Supplementary Information for:

Systematic Evaluation of the Electronic Effect of Aluminum-Containing Ligands in Iridium-Aluminum and Rhodium-Aluminum Bimetallic Complexes

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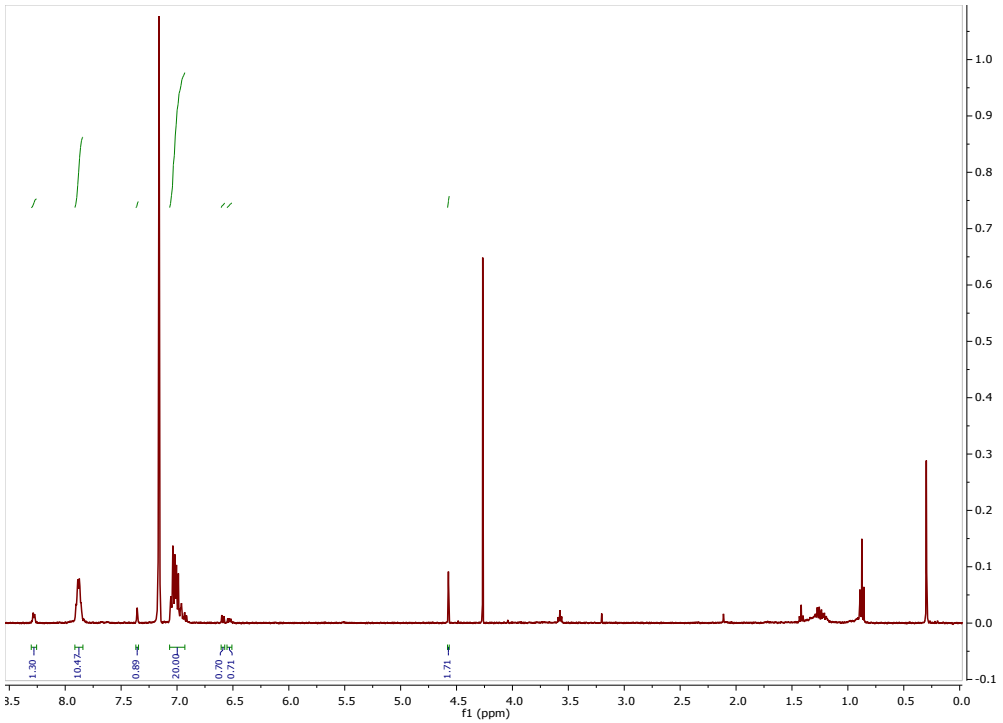

Figure S1. ^{1}H NMR spectrum of $[Ir(PPh_3)_2(CO)(2\text{-pyridinemethanol})][NO_3]$ (**8a**) in C_6D_6. Solvent impurity at 0.8 ppm and 1.2 ppm is pentane. Solvent impurity at 1.4 ppm and 3.5 ppm is tetrahydrofuran. Solvent impurity at 4.2 is dichloromethane. Signal at 0.3 ppm is silicone grease.

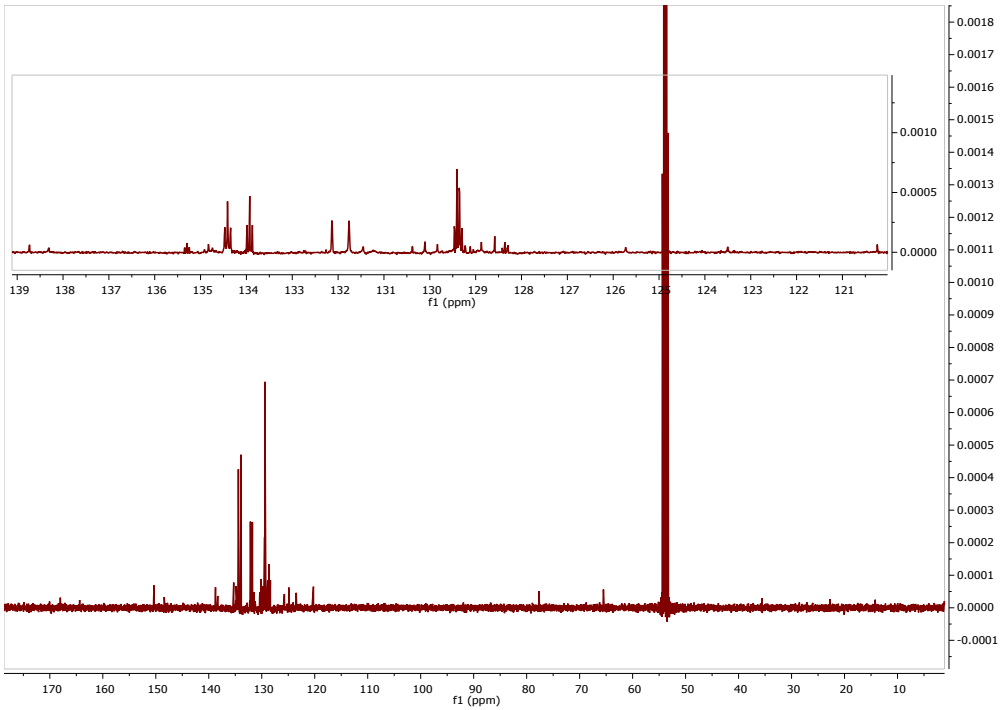

Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum of $[Ir(PPh_3)_2(CO)(2\text{-pyridinemethanol})][NO_3]$ (**8a**) in CD_2Cl_2. Inset is expansion of ppm range 139 ppm to 120.5 ppm. Solvent impurity upfield of 40 ppm is pentane. Number, multiplicity and chemical shift of signals supports existence of one N-bound isomer and one O-bound isomer.

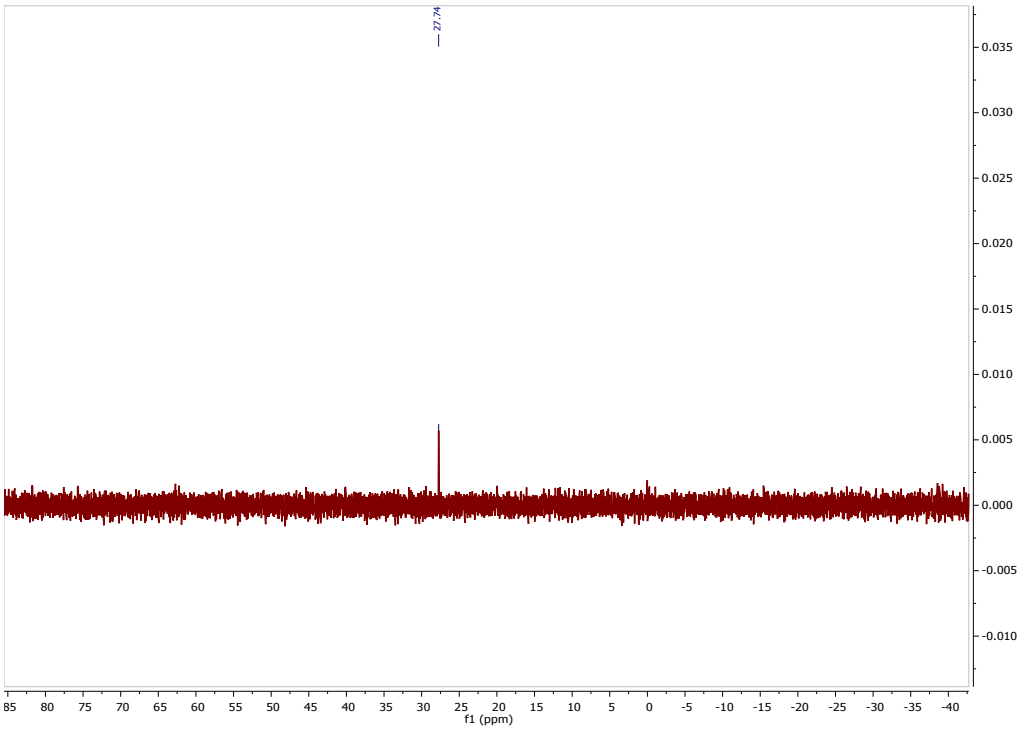

Figure S3. $^{31}P\{^{1}H\}$ NMR spectrum of $[Ir(PPh_3)_2(CO)(2\text{-pyridinemethanol})][NO_3]$ (**8a**) in C_6D_6.

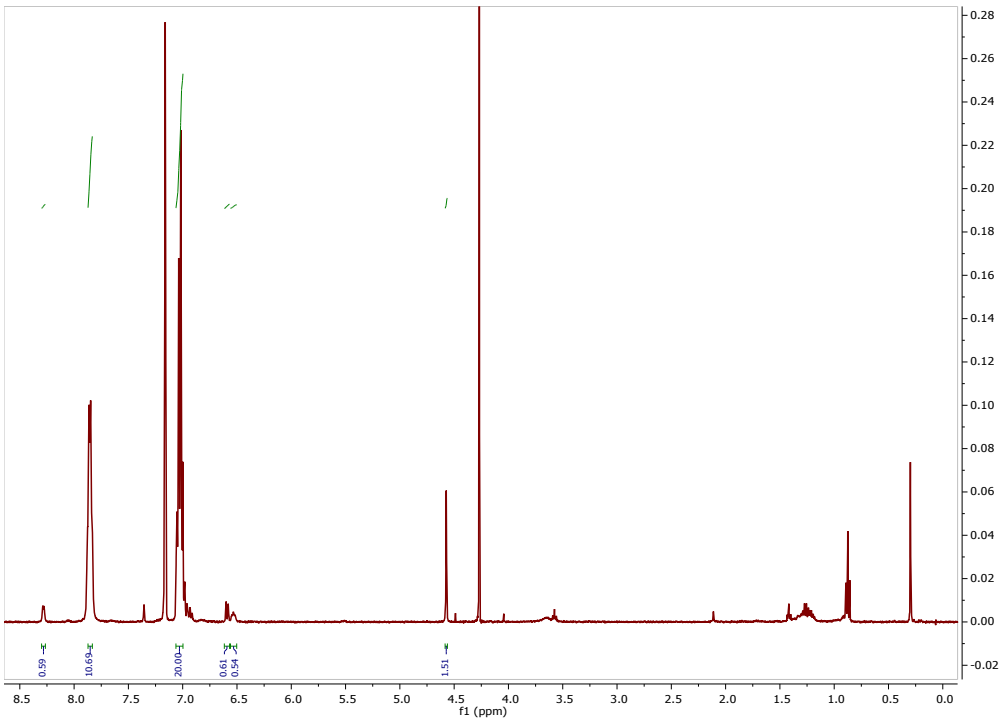

Figure S4. ^{1}H NMR spectrum of $[Rh(PPh_3)_2(CO)(2\text{-pyridinemethanol})][NO_3]$ (**8b**) in C_6D_6. Solvent impurity at 0.8 ppm and 1.2 ppm is pentane. Solvent impurity at 1.4 ppm and 3.57 ppm is tetrahydrofuran. Solvent impurity at 4.27 ppm is dichloromethane. Solvent impurity at 0.29 ppm is silicone grease.

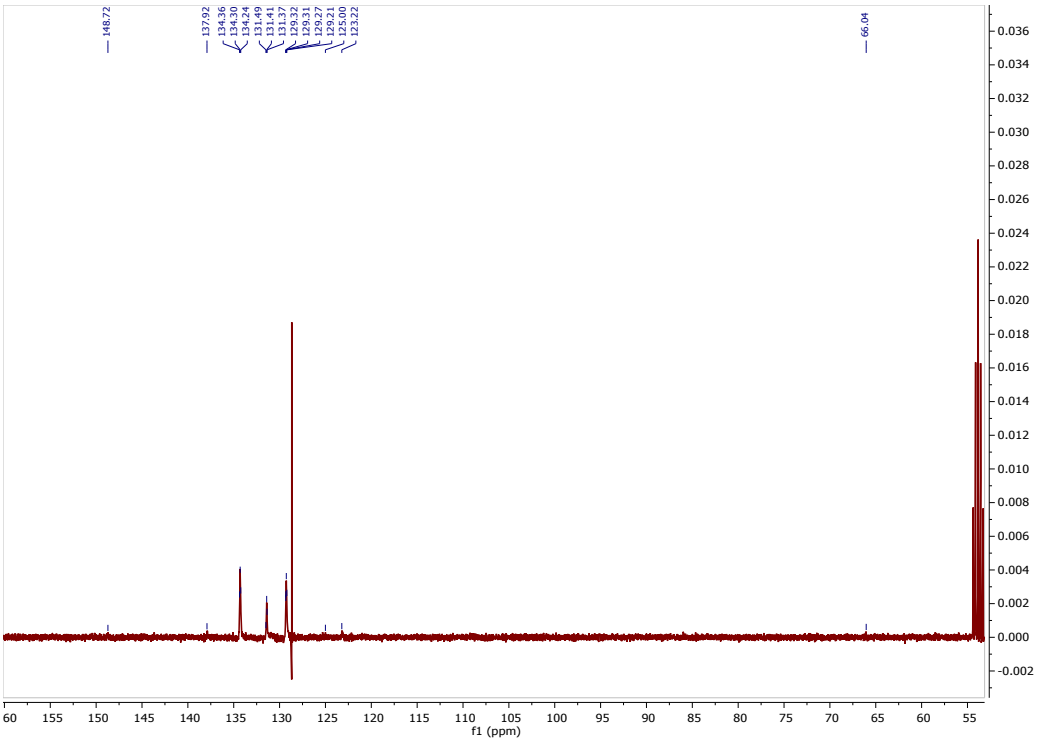

Figure S5. $^{13}C\{^{1}H\}$ NMR spectrum of $[Rh(PPh_3)_2(CO)(2\text{-pyridinemethanol})][NO_3]$ (**8b**) in CD_2Cl_2. Solvent impurity at 128 ppm is benzene.

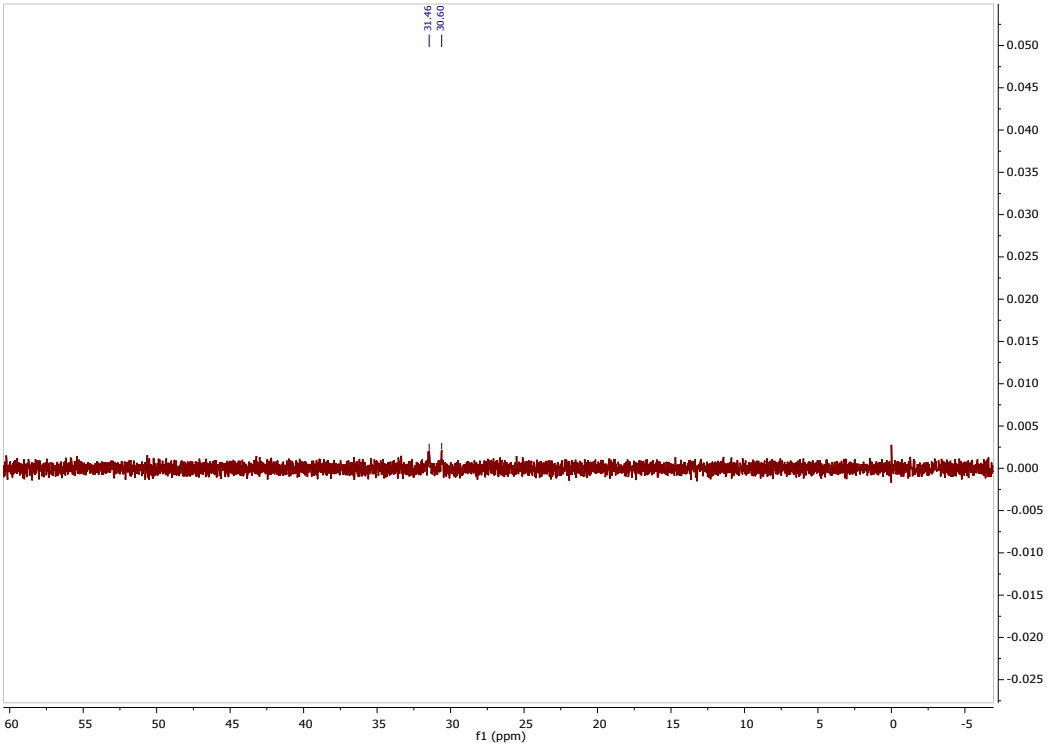

Figure S6. $^{31}P\{^{1}H\}$ NMR spectrum of $[Rh(PPh_3)_2(CO)(2\text{-pyridinemethanol})][NO_3]$ (**8b**) in C_6D_6. Signal at 0 ppm is an artifact.

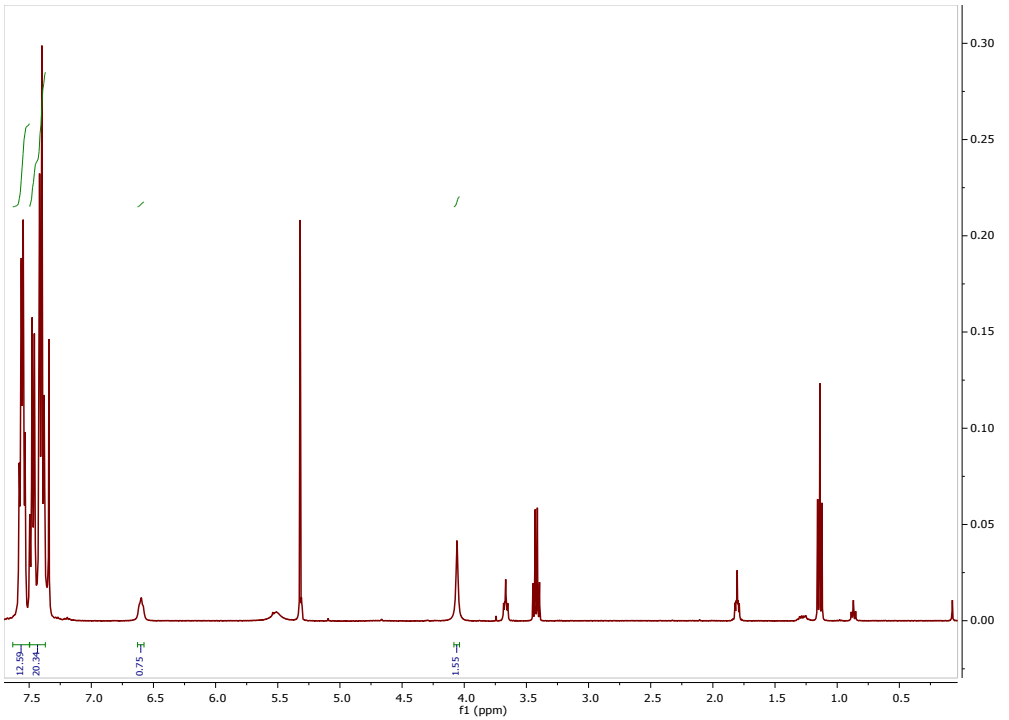

Figure S7. ^{1}H NMR spectrum of $[Ir(PPh_3)_2(CO)(3\text{-pyridinemethanol})][NO_3]$ (**9a**) in CD_2Cl_2. Solvent impurity at 0.8 ppm and 1.3 ppm is pentane. Solvent impurity at 1.8 ppm and 3.75 ppm is tetrahydrofuran. Solvent impurity at 1.15 ppm and 3.43 ppm is diethyl ether. Solvent impurity at 0.09 ppm is silicone grease.

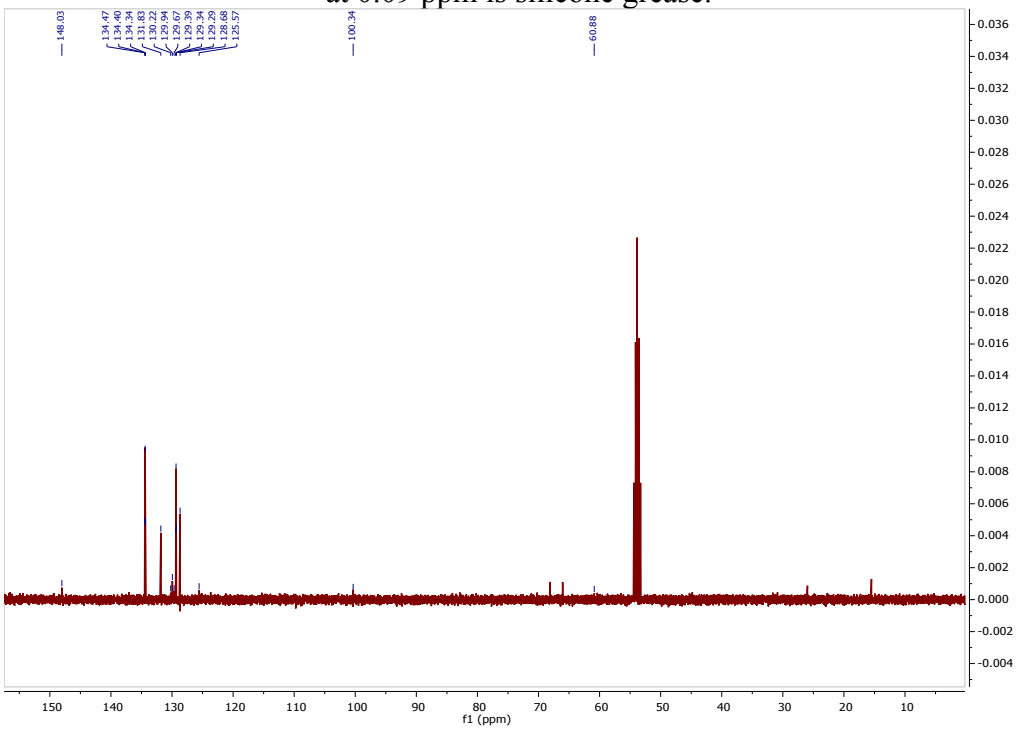

Figure S8. $^{13}C\{^{1}H\}$ NMR spectrum of $[Ir(PPh_3)_2(CO)(3\text{-pyridinemethanol})][NO_3]$ (**9a**) in CD_2Cl_2. Solvent impurity at 68 ppm and 25 is tetrahydrofuran. Solvent impurity at 66 ppm and 15 ppm is diethyl ether.

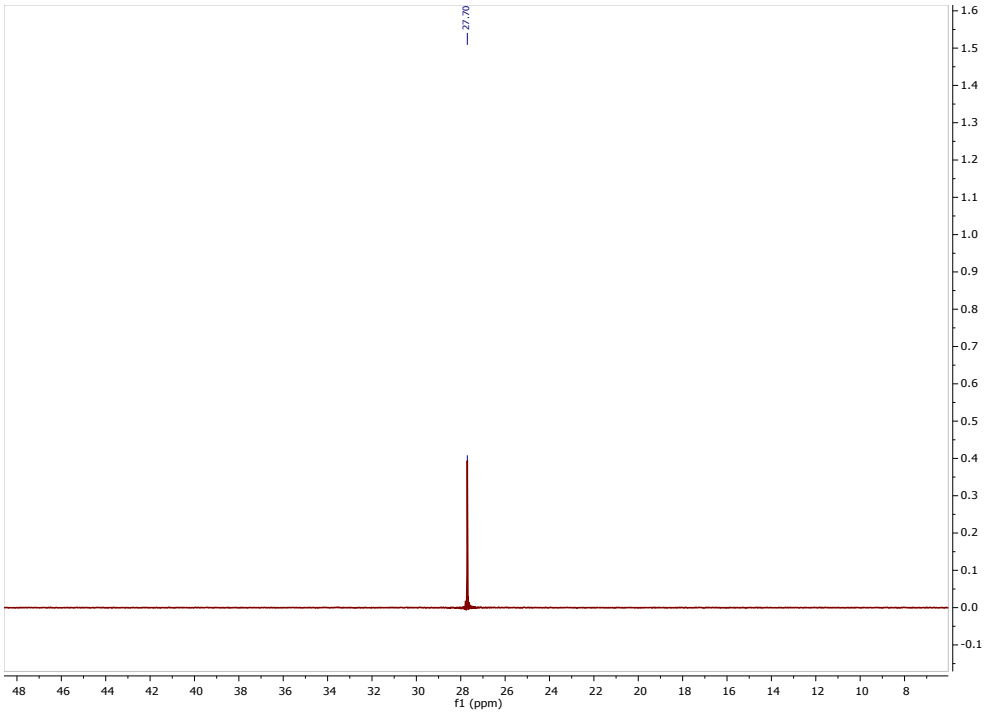

Figure S9. $^{31}P\{^{1}H\}$ NMR spectrum of $[Ir(PPh_3)_2(CO)(3\text{-pyridinemethanol})][NO_3]$ (**9a**) in CD_2Cl_2.

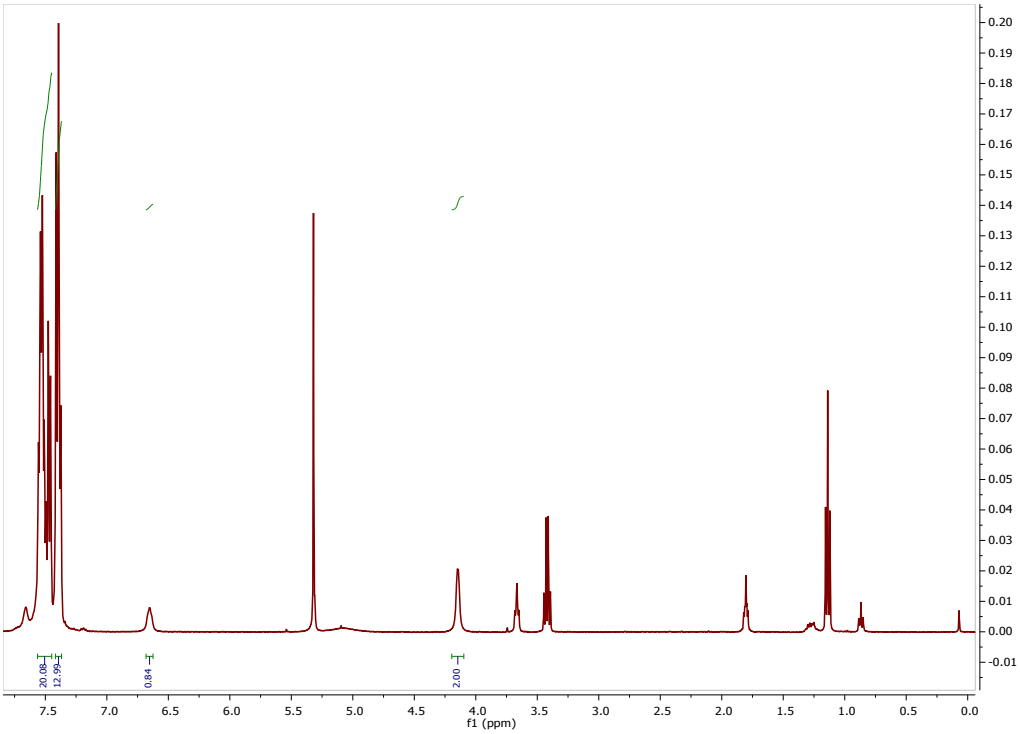

Figure S10. ^{1}H NMR spectrum of $[Rh(PPh_3)_2(CO)(3\text{-pyridinemethanol})][NO_3]$ (**9b**) in CD_2Cl_2. Solvent impurity at 0.8 ppm and 1.3 ppm is pentane. Solvent impurity at 1.8 ppm and 3.7 ppm is tetrahydrofuran. Solvent impurity at 1.15 ppm and 3.43 ppm is diethyl ether. Solvent impurity at 0.09 ppm is silicone grease.

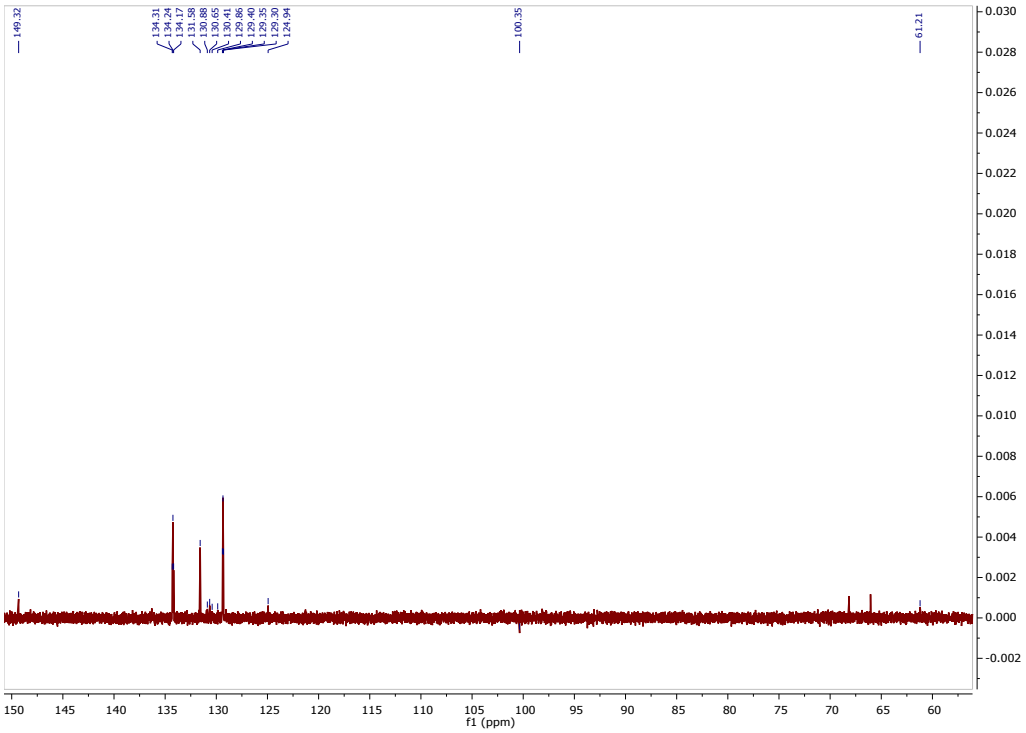

Figure S11. $^{13}C\{^{1}H\}$ NMR spectrum of $[Rh(PPh_3)_2(CO)(3\text{-pyridinemethanol})][NO_3]$ (**9b**) in CD_2Cl_2. Solvent impurities at 66 and 68 ppm are diethyl ether and THF.

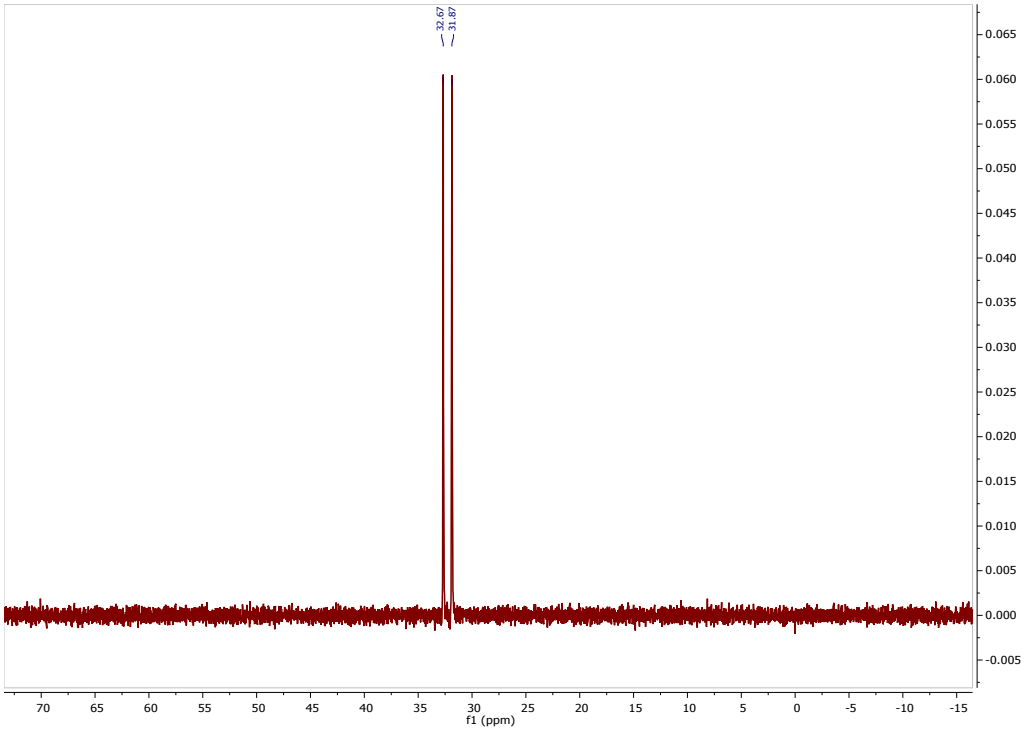

Figure S12. $^{31}P\{^{1}H\}$ NMR spectrum of $[Rh(PPh_3)_2(CO)(3\text{-pyridinemethanol})][NO_3]$ (**9b**) in CD_2Cl_2.

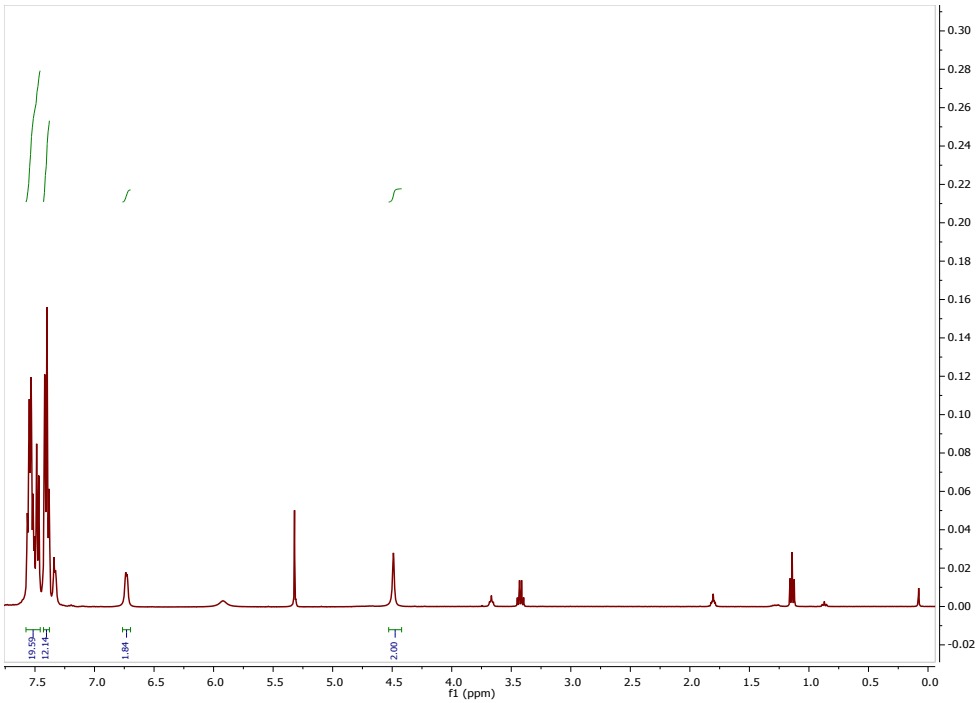

Figure S13. ^{1}H NMR spectrum of $[Ir(PPh_3)_2(CO)(4\text{-pyridinemethanol})][NO_3]$ (**10a**) in CD_2Cl_2. Solvent impurity at 0.8 ppm and 1.3 ppm is pentane. Solvent impurity at 1.8 ppm and 3.7 ppm is tetrahydrofuran. Solvent impurity at 1.15 ppm and 3.43 ppm is diethyl ether. Solvent impurity at 0.09 ppm is silicone grease.

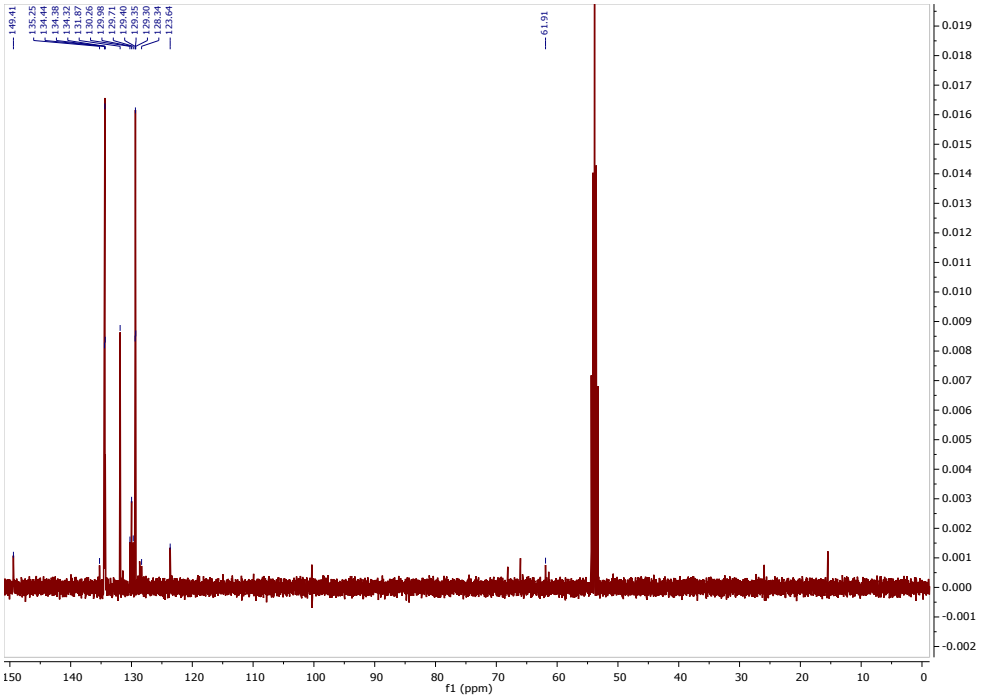

Figure S14. $^{13}C\{^{1}H\}$ NMR spectrum of $[Ir(PPh_3)_2(CO)(4\text{-pyridinemethanol})][NO_3]$ (**10a**) in CD_2Cl_2. Solvent impurity at 68 ppm and 25ppm is tetrahydrofuran. Solvent impurity at 66 ppm and 15 ppm is diethyl ether. Signal at 100 ppm is an artifact.

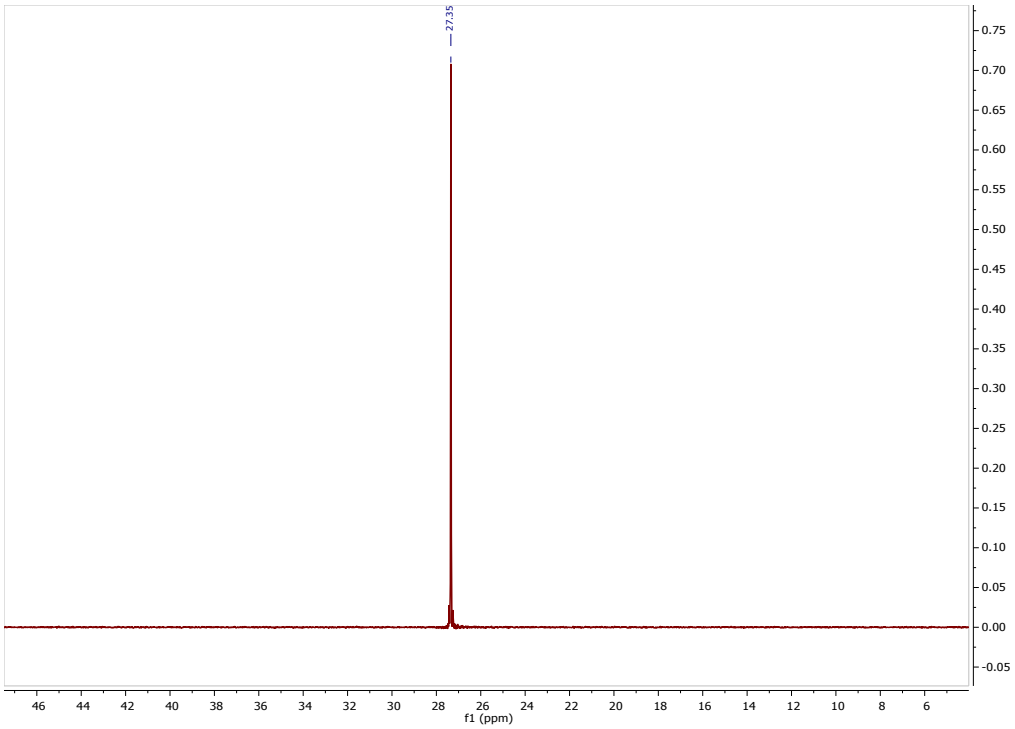

Figure S15. $^{31}P\{^{1}H\}$ NMR spectrum of $[Ir(PPh_3)_2(CO)(4\text{-pyridinemethanol})][NO_3]$ (**10a**) in CD_2Cl_2.

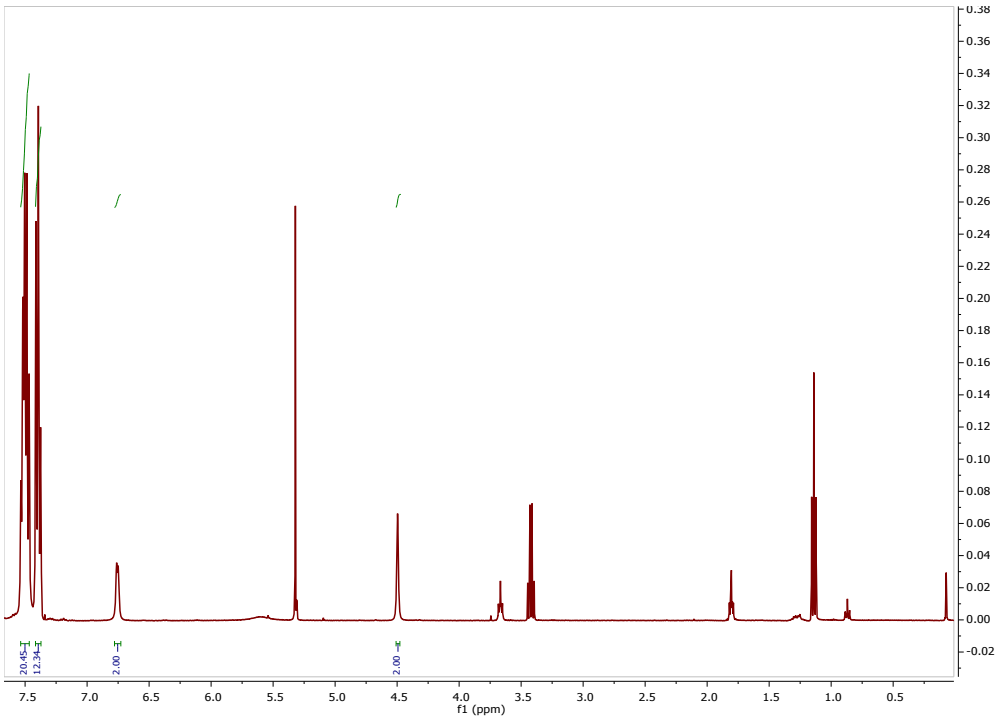

Figure S16. ^{1}H NMR spectrum of $[Rh(PPh_3)_2(CO)(4\text{-pyridinemethanol})][NO_3]$ (**10b**) in CD_2Cl_2. Solvent impurity at 0.8 ppm and 1.3 ppm is pentane. Solvent impurity at 1.8 ppm and 3.7 ppm is tetrahydrofuran. Solvent impurity at 1.15 ppm and 3.43 ppm is diethyl ether. Solvent impurity at 0.09 ppm is silicone grease.

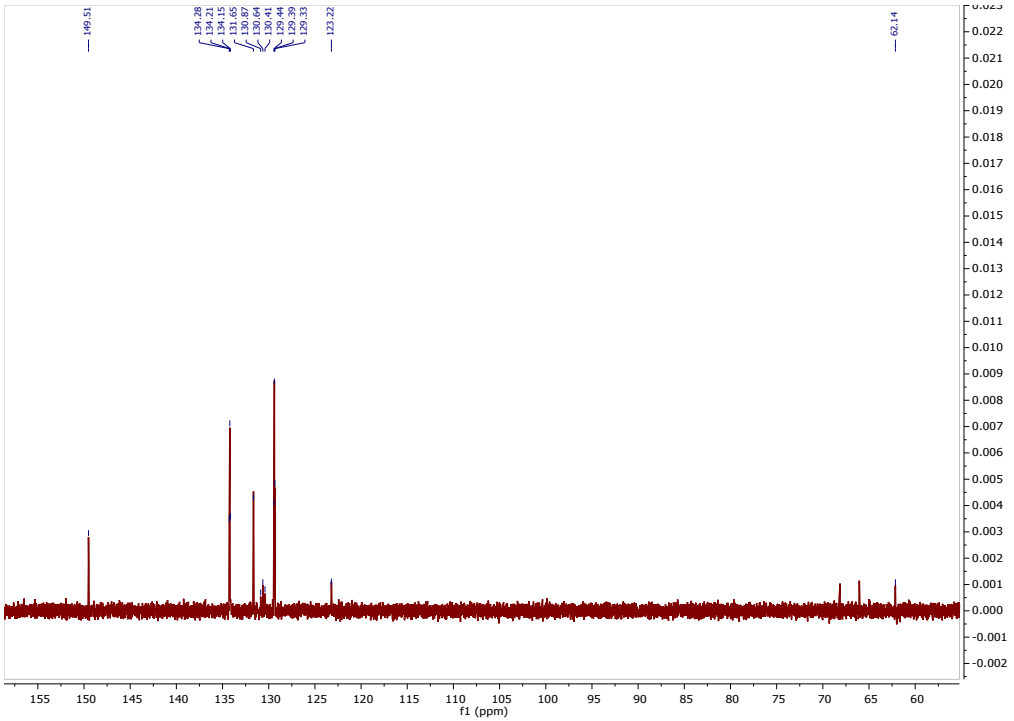

Figure S17. $^{13}C\{^{1}H\}$ NMR spectrum of $[Rh(PPh_3)_2(CO)(4\text{-pyridinemethanol})][NO_3]$ (**10b**) in CD_2Cl_2. Solvent impurity at 68 ppm is tetrahydrofuran. Solvent impurity at 66 ppm is diethyl ether.

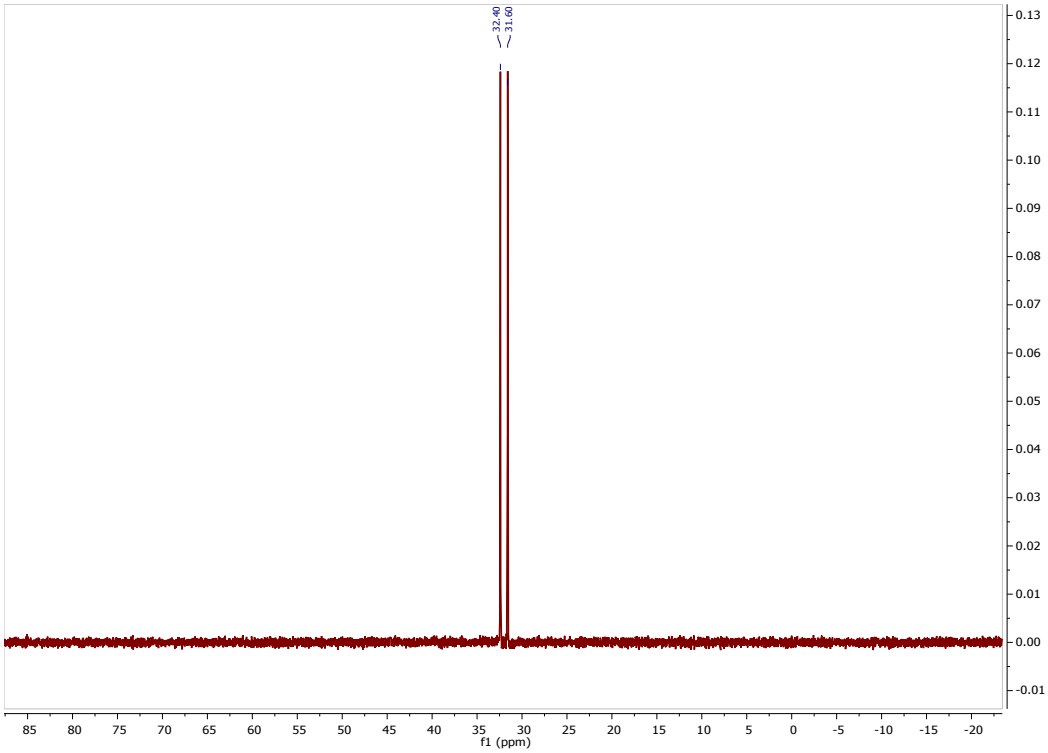

Figure S18. $^{31}P\{^{1}H\}$ NMR spectrum of $[Rh(PPh_3)_2(CO)(4\text{-pyridinemethanol})][NO_3]$ (**10b**) in CD_2Cl_2.

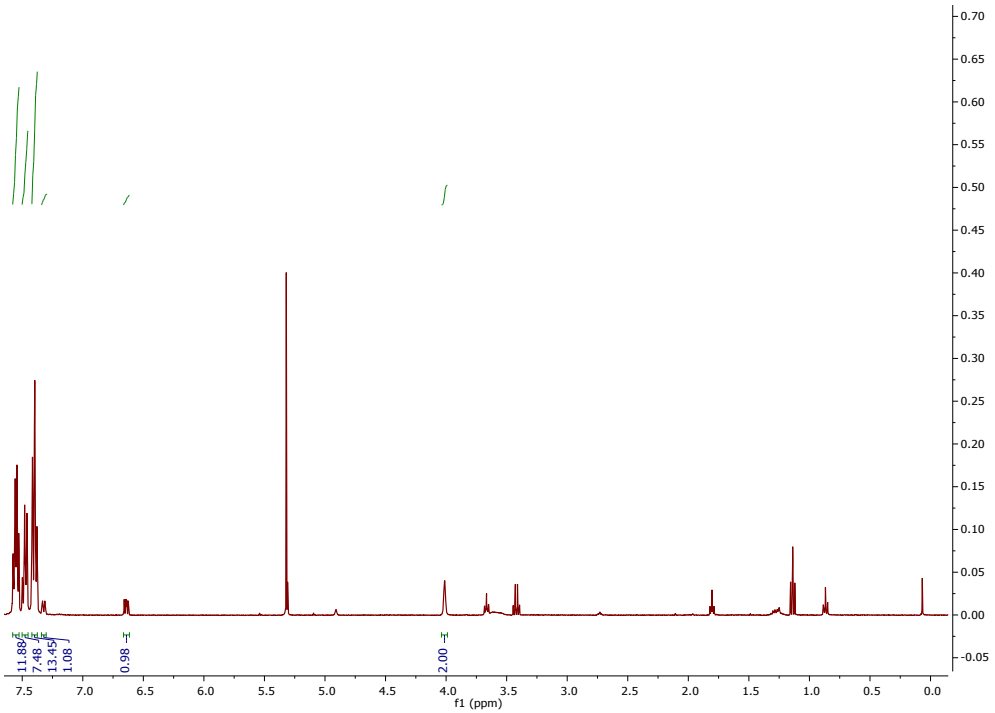

Figure S19. ^{1}H NMR spectrum of $[Ir(PPh_3)_2(CO)(3\text{-pyridinemethanol})][SO_3CF_3]$ (**11a**) in CD_2Cl_2. Solvent impurity at 0.84 ppm and 1.15 ppm is pentane. Solvent impurity at 1.25 ppm and 3.69 ppm is tetrahydrofuran. Solvent impurity at 5.32 is dichloromethane. Signal at 0.07 ppm is silicone grease.

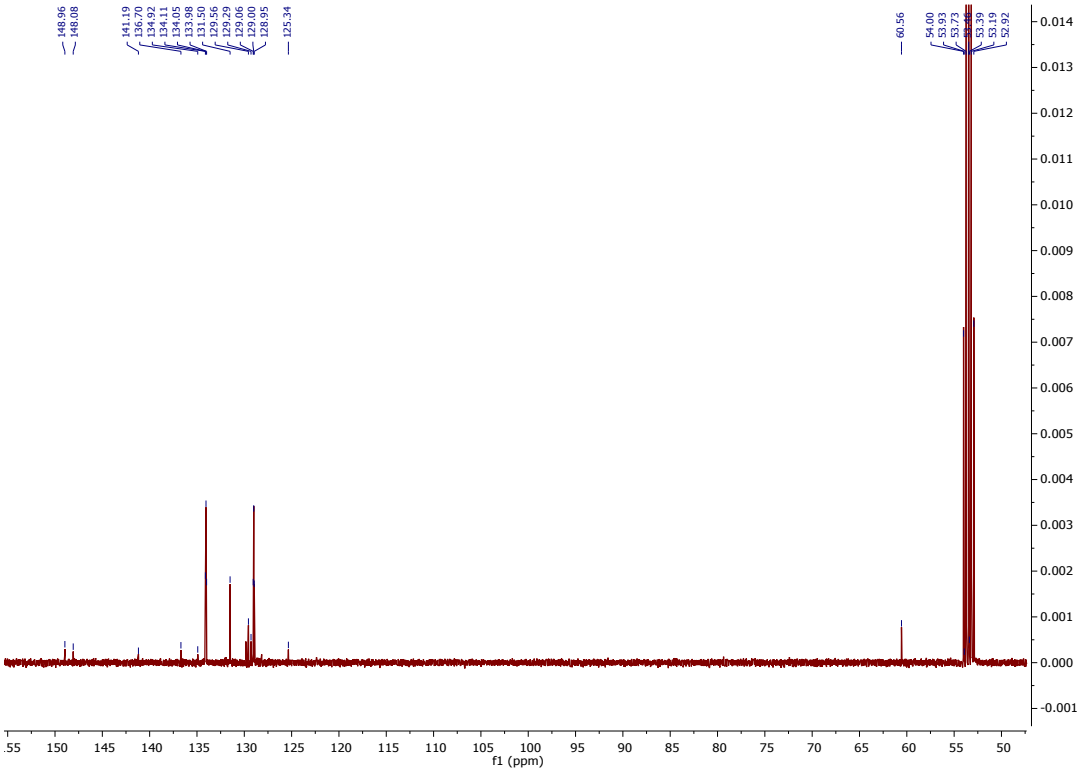

Figure S20. $^{13}C\{^{1}H\}$ NMR spectrum of $[Ir(PPh_3)_2(CO)(3\text{-pyridinemethanol})][SO_3CF_3]$ (**11a**) in CD_2Cl_2.

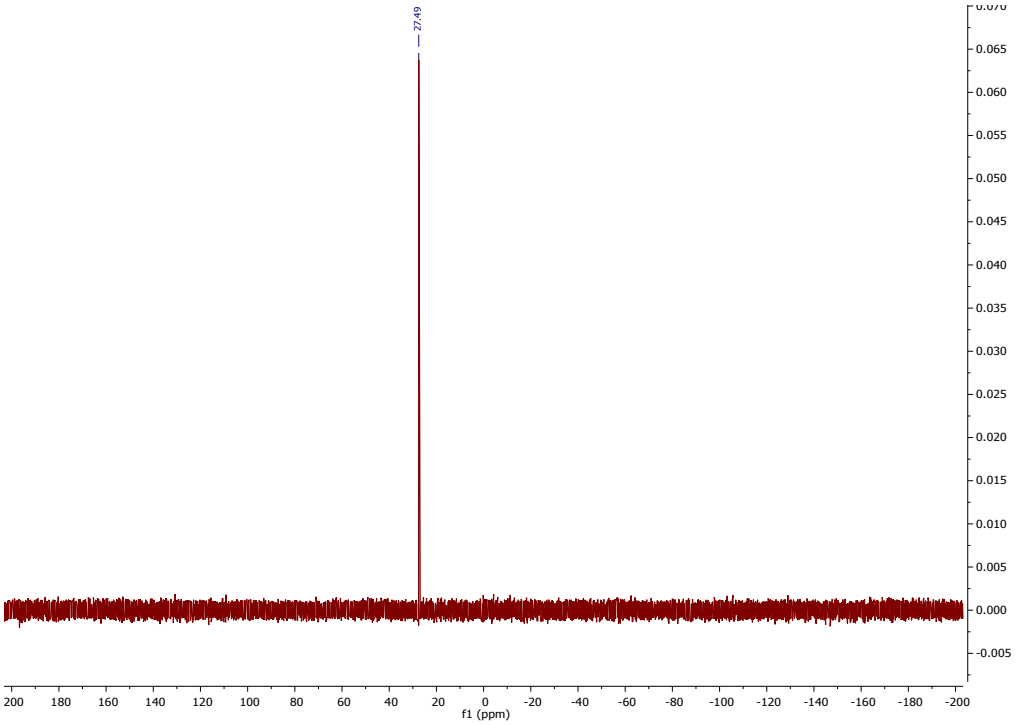

Figure S21. $^{31}P\{^{1}H\}$ NMR spectrum of $[Ir(PPh_3)_2(CO)(3\text{-pyridinemethanol})][SO_3CF_3]$ (**11a**) in CD_2Cl_2.

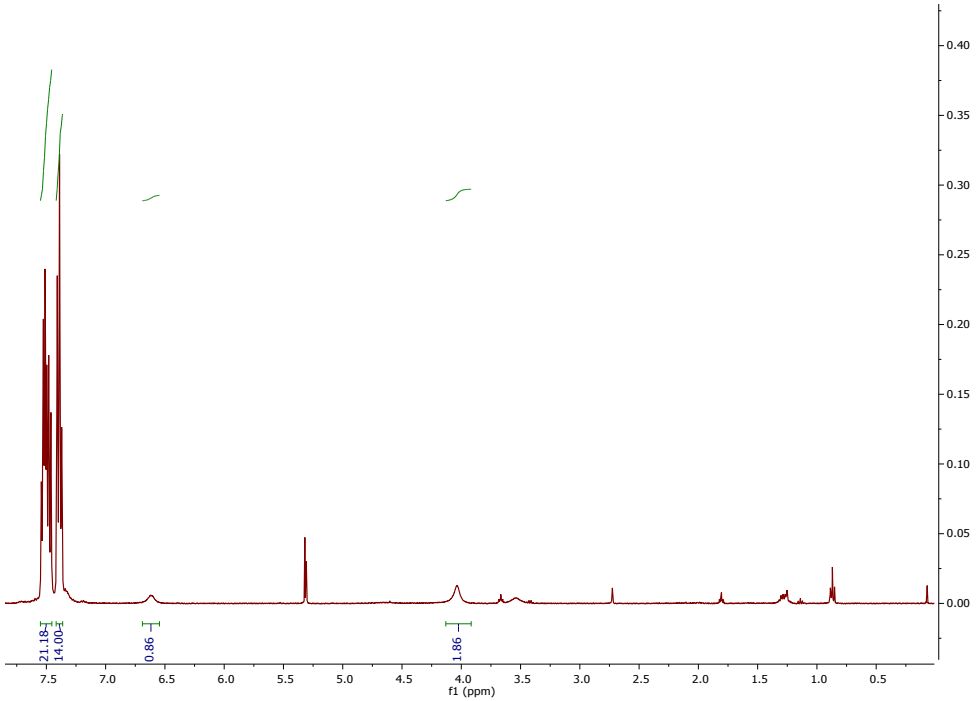

Figure S22. ^{1}H NMR spectrum of $[Rh(PPh_3)_2(CO)(3\text{-pyridinemethanol})][SO_3CF_3]$ (**11b**) in CD_2Cl_2. Solvent impurity at 1.28 ppm and 0.86 ppm is pentane. Solvent impurity at 1.8 ppm and 3.66 ppm is tetrahydrofuran. Solvent impurity at 5.32 is dichloromethane. Solvent impurity at 1.13 ppm is diethyl ether Signal at 0.069 ppm is silicone grease.

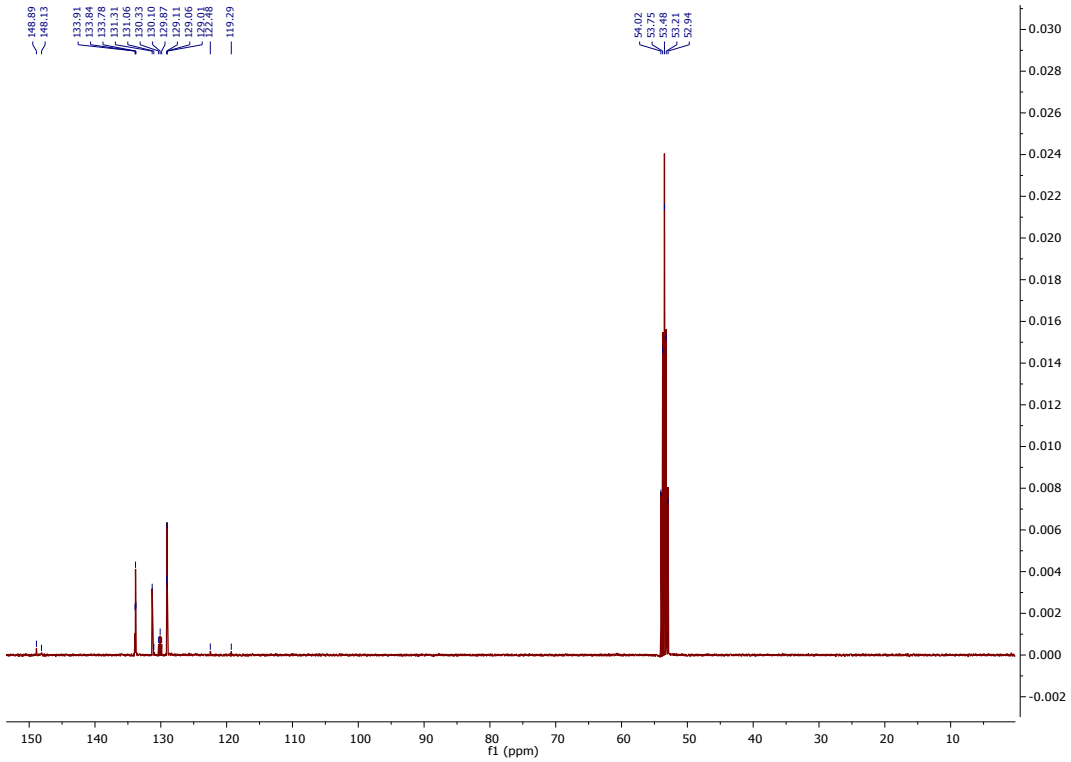

Figure S23. $^{13}C\{^{1}H\}$ NMR spectrum of $[Rh(PPh_3)_2(CO)(3\text{-pyridinemethanol})][SO_3CF_3]$ (**11b**) in CD_2Cl_2.

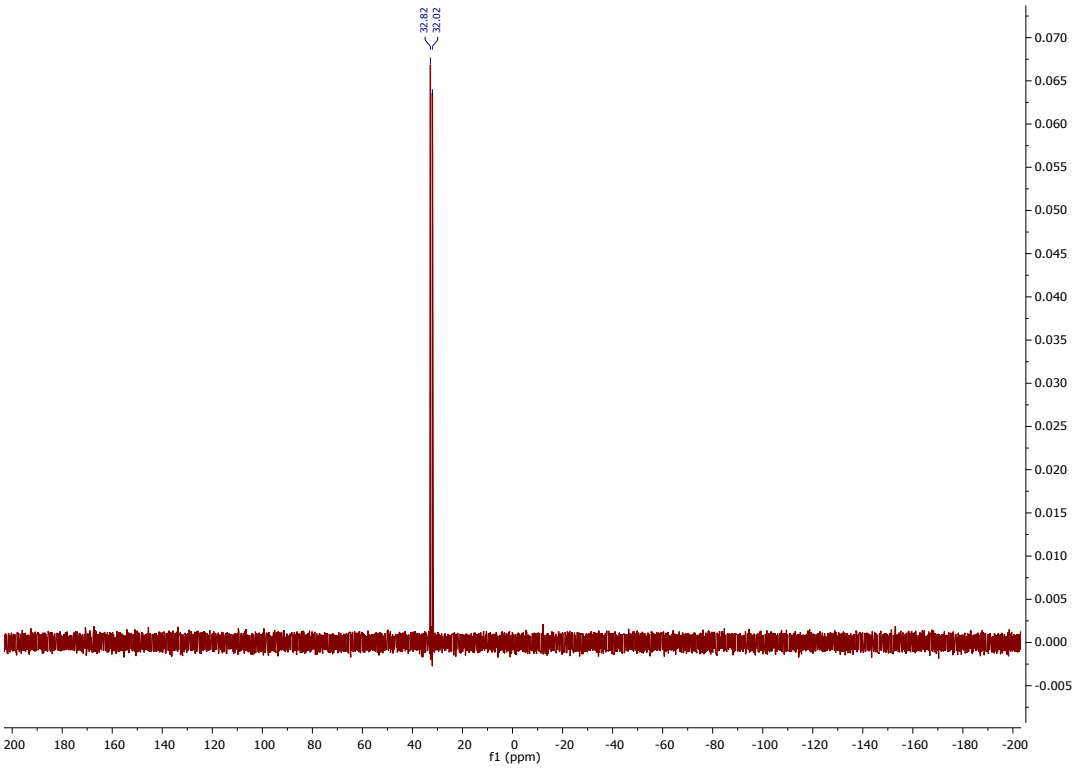

Figure S24. $^{31}P\{^{1}H\}$ NMR spectrum of $[Rh(PPh_3)_2(CO)(3\text{-pyridinemethanol})][SO_3CF_3]$ (**11b**) in CD_2Cl_2.

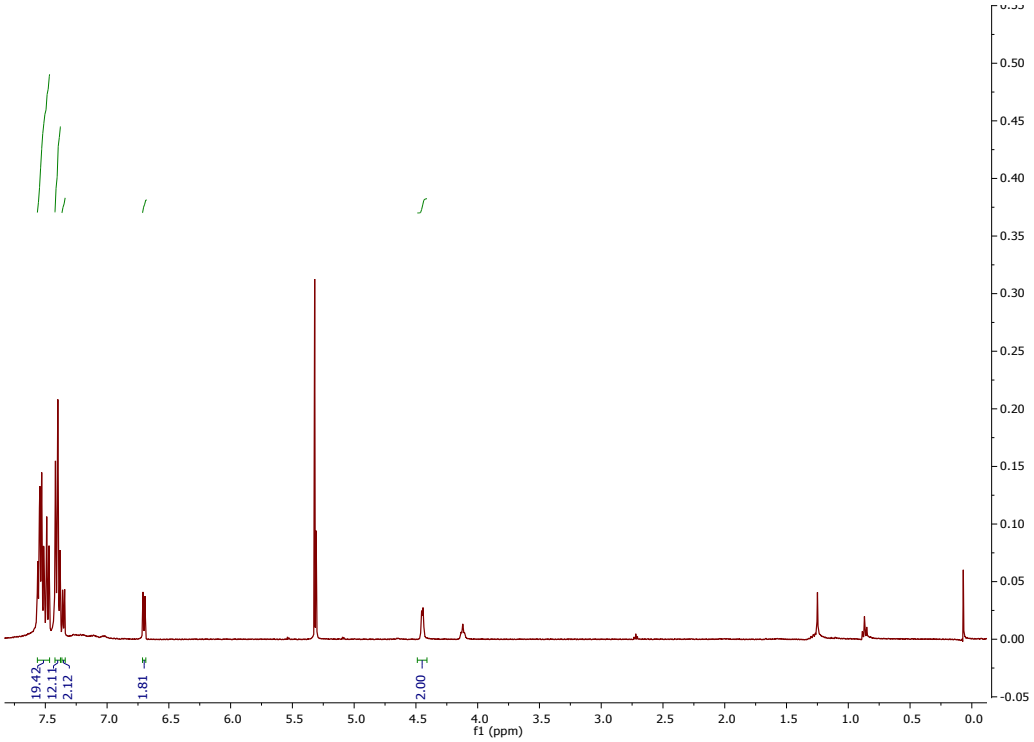

Figure S25. ^{1}H NMR spectrum of $[Ir(PPh_3)_2(CO)(4\text{-pyridinemethanol})][SO_3CF_3]$ (**12a**) in CD_2Cl_2. Solvent impurity at ppm 0.87 ppm is pentane. Solvent impurity at 1.24 ppm and 4.12 ppm is tetrahydrofuran. Solvent impurity at 5.32 is dichloromethane. Signal at 0.08 ppm is silicone grease.

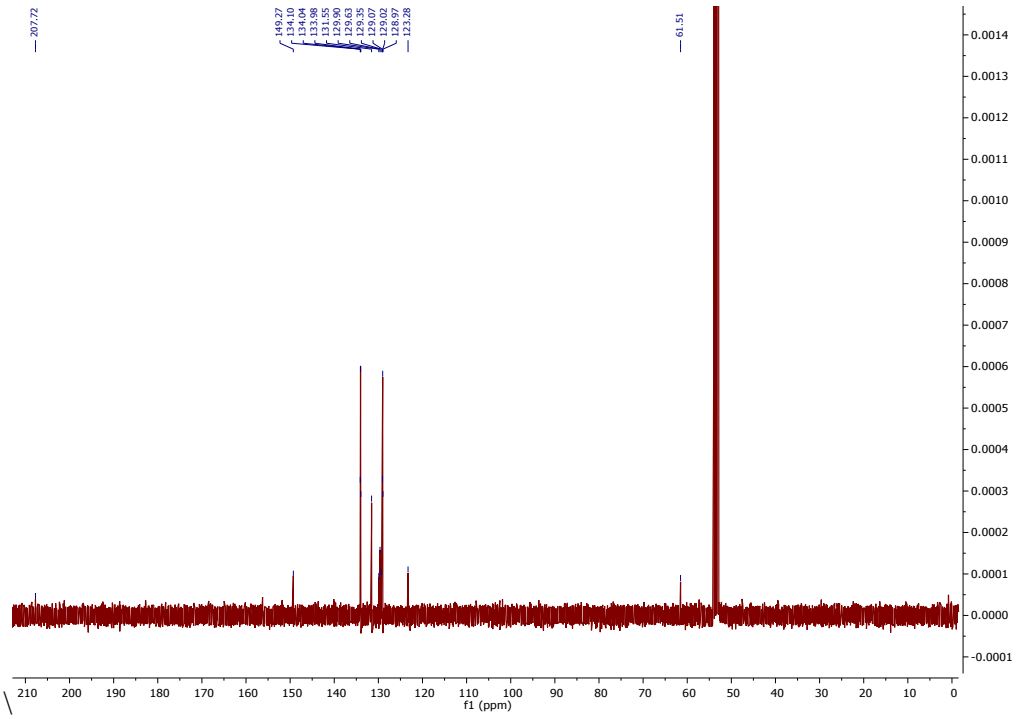

Figure S26. $^{13}C\{^{1}H\}$ NMR spectrum of $[Ir(PPh_3)_2(CO)(4\text{-pyridinemethanol})][SO_3CF_3]$ (**12a**) in CD_2Cl_2.

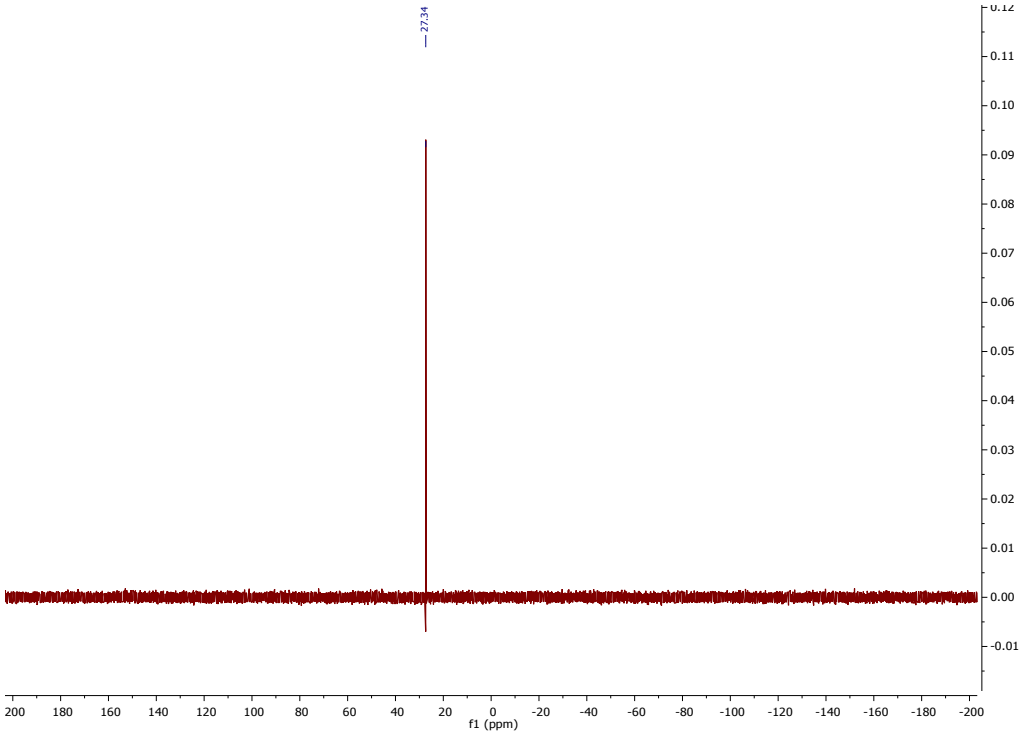

Figure S27. $^{31}P\{^{1}H\}$ NMR spectrum of $[Ir(PPh_3)_2(CO)(4\text{-pyridinemethanol})][SO_3CF_3]$ (**12a**) in CD_2Cl_2.

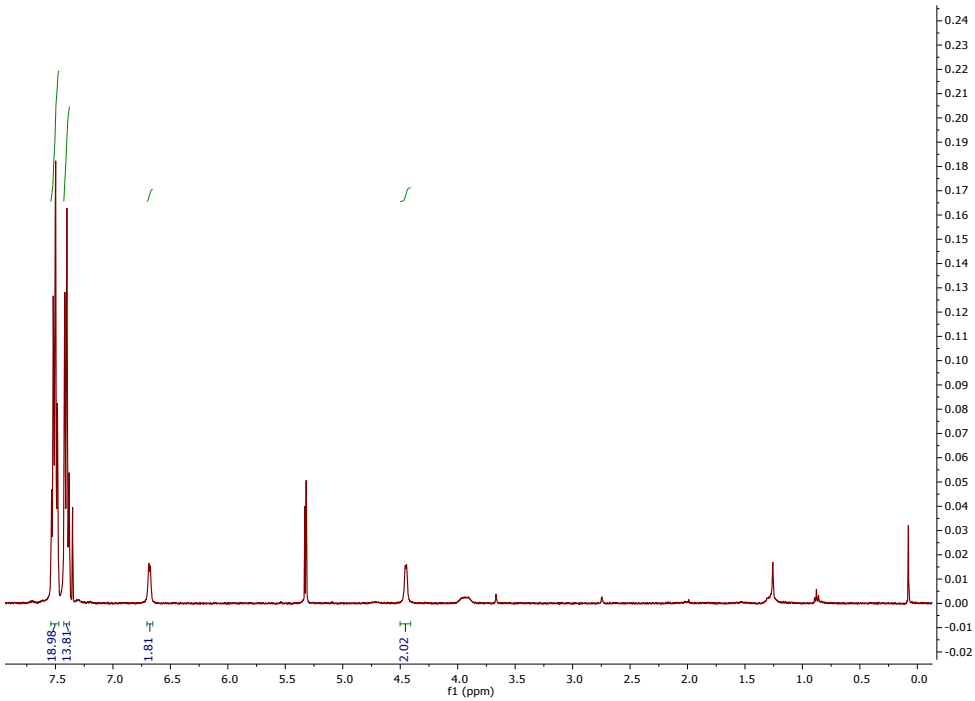

Figure S28. ^{1}H NMR spectrum of $[Rh(PPh_3)_2(CO)(4\text{-pyridinemethanol})][SO_3CF_3]$ (**12b**) in CD_2Cl_2. Solvent impurity at 0.87 ppm is pentane. Solvent impurity at 1.26 ppm and 3.66 ppm is tetrahydrofuran. Solvent impurity at 5.32 is dichloromethane. Signal at 0.07 ppm is silicone grease.

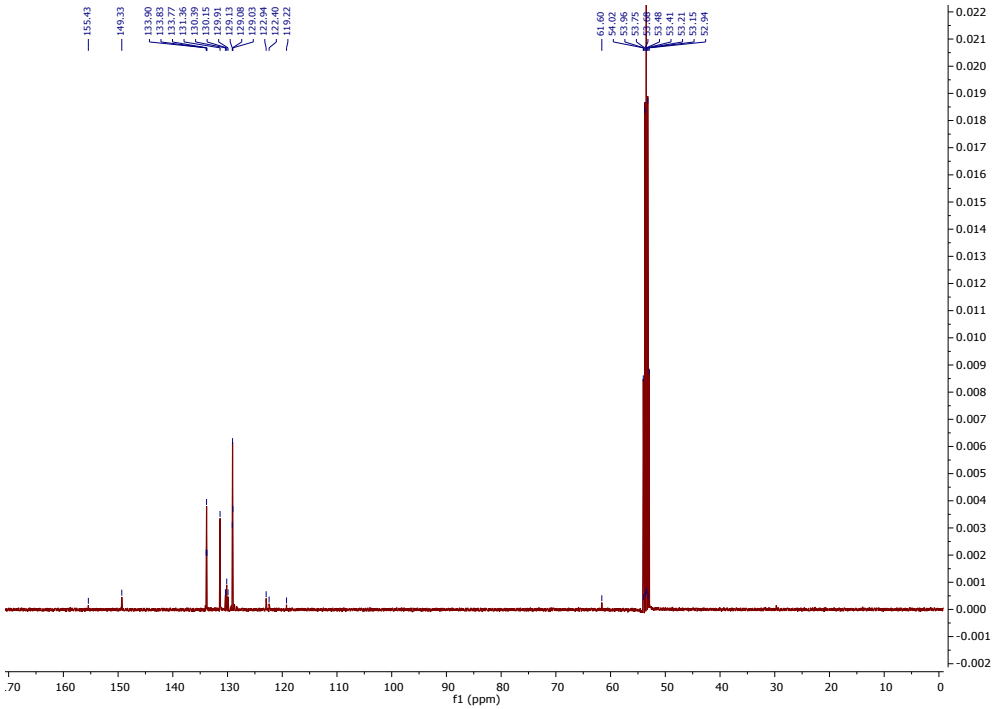

Figure S29. $^{13}C\{^{1}H\}$ NMR spectrum of $[Rh(PPh_3)_2(CO)(4\text{-pyridinemethanol})][SO_3CF_3]$ (**12b**) in CD_2Cl_2.

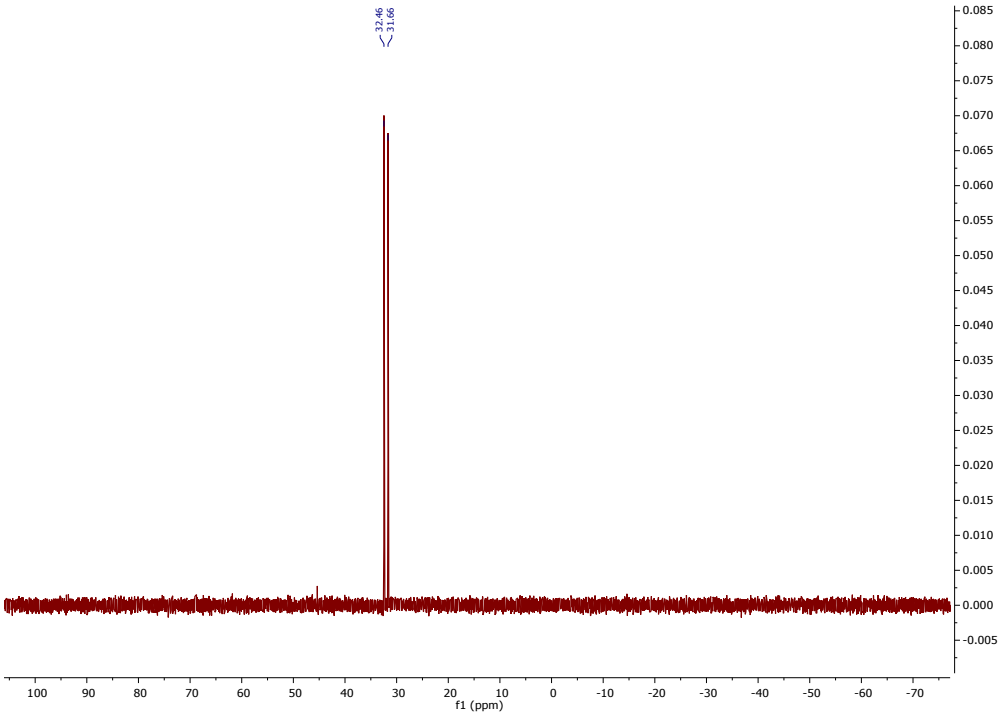

Figure S30. $^{31}P\{^{1}H\}$ NMR spectrum of $[Rh(PPh_3)_2(CO)(4\text{-pyridinemethanol})][SO_3CF_3]$ (**12b**) in CD_2Cl_2.

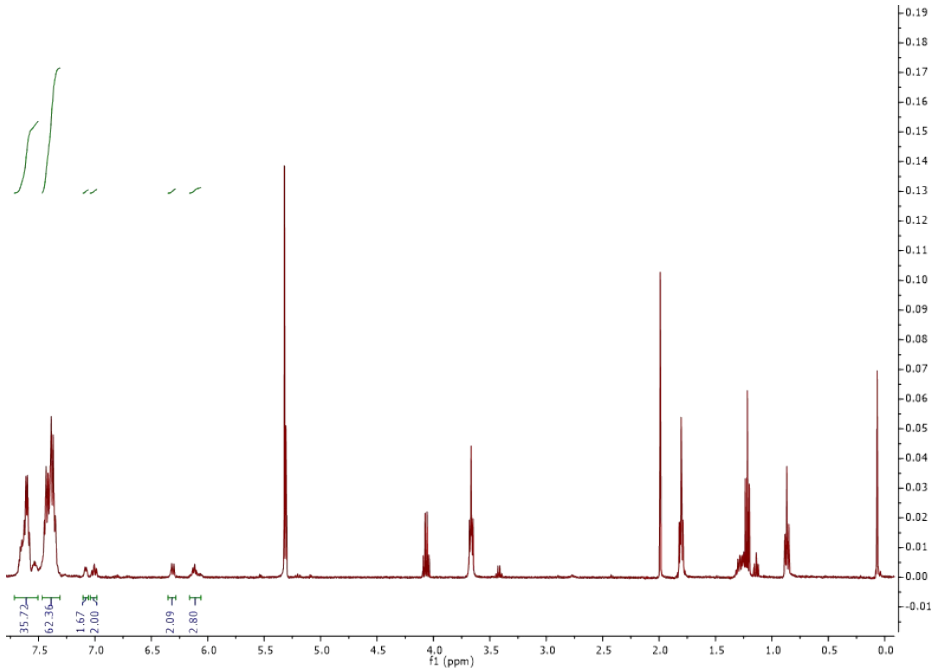

Figure S31. ^{1}H NMR spectrum of $[Ir(PPh_3)_2(CO)(2\text{-hydroxypyridine})][SO_3CF_3]$ (**13a**) in CD_2Cl_2. Solvent impurity at 0.86 ppm and1.21 ppm is pentane. Solvent impurity at 1.8 ppm and 3.66 ppm is tetrahydrofuran. Solvent impurity at 5.32 ppm is dichloromethane. Solvent impurity at 3.42 is diethyl ether. Solvent impurity at 4 ppm is ethyl acetate. Solvent impurity at 1.98 ppm is acetone. Signal at 0.07 ppm is silicone grease.

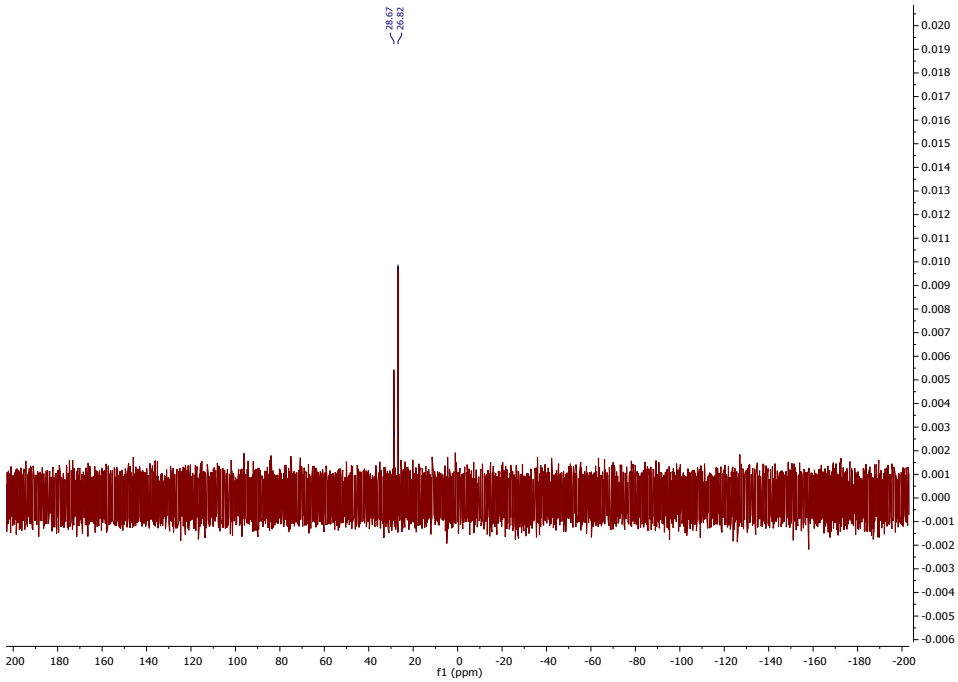

Figure S32. $^{31}P\{^{1}H\}$ NMR spectrum of $[Ir(PPh_3)_2(CO)(2\text{-hydroxypyridine})][SO_3CF_3]$ (**13a**) in CD_2Cl_2.

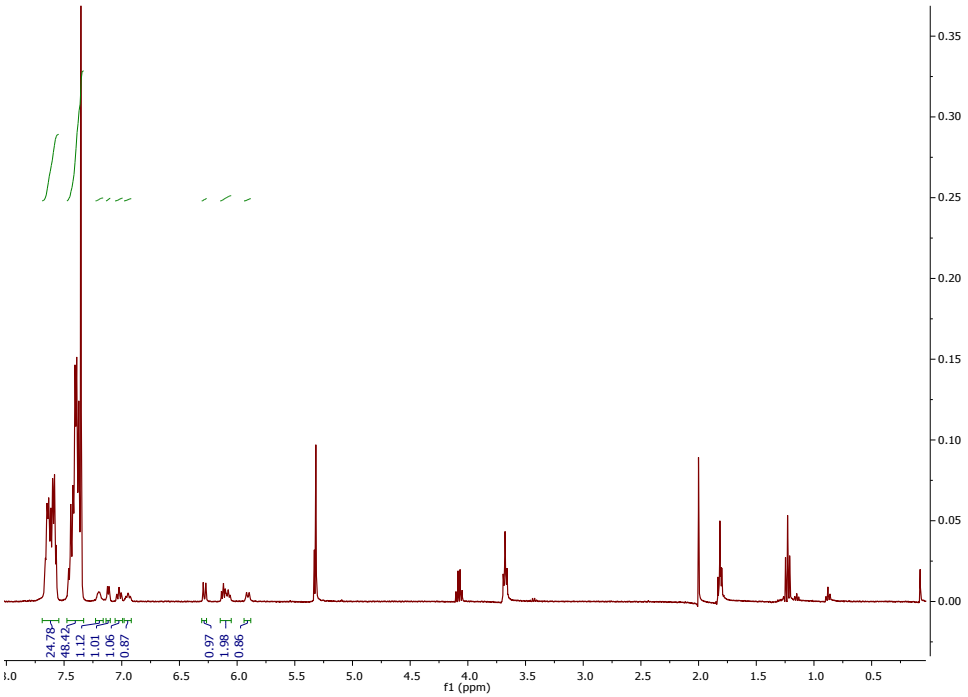

Figure S33. ^{1}H NMR spectrum of $[Rh(PPh_3)_2(CO)(2\text{-hydroxypyridine})][SO_3CF_3]$ (**13b**) in CD_2Cl_2. Solvent impurity at 0.87 ppm and 1.22 ppm is pentane. Solvent impurity at 3.66 ppm and 4.08 ppm is tetrahydrofuran. Solvent impurity at 5.32 ppm is dichloromethane. Solvent impurity at 2 is acetone. Signal at 0.079 ppm is silicone grease.

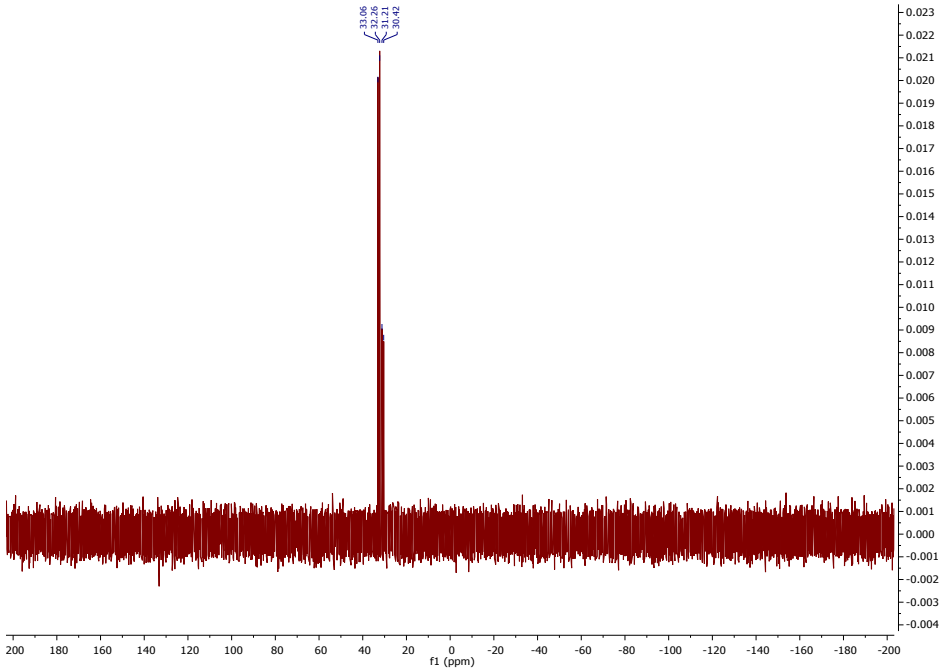

Figure S34. $^{31}P\{^{1}H\}$ NMR spectrum of $[Rh(PPh_3)_2(CO)(2\text{-hydroxypyridine})][SO_3CF_3]$ (**13b**) in CD_2Cl_2.

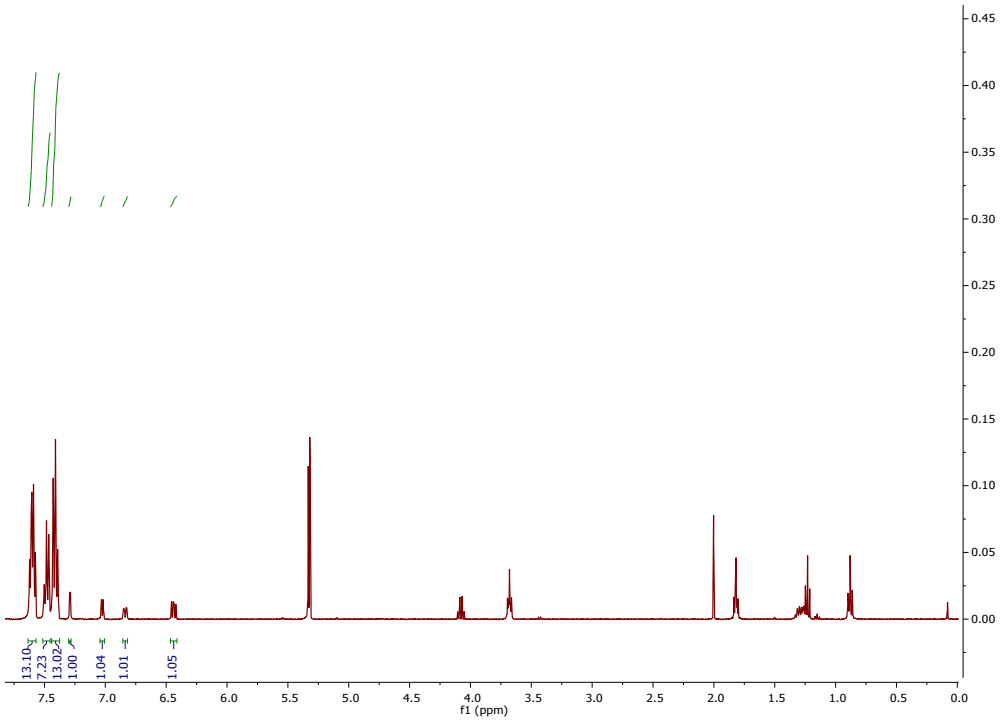

Figure S35. ^{1}H NMR spectrum of $[Ir(PPh_3)_2(CO)(3\text{-hydroxypyridine})][SO_3CF_3]$ (**14a**) in CD_2Cl_2. Solvent impurity at 0.88 ppm and 1.23 ppm is pentane. Solvent impurity at 1.81 ppm and 3.67 ppm is tetrahydrofuran. Solvent impurity at 5.32 is dichloromethane. Solvent impurity at 2 ppm is acetone. Solvent impurity at 4 ppm is ethyl acetate. Signal at 0.08 ppm is silicone grease.

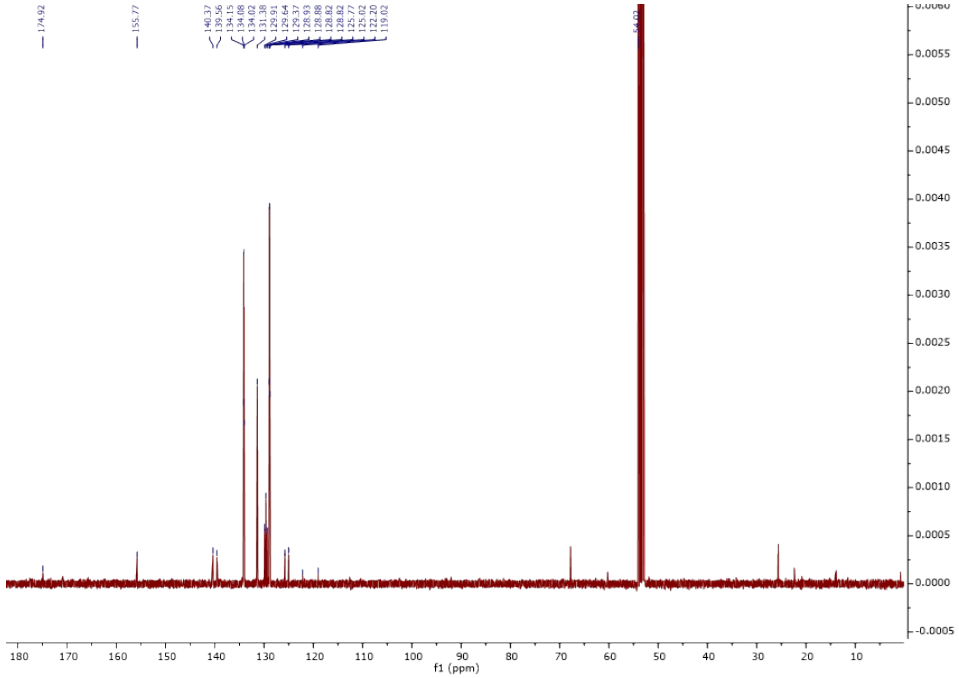

Figure S36. $^{13}C\{^{1}H\}$ NMR spectrum of $[Ir(PPh_3)_2(CO)(3\text{-hydroxypyridine})][SO_3CF_3]$ (**14a**) in CD_2Cl_2. Solvent impurity at 67 ppm and 25.6 ppm is tetrahydrofuran. Solvent impurity at 22 ppm is pentane Solvent impurity at 14 ppm is diethyl ether.

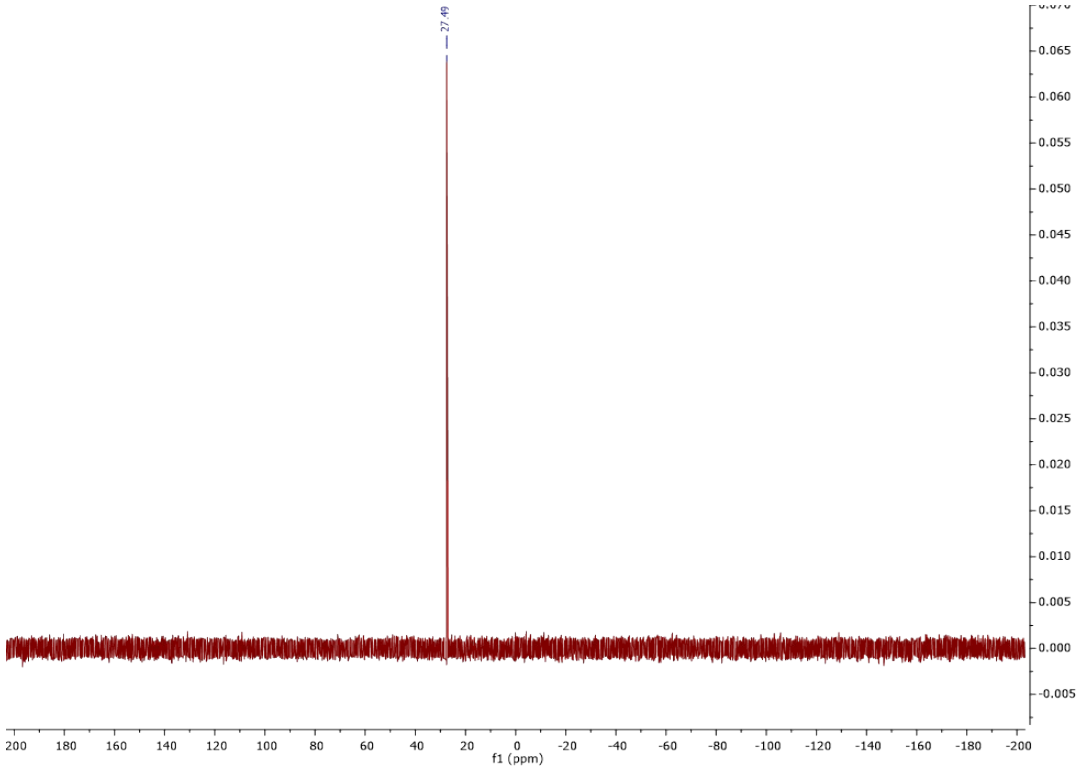

Figure S37. $^{31}P\{^{1}H\}$ NMR spectrum of $[Ir(PPh_3)_2(CO)(3\text{-hydroxypyridine})][SO_3CF_3]$ (**14a**) in CD_2Cl_2.

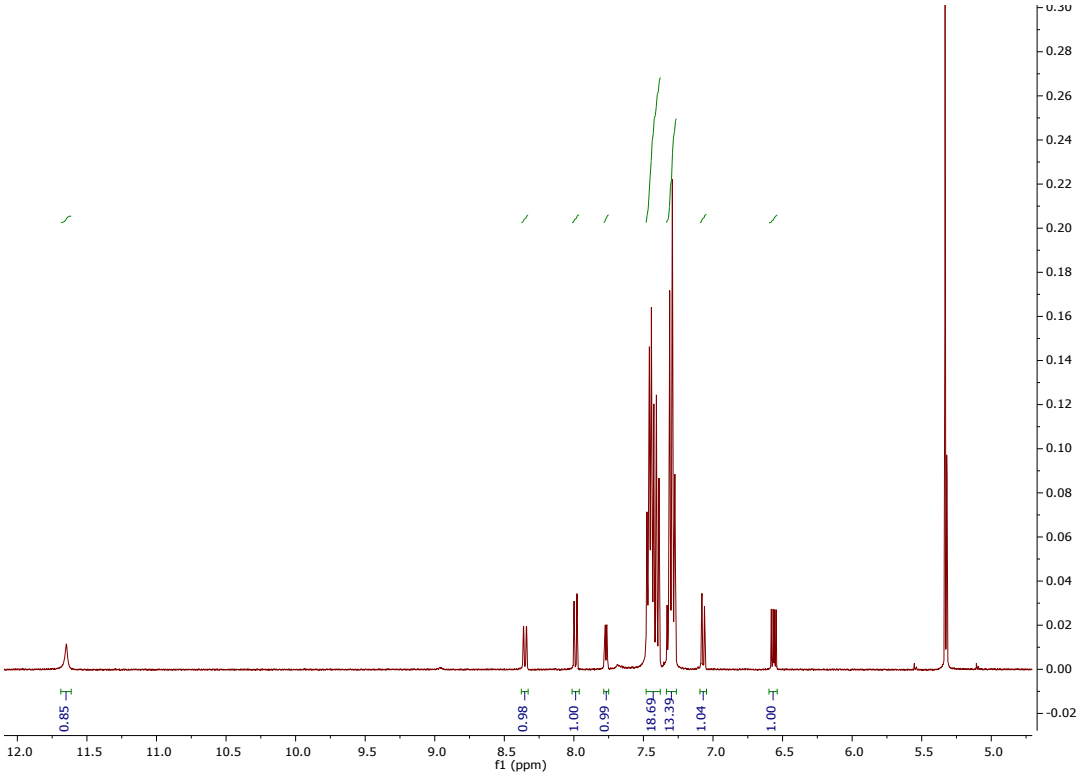

Figure S38. ^{1}H NMR spectrum of $[Ir(PPh_3)_2(CO)(5\text{-hydroxyquinoline})][NO_3]$ (**15a**) in CD_2Cl_2.

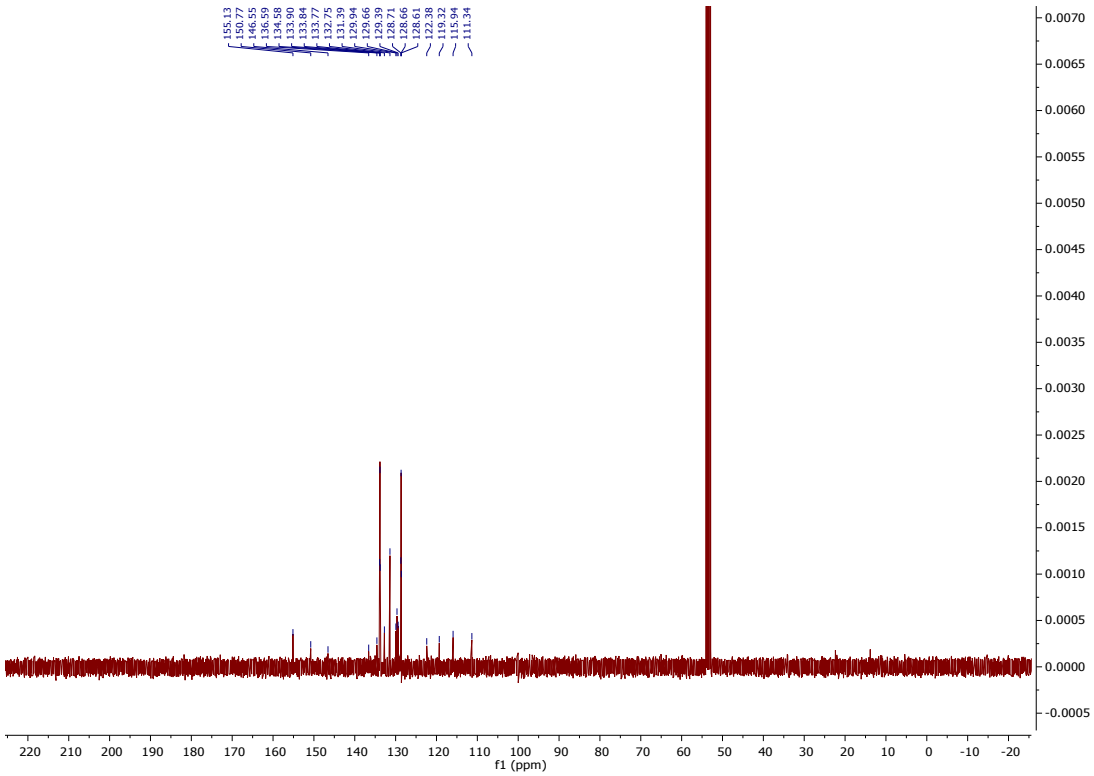

Figure S39. $^{13}C\{^{1}H\}$ NMR spectrum of $[Ir(PPh_3)_2(CO)(5\text{-hydroxyquinoline})][NO_3]$ (**15a**) in CD_2Cl_2.

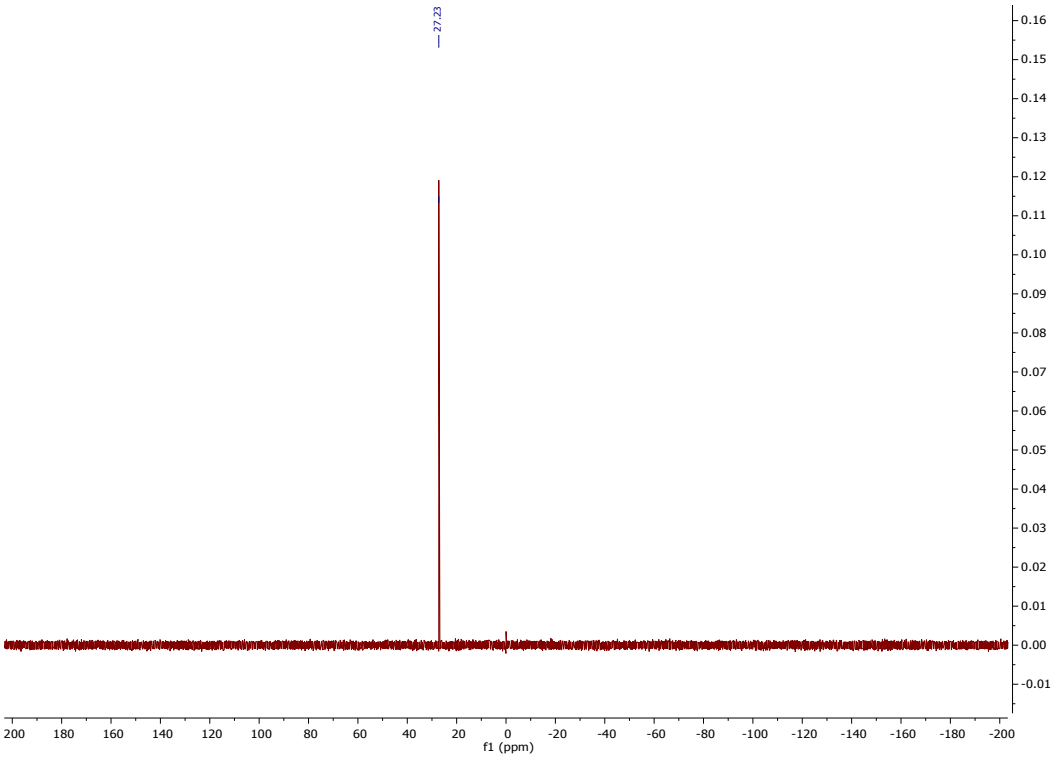

Figure S40. $^{31}P\{^{1}H\}$ NMR spectrum of $[Ir(PPh_3)_2(CO)(5\text{-hydroxyquinoline})][NO_3]$ (**15a**) in CD_2Cl_2.

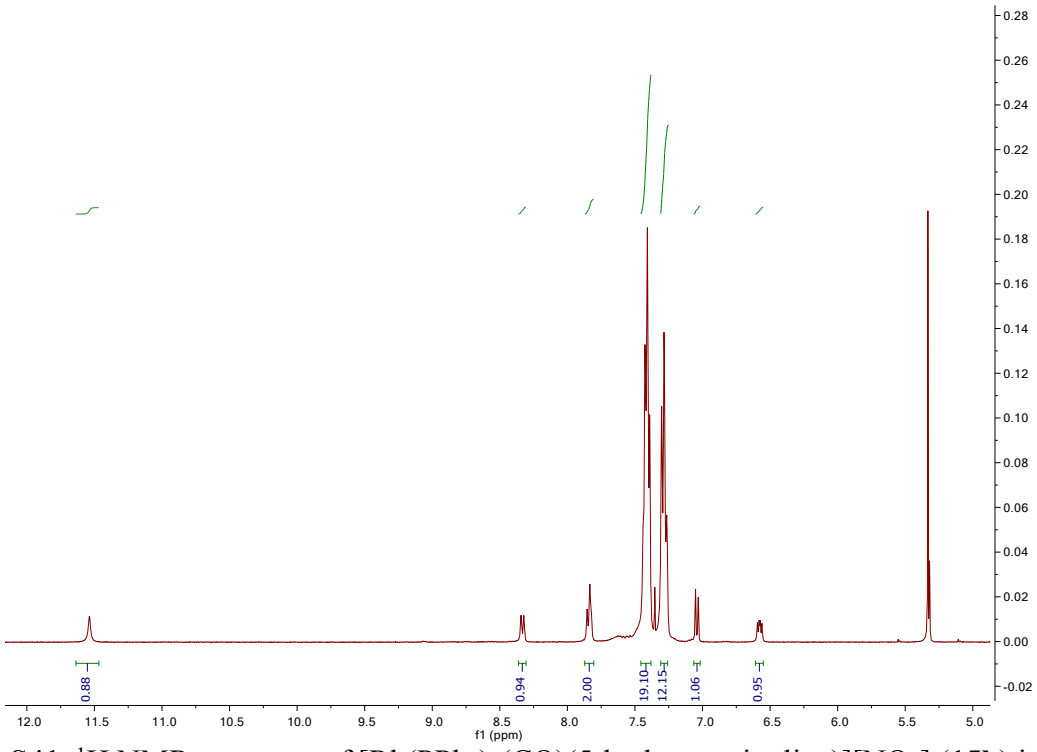

Figure S41. ^{1}H NMR spectrum of $[Rh(PPh_3)_2(CO)(5\text{-hydroxyquinoline})][NO_3]$ (**15b**) in CD_2Cl_2.

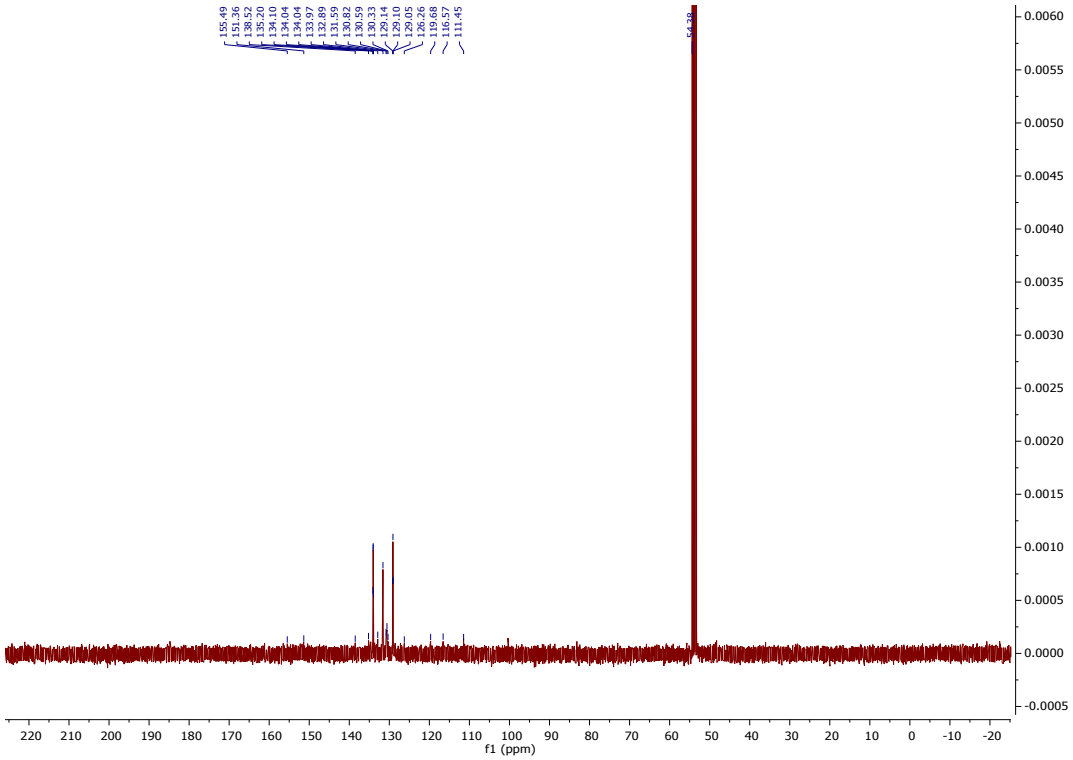

Figure S42. $^{13}C\{^{1}H\}$ NMR spectrum of $[Rh(PPh_3)_2(CO)(5\text{-hydroxyquinoline})][NO_3]$ (**15b**) in CD_2Cl_2.

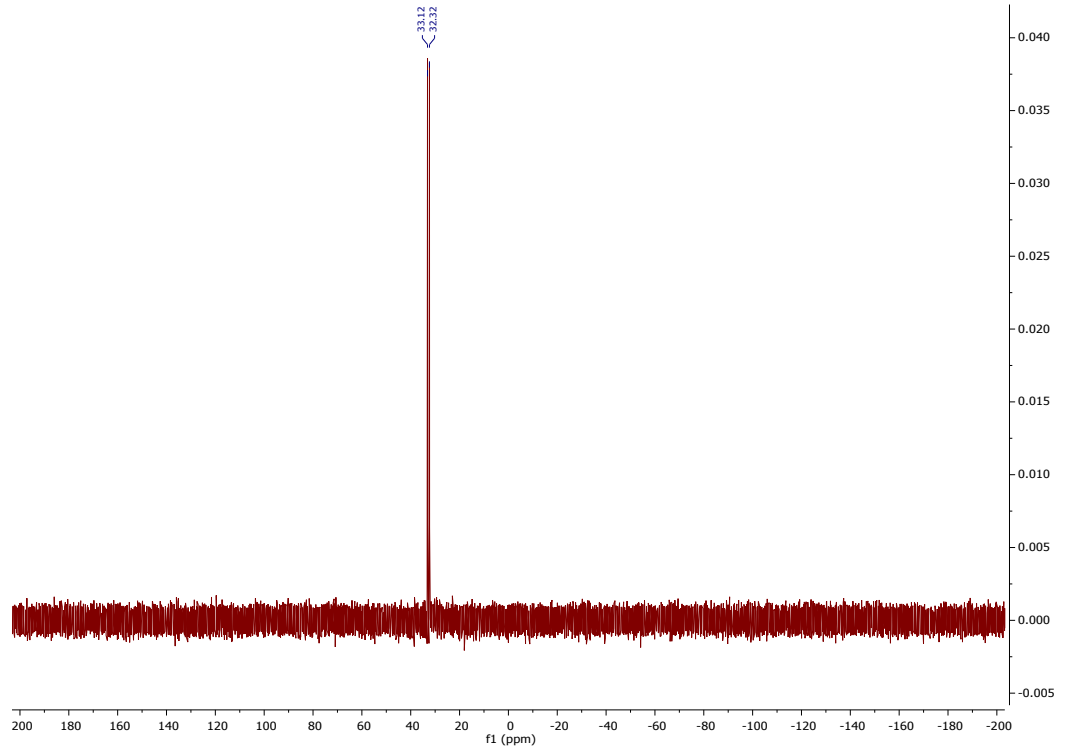

Figure S43. $^{31}P\{^{1}H\}$ NMR spectrum of $[Rh(PPh_3)_2(CO)(5\text{-hydroxyquinoline})][NO_3]$ (**15b**) in CD_2Cl_2.

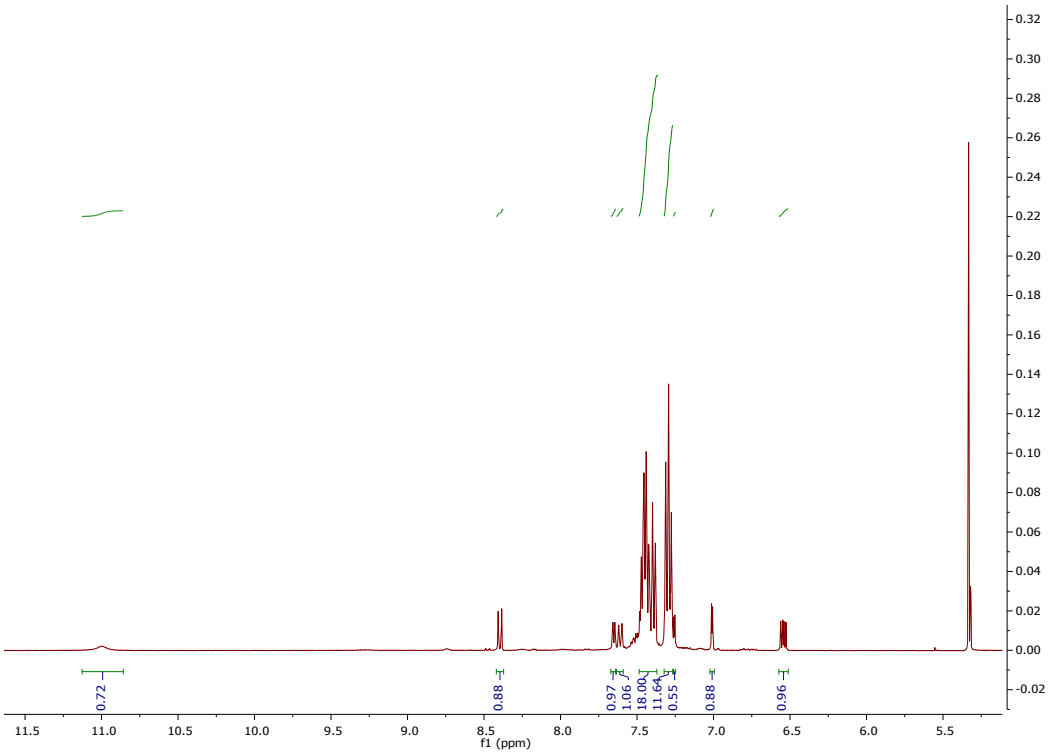

Figure S44. ^{1}H NMR spectrum of $[Ir(PPh_3)_2(CO)(6\text{-hydroxyquinoline})][NO_3]$ (**16a**) in CD_2Cl_2.

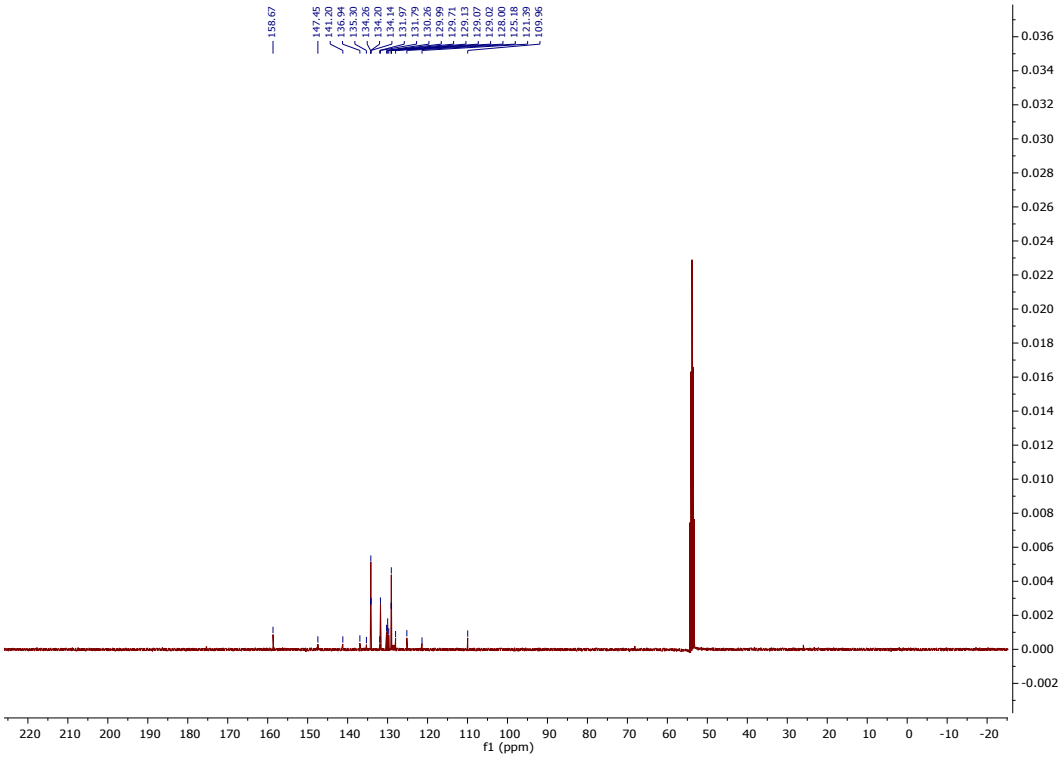

Figure S45. $^{13}C\{^{1}H\}$ NMR spectrum of $[Ir(PPh_3)_2(CO)(6\text{-hydroxyquinoline})][NO_3]$ (**16a**) in CD_2Cl_2. Solvent impurity at 67 ppm and 25.6 ppm is tetrahydrofuran.

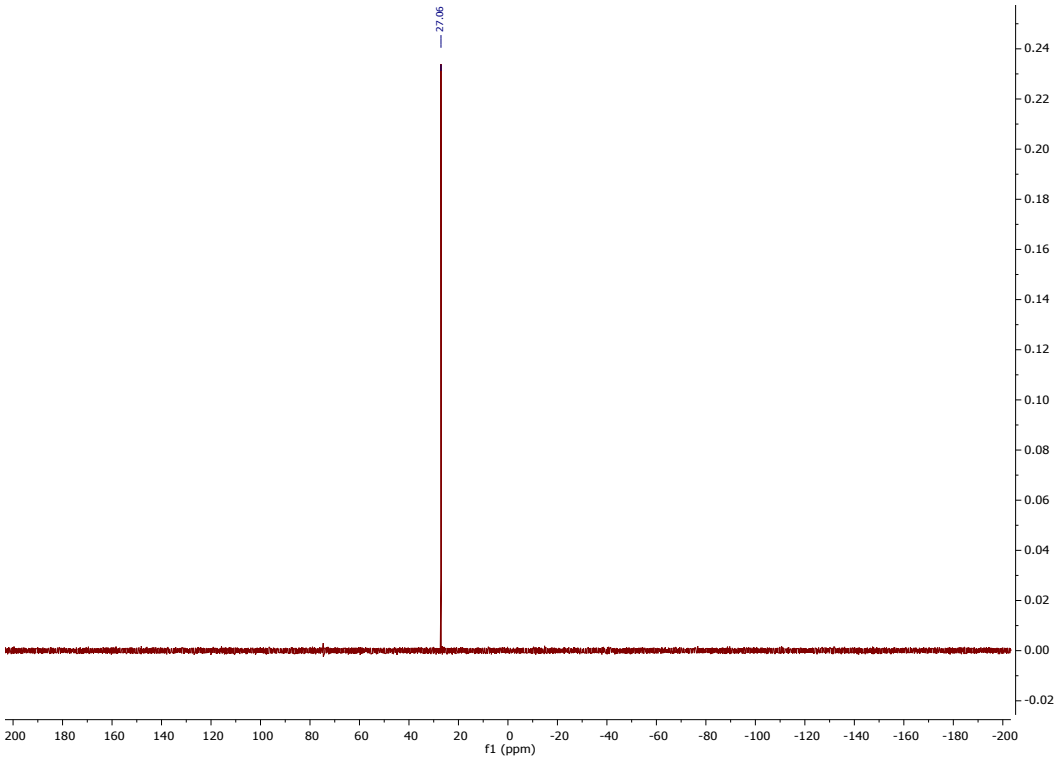

Figure S46. $^{31}P\{^{1}H\}$ NMR spectrum of $[Ir(PPh_3)_2(CO)(6\text{-hydroxyquinoline})][NO_3]$ (**16a**) in CD_2Cl_2.

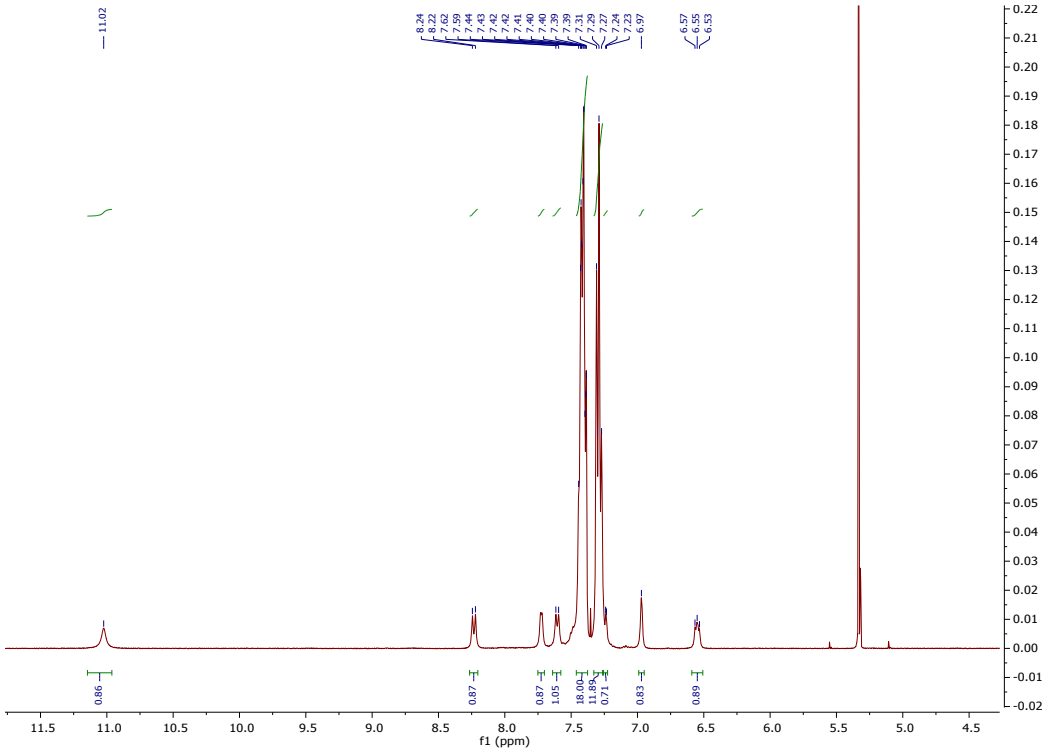

Figure S47. ^{1}H NMR spectrum of $[Rh(PPh_3)_2(CO)(6\text{-hydroxyquinoline})][NO_3]$ (**16b**) in CD_2Cl_2.

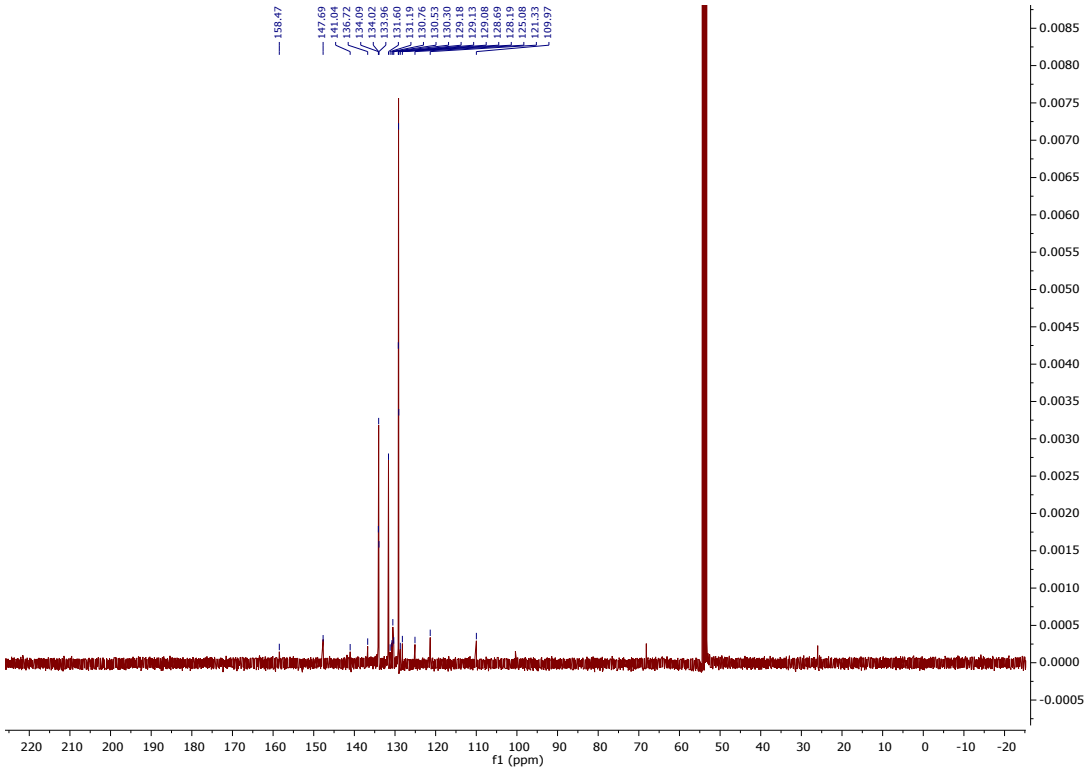

Figure S48. $^{13}C\{^{1}H\}$ NMR spectrum of $[Rh(PPh_3)_2(CO)(6\text{-hydroxyquinoline})][NO_3]$ (**16b**) in CD_2Cl_2. Solvent impurity at 67 ppm and 25.6 ppm is tetrahydrofuran.

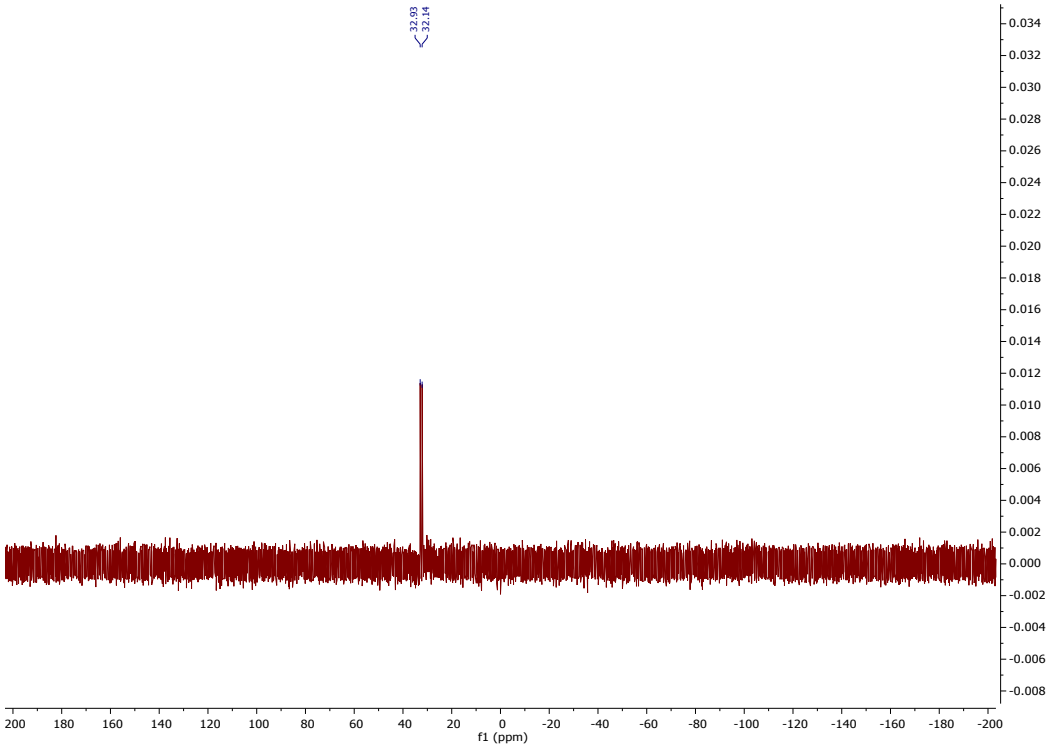

Figure S49. $^{31}P\{^{1}H\}$ NMR spectrum of $[Rh(PPh_3)_2(CO)(6\text{-hydroxyquinoline})][NO_3]$ (**16b**) in CD_2Cl_2.

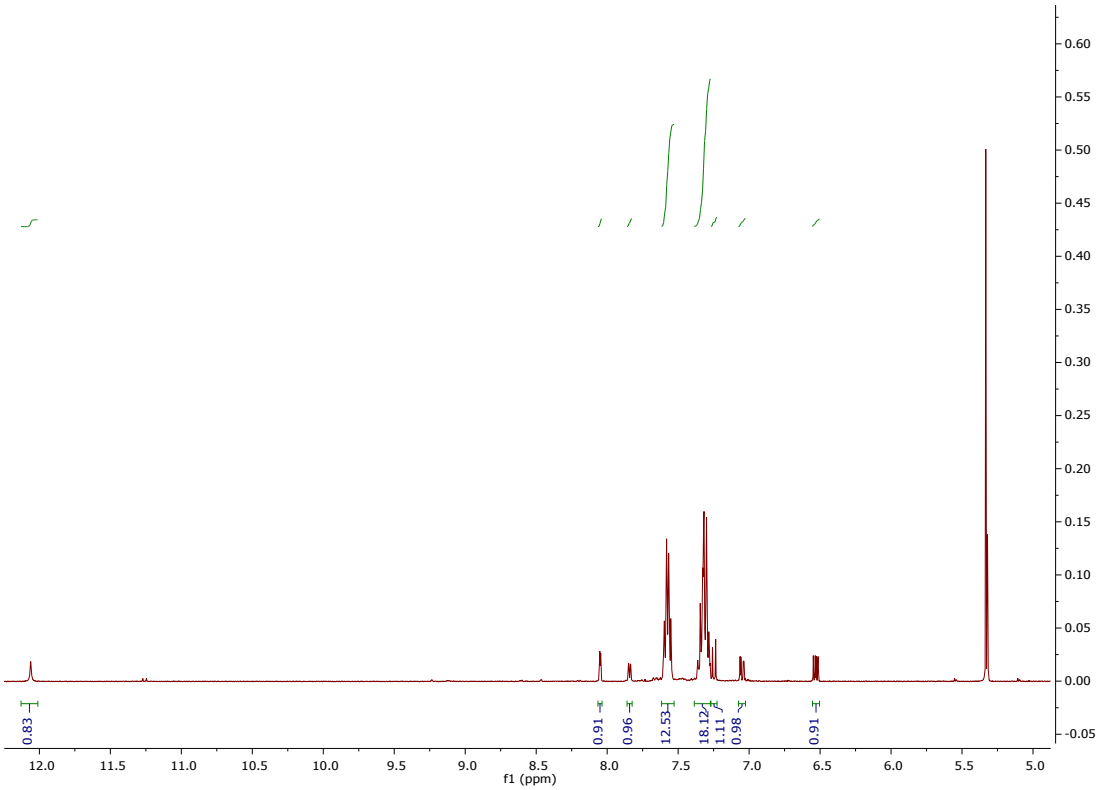

Figure S50. ^{1}H NMR spectrum of $[Ir(PPh_3)_2(CO)(7\text{-hydroxyquinoline})][NO_3]$ (**17a**) in CD_2Cl_2.

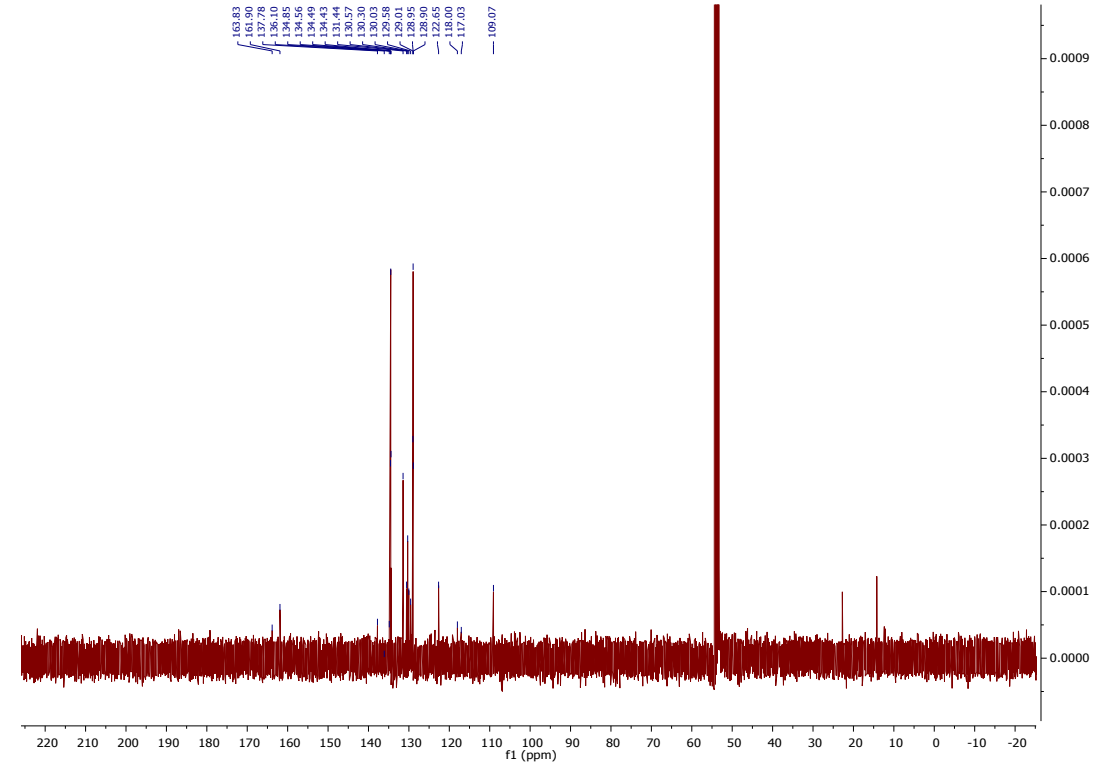

Figure S51. $^{13}C\{^{1}H\}$ NMR spectrum of $[Ir(PPh_3)_2(CO)(7\text{-hydroxyquinoline})][NO_3]$ (**17a**) in CD_2Cl_2. Solvent impurity at is pentane.

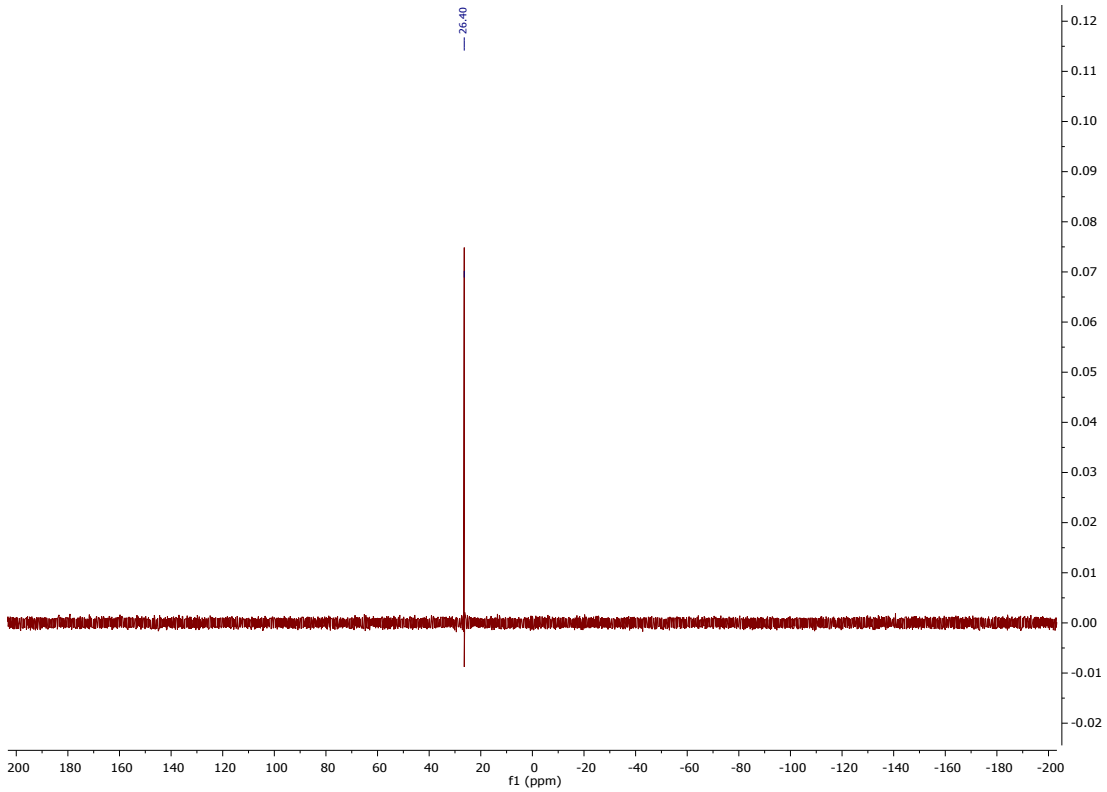

Figure S52. $^{31}P\{^{1}H\}$ NMR spectrum of $[Ir(PPh_3)_2(CO)(7\text{-hydroxyquinoline})][NO_3]$ (**17a**) in CD_2Cl_2.

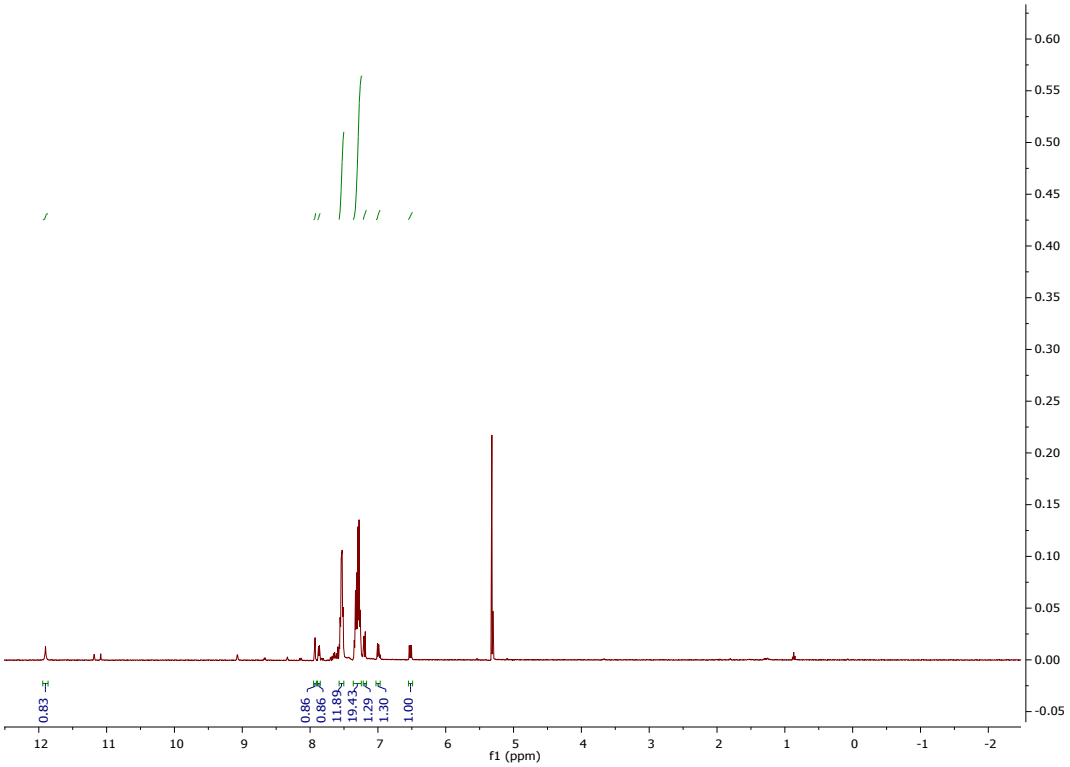

Figure S53. ^{1}H NMR spectrum of $[Rh(PPh_3)_2(CO)(7\text{-hydroxyquinoline})][NO_3]$ (**17b**) in CD_2Cl_2.

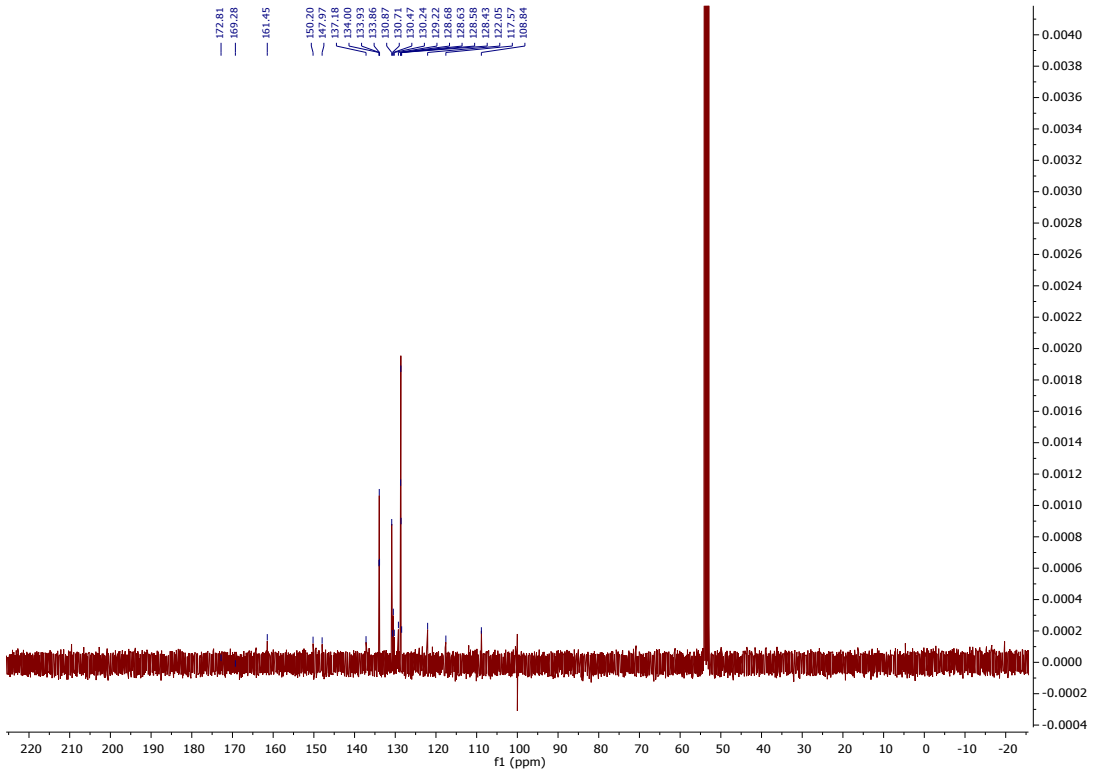

Figure S54. $^{13}C\{^{1}H\}$ NMR spectrum of $[Rh(PPh_3)_2(CO)(7\text{-hydroxyquinoline})][NO_3]$ (**17b**) in CD_2Cl_2. Signal at 100 ppm is a center-of-spectrum artifact.

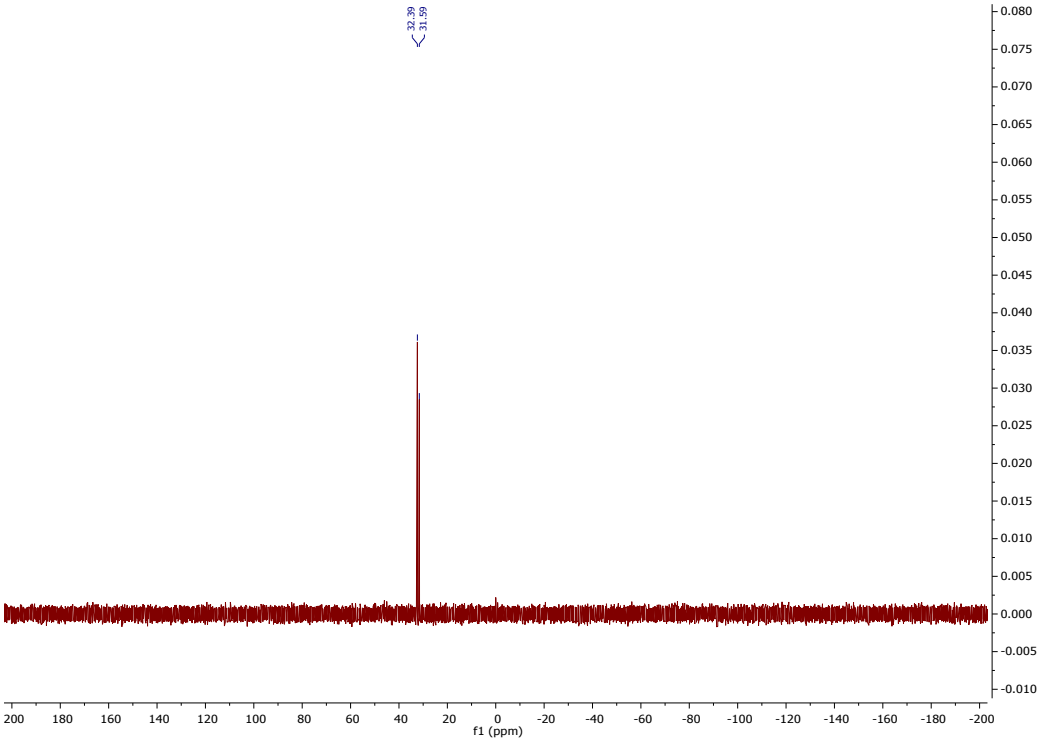

Figure S55. $^{31}P\{^{1}H\}$ NMR spectrum of $[Rh(PPh_3)_2(CO)(7\text{-hydroxyquinoline})][NO_3]$ (**17b**) in CD_2Cl_2.

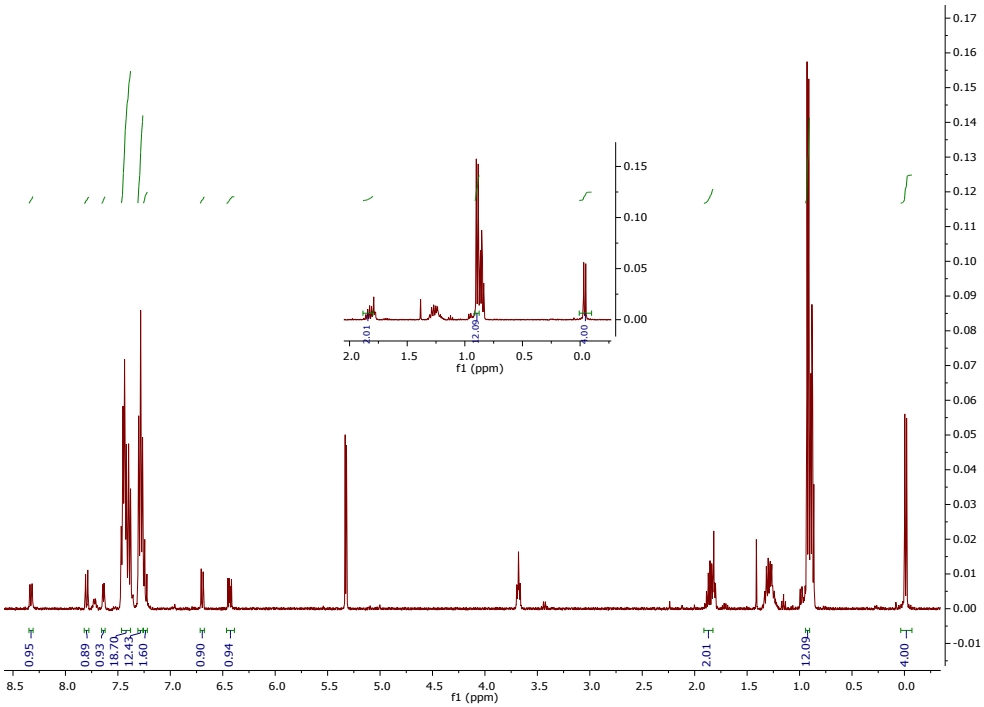

Figure S56. ^{1}H NMR spectrum of $Ir(PPh_3)_2(CO)$(5-oxyquinoline-[Al($^{i}Bu_2$)NO_3] (**18a**) in CD_2Cl_2. Solvent impurities are pentane and THF.

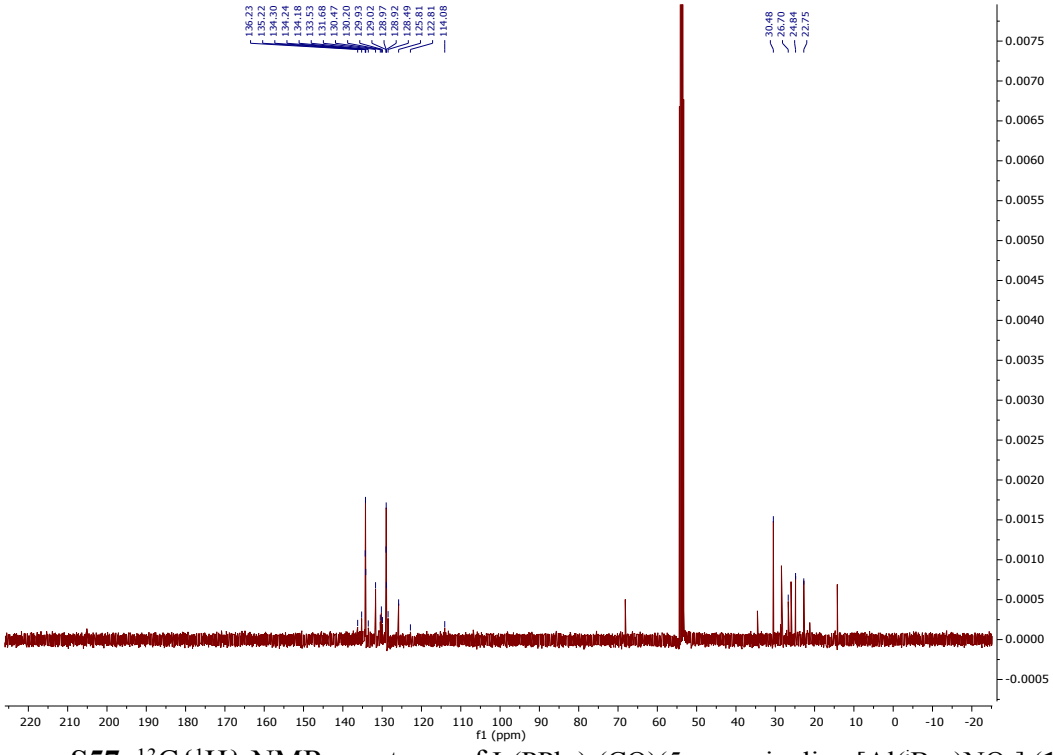

Figure S57. $^{13}C\{^{1}H\}$ NMR spectrum of $Ir(PPh_3)_2(CO)$(5-oxyquinoline-[Al($^{i}Bu_2$)NO_3] (**18a**) in CD_2Cl_2. Solvent impurities are pentane and THF.

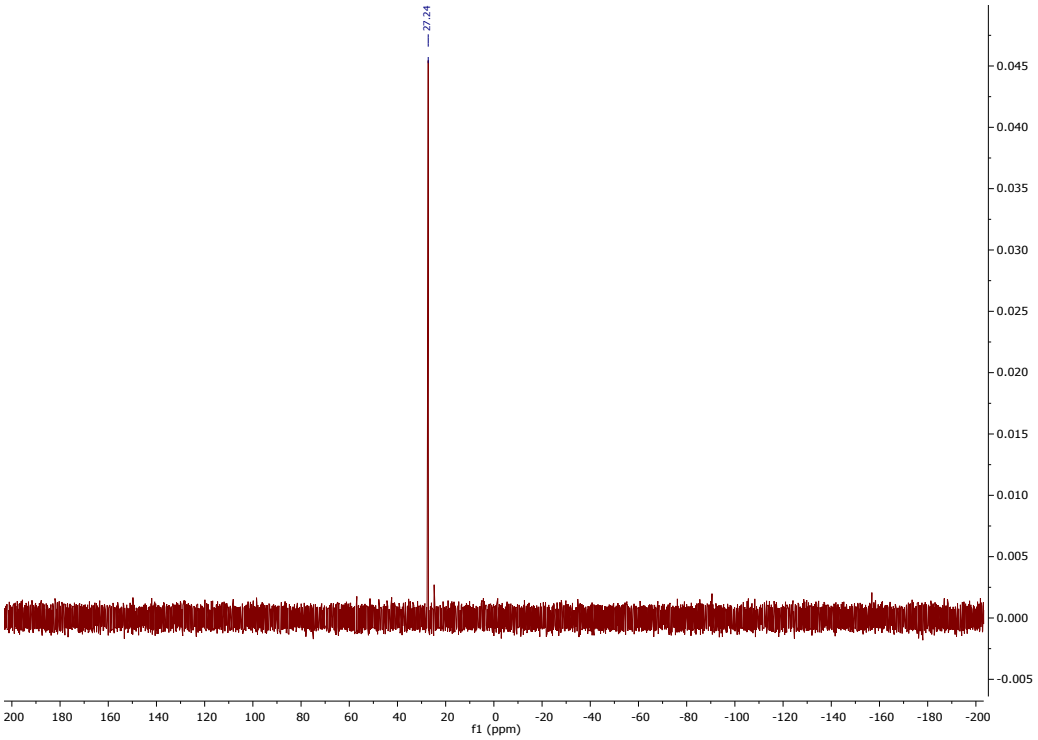

Figure S58. $^{31}P\{^{1}H\}$ NMR spectrum of $Ir(PPh_3)_2(CO)$(5-oxyquinoline-[$Al(^{i}Bu_2)NO_3$] (**18a**) in CD_2Cl_2.

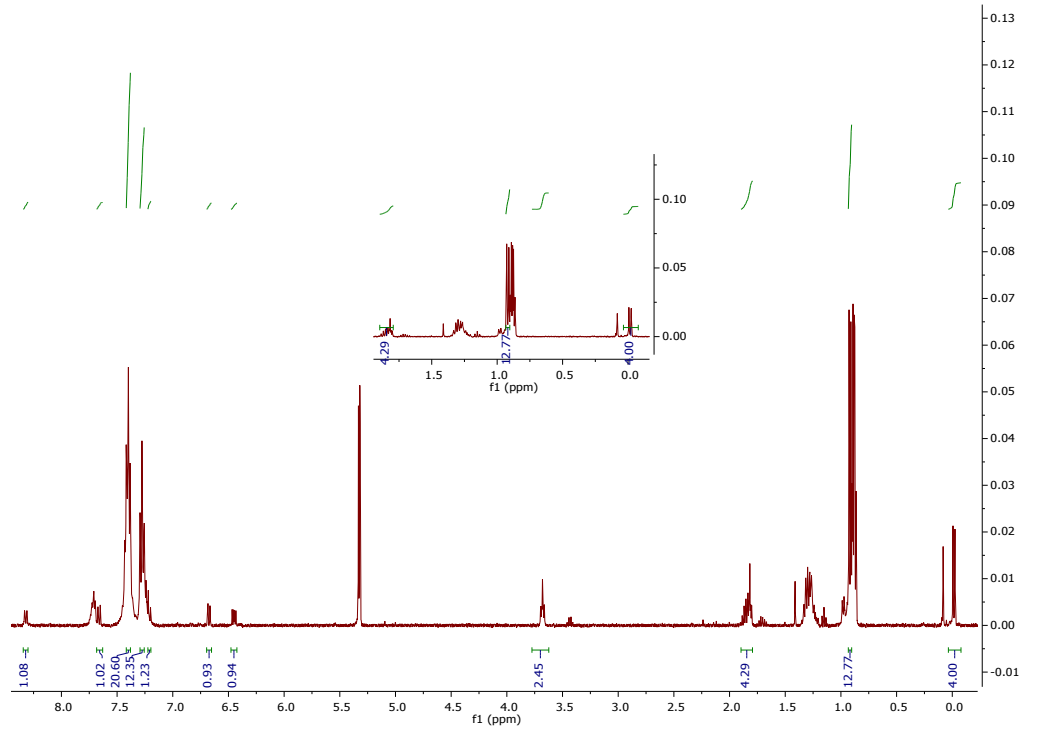

Figure S59. ^{1}H NMR spectrum of $Rh(PPh_3)_2(CO)$(5-oxyquinoline-[$Al(^{i}Bu_2)NO_3$] (**18b**) in CD_2Cl_2. Solvent impurities are pentane and THF.

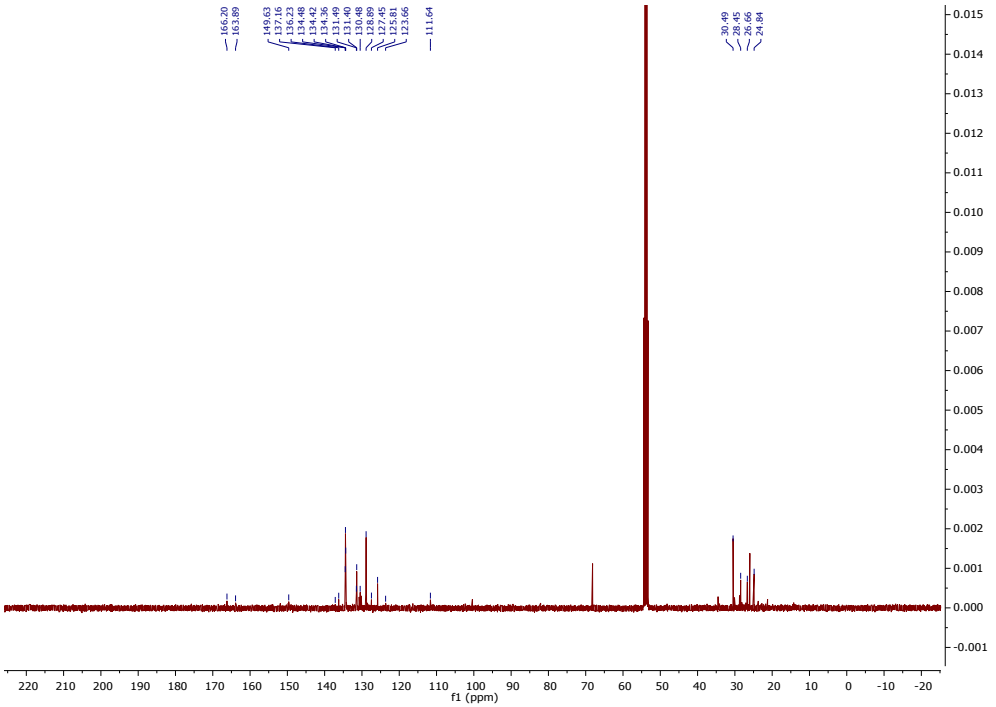

Figure S60. $^{13}C\{^{1}H\}$ NMR spectrum of $Rh(PPh_3)_2(CO)$(5-oxyquinoline-[Al($^{i}Bu_2$)NO_3] (**18b**) in CD_2Cl_2. Solvent impurities are pentane and THF.

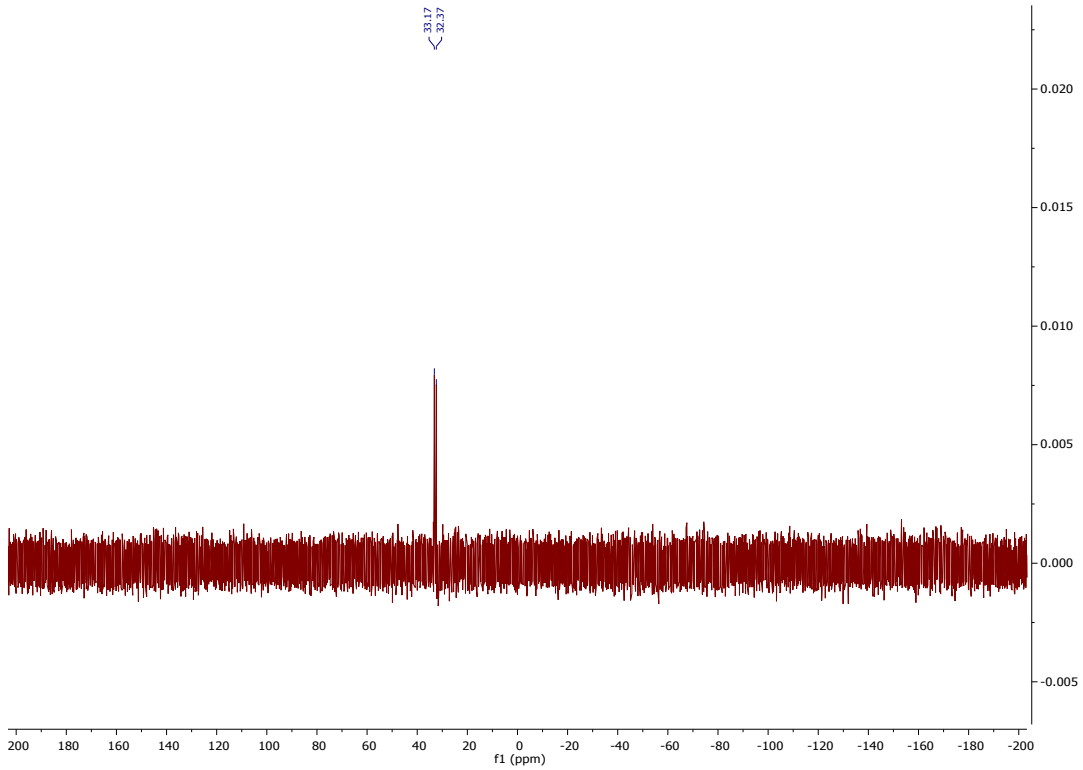

Figure S61. $^{31}P\{^{1}H\}$ NMR spectrum of $Rh(PPh_3)_2(CO)$(5-oxyquinoline-[Al($^{i}Bu_2$)NO_3] (**18b**) in CD_2Cl_2.

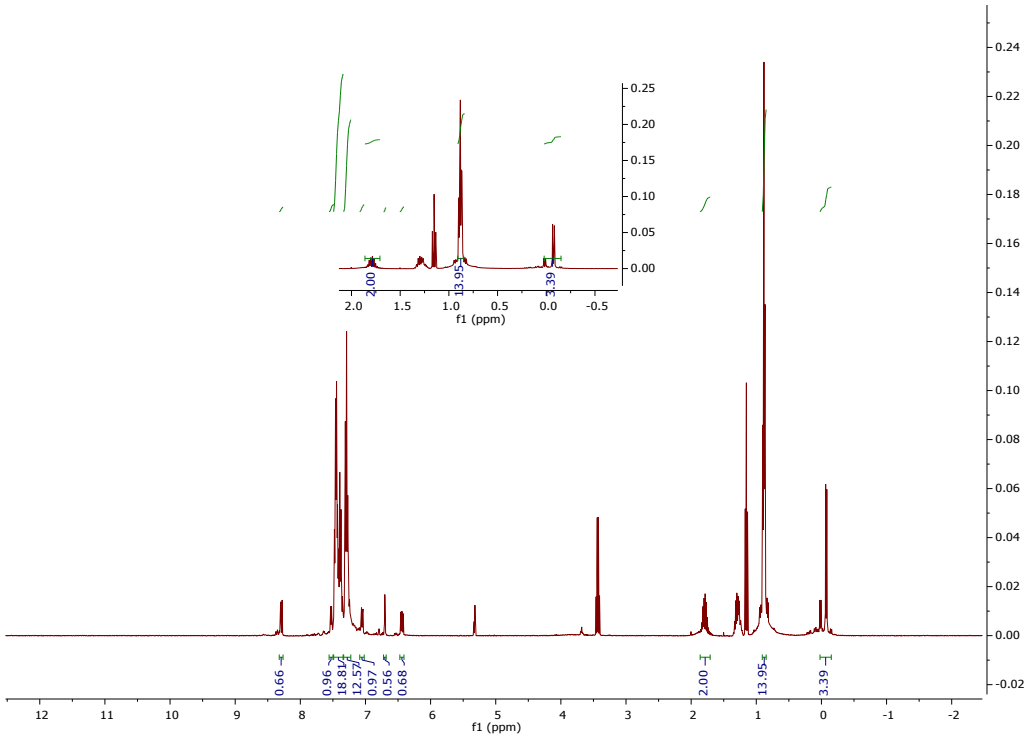

Figure S62. ^{1}H NMR spectrum of $Ir(PPh_3)_2(CO)$(6-oxyquinoline-[Al($^{i}Bu_2$)NO_3] (**19a**) in CD_2Cl_2. Solvent impurities are pentane and THF.

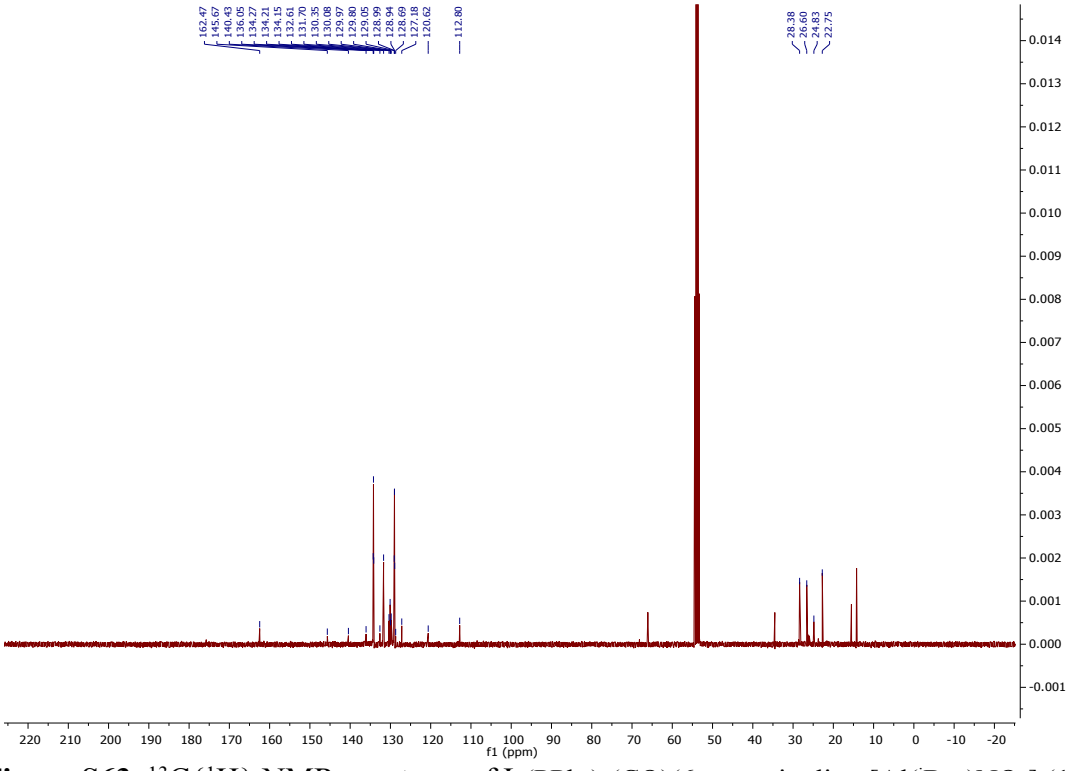

Figure S63. $^{13}C\{^{1}H\}$ NMR spectrum of $Ir(PPh_3)_2(CO)$(6-oxyquinoline-[Al($^{i}Bu_2$)NO_3] (**19a**) in CD_2Cl_2. Solvent impurities are pentane and THF.

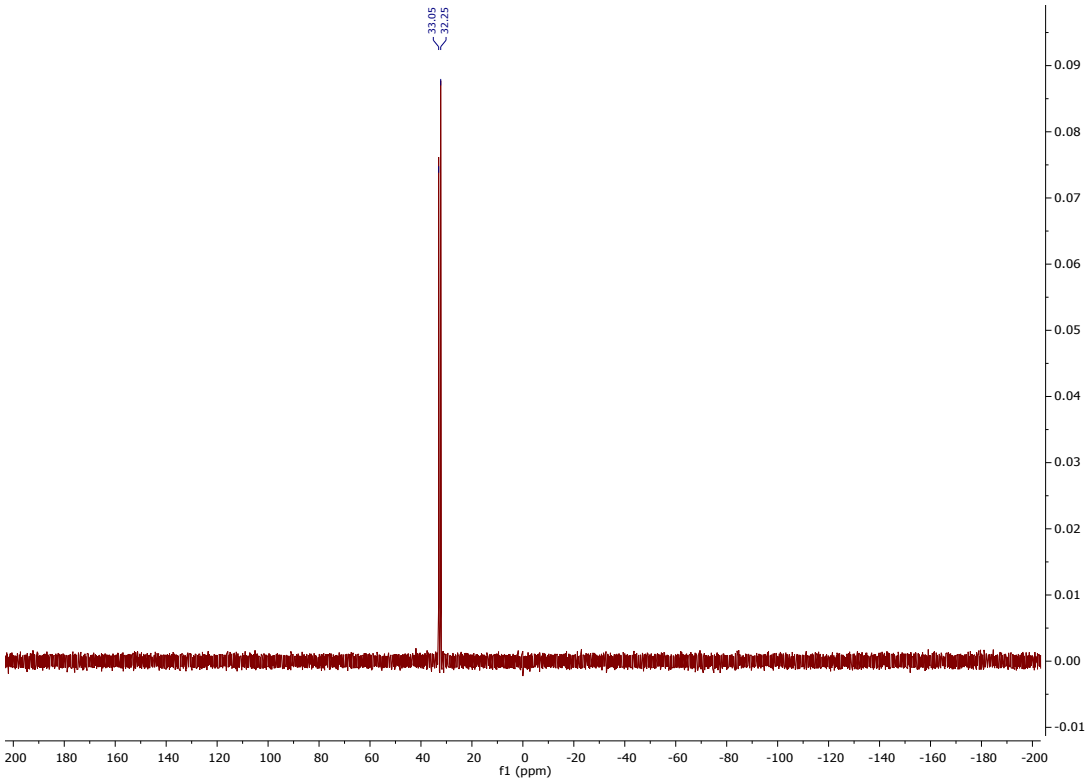

Figure S64. $^{31}P\{^{1}H\}$ NMR spectrum of $Ir(PPh_3)_2(CO)$(6-oxyquinoline-[$Al(^{i}Bu_2)NO_3$] (**19a**) in CD_2Cl_2.

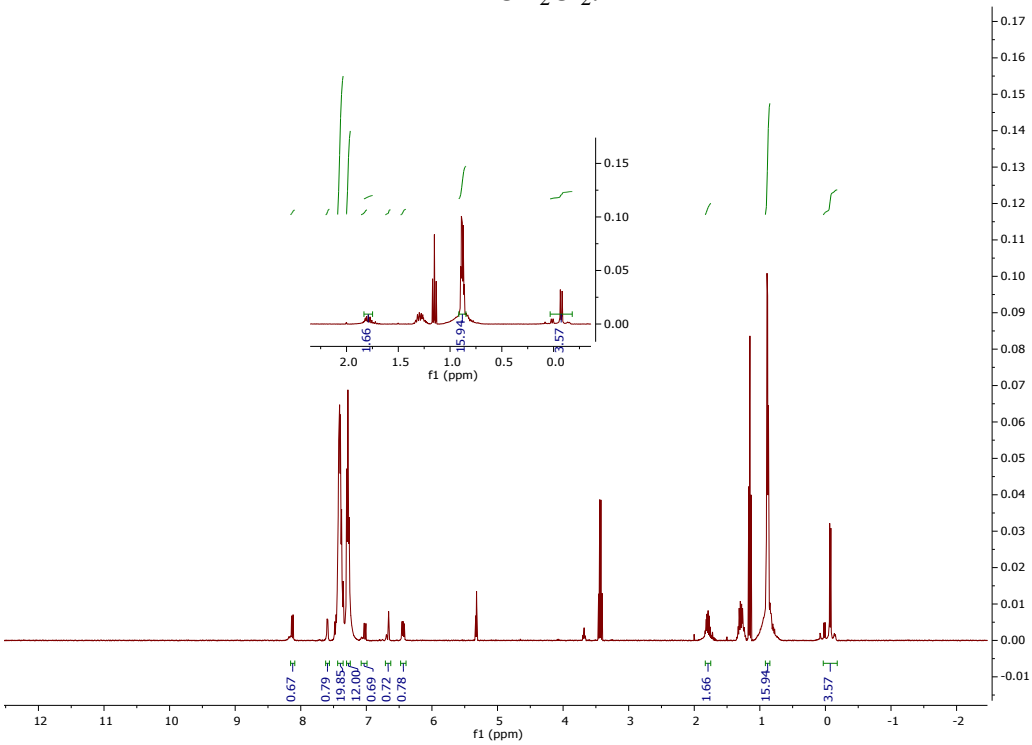

Figure S65. ^{1}H NMR spectrum of $Rh(PPh_3)_2(CO)$(6-oxyquinoline-[$Al(^{i}Bu_2)NO_3$] (**19b**) in CD_2Cl_2. Solvent impurities are pentane and THF.

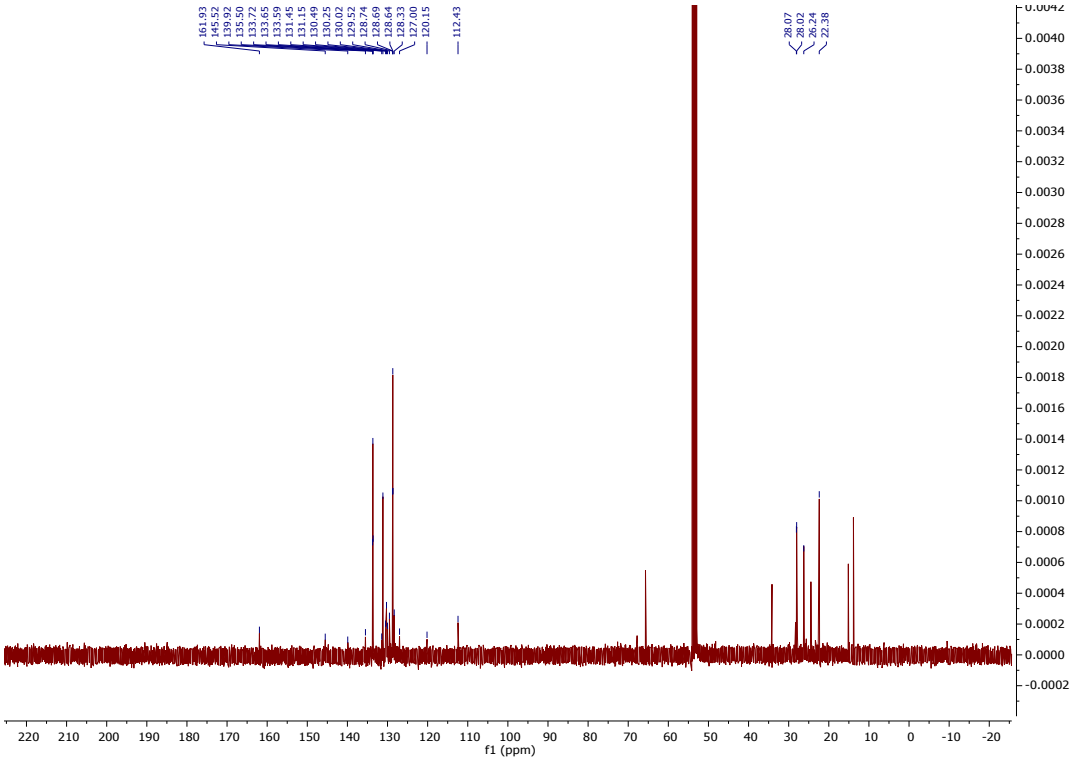

Figure S66. $^{13}C\{^{1}H\}$ NMR spectrum of $Rh(PPh_3)_2(CO)$(6-oxyquinoline-[Al($^{i}Bu_2$)NO_3] (**19b**) in CD_2Cl_2. Solvent impurities are pentane and THF.

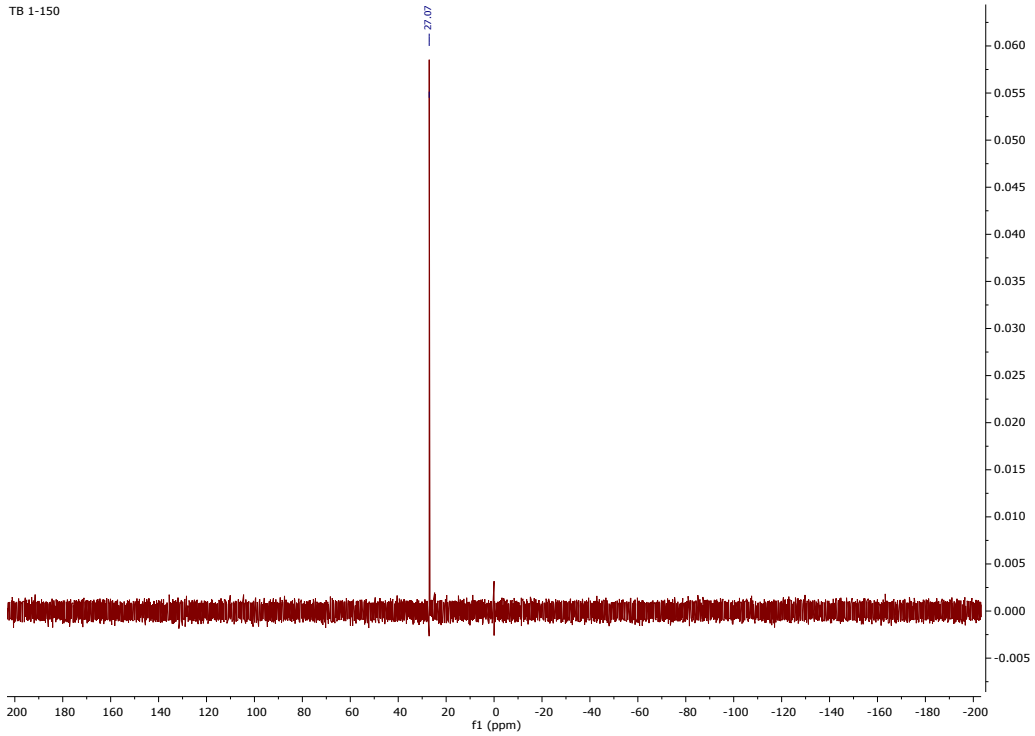

Figure S67. $^{31}P\{^{1}H\}$ NMR spectrum of $Rh(PPh_3)_2(CO)$(6-oxyquinoline-[Al($^{i}Bu_2$)NO_3] (**19b**) in CD_2Cl_2.

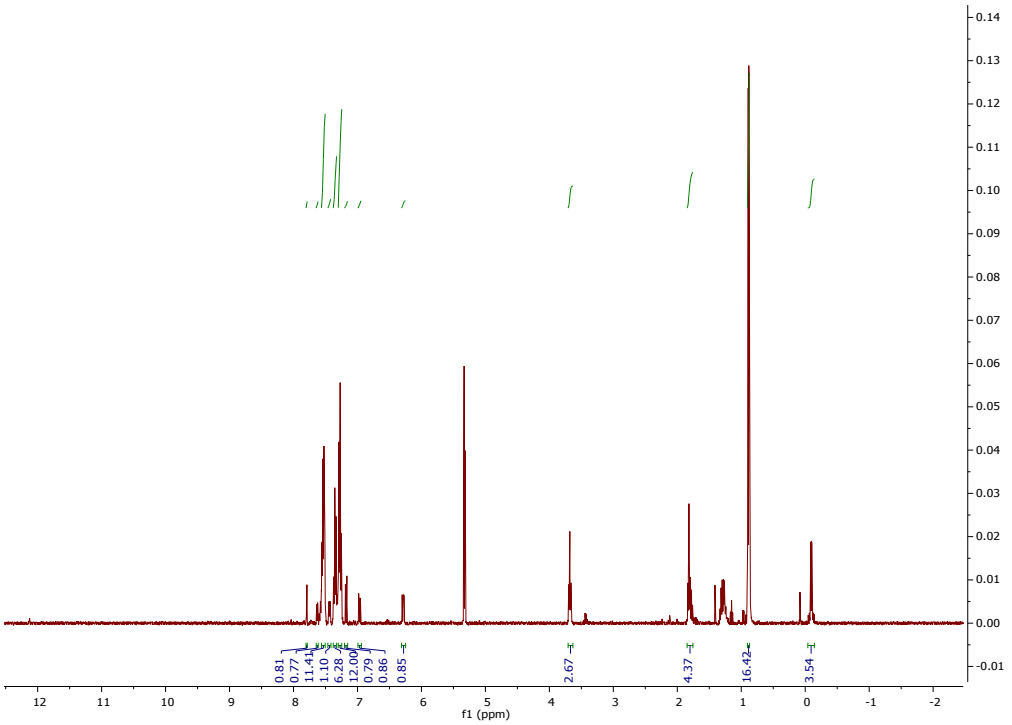

Figure S68. ^{1}H NMR spectrum of $Ir(PPh_3)_2(CO)$(7-oxyquinoline-[Al($^{i}Bu_2$)NO_3] (**20a**) in CD_2Cl_2. Solvent impurities are pentane and THF.

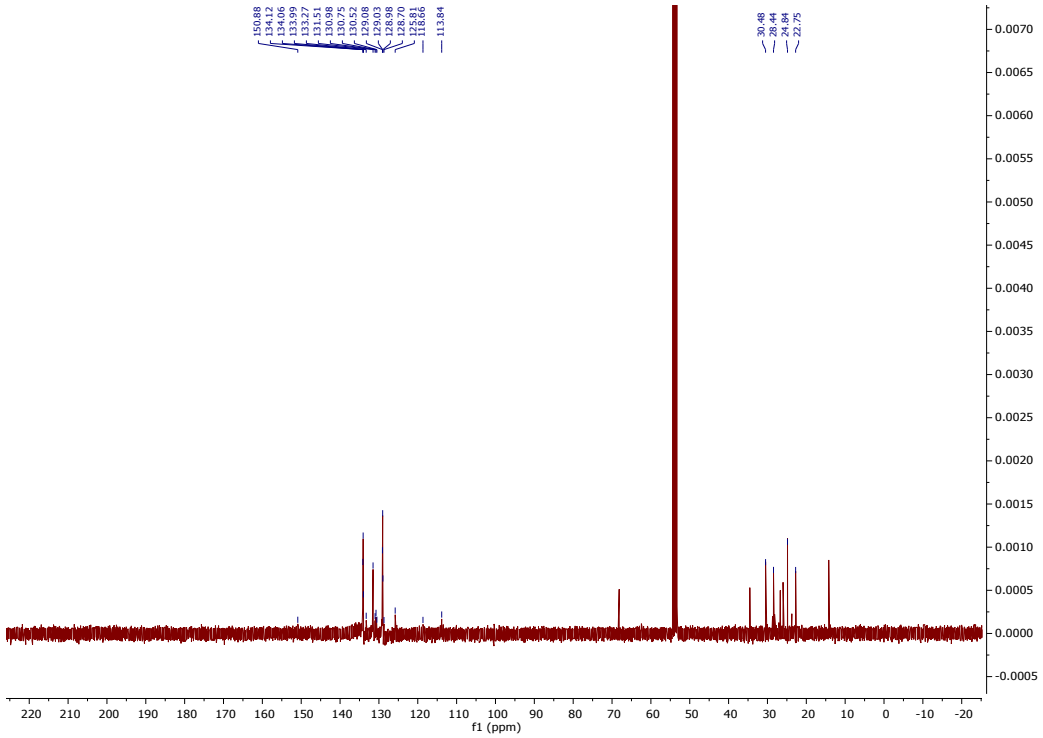

Figure S69. $^{13}C\{^{1}H\}$ NMR spectrum of $Ir(PPh_3)_2(CO)$(7-oxyquinoline-[Al($^{i}Bu_2$)NO_3] (**20a**) in CD_2Cl_2. Solvent impurities are pentane and THF.

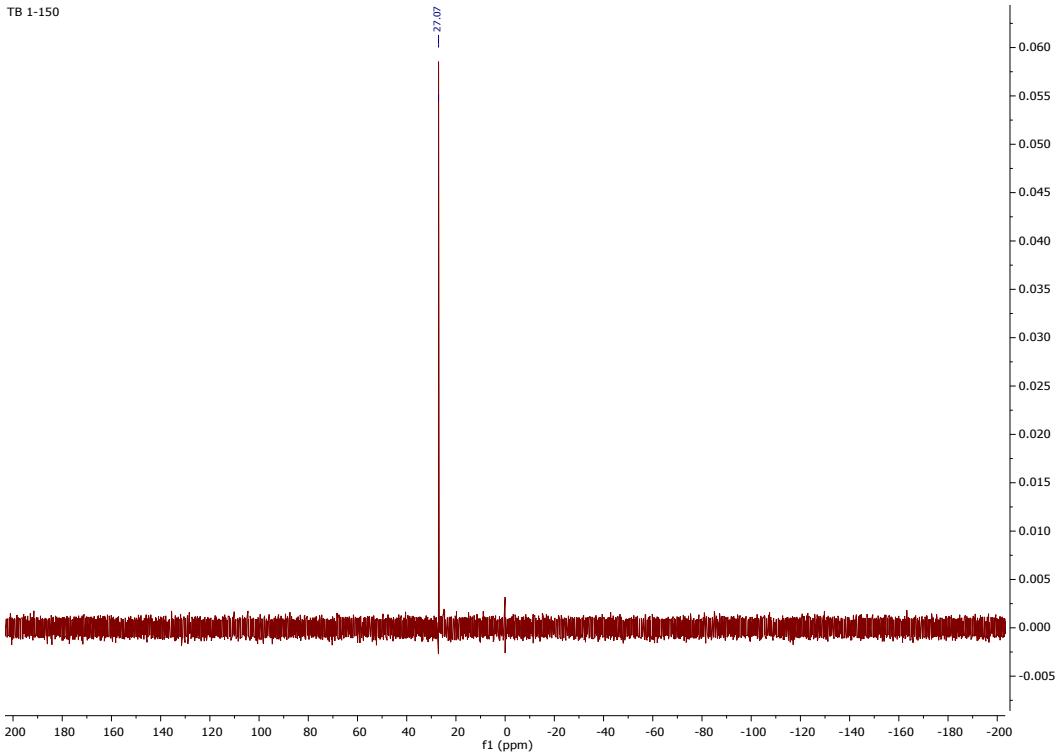

Figure S70. $^{31}P\{^{1}H\}$ NMR spectrum of $Ir(PPh_3)_2(CO)$(7-oxyquinoline-[$Al(^{i}Bu_2)NO_3$] (**20a**) in CD_2Cl_2.

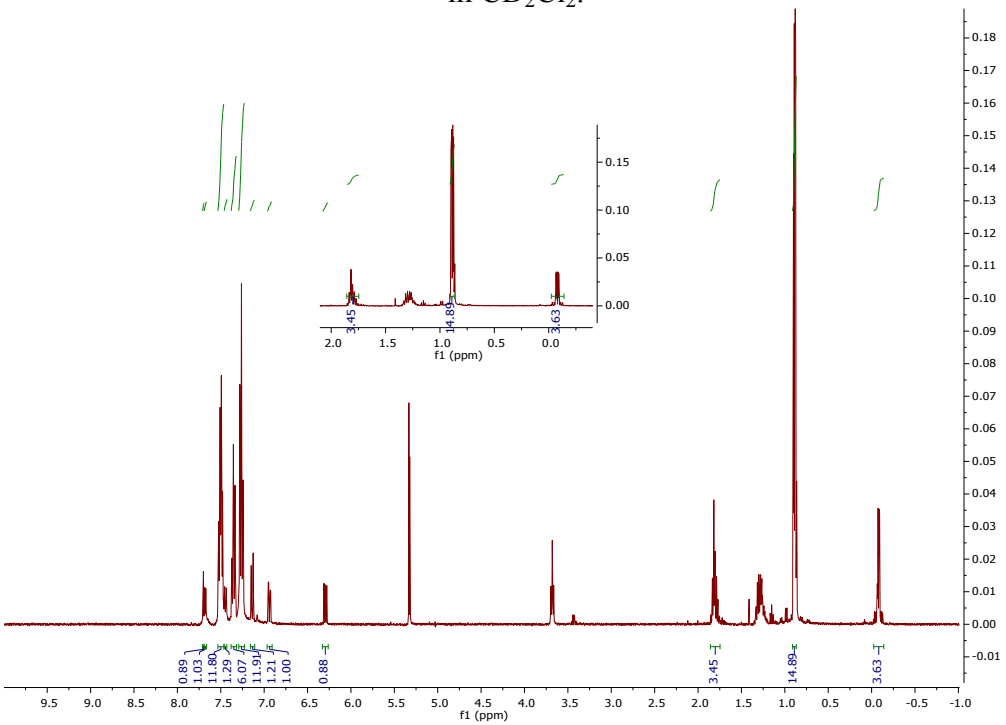

Figure S71. ^{1}H NMR spectrum of $Rh(PPh_3)_2(CO)$(7-oxyquinoline-[$Al(^{i}Bu_2)NO_3$] (**20b**) in CD_2Cl_2. Solvent impurities are pentane and THF.

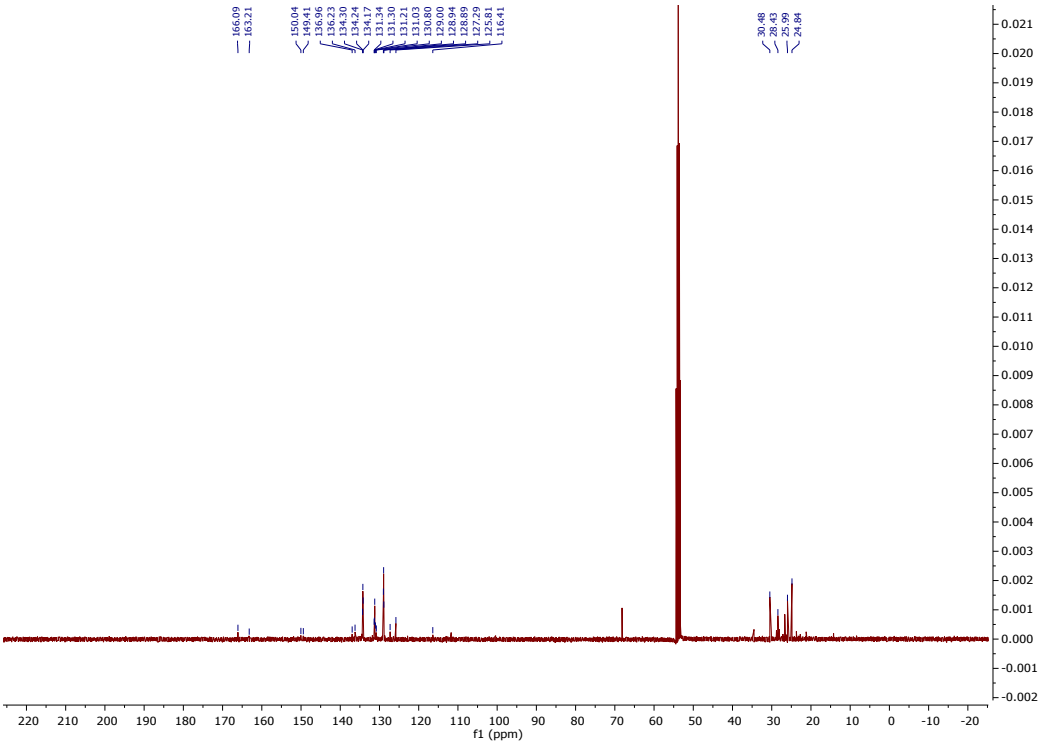

Figure S72. $^{13}C\{^{1}H\}$ NMR spectrum of $Rh(PPh_3)_2(CO)$(7-oxyquinoline-[Al($^{i}Bu_2$)NO_3] (**20b**) in CD_2Cl_2. Solvent impurities are pentane and THF.

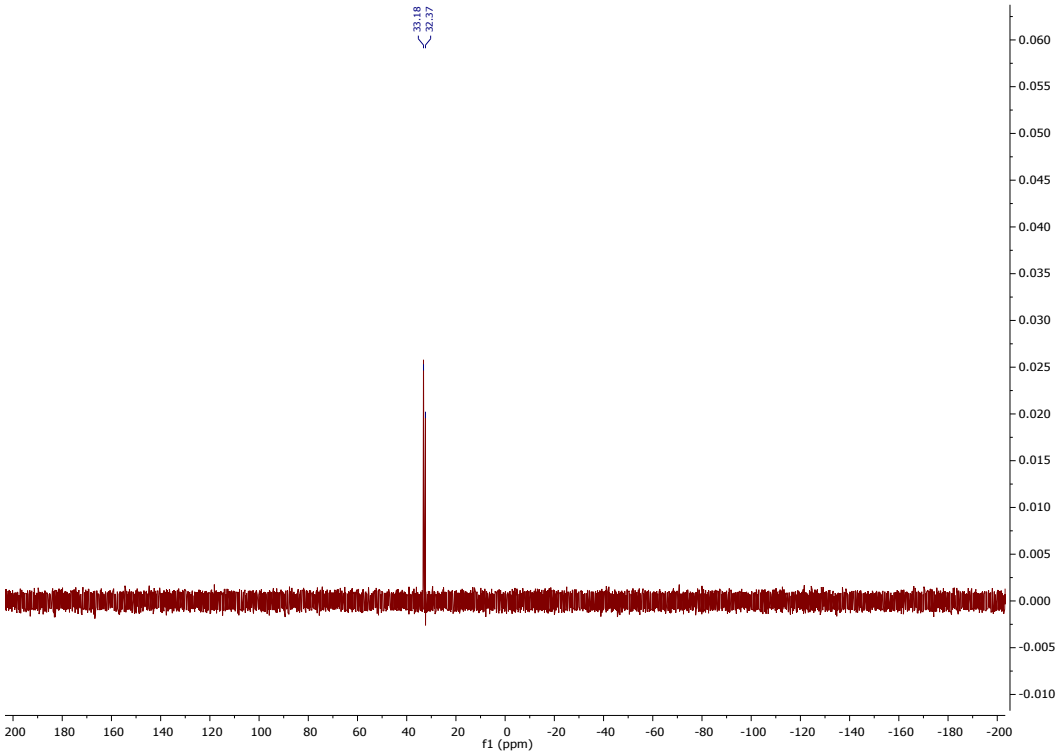

Figure S73. $^{31}P\{^{1}H\}$ NMR spectrum of $Rh(PPh_3)_2(CO)$(7-oxyquinoline-[Al($^{i}Bu_2$)NO_3] (**20b**) in CD_2Cl_2.

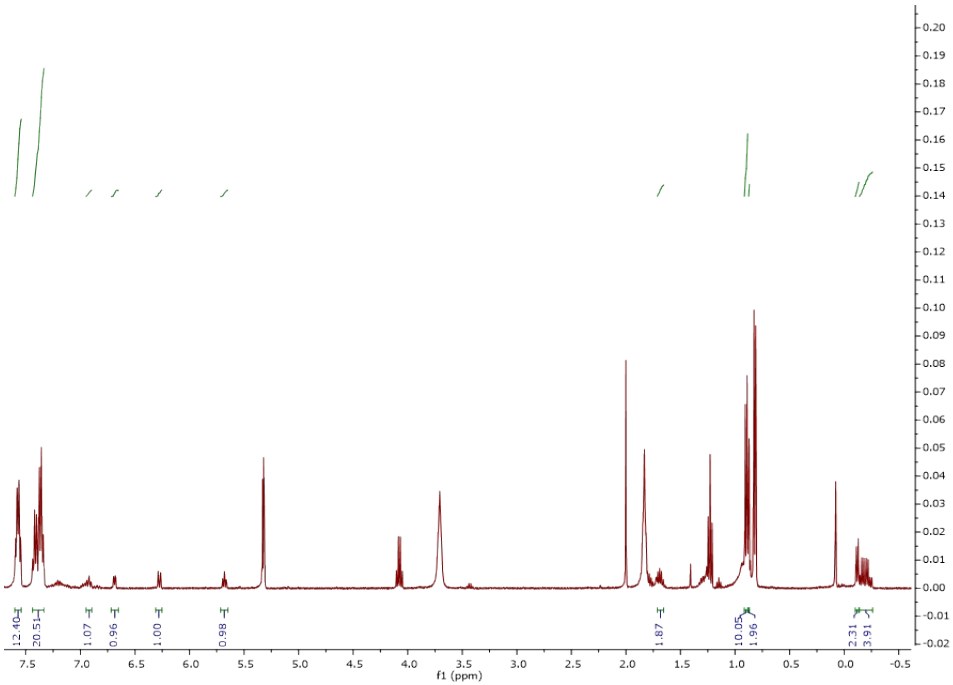

Figure S74. ^{1}H NMR spectrum of Ir(PPh$_3$)$_2$(CO)(2-oxypyridine-[Al(^{i}Bu$_2$)SO$_3$CF$_3$] (**21a**) in CD_2Cl_2. Solvent impurity at 0.81 and 1.26 ppm is pentane. Solvent impurity at 1.83 ppm and 3.7 ppm is tetrahydrofuran. Solvent impurity at 5.32 is dichloromethane. Signal impurity at 4..08 ppm is ethyl acetate. Signal impurity at 2 ppm is acetone. Signal at 0.077 ppm is silicone grease.

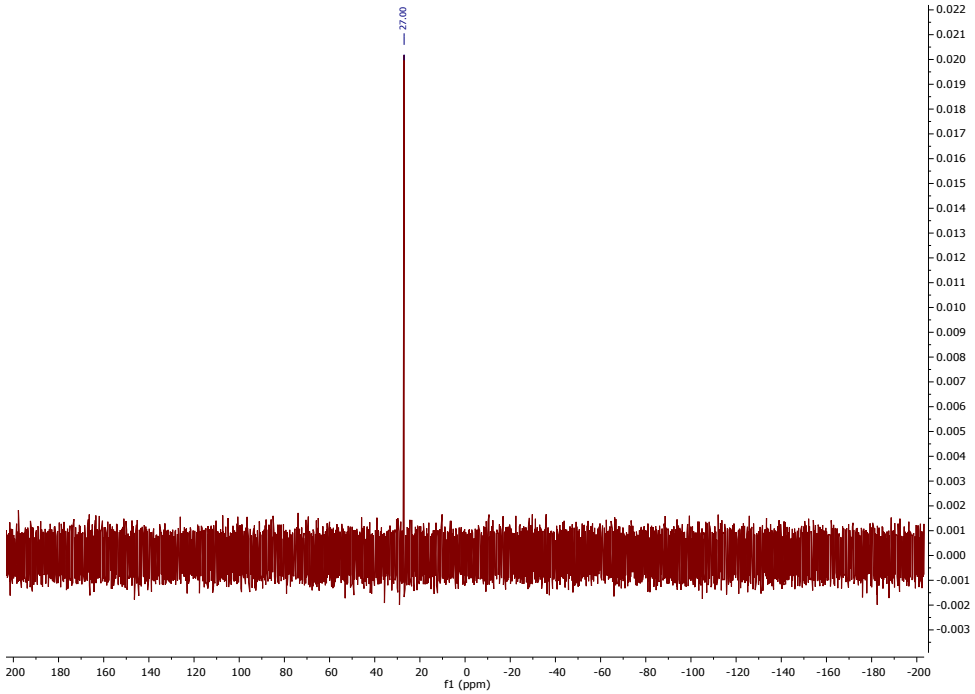

Figure S75. ^{31}P{H} NMR spectrum of Ir(PPh$_3$)$_2$(CO)(2-oxypyridine-[Al(^{i}Bu$_2$)SO$_3$CF$_3$] (**21a**) in CD_2Cl_2.

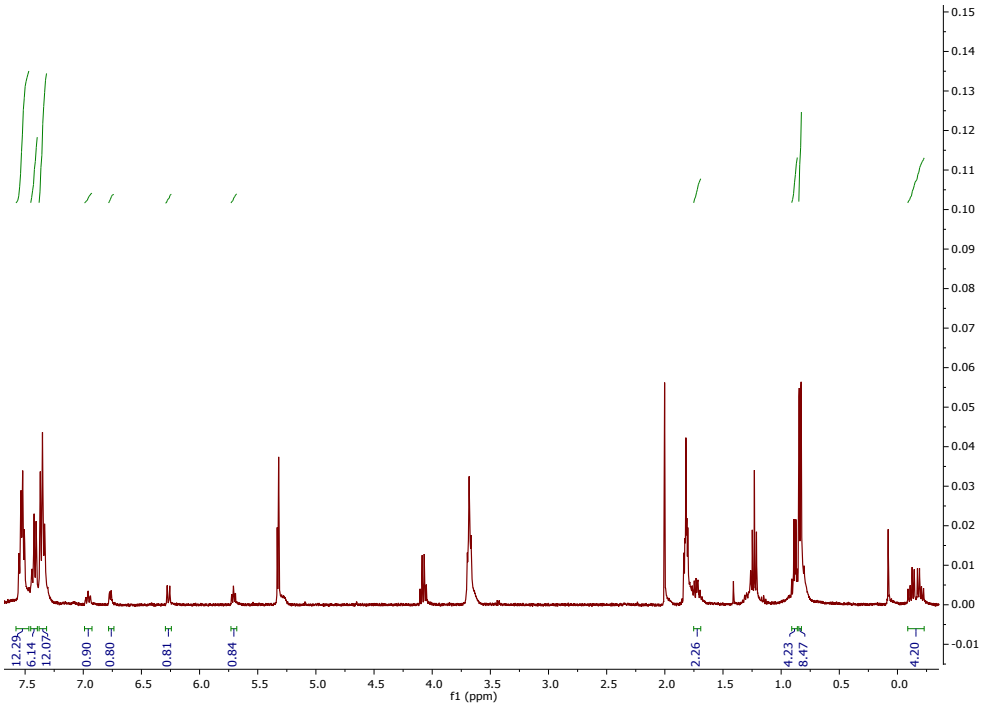

Figure S76. ^{1}H NMR spectrum of $Rh(PPh_3)_2(CO)$(2-oxypyridine-[Al($^{i}Bu_2$)SO_3CF_3] (**21b**) in CD_2Cl_2. Solvent impurity at 0.82 ppm and 1.23 ppm is pentane. Solvent impurity at 1.8 ppm and 3.68 ppm is tetrahydrofuran. Solvent impurity at 5.32 is dichloromethane. Solvent impurity at 4.08 ppm is ethyl acetate. Solvent impurity at 2 ppm is acetone. Signal at 0.08 ppm is silicone grease.

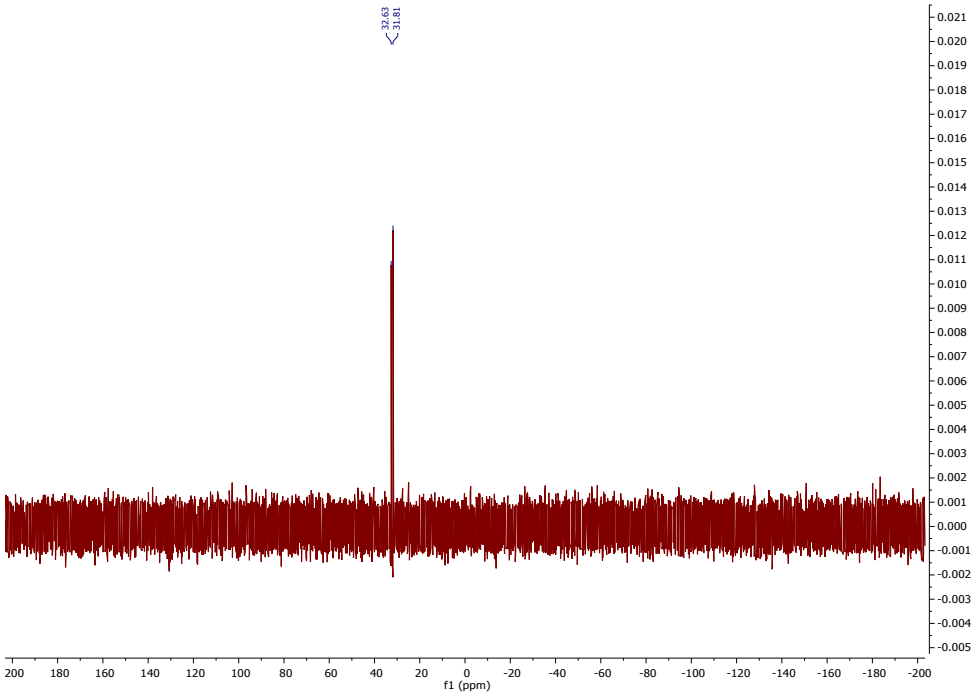

Figure S77. ^{31}P{H} NMR spectrum of $Rh(PPh_3)_2(CO)$(2-oxypyridine-[Al($^{i}Bu_2$)SO_3CF_3] (**21b**) in CD_2Cl_2.

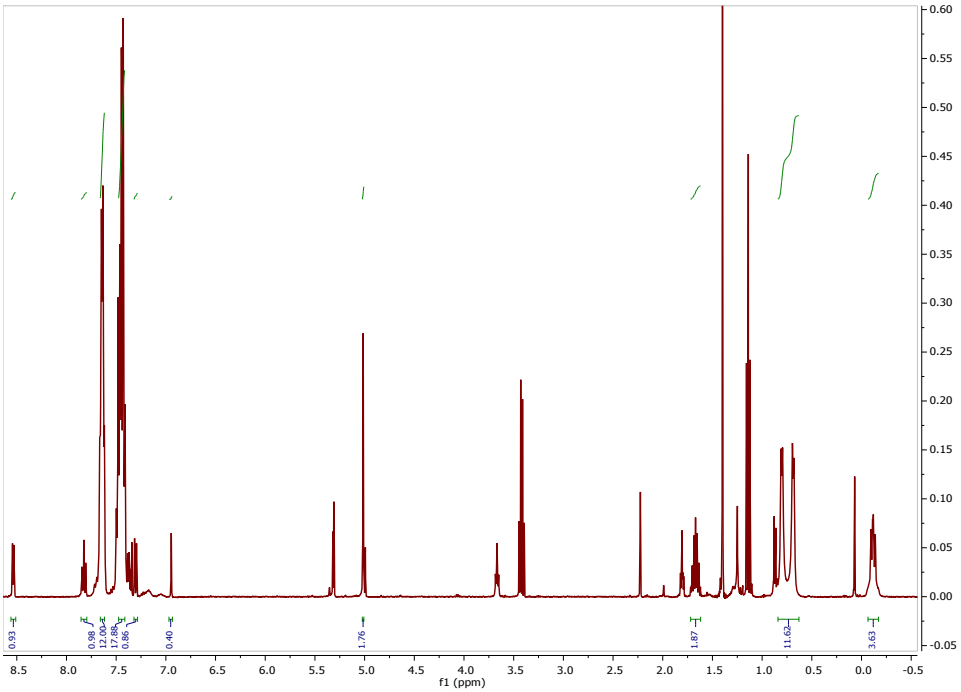

Figure S78. ^{1}H NMR spectrum of [Rh(PPh$_3$)$_2$(CO)(3-oxymethylpyridine-Al(ONO$_2$)(^{i}Bu)$_2$)] (**22b**) in CD_2Cl_2. Solvent impurity at 0.8 ppm and 1.3 ppm is pentane. Solvent impurity at 1.8 ppm and 3.7 ppm is tetrahydrofuran. Solvent impurity at 1.15 ppm and 3.43 ppm is diethyl ether. Solvent impurity at 0.09 ppm is silicone grease.

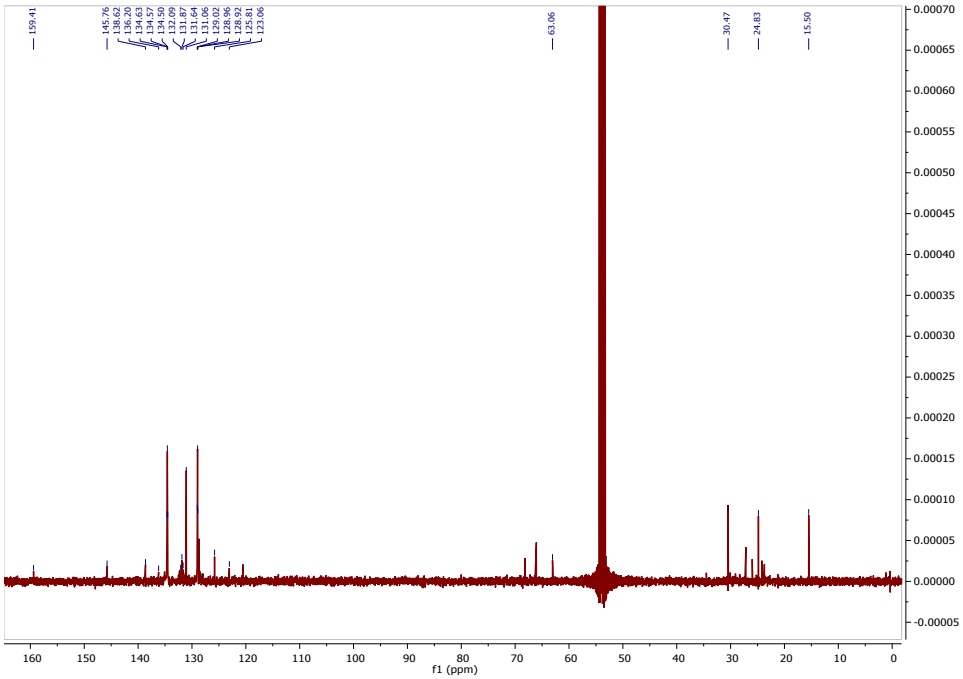

Figure S79. ^{13}C{^{1}H} NMR spectrum of [Rh(PPh$_3$)$_2$(CO)(3-oxymethylpyridine-Al(ONO$_2$)(^{i}Bu)$_2$)] (**22b**) in CD_2Cl_2. Solvent impurity at 68 ppm and 25 ppm is tetrahydrofuran 66 ppm and 15 ppm is diethyl ether.

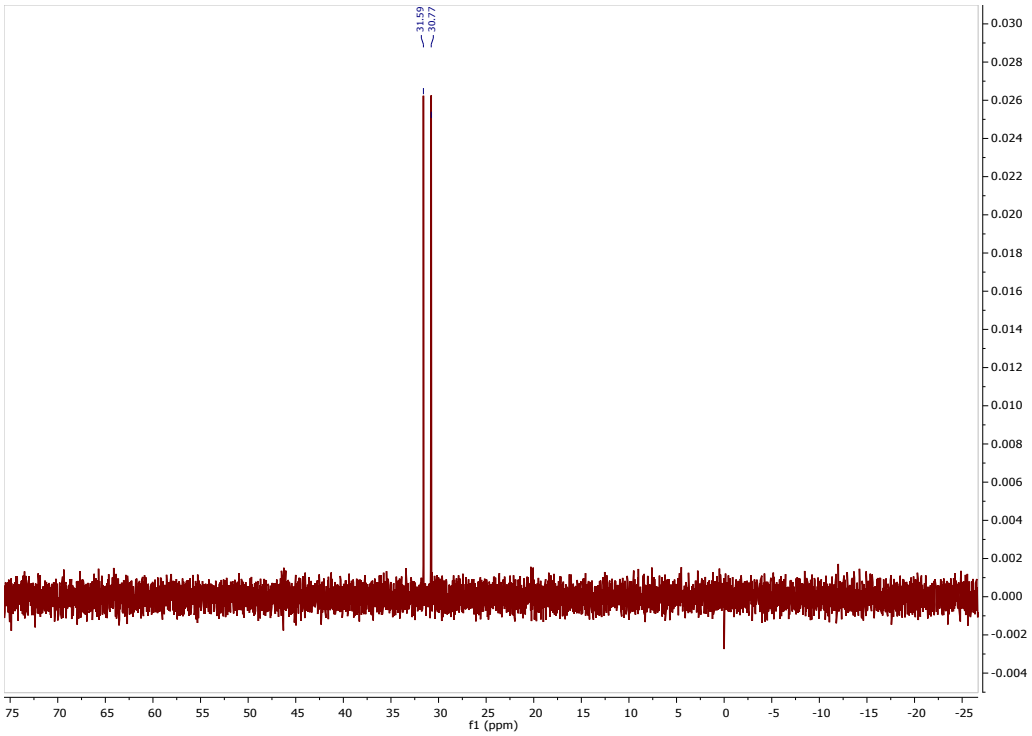

Figure S80. $^{31}P\{^{1}H\}$ NMR spectrum of $[Rh(PPh_3)_2(CO)(3\text{-oxymethylpyridine-Al}(ONO_2)(^{i}Bu)_2)]$ (**22b**) in CD_2Cl_2.

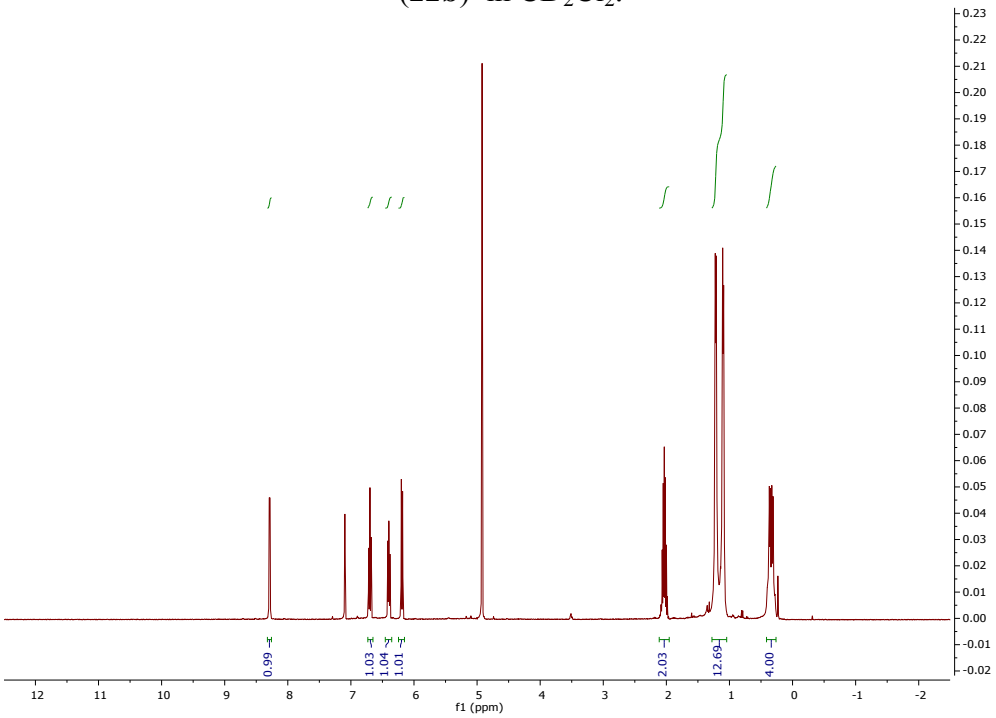

Figure S81. ^{1}H NMR spectrum of $Al(^{i}Bu_2)$(2-oxymethylpyridine) (**23**) in C_6D_6.

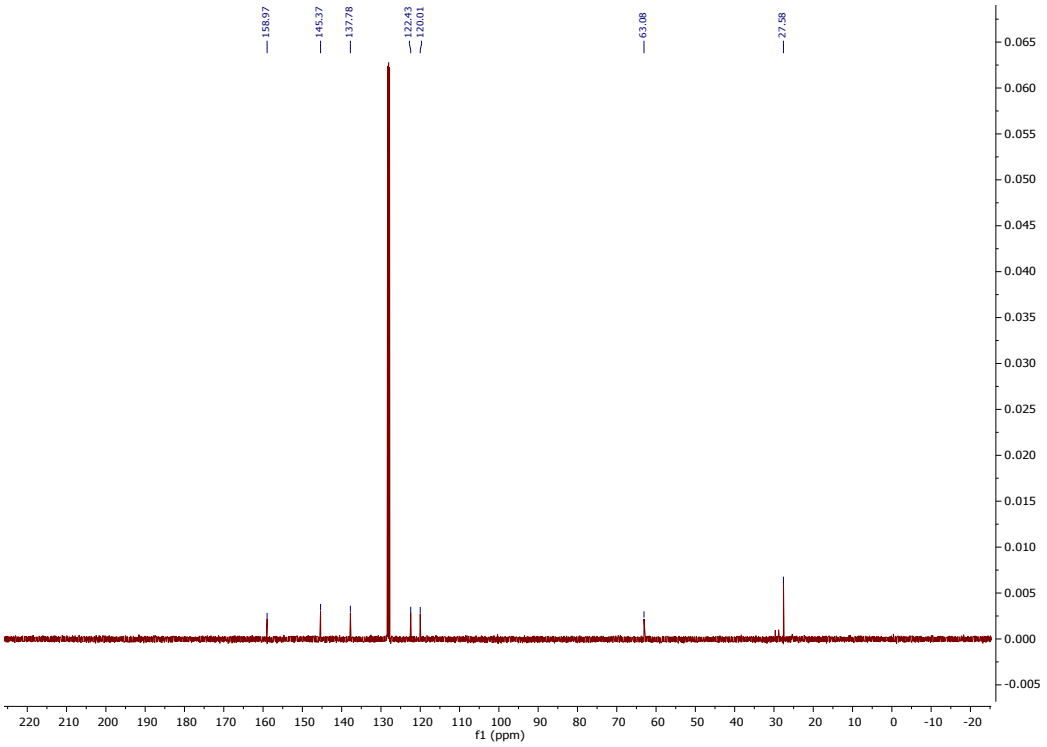

Figure S82. $^{13}C\{^{1}H\}$ NMR spectrum of Al($^{i}Bu_2$)(2-oxymethylpyridine) (**23**) in C_6D_6.

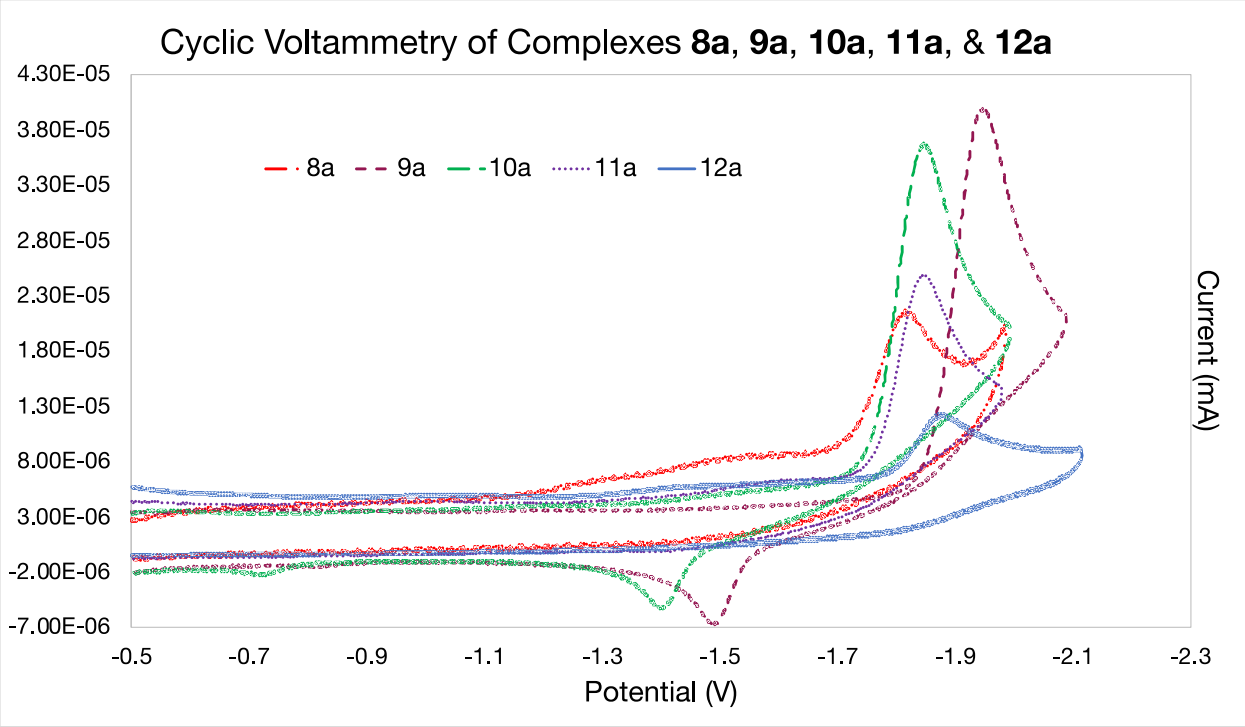

Figure S83. Voltammogram of complexes **8a** – **12a**.

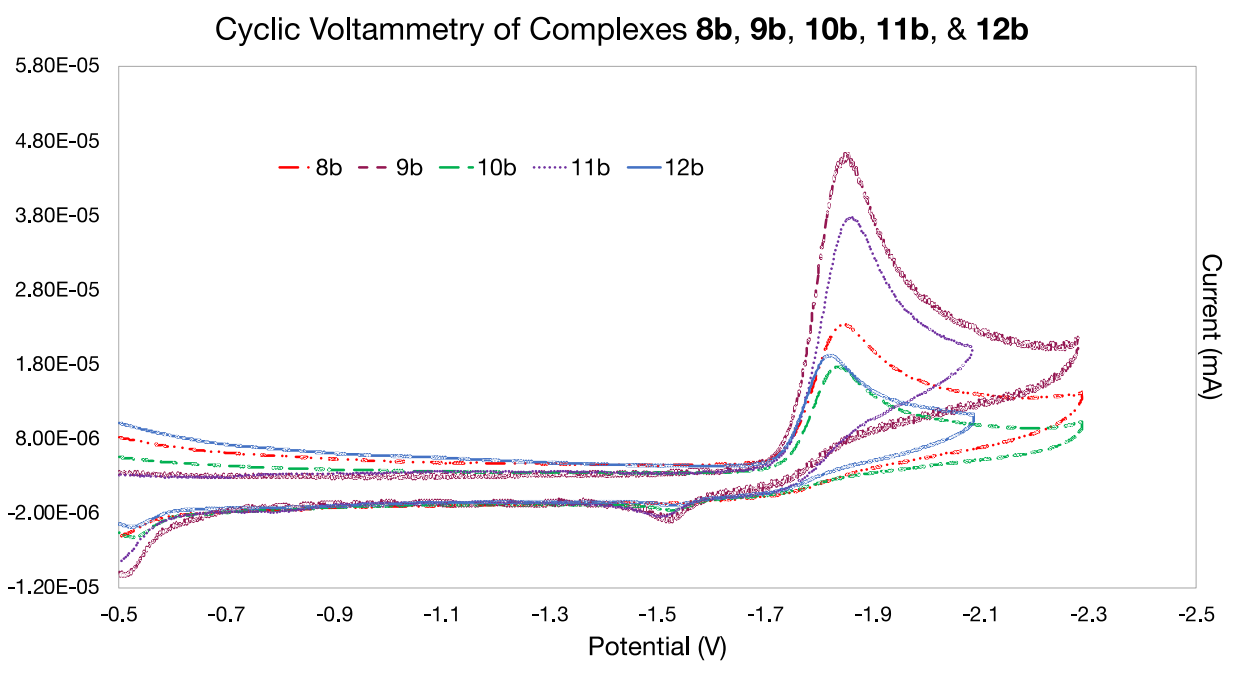

Figure S84. Voltammogram of complexes **8b** – **12b**.

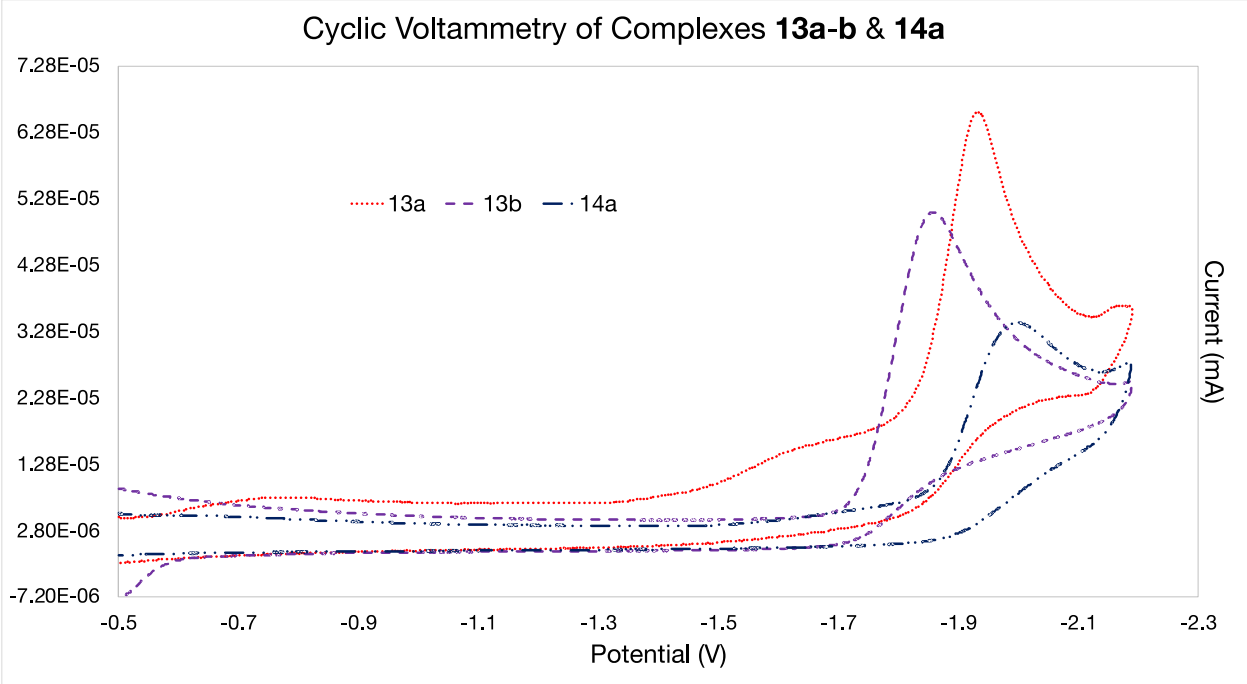

Figure S85. Voltammogram of complexes **13a-b**, **14a**.

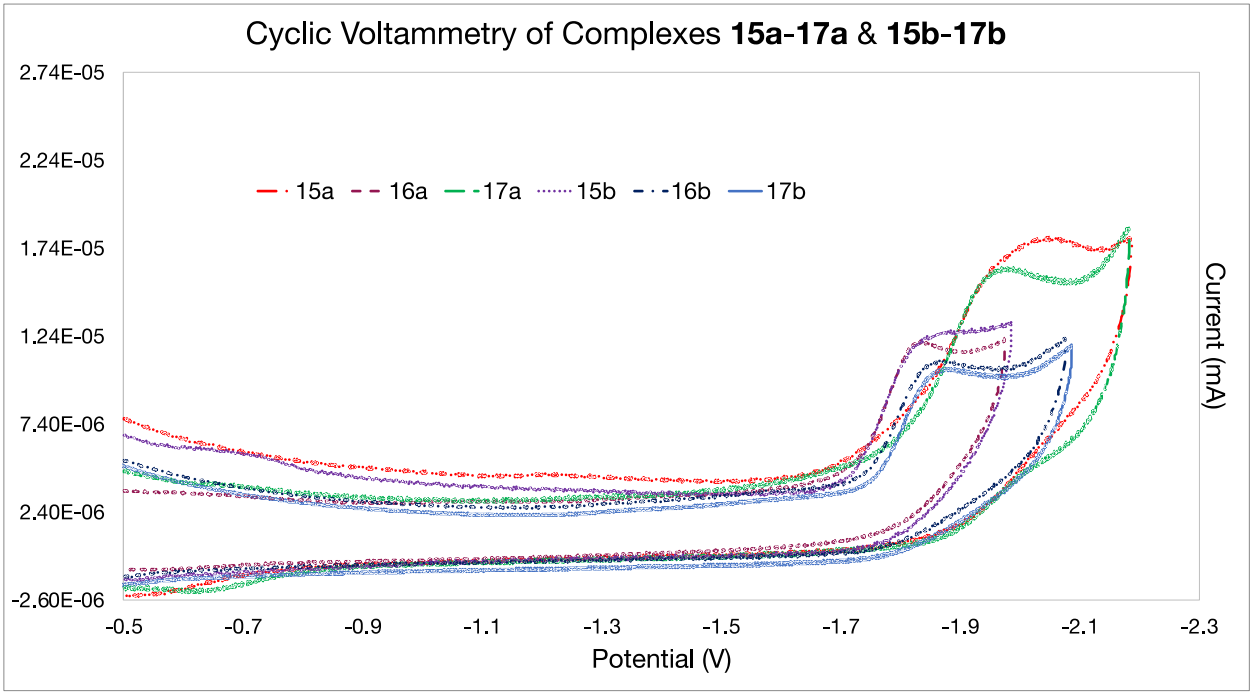

Figure S86. Voltammogram of complexes **15a-17a**, **15b-17b**.

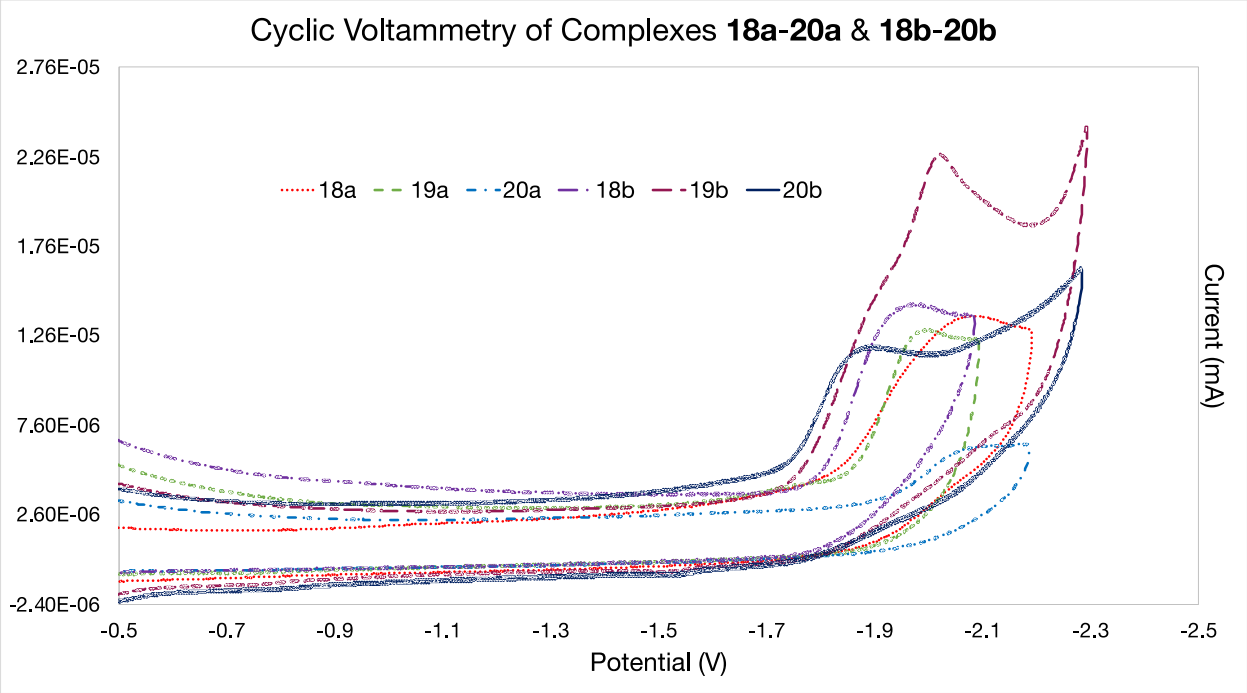

Figure S87. Voltammogram of complexes **18a-20a**, **18b-20b**.

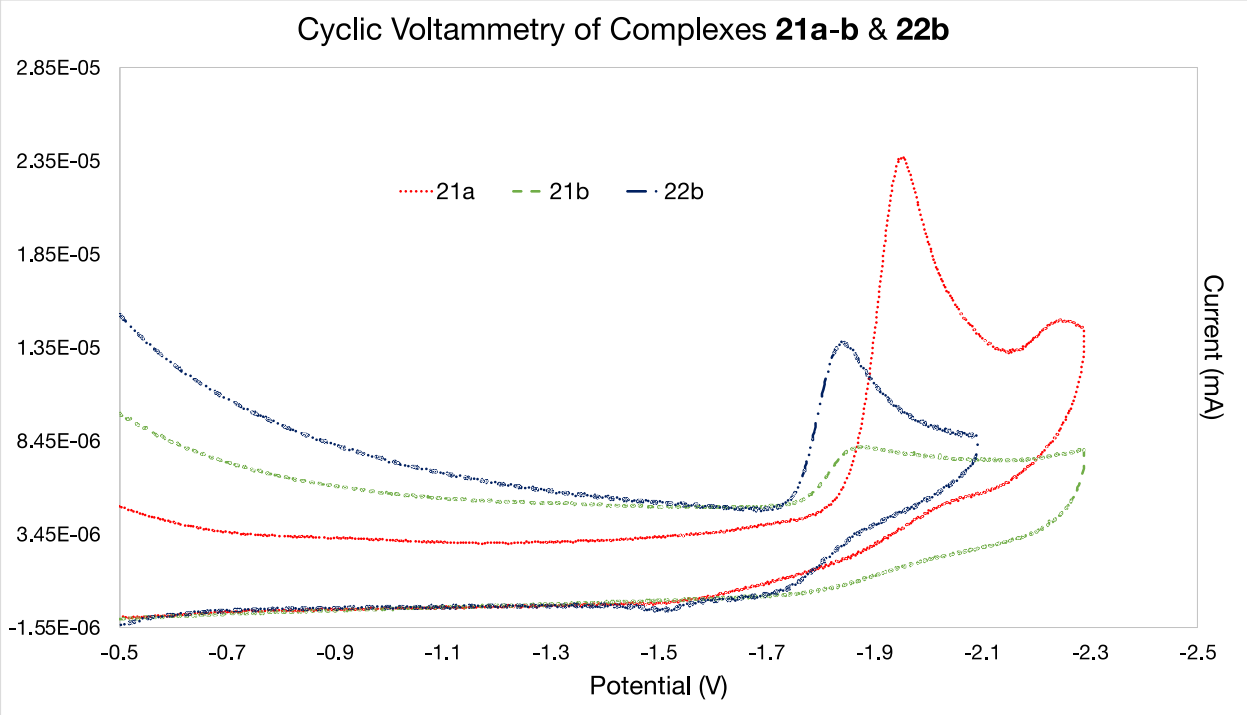

Figure S88. Voltammogram of complexes **21a-b**, **22b**.

X-Ray Crystallographic Data

Details of crystallographic refinement

General Methods. A suitable crystal of each sample was selected for analysis and mounted in a polyimide loop. All measurements were made on a Rigaku Oxford Diffraction Supernova Eos CCD with filtered Cu-Kα or Mo-Kα radiation at a temperature of 100 K. Using Olex2,[1] the structure was solved with the ShelXT structure solution program using Direct Methods and refined with the ShelXL refinement package[2] using Least Squares minimization.

Complex **8a**
The disordered nitrate anion was modeled over two positions with similarity restraints placed on the N-O bond distances and atom thermal parameters.

Complex **8b**
The model was refined without restraint.

Complexes **9a, 9b-1, 9b-2, 10a, 10b,**
The model was refined without restraint.

All structures have been uploaded to the CCDC, accession numbers 2013740-2013746.

Table 1. Crystal data and structure refinement **8a**.

Identification code	tj-11	
Empirical formula	C44 H39 Cl2 Ir N2 O5 P2	
Formula weight	1000.81	
Temperature	100.00(10) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 10.37212(18) Å	α = 90°
	b = 22.4932(4) Å	β = 97.1411(17)°
	c = 17.6765(3) Å	γ = 90°
Volume	4092.00(12) Å^3	
Z	4	
Density (calculated)	1.625 Mg/m^3	
Absorption coefficient	3.520 mm^{-1}	
F(000)	1992	
Crystal size	0.342 x 0.274 x 0.111 mm^3	
Theta range for data collection	2.322 to 30.010°.	
Index ranges	-13<=h<=14, -31<=k<=31, -22<=l<=24	
Reflections collected	48889	
Independent reflections	10737 [R(int) = 0.0424]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Gaussian	
Max. and min. transmission	1.000 and 0.250	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10737 / 117 / 537	
Goodness-of-fit on F^2	1.063	
Final R indices [I>2sigma(I)]	R1 = 0.0279, wR2 = 0.0530	
R indices (all data)	R1 = 0.0345, wR2 = 0.0552	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.966 and -0.947 e/Å^{-3}	

Table 2. Crystal data and structure refinement for **8b**.

Identification code	tj-10	
Empirical formula	C45 H41 Cl4 N2 O5 P2 Rh	
Formula weight	996.45	
Temperature	100.01(10) K	
Wavelength	1.54184 Å	
Crystal system	Orthorhombic	
Space group	Pbcm	
Unit cell dimensions	a = 10.32280(9) Å	α = 90°
	b = 18.37790(15) Å	β = 90°
	c = 23.0249(2) Å	γ = 90°
Volume	4368.08(7) Å^3	
Z	4	
Density (calculated)	1.515 Mg/m^3	
Absorption coefficient	6.498 mm^{-1}	
F(000)	2032	
Crystal size	0.179 x 0.113 x 0.101 mm^3	
Theta range for data collection	3.840 to 72.180°.	
Index ranges	-8<=h<=12, -18<=k<=22, -28<=l<=17	
Reflections collected	21772	
Independent reflections	4374 [R(int) = 0.0300]	
Completeness to theta = 67.684°	100.0 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.757 and 0.522	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4374 / 0 / 289	
Goodness-of-fit on F^2	1.077	
Final R indices [I>2sigma(I)]	R1 = 0.0372, wR2 = 0.0835	
R indices (all data)	R1 = 0.0398, wR2 = 0.0849	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.138 and -0.540 e/Å^{-3}	

Table 3. Crystal data and structure refinement for **9a**.

Identification code	tj-18	
Empirical formula	C43 H37 Ir N2 O5 P2	
Formula weight	915.88	
Temperature	100.00(10) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.8794(3) Å	α = 108.010(3)°
	b = 11.2620(3) Å	β = 95.694(2)°
	c = 17.7625(5) Å	γ = 94.789(2)°
Volume	1856.52(10) Å^3	
Z	2	
Density (calculated)	1.638 Mg/m^3	
Absorption coefficient	3.732 mm^{-1}	
F(000)	912	
Crystal size	0.259 x 0.164 x 0.019 mm^3	
Theta range for data collection	2.273 to 29.866°.	
Index ranges	-13<=h<=13, -15<=k<=15, -23<=l<=24	
Reflections collected	35005	
Independent reflections	9628 [R(int) = 0.0855]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Gaussian	
Max. and min. transmission	1.000 and 0.370	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9628 / 0 / 479	
Goodness-of-fit on F^2	1.040	
Final R indices [I>2sigma(I)]	R1 = 0.0433, wR2 = 0.0689	
R indices (all data)	R1 = 0.0548, wR2 = 0.0733	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.474 and -1.419 e/Å^{-3}	

Table 4. Crystal data and structure refinement for **9b-1**.

Identification code	tj-17	
Empirical formula	C46 H40 N2 O5 P2 Rh	
Formula weight	865.65	
Temperature	100.00(10) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	C 1 2/c 1	
Unit cell dimensions	a = 23.44630(10) Å	α = 90°
	b = 16.82500(10) Å	β = 110.0310(10)°
	c = 21.39890(10) Å	γ = 90°
Volume	7930.87(8) $Å^3$	
Z	8	
Density (calculated)	1.450 Mg/m^3	
Absorption coefficient	4.649 mm^{-1}	
F(000)	3560	
Crystal size	0.327 x 0.125 x 0.095 mm^3	
Theta range for data collection	3.305 to 72.263°.	
Index ranges	-28<=h<=28, -20<=k<=20, -25<=l<=25	
Reflections collected	46102	
Independent reflections	7785 [R(int) = 0.0238]	
Completeness to theta = 67.684°	100.0 %	
Absorption correction	Gaussian	
Max. and min. transmission	1.000 and 0.321	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7785 / 0 / 506	
Goodness-of-fit on F^2	1.187	
Final R indices [I>2sigma(I)]	R1 = 0.0293, wR2 = 0.0668	
R indices (all data)	R1 = 0.0294, wR2 = 0.0669	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.781 and -0.381 $e/Å^{-3}$	

Table 5. Crystal data and structure refinement for **9b-2**.

Identification code	tj-20	
Empirical formula	C43 H37 N2 O5 P2 Rh	
Formula weight	826.59	
Temperature	100.01(10) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.9080(4) Å	α = 108.050(4)°
	b = 11.2551(5) Å	β = 95.964(3)°
	c = 17.8041(7) Å	γ = 94.620(4)°
Volume	1864.11(14) Å^3	
Z	2	
Density (calculated)	1.473 Mg/m^3	
Absorption coefficient	0.593 mm^{-1}	
F(000)	848	
Crystal size	0.428 x 0.186 x 0.017 mm^3	
Theta range for data collection	2.263 to 29.853°.	
Index ranges	-13<=h<=13, -14<=k<=14, -24<=l<=24	
Reflections collected	32240	
Independent reflections	9518 [R(int) = 0.0688]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Gaussian	
Max. and min. transmission	1.000 and 0.422	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9518 / 0 / 479	
Goodness-of-fit on F^2	1.053	
Final R indices [I>2sigma(I)]	R1 = 0.0467, wR2 = 0.0875	
R indices (all data)	R1 = 0.0631, wR2 = 0.0945	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.891 and -1.272 e/Å^{-3}	

Table 6. Crystal data and structure refinement for **10a**.

Identification code	tj-21	
Empirical formula	C43 H37 Ir N2 O5 P2	
Formula weight	915.88	
Temperature	100.00(10) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 19.1415(5) Å	α = 90°
	b = 11.3474(3) Å	β = 110.521(3)°
	c = 18.5807(4) Å	γ = 90°
Volume	3779.77(16) Å^3	
Z	4	
Density (calculated)	1.609 Mg/m^3	
Absorption coefficient	3.666 mm^{-1}	
F(000)	1824	
Crystal size	0.272 x 0.121 x 0.084 mm^3	
Theta range for data collection	2.215 to 29.914°.	
Index ranges	-25<=h<=26, -15<=k<=15, -25<=l<=25	
Reflections collected	45522	
Independent reflections	9804 [R(int) = 0.0543]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Gaussian	
Max. and min. transmission	1.000 and 0.415	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9804 / 0 / 479	
Goodness-of-fit on F^2	1.063	
Final R indices [I>2sigma(I)]	R1 = 0.0330, wR2 = 0.0524	
R indices (all data)	R1 = 0.0442, wR2 = 0.0556	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.882 and -0.988 e/Å^{-3}	

Table 7. Crystal data and structure refinement for **10b**.

Identification code	tj-19	
Empirical formula	C43 H37 N2 O5 P2 Rh	
Formula weight	826.59	
Temperature	100.0(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 19.1625(6) Å	α = 90°
	b = 11.3328(3) Å	β = 110.478(3)°
	c = 18.6157(6) Å	γ = 90°
Volume	3787.2(2) $Å^3$	
Z	4	
Density (calculated)	1.450 Mg/m^3	
Absorption coefficient	0.584 mm^{-1}	
F(000)	1696	
Crystal size	0.395 x 0.227 x 0.176 mm^3	
Theta range for data collection	2.609 to 29.971°.	
Index ranges	-26<=h<=25, -14<=k<=15, -25<=l<=23	
Reflections collected	36911	
Independent reflections	9793 [R(int) = 0.0536]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Gaussian	
Max. and min. transmission	1.000 and 0.546	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9793 / 0 / 479	
Goodness-of-fit on F^2	1.038	
Final R indices [I>2sigma(I)]	R1 = 0.0368, wR2 = 0.0723	
R indices (all data)	R1 = 0.0461, wR2 = 0.0771	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.563 and -0.480 $e/Å^{-3}$	

(1) Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H., "OLEX2: a complete structure solution, refinement and analysis program." *J. Appl. Crystallogr.* **2009,** *42* (2), 339-341.
(2) Sheldrick, G., "A short history of SHELX." *Acta Crystallographica Section A* **2008,** *64* (1), 112-122.

Cartesian Coordinates for Calculated Structures

8a

Ir	0.031055	-0.332749	-0.013150
P	-2.369647	-0.395146	-0.045475
P	2.434048	-0.322459	-0.001291
O	0.079104	-3.279080	0.526808
C	0.058994	-2.138433	0.318838
N	0.004965	1.796943	-0.473260
C	-0.042053	2.778401	0.455913
C	-0.056731	4.125826	0.083406
C	-0.023030	4.474361	-1.262870
C	0.025124	3.455557	-2.217624
C	0.037977	2.137415	-1.783119
C	-0.100665	2.400690	1.917591
H	-0.107259	4.879963	0.862141
H	-0.034732	5.518711	-1.563927
H	0.049470	3.669751	-3.281598
H	0.070155	1.311398	-2.486464
O	-1.179758	3.118401	2.507642
C	-3.145471	-0.454414	1.633216
C	-4.481669	-0.067255	1.841717
H	-5.077214	0.315992	1.017362
C	-5.053022	-0.163155	3.112996
H	-6.087034	0.140181	3.260952
C	-4.299849	-0.644562	4.188294
H	-4.746295	-0.715065	5.177665
C	-2.971213	-1.029893	3.989590
H	-2.378083	-1.400503	4.822604
C	-2.395336	-0.933944	2.719983
H	-1.358254	-1.223999	2.574054
C	-2.996180	-1.895867	-0.934012
C	-4.155085	-2.578408	-0.531240
H	-4.710214	-2.252288	0.343808
C	-4.599833	-3.692234	-1.249545
H	-5.494337	-4.218180	-0.923303
C	-3.899765	-4.129569	-2.377700
H	-4.248655	-4.997138	-2.933306
C	-2.746550	-3.453041	-2.786161
H	-2.194068	-3.789467	-3.660611
C	-2.292432	-2.346325	-2.064718
H	-1.385306	-1.831610	-2.374696
C	-3.211310	1.023456	-0.890438
C	-3.686080	0.903235	-2.206596
H	-3.600415	-0.040693	-2.737623
C	-4.278800	1.996937	-2.845336
H	-4.646775	1.887952	-3.863177
C	-4.402471	3.218405	-2.178879
H	-4.866953	4.067227	-2.675844
C	-3.926019	3.345913	-0.870090
H	-4.016019	4.294429	-0.345157

C -3.331082 2.258343 -0.226686
H -2.961789 2.380553 0.788967
C 3.188931 -0.953823 -1.566143
C 2.407069 -1.730301 -2.437044
H 1.361737 -1.912170 -2.201688
C 2.962186 -2.257101 -3.606466
H 2.344954 -2.855339 -4.272930
C 4.301252 -2.009953 -3.920043
H 4.732250 -2.417541 -4.831787
C 5.085503 -1.231692 -3.062404
H 6.127363 -1.032535 -3.303000
C 4.534952 -0.703988 -1.892241
H 5.154395 -0.092792 -1.240707
C 3.119018 -1.380016 1.359112
C 2.433916 -1.415810 2.586610
H 1.506650 -0.859253 2.703549
C 2.931446 -2.167996 3.653631
H 2.392599 -2.183830 4.598359
C 4.109945 -2.904180 3.501985
H 4.493193 -3.497086 4.329432
C 4.790432 -2.882336 2.281163
H 5.703904 -3.459012 2.153877
C 4.302047 -2.122324 1.214437
H 4.843165 -2.119867 0.272711
C 3.232393 1.331554 0.258860
C 3.620153 1.752044 1.541957
H 3.506429 1.088534 2.395054
C 4.162569 3.026705 1.733332
H 4.464060 3.336226 2.731573
C 4.322493 3.893880 0.649301
H 4.747647 4.883645 0.799593
C 3.936537 3.482909 -0.630262
H 4.059528 4.150239 -1.480352
C 3.393114 2.211255 -0.826344
H 3.105088 1.904518 -1.828443
H -0.236567 1.311080 2.004852
H 0.855960 2.661966 2.396578
H -1.123750 3.006997 3.466881
el energy= -1983.71651276
zpe= -1983.033007
th energy= -1982.987063
th enthalpy= -1982.986119
free energy= -1983.119682

9a

Ir -0.009341 -0.427002 0.026162
P -2.407584 -0.416700 0.028912
P 2.389333 -0.471525 0.007364
O -0.047862 -3.284637 0.930347
C -0.031989 -2.177351 0.585568
N 0.020053 1.621041 -0.655267

C 0.158649 2.625263 0.234711
C 0.190704 3.967870 -0.137037
C 0.071750 4.271353 -1.497920
C -0.067470 3.235628 -2.420882
C -0.091279 1.920741 -1.965066
C 0.387109 5.049007 0.912618
H 0.085799 5.306908 -1.832548
H -0.163395 3.435968 -3.483666
H -0.202757 1.080715 -2.642875
C -3.156028 -0.296172 1.715748
C -4.502496 0.068697 1.901148
H -5.124404 0.326529 1.047565
C -5.050136 0.112574 3.185300
H -6.092631 0.394335 3.315289
C -4.261911 -0.202010 4.297112
H -4.690367 -0.164577 5.296198
C -2.921945 -0.557407 4.122031
H -2.301393 -0.795064 4.983108
C -2.369981 -0.602310 2.838729
H -1.323650 -0.864989 2.706586
C -3.092717 -1.964224 -0.726558
C -4.268532 -2.576605 -0.264678
H -4.806565 -2.166257 0.584972
C -4.752581 -3.729674 -0.889416
H -5.660387 -4.199608 -0.517540
C -4.074808 -4.277340 -1.982469
H -4.454795 -5.174802 -2.465499
C -2.903351 -3.673021 -2.448077
H -2.367072 -4.096308 -3.294459
C -2.409994 -2.527074 -1.819462
H -1.487644 -2.069056 -2.170936
C -3.214711 0.956421 -0.919005
C -3.665034 0.765853 -2.235169
H -3.589133 -0.210880 -2.705257
C -4.220936 1.830517 -2.951568
H -4.571501 1.667135 -3.968247
C -4.330408 3.093322 -2.364230
H -4.766317 3.919284 -2.921786
C -3.878738 3.291578 -1.055317
H -3.961244 4.271445 -0.590230
C -3.321877 2.232041 -0.336498
H -2.980331 2.399433 0.682090
C 3.106938 -1.275241 -1.494749
C 2.297251 -2.123886 -2.267576
H 1.254225 -2.264411 -1.995549
C 2.822035 -2.775408 -3.387171
H 2.183538 -3.427811 -3.978547
C 4.158186 -2.583056 -3.748251
H 4.565291 -3.087299 -4.621864
C 4.970367 -1.735591 -2.987771
H 6.010287 -1.579268 -3.265634

C 4.450186 -1.083057 -1.867683
H 5.090908 -0.419496 -1.292420
C 3.073853 -1.397283 1.459781
C 2.411637 -1.280680 2.694809
H 1.503992 -0.684530 2.765377
C 2.906518 -1.931741 3.827449
H 2.386027 -1.830536 4.777137
C 4.058491 -2.718273 3.735352
H 4.438932 -3.233502 4.614504
C 4.715985 -2.847199 2.508519
H 5.608616 -3.463683 2.428691
C 4.230826 -2.188039 1.375246
H 4.753051 -2.301382 0.429567
C 3.219487 1.184811 0.084915
C 3.621482 1.731952 1.314373
H 3.505898 1.162919 2.232830
C 4.179753 3.012762 1.368449
H 4.492463 3.420762 2.327042
C 4.340632 3.760654 0.198923
H 4.780409 4.754580 0.242189
C 3.937639 3.224018 -1.028295
H 4.060275 3.798406 -1.943831
C 3.378458 1.945626 -1.087027
H 3.073725 1.541623 -2.049089
H 0.244643 2.339940 1.277192
O 0.093706 4.622623 2.232711
H -0.866087 4.531556 2.319305
H 1.444580 5.342781 0.925560
H -0.193139 5.942197 0.635102
el energy= -1983.71756102
zpe= -1983.033363
th energy= -1982.987590
th enthalpy= -1982.986646
free energy= -1983.119517

10a

Ir 0.030504 -0.553257 0.022433
P 2.421406 -0.398196 -0.038033
P -2.367069 -0.637951 0.017436
O 0.083194 -3.532986 -0.264256
O -0.529939 6.588530 -0.620615
H -1.478909 6.466259 -0.765985
N -0.042487 1.608839 0.232598
C 0.074183 -2.378671 -0.155299
C -0.130160 2.389239 -0.864274
H -0.154318 1.873194 -1.817616
C -0.178151 3.776884 -0.794754
H -0.243803 4.363021 -1.705338
C -0.142435 4.408451 0.451034
C -0.061309 3.592665 1.587424
H -0.039396 4.019816 2.586852

C	-0.013887	2.213126	1.441239
H	0.044075	1.560195	2.304850
C	-0.168896	5.920891	0.573601
H	-0.817617	6.208603	1.415519
H	0.842730	6.270125	0.820317
C	3.329562	-1.921297	-0.592072
C	3.290041	-3.043173	0.256115
H	2.746857	-2.999113	1.197943
C	3.954850	-4.218681	-0.094744
H	3.916181	-5.077332	0.571809
C	4.665440	-4.291147	-1.297942
H	5.182497	-5.208029	-1.571788
C	4.710426	-3.180895	-2.143221
H	5.265271	-3.226132	-3.077777
C	4.048451	-1.998385	-1.793708
H	4.103659	-1.143345	-2.460434
C	2.927262	0.943754	-1.205251
C	2.476946	0.850965	-2.536843
H	1.878800	-0.002157	-2.851264
C	2.782221	1.853456	-3.459097
H	2.435291	1.763503	-4.485981
C	3.520376	2.972649	-3.059217
H	3.752505	3.757292	-3.775724
C	3.949327	3.083177	-1.734675
H	4.514070	3.955634	-1.413664
C	3.657237	2.074621	-0.809892
H	3.995501	2.181218	0.216284
C	3.233310	-0.060671	1.588838
C	4.627003	0.114856	1.679944
H	5.244288	0.088121	0.784761
C	5.230381	0.316048	2.922216
H	6.307371	0.456395	2.980671
C	4.454542	0.328329	4.087461
H	4.928585	0.481469	5.054390
C	3.074495	0.131221	4.007423
H	2.468496	0.123499	4.910574
C	2.465707	-0.064203	2.763323
H	1.395256	-0.246136	2.705261
C	-3.090719	-1.088289	1.657849
C	-2.274050	-1.720548	2.610260
H	-1.225230	-1.897633	2.384976
C	-2.799407	-2.109545	3.845603
H	-2.155645	-2.596293	4.574786
C	-4.142912	-1.867265	4.143834
H	-4.550759	-2.167319	5.106554
C	-4.961617	-1.232015	3.204443
H	-6.007136	-1.037172	3.432450
C	-4.441036	-0.842100	1.968285
H	-5.087086	-0.338965	1.253212
C	-3.017968	-1.881851	-1.192781
C	-4.177520	-2.635438	-0.950086

H -4.718510 -2.528962 -0.014184
C -4.641276 -3.540245 -1.909316
H -5.536271 -4.124253 -1.706452
C -3.959374 -3.696515 -3.119602
H -4.323355 -4.402118 -3.863087
C -2.804128 -2.949793 -3.368151
H -2.264040 -3.070457 -4.304547
C -2.330642 -2.052504 -2.407625
H -1.418678 -1.488917 -2.595045
C -3.220112 0.941312 -0.447854
C -3.610845 1.184041 -1.775007
H -3.466905 0.423240 -2.537456
C -4.194852 2.404585 -2.127038
H -4.498276 2.575792 -3.157496
C -4.392903 3.394919 -1.161385
H -4.851773 4.342015 -1.436392
C -4.001345 3.162319 0.160821
H -4.153336 3.926630 0.919781
C -3.416304 1.945183 0.517052
H -3.122359 1.778332 1.550072
el energy= -1983.71614517
zpe= -1983.031998
th energy= -1982.986200
th enthalpy= -1982.985255
free energy= -1983.119311

11a

Ir 1.268044 0.560616 -0.038885
P -0.441377 2.238389 0.100928
P 2.980393 -1.108107 -0.212707
O 2.868131 2.366163 -1.818430
C 2.247403 1.667024 -1.130943
N 0.122204 -0.736893 1.243939
C -0.678180 -1.676911 0.699905
C -1.452599 -2.548403 1.461877
C -1.380759 -2.433162 2.854835
C -0.550851 -1.466748 3.421649
C 0.185432 -0.631578 2.586384
C -2.329657 -3.588770 0.780176
H -1.971443 -3.090391 3.490689
H -0.473692 -1.349819 4.498481
H 0.838423 0.141671 2.978046
C -1.521577 2.332006 -1.395383
C -2.749757 3.018155 -1.373041
H -3.106604 3.476221 -0.453929
C -3.529033 3.104239 -2.528678
H -4.476821 3.636798 -2.499283
C -3.096859 2.501500 -3.714817
H -3.708546 2.565770 -4.611971
C -1.883076 1.809522 -3.742058
H -1.546711 1.329723 -4.658416

C	-1.098795	1.723727	-2.588235
H	-0.162069	1.172821	-2.606830
C	0.296458	3.927775	0.307523
C	-0.242755	5.072399	-0.300320
H	-1.114223	4.995270	-0.943967
C	0.345108	6.323639	-0.090975
H	-0.077750	7.201660	-0.574348
C	1.468779	6.446831	0.731052
H	1.923164	7.422094	0.891298
C	2.011628	5.311554	1.340214
H	2.889454	5.397513	1.976870
C	1.434361	4.058020	1.123675
H	1.871134	3.173225	1.582580
C	-1.633032	2.079418	1.510881
C	-1.452591	2.800609	2.702508
H	-0.630742	3.504799	2.800588
C	-2.334630	2.623601	3.773118
H	-2.187466	3.193145	4.688337
C	-3.400498	1.726276	3.665535
H	-4.087758	1.592865	4.498310
C	-3.581252	1.002118	2.482938
H	-4.406909	0.302068	2.383488
C	-2.703137	1.172492	1.410064
H	-2.870552	0.597807	0.502366
C	4.472738	-0.772407	0.827721
C	4.691296	0.527009	1.313832
H	3.963531	1.307176	1.106352
C	5.829120	0.816680	2.072257
H	5.984578	1.826805	2.444574
C	6.757199	-0.188445	2.356568
H	7.640831	0.036665	2.949705
C	6.544337	-1.487116	1.882787
H	7.260753	-2.275092	2.104191
C	5.408744	-1.780480	1.124259
H	5.251033	-2.796747	0.771944
C	3.598887	-1.271216	-1.952920
C	2.670880	-1.135153	-3.000660
H	1.631555	-0.907569	-2.773022
C	3.076533	-1.282426	-4.329367
H	2.347047	-1.178081	-5.129397
C	4.415673	-1.551613	-4.626663
H	4.734238	-1.657153	-5.661362
C	5.345816	-1.677541	-3.590790
H	6.390747	-1.879749	-3.815757
C	4.941825	-1.542513	-2.259251
H	5.678826	-1.641448	-1.467489
C	2.478349	-2.828892	0.260221
C	2.053088	-3.751620	-0.708981
H	2.066079	-3.486670	-1.762685
C	1.609670	-5.021811	-0.327656
H	1.287212	-5.727681	-1.089792

C 1.584101 -5.382626 1.021930
H 1.242062 -6.372309 1.316429
C 2.001473 -4.466517 1.993082
H 1.984436 -4.738908 3.046067
C 2.443751 -3.196536 1.617201
H 2.766513 -2.496268 2.383624
H -0.701681 -1.728640 -0.382211
O -2.419333 -3.427424 -0.617276
H -2.986063 -2.643764 -0.785158
H -1.897096 -4.582807 0.960079
H -3.324204 -3.582415 1.253308
F -7.554048 -2.040133 -0.078528
C -6.252521 -1.893475 0.199655
S -5.346793 -1.122899 -1.259718
O -3.913141 -1.120234 -0.788702
F -6.145349 -1.124863 1.295668
F -5.746499 -3.103753 0.489091
O -5.619651 -2.066629 -2.379207
O -5.951776 0.232039 -1.373345
el energy= -2557.23299940
zpe= -2556.520586
th energy= -2556.465887
th enthalpy= -2556.464942
free energy= -2556.621521

12a

Ir -1.586727 0.430728 0.010669
P -0.278261 2.442024 0.015727
P -2.928318 -1.558388 0.015264
O -4.068788 2.073321 0.365195
C -3.107375 1.438089 0.227138
N 0.194831 -0.762483 -0.241777
C 0.813203 -1.329324 0.815080
C 1.939764 -2.132657 0.679677
C 2.462518 -2.383243 -0.591816
C 1.818548 -1.785015 -1.684269
C 0.703871 -0.986688 -1.473900
C 3.667594 -3.284303 -0.793643
H 2.176750 -1.936834 -2.699690
H 0.185743 -0.507269 -2.298526
C -0.006067 3.145395 1.705211
C 1.017894 4.076337 1.959405
H 1.698271 4.374524 1.165778
C 1.177780 4.616458 3.237609
H 1.973484 5.334944 3.421278
C 0.322567 4.232371 4.275434
H 0.452116 4.651493 5.270829
C -0.692758 3.303475 4.032638
H -1.355638 2.993866 4.837547
C -0.855841 2.760422 2.755193
H -1.636184 2.026176 2.572908

C	-1.091056	3.786344	-0.968477
C	-1.041491	5.137209	-0.589760
H	-0.534303	5.434600	0.323706
C	-1.654356	6.112625	-1.381914
H	-1.615829	7.155165	-1.073756
C	-2.313922	5.752173	-2.560444
H	-2.789958	6.514038	-3.173786
C	-2.366045	4.409058	-2.944950
H	-2.881414	4.119721	-3.858120
C	-1.764699	3.430100	-2.150206
H	-1.822799	2.383332	-2.441856
C	1.425062	2.310136	-0.696462
C	1.704269	2.711290	-2.012712
H	0.927308	3.156586	-2.628269
C	2.988466	2.543410	-2.541493
H	3.193026	2.862982	-3.561168
C	4.000424	1.971806	-1.766383
H	4.997597	1.835161	-2.177113
C	3.728865	1.566094	-0.455181
H	4.503392	1.109591	0.155016
C	2.448905	1.733322	0.075688
H	2.252583	1.415861	1.096934
C	-3.813298	-1.865890	-1.579806
C	-3.970670	-0.808057	-2.490131
H	-3.537199	0.162630	-2.263784
C	-4.666984	-1.001620	-3.686477
H	-4.779123	-0.174275	-4.383650
C	-5.208853	-2.253872	-3.987653
H	-5.747753	-2.405250	-4.920363
C	-5.051020	-3.315168	-3.090386
H	-5.466726	-4.293520	-3.321022
C	-4.356129	-3.125666	-1.893624
H	-4.231487	-3.962753	-1.211300
C	-4.243810	-1.485761	1.320426
C	-3.924861	-0.882432	2.550017
H	-2.938318	-0.447366	2.696502
C	-4.868179	-0.830386	3.579142
H	-4.606447	-0.363721	4.526180
C	-6.144968	-1.365947	3.386151
H	-6.883197	-1.317454	4.183578
C	-6.472745	-1.957379	2.162771
H	-7.466822	-2.369468	2.003638
C	-5.527788	-2.022150	1.134482
H	-5.800627	-2.483819	0.189860
C	-2.037074	-3.148859	0.350317
C	-1.993258	-3.698263	1.641884
H	-2.526692	-3.221727	2.459862
C	-1.265857	-4.867000	1.887213
H	-1.244558	-5.283761	2.891750
C	-0.574437	-5.496821	0.849446
H	-0.010240	-6.406595	1.041867

C -0.609723 -4.952368 -0.438328
H -0.073736 -5.435852 -1.252037
C -1.333545 -3.784788 -0.688090
H -1.353431 -3.375762 -1.695063
H 0.376342 -1.126601 1.788096
H 2.409468 -2.573314 1.552268
O 4.155688 -3.836857 0.405463
H 5.013136 -3.404883 0.602922
H 3.366549 -4.099653 -1.471898
H 4.447740 -2.714314 -1.318991
C 7.032673 -0.448254 -0.757734
S 6.786742 -1.225478 0.940946
F 8.160521 -0.887262 -1.325807
F 7.100393 0.890146 -0.658732
F 6.006915 -0.744225 -1.576012
O 5.544948 -0.582612 1.460529
O 8.045303 -0.890689 1.661325
O 6.631590 -2.685060 0.602396
el energy= -2557.23203059
zpe= -2556.520088
th energy= -2556.465304
th enthalpy= -2556.464360
free energy= -2556.620206

13a

Ir 1.283908 0.435746 0.097181
P 2.751976 -1.468654 0.167825
P -0.124082 2.386749 -0.009557
O 3.004797 1.799845 2.141165
C 2.347672 1.281721 1.340542
N -0.054329 -0.623500 -1.230104
C -1.089212 -1.312218 -0.709159
C -2.012087 -1.995762 -1.514995
C -1.833783 -1.967532 -2.888569
C -0.748076 -1.264975 -3.437233
C 0.111399 -0.607222 -2.577625
O -1.223040 -1.347930 0.621455
H -2.840252 -2.512145 -1.043825
H -2.534770 -2.488453 -3.535705
H -0.578025 -1.225047 -4.508047
H 0.965198 -0.041064 -2.936359
C 2.612411 -2.512405 1.687399
C 3.088100 -3.836545 1.710664
H 3.513225 -4.283584 0.815796
C 3.008441 -4.593237 2.881992
H 3.378902 -5.615849 2.886462
C 2.453124 -4.040338 4.040174
H 2.388227 -4.633396 4.949642
C 1.976066 -2.727068 4.024379
H 1.536606 -2.292867 4.919458
C 2.053123 -1.966563 2.854560

H	1.669276	-0.950188	2.847738
C	4.523536	-0.934890	0.081033
C	5.549013	-1.611158	0.760720
H	5.322322	-2.469319	1.387019
C	6.872958	-1.177948	0.644277
H	7.658365	-1.704970	1.181456
C	7.186550	-0.074022	-0.153968
H	8.217923	0.260414	-0.240707
C	6.170733	0.603134	-0.835036
H	6.406094	1.465385	-1.454831
C	4.844967	0.179871	-0.713343
H	4.054958	0.718092	-1.233307
C	2.553748	-2.664759	-1.232364
C	3.378465	-2.594794	-2.366593
H	4.183785	-1.866994	-2.416379
C	3.173797	-3.465764	-3.441321
H	3.823732	-3.404740	-4.311428
C	2.145081	-4.409864	-3.396251
H	1.988643	-5.087600	-4.232467
C	1.316652	-4.481120	-2.271537
H	0.512907	-5.212588	-2.228181
C	1.516359	-3.613760	-1.195871
H	0.868483	-3.687495	-0.325730
C	0.588705	3.714827	-1.081216
C	1.970198	3.724280	-1.336624
H	2.598891	2.931566	-0.940230
C	2.541382	4.742987	-2.103951
H	3.612123	4.736286	-2.294987
C	1.739379	5.760787	-2.627099
H	2.183924	6.552090	-3.226581
C	0.362546	5.756802	-2.382906
H	-0.268171	6.544126	-2.789523
C	-0.212441	4.740518	-1.616120
H	-1.285593	4.745407	-1.444058
C	-0.382882	3.168235	1.651782
C	-0.480367	2.340572	2.783749
H	-0.362596	1.264557	2.680604
C	-0.721603	2.890650	4.045250
H	-0.798320	2.236856	4.911037
C	-0.854497	4.273974	4.192172
H	-1.034678	4.703520	5.175075
C	-0.749082	5.104684	3.072707
H	-0.845462	6.182764	3.180543
C	-0.517988	4.557597	1.807636
H	-0.437765	5.218666	0.949502
C	-1.830004	2.106523	-0.665646
C	-2.897136	1.842835	0.209546
H	-2.744643	1.872466	1.285242
C	-4.161328	1.525935	-0.294873
H	-4.976103	1.290148	0.385027
C	-4.374283	1.479594	-1.675624

H -5.355671 1.208278 -2.055037
C -3.319645 1.751670 -2.552238
H -3.477824 1.717665 -3.628098
C -2.050744 2.054715 -2.053521
H -1.237923 2.253912 -2.747286
H -0.486481 -0.814428 1.015185
F -4.454181 -1.464922 0.661337
C -5.557606 -2.230761 0.617053
S -7.087626 -1.208240 0.206196
O -8.200903 -2.181750 0.414032
F -5.350814 -3.185324 -0.309033
F -5.689094 -2.831740 1.808831
O -7.023561 -0.095607 1.204552
O -6.859713 -0.801603 -1.214242
el energy= -2517.92668284
zpe= -2517.243721
th energy= -2517.190305
th enthalpy= -2517.189361
free energy= -2517.342453

14a

Ir -1.028363 -0.531709 -0.114079
P 0.377258 -2.474536 -0.065127
P -2.412514 1.423044 -0.224769
O -2.402430 -1.619863 -2.545593
C -1.860754 -1.192921 -1.611845
N -0.109553 0.216786 1.688367
C 0.915305 1.082360 1.595713
C 1.565738 1.601901 2.726167
C 1.107773 1.203777 3.990900
C 0.043606 0.310367 4.070644
C -0.545440 -0.172079 2.903722
O 2.596685 2.454927 2.634048
H 1.592272 1.595269 4.881507
H -0.333991 -0.019740 5.034045
H -1.371018 -0.875310 2.919873
C 1.672348 -2.508537 -1.385578
C 2.784042 -3.366333 -1.294937
H 2.917820 -4.001052 -0.422582
C 3.733038 -3.400998 -2.319004
H 4.587982 -4.068459 -2.236739
C 3.587305 -2.578412 -3.440793
H 4.330166 -2.603631 -4.235001
C 2.490339 -1.717883 -3.534335
H 2.376812 -1.066766 -4.398065
C 1.538532 -1.680438 -2.511407
H 0.698433 -0.995126 -2.580113
C -0.622385 -4.019165 -0.300097

C	-0.151664	-5.125398	-1.024828
H	0.826434	-5.098172	-1.496630
C	-0.943523	-6.270292	-1.155065
H	-0.570512	-7.117808	-1.726026
C	-2.206386	-6.326047	-0.558609
H	-2.819809	-7.218361	-0.662619
C	-2.681867	-5.228761	0.165704
H	-3.665700	-5.262119	0.628642
C	-1.898365	-4.078655	0.288207
H	-2.278800	-3.218309	0.835233
C	1.330843	-2.768470	1.495447
C	0.909994	-3.713127	2.444812
H	0.026402	-4.318903	2.262891
C	1.627362	-3.885428	3.632939
H	1.293884	-4.624613	4.358203
C	2.766765	-3.116902	3.883595
H	3.325556	-3.253967	4.806907
C	3.186898	-2.170691	2.942827
H	4.072204	-1.567061	3.131207
C	2.474954	-1.991226	1.754653
H	2.819682	-1.250559	1.036272
C	-4.143992	1.163653	0.371432
C	-4.639400	-0.145249	0.488974
H	-3.988885	-0.987150	0.266004
C	-5.954967	-0.369156	0.904900
H	-6.324968	-1.388149	0.994009
C	-6.786860	0.710732	1.211822
H	-7.809587	0.536094	1.538706
C	-6.299723	2.017574	1.105268
H	-6.940760	2.862306	1.347521
C	-4.985837	2.245444	0.689767
H	-4.617001	3.265967	0.623293
C	-2.556090	2.045831	-1.964934
C	-1.422190	1.959757	-2.792454
H	-0.509749	1.506315	-2.410483
C	-1.463347	2.444836	-4.101944
H	-0.577475	2.375640	-4.729222
C	-2.641267	3.006006	-4.603875
H	-2.676917	3.375500	-5.626344
C	-3.775437	3.084596	-3.790551
H	-4.697233	3.513444	-4.177599
C	-3.735084	2.611475	-2.475601
H	-4.626428	2.679100	-1.858483
C	-1.815281	2.886814	0.742110
C	-1.037418	3.886447	0.135976
H	-0.823163	3.846304	-0.928490
C	-0.531165	4.944646	0.896935
H	0.067161	5.713608	0.413391
C	-0.792775	5.014197	2.267583
H	-0.398325	5.838332	2.857774
C	-1.563536	4.019693	2.878334

H -1.771550 4.065893 3.945033
C -2.070905 2.960614 2.122853
H -2.667933 2.194851 2.611610
H 1.230807 1.366855 0.599439
H 2.834962 2.617884 1.683950
C 5.676930 2.516591 -0.619252
S 3.915125 1.870749 -0.751901
O 3.133421 2.899032 0.037015
O 3.981153 0.532118 -0.099449
O 3.622149 1.888931 -2.209701
F 6.520186 1.708536 -1.275139
F 5.769970 3.744168 -1.146462
F 6.058997 2.576007 0.662676
el energy= -2517.93167939
zpe= -2517.248360
th energy= -2517.195118
th enthalpy= -2517.194174
free energy= -2517.346538

15a

Ir -0.022817 -0.578447 0.046064
P -2.422833 -0.566036 0.017322
P 2.378704 -0.669865 0.002551
O -0.089301 -3.396756 1.060901
C -0.062014 -2.306850 0.665210
N 0.018814 1.456252 -0.714729
C 0.080452 2.572150 0.096235
C 0.134623 3.885511 -0.484807
C 0.096705 3.995125 -1.894840
C 0.020000 2.859771 -2.672120
C -0.014132 1.606598 -2.036878
H 0.115647 4.964384 -2.388367
H -0.016020 2.911521 -3.755210
H -0.069082 0.692057 -2.620341
C -3.207293 -0.379964 1.681947
C -4.544613 0.033204 1.825263
H -5.136391 0.292055 0.950989
C -5.122133 0.123452 3.093998
H -6.156976 0.443920 3.191310
C -4.373793 -0.195083 4.231653
H -4.825234 -0.121414 5.218523
C -3.043683 -0.602292 4.097892
H -2.454007 -0.845088 4.979011
C -2.461586 -0.692231 2.830602
H -1.422715 -0.995885 2.732711
C -3.098247 -2.144435 -0.681715
C -4.281465 -2.732883 -0.207667
H -4.829121 -2.282870 0.615420
C -4.760914 -3.911932 -0.785786
H -5.674479 -4.362665 -0.404379
C -4.071186 -4.509617 -1.844544

H -4.447318 -5.427300 -2.291218
C -2.893117 -3.928592 -2.322997
H -2.348159 -4.390030 -3.143495
C -2.404506 -2.756492 -1.740604
H -1.478072 -2.315896 -2.103022
C -3.206014 0.764321 -1.008734
C -3.638070 0.510613 -2.320416
H -3.562159 -0.488816 -2.739892
C -4.175758 1.541316 -3.097901
H -4.511852 1.328876 -4.110395
C -4.285573 2.832675 -2.576537
H -4.707343 3.632152 -3.181554
C -3.852309 3.093623 -1.272403
H -3.934421 4.095966 -0.858035
C -3.313209 2.068349 -0.492681
H -2.984603 2.285948 0.520531
C 3.051938 -1.566037 -1.469445
C 2.217113 -2.443067 -2.181312
H 1.177095 -2.552971 -1.886180
C 2.712836 -3.163494 -3.271516
H 2.054510 -3.837490 -3.815032
C 4.045234 -3.012686 -3.664594
H 4.429793 -3.571042 -4.515195
C 4.882363 -2.137020 -2.965759
H 5.919570 -2.012392 -3.268646
C 4.391005 -1.415434 -1.875366
H 5.051252 -0.730965 -1.348886
C 3.063331 -1.546926 1.485518
C 2.418090 -1.371190 2.722357
H 1.519102 -0.761391 2.780353
C 2.918095 -1.982209 3.874986
H 2.410453 -1.835063 4.825639
C 4.058523 -2.787182 3.802137
H 4.443022 -3.270819 4.697326
C 4.699171 -2.975107 2.573975
H 5.582712 -3.606254 2.509073
C 4.208731 -2.356471 1.420415
H 4.718117 -2.515546 0.474348
C 3.265052 0.958261 -0.017475
C 3.757483 1.528236 1.167455
H 3.665750 0.997546 2.111145
C 4.374048 2.782887 1.144019
H 4.755675 3.209498 2.068986
C 4.502716 3.482007 -0.058785
H 4.985134 4.456737 -0.075164
C 4.011300 2.922234 -1.242381
H 4.109644 3.457875 -2.183986
C 3.394903 1.669221 -1.223912
H 3.028300 1.243309 -2.154396
C 0.208012 5.016943 0.392952
C 0.198231 4.835480 1.764703

C 0.127943 3.538512 2.309234
C 0.075994 2.418761 1.500656
O 0.276457 6.294813 -0.059316
H 0.025948 1.416328 1.916888
H 0.120484 3.421188 3.390153
H 0.248414 5.709827 2.407261
H 0.361579 6.333134 -1.021094
el energy= -2098.04837800
zpe= -2097.346367
th energy= -2097.299404
th enthalpy= -2097.298460
free energy= -2097.433066

16a

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P -2.414267 -0.578199 0.049661
P 2.386460 -0.647814 0.032255
O -0.057915 -3.218278 1.474018
C -0.039270 -2.195331 0.927724
N 0.009933 1.348399 -0.951074
C 0.058038 2.560478 -0.298776
C 0.077862 3.789911 -1.031914
C 0.046100 3.724342 -2.447835
C -0.008119 2.497541 -3.070911
C -0.026655 1.330585 -2.283617
H 0.060790 4.645289 -3.026404
H -0.037883 2.407022 -4.152211
H -0.070041 0.350882 -2.749807
C -3.197148 -0.156615 1.671649
C -4.539463 0.256428 1.757861
H -5.137074 0.374107 0.857495
C -5.114495 0.528249 3.001576
H -6.153189 0.846594 3.054862
C -4.358741 0.393403 4.170528
H -4.808327 0.608539 5.137357
C -3.023767 -0.012346 4.092959
H -2.428371 -0.112777 4.997645
C -2.444263 -0.283897 2.850590
H -1.401812 -0.585846 2.794293
C -3.076941 -2.247765 -0.408564
C -4.251299 -2.773759 0.153090
H -4.800412 -2.215315 0.905792
C -4.719816 -4.029250 -0.245213
H -5.626419 -4.429725 0.203026
C -4.028202 -4.766848 -1.210377
H -4.395811 -5.743569 -1.516999
C -2.859014 -4.248906 -1.775210
H -2.312423 -4.818526 -2.523456
C -2.381251 -2.999688 -1.371779
H -1.461507 -2.606776 -1.800129
C -3.212970 0.580219 -1.157084

C	-3.644153	0.132861	-2.416286
H	-3.556762	-0.916028	-2.685995
C	-4.195819	1.032642	-3.333805
H	-4.530991	0.670870	-4.303365
C	-4.320628	2.384813	-3.005774
H	-4.753226	3.082462	-3.719387
C	-3.888410	2.838186	-1.755167
H	-3.982045	3.889226	-1.491166
C	-3.335345	1.944100	-0.836205
H	-3.008574	2.311070	0.133533
C	3.055404	-1.734114	-1.307885
C	2.221516	-2.708830	-1.880195
H	1.185771	-2.784058	-1.560136
C	2.712422	-3.571051	-2.864435
H	2.054793	-4.319849	-3.300223
C	4.039117	-3.466100	-3.290439
H	4.420022	-4.135122	-4.058868
C	4.875099	-2.494380	-2.731139
H	5.907736	-2.405064	-3.060903
C	4.388527	-1.631088	-1.746645
H	5.047754	-0.874315	-1.329117
C	3.088688	-1.307393	1.616292
C	2.442780	-0.981041	2.821722
H	1.531643	-0.387048	2.802246
C	2.957404	-1.423190	4.043105
H	2.448785	-1.160912	4.968102
C	4.113953	-2.207537	4.072706
H	4.510283	-2.559590	5.022499
C	4.755826	-2.544716	2.877471
H	5.652059	-3.160949	2.893027
C	4.250296	-2.095434	1.654228
H	4.760638	-2.369463	0.735366
C	3.259526	0.968071	-0.217775
C	3.754570	1.699332	0.873905
H	3.673262	1.302760	1.882277
C	4.360231	2.943496	0.673349
H	4.744276	3.496224	1.527872
C	4.474912	3.471335	-0.615178
H	4.948755	4.438213	-0.769276
C	3.980428	2.750471	-1.706778
H	4.067337	3.152481	-2.713759
C	3.375164	1.507259	-1.511450
H	3.004516	0.955164	-2.371205
C	0.119640	5.024119	-0.334544
C	0.136651	5.043574	1.047095
C	0.114398	3.822103	1.775311
C	0.078190	2.614075	1.120122
H	0.134452	5.951094	-0.904872
O	0.172664	6.178238	1.789416
H	0.059645	1.681767	1.679177
H	0.127395	3.868519	2.860994

H 0.181563 6.956195 1.212285
el energy= -2098.05342544
zpe= -2097.351475
th energy= -2097.304518
th enthalpy= -2097.303574
free energy= -2097.439187

17a

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P -2.414437 -0.537151 0.033229
P 2.385098 -0.601801 0.015782
O -0.051299 -3.153344 1.494926
C -0.036365 -2.137616 0.934957
N 0.009520 1.371858 -1.000309
C 0.061745 2.597969 -0.367125
C 0.087068 3.806868 -1.138291
C 0.052866 3.717208 -2.546722
C -0.007907 2.476835 -3.149294
C -0.029302 1.332834 -2.334111
H 0.071080 4.628236 -3.141071
H -0.040254 2.362564 -4.227914
H -0.076686 0.343097 -2.779298
C -3.198086 -0.101705 1.651288
C -4.543092 0.303361 1.733725
H -5.142453 0.405304 0.832564
C -5.118598 0.587436 2.974449
H -6.159456 0.899153 3.024893
C -4.360432 0.473416 4.144107
H -4.810375 0.698080 5.108615
C -3.022612 0.076592 4.070108
H -2.425140 -0.006901 4.975140
C -2.442716 -0.207395 2.830674
H -1.397913 -0.501517 2.776856
C -3.073298 -2.212341 -0.409856
C -4.242905 -2.739322 0.160655
H -4.791354 -2.177591 0.911387
C -4.707359 -4.000005 -0.225955
H -5.610267 -4.401091 0.229156
C -4.016384 -4.741940 -1.188204
H -4.380779 -5.722677 -1.485729
C -2.851832 -4.223107 -1.761812
H -2.305693 -4.796078 -2.507838
C -2.378088 -2.968688 -1.370017
H -1.461756 -2.575058 -1.804988
C -3.217261 0.609714 -1.181695
C -3.663275 0.150476 -2.431271
H -3.584080 -0.901857 -2.689869
C -4.219213 1.042973 -3.353484
H -4.565946 0.672173 -4.315546
C -4.333453 2.399344 -3.039541
H -4.769315 3.091314 -3.756697

C -3.886125 2.864508 -1.798495
H -3.971010 3.919090 -1.545883
C -3.328753 1.977851 -0.875053
H -2.988294 2.353778 0.086634
C 3.056952 -1.721001 -1.295663
C 2.222358 -2.703959 -1.852530
H 1.184236 -2.767745 -1.537807
C 2.715572 -3.589141 -2.815058
H 2.057238 -4.344062 -3.239072
C 4.045381 -3.499268 -3.234617
H 4.428114 -4.186184 -3.986171
C 4.882246 -2.519565 -2.690697
H 5.917360 -2.441862 -3.015615
C 4.393309 -1.633304 -1.728085
H 5.053383 -0.870715 -1.322562
C 3.085381 -1.220434 1.617261
C 2.435510 -0.863734 2.811928
H 1.523764 -0.271594 2.773886
C 2.946918 -1.273394 4.045918
H 2.435234 -0.987682 4.962246
C 4.104204 -2.055397 4.099257
H 4.498144 -2.382231 5.059014
C 4.749926 -2.422803 2.915042
H 5.646689 -3.037524 2.949243
C 4.247626 -2.005997 1.679020
H 4.760998 -2.303475 0.769201
C 3.259192 1.006996 -0.274564
C 3.750758 1.766836 0.798982
H 3.665308 1.397399 1.817268
C 4.358378 3.004613 0.567529
H 4.740135 3.579452 1.408409
C 4.478206 3.497901 -0.734206
H 4.953681 4.459852 -0.912333
C 3.986663 2.748772 -1.807901
H 4.077159 3.123856 -2.824914
C 3.379477 1.511702 -1.581572
H 3.011243 0.937401 -2.427743
C 0.136098 5.051505 -0.452686
C 0.154484 5.104759 0.919876
C 0.124832 3.899902 1.675263
C 0.079994 2.668530 1.041377
H 0.156188 5.969392 -1.035500
O 0.139917 3.908384 3.030247
H 0.190501 6.062578 1.435359
H 0.056350 1.756422 1.631021
H 0.166026 4.818178 3.361107
el energy= -2098.05430575
zpe= -2097.352502
th energy= -2097.305505
th enthalpy= -2097.304561
free energy= -2097.440093

18a

Ir	2.096456	-0.061664	0.028204
P	1.902639	-2.453175	0.013361
P	2.337183	2.325969	-0.005974
O	4.943928	-0.324522	0.927980
C	3.841009	-0.221368	0.580625
N	0.057202	0.119578	-0.676045
C	-1.034162	0.207836	0.166845
C	-2.352661	0.316993	-0.384395
C	-2.507182	0.336331	-1.784441
C	-1.393925	0.240768	-2.598691
C	-0.131003	0.130030	-1.997559
H	-3.508738	0.423906	-2.196049
H	-1.471072	0.246791	-3.681419
H	0.766745	0.049968	-2.604887
C	1.736655	-3.215587	1.691570
C	1.231375	-4.517282	1.863500
H	0.888248	-5.090477	1.006099
C	1.155927	-5.081691	3.139181
H	0.762808	-6.088882	3.258292
C	1.580892	-4.355158	4.255919
H	1.517935	-4.795677	5.248499
C	2.079784	-3.059841	4.094069
H	2.404912	-2.486091	4.959087
C	2.155377	-2.491237	2.819741
H	2.529583	-1.478007	2.700470
C	3.397350	-3.246317	-0.745869
C	3.914938	-4.470682	-0.294063
H	3.459608	-4.983958	0.548140
C	5.029828	-5.036756	-0.919323
H	5.426296	-5.981915	-0.554829
C	5.633094	-4.393092	-2.003676
H	6.500642	-4.836689	-2.487233
C	5.122440	-3.174485	-2.460330
H	5.588713	-2.664957	-3.300695
C	4.015397	-2.599955	-1.830832
H	3.630580	-1.642534	-2.176047
C	0.479135	-3.153440	-0.945113
C	0.648480	-3.633169	-2.253880
H	1.632996	-3.639305	-2.713586
C	-0.448883	-4.111406	-2.977030
H	-0.302522	-4.484474	-3.988346
C	-1.722974	-4.113639	-2.403874
H	-2.575003	-4.487565	-2.967210
C	-1.899540	-3.632249	-1.102589
H	-2.888309	-3.627448	-0.649232
C	-0.807369	-3.152238	-0.376992
H	-0.960246	-2.780370	0.632909
C	3.210159	2.953534	-1.512985
C	4.009657	2.071088	-2.258007

H	4.071134	1.026335	-1.965186
C	4.713135	2.525639	-3.376826
H	5.326245	1.830288	-3.945850
C	4.622300	3.864674	-3.765980
H	5.166629	4.217396	-4.639232
C	3.824218	4.749513	-3.033891
H	3.746224	5.792265	-3.333481
C	3.120176	4.299163	-1.914535
H	2.495883	4.996778	-1.362091
C	3.324619	2.944719	1.437056
C	3.166347	2.303529	2.678238
H	2.503612	1.444786	2.760682
C	3.860890	2.756029	3.802897
H	3.726192	2.252165	4.757440
C	4.731816	3.844240	3.697077
H	5.279895	4.191403	4.570174
C	4.901729	4.480759	2.464146
H	5.583080	5.323877	2.373304
C	4.200079	4.038050	1.339084
H	4.345589	4.543428	0.388618
C	0.772579	3.317750	0.054888
C	0.295061	3.842025	1.266689
H	0.863639	3.711580	2.183334
C	-0.916856	4.538129	1.305617
H	-1.272439	4.942124	2.250933
C	-1.665014	4.715376	0.139057
H	-2.607393	5.257542	0.171270
C	-1.197236	4.193110	-1.070881
H	-1.772962	4.325931	-1.984094
C	0.012775	3.497463	-1.114590
H	0.365086	3.103628	-2.064289
C	-3.503286	0.391598	0.490607
C	-3.281414	0.362206	1.869690
C	-1.976545	0.252293	2.386683
C	-0.860575	0.174685	1.568985
O	-4.689888	0.492441	-0.066147
H	0.141389	0.086571	1.979940
H	-1.843672	0.227640	3.466811
H	-4.131577	0.421289	2.544388
Al	-6.480055	0.259494	0.338101
O	-7.063769	-0.786797	-1.177601
N	-6.987344	-0.362494	-2.424418
O	-6.562901	0.775621	-2.633609
O	-7.349060	-1.137177	-3.298582
C	-6.756756	-1.085037	1.810715
C	-7.378415	2.053816	0.432343
C	-8.851701	2.049381	-0.021365
C	-7.250084	2.664204	1.844295
H	-6.396888	-0.614063	2.744055
H	-6.828341	2.713990	-0.259478
H	-8.956394	1.710121	-1.060987

H -9.470378 1.385692 0.601322
H -9.304849 3.054058 0.041602
H -6.200764 2.760109 2.160811
H -7.698404 3.671141 1.902008
H -7.758803 2.047867 2.601038
C -8.250757 -1.409634 2.023932
C -5.951896 -2.385895 1.617842
H -8.403971 -2.122021 2.853222
H -8.695586 -1.866733 1.127530
H -8.841458 -0.511690 2.255209
H -4.871055 -2.196124 1.555793
H -6.111451 -3.098117 2.446340
H -6.244499 -2.903493 0.692521
el energy= -2617.05946608
zpe= -2616.165644
th energy= -2616.102410
th enthalpy= -2616.101466
free energy= -2616.277302

19a

Ir 1.950190 -0.139119 0.136689
P 1.563048 -2.505726 0.127785
P 2.397747 2.219985 0.135170
O 3.901034 -0.495125 2.384655
C 3.145786 -0.356226 1.514451
N 0.573860 0.110224 -1.518363
C -0.772496 0.341648 -1.355792
C -1.638216 0.501011 -2.488765
C -1.056162 0.412858 -3.780183
C 0.294803 0.174136 -3.909718
C 1.079047 0.026249 -2.749893
H -1.688555 0.530708 -4.657796
H 0.769705 0.096528 -4.883107
H 2.146330 -0.162648 -2.818778
C 0.460224 -3.099043 1.489718
C -0.188871 -4.345638 1.425025
H -0.082595 -4.975351 0.545428
C -0.985792 -4.781167 2.486475
H -1.483301 -5.746390 2.423518
C -1.145749 -3.979555 3.621130
H -1.770913 -4.318865 4.444031
C -0.507117 -2.738617 3.691618
H -0.633910 -2.106381 4.567518
C 0.289898 -2.298741 2.631416
H 0.772365 -1.326407 2.683907
C 3.144956 -3.454869 0.319797
C 3.221034 -4.654405 1.045254
H 2.342062 -5.052419 1.544308
C 4.433736 -5.343468 1.140373
H 4.481427 -6.267649 1.712159
C 5.577811 -4.848482 0.507979

H 6.519667 -5.387205 0.584883
C 5.509566 -3.655522 -0.217677
H 6.396241 -3.261099 -0.709079
C 4.302185 -2.958191 -0.305641
H 4.256462 -2.020771 -0.856014
C 0.798771 -3.202167 -1.410936
C 1.586111 -3.800726 -2.407693
H 2.659449 -3.902152 -2.272747
C 0.995319 -4.277271 -3.582231
H 1.616972 -4.743619 -4.343462
C -0.383519 -4.160199 -3.774285
H -0.841881 -4.534546 -4.686968
C -1.172935 -3.560278 -2.787912
H -2.247058 -3.463410 -2.929033
C -0.587528 -3.080963 -1.614272
H -1.215155 -2.619486 -0.856261
C 3.957128 2.666708 -0.757155
C 4.932221 1.677608 -0.967410
H 4.741598 0.658410 -0.641535
C 6.136156 1.993656 -1.602968
H 6.880980 1.216853 -1.761147
C 6.377375 3.299070 -2.039294
H 7.312776 3.544022 -2.537614
C 5.410181 4.289313 -1.839751
H 5.589912 5.306656 -2.180187
C 4.205971 3.977617 -1.204017
H 3.459917 4.756018 -1.066008
C 2.591185 2.894152 1.851811
C 1.775398 2.371667 2.870748
H 1.080078 1.565923 2.645819
C 1.857782 2.874401 4.171699
H 1.217663 2.463002 4.948921
C 2.765966 3.893537 4.472356
H 2.836942 4.279322 5.486914
C 3.587647 4.410918 3.466730
H 4.301381 5.199411 3.695254
C 3.500133 3.918583 2.161379
H 4.147206 4.331574 1.392814
C 1.108076 3.304700 -0.636931
C 0.135473 3.943473 0.148956
H 0.153448 3.847273 1.231051
C -0.866064 4.710866 -0.453345
H -1.611179 5.202111 0.168432
C -0.909026 4.846729 -1.843186
H -1.688635 5.444845 -2.309615
C 0.054331 4.210643 -2.632380
H 0.028901 4.310955 -3.715202
C 1.056247 3.442755 -2.035340
H 1.800497 2.959026 -2.662407
C -3.020293 0.723958 -2.290742
C -3.572692 0.787981 -1.011415

C -2.687245 0.635935 0.108892
C -1.339122 0.420533 -0.057728
H -3.670744 0.842118 -3.154614
O -4.860454 1.015151 -0.828939
H -0.682322 0.308750 0.802609
H -3.110927 0.721700 1.105974
Al -6.355451 0.350468 0.004778
C -7.592228 1.898105 0.332778
C -8.862592 1.523009 1.122624
C -6.908350 -1.335159 -0.945396
C -8.037026 -2.110890 -0.236923
C -7.267718 -1.098638 -2.426657
C -7.968721 2.632442 -0.970982
O -5.848382 -0.431194 1.703701
N -5.374728 0.233910 2.737895
O -4.969233 1.386186 2.561904
O -5.356366 -0.346427 3.813796
H -7.023544 2.611419 0.953486
H -8.627696 1.060737 2.092067
H -9.495264 2.404007 1.327703
H -9.488544 0.807425 0.568668
H -6.013736 -1.985499 -0.932277
H -8.972088 -1.531145 -0.212205
H -8.269088 -3.061739 -0.747963
H -6.449091 -0.614643 -2.977920
H -7.503408 -2.040632 -2.952119
H -8.152172 -0.451612 -2.529944
H -8.540304 1.983450 -1.651967
H -8.597630 3.519074 -0.778365
H -7.081248 2.975223 -1.521138
H -7.779716 -2.352618 0.803320
el energy= -2617.05668357
zpe= -2616.163110
th energy= -2616.099821
th enthalpy= -2616.098877
free energy= -2616.274940

20a

Ir 1.312400 0.132982 -0.269864
P 1.067113 2.518022 -0.323464
P 1.746135 -2.228518 -0.191043
O 2.160752 0.237513 -3.141826
C 1.820390 0.187333 -2.033269
N 0.828744 0.098298 1.845195
C -0.434456 -0.110140 2.367872
C -0.616679 -0.118264 3.794583
C 0.494435 0.095447 4.629638
C 1.744011 0.307027 4.072313
C 1.858205 0.300385 2.676156
H 0.357970 0.090748 5.709472
H 2.626201 0.476250 4.681315

H	2.822687	0.458378	2.201581
C	-0.423760	3.140513	-1.219101
C	-0.851072	4.476270	-1.092546
H	-0.326368	5.160841	-0.430331
C	-1.957932	4.930616	-1.811973
H	-2.278354	5.965113	-1.708890
C	-2.654086	4.058219	-2.656942
H	-3.519445	4.414500	-3.211765
C	-2.244428	2.728314	-2.775308
H	-2.789377	2.028258	-3.401780
C	-1.134465	2.270509	-2.059023
H	-0.838453	1.228747	-2.142182
C	2.523756	3.297042	-1.170517
C	2.399167	4.373599	-2.062241
H	1.421096	4.783019	-2.297031
C	3.534300	4.923317	-2.666645
H	3.422106	5.752067	-3.362344
C	4.803035	4.411524	-2.382422
H	5.683588	4.841556	-2.854631
C	4.935985	3.339158	-1.494832
H	5.919189	2.930568	-1.271878
C	3.803342	2.779493	-0.899382
H	3.909578	1.931585	-0.226301
C	0.975924	3.375541	1.318346
C	2.080817	4.040529	1.872189
H	3.020132	4.091816	1.328682
C	1.981315	4.648658	3.128133
H	2.844190	5.165261	3.542957
C	0.781897	4.597413	3.841976
H	0.705552	5.073262	4.817206
C	-0.321781	3.931685	3.297814
H	-1.259176	3.884844	3.847671
C	-0.226838	3.321994	2.045590
H	-1.092048	2.806668	1.635505
C	3.493813	-2.594733	0.300256
C	4.476450	-1.613816	0.085241
H	4.186378	-0.647677	-0.320349
C	5.814527	-1.871225	0.395480
H	6.564263	-1.101545	0.225691
C	6.185448	-3.109572	0.926757
H	7.226325	-3.308518	1.172503
C	5.214363	-4.091826	1.145152
H	5.496150	-5.057877	1.558246
C	3.875904	-3.838787	0.834075
H	3.131956	-4.610408	1.013959
C	1.512299	-3.085873	-1.817412
C	0.429441	-2.701383	-2.624934
H	-0.230289	-1.896041	-2.317091
C	0.184888	-3.350039	-3.837565
H	-0.666050	-3.040134	-4.439421
C	1.029435	-4.377828	-4.265272

H 0.845567 -4.878044 -5.213714
C 2.116256 -4.758624 -3.471732
H 2.781664 -5.553957 -3.800825
C 2.356582 -4.121368 -2.250964
H 3.204262 -4.431571 -1.646582
C 0.712965 -3.217585 0.991104
C -0.443735 -3.880302 0.548548
H -0.727456 -3.852799 -0.499470
C -1.250474 -4.573533 1.455651
H -2.142075 -5.083252 1.097191
C -0.914933 -4.612017 2.811548
H -1.543088 -5.154039 3.515041
C 0.230838 -3.948469 3.260257
H 0.499302 -3.969721 4.314240
C 1.038749 -3.252089 2.358432
H 1.925994 -2.742954 2.725446
C -1.925161 -0.348612 4.309524
C -2.984972 -0.564020 3.470634
C -2.817407 -0.556426 2.042717
C -1.540593 -0.317781 1.518023
H -2.064434 -0.353867 5.388880
O -3.870511 -0.804039 1.297743
H -3.983641 -0.748528 3.859048
H -1.393581 -0.319367 0.441199
Al -4.884798 -0.383880 -0.170593
C -6.123602 -1.929025 -0.497530
C -6.634935 -2.025126 -1.949178
C -5.528134 1.514168 -0.005834
C -6.428660 1.945948 -1.181343
C -6.220707 1.808156 1.340216
C -7.310208 -1.934986 0.489492
O -3.689166 -0.144297 -1.682729
N -2.931845 -1.086264 -2.192011
O -2.916180 -2.192930 -1.651617
O -2.269873 -0.794584 -3.185547
H -5.533353 -2.840139 -0.300900
H -5.811490 -2.127381 -2.669436
H -7.301131 -2.893387 -2.092824
H -7.211418 -1.134015 -2.239662
H -4.621211 2.144829 -0.046894
H -7.357169 1.356131 -1.217272
H -6.729788 3.005254 -1.104324
H -5.569845 1.581517 2.196366
H -6.520650 2.866901 1.428616
H -7.136106 1.210163 1.464548
H -7.949025 -1.048081 0.361650
H -7.959862 -2.815885 0.346820
H -6.977713 -1.944497 1.537621
H -5.928276 1.819678 -2.151739
el energy= -2617.06442002
zpe= -2616.170709

th energy= -2616.107495
th enthalpy= -2616.106551
free energy= -2616.280534

21a

Ir	-1.465748	0.500635	0.158969
P	-0.358759	2.625184	0.190359
P	-2.811816	-1.485951	-0.019561
O	-3.163072	1.428219	2.447012
C	-2.506105	1.063892	1.560466
N	-0.276173	-0.127623	-1.538791
C	0.877946	-0.840617	-1.410822
C	1.583986	-1.238964	-2.576375
C	1.112773	-0.894472	-3.829134
C	-0.069363	-0.143488	-3.942024
C	-0.719080	0.213889	-2.776511
H	2.503814	-1.802137	-2.460099
H	1.660383	-1.200469	-4.717786
H	-0.471555	0.156213	-4.904295
H	-1.638717	0.791325	-2.795832
O	1.288888	-1.113375	-0.202471
C	0.881447	2.861906	1.541165
C	1.849735	3.881051	1.486051
H	1.917155	4.527593	0.614694
C	2.741415	4.063069	2.545649
H	3.486752	4.853439	2.490890
C	2.677897	3.231769	3.668802
H	3.375708	3.373668	4.491127
C	1.722425	2.213787	3.728099
H	1.674135	1.556849	4.593517
C	0.829885	2.027084	2.668541
H	0.100608	1.222287	2.709093
C	-1.588791	3.998588	0.416566
C	-1.324844	5.127816	1.207320
H	-0.381066	5.220096	1.736846
C	-2.279840	6.142177	1.329258
H	-2.065020	7.007738	1.952252
C	-3.501892	6.045261	0.658415
H	-4.242405	6.836132	0.755855
C	-3.771984	4.924633	-0.132935
H	-4.722183	4.838488	-0.655499
C	-2.825153	3.904045	-0.246920
H	-3.045812	3.024733	-0.848101
C	0.555285	3.088634	-1.353072
C	-0.022744	3.916048	-2.329240
H	-1.011944	4.338807	-2.177082
C	0.672978	4.207963	-3.506893
H	0.215585	4.854799	-4.252617
C	1.946884	3.676005	-3.722307
H	2.486270	3.905374	-4.638898
C	2.526546	2.848084	-2.755400

H	3.514220	2.419762	-2.908506
C	1.835612	2.553590	-1.577944
H	2.309136	1.920512	-0.832320
C	-4.347674	-1.193280	-1.017638
C	-4.863053	0.109942	-1.114765
H	-4.331446	0.931539	-0.642698
C	-6.044299	0.354455	-1.820040
H	-6.429504	1.369471	-1.888680
C	-6.722182	-0.698856	-2.440169
H	-7.638869	-0.507629	-2.993798
C	-6.215952	-1.999090	-2.350800
H	-6.737582	-2.824002	-2.831193
C	-5.036172	-2.247563	-1.644241
H	-4.652869	-3.262896	-1.588488
C	-3.420783	-2.093044	1.623357
C	-2.546122	-2.036397	2.721894
H	-1.552621	-1.611317	2.599212
C	-2.946378	-2.516017	3.971481
H	-2.257447	-2.468668	4.811878
C	-4.229788	-3.044017	4.140304
H	-4.545594	-3.409293	5.115059
C	-5.108414	-3.095723	3.054210
H	-6.110345	-3.500329	3.180174
C	-4.707216	-2.627216	1.799633
H	-5.401824	-2.675294	0.965602
C	-2.073121	-2.997802	-0.803065
C	-1.718505	-4.120700	-0.038719
H	-1.875273	-4.125162	1.036067
C	-1.164760	-5.248264	-0.654097
H	-0.901119	-6.112376	-0.048865
C	-0.952240	-5.265230	-2.034547
H	-0.523154	-6.143918	-2.510943
C	-1.295968	-4.147342	-2.801621
H	-1.133999	-4.149557	-3.877259
C	-1.852771	-3.021607	-2.192167
H	-2.125606	-2.167948	-2.806206
Al	2.714418	-2.081063	0.541925
C	2.871844	-1.525152	2.457394
C	4.111187	-2.129326	3.151678
C	2.699771	-4.002314	-0.056089
C	4.074203	-4.512477	-0.536574
C	2.142319	-4.939736	1.036932
C	1.601991	-1.814870	3.283072
O	4.223586	-1.345001	-0.424631
S	4.885234	0.028425	-0.646677
O	4.430729	1.059091	0.313773
O	4.944858	0.381106	-2.081750
H	3.007162	-0.430597	2.446884
H	5.043243	-1.865313	2.635192
H	4.205199	-1.778126	4.193361
H	4.061365	-3.227662	3.192630

H 2.010441 -4.066839 -0.916093
H 4.826020 -4.469073 0.265866
H 4.465181 -3.921902 -1.375146
H 4.023134 -5.564128 -0.866411
H 2.776275 -4.934915 1.935720
H 2.092196 -5.985706 0.689504
H 1.129221 -4.656250 1.353505
H 1.700997 -1.460539 4.323519
H 1.383426 -2.891615 3.335232
H 0.717235 -1.323418 2.855335
C 6.660348 -0.365914 -0.160886
F 6.730460 -0.706710 1.127672
F 7.413231 0.718792 -0.362240
F 7.132612 -1.367894 -0.903062
el energy= -2756.48514287
zpe= -2755.625272
th energy= -2755.560497
th enthalpy= -2755.559553
free energy= -2755.736477

8b

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P -2.384900 -0.419708 -0.041935
P 2.452991 -0.351359 -0.005814
O 0.070055 -3.298579 0.477356
C 0.055680 -2.160655 0.290389
N 0.014082 1.795919 -0.471500
C -0.022710 2.764629 0.467663
C -0.042180 4.118075 0.115577
C -0.020550 4.482100 -1.227328
C 0.021104 3.475024 -2.195108
C 0.037214 2.150688 -1.774824
C -0.062221 2.359380 1.922765
H -0.084494 4.864011 0.903076
H -0.035551 5.530005 -1.516048
H 0.037485 3.703424 -3.256450
H 0.064436 1.333435 -2.489313
O -1.169136 3.019790 2.529950
C -3.143874 -0.513013 1.643140
C -4.480609 -0.139840 1.873791
H -5.088980 0.249351 1.061584
C -5.035310 -0.257551 3.150513
H -6.070064 0.034492 3.315223
C -4.264903 -0.746489 4.210239
H -4.698579 -0.834032 5.203917
C -2.935357 -1.116616 3.990488
H -2.328447 -1.492268 4.811256
C -2.376426 -0.998229 2.715120
H -1.337931 -1.276130 2.554998
C -3.013767 -1.905961 -0.954276
C -4.157632 -2.613412 -0.551513

H	-4.705076	-2.313778	0.337879
C	-4.596997	-3.717342	-1.288342
H	-5.479702	-4.262820	-0.961913
C	-3.907234	-4.119625	-2.435754
H	-4.252151	-4.979238	-3.006001
C	-2.769053	-3.418252	-2.844717
H	-2.224640	-3.726938	-3.734359
C	-2.319699	-2.322420	-2.103894
H	-1.424029	-1.789216	-2.417001
C	-3.248253	1.007927	-0.850161
C	-3.764942	0.904906	-2.151880
H	-3.699965	-0.032982	-2.696418
C	-4.373543	2.008089	-2.758965
H	-4.774044	1.911952	-3.765816
C	-4.471608	3.222293	-2.075251
H	-4.948256	4.078443	-2.547550
C	-3.953056	3.332763	-0.780845
H	-4.022588	4.275490	-0.242413
C	-3.341262	2.236197	-0.169618
H	-2.937652	2.345861	0.834395
C	3.185406	-0.900557	-1.612004
C	2.389943	-1.642414	-2.500989
H	1.351838	-1.847456	-2.251417
C	2.921031	-2.108494	-3.706773
H	2.293234	-2.680718	-4.386114
C	4.249974	-1.833307	-4.039703
H	4.662358	-2.192589	-4.979926
C	5.047679	-1.088972	-3.164540
H	6.081730	-0.868564	-3.419982
C	4.521055	-0.622927	-1.957686
H	5.150313	-0.037339	-1.292184
C	3.152721	-1.481957	1.287079
C	2.482717	-1.580041	2.519399
H	1.561736	-1.023325	2.680859
C	2.987493	-2.392342	3.537992
H	2.460567	-2.455395	4.487461
C	4.157818	-3.128159	3.331042
H	4.546291	-3.768520	4.119770
C	4.823407	-3.044582	2.104601
H	5.730654	-3.620132	1.934537
C	4.328232	-2.223530	1.087395
H	4.857830	-2.172036	0.140327
C	3.264044	1.281564	0.336844
C	3.678404	1.625811	1.634301
H	3.579956	0.913825	2.449328
C	4.227386	2.886444	1.889595
H	4.549405	3.135933	2.898231
C	4.367746	3.816187	0.855855
H	4.798026	4.794910	1.055746
C	3.954246	3.481855	-0.437496
H	4.060962	4.198211	-1.249055

C 3.403107 2.225116 -0.696807
H 3.090848 1.979997 -1.708600
H -0.153698 1.263684 1.989695
H 0.882759 2.650803 2.407181
H -1.106318 2.890971 3.486640
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zpe= -1987.823952
th energy= -1987.777861
th enthalpy= -1987.776917
free energy= -1987.910112

9b

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P -2.426683 -0.451524 0.031150
P 2.405286 -0.511136 0.005838
O -0.046997 -3.316000 0.893815
C -0.032443 -2.211596 0.561542
N 0.017802 1.607093 -0.663448
C 0.165356 2.607969 0.225985
C 0.200779 3.953372 -0.140111
C 0.075583 4.261624 -1.499261
C -0.072579 3.229065 -2.424475
C -0.099155 1.912793 -1.969596
C 0.407704 5.030658 0.911246
H 0.091839 5.298271 -1.830765
H -0.173534 3.433085 -3.486281
H -0.219293 1.077346 -2.652409
C -3.155182 -0.319351 1.725962
C -4.498342 0.048851 1.929204
H -5.132578 0.299526 1.082556
C -5.026232 0.104770 3.221075
H -6.066359 0.388849 3.364507
C -4.221622 -0.200922 4.323645
H -4.634743 -0.153903 5.328760
C -2.884921 -0.559585 4.131464
H -2.251573 -0.790571 4.985018
C -2.352990 -0.615979 2.840110
H -1.308805 -0.882262 2.696824
C -3.120111 -2.005695 -0.704980
C -4.281187 -2.626563 -0.217748
H -4.807046 -2.215380 0.639237
C -4.765812 -3.788189 -0.826094
H -5.661892 -4.264431 -0.434238
C -4.103985 -4.336051 -1.928778
H -4.484367 -5.240047 -2.399119
C -2.947598 -3.723278 -2.420407
H -2.423796 -4.146099 -3.274818
C -2.453061 -2.569452 -1.807149
H -1.542308 -2.106229 -2.182265
C -3.252510 0.910448 -0.917645
C -3.730647 0.706950 -2.222068

H -3.668462 -0.275349 -2.682533
C -4.297208 1.765529 -2.939302
H -4.669253 1.591529 -3.946597
C -4.390056 3.035599 -2.364922
H -4.834105 3.856790 -2.923105
C -3.910260 3.246992 -1.068014
H -3.979115 4.232556 -0.612765
C -3.341676 2.193918 -0.349093
H -2.976009 2.372622 0.659199
C 3.119050 -1.315646 -1.497883
C 2.301740 -2.153223 -2.274820
H 1.257304 -2.288221 -2.004613
C 2.819381 -2.804480 -3.397996
H 2.174606 -3.448723 -3.991520
C 4.156653 -2.621739 -3.759670
H 4.558492 -3.125389 -4.636047
C 4.976555 -1.784148 -2.996445
H 6.017347 -1.635042 -3.275103
C 4.463231 -1.132568 -1.872727
H 5.109617 -0.476468 -1.295176
C 3.086216 -1.442765 1.457360
C 2.422290 -1.322517 2.691099
H 1.520685 -0.717006 2.762990
C 2.908181 -1.979096 3.824549
H 2.386627 -1.873599 4.773204
C 4.052561 -2.776818 3.734041
H 4.425807 -3.297016 4.613340
C 4.711480 -2.910437 2.508416
H 5.598279 -3.535509 2.429916
C 4.235752 -2.244642 1.374978
H 4.759290 -2.361141 0.430298
C 3.248591 1.138417 0.087594
C 3.668244 1.676673 1.315071
H 3.560848 1.103128 2.231766
C 4.233727 2.954412 1.369705
H 4.560079 3.355124 2.326880
C 4.384301 3.708565 0.202884
H 4.829446 4.700081 0.246584
C 3.963237 3.181023 -1.022382
H 4.077425 3.760176 -1.936050
C 3.396006 1.906392 -1.081426
H 3.075197 1.510484 -2.041745
H 0.257141 2.322115 1.268323
O 0.102541 4.607855 2.230432
H -0.858244 4.519898 2.308739
H 1.468942 5.310383 0.930325
H -0.159075 5.932272 0.632642
el energy= -1988.50690230
zpe= -1987.823675
th energy= -1987.777563
th enthalpy= -1987.776619

free energy= -1987.911048

10b

Rh	0.004549	-0.522203	-0.011494
P	2.421523	-0.547440	-0.020925
P	-2.412902	-0.568169	0.005123
O	0.016979	-3.516102	-0.209535
C	0.012197	-2.365262	-0.131959
N	-0.003565	1.637205	0.123276
C	-0.136784	2.401658	-0.977065
C	-0.139854	3.792802	-0.932544
C	-0.007586	4.440154	0.299027
C	0.125951	3.640442	1.441942
C	0.127122	2.257774	1.314542
C	-0.006860	5.944880	0.412833
H	0.232038	4.083279	2.429190
H	0.236912	1.614192	2.182113
C	3.151751	-0.784743	-1.703149
C	4.496444	-0.475251	-1.980277
H	5.133005	-0.052696	-1.206871
C	5.022723	-0.698718	-3.254600
H	6.063891	-0.456654	-3.455859
C	4.215196	-1.228534	-4.266353
H	4.627165	-1.398414	-5.258609
C	2.877171	-1.531952	-4.001687
H	2.241699	-1.936658	-4.786194
C	2.346815	-1.308959	-2.727883
H	1.301692	-1.533450	-2.529805
C	3.103695	-1.913403	1.031417
C	4.260171	-2.632810	0.690540
H	4.790129	-2.417950	-0.233098
C	4.734641	-3.642019	1.533688
H	5.626906	-4.198106	1.254525
C	4.067544	-3.937251	2.726155
H	4.439860	-4.723518	3.379040
C	2.916066	-3.224571	3.073224
H	2.387910	-3.451461	3.996650
C	2.431633	-2.224155	2.226887
H	1.524273	-1.684811	2.492375
C	3.253548	0.980469	0.620721
C	3.709999	1.059234	1.946425
H	3.629858	0.199866	2.606631
C	4.277881	2.242789	2.428539
H	4.632739	2.286760	3.455918
C	4.394108	3.358440	1.595682
H	4.839359	4.276969	1.971480
C	3.936550	3.288955	0.275657
H	4.023529	4.152278	-0.380375
C	3.366557	2.110287	-0.209389
H	3.017806	2.071773	-1.238411
C	-3.134896	-1.040727	1.640868

C -2.325329 -1.701654 2.579308
H -1.280124 -1.892784 2.349553
C -2.851279 -2.104697 3.809962
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C -4.189516 -1.846831 4.118218
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C -5.001551 -1.181793 3.193728
H -6.042941 -0.974455 3.429643
C -4.479693 -0.778198 1.962626
H -5.119970 -0.252320 1.258770
C -3.090682 -1.781176 -1.222915
C -2.418682 -1.923675 -2.449902
H -1.513185 -1.350161 -2.639533
C -2.901250 -2.800251 -3.424922
H -2.373461 -2.897122 -4.371074
C -4.050584 -3.556785 -3.178070
H -4.421642 -4.247117 -3.932306
C -4.717352 -3.429456 -1.956032
H -5.608036 -4.020751 -1.755113
C -4.244776 -2.543887 -0.983003
H -4.774709 -2.458747 -0.038510
C -3.257751 1.027405 -0.416246
C -3.723092 1.285086 -1.715835
H -3.642065 0.525609 -2.488820
C -4.300980 2.520054 -2.026765
H -4.662462 2.703129 -3.036294
C -4.418317 3.509383 -1.047383
H -4.870938 4.468090 -1.290523
C -3.951572 3.261705 0.247778
H -4.039162 4.025964 1.016908
C -3.371431 2.031355 0.562286
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H -0.244973 1.871820 -1.918884
H -0.246710 4.366057 -1.846288
O -0.141490 6.519065 -0.873748
H -0.142753 7.480045 -0.775282
H -0.830999 6.249686 1.080105
H 0.930023 6.262396 0.901367
el energy= -1988.50697473
zpe= -1987.824209
th energy= -1987.777918
th enthalpy= -1987.776973
free energy= -1987.912286

11b

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P 2.895112 -0.699440 -0.316144
O 1.979348 2.431837 -2.274136
C 1.572723 1.757345 -1.430279
N 0.209864 -0.551819 1.548864

C	-0.391025	-1.729279	1.284091
C	-0.857739	-2.588266	2.278488
C	-0.682961	-2.193868	3.609885
C	-0.063404	-0.976955	3.890441
C	0.370030	-0.180630	2.833263
C	-1.528687	-3.903843	1.916640
H	-1.024208	-2.835489	4.420708
H	0.089422	-0.642975	4.912600
H	0.856702	0.774442	3.004827
C	-2.125947	2.210331	-1.269238
C	-3.391622	2.813598	-1.151223
H	-3.702890	3.253396	-0.206655
C	-4.263234	2.841971	-2.241535
H	-5.238594	3.312334	-2.138036
C	-3.886669	2.262539	-3.457510
H	-4.569397	2.281525	-4.304197
C	-2.637323	1.649271	-3.578781
H	-2.343746	1.184614	-4.517442
C	-1.761802	1.620330	-2.489541
H	-0.800096	1.123481	-2.584840
C	-0.310175	3.943861	0.286694
C	-0.929817	5.035286	-0.341557
H	-1.815860	4.887623	-0.952245
C	-0.405751	6.323640	-0.194881
H	-0.891518	7.159447	-0.693834
C	0.733941	6.537440	0.584949
H	1.138541	7.540990	0.696638
C	1.357115	5.455614	1.215116
H	2.247584	5.612073	1.820089
C	0.844008	4.165911	1.059803
H	1.345104	3.325086	1.535797
C	-2.027289	1.977948	1.626807
C	-2.003574	2.862948	2.715845
H	-1.349787	3.730726	2.705203
C	-2.825892	2.635500	3.824944
H	-2.801825	3.331519	4.660872
C	-3.675053	1.526637	3.856880
H	-4.314986	1.354237	4.719664
C	-3.698356	0.637465	2.776426
H	-4.349282	-0.233307	2.782950
C	-2.877093	0.857787	1.670016
H	-2.905879	0.151906	0.845573
C	4.446160	0.077213	0.330550
C	4.473551	1.457336	0.588721
H	3.576634	2.052565	0.438762
C	5.642052	2.068940	1.052192
H	5.647099	3.138533	1.250019
C	6.793747	1.308005	1.267624
H	7.701969	1.783434	1.631479
C	6.774153	-0.068954	1.022136
H	7.665845	-0.668147	1.192759

C 5.608346 -0.683205 0.559432
H 5.604203 -1.756245 0.384629
C 3.213433 -1.072894 -2.104244
C 2.099234 -1.307771 -2.929881
H 1.095456 -1.241906 -2.513855
C 2.271904 -1.617620 -4.281096
H 1.401456 -1.801969 -4.906784
C 3.558011 -1.678302 -4.826197
H 3.693015 -1.909225 -5.880557
C 4.669456 -1.433852 -4.014450
H 5.672181 -1.472361 -4.434554
C 4.501501 -1.136979 -2.658505
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C 3.010683 -3.672375 2.547401
H 3.161482 -3.718464 3.623727
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H 3.255150 -1.538206 2.474674
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H -2.182460 -4.143424 0.090525
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H -2.600028 -3.826668 2.152682
C -3.988514 -1.532160 -1.521651
S -4.653349 -2.849203 -0.351438
O -3.779578 -4.033514 -0.670119
O -6.073618 -3.009854 -0.765926
O -4.427286 -2.261084 1.001433
F -2.692490 -1.279217 -1.248444
F -4.672417 -0.389174 -1.381501
F -4.073951 -1.924651 -2.796995
el energy= -2562.02255005
zpe= -2561.311518
th energy= -2561.256442
th enthalpy= -2561.255498
free energy= -2561.411796

12b

Rh 1.788931 0.363136 0.039694
P 2.875868 -1.794809 0.118608
P 0.753648 2.546377 -0.037070
O 4.450225 1.664017 0.514865
C 3.424311 1.165990 0.339686
N -0.112504 -0.586251 -0.361081
C -0.971670 -0.897903 0.629570

C -2.187324 -1.533623 0.398819
C -2.554894 -1.865025 -0.908912
C -1.658642 -1.536107 -1.934841
C -0.460308 -0.906342 -1.625351
C -3.879906 -2.528384 -1.214730
H -1.882535 -1.772990 -2.972174
H 0.256151 -0.647899 -2.399446
C 3.197201 -2.382578 1.842617
C 3.473309 -3.732013 2.131129
H 3.471073 -4.474450 1.337022
C 3.741917 -4.131663 3.442266
H 3.954284 -5.177620 3.652174
C 3.734903 -3.193168 4.479348
H 3.940829 -3.508157 5.499944
C 3.455248 -1.852365 4.202651
H 3.439984 -1.118847 5.005680
C 3.184971 -1.448996 2.892021
H 2.953194 -0.407648 2.682239
C 4.524764 -1.782522 -0.731100
C 5.628962 -2.510972 -0.260868
H 5.552731 -3.100108 0.648655
C 6.842130 -2.476236 -0.954777
H 7.692671 -3.038490 -0.575522
C 6.963624 -1.723851 -2.126625
H 7.909341 -1.699334 -2.663461
C 5.868403 -0.996857 -2.602247
H 5.955598 -0.404740 -3.510526
C 4.658345 -1.018936 -1.904280
H 3.814151 -0.436677 -2.268901
C 1.968700 -3.201648 -0.678780
C 2.267644 -3.611284 -1.988442
H 3.077121 -3.140655 -2.539813
C 1.529716 -4.632823 -2.594488
H 1.776768 -4.943308 -3.607417
C 0.486000 -5.253129 -1.903244
H -0.085678 -6.048863 -2.375586
C 0.178760 -4.846279 -0.600810
H -0.633289 -5.321996 -0.055480
C 0.911846 -3.825777 0.007981
H 0.661239 -3.522731 1.021419
C 0.863943 3.328223 -1.709666
C 1.856037 2.885475 -2.600326
H 2.514991 2.070890 -2.309044
C 1.993702 3.477789 -3.858612
H 2.765142 3.124030 -4.538998
C 1.138202 4.514144 -4.242341
H 1.242059 4.972079 -5.223547
C 0.143465 4.957428 -3.364812
H -0.527296 5.761532 -3.659237
C 0.004219 4.369154 -2.105385
H -0.778691 4.717508 -1.436554

C 1.532815 3.755027 1.134181
C 1.927320 3.292698 2.402178
H 1.797448 2.243391 2.660478
C 2.489283 4.169526 3.333317
H 2.785530 3.798482 4.311963
C 2.678886 5.514461 3.002106
H 3.125456 6.195993 3.722693
C 2.299066 5.979327 1.739779
H 2.449471 7.023337 1.473676
C 1.724358 5.107483 0.810089
H 1.434108 5.485485 -0.166216
C -1.049957 2.614032 0.384549
C -1.485496 3.004286 1.661364
H -0.769308 3.328773 2.411103
C -2.846937 2.982051 1.980254
H -3.169488 3.290757 2.972276
C -3.785543 2.566014 1.033617
H -4.842231 2.535384 1.285033
C -3.358748 2.173420 -0.239465
H -4.082965 1.834449 -0.975710
C -2.001442 2.195852 -0.563445
H -1.686591 1.886454 -1.556922
H -0.663014 -0.622968 1.634134
H -2.848145 -1.774217 1.224136
O -4.431584 -3.128212 -0.065271
H -5.393239 -2.946331 -0.070533
H -4.556039 -1.762809 -1.627535
H -3.724695 -3.270003 -2.017891
C -6.501234 0.058891 0.200880
S -7.774721 -1.326434 0.302614
F -6.971764 1.188742 0.748874
F -5.375627 -0.281712 0.847654
F -6.177437 0.321204 -1.079035
O -8.940901 -0.782829 -0.446255
O -7.958833 -1.514127 1.768881
O -7.076902 -2.464659 -0.395003
el energy= -2562.01906582
zpe= -2561.307987
th energy= -2561.252916
th enthalpy= -2561.251972
free energy= -2561.408864

13b

Rh 0.263997 -0.597948 -0.294600
P 2.620807 -0.082350 -0.322462
P -2.025583 -1.383445 -0.368140
O 0.270741 -0.230632 -3.270955
C 0.256934 -0.365717 -2.125414
N 0.295250 -0.960490 1.849332
C 0.045388 -0.033002 2.792094
C 0.136964 -0.332267 4.167515

C	0.486519	-1.610306	4.560003
C	0.741287	-2.583861	3.578639
C	0.635377	-2.214433	2.251136
O	-0.274784	1.217113	2.470940
H	-0.076591	0.457970	4.879862
H	0.558416	-1.857156	5.616413
H	1.016395	-3.600935	3.838757
H	0.818906	-2.926130	1.452349
C	3.065720	1.687856	-0.616034
C	4.381046	2.148042	-0.413726
H	5.149206	1.469304	-0.050480
C	4.709047	3.479726	-0.673333
H	5.729224	3.823373	-0.516542
C	3.728131	4.367190	-1.129729
H	3.984541	5.405601	-1.328507
C	2.417896	3.921983	-1.317234
H	1.646513	4.610586	-1.648927
C	2.084093	2.588070	-1.058792
H	1.054989	2.258703	-1.175209
C	3.459129	-1.043277	-1.671966
C	4.407199	-0.480159	-2.539974
H	4.689770	0.563936	-2.443484
C	4.990256	-1.256472	-3.547021
H	5.717508	-0.804214	-4.217857
C	4.641305	-2.601349	-3.693362
H	5.096997	-3.201664	-4.477691
C	3.697429	-3.170760	-2.832603
H	3.415011	-4.215544	-2.942065
C	3.102976	-2.394669	-1.835458
H	2.354267	-2.839053	-1.182955
C	3.576476	-0.502472	1.211075
C	4.414240	-1.625277	1.291938
H	4.545113	-2.276367	0.432145
C	5.094850	-1.913255	2.479992
H	5.745555	-2.783884	2.526584
C	4.944690	-1.087052	3.595986
H	5.476600	-1.311578	4.517906
C	4.106683	0.031218	3.523689
H	3.981929	0.679307	4.388356
C	3.424307	0.321484	2.341201
H	2.778499	1.195921	2.298067
C	-2.078290	-3.231338	-0.463566
C	-0.968093	-3.907655	-0.996707
H	-0.092479	-3.339574	-1.302592
C	-0.982148	-5.298509	-1.132553
H	-0.114451	-5.808402	-1.545385
C	-2.104596	-6.029394	-0.733652
H	-2.114592	-7.112508	-0.834198
C	-3.214797	-5.365285	-0.202081
H	-4.092132	-5.928506	0.108411
C	-3.205059	-3.974537	-0.068116

H -4.074086 -3.471799 0.348396
C -3.003608 -0.801645 -1.832006
C -2.919261 0.554405 -2.193696
H -2.301636 1.235674 -1.614341
C -3.648405 1.037503 -3.283424
H -3.583401 2.091465 -3.544433
C -4.451114 0.172801 -4.032963
H -5.010401 0.548901 -4.886961
C -4.531812 -1.177962 -3.682347
H -5.152302 -1.858029 -4.262188
C -3.815956 -1.665322 -2.584673
H -3.891863 -2.717213 -2.324353
C -3.082240 -0.957872 1.097864
C -3.940304 0.154262 1.070481
H -4.024823 0.767709 0.178961
C -4.684243 0.499259 2.203071
H -5.346403 1.361431 2.163426
C -4.579357 -0.254825 3.374747
H -5.161241 0.015229 4.253201
C -3.719257 -1.356343 3.412887
H -3.626528 -1.948830 4.320514
C -2.971954 -1.704457 2.285196
H -2.310575 -2.565458 2.333714
H -0.519830 1.399509 1.526855
S -2.154782 3.516019 0.459016
C -1.197980 4.982580 -0.231653
O -1.189855 2.376777 0.227831
O -3.374280 3.460034 -0.394598
O -2.369148 3.867640 1.889771
F -0.072783 5.188679 0.465987
F -1.940057 6.096353 -0.174926
F -0.860801 4.767751 -1.515038
el energy= -2522.72744606
zpe= -2522.045473
th energy= -2521.991950
th enthalpy= -2521.991006
free energy= -2522.142910

15b

Rh -0.002097 -0.610147 0.041886
P -2.420304 -0.660034 0.023977
P 2.417983 -0.669277 0.008049
O -0.013865 -3.443825 1.023840
C -0.007830 -2.353594 0.647558
N -0.000055 1.429974 -0.726311
C 0.011772 2.542267 0.086704
C 0.010963 3.861230 -0.483945
C 0.013487 3.976161 -1.894789
C -0.003701 2.842385 -2.677584
C -0.015817 1.584604 -2.045534
H 0.033810 4.948083 -2.383685

H -0.006183 2.898194 -3.761260
H -0.032240 0.672646 -2.636399
C -3.192318 -0.494367 1.696743
C -4.537322 -0.113576 1.858681
H -5.146913 0.129635 0.992146
C -5.099290 -0.035691 3.135132
H -6.140309 0.259293 3.246404
C -4.327877 -0.334057 4.262888
H -4.767418 -0.270098 5.255778
C -2.989958 -0.707864 4.111405
H -2.382196 -0.934326 4.984560
C -2.423640 -0.784680 2.836055
H -1.378298 -1.061822 2.726439
C -3.068590 -2.251173 -0.674322
C -4.230697 -2.872930 -0.190543
H -4.781914 -2.439548 0.639186
C -4.684007 -4.062987 -0.767234
H -5.581213 -4.539262 -0.378023
C -3.989637 -4.638851 -1.835062
H -4.345540 -5.565011 -2.280790
C -2.832644 -4.024881 -2.323714
H -2.284140 -4.468702 -3.151553
C -2.369542 -2.842199 -1.741663
H -1.459131 -2.377205 -2.115008
C -3.247500 0.651928 -0.991958
C -3.693021 0.390222 -2.297706
H -3.603616 -0.607435 -2.718825
C -4.262291 1.409933 -3.067158
H -4.608618 1.190524 -4.074754
C -4.390562 2.699046 -2.544301
H -4.836779 3.489905 -3.143083
C -3.943495 2.968374 -1.246526
H -4.039538 3.968858 -0.830549
C -3.372231 1.954279 -0.475196
H -3.032304 2.179169 0.532701
C 3.094410 -1.500408 -1.499930
C 2.263855 -2.362384 -2.235060
H 1.228715 -2.500331 -1.933209
C 2.756153 -3.035091 -3.356898
H 2.101021 -3.698226 -3.917387
C 4.081358 -2.849912 -3.759466
H 4.463455 -3.370298 -4.634888
C 4.914323 -1.988579 -3.038068
H 5.945935 -1.837757 -3.348171
C 4.426215 -1.315542 -1.915680
H 5.082835 -0.642146 -1.370643
C 3.125939 -1.590766 1.453511
C 2.491377 -1.459593 2.701325
H 1.592236 -0.853256 2.790494
C 3.003074 -2.107266 3.828577
H 2.503880 -1.993123 4.788208

C 4.144461 -2.906686 3.718312
H 4.537842 -3.419610 4.593089
C 4.774494 -3.051094 2.478807
H 5.658871 -3.677444 2.384796
C 4.272771 -2.394456 1.351323
H 4.774352 -2.519016 0.395828
C 3.284052 0.969866 0.048323
C 3.780559 1.499091 1.250512
H 3.707440 0.929325 2.172817
C 4.377876 2.763083 1.272318
H 4.763031 3.157127 2.210242
C 4.483079 3.513122 0.098248
H 4.950093 4.495267 0.117122
C 3.987015 2.994473 -1.102127
H 4.066637 3.569699 -2.021929
C 3.389177 1.732754 -1.128632
H 3.016627 1.340975 -2.071664
C 0.004375 4.988201 0.401878
C 0.011737 4.796395 1.772257
C 0.018427 3.493315 2.308130
C 0.016116 2.378724 1.491066
O -0.005725 6.271452 -0.042137
H 0.014360 1.372621 1.901779
H 0.021225 3.368633 3.388305
H 0.006184 5.667447 2.421279
H -0.086486 6.317704 -1.003991
el energy= -2102.83848106
zpe= -2102.137725
th energy= -2102.090268
th enthalpy= -2102.089324
free energy= -2102.225995

16b

Rh -0.012331 -0.593808 0.074587
P -2.430777 -0.625541 0.060827
P 2.405976 -0.684465 0.039694
O -0.047014 -3.262096 1.444492
C -0.032296 -2.235451 0.919073
N 0.009278 1.322611 -0.962478
C 0.050406 2.528779 -0.306052
C 0.065191 3.765602 -1.026250
C 0.037849 3.708684 -2.443195
C -0.007672 2.485172 -3.073892
C -0.022967 1.311798 -2.292090
H 0.049304 4.633169 -3.016415
H -0.033341 2.402412 -4.156125
H -0.060603 0.334908 -2.765845
C -3.207443 -0.225035 1.691081
C -4.550655 0.182181 1.792264
H -5.155629 0.305124 0.897481
C -5.116492 0.440692 3.042947

H -6.156025 0.754241 3.107616
C -4.350791 0.298463 4.204618
H -4.793357 0.503233 5.176911
C -3.014861 -0.100970 4.112751
H -2.411673 -0.207008 5.011626
C -2.444751 -0.358583 2.863008
H -1.401190 -0.655607 2.797377
C -3.087905 -2.294089 -0.412018
C -4.251859 -2.839454 0.152902
H -4.800983 -2.294772 0.915763
C -4.709706 -4.095715 -0.255405
H -5.608238 -4.511129 0.195558
C -4.018301 -4.814922 -1.234568
H -4.377730 -5.792156 -1.549107
C -2.859627 -4.277830 -1.803235
H -2.313321 -4.832653 -2.562747
C -2.392131 -3.028296 -1.388691
H -1.480698 -2.621605 -1.822577
C -3.247387 0.538172 -1.129389
C -3.699101 0.099759 -2.384582
H -3.619627 -0.947857 -2.661737
C -4.261280 1.006620 -3.288775
H -4.612383 0.651202 -4.255098
C -4.376208 2.357504 -2.951935
H -4.816708 3.060626 -3.655274
C -3.922974 2.802274 -1.705561
H -4.008352 3.852248 -1.434448
C -3.358722 1.901256 -0.800412
H -3.014163 2.262176 0.165521
C 3.057588 -1.727780 -1.342269
C 2.209508 -2.675823 -1.938181
H 1.176959 -2.756551 -1.608174
C 2.680990 -3.507373 -2.957709
H 2.012320 -4.235981 -3.410602
C 4.002972 -3.396887 -3.396722
H 4.369118 -4.041374 -4.192787
C 4.853127 -2.450908 -2.814927
H 5.882158 -2.357625 -3.154797
C 4.385746 -1.619012 -1.794777
H 5.055505 -0.881794 -1.359332
C 3.114318 -1.404827 1.595126
C 2.488440 -1.098187 2.816286
H 1.594225 -0.478220 2.826260
C 3.002037 -1.589451 4.019215
H 2.509500 -1.340599 4.956559
C 4.136621 -2.405926 4.014076
H 4.531445 -2.797105 4.949059
C 4.758041 -2.724369 2.803033
H 5.637153 -3.364938 2.791514
C 4.254378 -2.224531 1.598627
H 4.749050 -2.483346 0.666735

C 3.294635 0.930943 -0.155823
C 3.819278 1.611622 0.954675
H 3.753792 1.175033 1.947531
C 4.434890 2.856711 0.793370
H 4.841757 3.369415 1.662229
C 4.530636 3.436439 -0.474191
H 5.012080 4.403954 -0.597679
C 4.006389 2.766390 -1.584288
H 4.077898 3.208780 -2.575466
C 3.390208 1.523185 -1.427978
H 2.994325 1.012186 -2.301827
C 0.098390 4.992005 -0.314610
C 0.113053 4.994859 1.067452
C 0.097456 3.765531 1.783495
C 0.068709 2.565465 1.113578
H 0.108804 5.926298 -0.873195
O 0.141110 6.122034 1.822635
H 0.055171 1.623893 1.658042
H 0.109496 3.801033 2.869642
H 0.146773 6.905933 1.253588
el energy= -2102.84350051
zpe= -2102.142240
th energy= -2102.095086
th enthalpy= -2102.094141
free energy= -2102.230026

17b

Rh -0.010880 -0.541623 0.060981
P -2.427937 -0.582484 0.042948
P 2.406863 -0.629452 0.021471
O -0.041958 -3.191712 1.466866
C -0.028160 -2.171237 0.929358
N 0.006928 1.353240 -1.008805
C 0.045775 2.570678 -0.365599
C 0.060764 3.791181 -1.117500
C 0.033249 3.716611 -2.527974
C -0.011726 2.482373 -3.144124
C -0.025511 1.327438 -2.339692
H 0.044330 4.634164 -3.112609
H -0.037959 2.380809 -4.224381
H -0.061695 0.342195 -2.796983
C -3.211026 -0.179604 1.669653
C -4.559329 0.211963 1.765577
H -5.164474 0.319840 0.868914
C -5.130142 0.474031 3.013203
H -6.173652 0.774953 3.073887
C -4.364188 0.351624 4.177032
H -4.810645 0.559143 5.146974
C -3.023092 -0.031090 4.090245
H -2.419502 -0.120814 4.990617
C -2.448098 -0.292514 2.843487

H -1.400443 -0.575535 2.781746
C -3.073940 -2.256601 -0.425774
C -4.230805 -2.811802 0.143969
H -4.782181 -2.271013 0.907947
C -4.678514 -4.072924 -0.260759
H -5.571611 -4.495841 0.194024
C -3.983967 -4.787321 -1.241155
H -4.335491 -5.768310 -1.552947
C -2.832166 -4.240507 -1.814612
H -2.283352 -4.791527 -2.575097
C -2.374705 -2.986151 -1.403576
H -1.468332 -2.571995 -1.841004
C -3.250023 0.573546 -1.150941
C -3.713322 0.128511 -2.399415
H -3.638273 -0.920910 -2.670912
C -4.281445 1.031241 -3.304198
H -4.641546 0.670844 -4.265357
C -4.390738 2.384260 -2.974413
H -4.835797 3.084140 -3.678125
C -3.925640 2.835596 -1.734674
H -4.006103 3.887475 -1.469482
C -3.355454 1.938853 -0.829102
H -2.999721 2.304675 0.131039
C 3.055910 -1.685471 -1.352058
C 2.206501 -2.639033 -1.937177
H 1.174870 -2.716906 -1.603561
C 2.675481 -3.479598 -2.950456
H 2.005750 -4.212335 -3.395063
C 3.996287 -3.372788 -3.393927
H 4.360472 -4.024222 -4.185228
C 4.847812 -2.421591 -2.822722
H 5.875960 -2.331212 -3.166048
C 4.382908 -1.580701 -1.808822
H 5.053660 -0.839597 -1.381573
C 3.119328 -1.334666 1.581956
C 2.497228 -1.014105 2.801488
H 1.604249 -0.392267 2.807262
C 3.013138 -1.493856 4.008072
H 2.523572 -1.234307 4.944074
C 4.146145 -2.312565 4.008381
H 4.542687 -2.694866 4.946315
C 4.763794 -2.644698 2.799084
H 5.641667 -3.287043 2.791912
C 4.257879 -2.156371 1.590884
H 4.749550 -2.425742 0.660376
C 3.295160 0.984277 -0.190896
C 3.820506 1.675789 0.912564
H 3.755853 1.248833 1.909636
C 4.435784 2.919330 0.738864
H 4.843491 3.440227 1.602471
C 4.530413 3.487051 -0.534253

H 5.011663 4.453390 -0.667420
C 4.005239 2.806384 -1.637362
H 4.075584 3.239331 -2.632790
C 3.389360 1.564599 -1.468565
H 2.992833 1.045430 -2.337291
C 0.093877 5.024425 -0.411098
C 0.108074 5.053683 0.962847
C 0.090630 3.836666 1.699624
C 0.060539 2.616577 1.044536
H 0.105368 5.953123 -0.976986
O 0.103200 3.824586 3.055583
H 0.131988 6.003196 1.494295
H 0.046350 1.690494 1.613330
H 0.119400 4.729615 3.399769
el energy= -2102.84433929
zpe= -2102.143197
th energy= -2102.095994
th enthalpy= -2102.095050
free energy= -2102.231134

18b

Rh -2.210722 0.075330 0.038150
P -2.005913 2.484413 0.023030
P -2.501471 -2.324457 0.000126
O -5.055255 0.376276 0.945580
C -3.959747 0.258550 0.601639
N -0.179330 -0.130132 -0.694115
C 0.909644 -0.228823 0.145301
C 2.229520 -0.342499 -0.400800
C 2.384484 -0.359761 -1.801866
C 1.271981 -0.257299 -2.615717
C 0.007831 -0.139448 -2.012632
H 3.385512 -0.451650 -2.213935
H 1.350025 -0.262414 -3.698597
H -0.888190 -0.052403 -2.622377
C -1.832012 3.243964 1.701572
C -1.329125 4.546483 1.876091
H -0.996533 5.125007 1.018018
C -1.243177 5.104195 3.153903
H -0.852671 6.112217 3.274777
C -1.654471 4.370056 4.270964
H -1.583219 4.805466 5.265231
C -2.149651 3.073653 4.107253
H -2.463586 2.493796 4.972341
C -2.235291 2.511997 2.830355
H -2.606243 1.497302 2.711170
C -3.497824 3.286017 -0.734829
C -4.028254 4.499909 -0.269948
H -3.580321 5.006301 0.580451
C -5.145786 5.064145 -0.892428
H -5.552082 6.001017 -0.517421

C	-5.738824	4.429726	-1.987759
H	-6.608240	4.871907	-2.469230
C	-5.215384	3.221704	-2.458162
H	-5.673131	2.719327	-3.307489
C	-4.106672	2.648525	-1.830377
H	-3.713214	1.699381	-2.189401
C	-0.581564	3.184507	-0.935140
C	-0.749618	3.687569	-2.235259
H	-1.735797	3.714712	-2.690670
C	0.351077	4.162865	-2.955493
H	0.205170	4.554408	-3.959925
C	1.627654	4.138848	-2.388456
H	2.482222	4.510242	-2.949619
C	1.803101	3.633553	-1.095960
H	2.793683	3.607708	-0.647193
C	0.707819	3.155860	-0.373783
H	0.860288	2.763968	0.628679
C	-3.358960	-2.918403	-1.529119
C	-4.125902	-2.009362	-2.276540
H	-4.174229	-0.967347	-1.970613
C	-4.817252	-2.432618	-3.415082
H	-5.405540	-1.716692	-3.984805
C	-4.745492	-3.767294	-3.822666
H	-5.279862	-4.095996	-4.711291
C	-3.979055	-4.678687	-3.089234
H	-3.916094	-5.718242	-3.403221
C	-3.287956	-4.259372	-1.949976
H	-2.688312	-4.977166	-1.396011
C	-3.527207	-2.939836	1.418709
C	-3.372624	-2.316866	2.669589
H	-2.686917	-1.478570	2.775073
C	-4.097046	-2.762211	3.778228
H	-3.963627	-2.273008	4.740563
C	-4.996042	-3.824411	3.645931
H	-5.567890	-4.165572	4.506044
C	-5.163164	-4.442321	2.403138
H	-5.865989	-5.265166	2.291888
C	-4.430781	-4.007401	1.294658
H	-4.573678	-4.498460	0.336193
C	-0.960572	-3.352171	0.082180
C	-0.522620	-3.909604	1.294264
H	-1.110971	-3.786749	2.199458
C	0.674883	-4.629381	1.348666
H	0.999144	-5.058722	2.294134
C	1.448531	-4.797985	0.197584
H	2.379703	-5.358359	0.241868
C	1.020509	-4.242649	-1.012472
H	1.616135	-4.368134	-1.913930
C	-0.174218	-3.522362	-1.071294
H	-0.493979	-3.100672	-2.020577
C	3.375437	-0.424114	0.478671

C 3.147292 -0.398934 1.856819
C 1.840281 -0.287631 2.370508
C 0.729158 -0.202326 1.547774
O 4.565502 -0.527913 -0.072545
H -0.275866 -0.114398 1.952674
H 1.703993 -0.268470 3.450393
H 3.994594 -0.463424 2.534753
Al 6.350898 -0.284672 0.342205
O 6.945064 0.751301 -1.177083
N 6.884183 0.314909 -2.420510
O 6.467400 -0.827130 -2.623548
O 7.251742 1.083053 -3.298116
C 6.611189 1.074611 1.804580
C 7.258918 -2.073062 0.459862
C 8.734681 -2.065234 0.014400
C 7.126137 -2.669387 1.877439
H 6.249232 0.609780 2.740180
H 6.716498 -2.743714 -0.227963
H 8.843284 -1.736939 -1.028331
H 9.346086 -1.391167 0.633115
H 9.193188 -3.066554 0.091033
H 6.075610 -2.768270 2.189010
H 7.580049 -3.672990 1.948372
H 7.626834 -2.042094 2.630532
C 8.101701 1.411476 2.022780
C 5.798606 2.368191 1.595582
H 8.245652 2.132319 2.846449
H 8.548038 1.863664 1.124634
H 8.697467 0.519821 2.265160
H 4.719372 2.170347 1.530773
H 5.949763 3.089571 2.417748
H 6.091767 2.878753 0.666482
el energy= -2621.84892363
zpe= -2620.955955
th energy= -2620.892445
th enthalpy= -2620.891500
free energy= -2621.068285

19b

Rh 2.053102 -0.159141 0.138864
P 1.645606 -2.541674 0.142255
P 2.548352 2.207817 0.149644
O 4.004249 -0.544686 2.385775
C 3.251241 -0.394729 1.524247
N 0.691763 0.107323 -1.532205
C -0.649053 0.353253 -1.369511
C -1.518978 0.519299 -2.498357

C -0.940094 0.424006 -3.791285
C 0.408332 0.172344 -3.922837
C 1.193272 0.017379 -2.761871
H -1.572934 0.546812 -4.668053
H 0.880072 0.089519 -4.897560
H 2.258722 -0.182901 -2.835416
C 0.536002 -3.114593 1.507439
C -0.125796 -4.355248 1.454035
H -0.022044 -4.995063 0.581380
C -0.930925 -4.771304 2.517000
H -1.437670 -5.732267 2.462760
C -1.087277 -3.955887 3.642393
H -1.718922 -4.279994 4.466461
C -0.437105 -2.720460 3.701804
H -0.561158 -2.077283 4.570102
C 0.367825 -2.300239 2.639488
H 0.858334 -1.331342 2.685389
C 3.217791 -3.507360 0.339006
C 3.289250 -4.698414 1.078817
H 2.408872 -5.085291 1.584331
C 4.498452 -5.392876 1.179806
H 4.542468 -6.310204 1.762876
C 5.643782 -4.912505 0.538389
H 6.582782 -5.455519 0.619747
C 5.580461 -3.728306 -0.201990
H 6.467931 -3.345199 -0.700887
C 4.376755 -3.025144 -0.294496
H 4.336780 -2.094803 -0.857758
C 0.874323 -3.244829 -1.390221
C 1.650008 -3.875935 -2.376005
H 2.720088 -4.001976 -2.235745
C 1.051776 -4.353812 -3.546349
H 1.664615 -4.845726 -4.298654
C -0.323008 -4.205520 -3.745727
H -0.787099 -4.580628 -4.655197
C -1.100735 -3.572578 -2.770560
H -2.171624 -3.450903 -2.917227
C -0.507733 -3.091314 -1.601684
H -1.126138 -2.602440 -0.853218
C 4.106016 2.616975 -0.762916
C 5.049673 1.601159 -0.988542
H 4.837700 0.587226 -0.658580
C 6.252059 1.882431 -1.643222
H 6.972268 1.084969 -1.812258
C 6.522485 3.180300 -2.084799
H 7.456224 3.398648 -2.598357
C 5.586452 4.197307 -1.871124
H 5.789197 5.208963 -2.215646
C 4.384404 3.919980 -1.215814
H 3.662319 4.718682 -1.066304
C 2.778395 2.879897 1.863465

C	1.956149	2.380387	2.888740
H	1.231496	1.598918	2.669323
C	2.065186	2.876347	4.190395
H	1.418656	2.483525	4.971933
C	3.008429	3.864752	4.485857
H	3.100864	4.244715	5.500876
C	3.837283	4.358630	3.474267
H	4.577923	5.123150	3.698755
C	3.722112	3.873941	2.168128
H	4.374603	4.268856	1.394492
C	1.276980	3.327213	-0.604288
C	0.338978	4.002456	0.193222
H	0.374722	3.916192	1.275745
C	-0.650529	4.794187	-0.397567
H	-1.368338	5.313508	0.233537
C	-0.716308	4.918814	-1.787544
H	-1.486501	5.535780	-2.244976
C	0.212223	4.246274	-2.588388
H	0.169048	4.337161	-3.671513
C	1.201105	3.453209	-2.002921
H	1.916868	2.939512	-2.639305
C	-2.898212	0.755036	-2.293720
C	-3.442684	0.826194	-1.011490
C	-2.553438	0.669945	0.105445
C	-1.208309	0.441489	-0.068046
H	-3.552752	0.877523	-3.154024
O	-4.728464	1.064631	-0.821730
H	-0.548557	0.325959	0.790058
H	-2.972166	0.762538	1.104053
Al	-6.219832	0.387365	0.007028
C	-7.464627	1.926820	0.343373
C	-8.729983	1.542799	1.136881
C	-6.766426	-1.296732	-0.949896
C	-7.889447	-2.081495	-0.242417
C	-7.130703	-1.055170	-2.429167
C	-7.850025	2.662110	-0.957246
O	-5.707710	-0.401135	1.701925
N	-5.230391	0.259179	2.737239
O	-4.834739	1.415785	2.567335
O	-5.198929	-0.329542	3.808429
H	-6.897632	2.641889	0.963644
H	-8.488984	1.079927	2.104541
H	-9.367113	2.419643	1.345989
H	-9.353701	0.824680	0.583664
H	-5.868535	-1.942638	-0.942171
H	-8.827495	-1.506782	-0.213357
H	-8.117592	-3.031399	-0.756988
H	-6.315824	-0.564739	-2.980313
H	-7.363186	-1.995873	-2.958382
H	-8.018499	-0.411938	-2.527281
H	-8.420685	2.011588	-1.637540

H -8.482956 3.544932 -0.760285
H -6.966503 3.010905 -1.509968
H -7.628765 -2.326200 0.796283
el energy= -2621.84633596
zpe= -2620.953425
th energy= -2620.889927
th enthalpy= -2620.888983
free energy= -2621.065561

20b

Rh 1.786656 0.112055 -0.237938
P 1.521394 2.513136 -0.321732
P 2.119408 -2.281530 -0.188948
O 3.110664 0.216266 -2.928847
C 2.595897 0.173964 -1.896706
N 0.906109 0.049517 1.744217
C -0.453450 -0.070272 1.944126
C -0.986637 -0.087734 3.278138
C -0.096009 0.012417 4.364210
C 1.263127 0.133681 4.130380
C 1.714016 0.151520 2.800099
H -0.488430 -0.001315 5.379478
H 1.980377 0.218319 4.940725
H 2.774262 0.248883 2.579623
C 0.098834 3.069041 -1.366117
C -0.460651 4.353814 -1.238010
H -0.081149 5.045611 -0.490274
C -1.517413 4.747922 -2.062081
H -1.942154 5.743195 -1.951724
C -2.029409 3.866705 -3.019826
H -2.856236 4.174242 -3.656094
C -1.482048 2.587669 -3.151350
H -1.880882 1.894067 -3.888095
C -0.425440 2.189646 -2.327687
H -0.014651 1.187763 -2.423149
C 3.018437 3.352056 -1.028000
C 2.934882 4.476963 -1.863757
H 1.967002 4.885062 -2.140985
C 4.098162 5.076765 -2.355528
H 4.019321 5.942813 -3.009116
C 5.353912 4.567642 -2.012419
H 6.256588 5.036904 -2.397383
C 5.445856 3.449179 -1.178633
H 6.418866 3.043821 -0.909848
C 4.285079 2.839605 -0.696109
H 4.361815 1.958411 -0.061977
C 1.253101 3.369288 1.301425
C 2.310707 3.995527 1.980643
H 3.303978 4.026761 1.541271
C 2.094944 4.591195 3.227441
H 2.922813 5.077531 3.738964

C	0.824945	4.567220	3.809100
H	0.658113	5.034268	4.777248
C	-0.231537	3.939785	3.140971
H	-1.223611	3.914085	3.586285
C	-0.020584	3.340634	1.897452
H	-0.851567	2.855101	1.392107
C	3.813031	-2.746330	0.394772
C	4.836426	-1.785784	0.337883
H	4.610364	-0.781175	-0.011417
C	6.136117	-2.109764	0.737021
H	6.918127	-1.355146	0.689013
C	6.425996	-3.395021	1.202664
H	7.436438	-3.646287	1.517642
C	5.412372	-4.356503	1.269442
H	5.631027	-5.357713	1.634213
C	4.112694	-4.036544	0.869633
H	3.332990	-4.791116	0.935895
C	1.930512	-3.068377	-1.858441
C	0.918434	-2.587916	-2.708208
H	0.292531	-1.756803	-2.389387
C	0.711994	-3.166830	-3.962908
H	-0.078264	-2.787844	-4.607079
C	1.525380	-4.220532	-4.389912
H	1.371876	-4.665399	-5.370583
C	2.541107	-4.696112	-3.555591
H	3.182028	-5.511299	-3.884443
C	2.742021	-4.128067	-2.294064
H	3.536126	-4.510048	-1.658706
C	0.981683	-3.264420	0.897683
C	-0.142033	-3.919959	0.369129
H	-0.338479	-3.898935	-0.699174
C	-1.019663	-4.609156	1.211840
H	-1.882970	-5.115755	0.786226
C	-0.788630	-4.648764	2.589295
H	-1.472171	-5.186013	3.242945
C	0.325891	-3.994648	3.123496
H	0.514995	-4.019844	4.194456
C	1.204539	-3.304723	2.285630
H	2.067940	-2.805549	2.717261
C	-2.398551	-0.190133	3.435393
C	-3.232236	-0.266328	2.348710
C	-2.707575	-0.256386	1.009037
C	-1.321911	-0.159235	0.840446
H	-2.809795	-0.198709	4.443177
O	-3.493245	-0.326451	-0.045510
H	-4.309216	-0.327874	2.484601
H	-0.909784	-0.147257	-0.165795
Al	-5.279607	-0.610506	-0.427683
C	-5.548922	-0.085698	-2.345640
C	-6.977906	0.397297	-2.665033
C	-5.875715	-2.396637	0.282755

C -7.352475 -2.699928 -0.043894
C -4.974706 -3.566870 -0.161522
C -5.133350 -1.210053 -3.317821
O -6.253742 0.525556 0.800012
N -6.164689 1.843462 0.790414
O -5.424288 2.374462 -0.038968
O -6.829347 2.451747 1.616518
H -4.870655 0.765865 -2.524779
H -7.260208 1.266852 -2.056042
H -7.085701 0.691962 -3.723446
H -7.726265 -0.387895 -2.479257
H -5.796863 -2.329897 1.383125
H -7.519076 -2.776244 -1.129168
H -7.686603 -3.656081 0.395409
H -3.927254 -3.416255 0.136553
H -5.301705 -4.528389 0.271740
H -4.983599 -3.694591 -1.254383
H -5.763456 -2.104167 -3.197913
H -5.225277 -0.897728 -4.372664
H -4.091532 -1.527834 -3.164447
H -8.026430 -1.916721 0.331289
el energy= -2621.85019478
zpe= -2620.957247
th energy= -2620.893755
th enthalpy= -2620.892811
free energy= -2621.069443

21b

Rh -1.320250 0.060344 -0.289076
P -1.593716 -2.333354 -0.464802
P -1.372011 2.470764 -0.093109
O -2.000938 0.228699 -3.204356
C -1.725810 0.175326 -2.083863
N -0.964577 -0.085645 1.844264
C 0.298319 -0.190479 2.336964
C 0.495441 -0.313133 3.736947
C -0.590394 -0.318432 4.593767
C -1.888206 -0.205391 4.067897
C -2.018679 -0.097313 2.694257
H 1.508425 -0.396151 4.117161
H -0.434870 -0.410097 5.666535
H -2.768335 -0.206072 4.702868
H -2.995370 -0.007851 2.226469
O 1.276496 -0.175465 1.475376
C -0.193798 -3.233032 -1.269226
C -0.088332 -4.636097 -1.214688
H -0.830149 -5.221765 -0.676614
C 0.975202 -5.286364 -1.843399
H 1.045052 -6.371063 -1.798101
C 1.949993 -4.545314 -2.521720
H 2.782363 -5.054360 -3.003020

C	1.858732	-3.152489	-2.567988
H	2.624719	-2.564103	-3.066472
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22b

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H	-3.572422	-0.378050	3.033892
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zpe= -2506.630922
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free energy= -2506.739494