Electronic Supplementary Material (ESI) for Chemical Communications.

Highly Regioselective Osmium-Catalyzed Hydroformylation

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1. Analytical Methods

NMR spectra were recorded on Bruker Avance 300 (300 MHz) and Bruker Avance 400 (400 MHz) NMR spectrometers. Chemical shifts δ (ppm) are given relative to solvent: references for $CDCl_3$ were 7.26 ppm (^{1}H-NMR) and 77.16 ppm (^{13}C-NMR) ^{13}C-NMR spectra were acquired on a broad band decoupled mode. Multiplets were assigned as s (singlet), d (doublet), t (triplet), dd (doublet of doublet), m (multiplet) and br. s (broad singlet). All measurements were carried out at room temperature unless otherwise stated. Electron impact (EI) mass spectra were recorded on AMD 402 mass spectrometer (70 eV). High resolution mass spectra (HRMS) were recorded on Agilent 6210. The data are given as mass units per charge (*m/z*) and intensities of signals are given in brackets. For GC analyses, HP 7890 chromatograph with a 30 m HP5 column was used. The products were isolated from the reaction mixture by solvent evaporation and further purified by column chromatography on silica gel 60, 0.063-0.2 mm, 70-230 mesh (Merck) or distilled bulb-to-bulb using Büchi Glass oven B-585 wherever necessary. Isooctane was used as an internal standard for GC analysis. The purity of isolated compounds was determined by GC. Linear to branched ratio were determined by GC analysis of the crude reaction mixture.

2. Materials and Methods

All commercial reagents were ordered from Acros Organics, Alfa Aesar, Aldrich or Strem. Dry solvents were prepared according to standard procedures.[1] Ligands were synthesized according to reported literature.[2] Air- and moisture-sensitive syntheses were performed under argon atmosphere in heating gun vacuum dried glassware.

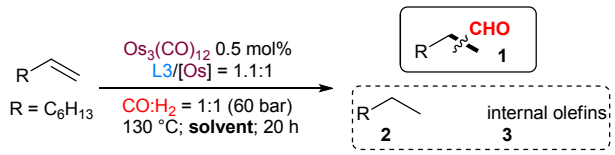
3. General Procedure for the Osmium-catalyzed Hydroformylation

Hydroformylation of alkenes were carried out in a Parr stainless steel autoclave (600 mL). In a typical experiment, a 4 mL vial was charged $Os_3(CO)_{12}$ (14.3 mg, 0.5 mol%), L (19.4 mg, 1.65 mol%), olefins (3.2 mmol), acetonitrile (2 mL) under argon atmosphere. Then the autoclave were pressurized with CO (30 bar) and hydrogen (30 bar) and the reaction was carried out at 130 °C for 20 hours. Then the autoclave was cooled to room temperature and depressurized. The content was

analyzed by gas chromatography using isooctane as internal standard.

4. Osmium-catalyzed hydroformylation: Solvent effects.[a]

Table S1:

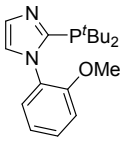


Entry	Solvent	Yield [%][b]		
		1 (*n:iso*)[b]	**2**	**3**
1	**MeCN**	64(97:3)	3	23
2	**MeOH**	56 (97:3)	2	19
3	**PC**	64 (97:3)	2	25
4	**NMP**	57 (97:3)	1	18
5	**DMA**	63 (97:3)	2	19
6	**THF**	40 (97:3)	3	15
7	**Tol**	6 (95:5)	1	4

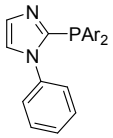
[a] 3.2 mmol 1-octene, $Os_3(CO)_{12}$ 0.5 mol%, L3 1.65 mol%, 2 mL solvent, CO/H_2 30:30 bar, 130 °C, 20 h. [b] Determined by GC with isooctane as internal standard.

5. Characterization of Ligands.

2-(Di-*tert*-butylphosphino)-1-(2-methoxyphenyl)-*1H*-imidazole (L1)



^{1}H NMR (300 MHz, CD_2Cl_2) δ = 7.41 (m, 1H,), 7.27 (d, 1H,), 7.17-7.14 (m, 1H), 7.07 (dd, 1H), 7.03-6.97 (m, 2H), 3.70 (s, 3H), 1.16 (d, 18H). **^{13}C NMR** (75 MHz, CD_2Cl_2) δ = 155.3 148.6, 130.7 (d, J = 3.0 Hz), 130.4, 129.9, 128.4, 124.1, 120.3, 111.9, 55.7, 33.7 (d, J = 16.7 Hz), 30.5 (d, J = 14.4 Hz). **^{31}P NMR** (121 MHz, CD_2Cl_2) δ/ppm: = 6.6. **MS** (EI) *m/z* (%): 318(17) $[M]^+$, 287 (30), 262 (39), 247 (28), 231 (71), 206 (46), 175 (100), 173 (35), 146 (10), 57 (10), 41 (8). **HRMS** (ESI) *m/z*: calcd. for $[C_{18}H_{27}N_2OP+H]^+$: 319.19338; found: 319.19396.

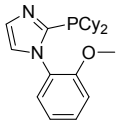


Ar = 3,5-bis(trifluoromethyl)benzene

2-(bis(3,5-bis(trifluoromethyl)phenyl)phosphino)-1-phenyl-1H-imidazole [L2]

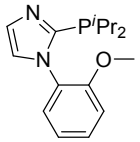
^{1}H NMR (300 MHz, $CDCl_3$) δ = 7.96-7.84 (m, 6H), 7.51-7.41 (m, 4H), 7.35 (dd, *J*=2.5, 1.1 Hz, 1H), 7.23-7.19 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ = 142.8, 138.1 (d, *J*=11.9 Hz), 138.0, 137.1, 133.7 (dd, *J*=22.6, 3.7 Hz), 132.1 (d, *J*=7.4 Hz), 131.8 (d, *J*=7.4 Hz), 126.3 (d, *J*=3.7 Hz), 123.8-123.6 (m), 121.6. **^{31}P NMR** (121 MHz, $CDCl_3$) δ -30.0. **^{19}F NMR** (282 MHz, $CDCl_3$) δ = -62.5. **MS (EI):** m/z = 600 $[M]^+$, 581, 523, 457, 387, 367, 319, 250, 175, 144,117, 77. **HRMS:** calcd. for $[C_{25}H_{13}F_{12}N_2P+H]^+$:601.06975 found:601.07018.

2-(Dicyclohexylphosphino)-1-(2-methoxyphenyl)-*1H*-imidazole [L3]



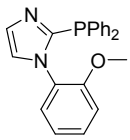
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.45-7.38 (m, 1H), 7.36 (d, *J* = 0.9 Hz, 1H), 7.19-7.16 (m, 1H), 7.07-7.05 (m, 1H), 7.04-6.98 (m, 2H), 3.75 (s, 3H), 2.12-2.04 (m, 2H), 1.70-1.60 (m, 10H), 1.33-0.98 (m, 10H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 154.6, 130.2, 129.5, 123.3, 120.1, 111.5, 55.3, 34.0 (d, *J* = 7.6), 30.1 (d, *J* = 15.8), 29.1, 27.1 (d, *J* = 12.6), 26.4. **^{31}P NMR** (121 MHz, $CDCl_3$) δ -23.1. **MS (EI):** 370 (9) $[M]^+$, 340 (16), 339 (77), 289 (6), 288 (60), 287 (100), 257 (26), 206 (11), 205 (13), 175 (31), 146 (12), 55 (15). **HRMS:** calcd. for $[C_{22}H_{32}N_2OP+H]^+$: 371.22468; found: 371.22457. **EA:** C (71.72%), H (8.665%), N (7.525%), P (8.361%).

2-(Diisopropylphosphino)-1-(2-methoxyphenyl)-*1H*-imidazole [L4]



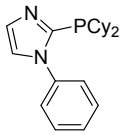
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.39-7.32 (m, 1H), 7.29 (d, *J* = 0.8 Hz, 1H), 7.16-7.11 (m, 1H), 7.01-6.97 (m, 1H), 6.96-6.95 (m, 2H), 3.69 (s, 3H), 2.25-2.16 (m, 2H), 0.98-0.88 (m, 12H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 154.7, 130.2, 129.4, 125.0, 123.4, 120.1, 111.5, 55.3, 24.5 (d, *J* = 7.3 Hz), 19.8 (d, *J* = 18.1 Hz), 19.3 (d, *J* = 8.7 Hz). **^{31}P NMR** (121 MHz, $CDCl_3$) δ -14.3. **MS (EI):** 290 (8) $[M]^+$, 260 (17), 248 (37), 247 (100), 217 (21), 205 (17), 190 (17), 174 (24), 146 (18), 41 (6). **HRMS:** calcd. for $[C_{16}H_{24}N_2OP+H]^+$: 291.16208; found: 291.16263.

2-(Diphenylphosphino)-1-(2-methoxyphenyl)-*1H*-imidazole [L5]



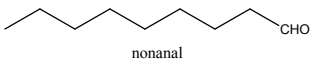
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.41-7.32 (m, 6H), 7.25-7.21 (m, 6H), 7.13-7,11 (m, 1H), 7.08 (dd, *J* = 2.3, 1.2 Hz, 1H), 6.94-6.88 (m, 1H), 6.86 (dd, *J* = 8.3, 1.1 Hz, 1H), 3.39 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 154.4, 136.0, 133.8 (d, *J* = 20.6 Hz), 130.3, 128.7, 128.6 (d, *J* = 2.5 Hz), 128.2 (d, *J* = 7.6 Hz), 124.0, 120.3, 111.6, 55.1. **^{31}P NMR** (121 MHz, $CDCl_3$) δ -29.6. **MS (EI):** 358 (13) $[M]^+$, 341(3), 327 (100), 250 (3), 219 (2), 183 (40), 173 (7), 152 (4). **HRMS:** calcd. for $[C_{22}H_{19}N_2OP+H]^+$: 359.1308; found: 359.131.

2-(Dicyclohexylphosphino)-1-phenyl-*1H*-imidazole [L6]



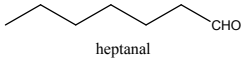
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.43-7.33 (m, 3H), 7.28 (s, 1H), 7.25-7.21 (m, 2H), 7.19-7.10 (m, 1H), 2.06 (t, *J* = 10.9 Hz, 2H), 1.69-1.49 (m, 10H), 1.26-0.90 (m, 10H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 147.3 (d, *J* = 19.4 Hz), 130.3, 128.8, 128.3, 127.3 (d, *J* = 3.9 Hz), 123.2, 34.3 (d, *J* = 8.0 Hz), 30.3 (d, *J* = 16.2 Hz), 29.2 (d, *J* = 7.4 Hz), 27.1, 26.4. **^{31}P NMR** (121 MHz, $CDCl_3$) δ -23.6. **MS (EI):** 340 (4) $[M]^+$, 258 (17), 257 (100), 206 (2), 176 (22), 175 (46), 174 (16), 149 (5), 55 (5). **HRMS:** calcd. for $[C_{21}H_{30}N_2P+H]^+$: 341.21411; found: 341.21459.

6. Characterization of the Selected Aldehydes.



nonanal

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.75 (t, *J* = 1.9 Hz, 1H), 2.44-2.38 (m, 2H), 1.70- 1.53 (m, 2H), 1.43-1.15 (m, 10H), 0.98-0.73 (m, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 203.0, 43.9, 31.8, 29.3, 29.1, 29.1, 22.6, 22.1, 14.1. **MS (EI):** m/z = 142, 124, 114, 98, 82, 70, 57, 41, 29.

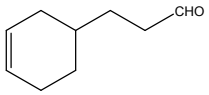


heptanal

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.74 (t, *J* = 1.9 Hz, 1H), 2.43-2.37 (m, 2H), 1.69- 1.51 (m, 2H), 1.29-

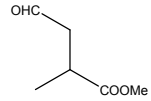
1.27 (m, 6H), 0.98-0.75 (m, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 203.0, 43.9, 31.5, 28.8, 22.4, 22.0, 14.0.

MS (EI): m/z = 114, 99, 86, 81, 70, 57, 44, 29.



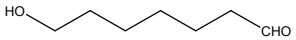
3-(cyclohex-3-en-1-yl)propanal

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.77 (t, *J* = 1.8 Hz, 1H), 5.65-5.62 (m, 2H), 2.49-2.43 (m, 2H), 2.08-1.97 (m, 2H), 1.81-1.46 (m, 6H), 1.31-1.12 (m, 1H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 202.8, 127.0, 126.0, 41.5, 33.0, 31.5, 28.6, 28.5, 25.0. **MS (EI):** m/z = 138 $[M]^+$, 120, 109, 94, 91, 81, 79, 77, 67, 54, 41.



methyl 2-methyl-4-oxobutanoate

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.69 (d, *J* = 1.1 Hz, 1H), 3.62 (s, 3H), 2.99 - 2.77 (m, 2H), 2.48 (dd, *J* = 17.5, 5.0 Hz, 1H), 1.16 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 199.9, 175.4, 51.8, 46.7, 33.3, 16.8. **MS (EI):** m/z = 102, 99, 87, 71, 59, 55, 43, 41, 39, 29. **HRMS:** calcd. for $[C_6H_{10}O_3 + Na^+]$: 153,05222; found: 153,05234.



7-hydroxyheptanal

^{1}H NMR (300 MHz, $CDCl_3$) δ 9.76 (t, *J* = 1.8 Hz, 1H), 3.64 (t, *J* = 6.5 Hz, 2H), 2.46-2.41 (m, 2H), 1.71-1.48 (m, 5H), 1.40 - 1.32 (m, 4H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 202.8, 62.8, 43.8, 32.5, 28.9, 25.5, 22.0. **MS (EI):** m/z = 112, 97, 87, 84, 79, 69, 57, 43, 41, 29.

7. X-ray crystal structure analysis of Os-L3 complex I

Summary of Data CCDC 1029506

Formula: C52 H62 N4 O10 Os3 P2,C2 H3 N1

Unit Cell Parameters: a 12.4416(9) b 15.7773(11) c 28.046(2) P21/c

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Data were collected on a Bruker Kappa APEX II Duo diffractometer. The structure was solved by direct methods and refined by full-matrix least-squares procedures on F^2 with the SHELXTL software package (Sheldrick, G. M. *Acta Crystallogr.* **2008**, *A64*, 112.). XP (Bruker AXS) was used for graphical representation.

Crystal data for Os-L3 complex **I**: $C_{54}H_{65}N_5O_{10}Os_3P_2$, *M* = 1576.65, monoclinic, space group $P2_1/c$, *a* = 12.4416(9), *b* = 15.7773(11), *c* = 28.046(2) Å, *β* = 102.532(2)°, *V* = 5374.1(7) Å^3, *T* = 150(2) K, *Z* = 4, 89727 reflections measured, 12988 independent reflections (R_{int} = 0.0352), final *R* values ($I > 2\sigma(I)$): R_1 = 0.0198, wR_2 = 0.0408, final *R* values (all data): R_1 = 0.0265, wR_2 = 0.0430, GOF on F^2: 1.049, 670

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The symmetry employed for this shelxl refinement is uniquely defined
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symmetry information in preference to the above space-group names.
They are only intended as comments.

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 Reflections were merged by SHELXL according to the crystal
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 _reflns_Friedel_fraction is defined as the number of unique
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'w=1/[\s^2^(Fo^2^)+(0.0163P)^2^+6.4379P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary ?
_atom_sites_solution_secondary ?
_atom_sites_solution_hydrogens geom
_refine_ls_hydrogen_treatment constr
_refine_ls_extinction_method none
_refine_ls_extinction_coef .
_refine_ls_number_reflns 12988
_refine_ls_number_parameters 670
_refine_ls_number_restraints 0
_refine_ls_R_factor_all 0.0265
_refine_ls_R_factor_gt 0.0198
_refine_ls_wR_factor_ref 0.0430
_refine_ls_wR_factor_gt 0.0408
_refine_ls_goodness_of_fit_ref 1.049
_refine_ls_restrained_S_all 1.049
_refine_ls_shift/su_max 0.006
_refine_ls_shift/su_mean 0.000

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_atom_site_site_symmetry_order
_atom_site_calc_flag
_atom_site_refinement_flags_posn
_atom_site_refinement_flags_adp
_atom_site_refinement_flags_occupancy
_atom_site_disorder_assembly
_atom_site_disorder_group
C1 C 0.8060(2) 0.73339(16) 1.06109(10) 0.0148(6) Uani 1 1 d . . . . .
C2 C 0.9828(2) 0.70934(17) 1.07040(10) 0.0165(6) Uani 1 1 d . . . . .
H2 H 1.0554 0.7095 1.0647 0.020 Uiso 1 1 calc R U . . .
C3 C 0.9524(2) 0.67469(17) 1.10963(11) 0.0187(6) Uani 1 1 d . . . . .

H3 H 0.9987 0.6451 1.1357 0.022 Uiso 1 1 calc R U . . .
C4 C 0.7784(2) 0.64383(18) 1.13318(10) 0.0188(6) Uani 1 1 d . . . . .
C5 C 0.7502(3) 0.56034(19) 1.11821(11) 0.0235(7) Uani 1 1 d . . . . .
C6 C 0.6917(3) 0.5115(2) 1.14535(12) 0.0283(7) Uani 1 1 d . . . . .
H6 H 0.6711 0.4550 1.1356 0.034 Uiso 1 1 calc R U . . .
C7 C 0.6638(3) 0.5451(2) 1.18623(13) 0.0321(8) Uani 1 1 d . . . . .
H7 H 0.6239 0.5115 1.2045 0.039 Uiso 1 1 calc R U . . .
C8 C 0.6929(3) 0.6272(2) 1.20120(12) 0.0300(7) Uani 1 1 d . . . . .
H8 H 0.6731 0.6497 1.2295 0.036 Uiso 1 1 calc R U . . .
C9 C 0.7509(3) 0.67623(19) 1.17464(11) 0.0226(7) Uani 1 1 d . . . . .
H9 H 0.7719 0.7323 1.1849 0.027 Uiso 1 1 calc R U . . .
C10 C 0.7434(3) 0.4547(2) 1.05632(13) 0.0338(8) Uani 1 1 d . . . . .
H10A H 0.7743 0.4090 1.0788 0.051 Uiso 1 1 calc R U . . .
H10B H 0.7662 0.4471 1.0253 0.051 Uiso 1 1 calc R U . . .
H10C H 0.6629 0.4533 1.0505 0.051 Uiso 1 1 calc R U . . .
C11 C 0.5680(2) 0.74138(18) 1.06170(11) 0.0179(6) Uani 1 1 d . . . . .
H11 H 0.5989 0.7357 1.0976 0.021 Uiso 1 1 calc R U . . .
C12 C 0.4655(2) 0.79904(19) 1.05494(11) 0.0214(6) Uani 1 1 d . . . . .
H12A H 0.4872 0.8548 1.0703 0.026 Uiso 1 1 calc R U . . .
H12B H 0.4359 0.8085 1.0196 0.026 Uiso 1 1 calc R U . . .
C13 C 0.3763(3) 0.7604(2) 1.07757(12) 0.0272(7) Uani 1 1 d . . . . .
H13A H 0.4033 0.7565 1.1134 0.033 Uiso 1 1 calc R U . . .
H13B H 0.3108 0.7977 1.0711 0.033 Uiso 1 1 calc R U . . .
C14 C 0.3437(3) 0.6729(2) 1.05714(13) 0.0296(7) Uani 1 1 d . . . . .
H14A H 0.3102 0.6772 1.0218 0.036 Uiso 1 1 calc R U . . .
H14B H 0.2883 0.6483 1.0737 0.036 Uiso 1 1 calc R U . . .
C15 C 0.4448(3) 0.6148(2) 1.06471(12) 0.0276(7) Uani 1 1 d . . . . .
H15A H 0.4744 0.6065 1.1001 0.033 Uiso 1 1 calc R U . . .
H15B H 0.4228 0.5586 1.0500 0.033 Uiso 1 1 calc R U . . .
C16 C 0.5341(2) 0.65256(18) 1.04149(11) 0.0209(6) Uani 1 1 d . . . . .
H16A H 0.5065 0.6560 1.0057 0.025 Uiso 1 1 calc R U . . .
H16B H 0.5993 0.6149 1.0480 0.025 Uiso 1 1 calc R U . . .
C17 C 0.7097(2) 0.89336(17) 1.06554(10) 0.0164(6) Uani 1 1 d . . . . .
H17 H 0.7861 0.9073 1.0623 0.020 Uiso 1 1 calc R U . . .
C18 C 0.6377(3) 0.96711(18) 1.04110(11) 0.0229(7) Uani 1 1 d . . . . .
H18A H 0.6422 0.9710 1.0064 0.028 Uiso 1 1 calc R U . . .
H18B H 0.5600 0.9565 1.0424 0.028 Uiso 1 1 calc R U . . .
C19 C 0.6762(3) 1.05064(19) 1.06702(12) 0.0288(7) Uani 1 1 d . . . . .
H19A H 0.7515 1.0637 1.0629 0.035 Uiso 1 1 calc R U . . .
H19B H 0.6269 1.0970 1.0518 0.035 Uiso 1 1 calc R U . . .
C20 C 0.6762(3) 1.0463(2) 1.12125(12) 0.0286(7) Uani 1 1 d . . . . .
H20A H 0.6002 1.0372 1.1255 0.034 Uiso 1 1 calc R U . . .
H20B H 0.7031 1.1008 1.1370 0.034 Uiso 1 1 calc R U . . .
C21 C 0.7498(3) 0.9743(2) 1.14560(11) 0.0248(7) Uani 1 1 d . . . . .

H21A H 0.7459 0.9708 1.1804 0.030 Uiso 1 1 calc R U . . .
H21B H 0.8271 0.9865 1.1441 0.030 Uiso 1 1 calc R U . . .
C22 C 0.7151(3) 0.88932(19) 1.12072(11) 0.0206(6) Uani 1 1 d . . . . .
H22A H 0.6419 0.8732 1.1263 0.025 Uiso 1 1 calc R U . . .
H22B H 0.7684 0.8451 1.1355 0.025 Uiso 1 1 calc R U . . .
C23 C 0.8294(2) 0.64719(17) 0.89843(10) 0.0150(6) Uani 1 1 d . . . . .
C24 C 0.9704(2) 0.60706(18) 0.95737(11) 0.0199(6) Uani 1 1 d . . . . .
H24 H 1.0268 0.6086 0.9862 0.024 Uiso 1 1 calc R U . . .
C25 C 0.9482(3) 0.54143(19) 0.92647(11) 0.0233(7) Uani 1 1 d . . . . .
H25 H 0.9853 0.4884 0.9292 0.028 Uiso 1 1 calc R U . . .
C26 C 0.8100(2) 0.51086(18) 0.85066(11) 0.0200(6) Uani 1 1 d . . . . .
C27 C 0.8647(3) 0.49231(18) 0.81331(11) 0.0213(6) Uani 1 1 d . . . . .
C28 C 0.8169(3) 0.43572(19) 0.77692(12) 0.0252(7) Uani 1 1 d . . . . .
H28 H 0.8526 0.4230 0.7511 0.030 Uiso 1 1 calc R U . . .
C29 C 0.7168(3) 0.3976(2) 0.77823(13) 0.0305(8) Uani 1 1 d . . . . .
H29 H 0.6852 0.3585 0.7534 0.037 Uiso 1 1 calc R U . . .
C30 C 0.6630(3) 0.4157(2) 0.81500(13) 0.0331(8) Uani 1 1 d . . . . .
H30 H 0.5945 0.3896 0.8156 0.040 Uiso 1 1 calc R U . . .
C31 C 0.7103(3) 0.47288(19) 0.85132(12) 0.0253(7) Uani 1 1 d . . . . .
H31 H 0.6736 0.4859 0.8768 0.030 Uiso 1 1 calc R U . . .
C32 C 1.0212(3) 0.5124(2) 0.77885(13) 0.0319(8) Uani 1 1 d . . . . .
H32A H 1.0390 0.4518 0.7799 0.048 Uiso 1 1 calc R U . . .
H32B H 1.0894 0.5455 0.7840 0.048 Uiso 1 1 calc R U . . .
H32C H 0.9749 0.5265 0.7469 0.048 Uiso 1 1 calc R U . . .
C33 C 0.9718(2) 0.77916(18) 0.85150(10) 0.0181(6) Uani 1 1 d . . . . .
H33 H 0.9504 0.7182 0.8462 0.022 Uiso 1 1 calc R U . . .
C34 C 0.9620(2) 0.81389(19) 0.79945(11) 0.0202(6) Uani 1 1 d . . . . .
H34A H 0.8834 0.8167 0.7827 0.024 Uiso 1 1 calc R U . . .
H34B H 0.9925 0.8720 0.8011 0.024 Uiso 1 1 calc R U . . .
C35 C 1.0241(3) 0.7572(2) 0.77012(12) 0.0264(7) Uani 1 1 d . . . . .
H35A H 0.9888 0.7007 0.7655 0.032 Uiso 1 1 calc R U . . .
H35B H 1.0203 0.7824 0.7375 0.032 Uiso 1 1 calc R U . . .
C36 C 1.1435(3) 0.7475(2) 0.79624(12) 0.0283(7) Uani 1 1 d . . . . .
H36A H 1.1815 0.8026 0.7961 0.034 Uiso 1 1 calc R U . . .
H36B H 1.1798 0.7061 0.7784 0.034 Uiso 1 1 calc R U . . .
C37 C 1.1548(3) 0.7178(2) 0.84863(12) 0.0245(7) Uani 1 1 d . . . . .
H37A H 1.2337 0.7168 0.8650 0.029 Uiso 1 1 calc R U . . .
H37B H 1.1260 0.6593 0.8486 0.029 Uiso 1 1 calc R U . . .
C38 C 1.0922(2) 0.7756(2) 0.87751(12) 0.0246(7) Uani 1 1 d . . . . .
H38A H 1.0988 0.7531 0.9110 0.030 Uiso 1 1 calc R U . . .
H38B H 1.1242 0.8333 0.8800 0.030 Uiso 1 1 calc R U . . .
C39 C 0.8530(2) 0.94049(17) 0.87074(10) 0.0160(6) Uani 1 1 d . . . . .
H39 H 0.8067 0.9626 0.8930 0.019 Uiso 1 1 calc R U . . .
C40 C 0.7972(2) 0.97250(18) 0.81987(11) 0.0204(6) Uani 1 1 d . . . . .

H40A H 0.7247 0.9445 0.8091 0.025 Uiso 1 1 calc R U . . .
H40B H 0.8430 0.9579 0.7963 0.025 Uiso 1 1 calc R U . . .
C41 C 0.7813(3) 1.06878(19) 0.82069(12) 0.0270(7) Uani 1 1 d . . . . .
H41A H 0.7469 1.0886 0.7874 0.032 Uiso 1 1 calc R U . . .
H41B H 0.7308 1.0827 0.8424 0.032 Uiso 1 1 calc R U . . .
C42 C 0.8903(3) 1.1148(2) 0.83852(13) 0.0293(7) Uani 1 1 d . . . . .
H42A H 0.8763 1.1763 0.8410 0.035 Uiso 1 1 calc R U . . .
H42B H 0.9374 1.1070 0.8146 0.035 Uiso 1 1 calc R U . . .
C43 C 0.9502(3) 1.08131(19) 0.88824(12) 0.0249(7) Uani 1 1 d . . . . .
H43A H 0.9076 1.0961 0.9131 0.030 Uiso 1 1 calc R U . . .
H43B H 1.0233 1.1087 0.8977 0.030 Uiso 1 1 calc R U . . .
C44 C 0.9650(2) 0.98503(18) 0.88728(11) 0.0196(6) Uani 1 1 d . . . . .
H44A H 1.0012 0.9649 0.9203 0.024 Uiso 1 1 calc R U . . .
H44B H 1.0131 0.9704 0.8646 0.024 Uiso 1 1 calc R U . . .
C45 C 0.8750(2) 0.91122(18) 0.98439(10) 0.0165(6) Uani 1 1 d . . . . .
C46 C 1.0464(2) 0.81004(18) 0.98423(10) 0.0178(6) Uani 1 1 d . . . . .
C47 C 0.6395(2) 0.89288(18) 0.92837(11) 0.0179(6) Uani 1 1 d . . . . .
C48 C 0.5000(2) 0.75529(19) 0.93058(11) 0.0212(6) Uani 1 1 d . . . . .
C49 C 0.6871(2) 0.65752(18) 0.96105(10) 0.0178(6) Uani 1 1 d . . . . .
C50 C 0.7428(2) 0.69524(18) 0.79721(11) 0.0181(6) Uani 1 1 d . . . . .
C51 C 0.6025(2) 0.81676(18) 0.82919(11) 0.0194(6) Uani 1 1 d . . . . .
C52 C 0.5872(3) 0.65124(19) 0.85272(11) 0.0222(6) Uani 1 1 d . . . . .
C53 C 0.4920(3) 0.8441(3) 0.21894(15) 0.0447(10) Uani 1 1 d . . . . .
C54 C 0.5175(3) 0.9316(3) 0.21469(18) 0.0518(11) Uani 1 1 d . . . . .
H54A H 0.4921 0.9641 0.2399 0.078 Uiso 1 1 calc R U . . .
H54B H 0.4805 0.9525 0.1824 0.078 Uiso 1 1 calc R U . . .
H54C H 0.5973 0.9384 0.2189 0.078 Uiso 1 1 calc R U . . .
N1 N 0.89115(19) 0.74450(14) 1.03994(8) 0.0137(5) Uani 1 1 d . . . . .
N2 N 0.84150(19) 0.69038(15) 1.10453(9) 0.0170(5) Uani 1 1 d . . . . .
N3 N 0.89768(19) 0.67221(14) 0.94035(8) 0.0153(5) Uani 1 1 d . . . . .
N4 N 0.8609(2) 0.56618(15) 0.88990(9) 0.0189(5) Uani 1 1 d . . . . .
N5 N 0.4732(4) 0.7753(3) 0.22260(18) 0.0835(16) Uani 1 1 d . . . . .
O1 O 0.78255(18) 0.53454(13) 1.07721(8) 0.0252(5) Uani 1 1 d . . . . .
O2 O 0.96357(18) 0.53185(14) 0.81623(8) 0.0277(5) Uani 1 1 d . . . . .
O3 O 0.86648(17) 0.98233(13) 0.99308(8) 0.0236(5) Uani 1 1 d . . . . .
O4 O 1.13912(17) 0.82119(15) 0.99774(8) 0.0295(5) Uani 1 1 d . . . . .
O5 O 0.62631(17) 0.96122(13) 0.91378(8) 0.0246(5) Uani 1 1 d . . . . .
O6 O 0.40712(18) 0.73983(16) 0.91975(10) 0.0360(6) Uani 1 1 d . . . . .
O7 O 0.70242(18) 0.58616(13) 0.96759(8) 0.0252(5) Uani 1 1 d . . . . .
O8 O 0.75814(19) 0.67191(14) 0.76027(8) 0.0271(5) Uani 1 1 d . . . . .
O9 O 0.53922(18) 0.86695(14) 0.81294(8) 0.0300(5) Uani 1 1 d . . . . .
O10 O 0.5126(2) 0.60761(16) 0.84933(10) 0.0386(6) Uani 1 1 d . . . . .
Os1 Os 0.89194(2) 0.79793(2) 0.96802(2) 0.01238(3) Uani 1 1 d . . . . .
Os2 Os 0.65314(2) 0.77604(2) 0.94941(2) 0.01367(3) Uani 1 1 d . . . . .

Os3 Os 0.70742(2) 0.72983(2) 0.85653(2) 0.01404(3) Uani 1 1 d . . . . .
P1 P 0.67627(6) 0.78925(4) 1.03374(3) 0.01421(14) Uani 1 1 d . . . . .
P2 P 0.86459(6) 0.82441(4) 0.88309(3) 0.01340(14) Uani 1 1 d . . . . .

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C1 0.0176(14) 0.0120(13) 0.0137(14) -0.0009(10) 0.0009(11) -0.0005(10)
C2 0.0171(14) 0.0156(13) 0.0155(14) -0.0002(11) 0.0005(11) 0.0014(11)
C3 0.0211(15) 0.0169(14) 0.0159(15) 0.0031(11) -0.0009(12) 0.0020(11)
C4 0.0216(15) 0.0216(15) 0.0123(14) 0.0077(11) 0.0017(11) -0.0007(11)
C5 0.0232(16) 0.0235(16) 0.0211(16) 0.0043(12) -0.0009(13) 0.0008(12)
C6 0.0266(17) 0.0281(17) 0.0275(19) 0.0074(14) 0.0002(14) -0.0085(13)
C7 0.0289(18) 0.041(2) 0.0274(19) 0.0121(15) 0.0075(15) -0.0063(15)
C8 0.0325(18) 0.041(2) 0.0174(16) 0.0033(14) 0.0072(14) 0.0008(15)
C9 0.0308(17) 0.0205(15) 0.0160(15) 0.0020(12) 0.0037(13) 0.0015(12)
C10 0.047(2) 0.0191(16) 0.0310(19) -0.0022(14) 0.0000(16) -0.0039(14)
C11 0.0158(14) 0.0233(15) 0.0150(14) 0.0000(11) 0.0042(11) -0.0024(11)
C12 0.0190(15) 0.0240(15) 0.0216(16) -0.0011(12) 0.0054(12) -0.0008(12)
C13 0.0192(15) 0.0382(19) 0.0259(18) 0.0011(14) 0.0088(13) 0.0022(13)
C14 0.0204(16) 0.0373(19) 0.0320(19) 0.0058(15) 0.0075(14) -0.0058(14)
C15 0.0269(17) 0.0302(17) 0.0264(18) 0.0045(14) 0.0072(14) -0.0082(13)
C16 0.0202(15) 0.0221(15) 0.0202(16) 0.0007(12) 0.0037(12) -0.0020(12)
C17 0.0176(14) 0.0160(14) 0.0155(14) -0.0025(11) 0.0033(11) -0.0007(11)
C18 0.0312(17) 0.0185(15) 0.0183(16) -0.0033(12) 0.0037(13) 0.0018(12)
C19 0.044(2) 0.0173(15) 0.0274(18) -0.0022(13) 0.0117(15) 0.0019(13)
C20 0.0351(19) 0.0237(16) 0.0287(19) -0.0100(14) 0.0103(15) -0.0032(14)
C21 0.0231(16) 0.0337(18) 0.0179(16) -0.0080(13) 0.0051(13) -0.0060(13)
C22 0.0242(16) 0.0221(15) 0.0151(15) -0.0028(12) 0.0034(12) -0.0026(12)
C23 0.0199(14) 0.0151(13) 0.0113(13) 0.0010(10) 0.0060(11) -0.0024(11)
C24 0.0214(15) 0.0193(14) 0.0180(15) 0.0010(12) 0.0021(12) 0.0061(11)
C25 0.0305(17) 0.0166(14) 0.0219(16) 0.0010(12) 0.0037(13) 0.0080(12)
C26 0.0296(16) 0.0143(14) 0.0157(15) -0.0016(11) 0.0044(13) -0.0005(11)
C27 0.0275(16) 0.0172(14) 0.0191(16) -0.0014(11) 0.0045(13) -0.0006(12)
C28 0.0335(18) 0.0231(16) 0.0199(16) -0.0057(12) 0.0077(14) 0.0022(13)
C29 0.0378(19) 0.0254(17) 0.0280(19) -0.0105(14) 0.0066(15) -0.0057(14)
C30 0.0352(19) 0.0294(18) 0.037(2) -0.0079(15) 0.0119(16) -0.0109(15)
C31 0.0341(18) 0.0222(16) 0.0229(17) -0.0036(13) 0.0137(14) -0.0016(13)
C32 0.0326(19) 0.038(2) 0.0279(19) -0.0085(15) 0.0130(15) -0.0019(15)

C33 0.0192(14) 0.0210(15) 0.0137(14) 0.0016(11) 0.0027(11) 0.0001(11)
C34 0.0227(15) 0.0235(15) 0.0149(15) 0.0029(12) 0.0055(12) 0.0001(12)
C35 0.0328(18) 0.0301(17) 0.0177(16) 0.0017(13) 0.0088(14) 0.0037(14)
C36 0.0296(18) 0.0290(17) 0.0304(19) 0.0032(14) 0.0157(15) 0.0042(14)
C37 0.0198(15) 0.0268(16) 0.0267(17) 0.0017(13) 0.0049(13) 0.0034(12)
C38 0.0215(16) 0.0297(17) 0.0215(16) 0.0019(13) 0.0022(13) 0.0002(12)
C39 0.0200(14) 0.0139(13) 0.0135(14) 0.0004(11) 0.0020(11) -0.0007(11)
C40 0.0229(15) 0.0179(14) 0.0175(15) 0.0010(11) -0.0022(12) -0.0019(11)
C41 0.0327(18) 0.0210(16) 0.0238(17) 0.0056(13) -0.0013(14) 0.0030(13)
C42 0.0381(19) 0.0160(15) 0.0331(19) 0.0027(13) 0.0060(15) -0.0040(13)
C43 0.0297(17) 0.0197(15) 0.0238(17) -0.0009(12) 0.0025(14) -0.0072(12)
C44 0.0217(15) 0.0190(14) 0.0168(15) 0.0020(11) 0.0011(12) -0.0035(11)
C45 0.0153(14) 0.0205(15) 0.0132(14) 0.0018(11) 0.0021(11) -0.0020(11)
C46 0.0215(15) 0.0181(14) 0.0141(14) 0.0012(11) 0.0042(12) -0.0001(11)
C47 0.0137(14) 0.0230(15) 0.0174(15) -0.0036(12) 0.0041(11) -0.0005(11)
C48 0.0234(16) 0.0200(15) 0.0193(16) -0.0008(12) 0.0029(12) 0.0010(12)
C49 0.0210(15) 0.0217(15) 0.0114(14) -0.0018(11) 0.0050(11) -0.0044(11)
C50 0.0226(15) 0.0164(14) 0.0143(15) 0.0019(11) 0.0017(12) -0.0044(11)
C51 0.0214(15) 0.0208(15) 0.0149(15) -0.0029(11) 0.0017(12) -0.0048(12)
C52 0.0275(16) 0.0222(15) 0.0166(15) -0.0035(12) 0.0040(13) -0.0035(13)
C53 0.043(2) 0.039(2) 0.043(2) 0.0055(18) -0.0092(18) 0.0030(18)
C54 0.046(2) 0.038(2) 0.076(3) 0.007(2) 0.023(2) 0.0016(18)
N1 0.0174(12) 0.0122(11) 0.0111(11) 0.0003(9) 0.0022(9) 0.0004(9)
N2 0.0206(12) 0.0168(12) 0.0135(12) 0.0022(9) 0.0031(10) 0.0000(9)
N3 0.0198(12) 0.0149(11) 0.0117(12) -0.0005(9) 0.0045(9) -0.0003(9)
N4 0.0277(14) 0.0137(12) 0.0157(13) -0.0026(9) 0.0059(10) 0.0002(10)
N5 0.088(3) 0.043(2) 0.091(4) 0.011(2) -0.041(3) -0.011(2)
O1 0.0349(13) 0.0199(11) 0.0217(12) -0.0030(9) 0.0082(10) -0.0031(9)
O2 0.0276(12) 0.0319(12) 0.0263(13) -0.0102(10) 0.0114(10) -0.0062(10)
O3 0.0314(12) 0.0171(11) 0.0230(12) -0.0033(9) 0.0075(10) -0.0010(9)
O4 0.0187(11) 0.0347(13) 0.0318(13) -0.0009(10) -0.0013(10) -0.0024(9)
O5 0.0275(12) 0.0196(11) 0.0267(12) 0.0035(9) 0.0060(10) 0.0034(9)
O6 0.0193(12) 0.0402(14) 0.0446(16) -0.0040(12) -0.0020(11) -0.0042(10)
O7 0.0353(13) 0.0176(11) 0.0257(12) 0.0013(9) 0.0134(10) -0.0003(9)
O8 0.0361(13) 0.0293(12) 0.0172(12) -0.0033(9) 0.0085(10) -0.0016(10)
O9 0.0275(12) 0.0299(12) 0.0288(13) 0.0040(10) -0.0023(10) 0.0077(10)
O10 0.0344(14) 0.0366(14) 0.0457(16) -0.0085(12) 0.0102(12) -0.0178(11)
Os1 0.01440(5) 0.01222(5) 0.01015(5) -0.00001(4) 0.00188(4) -0.00097(4)
Os2 0.01471(5) 0.01447(5) 0.01137(5) -0.00032(4) 0.00179(4) -0.00018(4)
Os3 0.01706(6) 0.01363(5) 0.01075(5) -0.00084(4) 0.00153(4) -0.00242(4)
P1 0.0147(3) 0.0156(3) 0.0124(3) -0.0002(3) 0.0029(3) -0.0002(3)
P2 0.0155(3) 0.0130(3) 0.0112(3) 0.0003(3) 0.0018(3) -0.0015(3)

_geom_special_details

All esds (except the esd in the dihedral angle between two l.s. planes)
are estimated using the full covariance matrix. The cell esds are taken
into account individually in the estimation of esds in distances, angles
and torsion angles; correlations between esds in cell parameters are only
used when they are defined by crystal symmetry. An approximate (isotropic)
treatment of cell esds is used for estimating esds involving l.s. planes.

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C1 N2 1.381(3) . ?
C1 P1 1.853(3) . ?
C2 C3 1.354(4) . ?
C2 N1 1.384(3) . ?
C2 H2 0.9500 . ?
C3 N2 1.378(4) . ?
C3 H3 0.9500 . ?
C4 C9 1.379(4) . ?
C4 C5 1.404(4) . ?
C4 N2 1.441(4) . ?
C5 O1 1.361(4) . ?
C5 C6 1.395(4) . ?
C6 C7 1.374(5) . ?
C6 H6 0.9500 . ?
C7 C8 1.386(5) . ?
C7 H7 0.9500 . ?
C8 C9 1.380(4) . ?
C8 H8 0.9500 . ?
C9 H9 0.9500 . ?
C10 O1 1.429(4) . ?
C10 H10A 0.9800 . ?
C10 H10B 0.9800 . ?
C10 H10C 0.9800 . ?
C11 C16 1.536(4) . ?
C11 C12 1.544(4) . ?
C11 P1 1.860(3) . ?
C11 H11 1.0000 . ?
C12 C13 1.521(4) . ?
C12 H12A 0.9900 . ?

C12 H12B 0.9900 . ?
C13 C14 1.516(5) . ?
C13 H13A 0.9900 . ?
C13 H13B 0.9900 . ?
C14 C15 1.533(5) . ?
C14 H14A 0.9900 . ?
C14 H14B 0.9900 . ?
C15 C16 1.525(4) . ?
C15 H15A 0.9900 . ?
C15 H15B 0.9900 . ?
C16 H16A 0.9900 . ?
C16 H16B 0.9900 . ?
C17 C22 1.535(4) . ?
C17 C18 1.536(4) . ?
C17 P1 1.872(3) . ?
C17 H17 1.0000 . ?
C18 C19 1.531(4) . ?
C18 H18A 0.9900 . ?
C18 H18B 0.9900 . ?
C19 C20 1.522(5) . ?
C19 H19A 0.9900 . ?
C19 H19B 0.9900 . ?
C20 C21 1.524(5) . ?
C20 H20A 0.9900 . ?
C20 H20B 0.9900 . ?
C21 C22 1.530(4) . ?
C21 H21A 0.9900 . ?
C21 H21B 0.9900 . ?
C22 H22A 0.9900 . ?
C22 H22B 0.9900 . ?
C23 N3 1.351(3) . ?
C23 N4 1.373(4) . ?
C23 Os3 2.147(3) . ?
C24 C25 1.340(4) . ?
C24 N3 1.384(3) . ?
C24 H24 0.9500 . ?
C25 N4 1.379(4) . ?
C25 H25 0.9500 . ?
C26 C31 1.381(4) . ?
C26 C27 1.399(4) . ?
C26 N4 1.439(4) . ?
C27 O2 1.366(4) . ?
C27 C28 1.389(4) . ?
C28 C29 1.390(5) . ?

C28 H28 0.9500 . ?
C29 C30 1.376(5) . ?
C29 H29 0.9500 . ?
C30 C31 1.392(4) . ?
C30 H30 0.9500 . ?
C31 H31 0.9500 . ?
C32 O2 1.426(4) . ?
C32 H32A 0.9800 . ?
C32 H32B 0.9800 . ?
C32 H32C 0.9800 . ?
C33 C38 1.518(4) . ?
C33 C34 1.539(4) . ?
C33 P2 1.894(3) . ?
C33 H33 1.0000 . ?
C34 C35 1.533(4) . ?
C34 H34A 0.9900 . ?
C34 H34B 0.9900 . ?
C35 C36 1.514(5) . ?
C35 H35A 0.9900 . ?
C35 H35B 0.9900 . ?
C36 C37 1.519(5) . ?
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C36 H36B 0.9900 . ?
C37 C38 1.539(4) . ?
C37 H37A 0.9900 . ?
C37 H37B 0.9900 . ?
C38 H38A 0.9900 . ?
C38 H38B 0.9900 . ?
C39 C40 1.531(4) . ?
C39 C44 1.539(4) . ?
C39 P2 1.864(3) . ?
C39 H39 1.0000 . ?
C40 C41 1.533(4) . ?
C40 H40A 0.9900 . ?
C40 H40B 0.9900 . ?
C41 C42 1.524(4) . ?
C41 H41A 0.9900 . ?
C41 H41B 0.9900 . ?
C42 C43 1.526(4) . ?
C42 H42A 0.9900 . ?
C42 H42B 0.9900 . ?
C43 C44 1.531(4) . ?
C43 H43A 0.9900 . ?
C43 H43B 0.9900 . ?

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C44 H44B 0.9900 . ?
C45 O3 1.158(3) . ?
C45 Os1 1.869(3) . ?
C46 O4 1.147(3) . ?
C46 Os1 1.886(3) . ?
C47 O5 1.152(3) . ?
C47 Os2 1.932(3) . ?
C48 O6 1.156(4) . ?
C48 Os2 1.892(3) . ?
C49 O7 1.150(3) . ?
C49 Os2 1.929(3) . ?
C50 O8 1.154(4) . ?
C50 Os3 1.891(3) . ?
C51 O9 1.140(4) . ?
C51 Os3 1.933(3) . ?
C52 O10 1.143(4) . ?
C52 Os3 1.927(3) . ?
C53 N5 1.121(5) . ?
C53 C54 1.428(6) . ?
C54 H54A 0.9800 . ?
C54 H54B 0.9800 . ?
C54 H54C 0.9800 . ?
N1 Os1 2.188(2) . ?
N3 Os1 2.137(2) . ?
Os1 P2 2.3690(7) . ?
Os1 Os2 2.9232(3) . ?
Os2 P1 2.3289(8) . ?
Os2 Os3 2.9218(2) . ?
Os3 P2 2.4440(7) . ?

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N2 C1 P1 133.0(2) . . ?
C3 C2 N1 109.0(3) . . ?
C3 C2 H2 125.5 . . ?

N1 C2 H2 125.5 . . ?
C2 C3 N2 107.1(2) . . ?
C2 C3 H3 126.5 . . ?
N2 C3 H3 126.5 . . ?
C9 C4 C5 120.6(3) . . ?
C9 C4 N2 123.1(3) . . ?
C5 C4 N2 116.3(3) . . ?
O1 C5 C6 125.5(3) . . ?
O1 C5 C4 115.7(3) . . ?
C6 C5 C4 118.8(3) . . ?
C7 C6 C5 119.9(3) . . ?
C7 C6 H6 120.1 . . ?
C5 C6 H6 120.1 . . ?
C6 C7 C8 121.2(3) . . ?
C6 C7 H7 119.4 . . ?
C8 C7 H7 119.4 . . ?
C9 C8 C7 119.5(3) . . ?
C9 C8 H8 120.2 . . ?
C7 C8 H8 120.2 . . ?
C4 C9 C8 120.1(3) . . ?
C4 C9 H9 120.0 . . ?
C8 C9 H9 120.0 . . ?
O1 C10 H10A 109.5 . . ?
O1 C10 H10B 109.5 . . ?
H10A C10 H10B 109.5 . . ?
O1 C10 H10C 109.5 . . ?
H10A C10 H10C 109.5 . . ?
H10B C10 H10C 109.5 . . ?
C16 C11 C12 109.8(2) . . ?
C16 C11 P1 112.4(2) . . ?
C12 C11 P1 111.3(2) . . ?
C16 C11 H11 107.7 . . ?
C12 C11 H11 107.7 . . ?
P1 C11 H11 107.7 . . ?
C13 C12 C11 111.7(3) . . ?
C13 C12 H12A 109.3 . . ?
C11 C12 H12A 109.3 . . ?
C13 C12 H12B 109.3 . . ?
C11 C12 H12B 109.3 . . ?
H12A C12 H12B 107.9 . . ?
C14 C13 C12 111.5(3) . . ?
C14 C13 H13A 109.3 . . ?
C12 C13 H13A 109.3 . . ?
C14 C13 H13B 109.3 . . ?

C12 C13 H13B 109.3 . . ?
H13A C13 H13B 108.0 . . ?
C13 C14 C15 110.4(3) . . ?
C13 C14 H14A 109.6 . . ?
C15 C14 H14A 109.6 . . ?
C13 C14 H14B 109.6 . . ?
C15 C14 H14B 109.6 . . ?
H14A C14 H14B 108.1 . . ?
C16 C15 C14 111.0(3) . . ?
C16 C15 H15A 109.4 . . ?
C14 C15 H15A 109.4 . . ?
C16 C15 H15B 109.4 . . ?
C14 C15 H15B 109.4 . . ?
H15A C15 H15B 108.0 . . ?
C15 C16 C11 111.5(3) . . ?
C15 C16 H16A 109.3 . . ?
C11 C16 H16A 109.3 . . ?
C15 C16 H16B 109.3 . . ?
C11 C16 H16B 109.3 . . ?
H16A C16 H16B 108.0 . . ?
C22 C17 C18 112.0(2) . . ?
C22 C17 P1 113.6(2) . . ?
C18 C17 P1 113.86(19) . . ?
C22 C17 H17 105.5 . . ?
C18 C17 H17 105.5 . . ?
P1 C17 H17 105.5 . . ?
C19 C18 C17 110.4(2) . . ?
C19 C18 H18A 109.6 . . ?
C17 C18 H18A 109.6 . . ?
C19 C18 H18B 109.6 . . ?
C17 C18 H18B 109.6 . . ?
H18A C18 H18B 108.1 . . ?
C20 C19 C18 111.6(3) . . ?
C20 C19 H19A 109.3 . . ?
C18 C19 H19A 109.3 . . ?
C20 C19 H19B 109.3 . . ?
C18 C19 H19B 109.3 . . ?
H19A C19 H19B 108.0 . . ?
C19 C20 C21 110.5(3) . . ?
C19 C20 H20A 109.5 . . ?
C21 C20 H20A 109.5 . . ?
C19 C20 H20B 109.5 . . ?
C21 C20 H20B 109.5 . . ?
H20A C20 H20B 108.1 . . ?

C20 C21 C22 111.5(3) . . ?
C20 C21 H21A 109.3 . . ?
C22 C21 H21A 109.3 . . ?
C20 C21 H21B 109.3 . . ?
C22 C21 H21B 109.3 . . ?
H21A C21 H21B 108.0 . . ?
C21 C22 C17 111.7(2) . . ?
C21 C22 H22A 109.3 . . ?
C17 C22 H22A 109.3 . . ?
C21 C22 H22B 109.3 . . ?
C17 C22 H22B 109.3 . . ?
H22A C22 H22B 107.9 . . ?
N3 C23 N4 105.9(2) . . ?
N3 C23 Os3 122.35(19) . . ?
N4 C23 Os3 131.6(2) . . ?
C25 C24 N3 108.9(3) . . ?
C25 C24 H24 125.6 . . ?
N3 C24 H24 125.6 . . ?
C24 C25 N4 106.3(3) . . ?
C24 C25 H25 126.9 . . ?
N4 C25 H25 126.9 . . ?
C31 C26 C27 120.3(3) . . ?
C31 C26 N4 120.0(3) . . ?
C27 C26 N4 119.7(3) . . ?
O2 C27 C28 125.0(3) . . ?
O2 C27 C26 116.0(3) . . ?
C28 C27 C26 119.0(3) . . ?
C27 C28 C29 120.1(3) . . ?
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C29 C28 H28 119.9 . . ?
C30 C29 C28 120.9(3) . . ?
C30 C29 H29 119.5 . . ?
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C29 C30 C31 119.1(3) . . ?
C29 C30 H30 120.5 . . ?
C31 C30 H30 120.5 . . ?
C26 C31 C30 120.6(3) . . ?
C26 C31 H31 119.7 . . ?
C30 C31 H31 119.7 . . ?
O2 C32 H32A 109.5 . . ?
O2 C32 H32B 109.5 . . ?
H32A C32 H32B 109.5 . . ?
O2 C32 H32C 109.5 . . ?
H32A C32 H32C 109.5 . . ?

H32B C32 H32C 109.5 . . ?
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C38 C33 P2 120.7(2) . . ?
C34 C33 P2 112.97(19) . . ?
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C34 C33 H33 103.8 . . ?
P2 C33 H33 103.8 . . ?
C35 C34 C33 110.8(2) . . ?
C35 C34 H34A 109.5 . . ?
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C35 C34 H34B 109.5 . . ?
C33 C34 H34B 109.5 . . ?
H34A C34 H34B 108.1 . . ?
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C36 C35 H35B 109.5 . . ?
C34 C35 H35B 109.5 . . ?
H35A C35 H35B 108.1 . . ?
C35 C36 C37 112.0(3) . . ?
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C37 C36 H36A 109.2 . . ?
C35 C36 H36B 109.2 . . ?
C37 C36 H36B 109.2 . . ?
H36A C36 H36B 107.9 . . ?
C36 C37 C38 112.1(3) . . ?
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C38 C37 H37A 109.2 . . ?
C36 C37 H37B 109.2 . . ?
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H37A C37 H37B 107.9 . . ?
C33 C38 C37 109.1(3) . . ?
C33 C38 H38A 109.9 . . ?
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H38A C38 H38B 108.3 . . ?
C40 C39 C44 109.2(2) . . ?
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C44 C39 P2 111.36(19) . . ?
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P2 C39 H39 105.0 . . ?
C39 C40 C41 110.3(2) . . ?

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C39 C40 H40B 109.6 . . ?
C41 C40 H40B 109.6 . . ?
H40A C40 H40B 108.1 . . ?
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C43 C42 H42B 109.4 . . ?
H42A C42 H42B 108.0 . . ?
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C44 C43 H43A 109.3 . . ?
C42 C43 H43B 109.3 . . ?
C44 C43 H43B 109.3 . . ?
H43A C43 H43B 108.0 . . ?
C43 C44 C39 110.7(2) . . ?
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C39 C44 H44A 109.5 . . ?
C43 C44 H44B 109.5 . . ?
C39 C44 H44B 109.5 . . ?
H44A C44 H44B 108.1 . . ?
O3 C45 Os1 177.3(3) . . ?
O4 C46 Os1 173.9(3) . . ?
O5 C47 Os2 176.1(3) . . ?
O6 C48 Os2 177.6(3) . . ?
O7 C49 Os2 177.0(3) . . ?
O8 C50 Os3 175.8(3) . . ?
O9 C51 Os3 178.8(3) . . ?
O10 C52 Os3 176.7(3) . . ?
N5 C53 C54 179.2(5) . . ?
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C53 C54 H54B 109.5 . . ?
H54A C54 H54B 109.5 . . ?
C53 C54 H54C 109.5 . . ?
H54A C54 H54C 109.5 . . ?
H54B C54 H54C 109.5 . . ?

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C1 N1 Os1 128.58(18) . . ?
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C46 Os1 P2 98.11(9) . . ?
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N1 Os1 P2 165.11(6) . . ?
C45 Os1 Os2 89.57(9) . . ?
C46 Os1 Os2 176.31(9) . . ?
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C1 P1 Os2 106.40(9) . . ?
C11 P1 Os2 116.78(9) . . ?
C17 P1 Os2 121.88(9) . . ?
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C39 P2 Os1 110.40(9) . . ?
C33 P2 Os1 116.22(9) . . ?
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Os1 P2 Os3 97.45(3) . . ?

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  _geom_torsion_site_symmetry_4
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C9 C4 C5 O1 -179.2(3) . . . . ?
N2 C4 C5 O1 -2.4(4) . . . . ?
C9 C4 C5 C6 1.5(4) . . . . ?
N2 C4 C5 C6 178.3(3) . . . . ?

O1 C5 C6 C7 -180.0(3) . . . . ?
C4 C5 C6 C7 -0.7(5) . . . . ?
C5 C6 C7 C8 0.0(5) . . . . ?
C6 C7 C8 C9 0.0(5) . . . . ?
C5 C4 C9 C8 -1.6(5) . . . . ?
N2 C4 C9 C8 -178.1(3) . . . . ?
C7 C8 C9 C4 0.8(5) . . . . ?
C16 C11 C12 C13 54.8(3) . . . . ?
P1 C11 C12 C13 179.9(2) . . . . ?
C11 C12 C13 C14 -56.2(3) . . . . ?
C12 C13 C14 C15 56.5(4) . . . . ?
C13 C14 C15 C16 -56.8(4) . . . . ?
C14 C15 C16 C11 56.9(3) . . . . ?
C12 C11 C16 C15 -55.2(3) . . . . ?
P1 C11 C16 C15 -179.7(2) . . . . ?
C22 C17 C18 C19 53.7(3) . . . . ?
P1 C17 C18 C19 -175.7(2) . . . . ?
C17 C18 C19 C20 -56.4(4) . . . . ?
C18 C19 C20 C21 57.9(4) . . . . ?
C19 C20 C21 C22 -56.3(4) . . . . ?
C20 C21 C22 C17 54.0(3) . . . . ?
C18 C17 C22 C21 -52.9(3) . . . . ?
P1 C17 C22 C21 176.3(2) . . . . ?
N3 C24 C25 N4 0.0(4) . . . . ?
C31 C26 C27 O2 -178.9(3) . . . . ?
N4 C26 C27 O2 -2.3(4) . . . . ?
C31 C26 C27 C28 0.4(5) . . . . ?
N4 C26 C27 C28 177.0(3) . . . . ?
O2 C27 C28 C29 178.5(3) . . . . ?
C26 C27 C28 C29 -0.8(5) . . . . ?
C27 C28 C29 C30 0.7(5) . . . . ?
C28 C29 C30 C31 -0.2(5) . . . . ?
C27 C26 C31 C30 0.1(5) . . . . ?
N4 C26 C31 C30 -176.5(3) . . . . ?
C29 C30 C31 C26 -0.2(5) . . . . ?
C38 C33 C34 C35 59.8(3) . . . . ?
P2 C33 C34 C35 -162.5(2) . . . . ?
C33 C34 C35 C36 -55.9(3) . . . . ?
C34 C35 C36 C37 53.1(4) . . . . ?
C35 C36 C37 C38 -54.4(4) . . . . ?
C34 C33 C38 C37 -59.4(3) . . . . ?
P2 C33 C38 C37 166.7(2) . . . . ?
C36 C37 C38 C33 57.2(3) . . . . ?
C44 C39 C40 C41 -58.7(3) . . . . ?

P2 C39 C40 C41 171.1(2) . . . . ?
C39 C40 C41 C42 57.5(4) . . . . ?
C40 C41 C42 C43 -54.7(4) . . . . ?
C41 C42 C43 C44 54.3(4) . . . . ?
C42 C43 C44 C39 -56.8(4) . . . . ?
C40 C39 C44 C43 58.7(3) . . . . ?
P2 C39 C44 C43 -166.7(2) . . . . ?
N2 C1 N1 C2 -0.8(3) . . . . ?
P1 C1 N1 C2 170.30(19) . . . . ?
N2 C1 N1 Os1 174.44(17) . . . . ?
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C3 C2 N1 C1 1.6(3) . . . . ?
C3 C2 N1 Os1 -173.92(18) . . . . ?
C2 C3 N2 C1 1.2(3) . . . . ?
C2 C3 N2 C4 164.0(2) . . . . ?
N1 C1 N2 C3 -0.2(3) . . . . ?
P1 C1 N2 C3 -169.5(2) . . . . ?
N1 C1 N2 C4 -160.9(3) . . . . ?
P1 C1 N2 C4 29.8(4) . . . . ?
C9 C4 N2 C3 100.3(3) . . . . ?
C5 C4 N2 C3 -76.4(3) . . . . ?
C9 C4 N2 C1 -101.2(4) . . . . ?
C5 C4 N2 C1 82.2(4) . . . . ?
N4 C23 N3 C24 0.0(3) . . . . ?
Os3 C23 N3 C24 -176.8(2) . . . . ?
N4 C23 N3 Os1 175.65(17) . . . . ?
Os3 C23 N3 Os1 -1.2(3) . . . . ?
C25 C24 N3 C23 0.0(3) . . . . ?
C25 C24 N3 Os1 -175.2(2) . . . . ?
N3 C23 N4 C25 0.0(3) . . . . ?
Os3 C23 N4 C25 176.4(2) . . . . ?
N3 C23 N4 C26 177.1(3) . . . . ?
Os3 C23 N4 C26 -6.5(4) . . . . ?
C24 C25 N4 C23 0.0(4) . . . . ?
C24 C25 N4 C26 -177.3(3) . . . . ?
C31 C26 N4 C23 -74.0(4) . . . . ?
C27 C26 N4 C23 109.4(3) . . . . ?
C31 C26 N4 C25 102.8(4) . . . . ?
C27 C26 N4 C25 -73.8(4) . . . . ?
C6 C5 O1 C10 7.8(4) . . . . ?
C4 C5 O1 C10 -171.5(3) . . . . ?
C28 C27 O2 C32 -0.4(4) . . . . ?
C26 C27 O2 C32 178.9(3) . . . . ?
N1 C1 P1 C11 167.0(2) . . . . ?

N2 C1 P1 C11 -24.5(3) . . . . ?
N1 C1 P1 C17 -84.7(2) . . . . ?
N2 C1 P1 C17 83.8(3) . . . . ?
N1 C1 P1 Os2 41.9(2) . . . . ?
N2 C1 P1 Os2 -149.6(2) . . . . ?
C16 C11 P1 C1 -74.2(2) . . . . ?
C12 C11 P1 C1 162.2(2) . . . . ?
C16 C11 P1 C17 -177.2(2) . . . . ?
C12 C11 P1 C17 59.1(2) . . . . ?
C16 C11 P1 Os2 44.2(2) . . . . ?
C12 C11 P1 Os2 -79.4(2) . . . . ?
C22 C17 P1 C1 -68.3(2) . . . . ?
C18 C17 P1 C1 161.8(2) . . . . ?
C22 C17 P1 C11 40.9(2) . . . . ?
C18 C17 P1 C11 -89.0(2) . . . . ?
C22 C17 P1 Os2 176.77(16) . . . . ?
C18 C17 P1 Os2 46.9(2) . . . . ?
C40 C39 P2 C33 72.6(3) . . . . ?
C44 C39 P2 C33 -56.6(2) . . . . ?
C40 C39 P2 Os1 -159.0(2) . . . . ?
C44 C39 P2 Os1 71.8(2) . . . . ?
C40 C39 P2 Os3 -46.2(3) . . . . ?
C44 C39 P2 Os3 -175.39(16) . . . . ?
C38 C33 P2 C39 89.4(2) . . . . ?
C34 C33 P2 C39 -43.2(2) . . . . ?
C38 C33 P2 Os1 -35.6(3) . . . . ?
C34 C33 P2 Os1 -168.22(17) . . . . ?
C38 C33 P2 Os3 -140.8(2) . . . . ?
C34 C33 P2 Os3 86.6(2) . . . . ?

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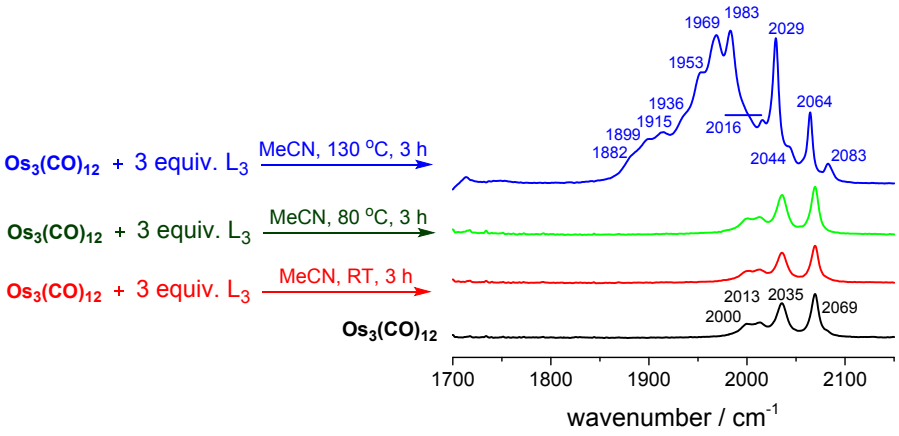


Figure S1. IR analysis of the reaction of $Os_3(CO)_{12}$ with L_3.

The IR study of the Os-L3 complex was also implemented as shown in the above figure. When we prepared the Os complex with 1:1 ratio of Os and L_3 at room temperature and 80 °C in MeCN for 3 h, there is no shift for the peak of carbonyl group in $Os_3(CO)_{12}$. When the reaction temperature is increased to 130 °C, an obvious red shift for the signal of carbonyl group was observed. These results indicate that the coordination of ligand can only happen at higher temperature, which again shows the stability of $Os_3(CO)_{12}$ in the presence of this ligand.

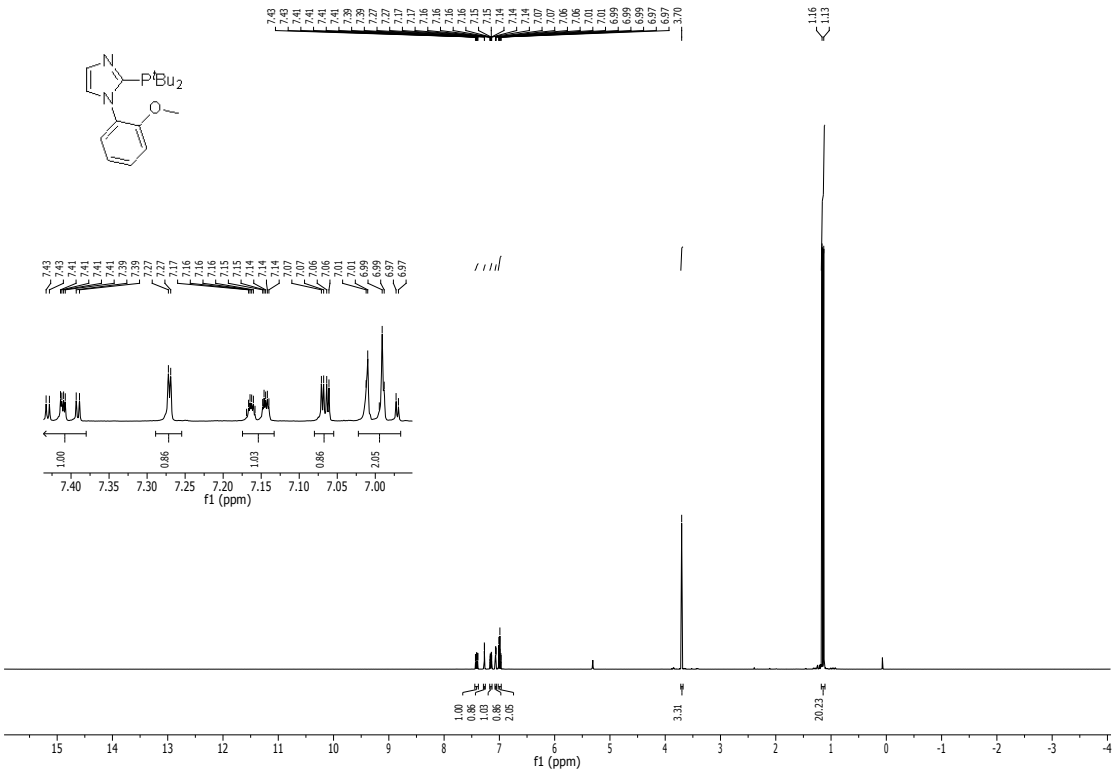
8. References

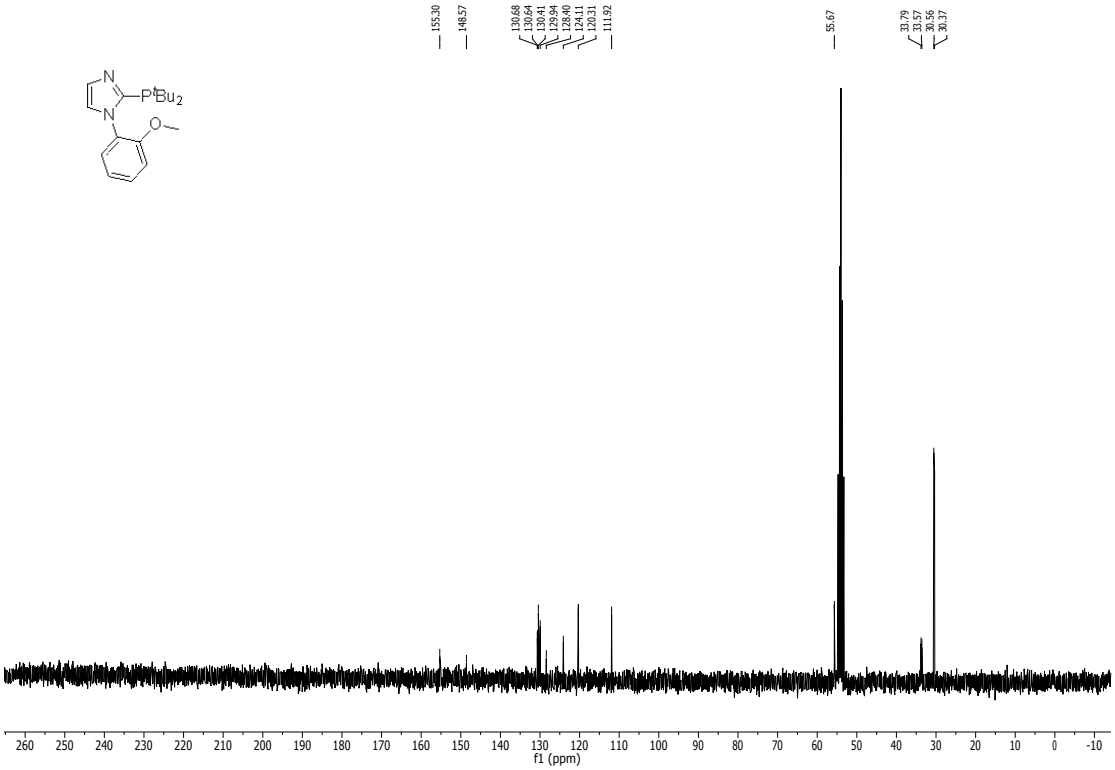
1. *Purification of Laboratory Chemicals* (Eds: D. D. Perrin, W. L. F.-. Armarego,). Pergamon Press, Oxford, 1988 (3).

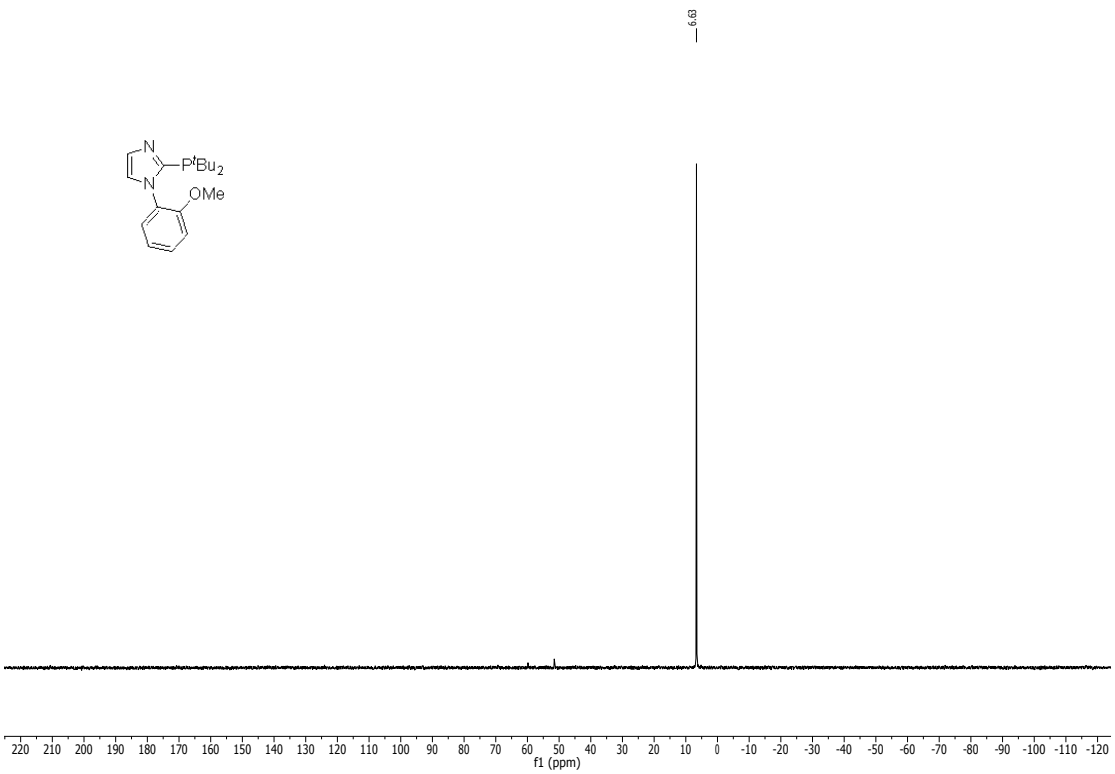
2. a) H. Zhang, Q. Cai, D. Ma, *J. Org. Chem.* **2005,** *70* (13), 5164-5173. b) T. Schulz, C. Torborg, B. Schäffner, J. Huang, A. Zapf, R. Kadyrov, A. Börner, M. Beller, *Angew. Chem. Int. Ed.* **2009,** *48*, 918-921.

9. NMR Spectra

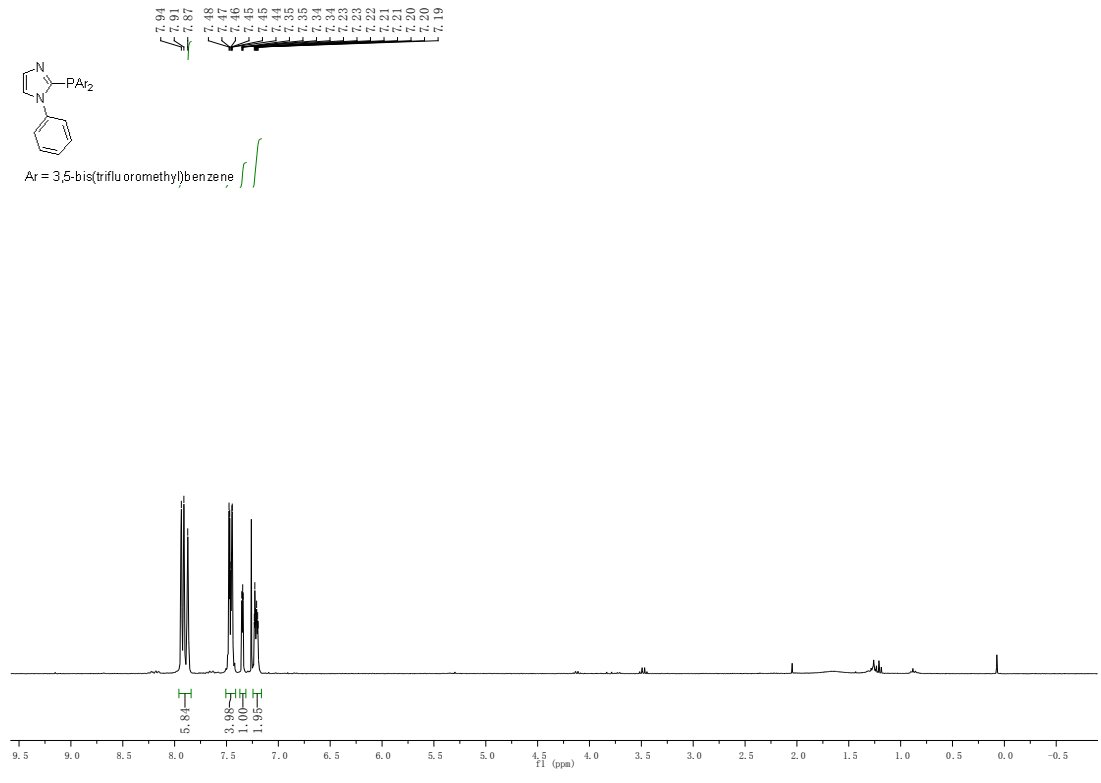
[L1]

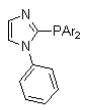




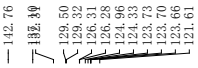

6.83
N
N
P^{t}Bu$_2$
OMe
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120
f1 (ppm)

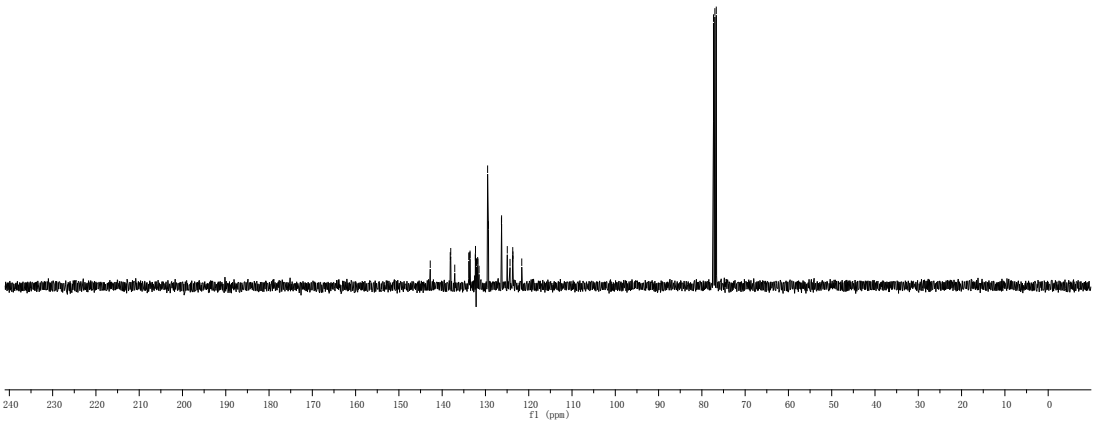
[**L2**]

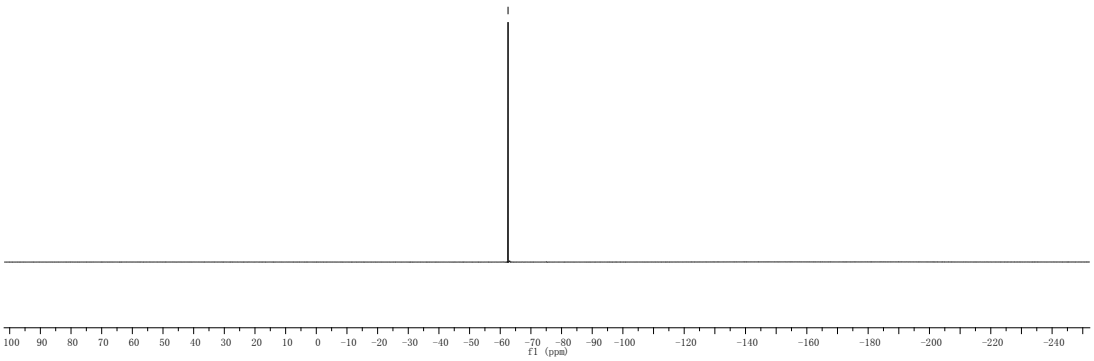

7.94
7.91
7.87
7.48
7.47
7.46
7.45
7.45
7.44
7.35
7.35
7.34
7.34
7.23
7.23
7.22
7.21
7.21
7.20
7.20
7.19
N
N
PAr$_2$
Ar = 3,5-bis(trifluoromethyl)benzene
5.84
3.98
1.00
1.95
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

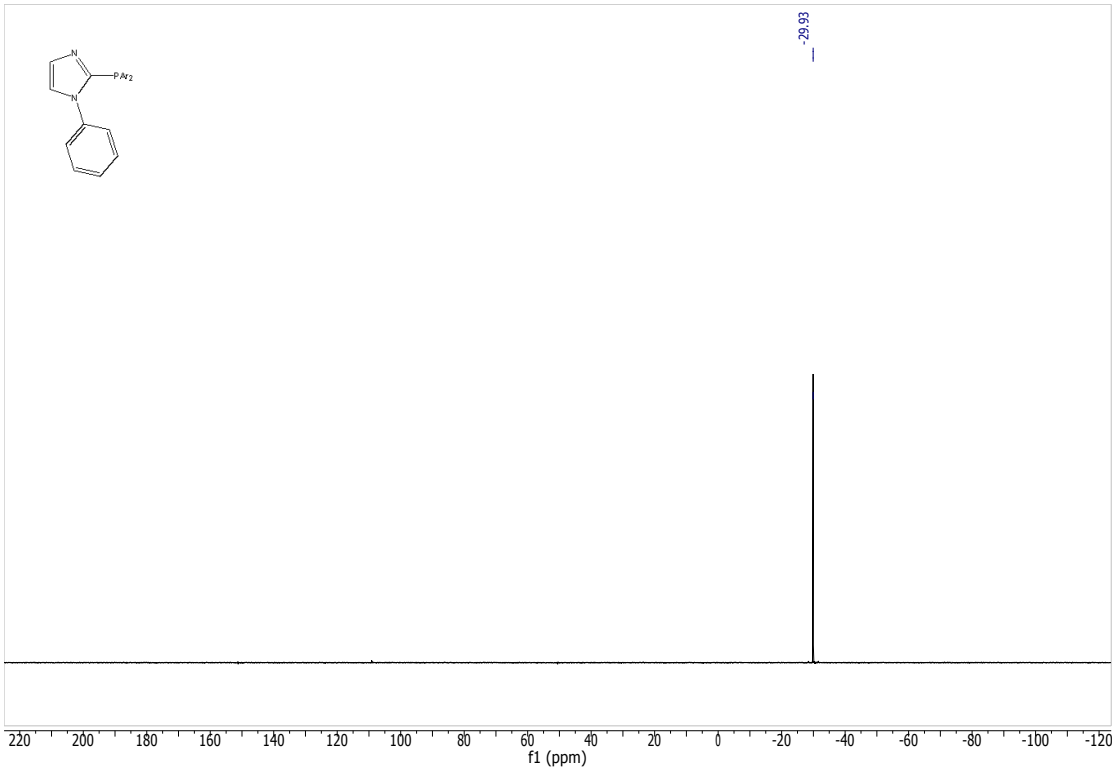


Ar = 3,5-bis(trifluoromethyl)benzene

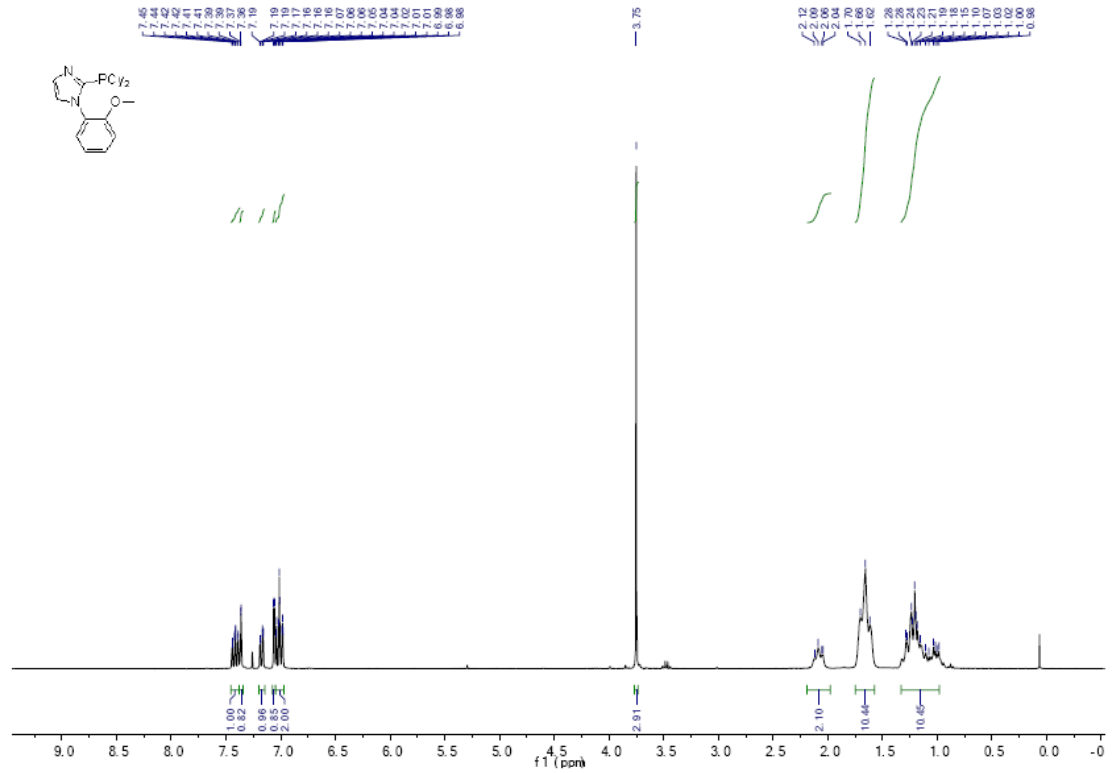


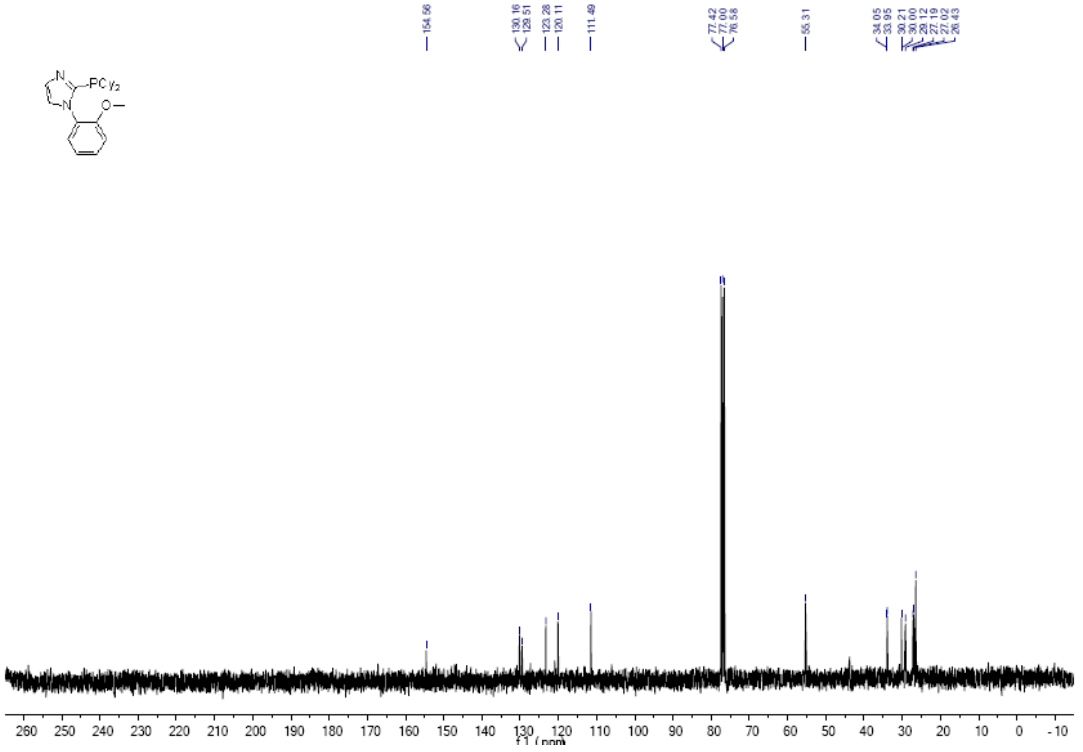


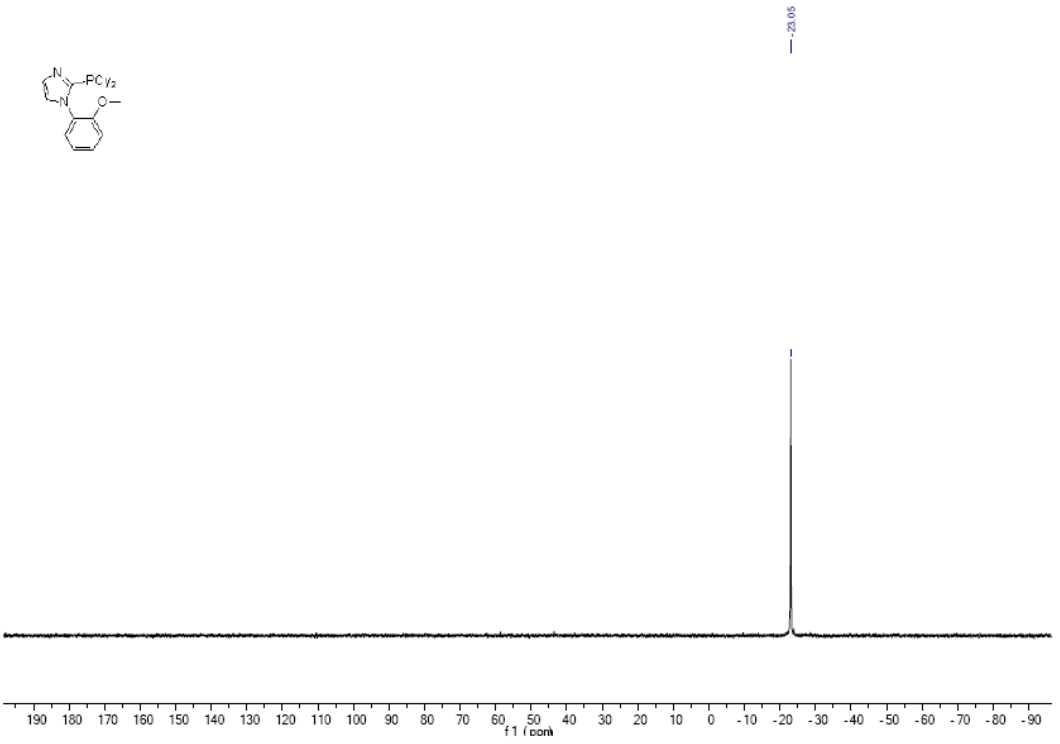



-29.93
PAr2
220 200 180 160 140 120 100 80 60 40 20 0 -20 -40 -60 -80 -100 -120
f1 (ppm)

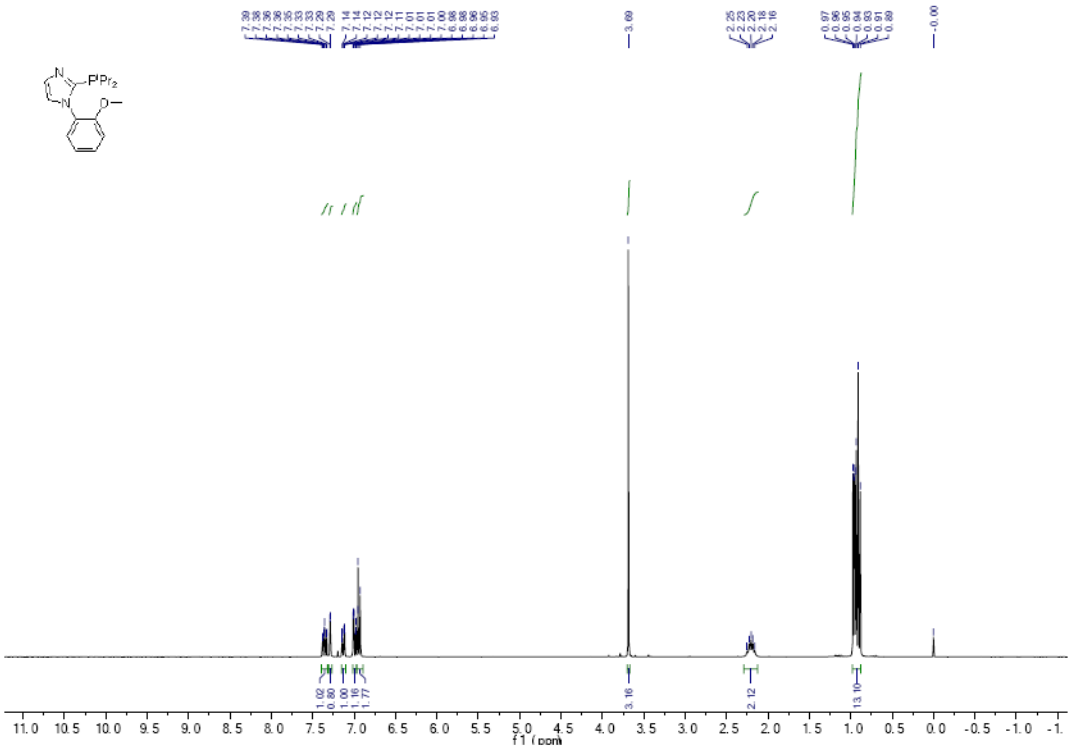
[L3]

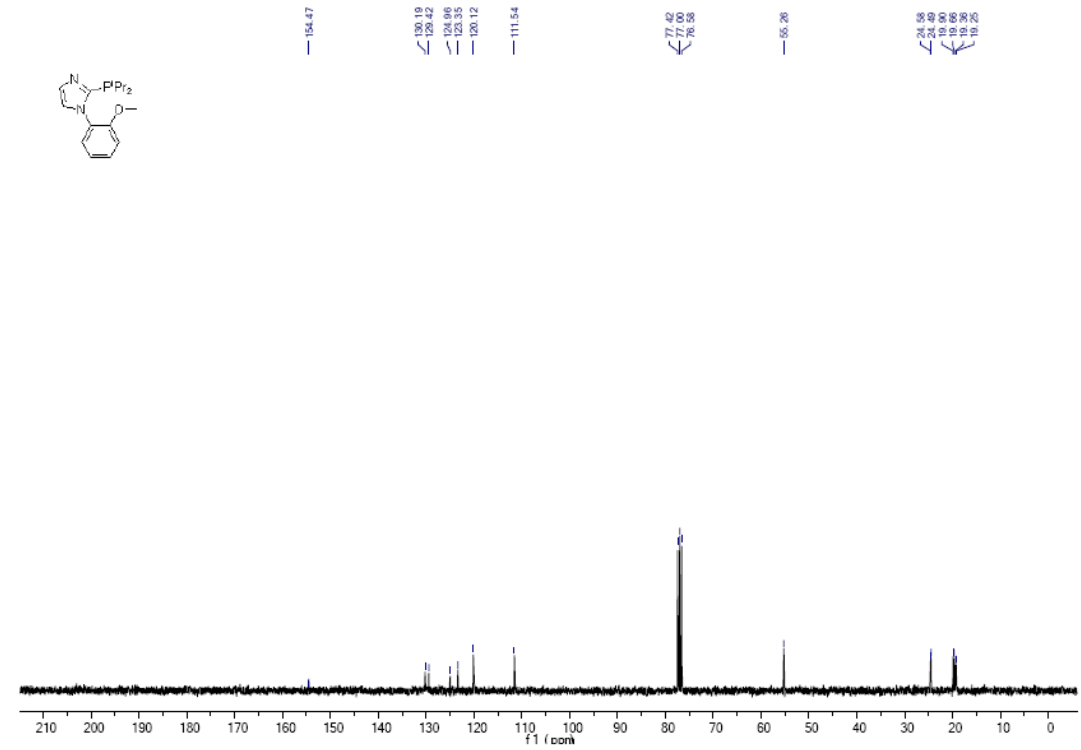

PCy2
O
3.75
2.91
2.10
10.44
10.45
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)

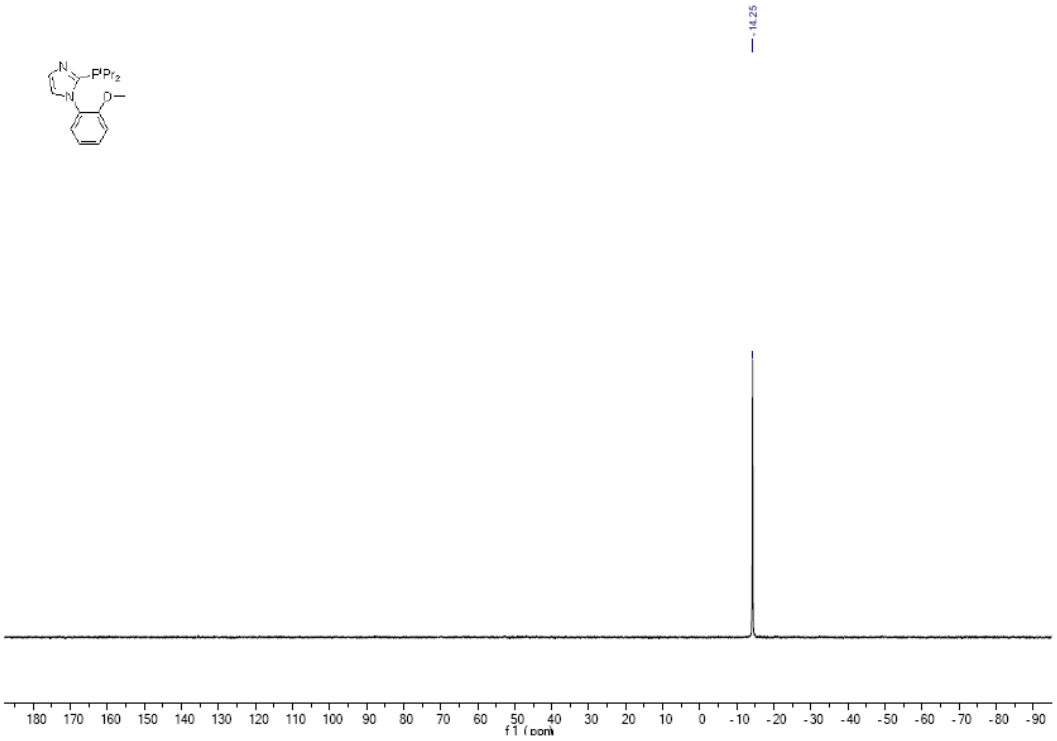

154.66
130.16
129.51
123.28
120.11
111.49
77.42
77.00
76.58
55.31
34.05
33.95
30.21
29.60
29.12
27.19
27.02
26.43
PCy2
O
260 250 240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


23.05
PCy2
O
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90
f1 (ppm)

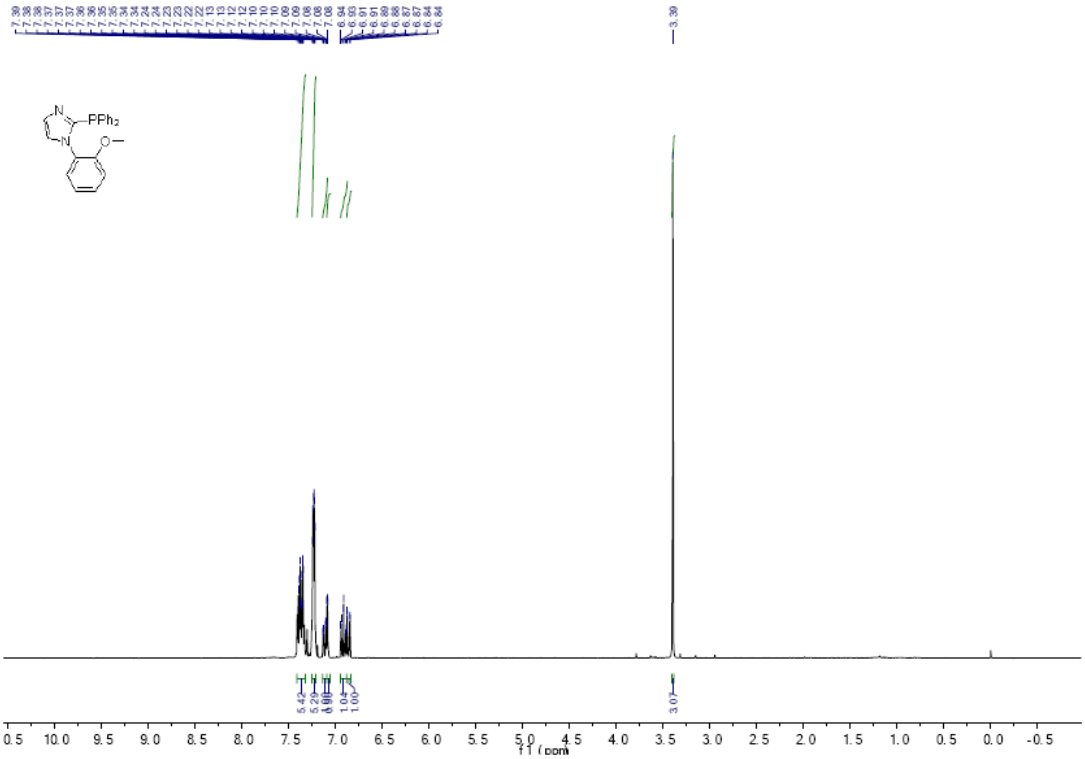
[L4]

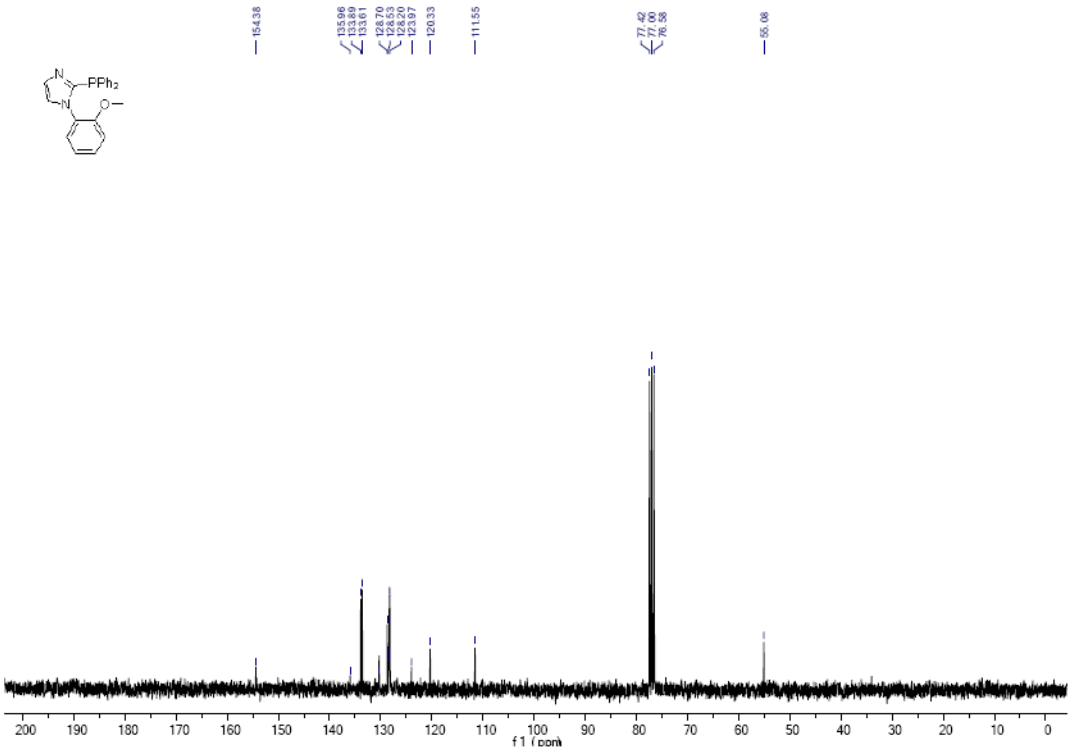


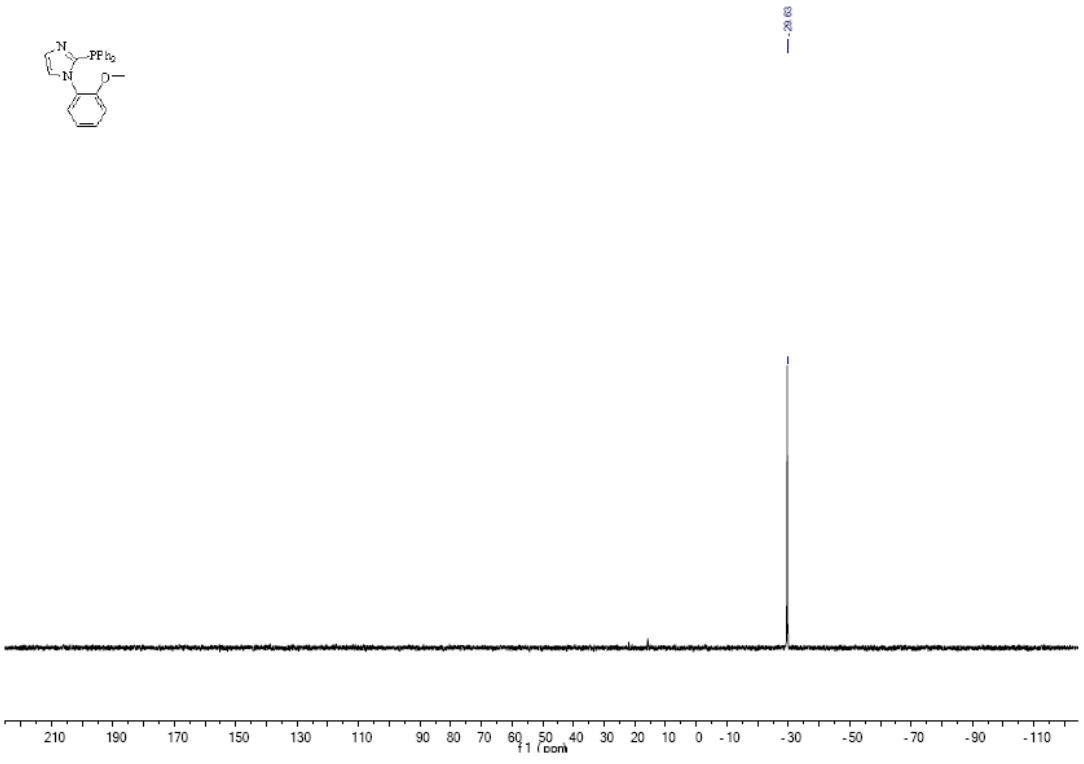



PPr2
O
14.25
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90
f1 (ppm)

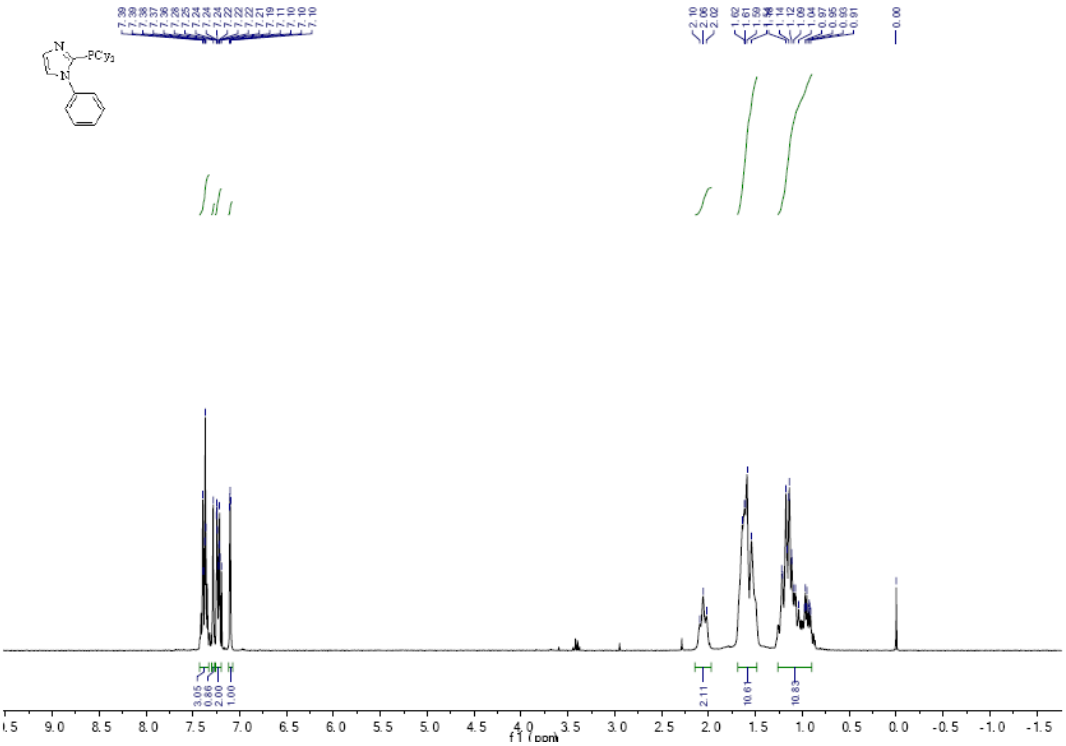
[L5]

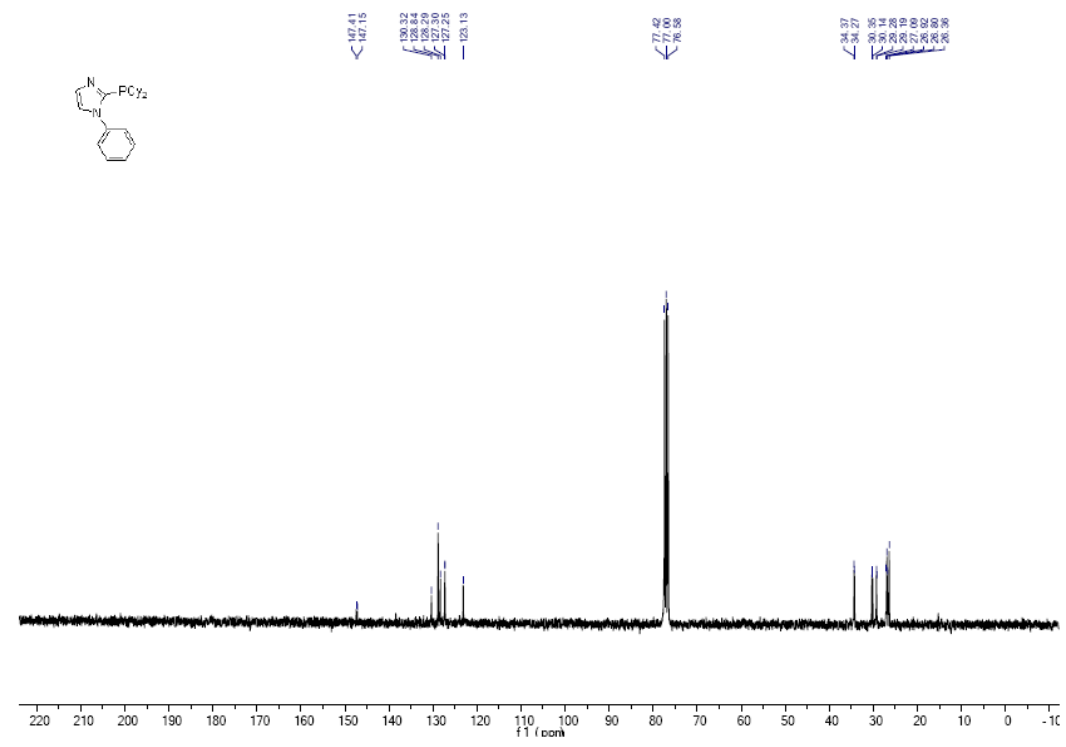

PPh2
O
3.39
5.42
5.29
1.04
1.00
3.07
0.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

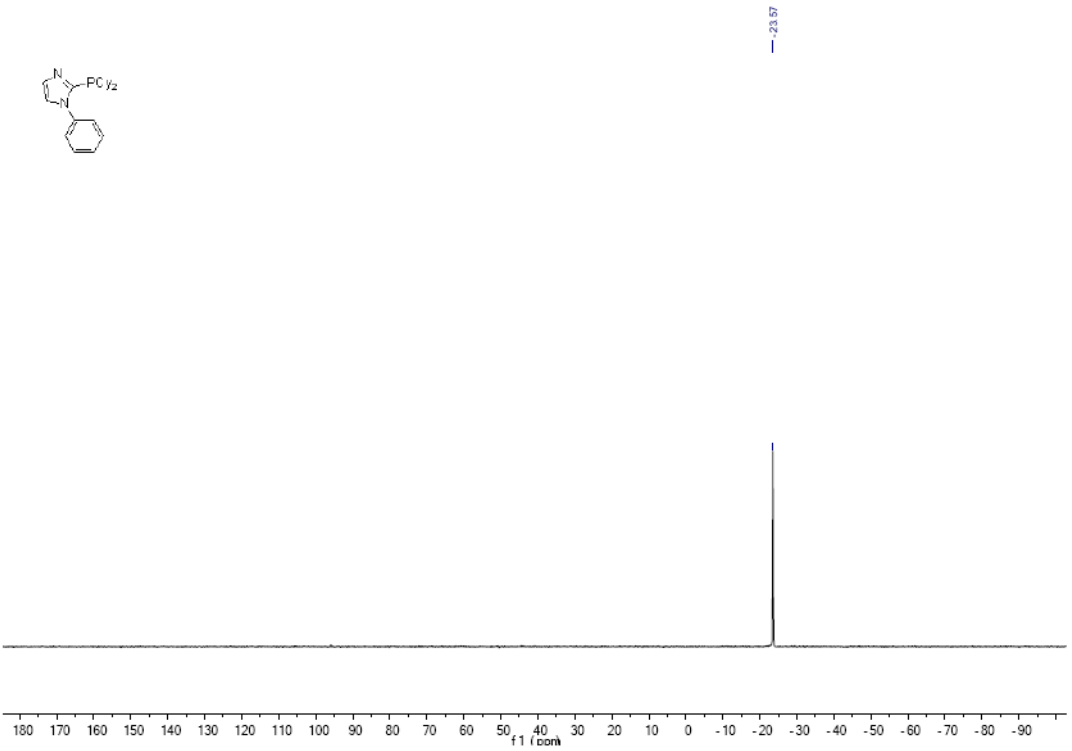

154.38
135.96
133.89
133.61
128.70
128.53
128.20
123.97
120.33
111.55
77.42
77.00
76.58
55.08
PPh2
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


29.63
PPh2
O
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -10 -30 -50 -70 -90 -110
f1 (ppm)

2-(Dicyclohexylphosphino)-1-phenyl-*1H*-imidazole [L6]






PCy2
N
N
23.57
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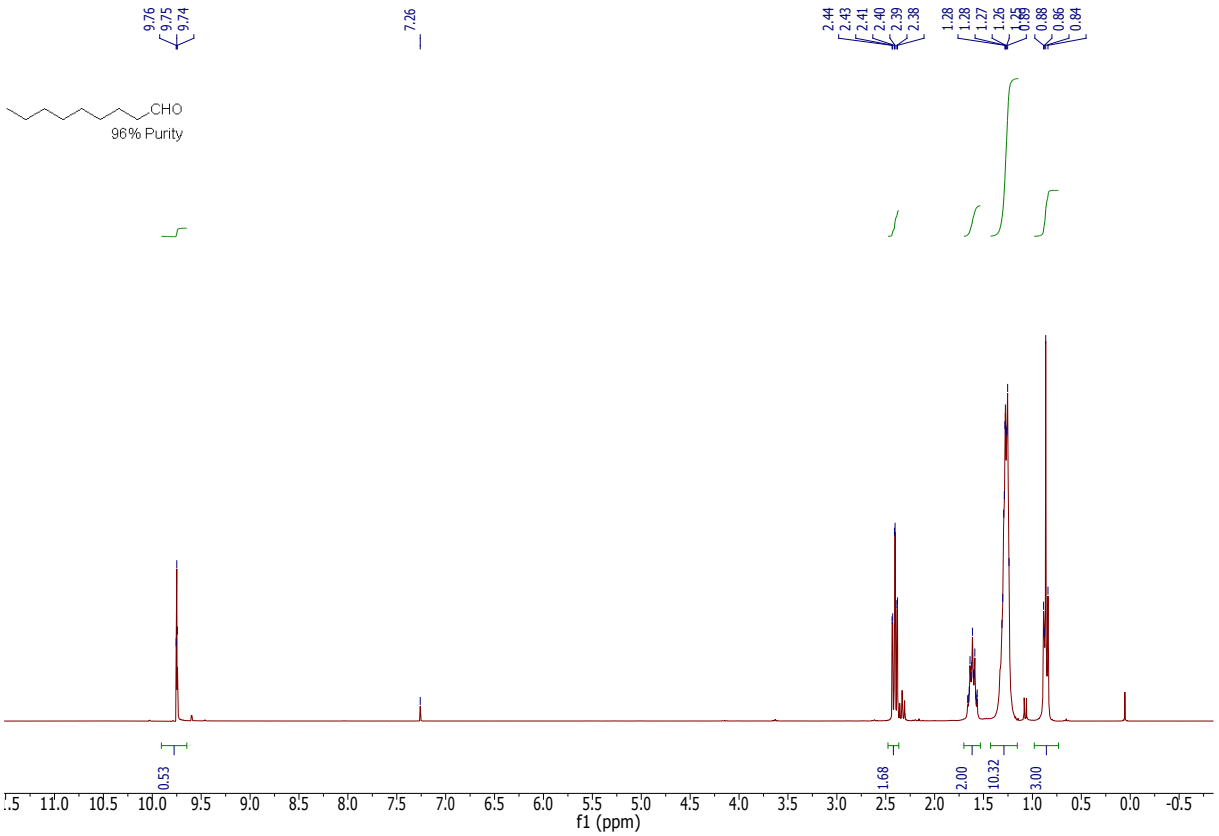
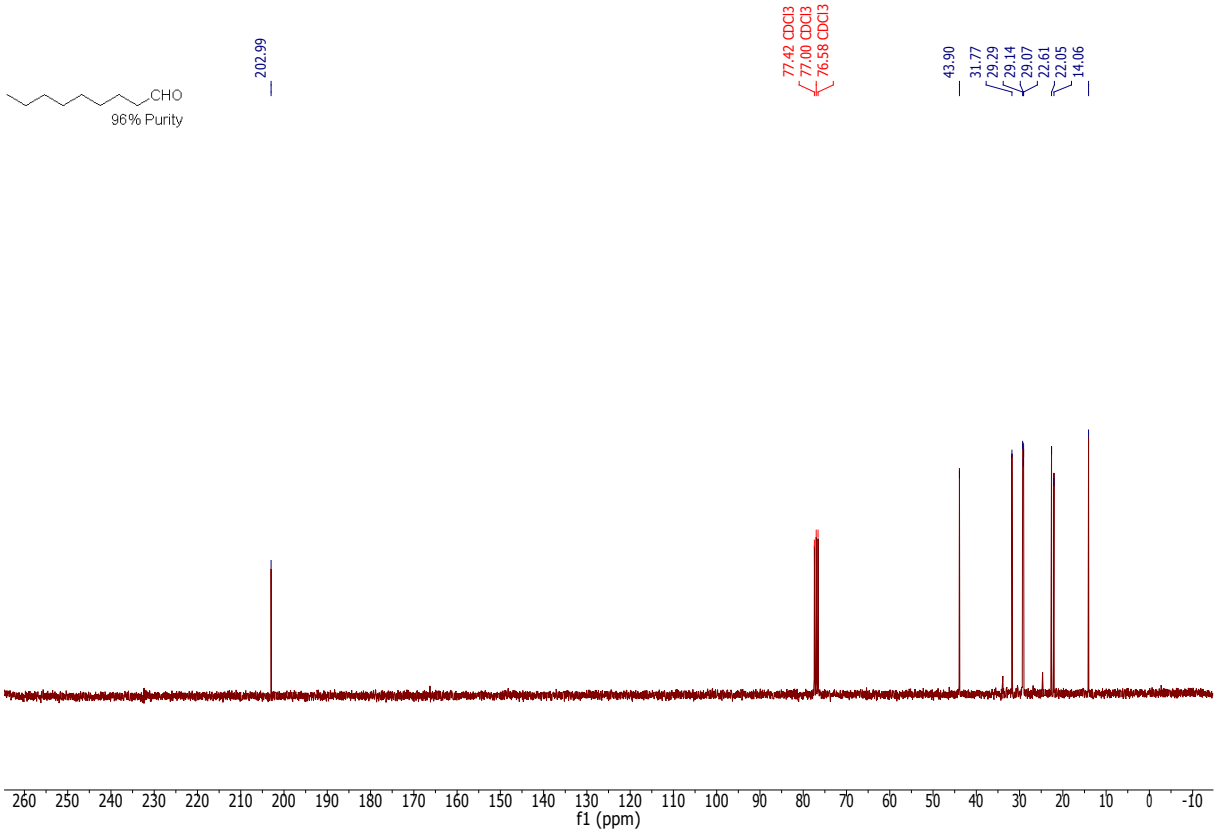
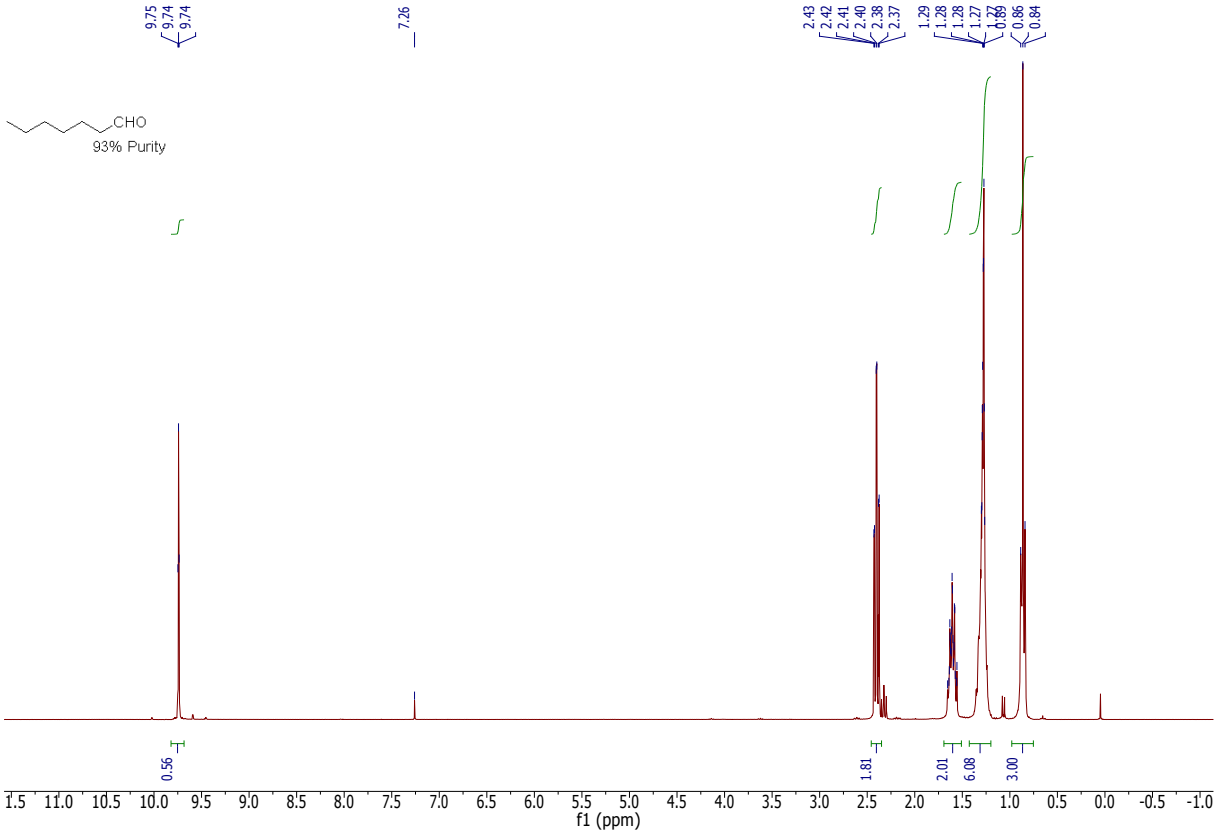
f1 (ppm)

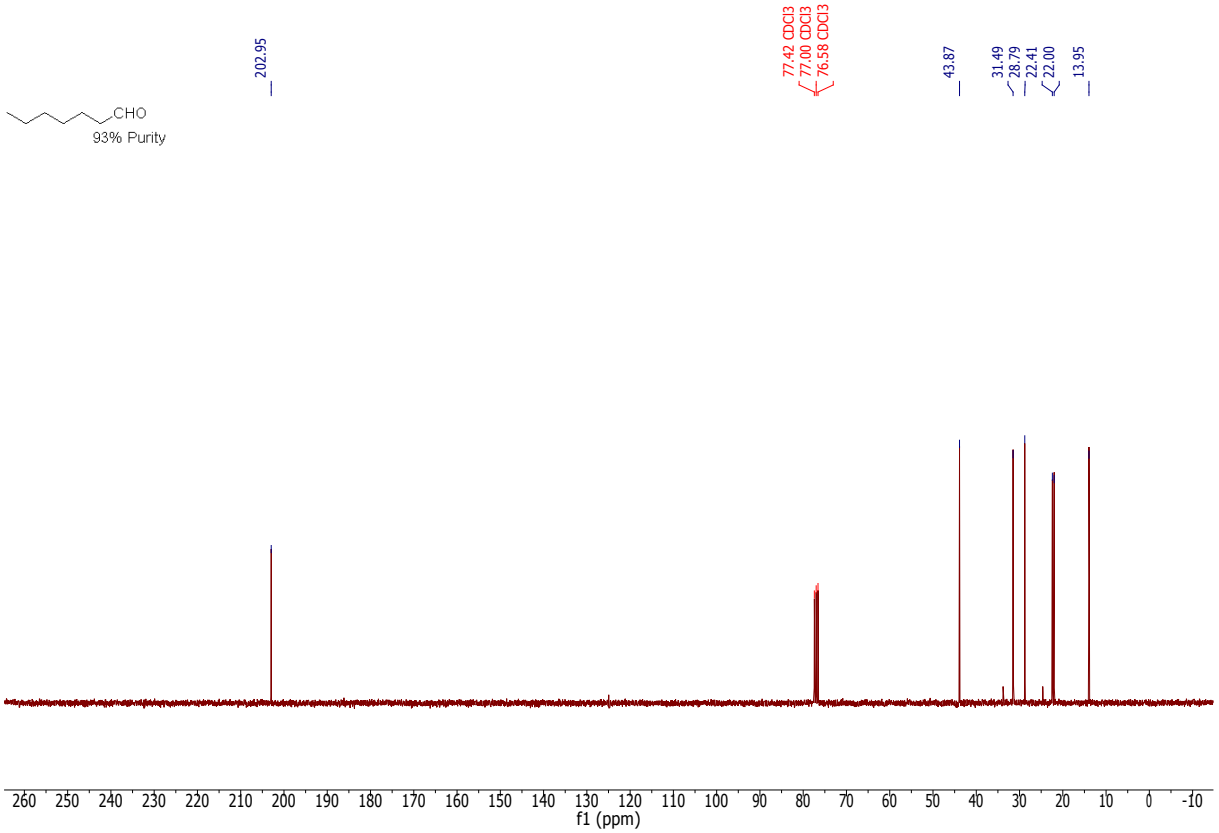
[1]


9.76
9.75
9.74
7.26
2.44
2.43
2.41
2.40
2.39
2.38
1.28
1.28
1.27
1.26
0.89
0.88
0.86
0.84
CHO
96% Purity
0.53
1.68
2.00
10.32
3.00
f1 (ppm)

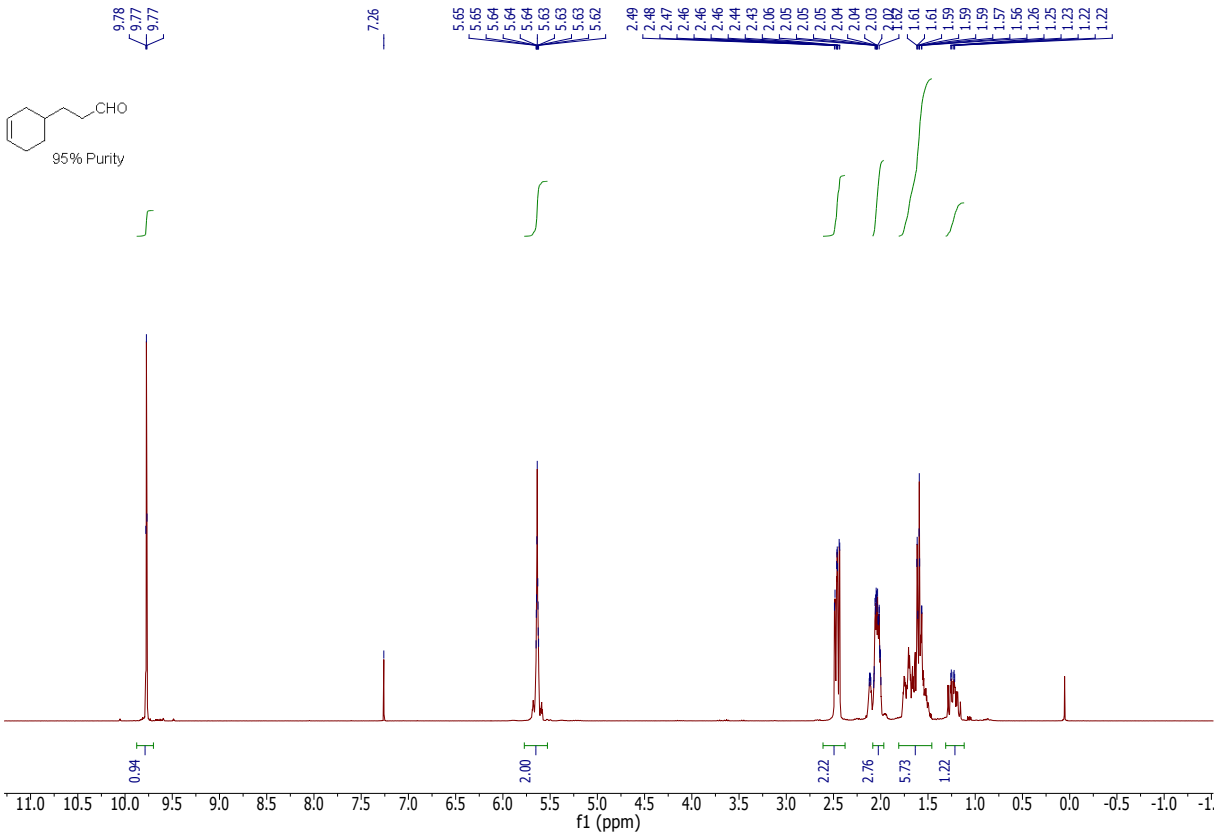

202.99
77.42 CDCl3
77.00 CDCl3
76.58 CDCl3
43.90
31.77
29.29
29.14
29.07
22.61
22.05
14.06
CHO
96% Purity
f1 (ppm)

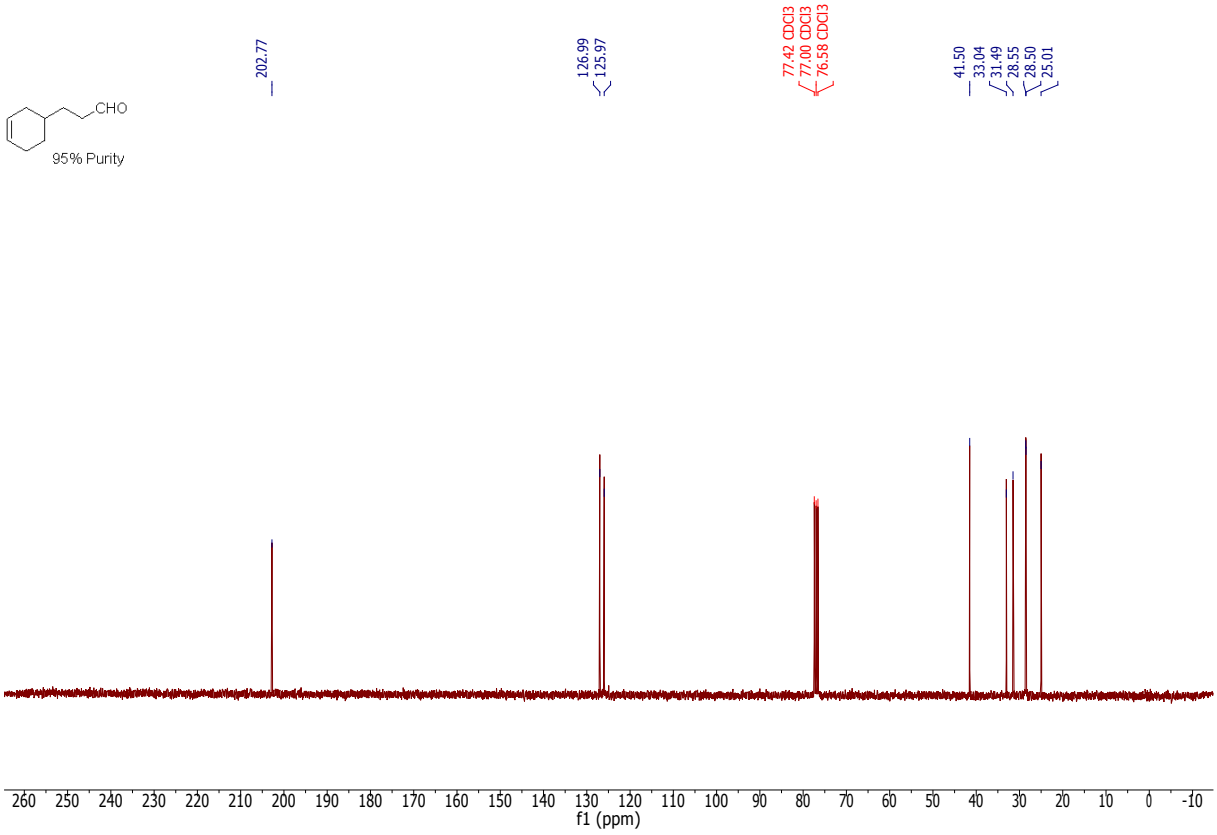
[4]


9.75
9.74
9.74
7.26
2.43
2.42
2.41
2.40
2.38
2.37
1.29
1.28
1.28
1.27
0.89
0.86
0.84
CHO
93% Purity
0.56
1.81
2.01
6.08
3.00
f1 (ppm)

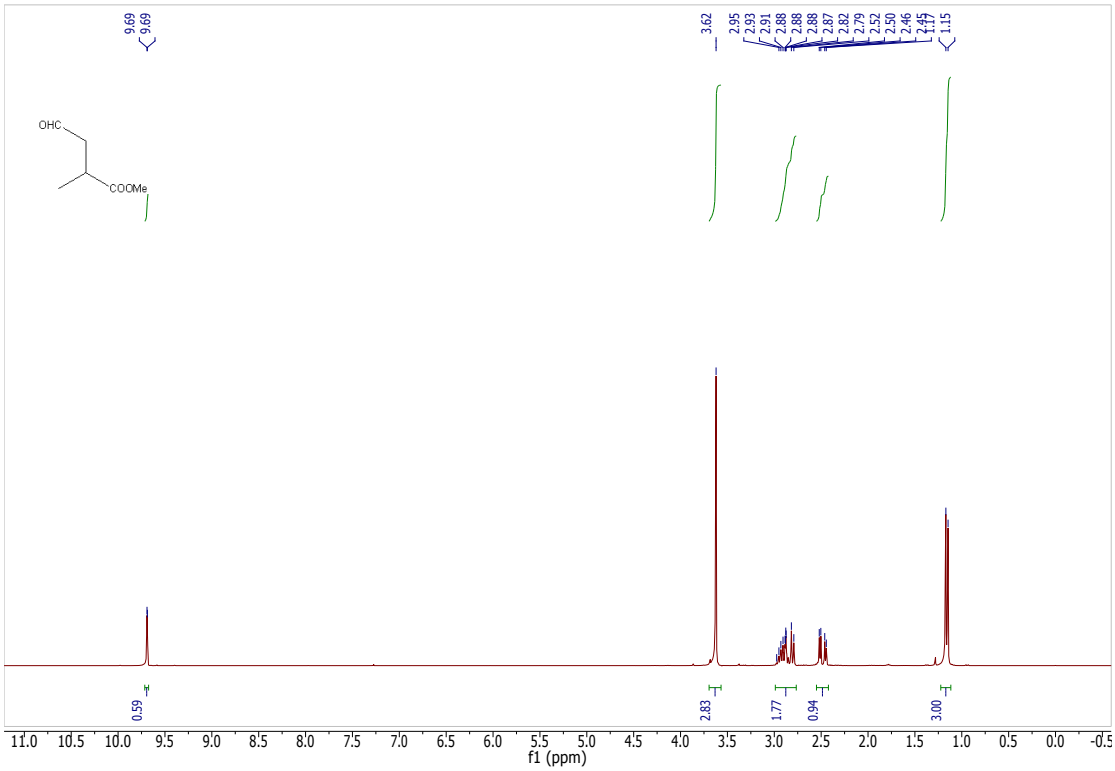

202.95
77.42 CDCl3
77.00 CDCl3
76.58 CDCl3
43.87
31.49
28.79
22.41
22.00
13.95
CHO
93% Purity
f1 (ppm)

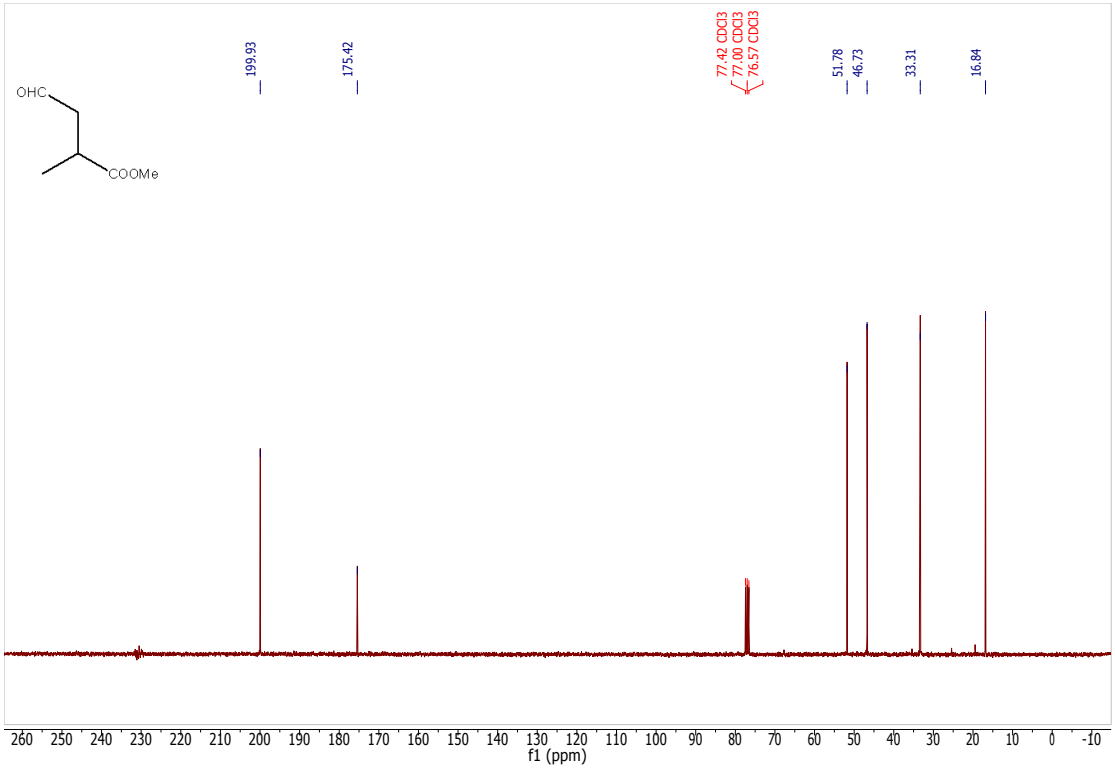
[7]


9.78
9.77
9.77
7.26
5.65
5.65
5.64
5.64
5.64
5.64
5.63
5.63
5.63
5.62
2.49
2.48
2.47
2.46
2.46
2.46
2.44
2.43
2.06
2.05
2.05
2.05
2.04
2.04
2.03
1.61
1.61
1.59
1.59
1.59
1.57
1.56
1.26
1.25
1.23
1.22
1.22
CHO
95% Purity
0.94
2.00
2.22
2.76
5.73
1.22
f1 (ppm)

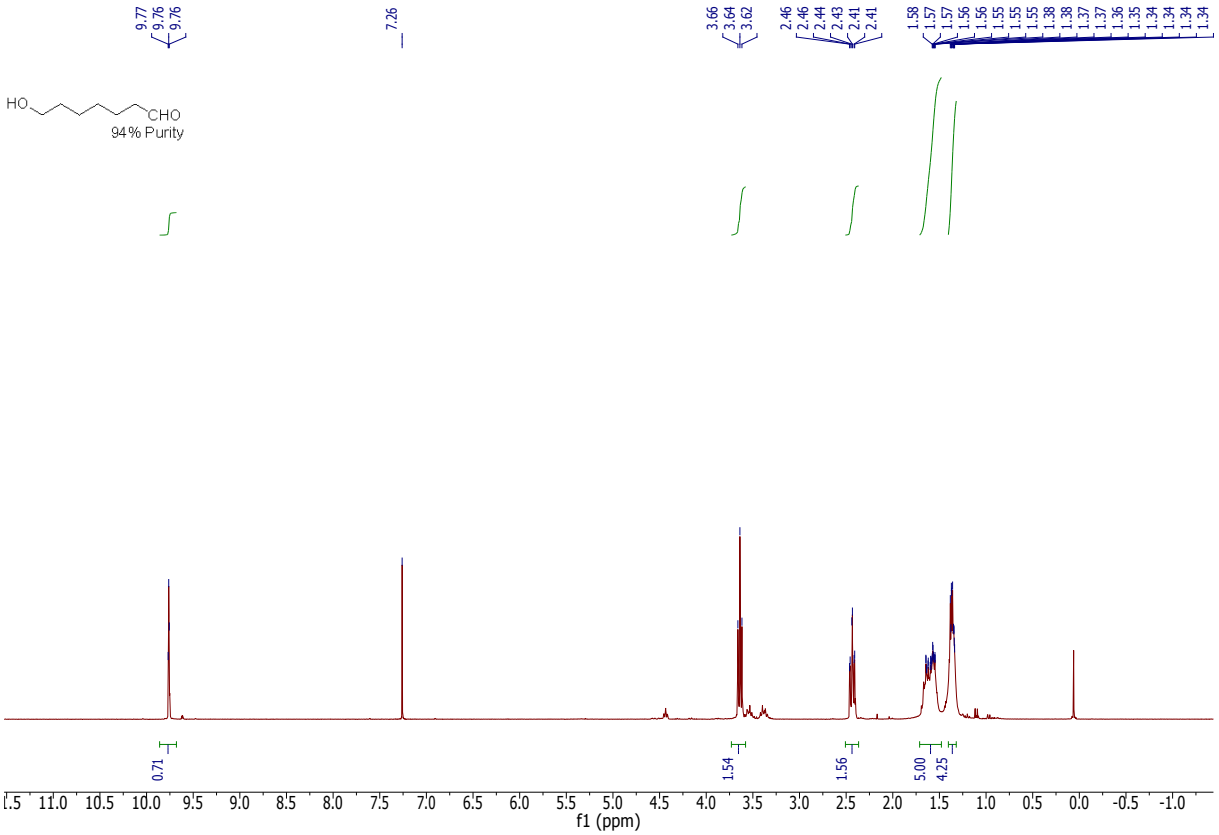

202.77
126.99
125.97
77.42 CDCl3
77.00 CDCl3
76.58 CDCl3
41.50
33.04
31.49
28.55
28.50
25.01
CHO
95% Purity
f1 (ppm)

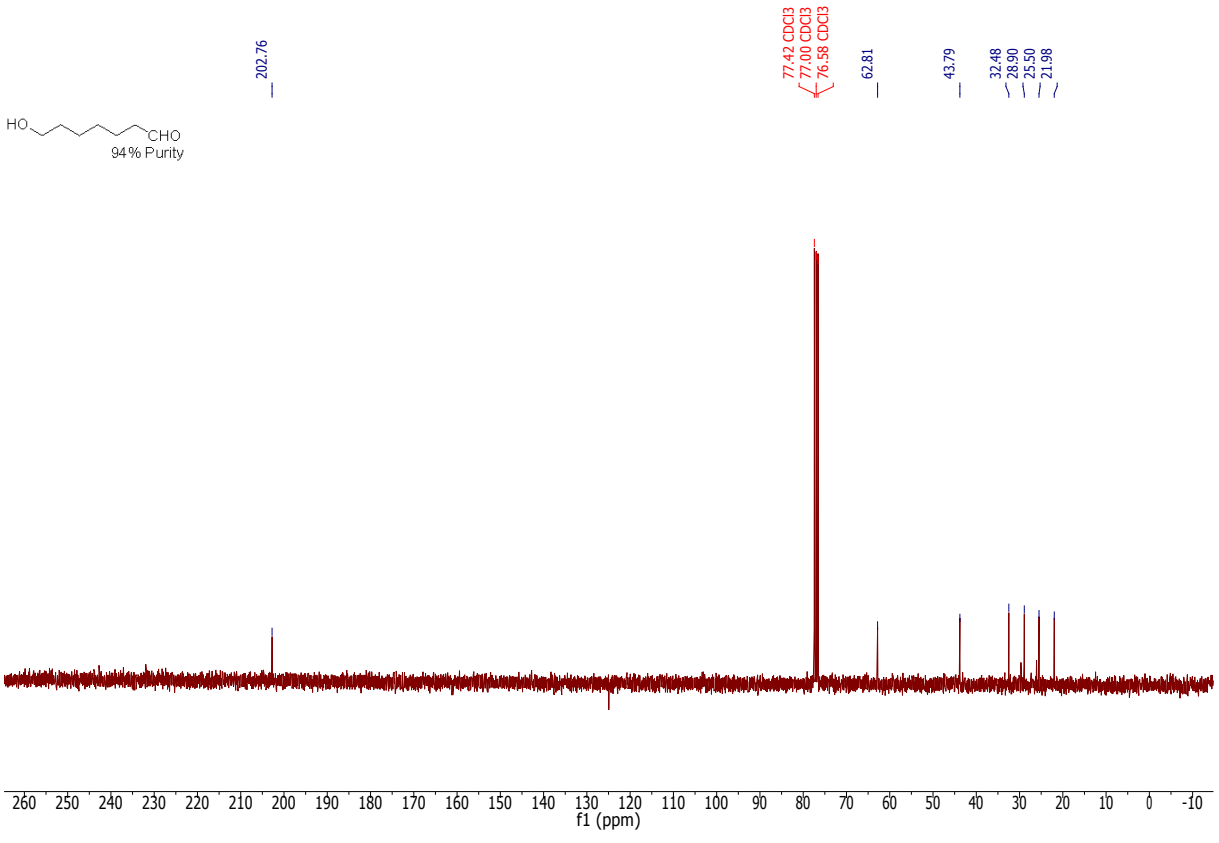
[9]


9.69
9.69
3.62
2.95
2.93
2.91
2.88
2.88
2.88
2.87
2.82
2.79
2.52
2.50
2.46
2.45
1.17
1.15
OHC
COOMe
0.59
2.83
1.77
0.94
3.00
f1 (ppm)


199.93
175.42
77.42 CDCl3
77.00 CDCl3
76.57 CDCl3
51.78
46.73
33.31
16.84
OHC
COOMe
f1 (ppm)

[10]


9.77
9.76
9.76
7.26
3.66
3.64
3.62
2.46
2.46
2.44
2.43
2.41
2.41
1.58
1.57
1.57
1.56
1.56
1.55
1.55
1.55
1.38
1.38
1.37
1.37
1.36
1.35
1.34
1.34
1.34
1.34
HO
CHO
94% Purity
0.71
1.54
1.56
5.00
4.25
f1 (ppm)


202.76
77.42 CDCl3
77.00 CDCl3
76.58 CDCl3
62.81
43.79
32.48
28.90
25.50
21.98
HO
CHO
94% Purity
f1 (ppm)