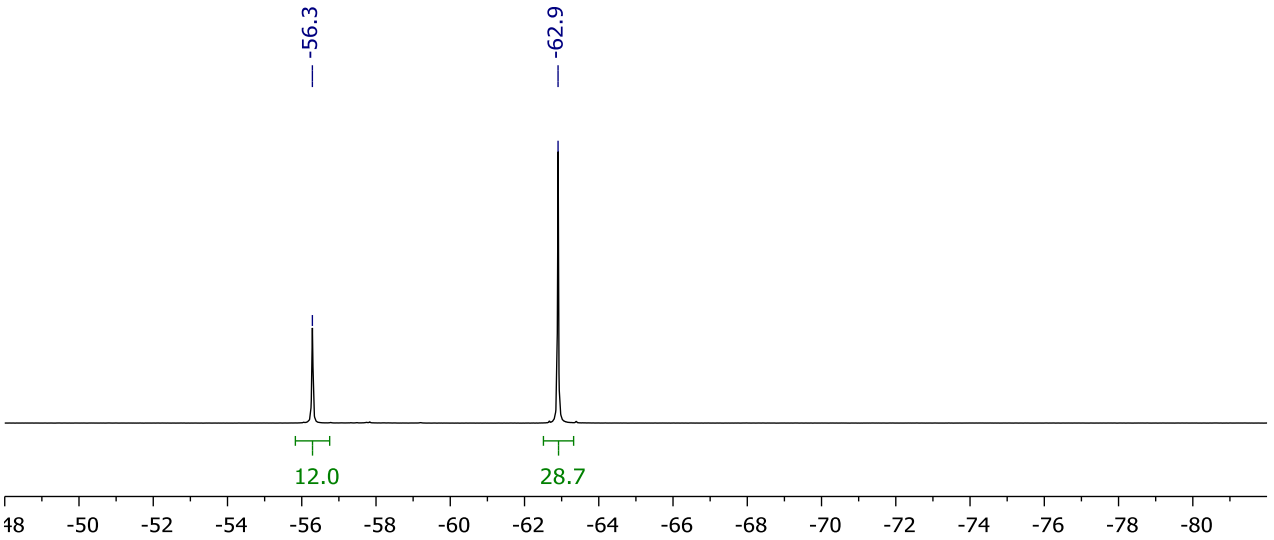
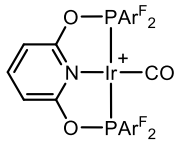


$^{31}P\{^{1}H\}$ NMR spectrum of [Ir(PONOP-Ar^{F})(CO)][BAr$^{f}_{4}$]: CD_2Cl_2, 162 MHz



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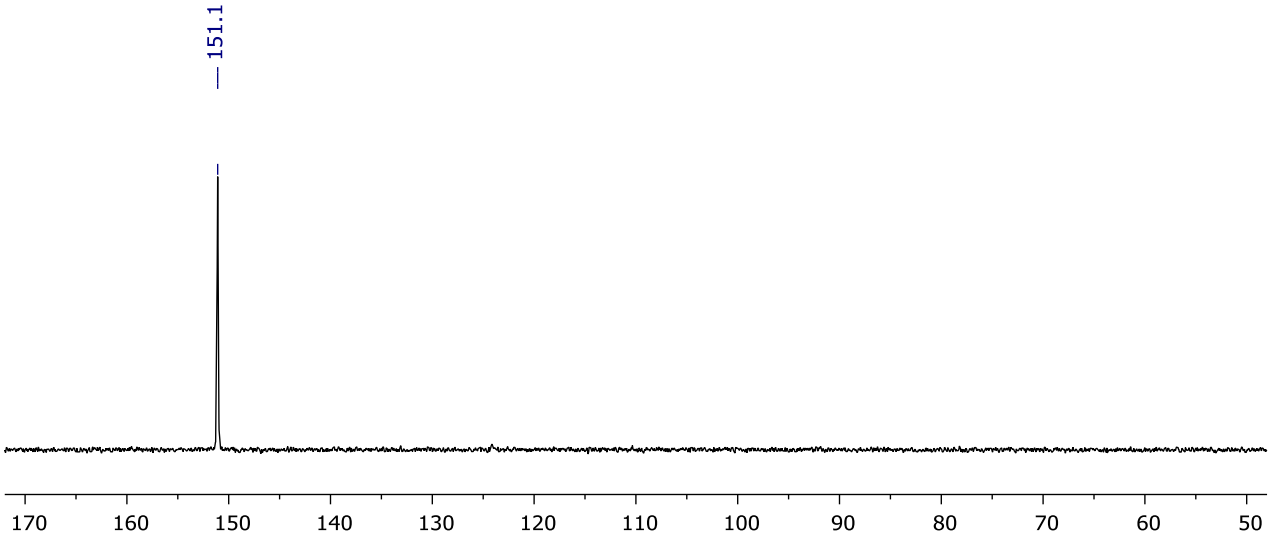
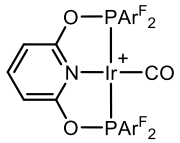


HR ESI-MS (positive ion, 4 kV) of [Ir(PONOP-Ar^F)(CO)][BAr$^f_4$]: 974.0448 ([M]$^+$, 974.0431 calcd) *m/z*



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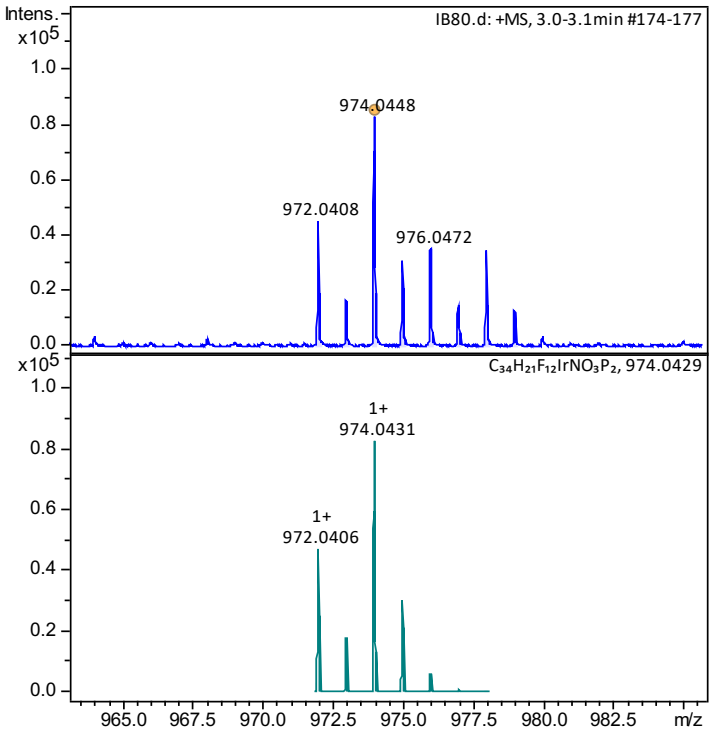
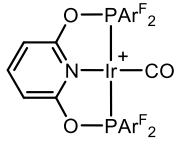


IR spectrum of [Ir(PONOP-Ar^F)(CO)][BAr$^f_4$]:



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