Supporting Information for:

Expanded scope for the asymmetric isomerization of primary allylic alcohols using readily accessible second-generation catalysts

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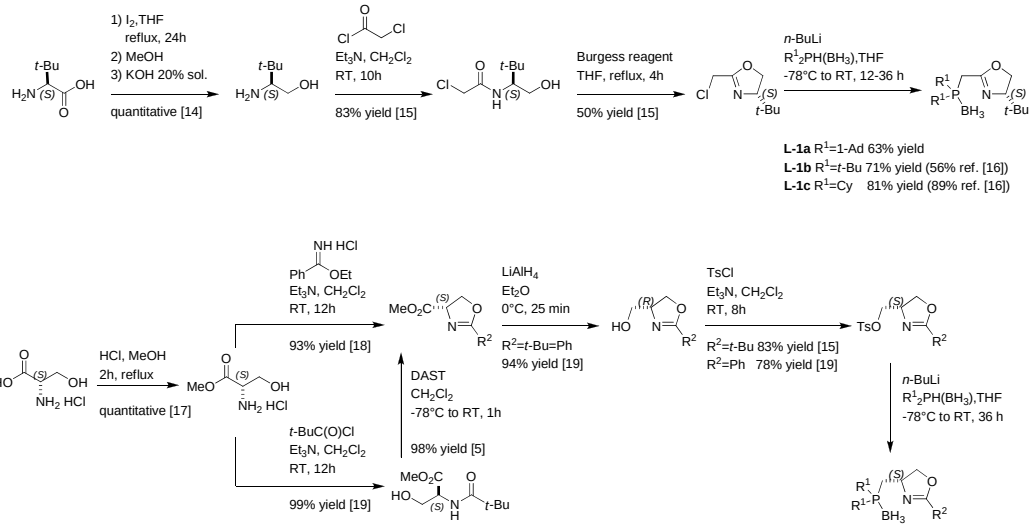
General Methods. All reactions were carried out under an inert atmosphere of argon or nitrogen using either two-manifold vacuum / inert gas lines or a MBraun glove-box, unless otherwise noted. Solvents were dried over activated alumina columns and further degassed by three successive "freeze-pump-thaw" cycles if necessary. NMR spectra were recorded on ARX-300, AMX-400 and AMX-500 Bruker Avance spectrometers. ^{1}H and ^{13}C NMR chemical shifts are given in ppm relative to $SiMe_4$, with the solvent resonance used as internal reference. ^{31}P NMR chemical shifts are reported in ppm relative to H_3PO_4. Infrared spectra were obtained on a Perkin-Elmer 1650 FT-IR spectrometer using neat samples on a diamond ATR Golden Gate sampler. Optical rotations were measured on a Perkin-Elmer 241 polarimeter equipped with a Na-lamp.
The mass spectrometric data were obtained at the mass spectrometry facility of the University of Geneva (http://www.ms.unige.ch/sms). Chiral GC analyses were performed on either a HP6890 or a HP6850 gas chromatograph. SFC analyses were run on a Berger SFC. Commercial reagents were purchased from Aldrich, Fluka, Acros or Strem and used without further purification, unless otherwise noted. Liquid reagents were transferred with stainless steel syringes or cannula. Flash chromatography was performed using silica gel 60 (230–400 mesh ASTM) from Fluka.
$IrCl_3 \cdot (H_2O)_x$ was generously provided by Johnson-Matthey. $[Ir(COD)Cl]_2$[1] was prepared according to literature procedures. New protected ligands **L-2a-f** and new precatalysts **2a-f** were fully characterized: data and ^{1}H, $^{31}P\{^{1}H\}$, $^{13}C\{^{1}H\}$ NMR ($CDCl_3$) spectra are reported below; ^{1}H, $^{31}P\{^{1}H\}$ NMR (THF-d_8) are reported. Substrates **3b-f** and **3h-j** were synthesized using our protocol;[2] **3g** was synthesized using a procedure reported for a similar substrate.[3] Compounds **3b**,[4b] **3c**,[2b,5] **3d**,[4b] **3e**,[2b,5,6] **3f**,[2] **3g**,[7] **3h**,[2a] **3i**,[2] **3j**,[5,8] **3k**,[9] **4b**,[2b,4b] **4c**,[2b,4a] **4d**,[2b,4b] **4e**,[2b,10] **4f**,[2b,4b] **4g**,[11] **4h**,[2] **4i**,[2,4] **4j**,[12] **4k**[13] match the spectroscopic and spectrometric data reported in the literature.

Representative procedure for the catalytic isomerization of allylic alcohols using (*S*)-2b. (*R*)-4-methyl-3-phenylpentanal (**4a**, Table 1, entry 3): a 25 mL Schlenk containing 7.4 mg of catalyst (*S*)-**2b** (5.0 mol%) was purged by three successive vacuum/N_2 sequences and refilled with N_2. Distilled THF (2 mL) was added next and H_2 gas was gently bubbled directly through the solution via a stainless-steel needle at room temperature. The orange solution rapidly discolored. After 5 minutes, bubbling was ceased, the Schlenk was refilled with N_2 and the rubber septum was replaced with a polyethylene stopper and the solution degassed by two successive freeze-pump-thaw

[1] J. Choudhury, S. Podder and S. Roy, *J. Am. Chem. Soc.*, 2005, **127**, 6162−6163.
[2] (a) L. Mantilli and C. Mazet, *Tetrahedron Lett.*, 2009, **50**, 4141-4144; (b) L. Mantilli, D. Gérard, S. Torche, C. Besnard and C. Mazet, *Angew. Chem. Int. Ed.*, 2009, **48**, 5143−5147.
[3] T. Nagano, J. Pospisil, G. Chollet, S. Shulthoff, V. Hickmann, E. Moulin, J. Herrmann, R. Müller and A. Fürstner, , *Chem. Eur. J.*, 2009, **15**, 9697-9707.
[4] (a) K. Tanaka, S. Qiao, M. Tobisu, M. M.-C. Lo, G. C. Fu, *J. Am. Chem. Soc.*, 2000, **122**, 9870−9871; (b) K. Tanaka and G. C. Fu, *J. Org. Chem.*, 2001, **66**, 8177−8186.
[5] For a full characterization, see this work.
[6] R_f, m.p. and b.p.can be found in G. Pinna, G. Cignarella, G. Loriga, G. Morineddu, J.-M. Mussinu, S. Ruiu, P. Fadda and W. Fratta, *Bioorg. Med. Chem.*, 1967, **32**, 1929−1937.
[7] H. Taguchi, K. Ghoroku, M. Tadaki, A. Tsubouchi and T. Takeda, *J. Org. Chem.*, 2002, **67**, 8450−8456.
[8] IR can be found in S. Bywater, P. Lachance and P. Black, *J. Organomet. Chem.*, 1985, **280**, 159−164; For a full characterization, see this work.
[9] Geraniol is commercially available from Aldrich.
[10] A. I. Meyers and M. Shipman, *J. Org. Chem.*, 1991, **56**, 7098−7102.
[11] T. K. Sarkar, S. K. Ghosh and T. K. Satapathi, *Tetrahedron*, 1990, **46**, 1885−1898.
[12] 3,5,5-trimethylhexanal is commercially available from Aldrich.
[13] Citronellal is commercially available from Aldrich.

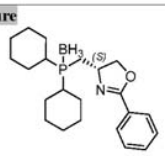
cycles. After the second cycle, 17.5 µL of (*E*)-3-phenylpent-2-en-1-ol (**3a**, 0.1 mmol) were added by micro-syringe and the reaction stirred at room temperature for 4h**.** Volatiles were removed under vacuum, the yellow residue was dissolved in $CDCl_3$ and conversions were assessed by either ^1H NMR spectroscopy or GC analysis using an internal standard. For purification, the residue was dissolved in cyclohexane/ethyl acetate (3:1) and filtered through a short plug of silica or Celite® (pasteur pipette) to remove the deactivated catalyst. The *ee* was determined by GC using a CP-Chirasil-Dex-CB chiral column. Yields match conversion in all cases.

Comparative synthetic routes to ligands L-1 and L-2.



[14] M. Nakamura, T. Hatakeyama, K. Hara and E. Nakamura, *J. Am. Chem. Soc*., 2003, **125**, 6362-6363.
[15] S. Nanchen and A. Pfaltz, *Chem. Eur. J.*, 2006, **12**, 4550-4558.
[16] M. G. Schrems, E. Neumann and A. Pfaltz, *Angew. Chem. Int. Ed.*, 2007, **46**, 8274−8276.
[17] F. Liu, J. Thomas and T. R. Burke Jr, *Synthesis*, 2008, **15**, 2432-2438.
[18] A. I. Meyers, W. Schmidt and M. J. McKennon, *Synthesis*, 1993, **2**, 250-262.
[19] M. Diéguez and O. Pàmies, *Chem. Eur. J.*, 2008, **14**, 3653-3669.

Structure	^{1}H	$^{13}C\{^1H\}$	$^{31}P\{^1H\}$	IR	HRMS	$[\alpha]_D$	MAZET GROUP DATA FORM



Name (*S*)-4-[(di-cyclohexylphosphanyl)-methyl]-2-(phenyl)-4,5-dihydrooxazoline-borane adduct.
LM-427

Properties white wax

Formula $C_{22}H_{35}BNOP$

Molecular Weight 371.30

tlc conditions: SiO_2, Pent / EtO_2 = 4:1
R_f =0.19 (UV)

$[\alpha]^{26}_D$ = + 17.7
c 1.0. *in* CH_2Cl_2.

^{1}H NMR (CDCl$_3$, 500 MHz, 298 K) δ (ppm) = 7.92 (m, 2H, H_{oPh}), 7.48 (m, 1H, H_{pPh}), 7.40 (m, 2H, H_{mPh}), 4.60 (*ap*.t, $^{2,3}J_{HH}$ = 9.0 Hz, 1H, C*H*O), 4.53 (m, 1H, C*H*N), 4.15 (dd, $^2J_{HH}$ = 9.0 Hz, $^3J_{HH}$ = 7.3 Hz, 1H, C*H*O), 2.23 (*ap*.td, $^2J_{HP}$ = $^2J_{HH}$ = 14.5 Hz, $^3J_{HH}$ = 3.8 Hz, 1H, C*H*P), 1.93-1.69 (m, 1H, C*H*P, 12H, H_{Cy}), 1.48-1.44 (m, 2H, H_{Cy}), 1.28-1.22 (m, 8H, H_{Cy}), 0.33 (bq, $^1J_{HB}$ = 107.8 Hz, 3H, BH_3).

^{13}C NMR (CDCl$_3$, 126 MHz, 298 K) δ (ppm) = 164.3 (s, *C*N), 131.6 (s, C_{pPh}), 128.5 (s, C_{mPh}), 128.4 (s, C_{oPh}), 127.6 (s, C_{ipsoPh}), 74.4 (d, $^3J_{CP}$ = 2.8 Hz, CH_2O), 63.3 (d, $^2J_{CP}$ = 2.8 Hz, CHN), 32.9 (d, $^1J_{CP}$ = 32.1 Hz, CH_{Cy}), 31.8 (d, $^1J_{CP}$ = 33.0 Hz, $CH_{Cy'}$), 27.1-26.8 (m, CH_{2Cy}), 26.6 (d, $^1J_{CP}$ = 32.1 Hz, CH_2P), 26.5 (d, $^4J_{CP}$ = 2.8 Hz, $CH_{2\,Cy}$), 26.0 (d, $^4J_{CP}$ = 3.7 Hz, $CH_{2\,Cy}$).

$^{31}P\{^1H\}$ NMR (CDCl$_3$, 202 MHz, 298 K) δ (ppm) = 21.5 (m).

IR spectrum (neat) ν (cm^{-1}) = 22923, 2852, 2369, 2352, 2269, 1652, 1579, 1492, 1471, 1449, 1361, 1301, 1264, 1208, 1174, 1135, 1078, 1065, 1016, 963, 933, 905, 851, 777, 694, 678.

HRMS *(method: ESI+)*
calculated for $C_{22}H_{36}BNP$ $[M+H]^+$: 372.2622,
found 372.2601.

relevant literature references: S. Nanchen, A. Pfaltz *Chem. Eur. J.* **2006**, *12*, 4550-4558; M. Diéguez, O. Pàmies *Chem. Eur. J.* **2008**, *14*, 3653-3669; D.-R. Hou, K. Burgess, *Org. Lett.* **1999**, *1*, 1745–1747; D.-R. Hou, J. H. Reibenspies, K. Burgess, *J. Org. Chem.* **2001**, *66*, 206–215.

Separation Conditions

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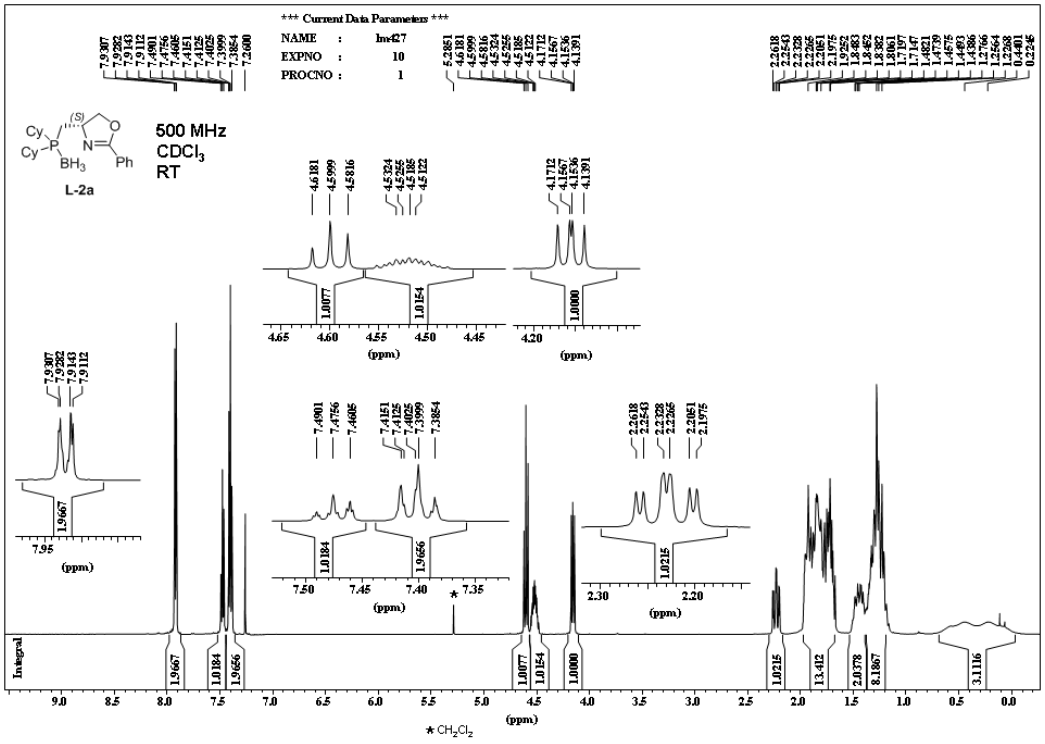
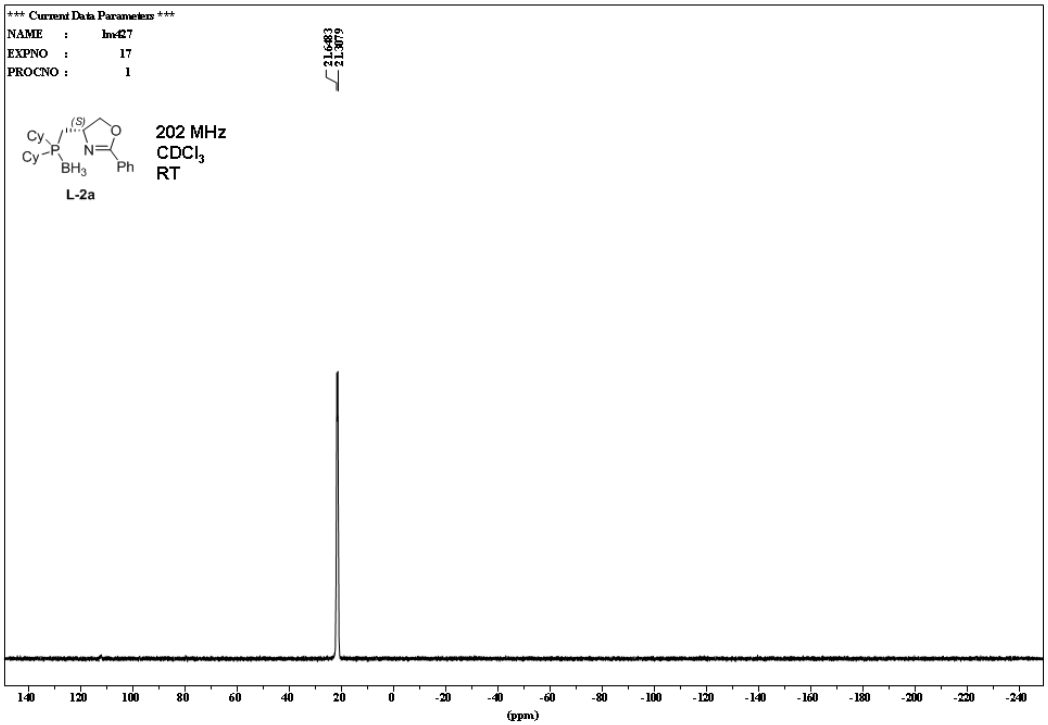
GC (column, method or sequence, retention time):

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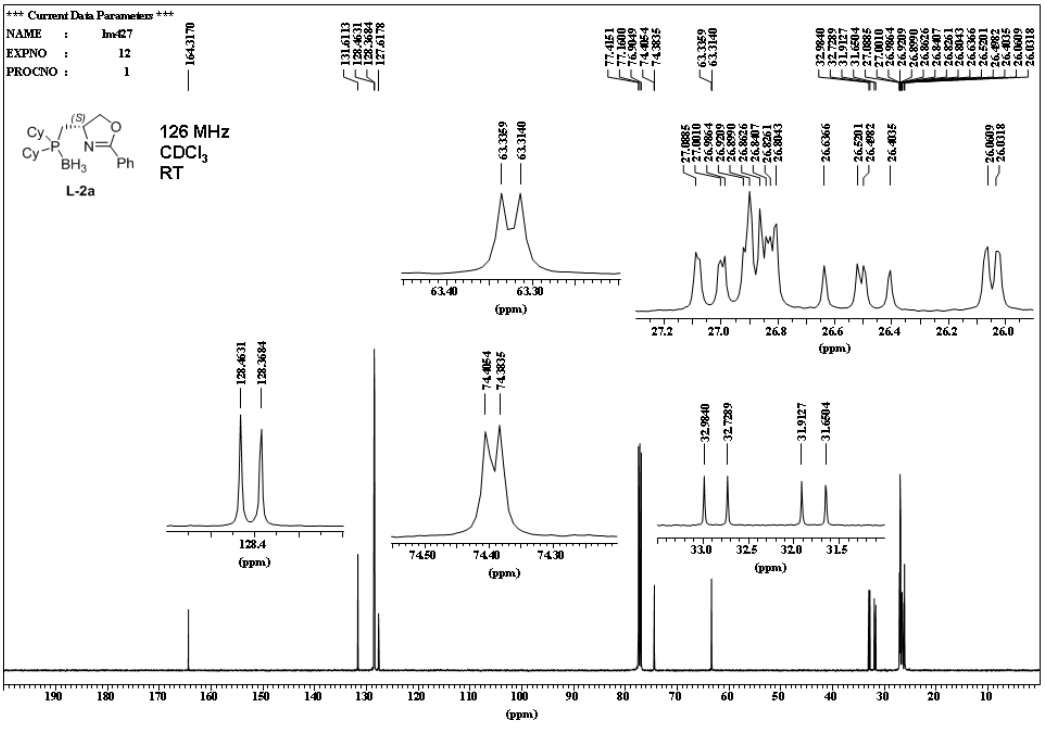
(ppm)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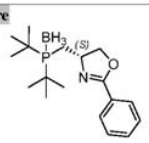
63.3359
63.3140
32.9840
32.7289
31.9127
31.6504
27.0885
27.0010
26.9864
26.9289
26.8990
26.8926
26.8407
26.8261
26.8043
26.6366
26.5291
26.4982
26.4035
26.0689
26.0318
126 MHz
CDCl3
RT
L-2a
(ppm)

Structure	^{1}H	^{13}C{^{1}H}	^{31}P{^{1}H}	IR	HRMS	$[\alpha]_D$	MAZET GROUP DATA FORM



Name (*S*)-4-[(di-*tert*-butylphosphanyl)-methyl]-2-(phenyl)-4,5-dihydrooxazoline-borane adduct.
LM-423

Properties white powder

Formula $C_{18}H_{31}BNOP$

Molecular Weight 319.23

tlc conditions: SiO_2, Pent / EtO_2 = 3:1
R_f =0.18 (UV)

$[\alpha]^{26}_D$ = - 5.2
c 1.0. *in* CH_2Cl_2.

Mp = 125°C

^{1}H NMR ($CDCl_3$, 500 MHz, 298 K) δ (ppm) = 7.93 (m, 2H, H_{oPh}), 7.47 (m, 1H, H_{pPh}), 7.40 (m, 2H, H_{mPh}), 4.67 (*ap*.t, $^{2,3}J_{HH}$ = 9.1 Hz, 1H, C*H*O), 4.55 (m, 1H, C*H*N), 4.20 (dd, $^2J_{HH}$ = 9.1 Hz, $^3J_{HH}$ = 7.3 Hz, 1H, C*H*O), 2.43 (*ap*.t, $^2J_{HP}$ = $^2J_{HH}$ = 15.2 Hz, 1H, C*H*P), 1.67 (ddd, $^2J_{HP}$ = 15.2 Hz, $^2J_{HH}$ = 11.1 Hz, $^3J_{HH}$ = 7.0 Hz, 1H, C*H*P), 1.34 (d, $^3J_{HP}$ = 12.6 Hz, 9H, CH_{3}tBu), 1.25 (d, $^3J_{HP}$ = 12.7 Hz, 9H, CH_{3}tBu'), 0.40 (bq, $^1J_{HB}$ = 103.7 Hz, 3H, BH_3).

^{13}C NMR ($CDCl_3$, 126 MHz, 298 K) δ (ppm) = 164.3 (s, *C*N), 131.6 (s, C_{pPh}), 128.5 (s, C_{mPh}), 128.4 (s, C_{oPh}), 127.7 (s, C_{ipsoPh}), 74.8 (s, CH_2O), 64.2 (d, $^2J_{CP}$ = 4.6 Hz, *C*HN), 33.0 (d, $^1J_{CP}$ = 26.6 Hz, C_{t}Bu), 31.9 (d, $^1J_{CP}$ = 28.5 Hz, C_{t}Bu'), 28.0 (s, CH_{3}tBu), 27.8 (s, CH_{3}tBu'), 25.4 (d, $^1J_{CP}$ = 26.6 Hz, CH_2P).

^{31}P{^{1}H} NMR ($CDCl_3$, 202 MHz, 298 K) δ (ppm) = 38.9 (m).

IR spectrum (neat) ν (cm^{-1}) = 2955, 2906, 2871, 2375, 2270, 1645, 1581, 1496, 1471, 1450, 1393, 1358, 1304, 1261, 1177, 1078, 1061, 1025, 961, 910, 772, 693, 679, 629.

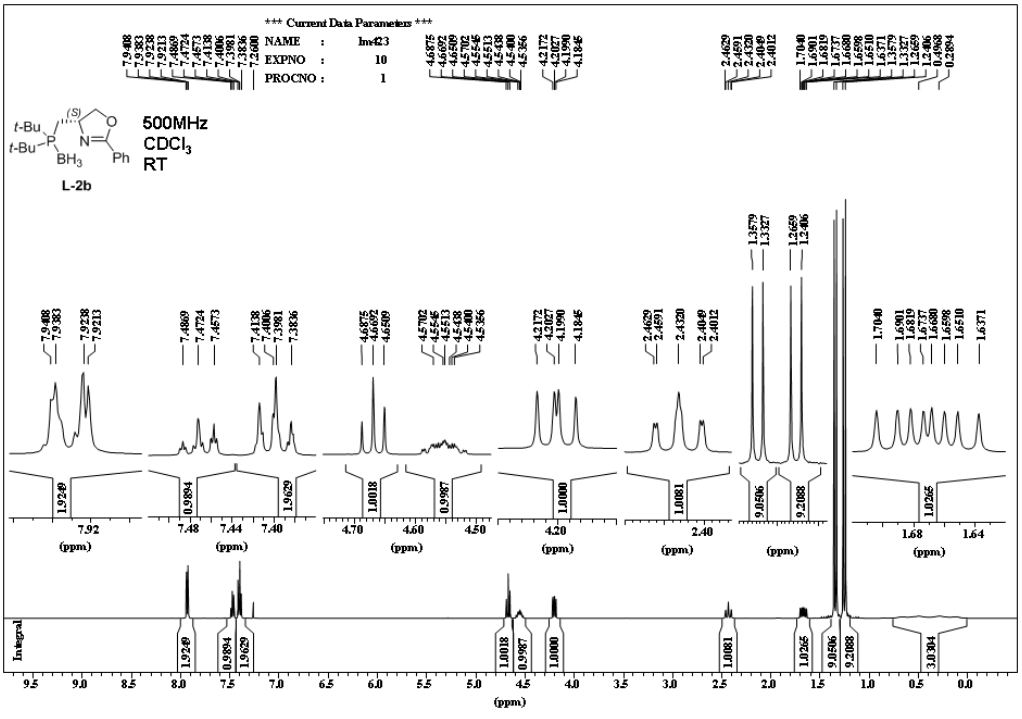
HRMS *(method: ESI+)*
calculated for $C_{18}H_{32}BNOP$ $[M+H]^+$: 320.2309,
found 320.2317.

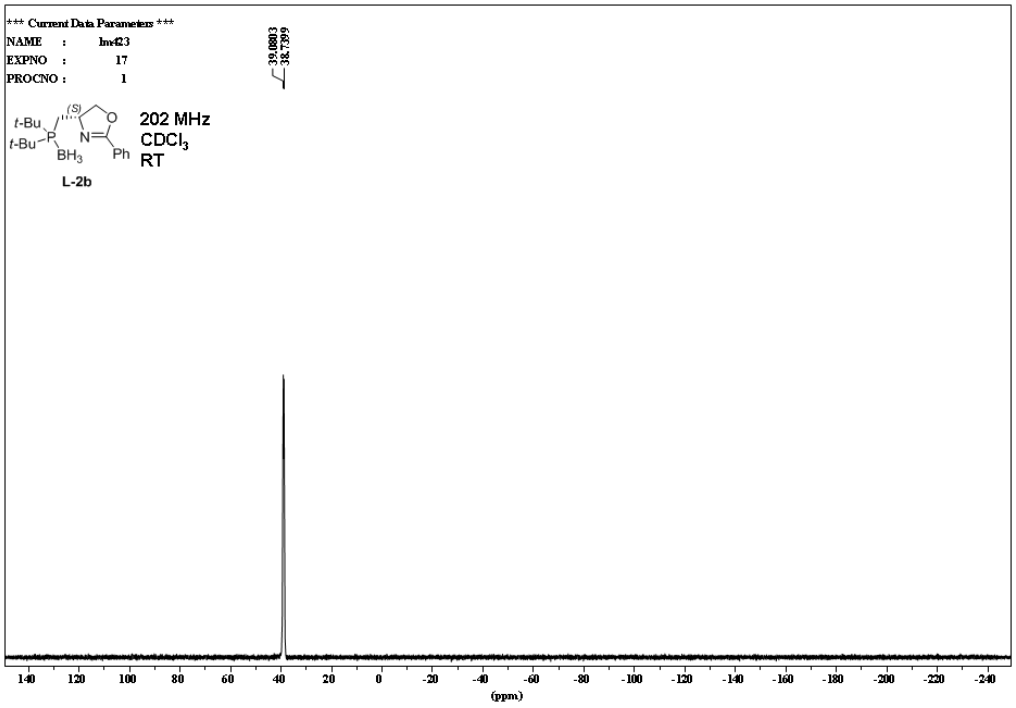
relevant literature references: S. Nanchen, A. Pfaltz *Chem. Eur. J.* **2006**, *12*, 4550-4558; M. Diéguez, O. Pàmies *Chem. Eur. J.* **2008**, *14*, 3653-3669; D.-R. Hou, K. Burgess, *Org. Lett.* **1999**, *1*, 1745–1747; D.-R. Hou, J. H. Reibenspies, K. Burgess, *J. Org. Chem.* **2001**, *66*, 206–215.

Separation Conditions

HPLC (column, λ_1, λ_2, eluent, flow rate, retention time):

GC (column, method or sequence, retention time):

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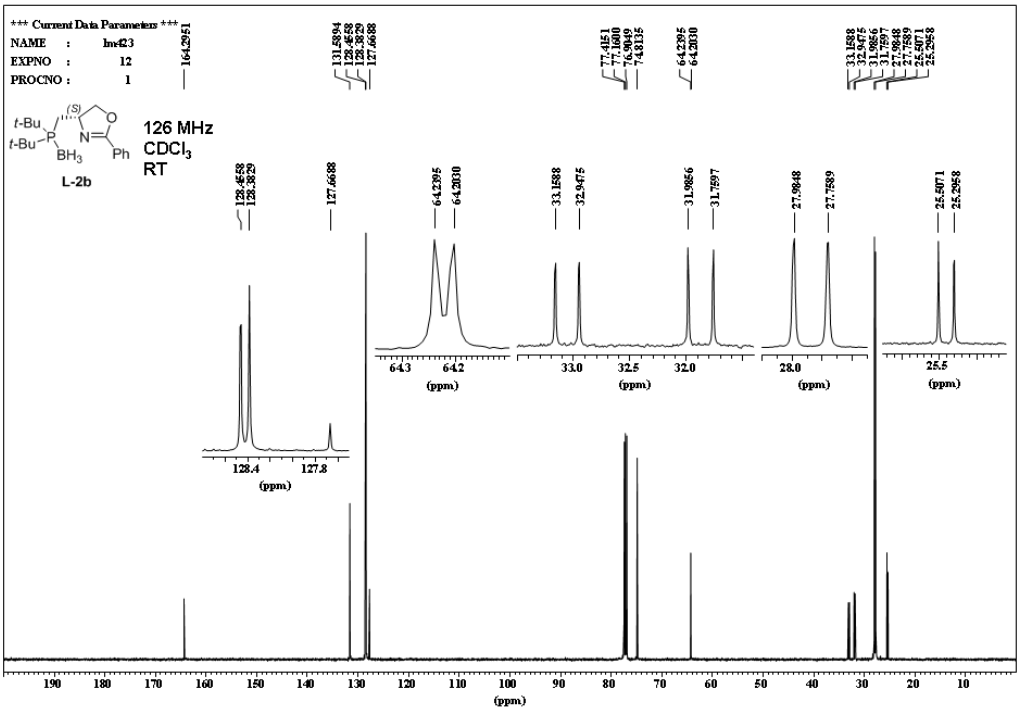
L-2b
(ppm)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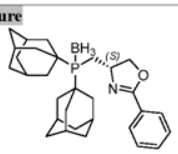
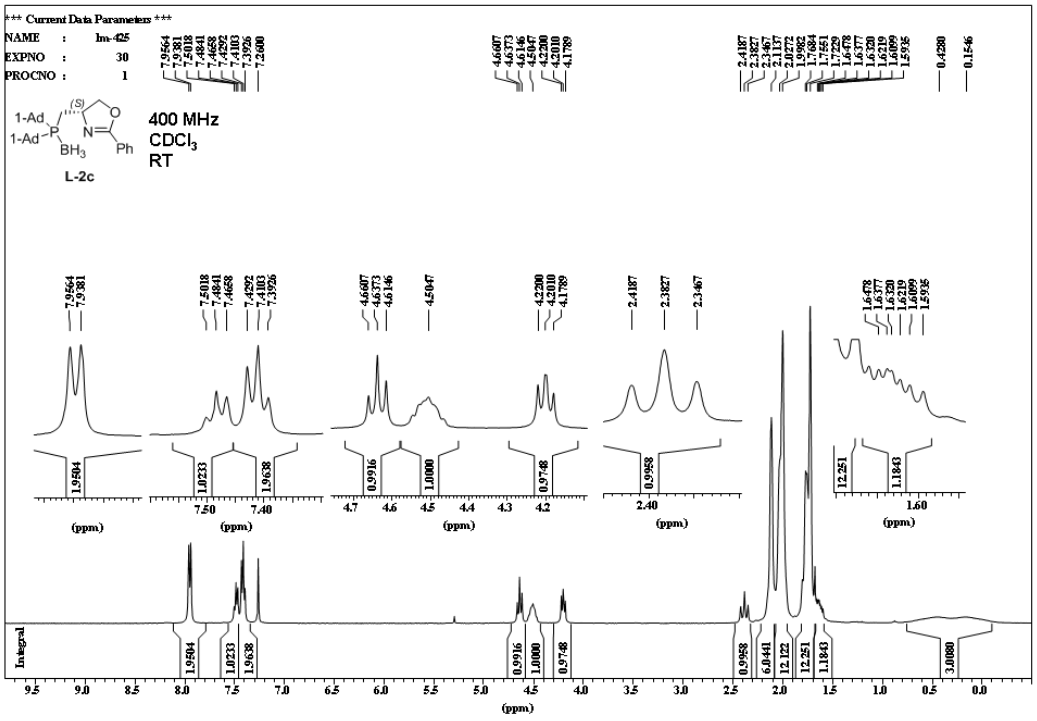
74.8135
64.2395
64.2030
33.1588
32.9475
31.9856
31.7597
27.9948
27.7589
25.6071
25.2958
126 MHz
CDCl3
RT
L-2b
(ppm)

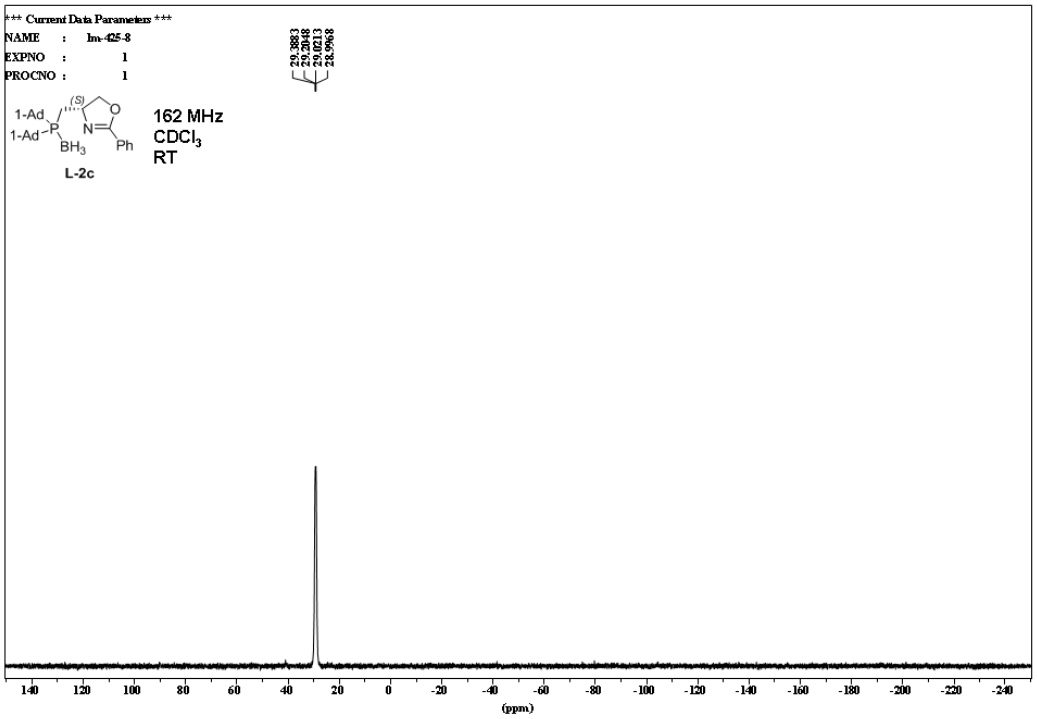
Structure	^{1}H	$^{13}C\{^{1}H\}$	$^{31}P\{^{1}H\}$	IR	HRMS	$[\alpha]_D$	MAZET GROUP DATA FORM
	**Name** (*S*)-4-[(di-1-adamantylphosphanyl)-methyl]-2-(phenyl)-4,5-dihydrooxazoline-borane adduct. LM-425						
	Properties white powder					**Formula** $C_{30}H_{43}BNOP$	
Molecular Weight 475.45	*tlc conditions:* SiO_2, Pent / EtO_2 = 3:1 R_f = 0.28 (UV)					$[\alpha]^{26}_D$ = + 1.6 *c* 1.0. *in* CH_2Cl_2.	*Mp* = 223-224 °C

^{1}H NMR ($CDCl_3$, 400 MHz, 298 K) δ (ppm) = 7.95 (d, $^{3}J_{HH}$ = 7.3 Hz, 2H, H_{oPh}), 7.48 (t, $^{3}J_{HH}$ = 7.3 Hz, 1H, H_{pPh}), 7.41 (t, $^{3}J_{HH}$ = 7.3 Hz, 2H, H_{mPh}), 4.64 (*ap*.t, $^{2,3}J_{HH}$ = 8.7 Hz, 1H, C*H*O), 4.50 (m, 1H, C*H*N), 4.20 (*ap*.t, $^{2,3}J_{HH}$ = 8.7 Hz, 1H, C*H*O), 2.38 (*ap*.t, $^{2}J_{HP}$ = $^{2}J_{HH}$ = 14.4 Hz, 1H, C*H*P), 2.11 (m, 6H, CH_2C_{Ad}), 2.03 (m, 6H, CH_2C_{Ad}, 6H, CHC_{Ad}), 1.76 (m, 12H, CH_2CH_{Ad}), 1.63 (m, 1H, CH_2P), 0.29 (bq, $^{1}J_{HB}$ = 109.4 Hz, 3H, BH_3).

^{13}C NMR ($CDCl_3$, 126 MHz, 298 K) δ (ppm) = 164.3 (s, *C*N), 131.6 (s, C_{pPh}), 128.5 (s, C_{mPh}), 128.4 (s, C_{oPh}), 127.8 (s, C_{ipsoPh}), 75.0 (s, *C*H$_2$O), 64.3 (d, $^{2}J_{CP}$ = 2.9 Hz, *C*HN), 38.0 (s, CH_2C_{Ad}), 37.8 (s, $CH_2C_{Ad'}$), 37.6 (d, $^{1}J_{CP}$ = 24.8 Hz, C_{Ad}P), 36.6 (s, CH_2CH_{Ad}), 36.5 (s, CH_2CH_{Ad}), 36.3 (d, $^{1}J_{CP}$ = 26.6 Hz, $C_{Ad'}$P), 28.2 (d, $^{2}J_{CP}$ = 1.8 Hz, CHC_{Ad}), 28.1 (d, $^{2}J_{CP}$ = 1.8 Hz, $CHC_{Ad'}$), 22.3 (d, $^{1}J_{CP}$ = 26.6 Hz, CH_2P).

$^{31}P\{^{1}H\}$ NMR ($CDCl_3$, 162 MHz, 298 K) δ (ppm) = 29.1 (m).	**IR spectrum (neat)** ν (cm^{-1}) = 2961, 2932, 2904, 2849, 2402, 2368, 2266, 1649, 1579, 1496, 1470, 1448, 1356, 1345, 1304, 1255, 1174, 1069, 1061, 1028, 958, 910, 837, 795, 772, 733, 691, 671, 646.
HRMS *(method: ESI+)* calculated for $C_{30}H_{44}BNOP$ $[M+H]^+$: 476.3248, found 476.3281.	**relevant literature references**: S. Nanchen, A. Pfaltz *Chem. Eur. J.* **2006**, *12*, 4550-4558; M. Diéguez, O. Pàmies *Chem. Eur. J.* **2008**, *14*, 3653-3669; D.-R. Hou, K. Burgess, *Org. Lett.* **1999**, *1*, 1745–1747; D.-R. Hou, J. H. Reibenspies, K. Burgess, *J. Org. Chem.* **2001**, *66*, 206–215.
Separation Conditions	
HPLC (column, λ_1, λ_2, eluent, flow rate, retention time):	**GC (column, method or sequence, retention time)**:

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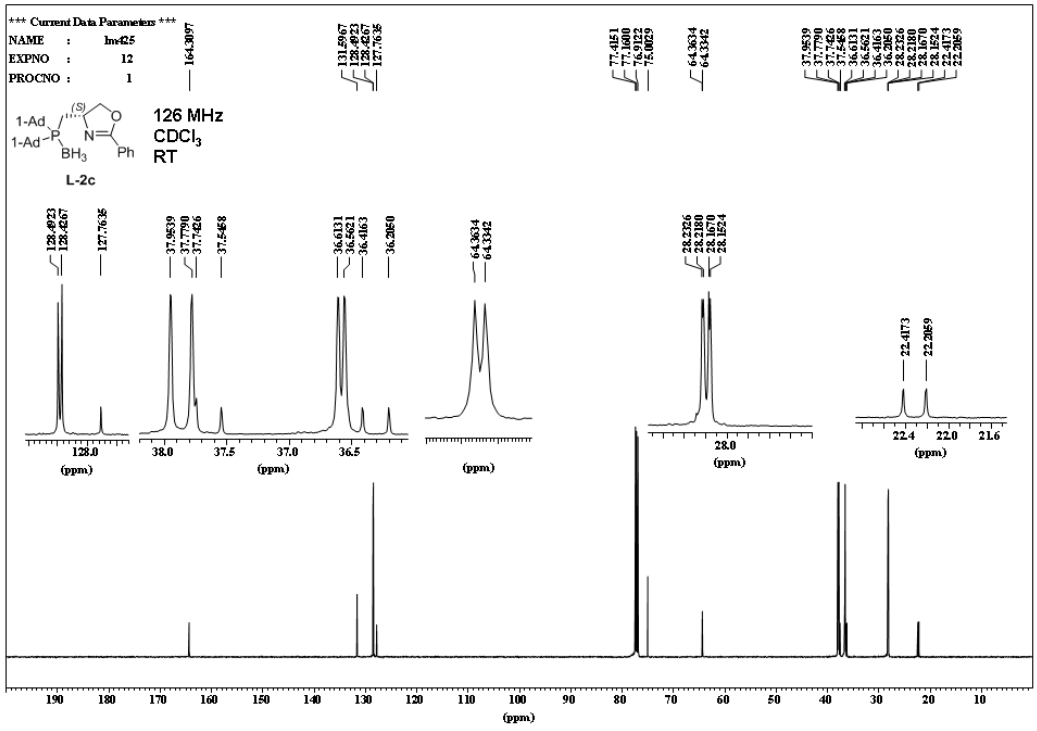
(ppm)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126 MHz
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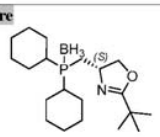
Structure	^{1}H	$^{13}C\{^1H\}$	$^{31}P\{^1H\}$	IR	HRMS	$[\alpha]_D$	MAZET GROUP DATA FORM



Name (*S*)-4-[(di-cyclohexylphosphanyl)-methyl]-2-(*tert*-butyl)-4,5-dihydrooxazoline-borane adduct. LM-519

Properties white wax

Formula $C_{20}H_{39}BNOP$

Molecular Weight 351.31

tlc conditions: SiO_2, Pent / EtO_2 = 6:1

R_f = 0.31 ($KMnO_4$)

$[\alpha]^{26}_D$ = + 30.9

c 1.0. *in* CH_2Cl_2.

^{1}H NMR ($CDCl_3$, 400 MHz, 298 K) δ (ppm) = 4.36 (*ap*.t, $^{2,3}J_{HH}$ = 9.1 Hz, 1H, C*H*O), 4.24 (m, 1H, C*H*N), 3.89 (dd, $^2J_{HH}$ = 9.1 Hz, $^3J_{HH}$ = 7.3 Hz, 1H, C*H*O), 2.10 (*ap*.td, $^2J_{HP}$ = $^2J_{HH}$ = 14.3 Hz, $^3J_{HH}$ = 3.8 Hz, 1H, C*H*P), 1.91-1.65 (m, 12H, H_{Cy}), 1.52 (ddd, $^2J_{HP}$ = 14.6 Hz, $^2J_{HH}$ = 9.8 Hz, $^3J_{HH}$ = 7.3 Hz, 1H, C*H*P), 1.42-1.22 (m, 10H, H_{Cy}), 1.17 (s, 9H, $CH_{3tBu\ Ox}$), 0.24 (bq, $^1J_{HB}$ = 112.4 Hz, 3H, BH_3).

^{13}C NMR ($CDCl_3$, 101 MHz, 298 K) δ (ppm) = 174.7 (s, *C*N), 74.2 (d, $^3J_{CP}$ = 1.8 Hz, CH_2O), 62.8 (d, $^2J_{CP}$ = 2.8 Hz, *C*HN), 33.3 (s, $C_{tBu\ Ox}$), 32.8 (d, $^1J_{CP}$ = 32.3 Hz, CH_{Cy}), 31.7 (d, $^1J_{CP}$ = 34.1 Hz, $CH_{Cy'}$), 28.0 (s, $CH_{3tBu\ Ox}$), 27.1-26.5 (m, $CH_{2\ Cy}$), 26.6 (d, $^1J_{CP}$ = 26.7 Hz, CH_2P), 26.0 (s, $CH_{2\ Cy}$).

^{31}P{^{1}H} NMR ($CDCl_3$, 162 MHz, 298 K) δ (ppm) = 21.2 (m).

IR spectrum (neat) ν (cm^{-1}) = 2928, 2853, 2369, 2380, 2263, 1654, 1480, 1449, 1394, 1362, 1344, 1302, 1271, 1211, 1173, 1140, 1064, 1004, 977, 924, 890, 854, 826, 781, 732.

HRMS *(method: ESI+)*

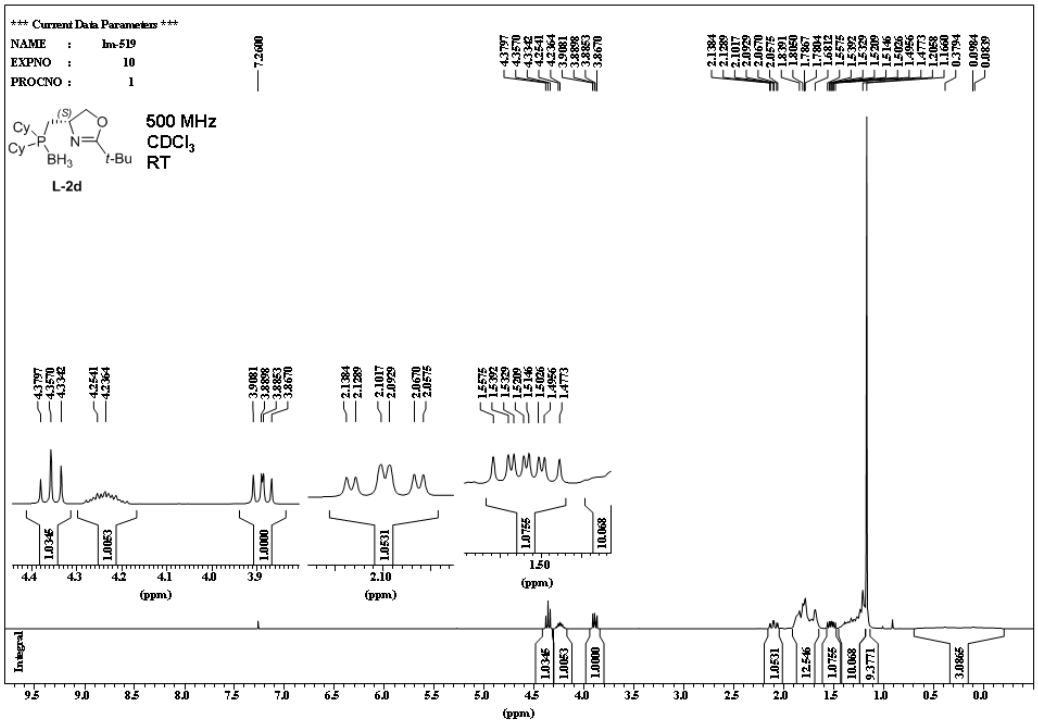
calculated for $C_{20}H_{38}BNP$ [M-H]: 350.2778,
found 350.2792.

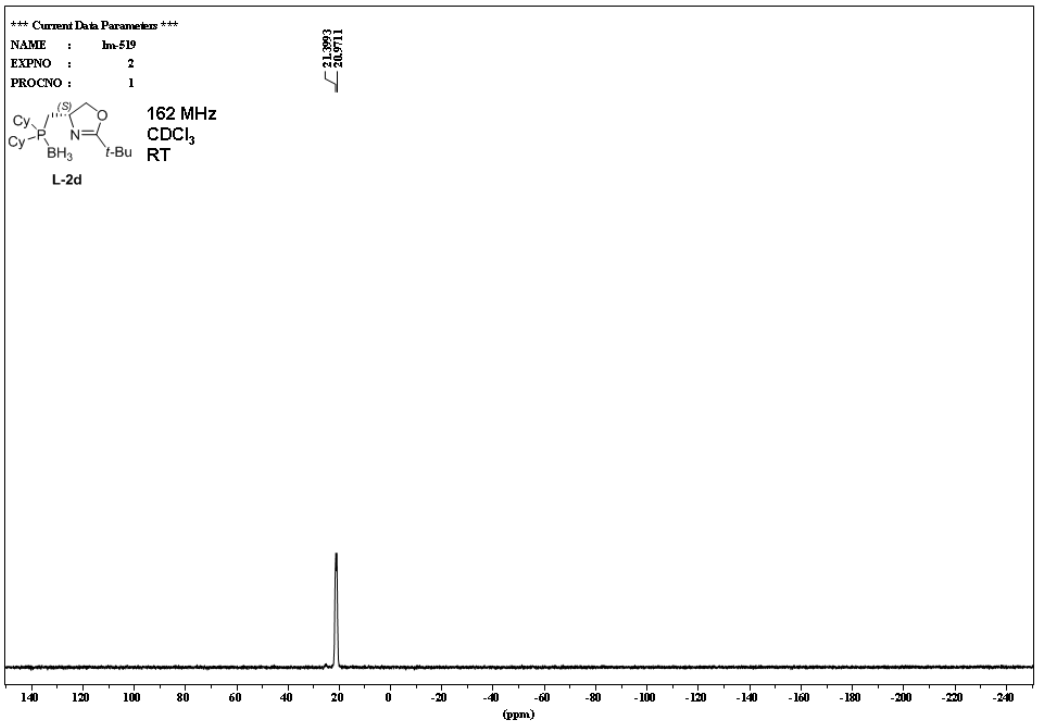
relevant literature references: S. Nanchen, A. Pfaltz *Chem. Eur. J.* **2006**, *12*, 4550-4558; M. Diéguez, O. Pàmies *Chem. Eur. J.* **2008**, *14*, 3653-3669; D.-R. Hou, K. Burgess *Org. Lett.* **1999**, *1*, 1745–1747; D.-R. Hou, J. H. Reibenspies, K. Burgess *J. Org. Chem.* **2001**, *66*, 206–215.

Separation Conditions

HPLC (column, λ_1, λ_2, eluent, flow rate, retention time):

GC (column, method or sequence, retention time):

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PROCNO : 1
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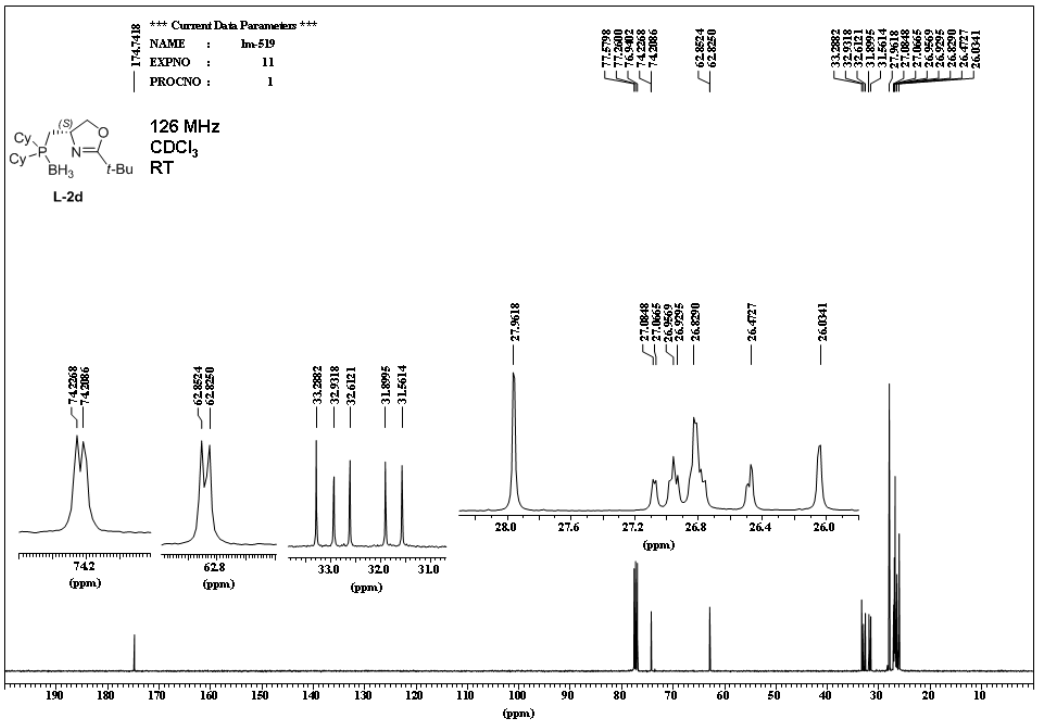
162 MHz
CDCl3
RT
L-2d
(ppm)


*** Current Data Parameters ***
NAME : lm-519
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PROCNO : 1
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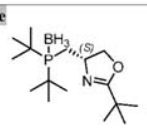
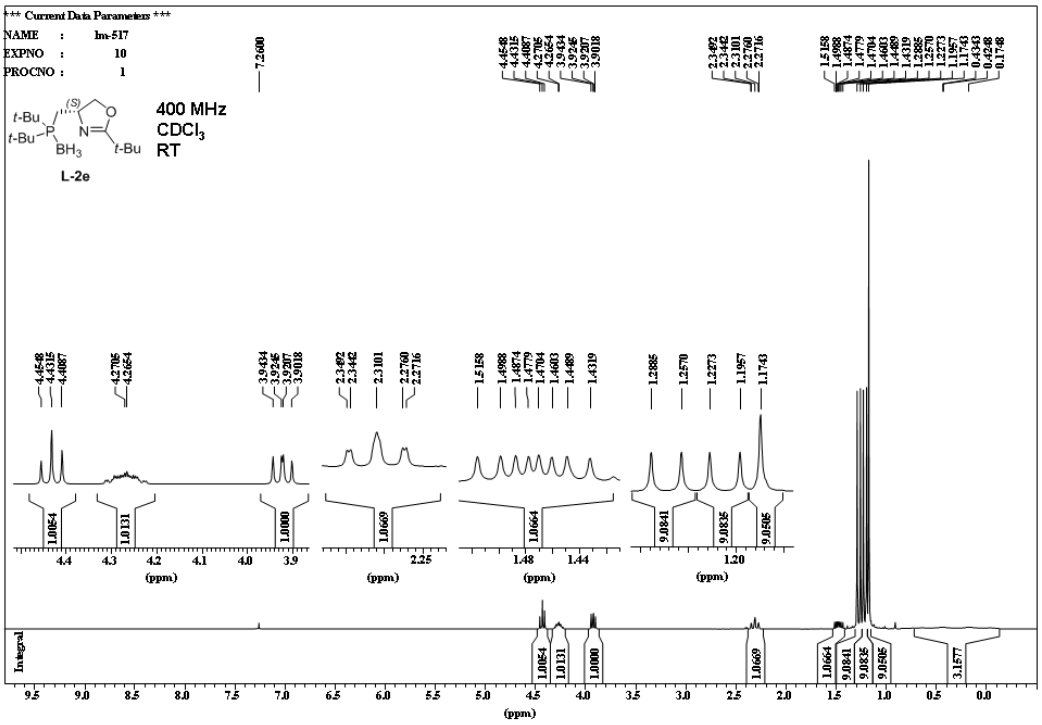
77.5798
77.2600
77.0402
74.2268
74.2886
62.8524
62.8250
33.2882
32.9318
32.6121
31.8995
31.5614
27.9618
27.0848
27.0665
26.9569
26.9295
26.8290
26.4727
26.0341
126 MHz
CDCl3
RT
L-2d
(ppm)

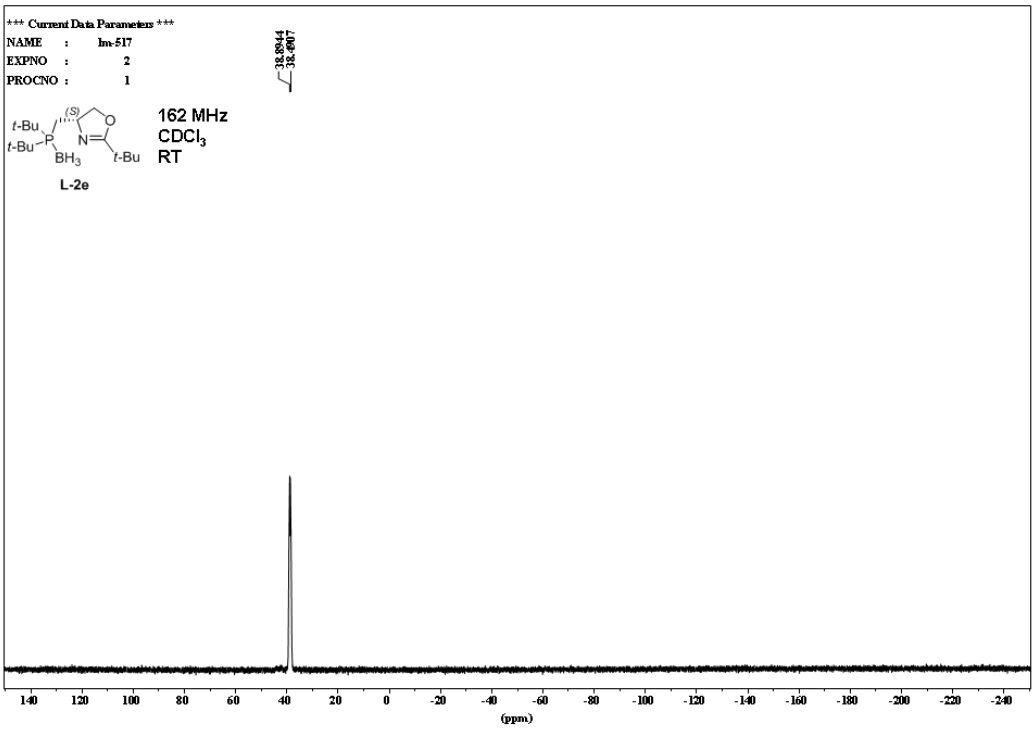
Structure	^{1}H | $^{13}C\{^{1}H\}$ | $^{31}P\{^{1}H\}$ | IR | HRMS | $[\alpha]_D$	MAZET GROUP DATA FORM
	**Name** (*S*)-4-[(di-*tert*-butylphosphanyl)-methyl]-2-(*tert*-butyl)-4,5-dihydrooxazoline-borane adduct. LM-517	
	Properties colourless oil	**Formula** $C_{16}H_{35}BNOP$
Molecular Weight 299.24	*tlc conditions:* SiO_2, Pent / EtO_2 = 3:1 R_f = 0.26 (UV)	$[\alpha]^{26}_D$ = + 11.9 *c* 1.0. *in* CH_2Cl_2.

^{1}H NMR (CDCl$_3$, 400 MHz, 298 K) δ (ppm) = 4.43 (*ap*.t, $^{2,3}J_{HH}$ = 9.2 Hz, 1H, C*H*O), 4.27 (m, 1H, C*H*N), 3.92 (dd, $^{2}J_{HH}$ = 9.2 Hz, $^{3}J_{HH}$ = 7.6 Hz, 1H, C*H*O), 2.43 (*ap*.t, $^{2}J_{HP}$ = $^{2}J_{HH}$ = 14.6 Hz, 1H, C*H*P), 1.47 (ddd, $^{2}J_{HP}$ = 18.2 Hz, $^{2}J_{HH}$ = 14.6 Hz, $^{3}J_{HH}$ = 6.8 Hz, 1H, C*H*P), 1.27 (d, $^{3}J_{HP}$ = 12.6 Hz, 9H, C$H_{3}$$_{t}$Bu), 1.21 (d, $^{3}J_{HP}$ = 12.6 Hz, 9H, C$H_{3}$$_{t}$Bu'), 1.17 (s, 9H, C$H_{3}$$_{t}$Bu Ox), 0.30 (bq, $^{1}J_{HB}$ = 103.8 Hz, 3H, BH_3).

^{13}C NMR (CDCl$_3$, 101 MHz, 298 K) δ (ppm) = 174.6 (s, *C*N), 74.5 (s, *C*H$_2$O), 63.7 (d, $^{2}J_{CP}$ = 3.7 Hz, *C*HN), 33.2 (s, C_{t}Bu Ox), 32.9 (d, $^{1}J_{CP}$ = 26.8 Hz, C_{t}Bu), 31.8 (d, $^{1}J_{CP}$ = 28.6 Hz, C_{t}Bu'), 28.0 (s, C$H_{3}$$_{t}$Bu), 27.9 (s, C$H_{3}$$_{t}$Bu Ox), 27.7 (s, C$H_{3}$$_{t}$Bu'), 25.3 (d, $^{1}J_{CP}$ = 26.8 Hz, *C*H$_2$P).

$^{31}P\{^{1}H\}$ NMR (CDCl$_3$, 162 MHz, 298 K) δ (ppm) = 38.7 (m).	**IR spectrum (neat)** ν (cm^{-1}) = 2967, 2873, 2376, 1654, 1478, 1452, 1394, 1369, 1348, 1265, 1189, 1142, 1072, 1021, 974, 928, 816, 777, 732, 667, 628.
HRMS *(method: ESI+)* calculated for $C_{16}H_{36}BNOP$ $[M+H]^+$: 300.2629, found 300.2622.	**relevant literature references**: S. Nanchen, A. Pfaltz *Chem. Eur. J.* **2006**, *12*, 4550-4558; M. Diéguez, O. Pàmies *Chem. Eur. J.* **2008**, *14*, 3653-3669; D.-R. Hou, K. Burgess *Org. Lett.* **1999**, *1*, 1745–1747; D.-R. Hou, J. H. Reibenspies, K. Burgess *J. Org. Chem.* **2001**, *66*, 206–215.
Separation Conditions	
HPLC (column, λ_1, λ_2, eluent, flow rate, retention time):	**GC (column, method or sequence, retention time)**:




*** Current Data Parameters ***
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PROCNO : 1
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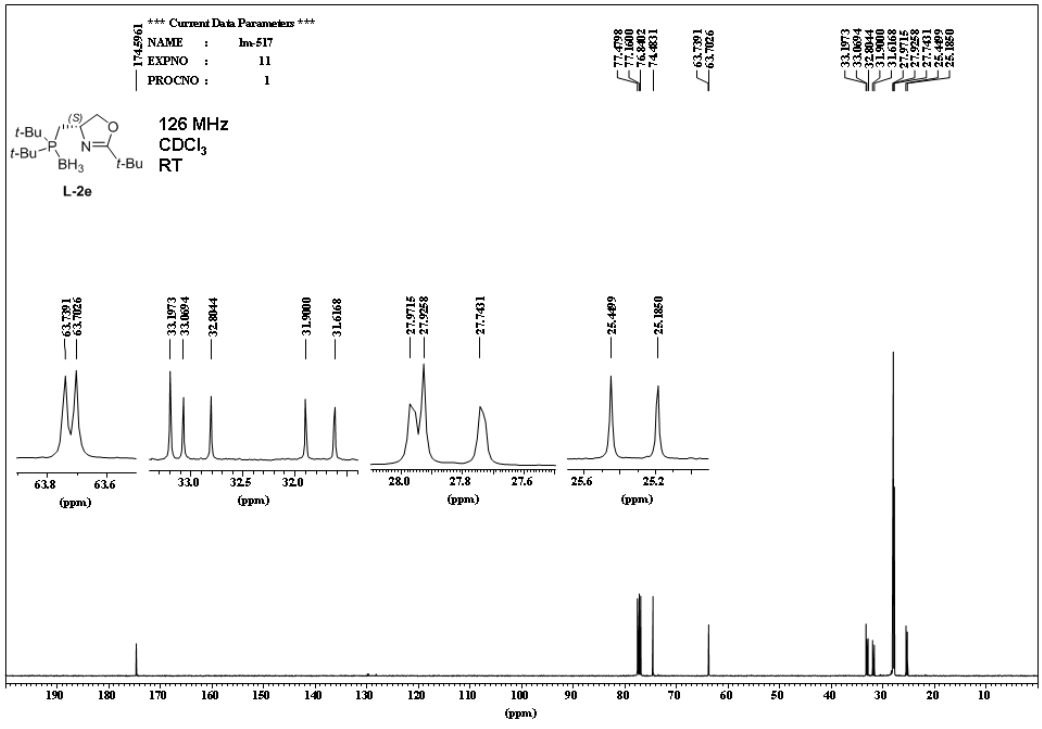
38.4907
162 MHz
CDCl3
RT
L-2e
(ppm)


*** Current Data Parameters ***
NAME : lm-517
EXPNO : 11
PROCNO : 1
174.5961
77.4798
77.1680
76.8402
74.4831
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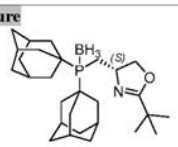
63.7026
33.1973
33.0694
32.8044
31.9000
31.6168
27.5715
27.5258
27.7431
25.4499
25.1850
126 MHz
CDCl3
RT
L-2e
(ppm)

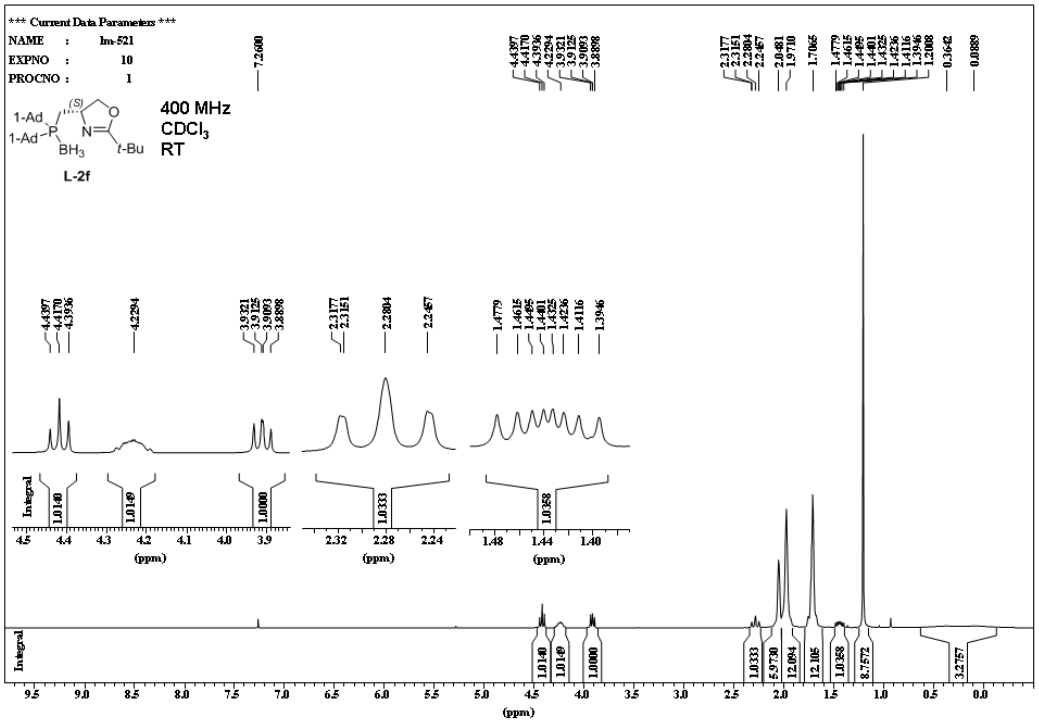
Structure	^{1}H	^{13}C{^{1}H}	^{31}P{^{1}H}	IR	HRMS	$[\alpha]_D$	MAZET GROUP DATA FORM
	**Name** (*S*)-4-[(di-1-adamantylphosphanyl)-methyl]-2-(*tert*-butyl)-4,5-dihydrooxazoline-borane adduct. LM-521						
	Properties white solid					**Formula** $C_{28}H_{47}BNOP$	
Molecular Weight 455.46	*tlc conditions:* SiO_2, Pent / EtO_2 = 8:1 R_f = 0.22 ($KMnO_4$)					$[\alpha]^{26}_D$ = + 6.6 *c* 1.0. *in* CH_2Cl_2.	*Mp* = 200 °C

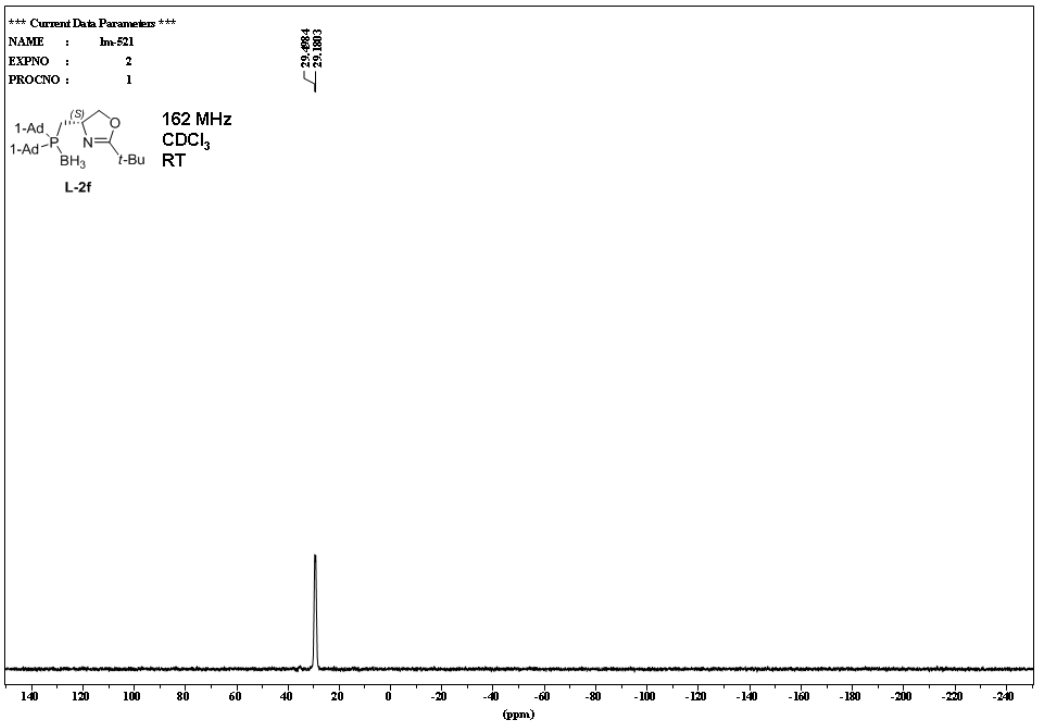
^{1}H NMR (CDCl$_3$, 400 MHz, 298 K) δ (ppm) = 4.42 (*ap*.t, $^{2,3}J_{HH}$ = 4.42 (*ap*.t, $^{2,3}J_{HH}$ = 9.1 Hz, 1H, C*H*O), 4.23 (m, 1H, C*H*N), 3.91 (dd, $^2J_{HH}$ = 9.1 Hz, $^3J_{HH}$ = 7.8 Hz, 1H, C*H*O), 2.28 (*ap*.t, $^2J_{HP}$ = $^2J_{HH}$ = 14.4 Hz, 1H, C*H*P), 2.05 (m, 6H, CH_2C$_{Ad}$), 1.97 (m, 6H, CH_2C$_{Ad}$, 6H, CHC$_{Ad}$), 1.76 (m, 12H, CH_2CH$_{Ad}$), 1.44 (ddd, $^2J_{HP}$ = 15.1 Hz, $^2J_{HH}$ = 11.4 Hz, $^3J_{HH}$ = 6.6 Hz, 1H, C*H*P), 0.23 (bq, $^1J_{HB}$ = 110.1 Hz, 3H, BH_3).

^{13}C NMR (CDCl$_3$, 101 MHz, 298 K) δ (ppm) = 174.6 (s, *C*N), 74.7 (s, *C*H$_2$O), 63.9 (d, $^2J_{CP}$ = 3.7 Hz, *C*HN), 37.8 (s, *C*H$_2$C$_{Ad}$), 37.7 (s, *C*H$_2$C$_{Ad'}$), 37.5 (d, $^1J_{CP}$ = 25.8 Hz, *C*$_{Ad}$P), 36.5 (s, *C*H$_2$CH$_{Ad}$), 36.4 (s, *C*H$_2$CH$_{Ad}$), 36.2 (d, $^1J_{CP}$ = 26.8 Hz, *C*$_{Ad'}$P), 33.2 (s, *C*$_{tBu\ OX}$), 28.1 (s, *C*HC$_{Ad}$), 28.1 (s, *C*HC$_{Ad'}$), 28.0 (s, *C*H$_{3tBu\ OX}$), 22.3 (d, $^1J_{CP}$ = 26.8 Hz, *C*H$_2$P).

^{31}P{^{1}H} NMR (CDCl$_3$, 162 MHz, 298 K) δ (ppm) = 29.3 (m).	**IR spectrum (neat)** ν (cm^{-1}) = 2903, 2849, 2409, 2383, 1656, 1478, 1469, 1450, 1411, 1359, 1343, 1304, 1269, 1183, 1144, 1103, 1077, 1052, 975, 930, 880, 836, 816, 801, 766.
HRMS *(method: ESI+)* calculated for $C_{28}H_{46}BNOP$ [M-H]: 454.3404, found 454.3389.	**relevant literature references**: S. Nanchen, A. Pfaltz *Chem. Eur. J.* **2006**, *12*, 4550-4558; M. Diéguez, O. Pàmies *Chem. Eur. J.* **2008**, *14*, 3653-3669; D.-R. Hou, K. Burgess *Org. Lett.* **1999**, *1*, 1745–1747; D.-R. Hou, J. H. Reibenspies, K. Burgess *J. Org. Chem.* **2001**, *66*, 206–215.

Separation Conditions	
HPLC (column, λ_1, λ_2, eluent, flow rate, retention time):	**GC (column, method or sequence, retention time)**:

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PROCNO : 1
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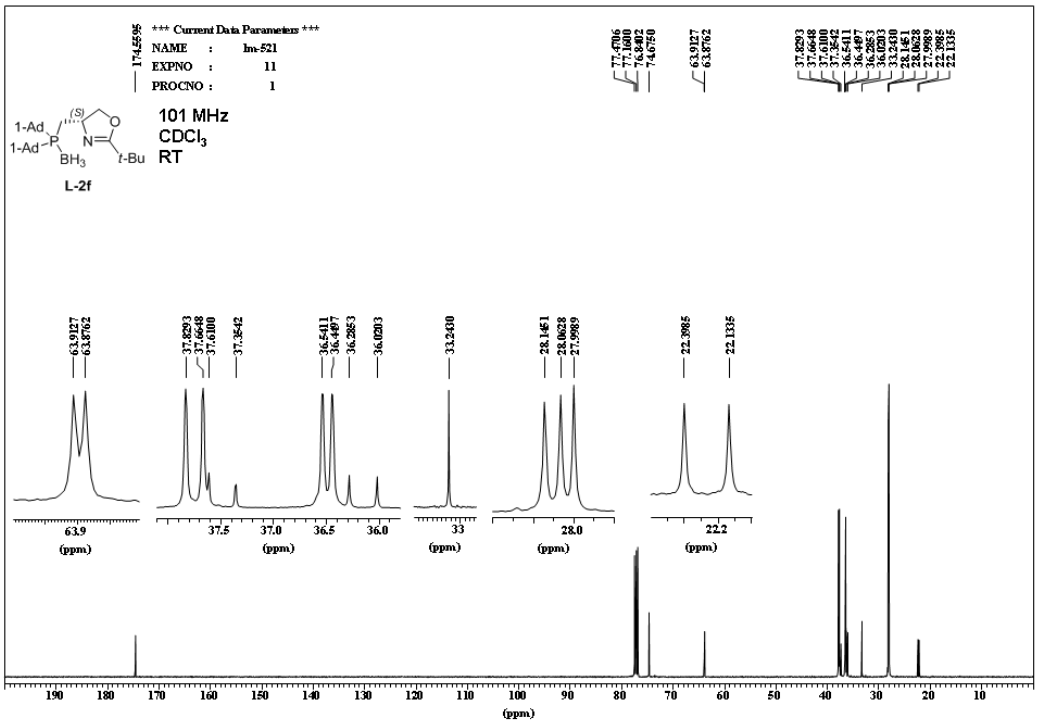
29.1803
1-Ad
1-Ad
P
BH3
(S)
N
O
t-Bu
162 MHz
CDCl3
RT
L-2f
140 120 100 80 60 40 20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220 -240
(ppm)


174.5595
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PROCNO : 1
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74.6750
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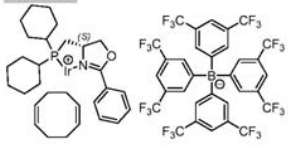
63.8762
37.8293
37.6648
37.6100
37.3542
36.5411
36.4497
36.2853
36.0203
33.2430
28.1451
28.0628
27.7989
22.3985
22.1335
1-Ad
1-Ad
P
BH3
(S)
N
O
t-Bu
101 MHz
CDCl3
RT
L-2f
63.9 (ppm)
37.5 37.0 36.5 36.0 (ppm)
33 (ppm)
28.0 (ppm)
22.2 (ppm)
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
(ppm)

Structure	^{1}H	$^{13}C\{^{1}H\}$	$^{31}P\{^{1}H\}$	IR	HRMS	$[\alpha]_D$	MAZET GROUP DATA FORM



Name (*S*)-4-[(Di-cyclohexylphosphanyl)-methyl]-2-(phenyl)-4,5-dihydrooxazoline-η^4-(1,5-cyclooctadiene) iridium(I) tetrakis-[3,5-bis(trifluoromethyl)phenyl]borate. LM-428

Properties orange-beige solid

Formula $C_{62}H_{56}BF_{24}IrNOP$

Molecular Weight 1521.08

tlc conditions: SiO_2, CH_2Cl_2

R_f = 0.89 (UV)

$[\alpha]^{26}_D$ = + 38.2

c 1.0. *in* CH_2Cl_2.

Mp = 73-75°C

^{1}H NMR (CDCl$_3$, 500 MHz, 298 K) δ(ppm) = 8.16 (m, 2H, H_{oPh}), 7.72 (s, 8H, H_{oBArF}, 1H, H_{pPh}), 7.53 (m, 4H, H_{pBArF} 2H, H_{mPh}), 5.05 (m, 1H, CH_{COD}), 4.80 (m, 1H, CH_{COD}), 4.57 (m, 2H, CH_2O), 4.37 (m, 1H, *CH*N), 3.73 (m, 1H, CH_{COD}), 3.60 (m, 1H, CH_{COD}), 2.49-1.22 (m, 22H, H_{Cy}, 8H, $CH_{2\,COD}$, 2H, CH_2P).

$^{13}C\{^{1}H\}$ NMR (CDCl$_3$, 126 MHz, 298 K) δ(ppm) = 170.4 (s, *C*N), 161.9 (q, $^{1}J_{CB}$ = 49.9 Hz, $C_{ipsoBArF}$), 135.1 (s, C_{pPh}), 135.0 (s, C_{oBArF}), 131.0 (s, C_{oPh}), 129.0 (q, $^{2}J_{CF}$ = 31.5 Hz, CCF_3), 128.9 (s, C_{mPh}), 124.7 (q, $^{1}J_{CF}$ = 273.3 Hz, CF_3), 123.2 (s, C_{ipsoPh}), 117.6 (s, C_{pBArF}), 94.6 (d, $^{2}J_{CP}$ = 8.3 Hz, CH_{COD}), 84.1 (d, $^{2}J_{CP}$ = 14.7 Hz, CH_{COD}), 72.0 (d, $^{3}J_{CP}$ = 11.9 Hz, CH_2O), 71.0 (d, $^{2}J_{CP}$ = 4.6 Hz, *C*HN), 66.7 (s, CH_{COD}), 63.0 (s, CH_{COD}), 36.5 (d, $^{3}J_{CP}$ = 3.7 Hz, $CH_{2\,COD}$), 34.7 (d, $^{1}J_{CP}$ = 25.7 Hz, CH_{Cy}), 32.2 (d, $^{1}J_{CP}$ = 28.5 Hz, $CH_{Cy'}$), 32.2 (s, $CH_{2\,COD}$), 30.4 (d, $^{2}J_{CP}$ = 1.8 Hz, $CH_{2\,Cy}$), 30.1 (d, $^{2}J_{CP}$ = 2.8 Hz, $CH_{2\,Cy}$), 29.3 (s, $CH_{2\,Cy}$), 29.1 (s, $CH_{2\,COD}$), 28.0 (s, $CH_{2\,Cy}$), 26.0 (s, $CH_{2\,Cy}$), 25.8 (s, $CH_{2\,COD}$), 25.0 (d, $^{1}J_{CP}$ = 28.5 Hz, CH_2P).

$^{31}P\{^{1}H\}$ NMR (CDCl$_3$, 202 MHz, 298 K) δ(ppm) = 28.5 (s).

IR spectrum (neat) ν (cm^{-1}) = 2935, 2859, 1610, 1577, 1495, 1450, 1353, 1273, 1158, 1116, 1002, 975, 934, 886, 839, 777, 744, 712, 682, 669.

HRMS *(method: ESI+)*

calculated for $C_{30}H_{44}IrNOP$ [M-BAr_F]$^+$: 658.2784,

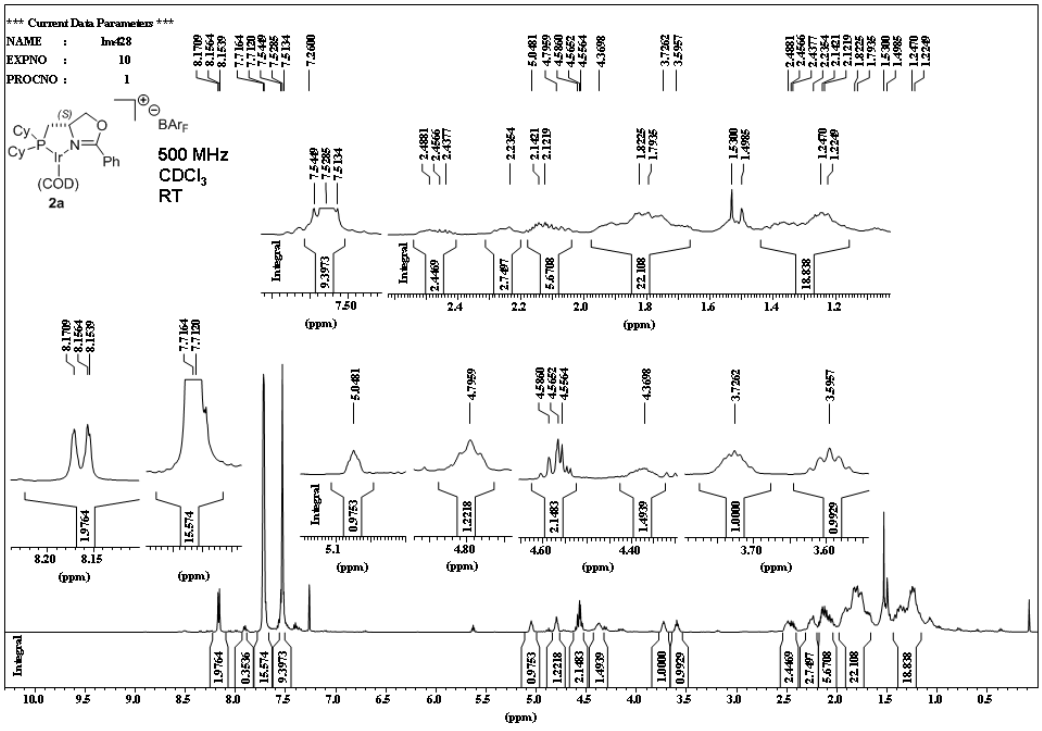
found 658.2805.

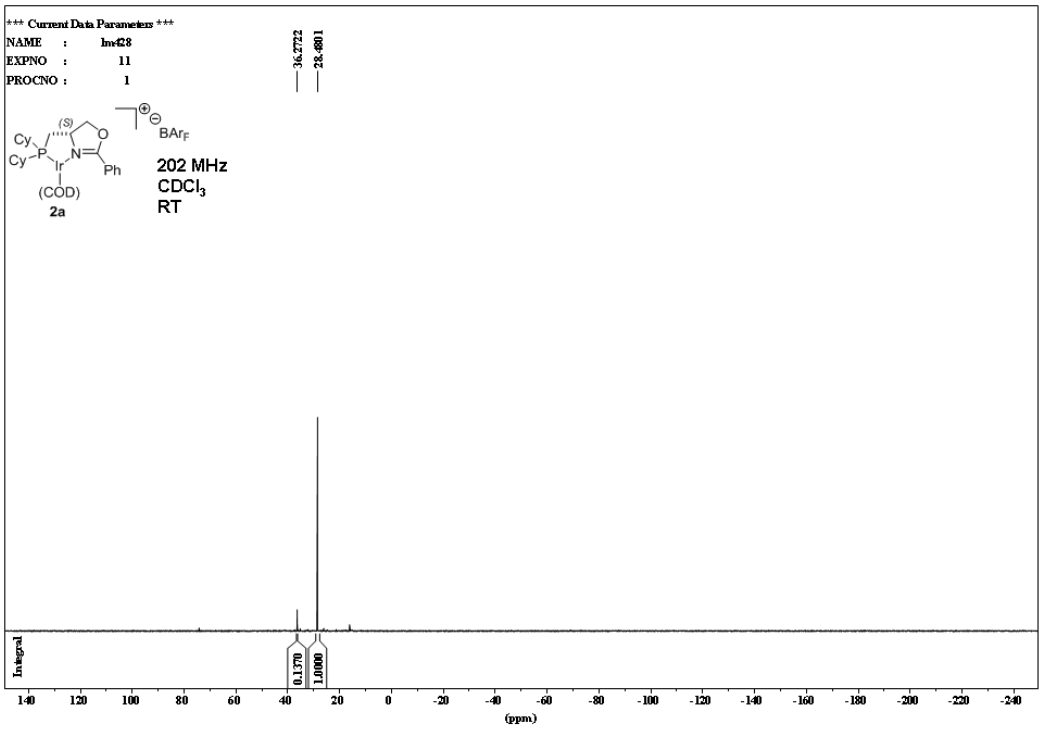
relevant literature references: S. Nanchen, A. Pfaltz *Chem. Eur. J.* **2006**, *12*, 4550-4558; M. Diéguez, O. Pàmies *Chem. Eur. J.* **2008**, *14*, 3653-3669; D.-R. Hou, K. Burgess *Org. Lett.* **1999**, *1*, 1745–1747; D.-R. Hou, J. H. Reibenspies, K. Burgess *J. Org. Chem.* **2001**, *66*, 206–215.

Separation Conditions

HPLC (column, λ_1, λ_2, eluent, flow rate, retention time):

GC (column, method or sequence, retention time):




*** Current Data Parameters ***
NAME : lmv428
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PROCNO : 1
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28.4891
202 MHz
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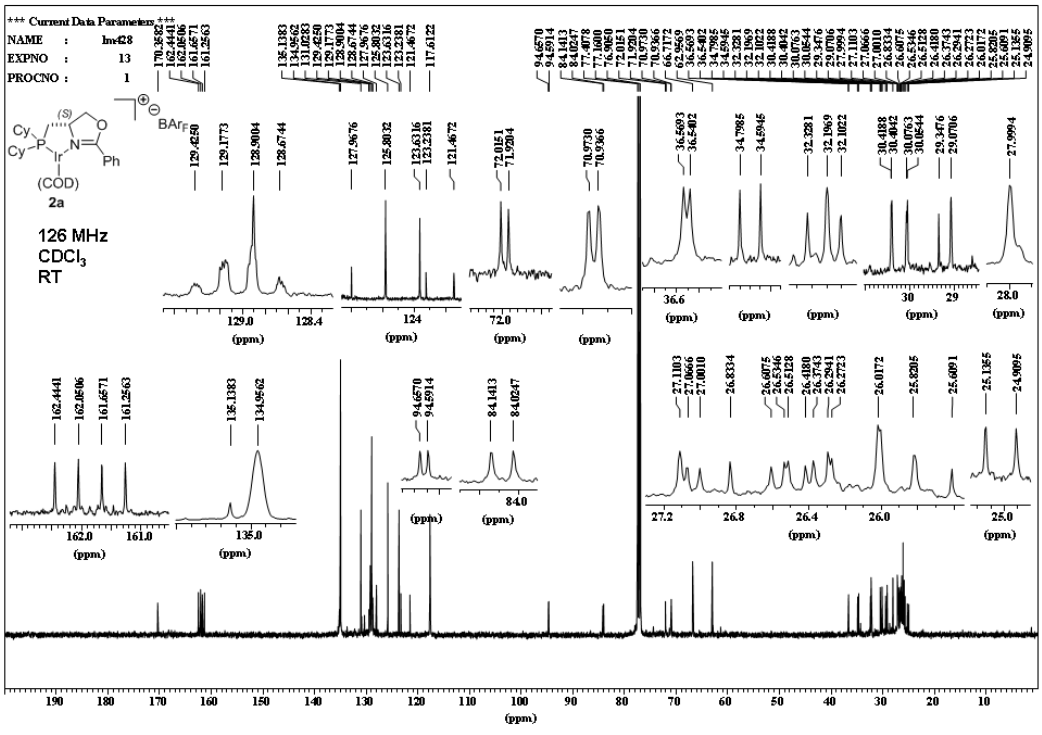
RT
2a
Integral
0.1370
1.0000
(ppm)


*** Current Data Parameters ***
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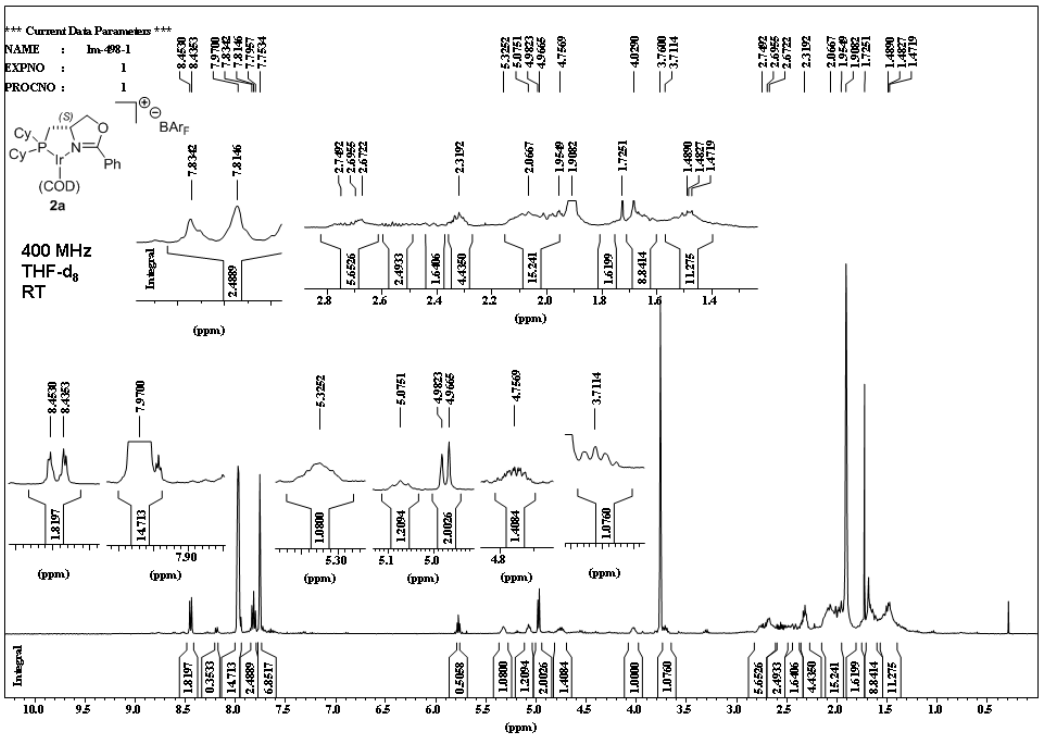
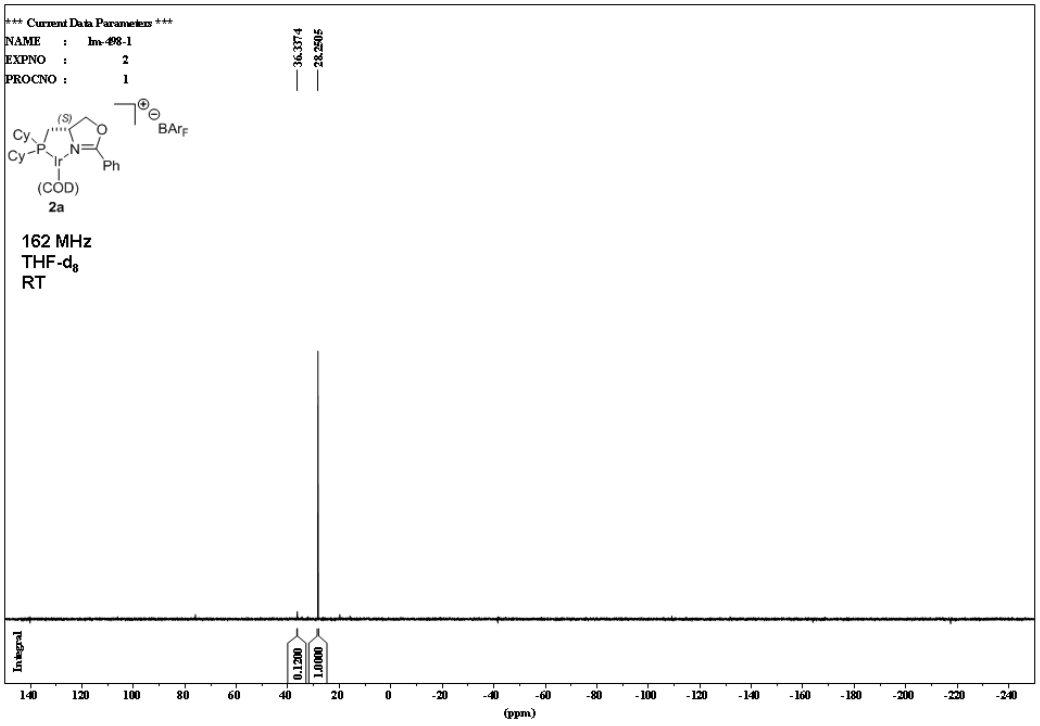
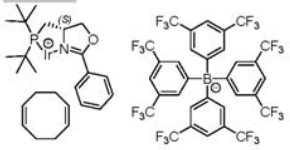
EXPNO : 13
PROCNO : 1
126 MHz
CDCl3
RT
2a
(ppm)


*** Current Data Parameters ***
NAME : lm-498-1
EXPNO : 1
PROCNO : 1
2a
400 MHz
THF-d8
RT
(ppm)
Integral


*** Current Data Parameters ***
NAME : lm-498-1
EXPNO : 2
PROCNO : 1
2a
162 MHz
THF-d8
RT
(ppm)
Integral

Structure	^{1}H	^{13}C{^{1}H}	^{31}P{^{1}H}	IR	HRMS	$[\alpha]_D$	MAZET GROUP DATA FORM



Name (*S*)-4-[(Di-*tert*-butylphosphanyl)-methyl]-2-(phenyl)-4,5-dihydrooxazoline-η^4-(1,5-cyclooctadiene) iridium(I) tetrakis-[3,5-bis(trifluoromethyl)phenyl]borate. LM-424

Properties orange solid

Formula $C_{58}H_{52}BF_{24}IrNOP$

Molecular Weight 1469.00

tlc conditions: SiO_2, CH_2Cl_2

R_f = 0.88 (UV)

$[\alpha]^{26}_D$ = + 33.7

c 1.0. *in* CH_2Cl_2.

Mp = 112-114°C

^{1}H NMR ($CDCl_3$, 500 MHz, 298 K) δ (ppm) = 8.25 (m, 2H, H_{oPh}), 7.72 (s, 8H, H_{oBArF}, 1H, H_{pPh}), 7.53 (s, 4H, H_{pBArF}), 7.50 (m, 2H, H_{mPh}), 5.18 (m, 1H, CH_{COD}), 4.92 (m, 1H, CH_{COD}), 4.62 (m, 2H, CH_2O), 4.46 (m, 1H, CHN), 4.38 (m, 1H, CH_{COD}), 3.43 (m, 1H, CH_{COD}), 2.54-2.14 (m, 4H, $CH_{2\,COD}$, 1H, CHP), 1.91-1.32 (m, 4H, $CH_{2\,COD}$, 1H, CHP), 1.44 (d, $^3J_{HP}$ = 13.9 Hz, 9H, CH_{3tBu}), 1.24 (d, $^3J_{HP}$ = 14.2 Hz, 9H, $CH_{3tBu'}$).

^{13}C{^{1}H} NMR ($CDCl_3$, 126 MHz, 298 K) δ (ppm) = 170.0 (s, *C*N), 161.8 (q, $^1J_{CB}$ = 49.9 Hz, $C_{ipsoBArF}$), 135.3 (s, C_{pPh}), 134.9 (s, C_{oBArF}), 131.2 (s, C_{oPh}), 129.1 (q, $^2J_{CF}$ = 31.5 Hz, CCF_3), 128.9 (s, C_{mPh}), 124.7 (q, $^1J_{CF}$ = 273.0 Hz, CF_3), 123.0 (s, C_{ipsoPh}), 117.6 (s, C_{pBArF}), 90.5 (d, $^2J_{CP}$ = 6.4 Hz, CH_{COD}), 78.5 (d, $^2J_{CP}$ = 16.5 Hz, CH_{COD}), 72.0 (d, $^3J_{CP}$ = 11.9 Hz, CH_2O), 71.0 (d, $^2J_{CP}$ = 5.5 Hz, *C*HN), 70.5 (s, CH_{COD}), 62.4 (s, CH_{COD}), 37.6 (d, $^3J_{CP}$ = 3.7 Hz, $CH_{2\,COD}$), 37.0 (d, $^1J_{CP}$ = 16.5 Hz, C_{tBu}), 36.3 (d, $^1J_{CP}$ = 19.3 Hz, $C_{tBu'}$), 33.5 (s, $CH_{2\,COD}$), 30.0 (s CH_{3tBu}), 29.9 (s $CH_{3tBu'}$), 29.2 (s, $CH_{2\,COD}$), 27.2 (d, $^1J_{CP}$ = 24.8 Hz, CH_2P), 25.2 (d, $^2J_{CP}$ = 2.7 Hz, $CH_{2\,COD}$).

^{31}P{^{1}H} NMR ($CDCl_3$, 202 MHz, 298 K) δ (ppm) = 46.5 (s).

IR spectrum (neat) ν (cm^{-1}) = 2967, 2917, 1610, 1597, 1495, 1473, 1452, 1353, 1272, 1159, 1114, 998, 934, 886, 839, 810, 778, 745, 712, 701, 681, 669.

HRMS *(method: ESI+)*

calculated for $C_{26}H_{40}IrNOP$ [M-BAr_F]$^+$: 606.2471,

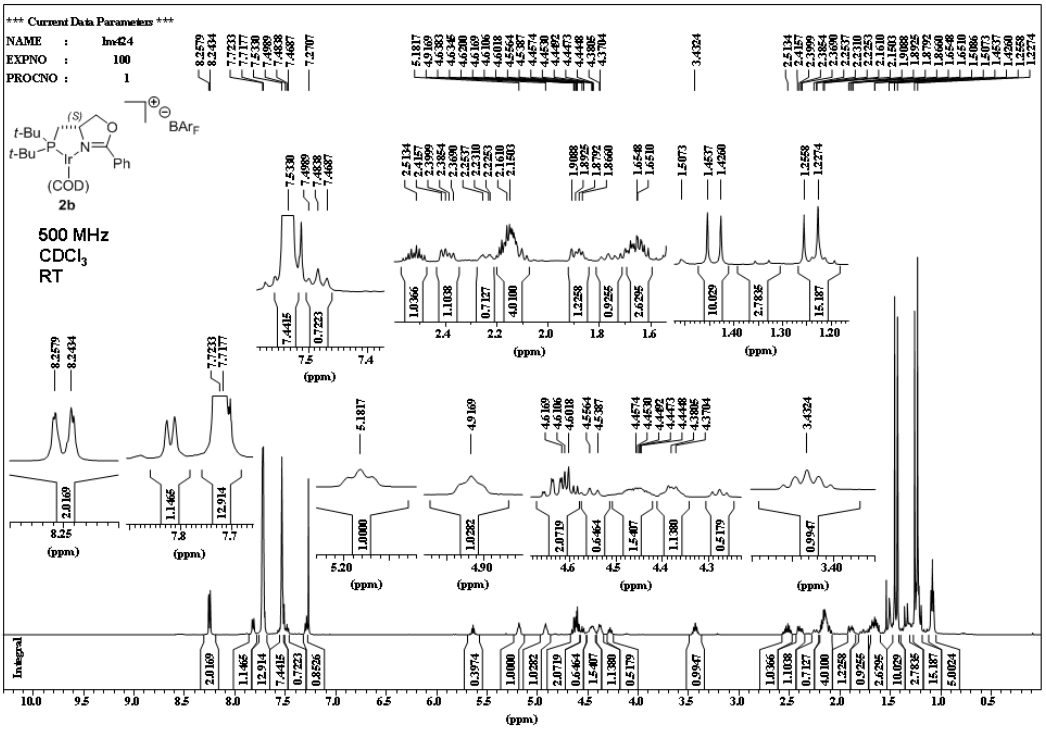
found. 606.2498.

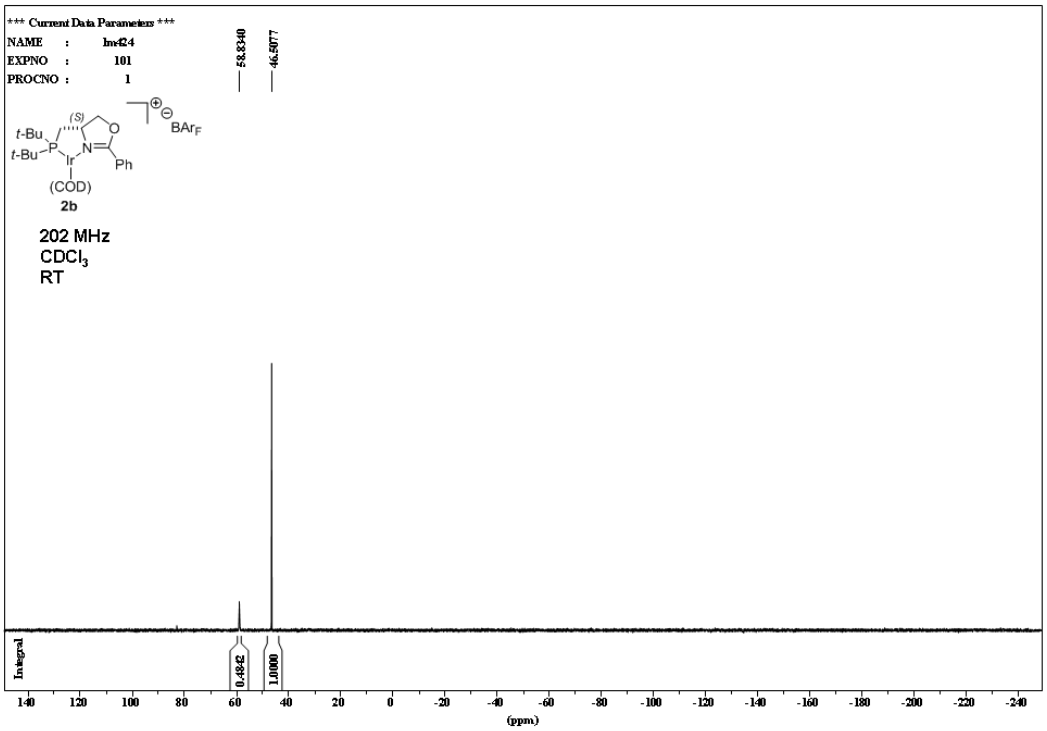
relevant literature references: S. Nanchen, A. Pfaltz *Chem. Eur. J.* **2006**, *12*, 4550-4558; M. Diéguez, O. Pàmies *Chem. Eur. J.* **2008**, *14*, 3653-3669; D.-R. Hou, K. Burgess *Org. Lett.* **1999**, *1*, 1745–1747; D.-R. Hou, J. H. Reibenspies, K. Burgess *J. Org. Chem.* **2001**, *66*, 206–215.

Separation Conditions

HPLC (column, λ_1, λ_2, eluent, flow rate, retention time):

GC (column, method or sequence, retention time):




*** Current Data Parameters ***
NAME : lmr424
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PROCNO : 1
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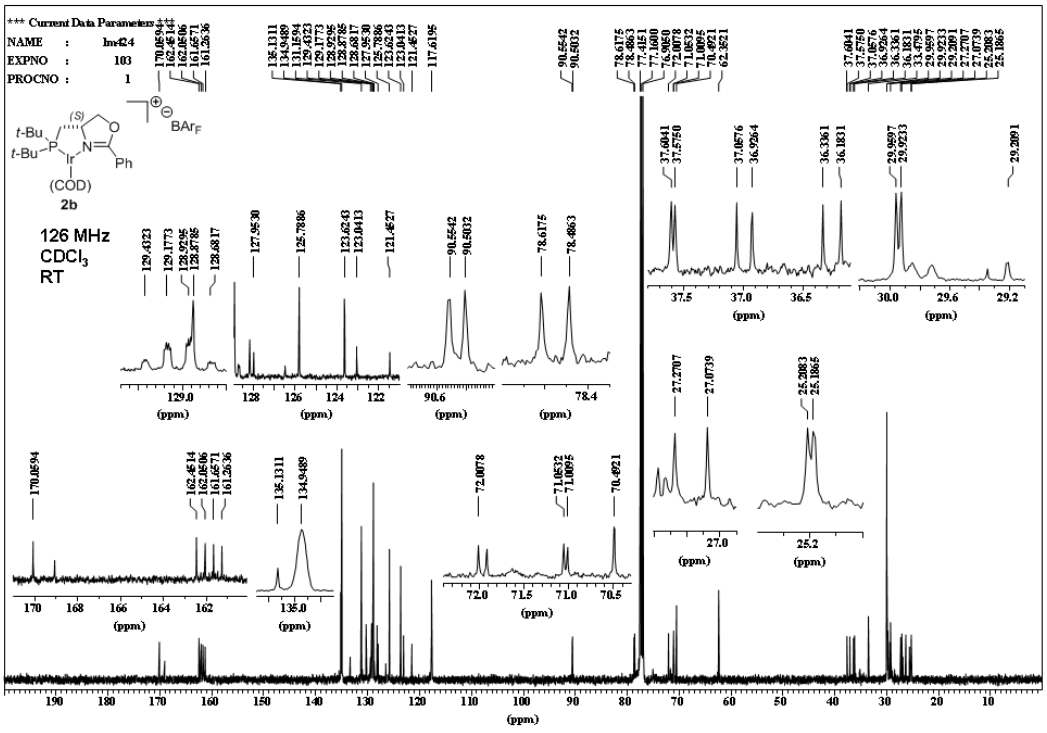
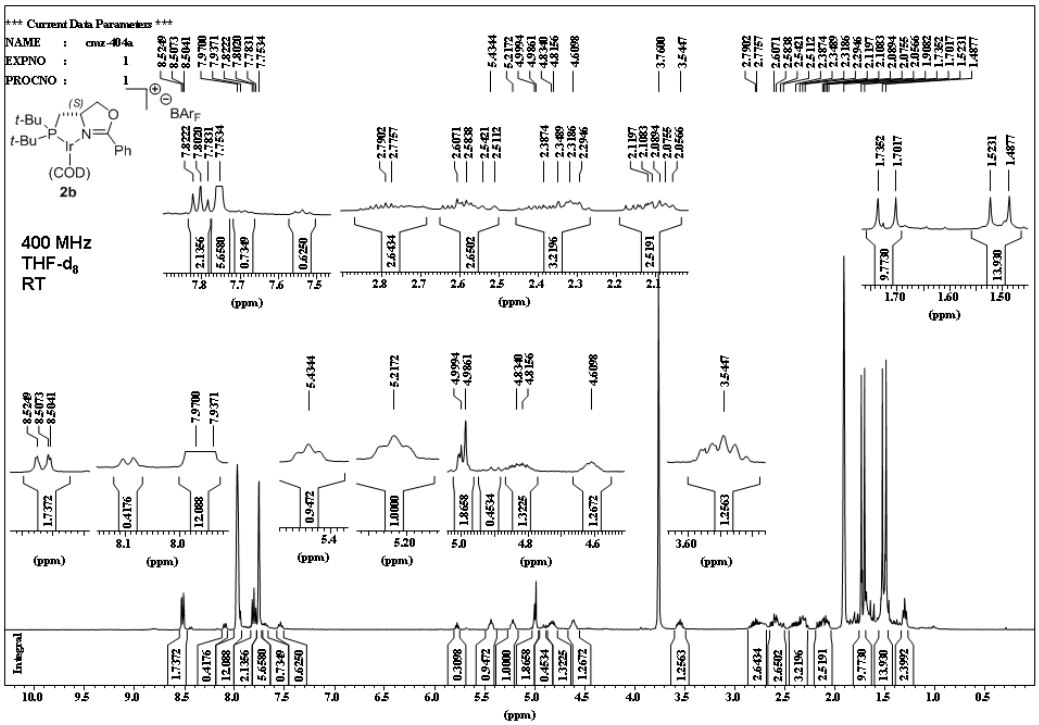
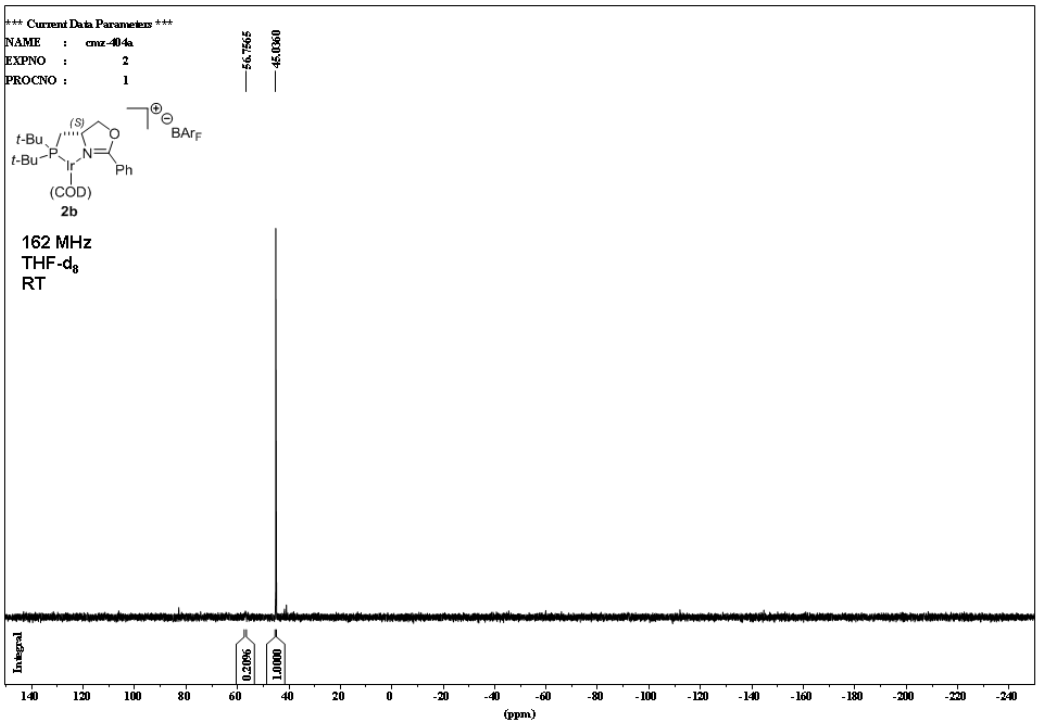
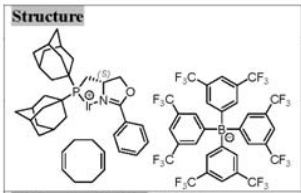
46.8077
2b
202 MHz
CDCl3
RT
Integral
0.4842
1.0000
(ppm)


*** Current Data Parameters ***
NAME : lmr424
EXPNO : 103
PROCNO : 1
2b
126 MHz
CDCl3
RT
(ppm)


*** Current Data Parameters ***
NAME : cmz-404a
EXPNO : 1
PROCNO : 1
400 MHz
THF-d8
RT
2b
(COD)
Integral
(ppm)


*** Current Data Parameters ***
NAME : cmz-404a
EXPNO : 2
PROCNO : 1
162 MHz
THF-d8
RT
2b
(COD)
Integral
(ppm)

Structure	^{1}H	^{13}C{^{1}H}	^{31}P{^{1}H}	IR	HRMS	$[\alpha]_D$	MAZET GROUP DATA FORM



Name (*S*)-4-[(di-1-adamantylphosphanyl)-methyl]-2-(phenyl)-4,5-dihydrooxazoline-η^4-(1,5-cyclooctadiene) iridium(I) tetrakis-[3,5-bis(trifluoromethyl)phenyl]borate. LM-426

Properties orange solid

Formula $C_{70}H_{64}BF_{24}IrNOP$

Molecular Weight 1625.23

tlc conditions: SiO_2, CH_2Cl_2

R_f = 0.86 (UV)

$[\alpha]^{26}_D$ = + 32.0

c 1.0. *in* CH_2Cl_2.

Mp = 94-96°C

^{1}H NMR ($CDCl_3$, 500 MHz, 298 K) δ (ppm) = 8.21 (m, 2H, H_{oPh}), 7.73 (s, 8H, H_{oBArF}), 7.70 (m, 1H, H_{pPh}), 7.53 (s, 4H, H_{pBArF}), 7.52 (m, 2H, H_{mPh}), 5.30 (m, 1H, CH_{COD}), 4.81 (m, 1H, CH_{COD}), 4.62 (m, 2H, CH_2O, 1H, CH_{COD}), 4.43 (m, 1H, CHN), 3.29 (m, 1H, CH_{COD}), 2.65-1.24 (m, 30H, H_{Ad}, 8H, $CH_{2\,COD}$, 2H, CH_2P).

^{13}C{^{1}H} NMR ($CDCl_3$, 126 MHz, 298 K) δ (ppm) = 169.9 (s, *C*N), 161.9 (q, $^1J_{CB}$ = 49.9 Hz, $C_{ipsoBArF}$), 134.9 (s, C_{oBArF}, C_{pPh}), 130.9 (s, C_{oPh}), 129.0 (q, $^2J_{CF}$ = 32.4 Hz, *C*CF_3), 128.8 (s, C_{mPh}), 124.7 (q, $^1J_{CF}$ = 273.3 Hz, *C*F_3), 123.3 (s, C_{ipsoPh}), 117.6 (s, C_{pBArF}), 88.3 (d, $^2J_{CP}$ = 6.4 Hz, CH_{COD}), 76.7 (d, $^2J_{CP}$ = 16.5 Hz, CH_{COD}), 72.0 (d, $^3J_{CP}$ = 11.1 Hz, CH_2O), 71.6 (d, $^2J_{CP}$ = 5.5 Hz, *C*HN), 71.2 (s, CH_{COD}), 62.1 (s, CH_{COD}), 42.9 (d, $^1J_{CP}$ = 15.6 Hz, C_{Ad}P), 42.6 (d, $^1J_{CP}$ = 13.8 Hz, $C_{Ad'}$P), 41.4 (s, CH_2C_{Ad}), 40.6 (s, $CH_2C_{Ad'}$), 37.7 (d, $^3J_{CP}$ = 4.6 Hz, $CH_{2\,COD}$), 36.3 (s, CH_2CH_{Ad}), 36.2 (s, $CH_2CH_{Ad'}$), 33.7 (s, $CH_{2\,COD}$), 29.1 (s, $CH_{2\,COD}$), 28.4 (d, $^3J_{CP}$ = 8.3 Hz, CHC_{Ad}), 28.3 (d, $^3J_{CP}$ = 9.2 Hz, $CHC_{Ad'}$), 25.2 (d, $^2J_{CP}$ = 2.7 Hz, $CH_{2\,COD}$), 23.2 (d, $^1J_{CP}$ = 24.8 Hz, CH_2P).

^{31}P{^{1}H} NMR ($CDCl_3$, 202 MHz, 298 K) δ (ppm) = 38.6 (s).

IR spectrum (neat) ν (cm^{-1}) = 2910, 2856, 1610, 1599, 1575, 1497, 1452, 1353, 1273, 1158, 1117, 971, 940, 886, 839, 777, 745, 712, 700, 682, 669.

HRMS *(method: ESI+)*

calculated for $C_{38}H_{52}IrNOP$ [M-BAr_F]$^+$: 762.3410,

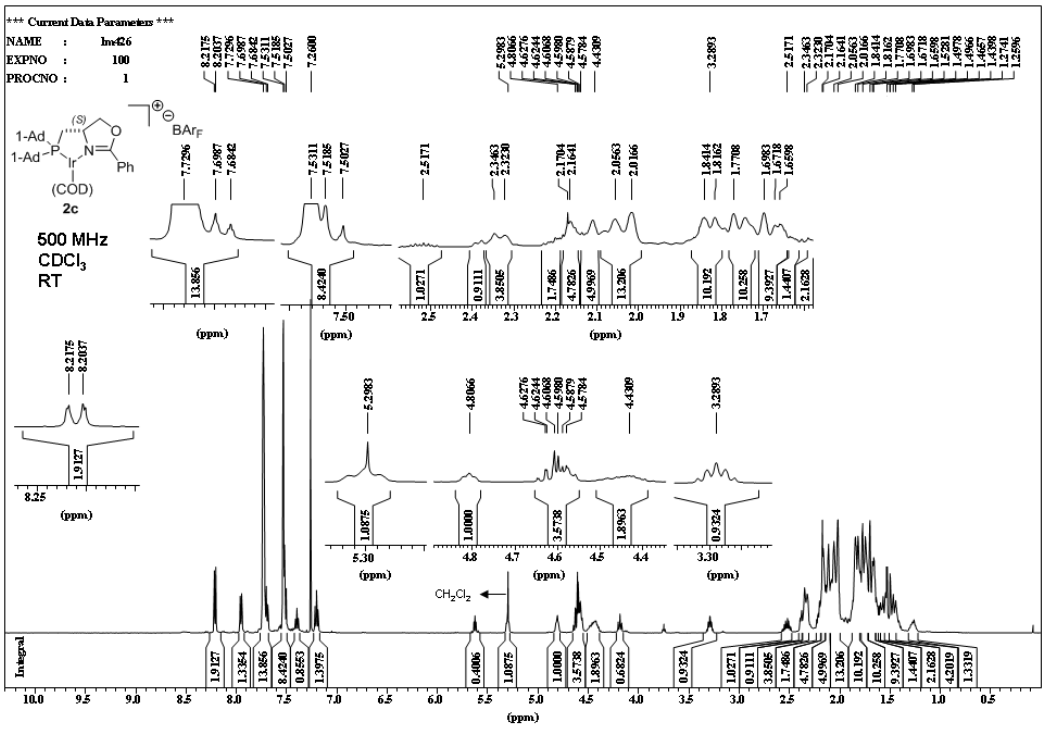
found 762.3414.

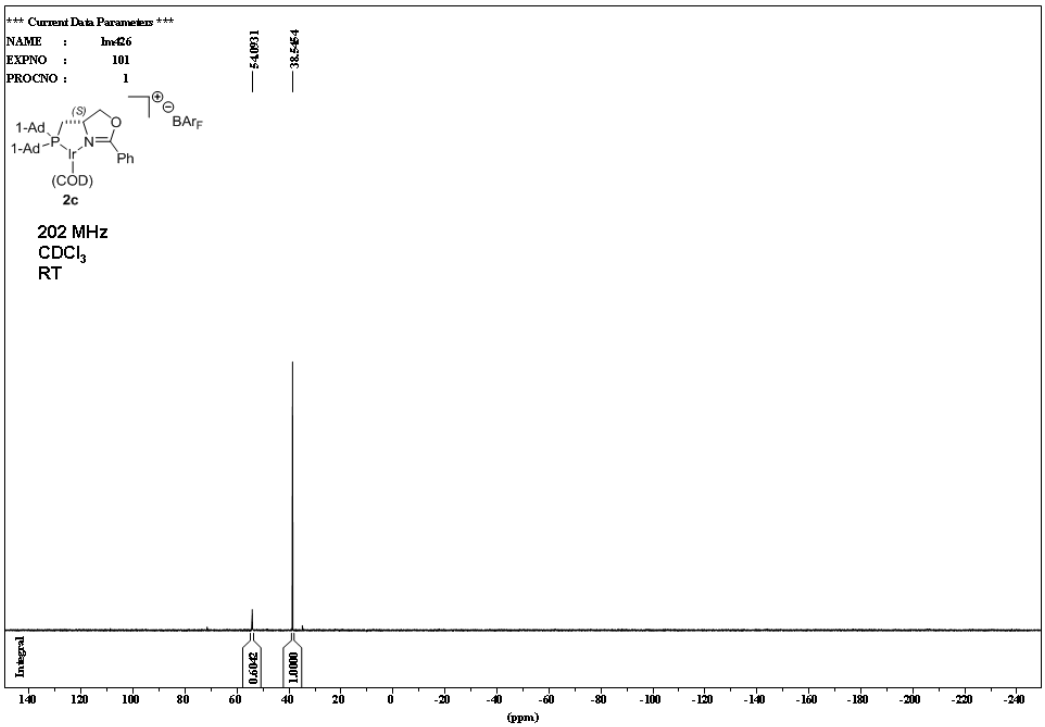
relevant literature references: S. Nanchen, A. Pfaltz *Chem. Eur. J.* **2006**, *12*, 4550-4558; M. Diéguez, O. Pàmies *Chem. Eur. J.* **2008**, *14*, 3653-3669; D.-R. Hou, K. Burgess *Org. Lett.* **1999**, *1*, 1745–1747; D.-R. Hou, J. H. Reibenspies, K. Burgess *J. Org. Chem.* **2001**, *66*, 206–215.

Separation Conditions

HPLC (column, λ_1, λ_2, eluent, flow rate, retention time):

GC (column, method or sequence, retention time):




*** Current Data Parameters ***
NAME : lnv426
EXPNO : 101
PROCNO : 1
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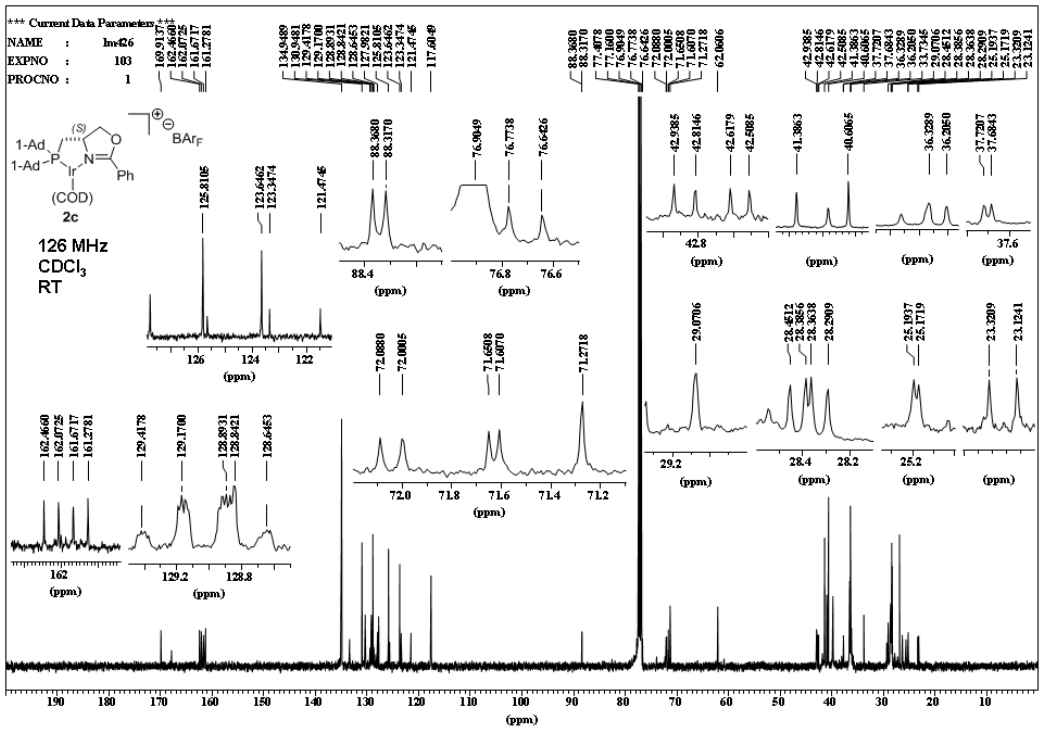
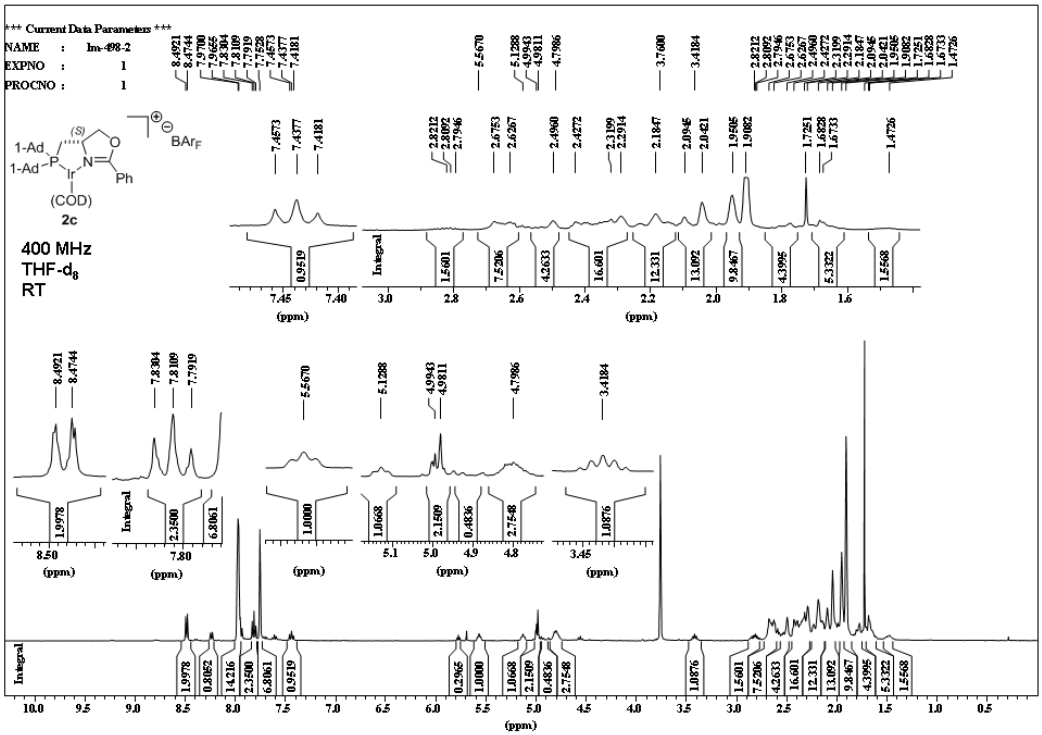
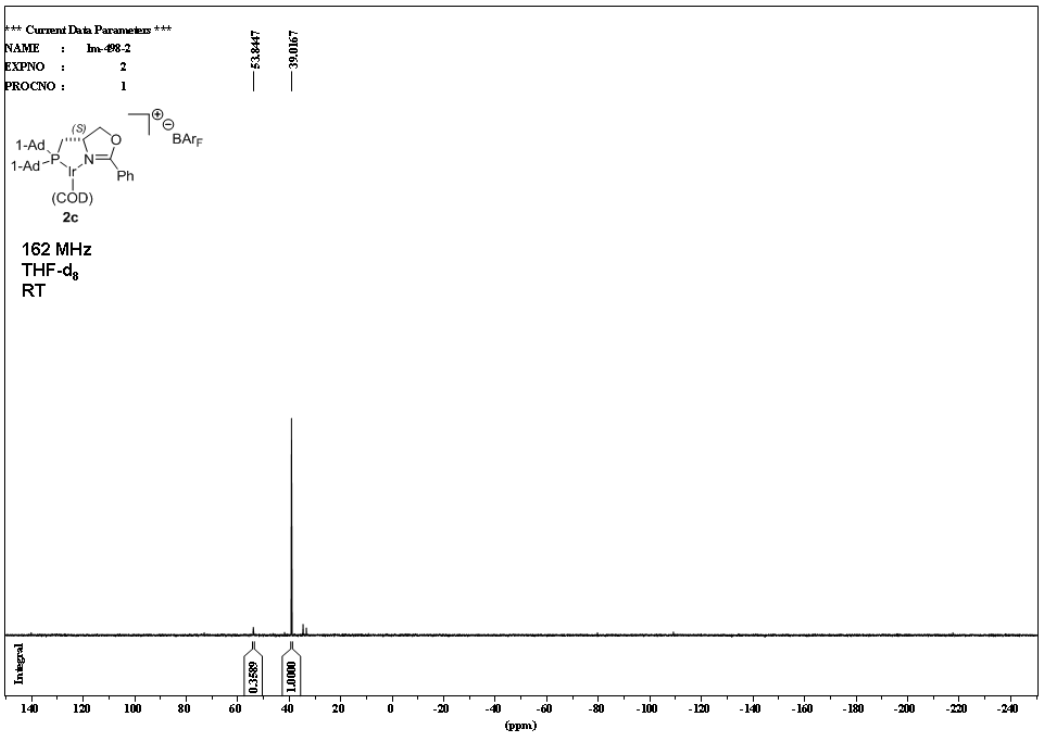
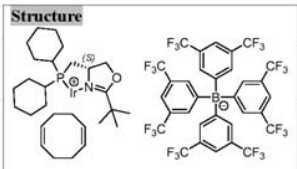
38.5454
1-Ad
1-Ad
P
Ir
N
O
(S)
Ph
(COD)
BArF
2c
202 MHz
CDCl3
RT
Integral
0.6042
1.0000
(ppm)


*** Current Data Parameters ***
NAME : lnv426
EXPNO : 103
PROCNO : 1
2c
126 MHz
CDCl3
RT
(ppm)


*** Current Data Parameters ***
NAME : lm-498-2
EXPNO : 1
PROCNO : 1
2c
400 MHz
THF-d8
RT
(ppm)
Integral


*** Current Data Parameters ***
NAME : lm-498-2
EXPNO : 2
PROCNO : 1
2c
162 MHz
THF-d8
RT
(ppm)
Integral

Structure	^{1}H	$^{13}C\{^1H\}$	$^{31}P\{^1H\}$	IR	HRMS	$[\alpha]_D$	MAZET GROUP DATA FORM



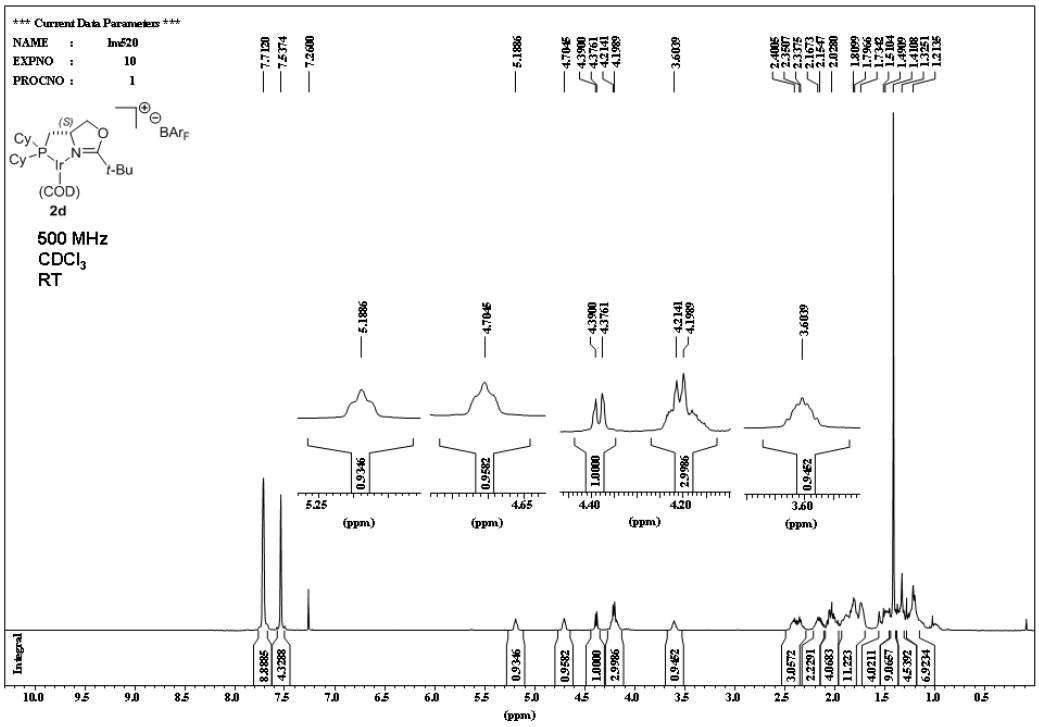
Name (*S*)-4-[(Di-cyclohexylphosphanyl)-methyl]-2-(*tert*-butyl)-4,5-dihydrooxazoline-η^4-(1,5-cyclooctadiene) iridium(I) tetrakis-[3,5-bis(trifluoromethyl)phenyl]borate. LM-520

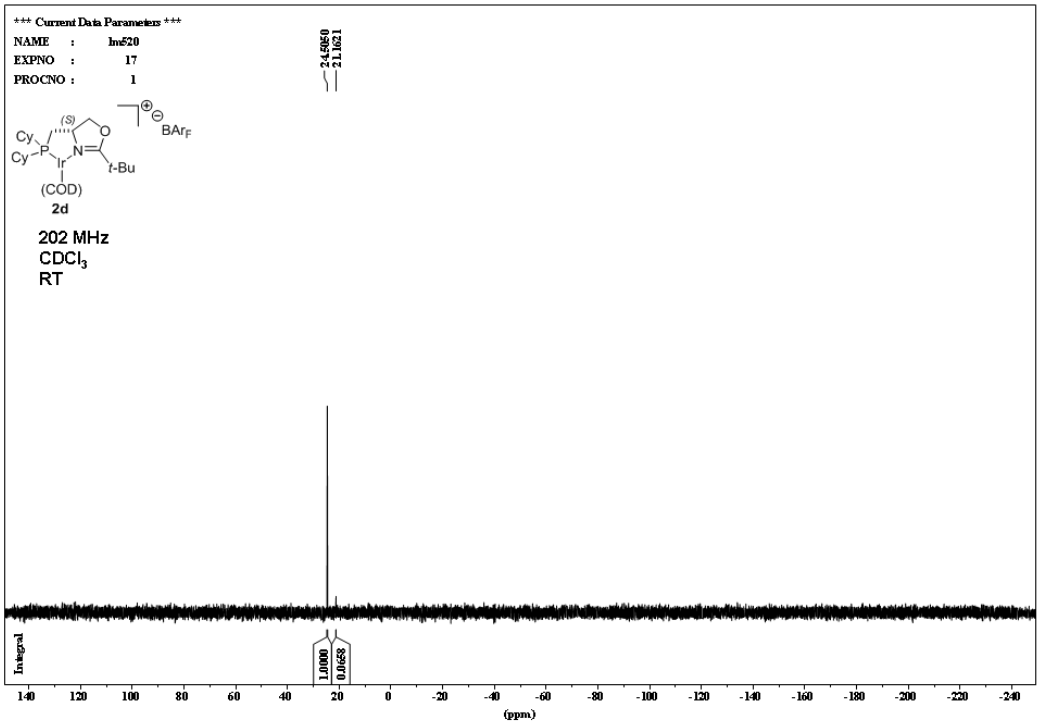
Properties orange solid	**Formula** $C_{60}H_{60}BF_{24}IrNOP$	
Molecular Weight 1501.09	*tlc conditions:* SiO_2, CH_2Cl_2 R_f = 0.86 (UV)	$[\alpha]^{26}_D$ = + 32.1 *c* 1.0. *in* CH_2Cl_2.	*Mp* = 144-146°C

^{1}H NMR (CDCl$_3$, 500 MHz, 298 K) δ (ppm) = 7.71 (s, 8H, H_{oBArF}), 7.54 (m, 4H, H_{pBArF}), 5.19 (m, 1H, CH_{COD}), 4.70 (m, 1H, CH_{COD}), 4.38 (d, $^2J_{HH}$ = 7.3 Hz, 1H, C*H*O), 4.20 (d, $^2J_{HH}$ = 7.3 Hz, 1H, C*H*O), 4.19 (m, 1H, C*H*N, 1H, CH_{COD}), 3.60 (m, 1H, CH_{COD}), 2.48-1.18 (m, 22H, H_{Cy}, 8H, $CH_{2\ COD}$, 2H, CH_2P), 1.41 (s, 9H, $CH_{3\ tBu\ Ox}$).

$^{13}C\{^1H\}$ NMR (CDCl$_3$, 126 MHz, 298 K) δ (ppm) = 181.4 (s, *C*N), 161.9 (q, $^1J_{CB}$ = 50.2 Hz, $C_{ipsoBArF}$), 134.9 (s, C_{oBArF}), 129.0 (q, $^2J_{CF}$ = 31.5 Hz, *C*CF$_3$), 124.7 (q, $^1J_{CF}$ = 273.3 Hz, *C*F$_3$), 117.6 (s, C_{pBArF}), 92.2 (d, $^2J_{CP}$ = 6.4 Hz, CH_{COD}), 81.2 (d, $^2J_{CP}$ = 17.5 Hz, CH_{COD}), 70.9 (d, $^3J_{CP}$ = 11.9 Hz, *C*H$_2$O), 69.8 (d, $^2J_{CP}$ = 5.5 Hz, *C*HN), 66.4 (s, CH_{COD}), 61.8 (s, CH_{COD}), 37.9 (d, $^3J_{CP}$ = 4.6 Hz, $CH_{2\ COD}$), 35.2 (d, $^1J_{CP}$ = 24.8 Hz, *C*H$_{Cy}$), 34.3 (s, $C_{tBu\ Ox}$), 33.7 (s, $CH_{2\ COD}$), 30.9 (d, $^1J_{CP}$ = 29.4 Hz, *C*H$_{Cy}$), 30.4 (d, $^2J_{CP}$ = 2.8 Hz, $CH_{2\ Cy}$), 29.1 (s, $CH_{3\ tBu\ Ox}$), 28.9 (s, $CH_{2\ COD}$), 28.6 (s, $CH_{2\ Cy}$), 27.9 (s, $CH_{2\ Cy}$), 26.9 (d, $^3J_{CP}$ = 12.9 Hz, $CH_{2\ Cy}$), 26.6 (d, $^3J_{CP}$ = 11.0 Hz, $CH_{2\ Cy}$), 26.5 (d, $^3J_{CP}$ = 14.7 Hz, $CH_{2\ Cy}$), 26.3 (d, $^3J_{CP}$ = 11.9 Hz, $CH_{2\ Cy}$), 26.0 (s, $CH_{2\ Cy}$), 25.8 (s, $CH_{2\ Cy}$), 25.2 (d, $^3J_{CP}$ = 2.8 Hz, $CH_{2\ COD}$), 24.0 (d, $^1J_{CP}$ = 29.4 Hz, *C*H$_2$P).

$^{31}P\{^1H\}$ NMR (CDCl$_3$, 202 MHz, 298 K) δ(ppm) = 24.5 (s).	**IR spectrum (neat)** ν (cm^{-1}) = 2938, 2861, 1598, 1481, 1451, 1353, 1272, 1161, 1118, 997, 970, 887, 839, 744, 715, 682, 668.
HRMS *(method: ESI+)* calculated for $C_{28}H_{48}IrNOP$ [M-BAr$_F$]$^+$: 638.3097, found. 638.3122.	**relevant literature references**: S. Nanchen, A. Pfaltz *Chem. Eur. J.* **2006**, *12*, 4550-4558; M. Diéguez, O. Pàmies *Chem. Eur. J.* **2008**, *14*, 3653-3669; D.-R. Hou, K. Burgess *Org. Lett.* **1999**, *1*, 1745–1747; D.-R. Hou, J. H. Reibenspies, K. Burgess *J. Org. Chem.* **2001**, *66*, 206–215.
Separation Conditions	
HPLC (column, λ_1, λ_2, eluent, flow rate, retention time):	**GC (column, method or sequence, retention time)**:

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PROCNO : 1
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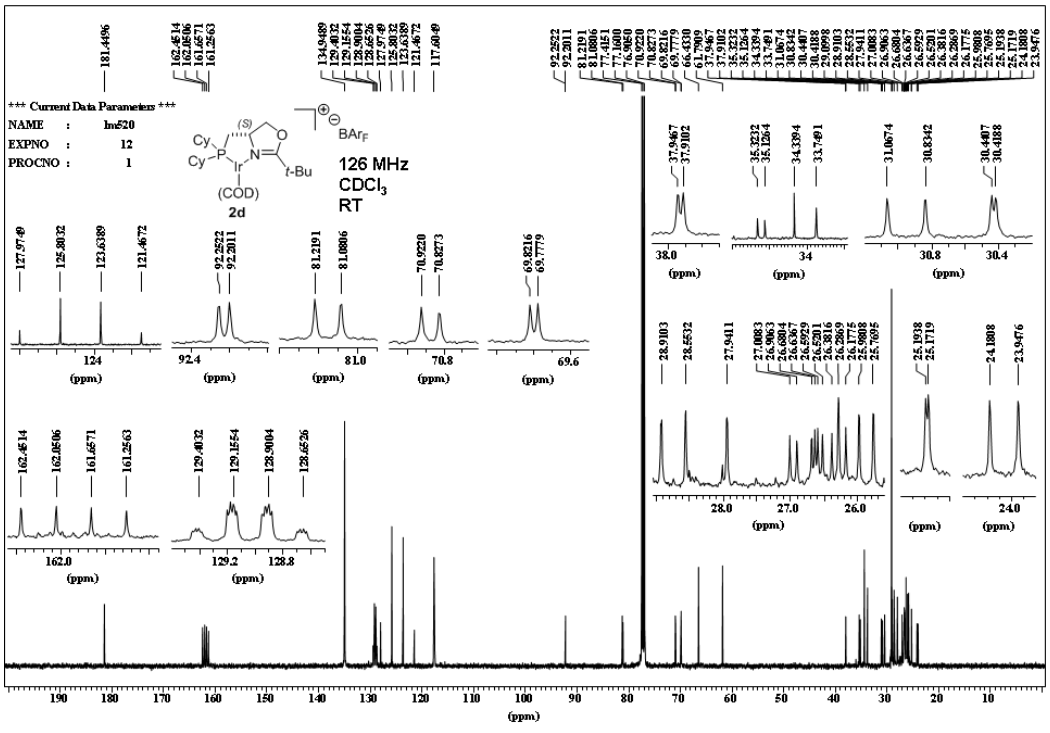
21.1621
Cy
Cy
P
Ir
(S)
O
N
t-Bu
(COD)
BArF
2d
202 MHz
CDCl3
RT
Integral
1.0000
0.0628
140 120 100 80 60 40 20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220 -240
(ppm)


*** Current Data Parameters ***
NAME : lm520
EXPNO : 12
PROCNO : 1
2d
126 MHz
CDCl3
RT
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162.4514
162.0586
161.6571
161.2563
134.9489
129.4032
129.1554
128.9084
128.6526
125.8032
123.6389
121.4672
117.6049
92.2522
92.2011
81.2191
81.0886
70.9220
70.8273
69.8216
69.7779
66.4330
61.7909
37.9467
37.9102
35.3232
35.1264
34.3394
33.7491
31.0674
30.8342
30.4487
30.4088
29.1098
28.9103
28.5532
27.9411
27.0083
26.9063
26.6804
26.6367
26.5929
26.5201
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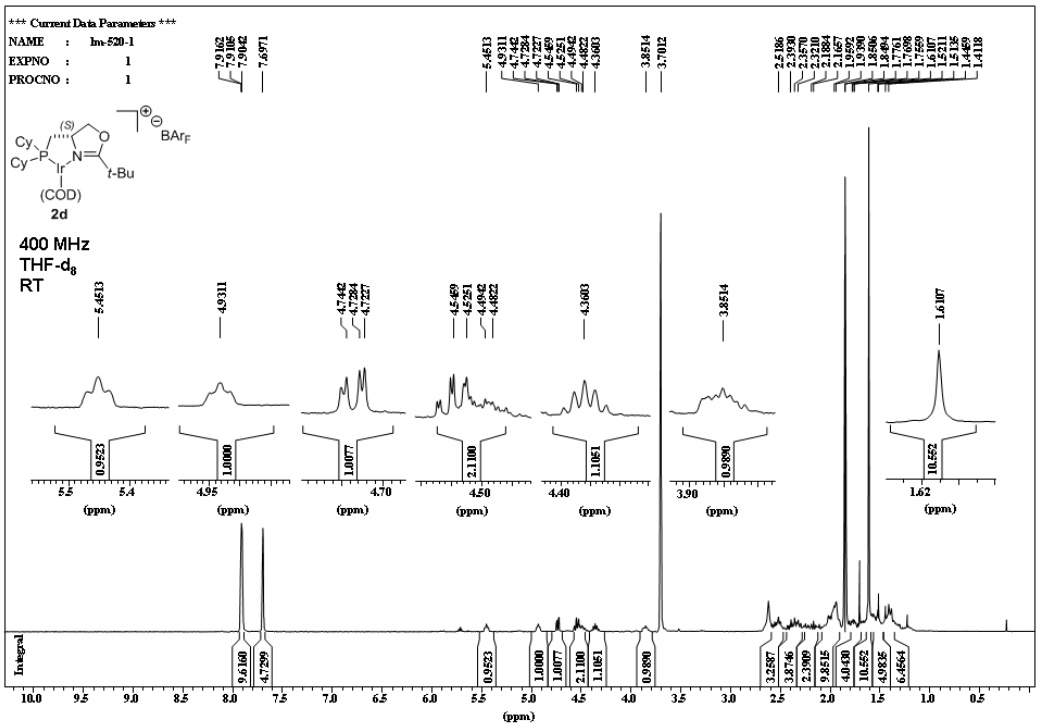
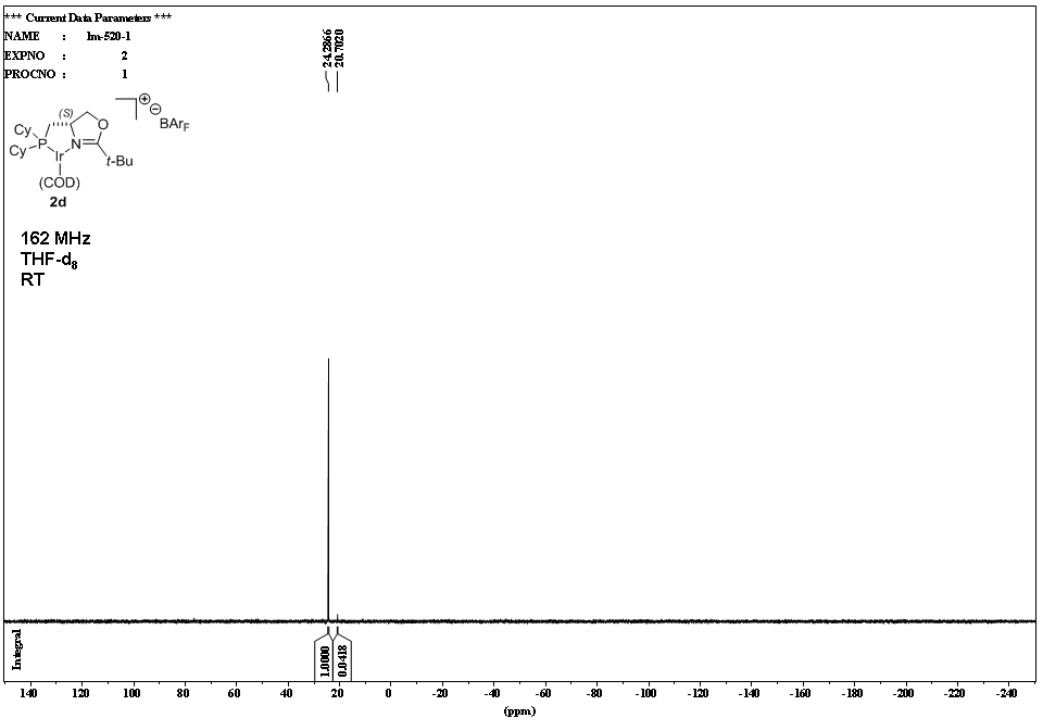
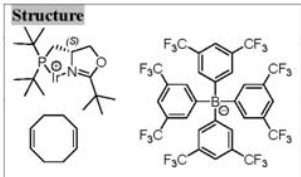
25.1938
25.1719
24.1808
23.9476
(ppm)


*** Current Data Parameters ***
NAME : lm-520-1
EXPNO : 1
PROCNO : 1
2d
400 MHz
THF-d8
RT
(ppm)
Integral


*** Current Data Parameters ***
NAME : lm-520-1
EXPNO : 2
PROCNO : 1
2d
162 MHz
THF-d8
RT
(ppm)
Integral

Structure	^{1}H	^{13}C{^{1}H}	^{31}P{^{1}H}	IR	HRMS	$[\alpha]_D$	MAZET GROUP DATA FORM



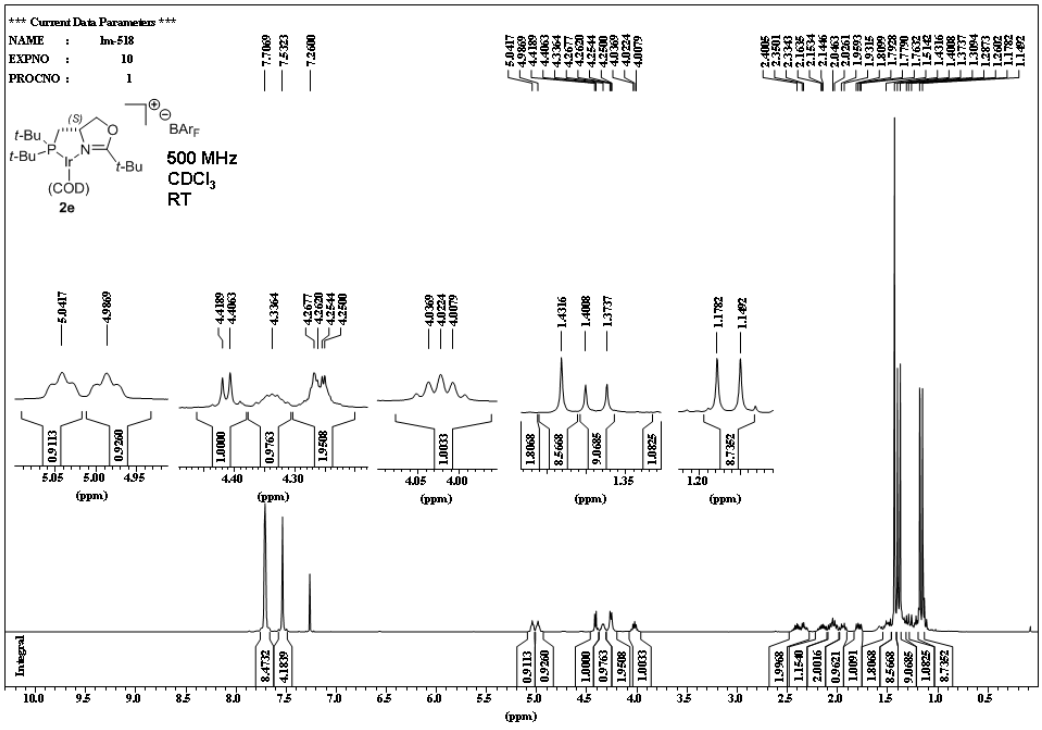
Name (*S*)-4-[(Di-*tert*-butylphosphanyl)-methyl]-2-(*tert*-butyl)-4,5-dihydrooxazoline-η^4-(1,5-cyclooctadiene) iridium(I) tetrakis-[3,5-bis(trifluoromethyl)phenyl]borate. LM-518

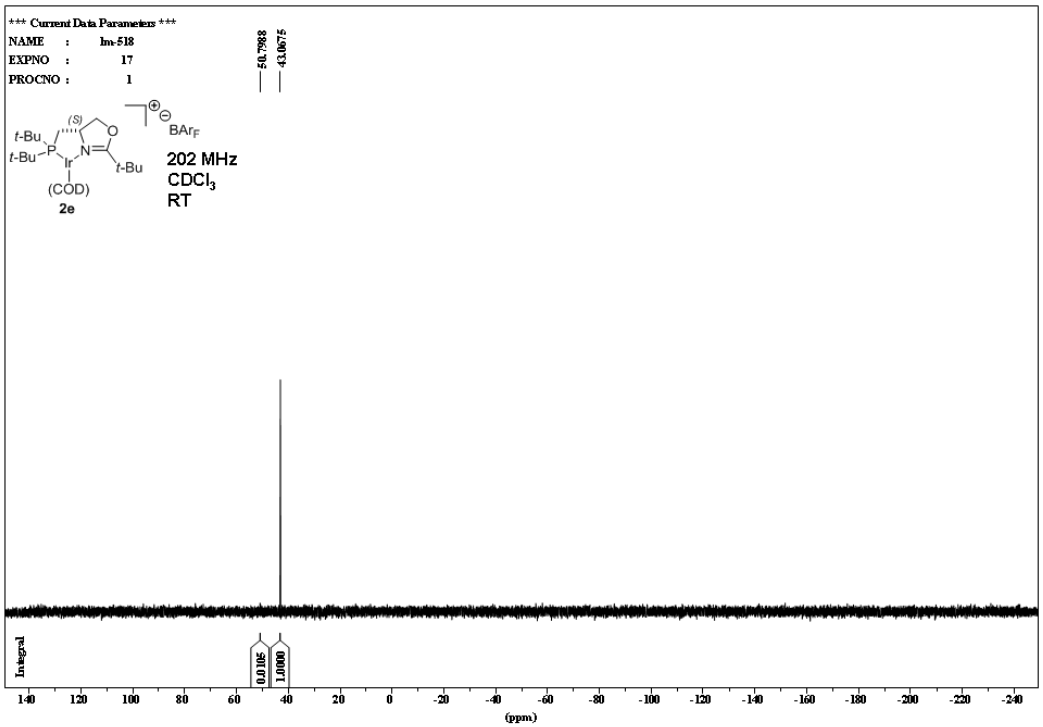
Properties orange solid	**Formula** $C_{56}H_{56}BF_{24}IrNOP$	
Molecular Weight 1449.01	*tlc conditions:* SiO_2, CH_2Cl_2 R_f = 0.89 (UV)	$[\alpha]^{26}_D$ = + 20.5 *c* 1.0. *in* CH_2Cl_2.	*Mp* = 214-216°C

^{1}H NMR (CDCl$_3$, 500 MHz, 298 K) δ (ppm) = 7.71 (s, 8H, H_{oBArF}), 7.53 (s, 4H, H_{pBArF}), 5.04 (m, 1H, CH_{COD}), 4.99 (m, 1H, CH_{COD}), 4.41 (m, 1H, CHO), 4.34 (m, 1H, CH_{COD}), 4.26 (m, 1H, CHN, 1H, CHO), 4.02 (m, 1H, CH_{COD}), 2.40 (m, 2H, $CH_{2\,COD}$), 2.22 (m, 1H, $CH_{2\,COD}$), 2.05 (m, 1H, $CH_{2\,COD}$, 1H, CHP), 1.94 (m, 1H, $CH_{2\,COD}$), 1.79 (m, 1H, $CH_{2\,COD}$), 1.48 (m, 1H, $CH_{2\,COD}$, 1H, CHP), 1.43 (s, 9H, $CH_{3\,tBu\,Ox}$), 1.38 (d, $^3J_{HP}$ = 13.6 Hz, 9H, $CH_{3\,tBu}$), 1.16 (d, $^3J_{HP}$ = 14.5 Hz, 9H, $CH_{3\,tBu'}$).

^{13}C{^{1}H} NMR (CDCl$_3$, 126 MHz, 298 K) δ (ppm) = 181.3 (s, CN), 161.0 (q, $^1J_{CB}$ = 50.2 Hz, $C_{ipsoBArF}$), 134.9 (s, C_{oBArF}), 129.0 (q, $^2J_{CF}$ = 31.5 Hz, CCF_3), 124.7 (q, $^1J_{CF}$ = 273.0 Hz, CF_3), 117.6 (s, C_{pBArF}), 88.1 (d, $^2J_{CP}$ = 6.4 Hz, CH_{COD}), 75.5 (d, $^2J_{CP}$ = 19.3 Hz, CH_{COD}), 70.9 (d, $^3J_{CP}$ = 11.9 Hz, CH_2O), 70.0 (s, CH_{COD}), 69.9 (d, $^2J_{CP}$ = 5.5 Hz, CHN), 60.5 (s, CH_{COD}), 37.9 (d, $^2J_{CP}$ = 4.6 Hz, $CH_{2\,COD}$), 37.3 (d, $^1J_{CP}$ = 16.4 Hz, C_{tBu}), 35.5 (d, $^1J_{CP}$ = 19.3 Hz, $C_{tBu'}$), 34.7 (s, $C_{tBu\,Ox}$), 34.3 (s, $CH_{2\,COD}$), 30.1 (d, $^2J_{CP}$ = 4.6 Hz, CH_{3tBu}), 29.8 (d, $^2J_{CP}$ = 3.7 Hz, $CH_{3tBu'}$), 29.3 (s, $CH_{3tBu\,Ox}$), 28.5 (s, CH_{2COD}), 26.4 (d, $^1J_{CP}$ = 24.8 Hz, CH_2P), 25.0 (d, $^2J_{CP}$ = 2.8 Hz, CH_{2COD}).

^{31}P{^{1}H} NMR (CDCl$_3$, 202 MHz, 298 K) δ (ppm) = 43.1 (s).	**IR spectrum (neat)** ν (cm^{-1}) = 2967, 2886, 1607, 1594, 1480, 1353, 1270, 1162, 1120, 974, 898, 887, 839, 744, 716, 681, 668.
HRMS *(method: ESI+)* calculated for calculated for $C_{24}H_{44}IrNOP$ [M-BAr_F]$^+$: 586.2784, found. 586.2726.	**relevant literature references**: S. Nanchen, A. Pfaltz *Chem. Eur. J.* **2006**, *12*, 4550-4558; M. Diéguez, O. Pàmies *Chem. Eur. J.* **2008**, *14*, 3653-3669; D.-R. Hou, K. Burgess *Org. Lett.* **1999**, *1*, 1745–1747; D.-R. Hou, J. H. Reibenspies, K. Burgess *J. Org. Chem.* **2001**, *66*, 206–215.
Separation Conditions	
HPLC (column, λ_1, λ_2, eluent, flow rate, retention time):	**GC (column, method or sequence, retention time)**:




*** Current Data Parameters ***
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PROCNO : 1
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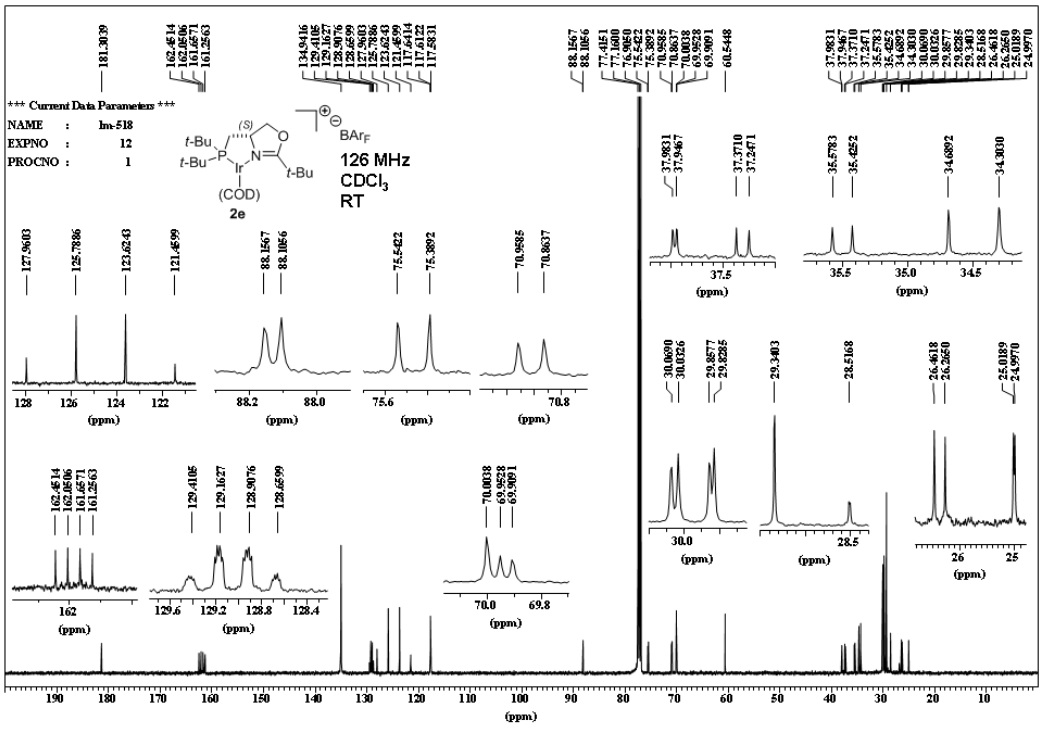
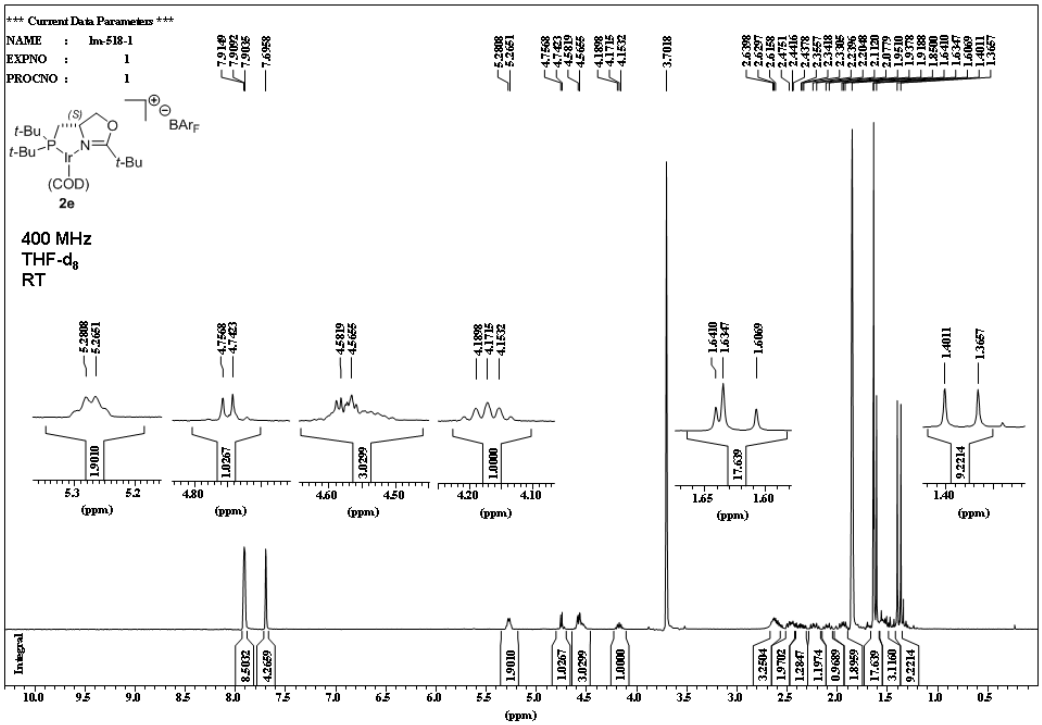
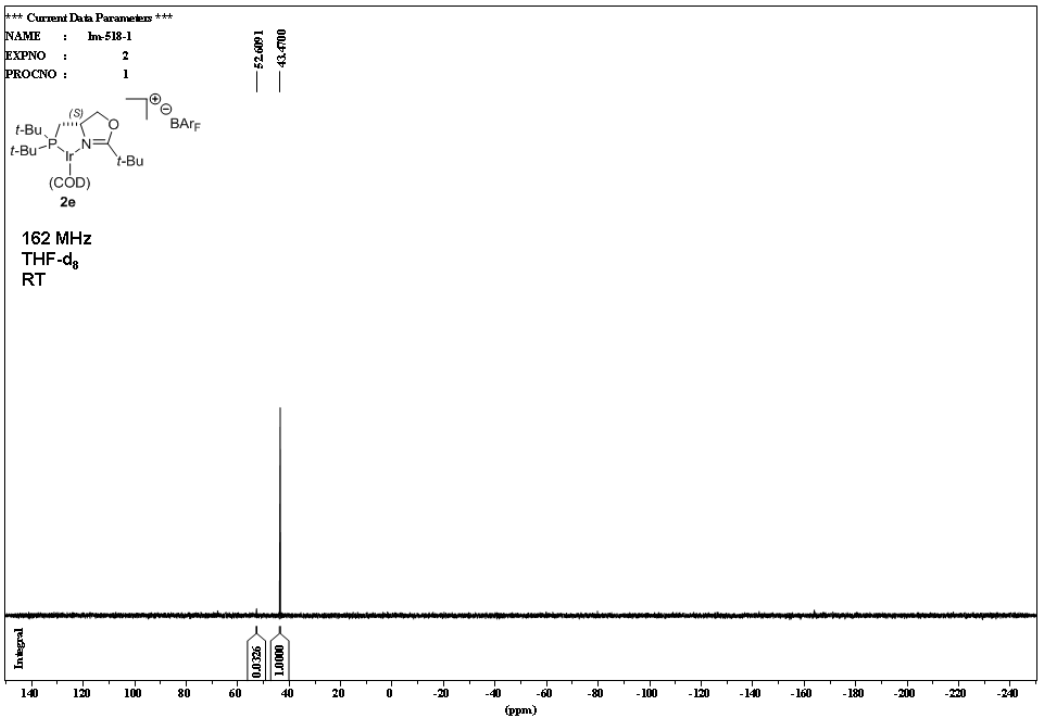
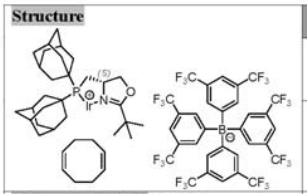
43.0675
BAr$_F$
202 MHz
CDCl$_3$
RT
2e
Integral
0.0105
1.0000
(ppm)


*** Current Data Parameters ***
NAME : lm-518
EXPNO : 12
PROCNO : 1
BAr$_F$
126 MHz
CDCl$_3$
RT
2e
(ppm)


*** Current Data Parameters ***
NAME : lm-518-1
EXPNO : 1
PROCNO : 1
2e
400 MHz
THF-d8
RT
(ppm)
Integral


*** Current Data Parameters ***
NAME : lm-518-1
EXPNO : 2
PROCNO : 1
2e
162 MHz
THF-d8
RT
(ppm)
Integral

Structure	^{1}H	$^{13}C\{^1H\}$	$^{31}P\{^1H\}$	IR	HRMS	$[\alpha]_D$	MAZET GROUP DATA FORM



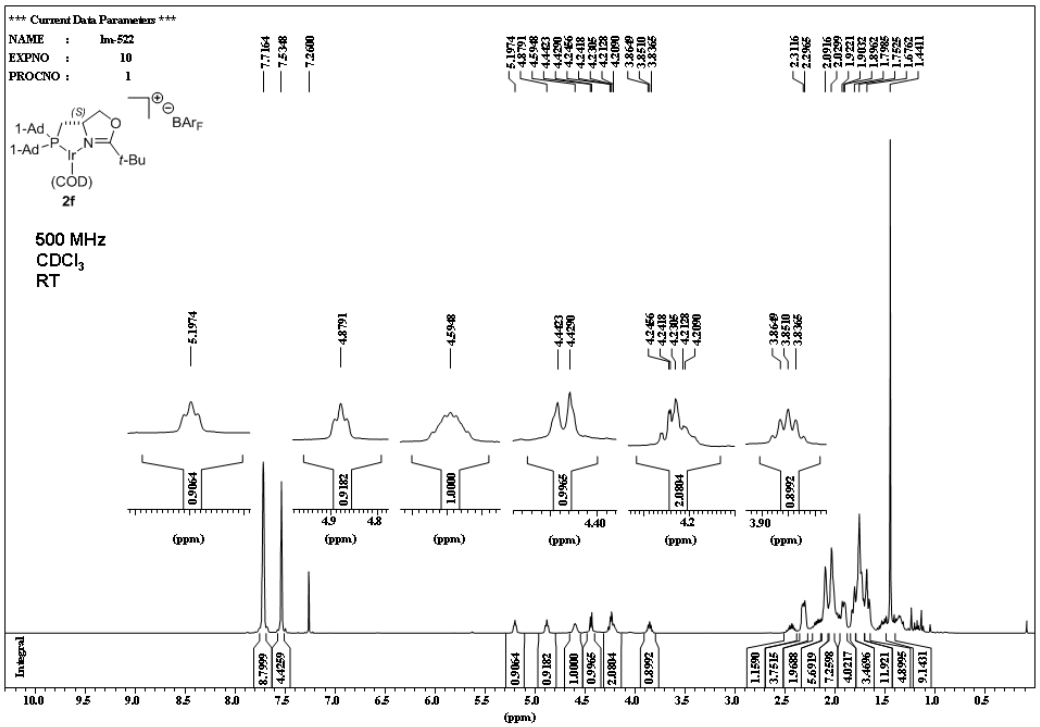
Name (*S*)-4-[(di-1-adamantylphosphanyl)-methyl]-2-(*tert*-butyl)-4,5-dihydrooxazoline-η^4-(1,5-cyclooctadiene) iridium(I) tetrakis-[3,5-bis(trifluoromethyl)phenyl]borate. LM-522

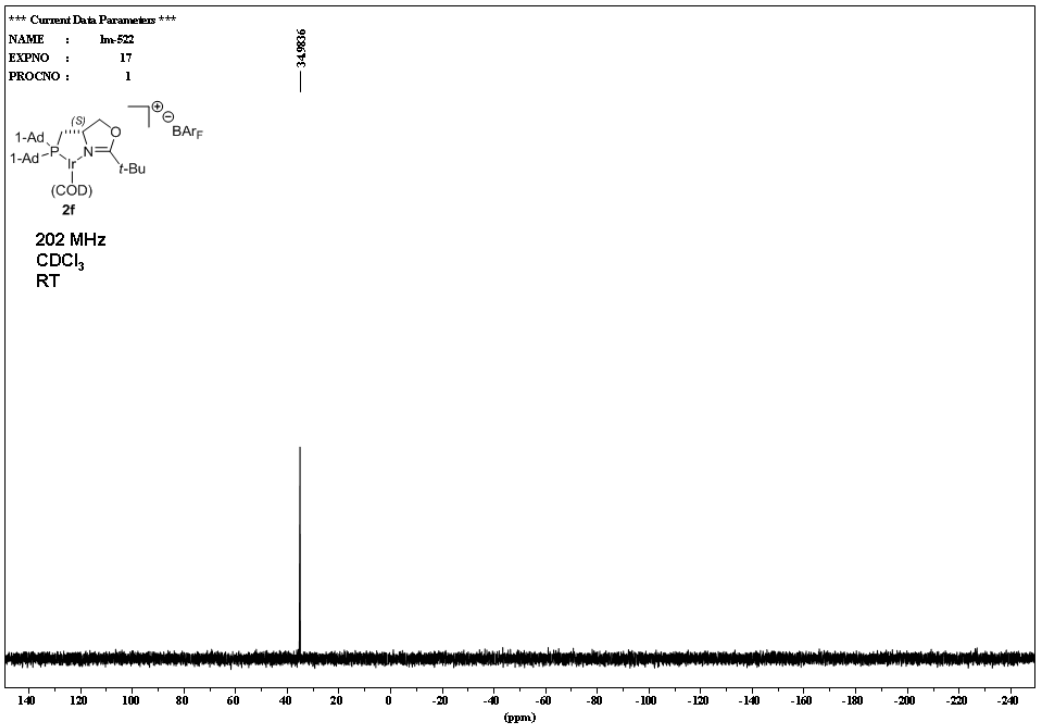
Properties orange solid	**Formula** $C_{68}H_{68}BF_{24}IrNOP$	
Molecular Weight 1605.24	*tlc conditions:* SiO_2, CH_2Cl_2 R_f = 0.89 (UV)	**$[\alpha]^{26}_D$** = + 41.1 *c* 1.0. *in* CH_2Cl_2.	*Mp* = 87-88°C

^{1}H NMR (CDCl$_3$, 500 MHz, 298 K) δ (ppm) = 7.72 (s, 8H, H_{oBArF}), 7.54 (s, 4H, H_{pBArF}), 5.20 (m, 1H, CH_{COD}), 4.88 (m, 1H, CH_{COD}), 4.59 (m, 1H, CH_{COD}), 4.43 (m, 1H, CHO), 4.24 (m, 1H, CHO, 1H, CHN), 3.85 (m, 1H, CH_{COD}), 2.35-1.24 (m, 30H, H_{Ad}, 8H, $CH_{2\,COD}$, 2H, CH_2P), 1.44 (s, 9H, $CH_{3\,tBu\,Ox}$).

$^{13}C\{^1H\}$ NMR (CDCl$_3$, 126 MHz, 298 K) δ (ppm) = 180.9 (s, *C*N), 161.9 (q, $^1J_{CB}$ = 49.9 Hz, $C_{ipso BArF}$), 135.0 (s, C_{oBArF}), 129.0 (q, $^2J_{CF}$ = 31.2 Hz, CCF_3), 124.7 (q, $^1J_{CF}$ = 273.3 Hz, CF_3), 117.6 (s, C_{pBArF}), 85.9 (d, $^2J_{CP}$ = 4.6 Hz, CH_{COD}), 73.1 (d, $^2J_{CP}$ = 19.3 Hz, CH_{COD}), 71.4 (s, CH_{COD}), 71.0 (d, $^3J_{CP}$ = 11.9 Hz, CH_2O), 70.3 (d, $^2J_{CP}$ = 6.4 Hz, CHN), 60.0 (s, CH_{COD}), 42.7 (d, $^1J_{CP}$ = 12.9 Hz, $C_{Ad}P$), 42.0 (d, $^1J_{CP}$ = 15.6 Hz, $C_{Ad'}P$), 41.7 (s, CH_2C_{Ad}), 40.3 (s, $CH_2C_{Ad'}$), 38.1 (d, $^3J_{CP}$ = 4.6 Hz, $CH_{2\,COD}$), 36.3 (s, CH_2CH_{Ad}), 36.2 (s, $CH_2CH_{Ad'}$), 34.8 (s, $C_{tBu\,Ox}$), 34.6 (s, $CH_{2\,COD}$), 29.3 (s, $CH_{3tBu\,Ox}$), 28.5 (s, $CH_{2\,COD}$), 28.4 (d, $^3J_{CP}$ = 8.3 Hz, CHC_{Ad}), 28.3 (d, $^3J_{CP}$ = 8.3 Hz, $CHC_{Ad'}$), 25.0 (d, $^2J_{CP}$ = 2.8 Hz, $CH_{2\,COD}$), 22.2 (d, $^1J_{CP}$ = 24.8 Hz, CH_2P).

$^{31}P\{^1H\}$ NMR (CDCl$_3$, 202 MHz, 298 K) δ (ppm) = 35.0 (s).	**IR spectrum (neat)** ν (cm^{-1}) = 2911, 2856, 1608, 1593, 1481, 1452, 1353, 1273, 1158, 1117, 973, 934, 886, 839, 745, 712, 682, 669.
HRMS *(method: ESI+)* calculated for $C_{36}H_{56}IrNOP$ $[M\text{-}BAr_F]^+$: 742.3723, found 742.3750.	**relevant literature references**: S. Nanchen, A. Pfaltz *Chem. Eur. J.* **2006**, *12*, 4550-4558; M. Diéguez, O. Pàmies *Chem. Eur. J.* **2008**, *14*, 3653-3669; D.-R. Hou, K. Burgess *Org. Lett.* **1999**, *1*, 1745–1747; D.-R. Hou, J. H. Reibenspies, K. Burgess *J. Org. Chem.* **2001**, *66*, 206–215.
Separation Conditions	
HPLC (column, λ_1, λ_2, eluent, flow rate, retention time):	**GC (column, method or sequence, retention time)**:




*** Current Data Parameters ***
NAME : lm-522
EXPNO : 17
PROCNO : 1
34.9836
1-Ad
1-Ad
(S)
P
Ir
N
O
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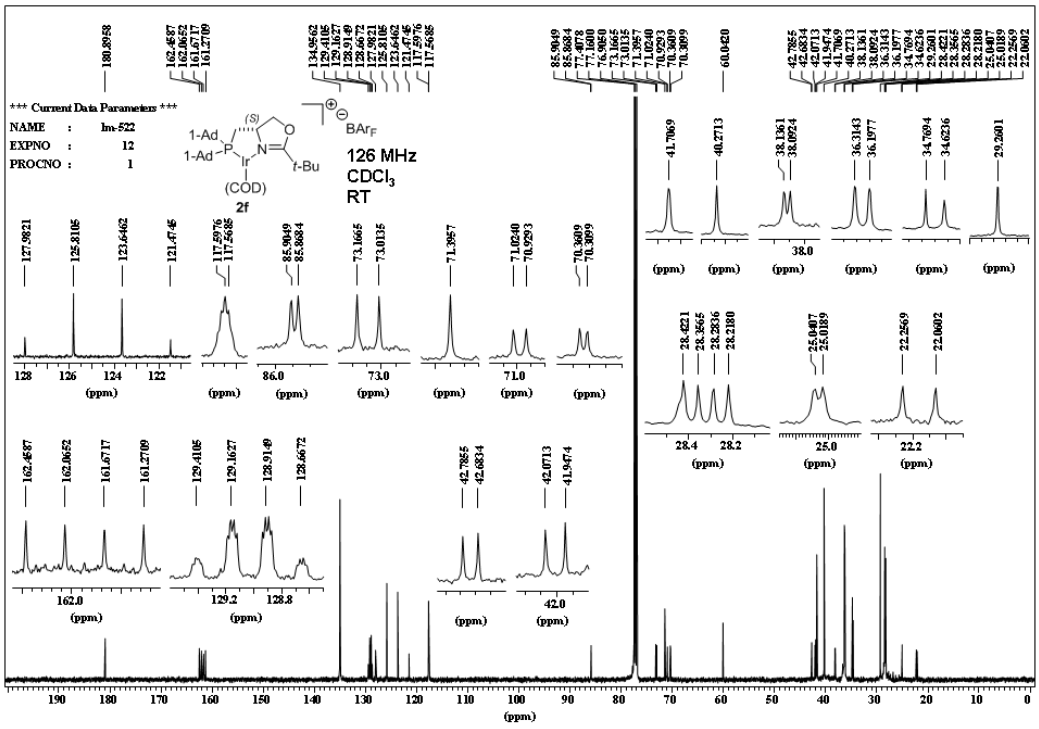
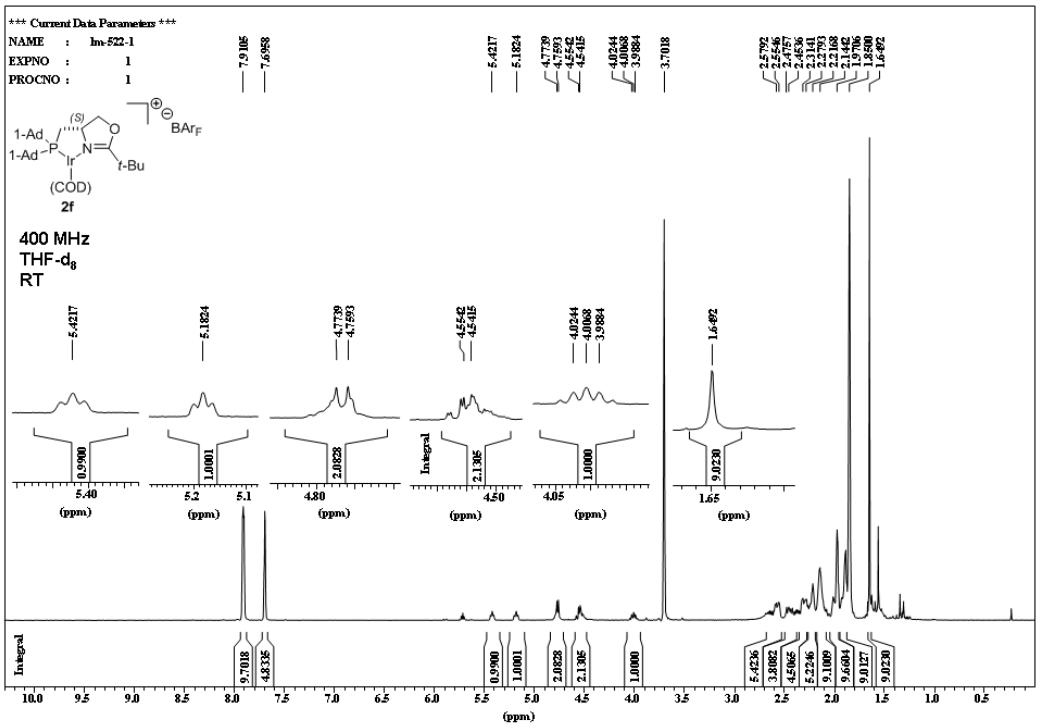
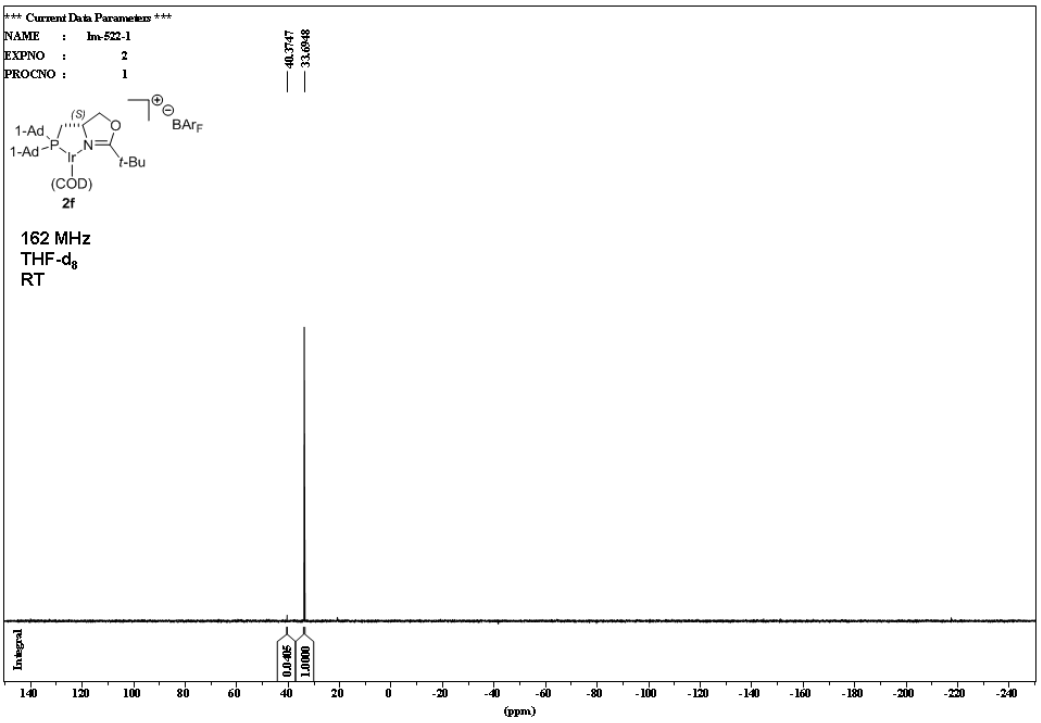
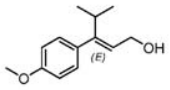
BAr$_F$
(COD)
2f
202 MHz
CDCl$_3$
RT
(ppm)


*** Current Data Parameters ***
NAME : lm-522
EXPNO : 12
PROCNO : 1
2f
126 MHz
CDCl$_3$
RT
(ppm)


*** Current Data Parameters ***
NAME : lm-522-1
EXPNO : 1
PROCNO : 1
2f
400 MHz
THF-d8
RT
(ppm)

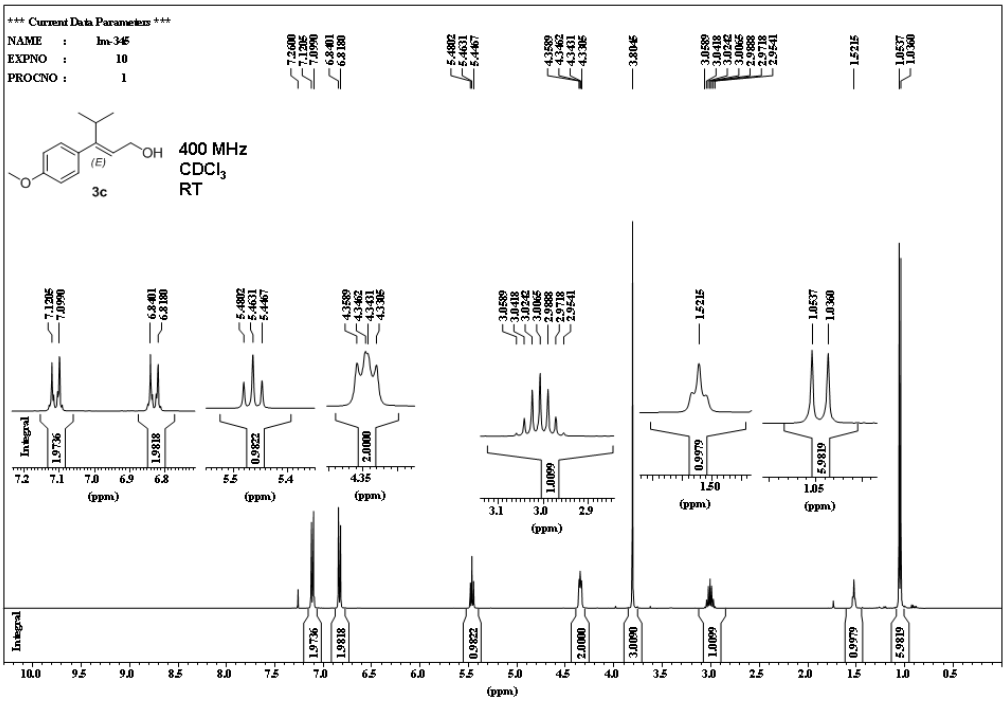

*** Current Data Parameters ***
NAME : lm-522-1
EXPNO : 2
PROCNO : 1
2f
162 MHz
THF-d8
RT
(ppm)

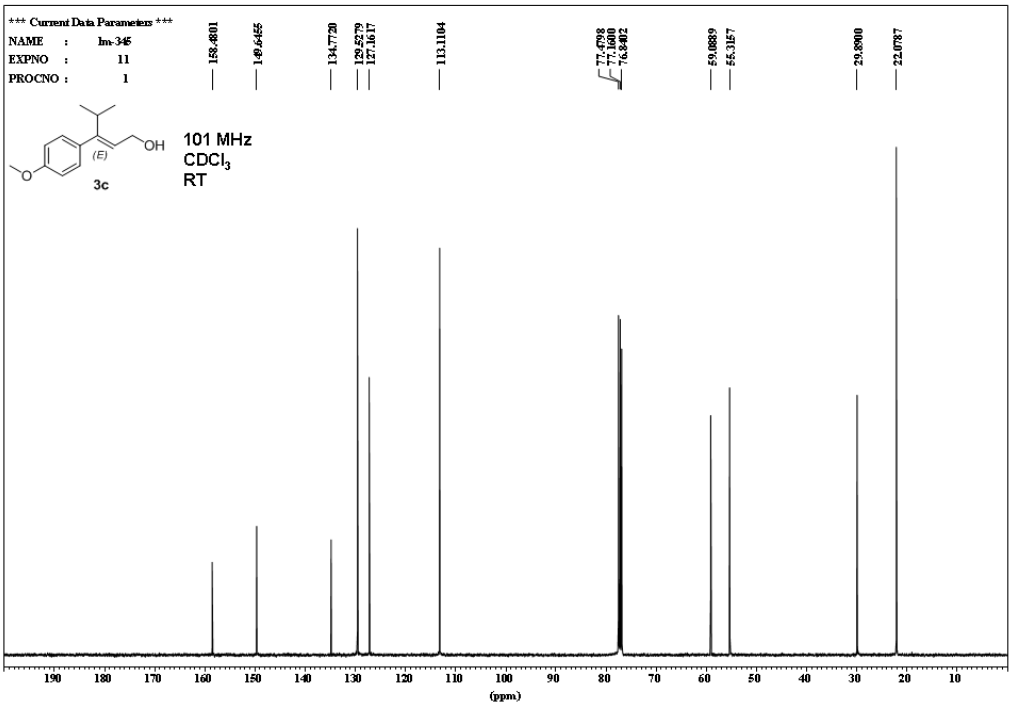
Structure	^{1}H	$^{13}C\{^1H\}$		IR	LRMS		MAZET GROUP DATA FORM
	**Name** (*E*)-3-(4-methoxyphenyl)-4-methylpent-2-en-1-ol. LM-345						
	Properties colourless oil					**Formula** $C_{13}H_{18}O_2$	
Molecular Weight 206.28	*tlc conditions:* SiO_2, Pent / Et_2O = 1:1 R_f = 0.32 (UV)						

^{1}H NMR (CDCl$_3$, 400 MHz, 298 K) δ (ppm) = 7.11 (d, $^3J_{HH}$ = 8.7 Hz, 2H, H_{oAr}), 6.83 (d, $^3J_{HH}$ = 8.7 Hz, 2H, H_{mAr}), 5.46 (t, $^3J_{HH}$ = 6.7 Hz, 1H, $CHCH_2$), 4.34 (dd, $^3J_{HH}$ = 6.4 Hz, $^3J_{HH}$ = 5.3 Hz, 2H, CH_2OH), 3.80 (s, OCH_3), 3.01 (hept, $^3J_{HH}$ = 7.0 Hz, 1H, CH_{iPr}), 1.52 (bs, 1H, OH), 1.05 (d, $^3J_{HH}$ = 7.0 Hz, 6H, CH_{3iPr}).

$^{13}C\{^1H\}$ NMR (CDCl$_3$, 101 MHz, 298 K) δ (ppm) = 158.5 (s, C_{pAr}), 149.6 (CCH_{iPr}), 134.8 (s, C_{ipsoAr}), 129.5 (s, C_{oAr}), 127.2 ($CHCH_2$), 113.1 (s, C_{mAr}), 59.1 (CH_2OH), 55.3 (s, OCH_3), 29.9 (s, CH_{iPr}), 22.1 (s, CH_{3iPr}).

	IR spectrum (neat) ν (cm^{-1}) = 3341, 2961, 2932, 2871, 2836, 1608, 1508, 1463, 1442, 1362, 1284, 1242, 1177, 1107, 1085, 1033, 828, 792, 733.
LRMS *(method: ESI)* calculated for $C_{13}H_{17}O$ $[M\text{-}OH]^+$: 189.3, found 189.4.	**relevant literature references**: L. Mantilli, D. Gérard, S. Torche, C. Besnard, C. Mazet *Angew. Chem. Int. Ed.* **2009**, *48*, 5143–5147.
Separation Conditions	
HPLC (column, λ_1, λ_2, eluent, flow rate, retention time):	**GC (column, method or sequence, retention time)**:




*** Current Data Parameters ***
NAME : lm-345
EXPNO : 11
PROCNO : 1
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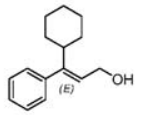
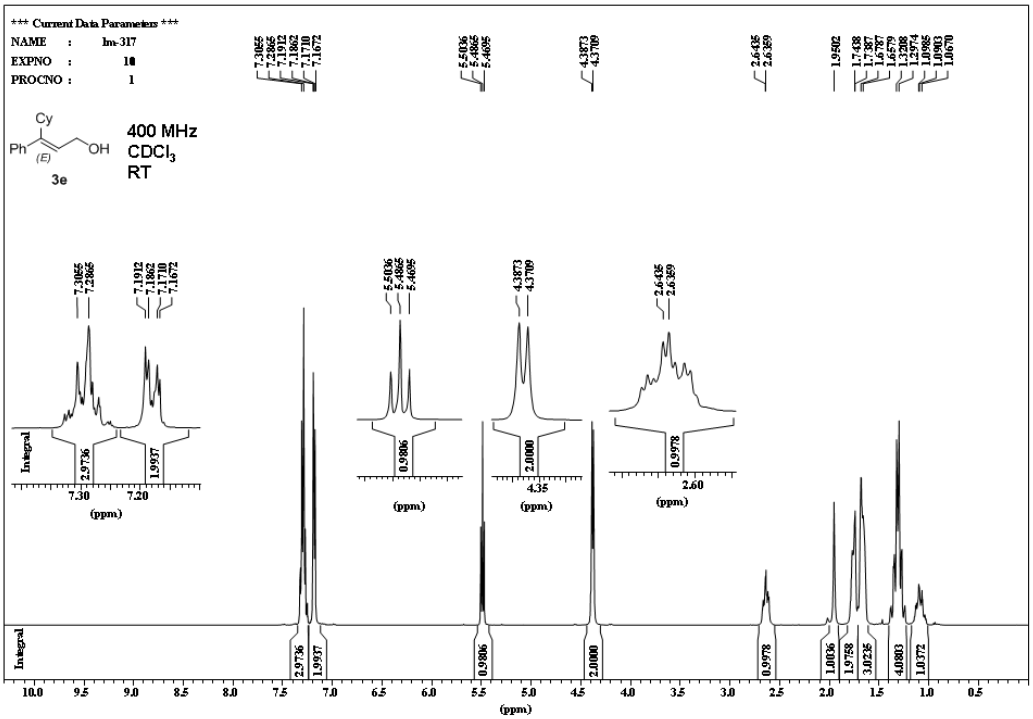
149.6455
134.7720
129.5279
127.1617
113.1104
77.4798
77.1680
76.8402
59.0889
55.3157
29.8900
22.0787
OH
(E)
O
3c
101 MHz
CDCl3
RT
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
(ppm)

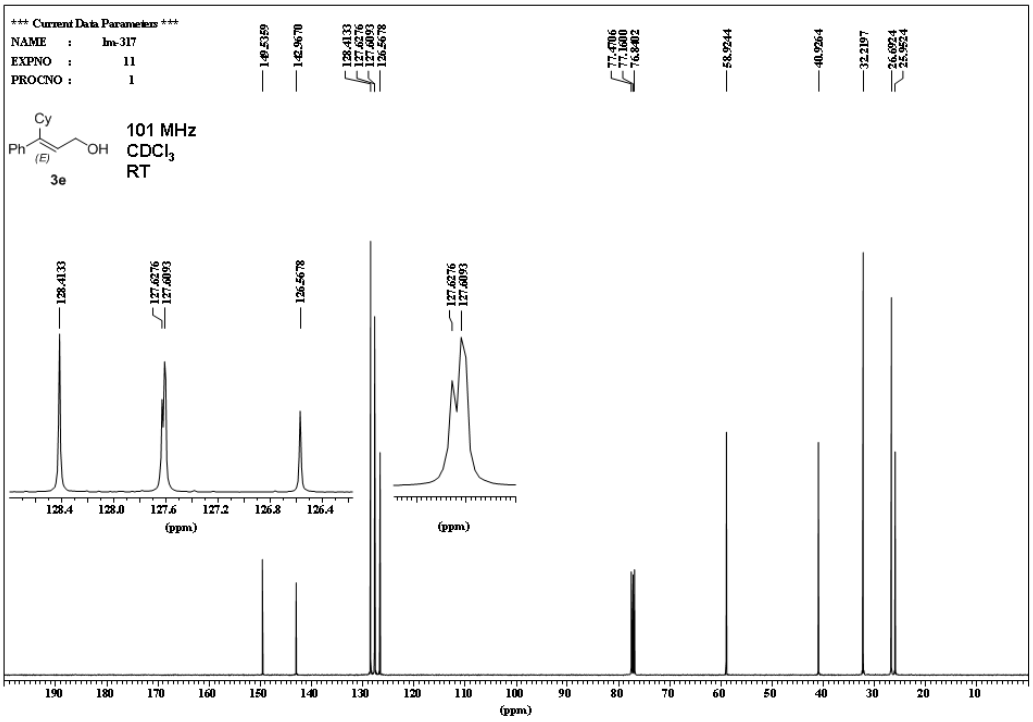
Structure	^{1}H	^{13}C{^{1}H}		IR	LRMS		MAZET GROUP DATA FORM
	**Name** (*E*)-3-cyclohexyl-3-phenylprop-2-en-1-ol LM-317						
	Properties colourless oil					**Formula** $C_{13}H_{18}O_2$	
Molecular Weight 216.32	*tlc conditions:* SiO_2, Pent / Et_2O = 2:1 R_f = 0.21 (UV)						

^{1}H NMR ($CDCl_3$, 400 MHz, 298 K) δ (ppm) = 7.33-7.26 (m, 3H, $H_{m,pPh}$), 7.19-7.17 (m, 2H, H_{oPh}), 5.49 (t, $^3J_{HH}$ = 6.7 Hz, 1H, $CHCH_2$), 4.38 (d, $^3J_{HH}$ = 6.6 Hz, 2H, CH_2OH), 2.64 (m ,1H, CH_{Cy}), 1.95 (m, 1H, H_{Cy}), 1.74 (m, 2H, H_{Cy}), 1.67 (m, 2H, H_{Cy}, 1H, OH), 1.30 (m, 4H, H_{Cy}), 1.08 (m, 1H, H_{Cy}).

^{13}C{^{1}H} NMR ($CDCl_3$, 101 MHz, 298 K) δ (ppm) = 149.5 (CCH_{Cy}), 143.0 (C_{ipsoPh}), 128.4 (s, C_{oPh}), 127.6 ($CHCH_2$), 127.6 (s, C_{mPh}), 126.6 (s, C_{pPh}), 58.9 (CH_2OH), 32.2 (s, $CH_{2\,Cy}$), 26.7 (s, $CH_{2\,Cy}$), 26.0 (s, $CH_{2\,Cy}$).

	IR spectrum (neat) ν (cm^{-1}) = 3310, 3054, 2925, 2852, 1599, 1490, 1448, 1264, 1109, 1073, 1050, 1008, 949, 891, 845, 765,737, 700.
LRMS *(method: ESI)* calculated for $C_{15}H_{19}$ $[M\text{-}OH]^+$: 199.3, found 199.1.	**relevant literature references**: L. Mantilli, D. Gérard, S. Torche, C. Besnard, C. Mazet *Angew. Chem. Int. Ed.* **2009**, *48*, 5143−5147; G. Pinna, G. Cignarella, G. Loriga, G. Morineddu, J.-M. Mussinu, S. Ruiu, P. Fadda and W. Fratta *Bioorg. Med. Chem.* **1967**, *32*, 1929−1937.
Separation Conditions	
HPLC (column, λ_1, λ_2, eluent, flow rate, retention time):	**GC (column, method or sequence, retention time)**:




*** Current Data Parameters ***
NAME : lm-317
EXPNO : 11
PROCNO : 1
101 MHz
CDCl3
RT
3e
Cy
Ph
(E)
OH
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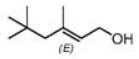
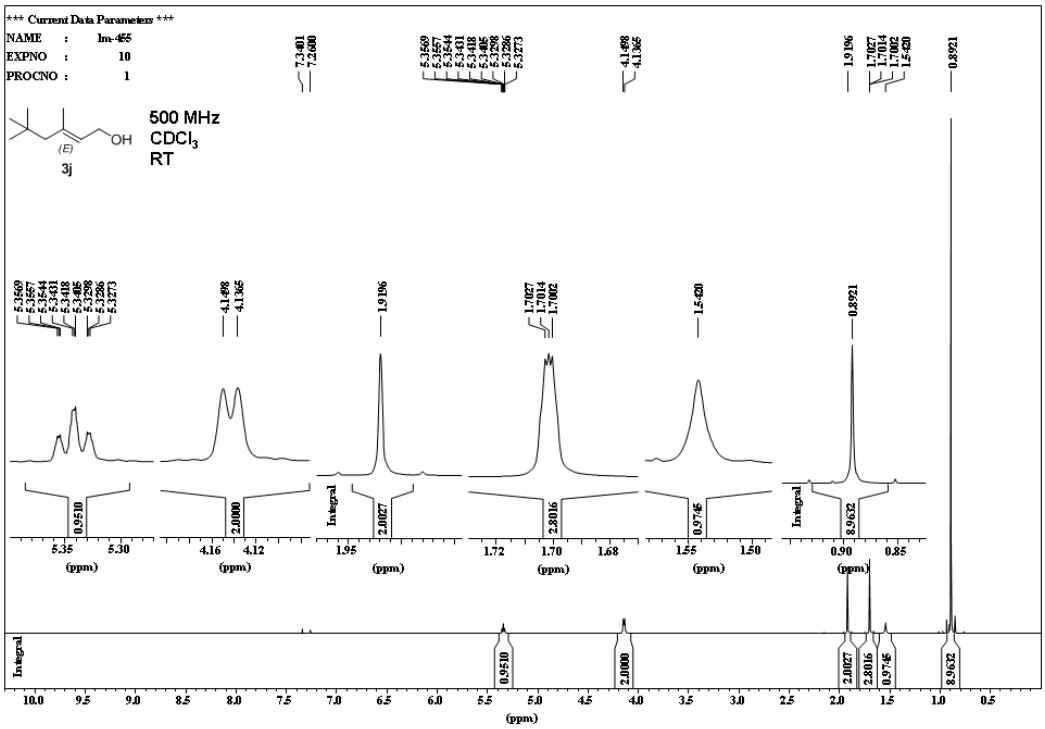
142.9670
128.4133
127.6276
127.6093
126.5678
77.4706
77.1600
76.8402
58.9244
40.9564
32.2197
26.6924
25.9524
(ppm)

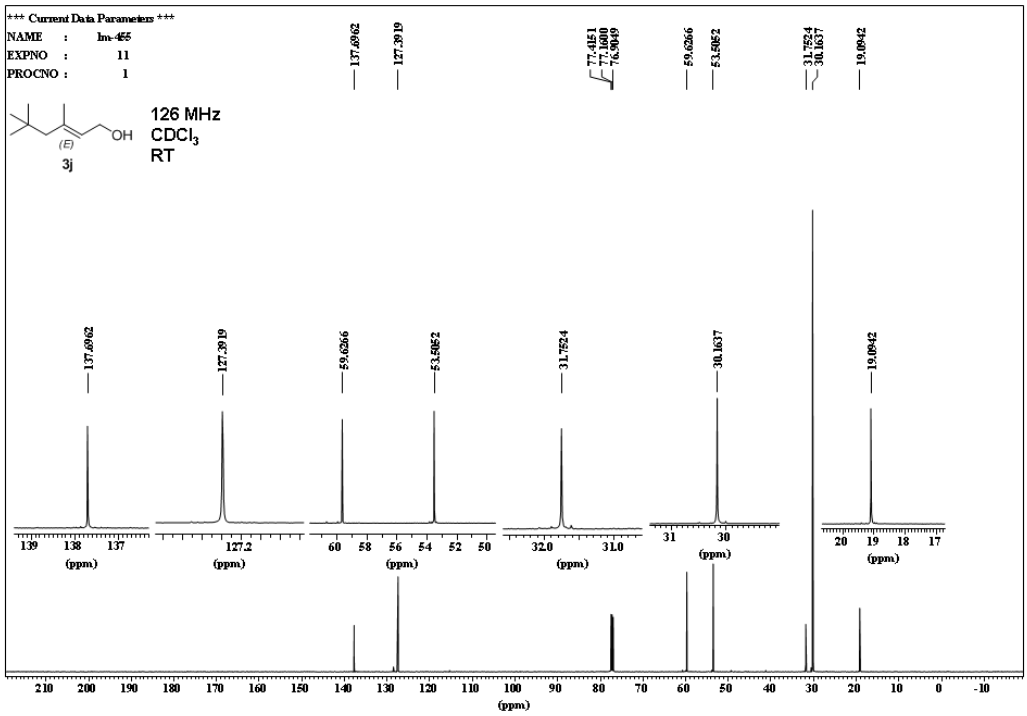
Structure	^{1}H | ^{13}C{^{1}H} | IR | HRMS	MAZET GROUP DATA FORM
	**Name** (*E*)-3,5,5-trimethylhex-2-en-1-ol. LM-455	
	Properties colourless oil	**Formula** $C_9H_{18}O$
Molecular Weight 142.24	*tlc conditions:* SiO_2, Pent / Et_2O = 5:2 R_f = 0.30 (UV)	

^{1}H NMR (CDCl$_3$, 500 MHz, 298 K) δ(ppm) = 5.34 (*ap.*tt, $^3J_{HH}$ = 6.6 Hz, $^4J_{HH}$ = 0.7 Hz, 1H, C*H*CH$_2$), 4.14 (d, $^3J_{HH}$ = 6.6 Hz, 2H, C*H*$_2$OH), 1.92 (s, 2H, C*H*$_2$C$_{quat}$), 1.70 (*ap.*t, $^4J_{HH}$ = 0.7 Hz, 3H, CC*H*$_3$), 1.54 (bs, 1H, OH), 0.89 (s, 9H, C*H*$_{3tBu}$).

^{13}C NMR (CDCl$_3$, 126 MHz, 298 K) δ (ppm) = 137.7 (*C*CH$_3$), 127.4 (*C*HCH$_2$), 59.6 (*C*H$_2$OH), 53.5 (*C*H$_2$C$_{quat}$), 31.8 (*C*CH$_{3tBu}$), 30.2 (*C*H$_{3tBu}$), 19.1 (CH$_3$).

	IR spectrum (neat) ν (cm^{-1}) = 3327, 2951, 2908, 2867, 1661, 1476, 1466, 1391, 1364, 1236, 1199, 1093, 1038, 995, 892, 792, 733.
LRMS *(method: EI)* calculated for, $C_8H_{16}O$ [M-CH$_2$]: 128.1, found 128.0.	**relevant literature references**: S. Bywater, P. Lachance, P. Black *J. Organomet. Chem.* **1985**, 280, 159-164 (only IR).
Separation Conditions	
HPLC (column, λ_1, λ_2, eluent, flow rate, retention time):	**GC (column, method or sequence, retention time)**:




*** Current Data Parameters ***
NAME : lm-455
EXPNO : 11
PROCNO : 1
126 MHz
CDCl3
RT
(E)
OH
3j
137.6962
127.3919
77.4151
77.1600
76.9049
59.6266
53.5052
31.7524
30.1637
19.0942
(ppm)