Supplementary Material (ESI) for Chemical Communications

Design and synthesis of a novel three hindered quadrant bisphosphine ligand and its application in asymmetric hydrogenation

Kexuan Huang,[a] Xiaowei Zhang,[ab] Thomas J. Emge,[a] Guohua Hou,[a] Bonan Cao[a] and Xumu Zhang*[a]

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General Methods. Starting materials, reagents and solvents were purchased fromcommercial sources and were used as received**.** All reactions and manipulations that were sensitive to moisture or air were performed in a nitrogen-filled glovebox or using standard Schlenk techniques, unless otherwise noted. Solvents were dried with standard procedures and degassed with N_2. Column chromatography was performed using 200-400 mesh silica gel supplied by Natland International Corp. Thin-layer chromatography (TLC) was performed on EM reagents 0.25 mm silica 60-F plates. ^{1}H, ^{13}C, and ^{31}P NMR spectra were recorded on BrukerAvance 400 MHz spectrometers or Varian Mercury 500 MHz FT-NMR spectrometer. Optical rotation was obtained on a Perkin-Elmer 341 MC polarimeter. HRMS were recorded on a Thermo LTQ Orbitrap hybrid mass spectrometer. GC analysis was carried out on Hewlett-Packard 7890 gas chromatography using chiral capillary columns. HPLC analysis was carried out on Agilent 1200 series. Compound

3((1*S*,2*S*)-1,2-cyclohexanedicarboxylic acid**)** is commercial available from TCI America or synthesized according reference.[1]

Ligand synthesis procedure

(1S,2S)-Cyclohexane-1,2-diyldimethanol (4). To a suspension of $LiAlH_4$ (6.76 g, 178.0 mmol) in anhydrous THF (150 mL) was added (*S*, *S*)-**3** (12.25 g, 71.2 mmol) in portions at 0 ˚C. The mixture was stirred at room temperature overnight and then heated at 60 ˚C for 5 h. The reaction was cooled to r.t. and quenched with H_2O (10 mL) slowly at 0 ˚C (Caution: vigorous gas evolved). An aqueous solution of NaOH (40 mL, 15 % w/w) was added and stirred for 1h. The organic layer was separated and the aqueous phase was extracted with ethyl acetate (150 mL) for three times. The combined organic extracts were dried over Na_2SO_4. Removing the solvent under vacuum afforded (*S*, *S*)-**4**as a white solid (9.85 g, 98 % yield, pure enough for next use). $[\alpha]^{24}_{D}$ = -21.7 (c = 1.2, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 4.09 (s, 2H), 3.61 (dd, *J* = 10.9, 6.4 Hz, 2H), 3.53 (dd, *J* = 10.9, 6.4 Hz, 2H), 1.75-1.73 (m, 2H), 3.61 (dd, *J* = 16.8, 1.6 Hz, 2H), 1.35-1.31 (m, 2H), 1.27-1.22 (m, 2H), 1.08-1.03 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 67.8, 44.6, 29.9, 26.1 ppm.

(5a*S*,9a*S*)-octahydrobenzo[*e*][1,3,2]dioxathiepine 3,3-dioxide (5). To a solution of (*S*, *S*)-**4** (5.16 g, 35.8 mmol) and triethylamine (19.95 mL, 143.2 mmol) in 120 mL of CH_2Cl_2 was added thionyl chloride (3.94 mL, 53.7 mmol) dropwise at 0 ˚C. The resulting dark brown solution was stirred at 0 ˚C for 1 h. The reaction was then quenched with water (30 mL). The organic layer was separated and the aqueous layer was extracted with CH_2Cl_2 (50 mL). The combined organic layers were dried over Na_2SO_4 and concentrated. The residue was passed a short silica gel plug (CH_2Cl_2 as eluent) to afford crystalline crude cyclic sulfite (6.61 g. 34.7 mmol). The crude product was dissolved in a mixture of acetonitrile, chloroform and water (50, 50, 75 mL respectively). $NaIO_4$ (11.50 g, 53.7 mmol) and $RuCl_3{\cdot}xH_2O$ (120 mg) were added at 0 ˚C. After vigorous stirring at 0 ˚C for 1.5 h, the reaction mixture was added brine (75 mL) and filtered. The organic layer of the

filtrate was separated. The aqueous layer was washed with CH_2Cl_2 (50 mL) twice. The combined organic layers were dried over Na_2SO_4 and concentrated. The resulting solid residue was purified by passing through a short silica gel plug (CH_2Cl_2 as eluent) to give (*S*, *S*)-**6** as a white solid (6.47 g, 88%). $[\alpha]^{24}_D$ = +64.6 (c = 1.1, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 4.30 (dd, *J* = 12.0, 9.6 Hz, 2H), 4.10 (dd, *J* = 12.0, 2.4 Hz, 2H), 1.91-1.82 (m, 2H), 1.78-1.68 (m, 2H), 1.65-1.62 (m, 2H), 1.40-1.26 (m, 2H), 1.06-0.96 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 75.6, 44.0, 27.4, 25.5 ppm; HRMS (ESI): *m*/*z*: calcd for $C_8H_{14}O_4NaS$ ([*M*+Na]$^+$): 229.0510; found: 229.0505.

(3a*S*,7a*S*)-2-(*tert*-butyl)octahydro-1*H*-isophosphindole 2-sulfide (6). To a mixture of *tert*-butyl phosphine solution (24.48 mL, 20 % v/v in octane, 30.0 mmol) and THF (80 mL) was added *n*-BuLi (12.0 mL, 2.5 M in hexane, 30.0 mmol) dropwise at -78 ˚C. The resulting yellow solution was allowed to warm to r.t. and stirred for 1 h. The reaction mixture was then cooled back to -78 ˚C and was added a solution of (*S*, *S*)-**6** (6.19 g, 30.0 mmol) in THF (50 mL) dropwise. The resulting solution was allowed to warm to r.t. and stirred for 4 h. After being cooled to -78 ˚C again, *n*-BuLi (12.0 mL, 2.5 M in hexane, 30.0 mmol) was added dropwise. The reaction mixture was warmed to r.t. and stirred overnight. After being quenched with degassed water (5.0 mL), sulfur powder (1.44 g, 45 mmol) was added as a portion. After being stirred for 2 h, the solvent was removed and the residue was dissolved in 200 mL ethyl acetate. The organic layer was washes with water (100 mL) and brine (100 mL) subsequently, and then dried over Na_2SO_4 and concentrated. The residue was passed a short alumina plug (ethyl acetate as eluent) and followed by recrystallization from hexane to give (*S*, *S*)-**7** as white crystals (5.59 g, 81%). $[\alpha]^{24}_D$ = -45.2 (c = 1.0, $CHCl_3$) at > 99 % *ee*; Enantiomeric excess was determined by HPLC analysis: Daicel ChiralPak AD, hexane/*i*PrOH = 99:1, flow rate = 1.0 mL/min, λ = 205 nm, t_{major} = 11.4 min, t_{minor} = 13.2 min; ^{1}H NMR (400 MHz, CD_2Cl_2) δ: 2.53 (ddd, *J* = 14.8, 6.8, 2.8 Hz, 1H), 2.01-1.76 (m, 7H), 1.57-1.46 (m, 1H), 1.37-1.10 (m, 14H); ^{13}C NMR (100 MHz, CD_2Cl_2) δ: 46.8 (d, J_{CP} = 3.3 Hz), 43.7 (d, J_{CP} = 4.4 Hz), 38.5 (d, J_{CP} = 47.1 Hz), 36.9 (d, J_{CP} = 48.5 Hz), 33.7 (d, J_{CP} = 14.3 Hz), 33.4 (d, J_{CP} = 13.2 Hz), 33.1 (d, J_{CP} = 15.6 Hz), 26.4 (d, J_{CP} = 1.5 Hz), 26.3 (d, J_{CP} = 1.5 Hz), 25.1 (d, J_{CP} = 2.1 Hz) ppm; ^{31}P NMR (162 MHz, CD_2Cl_2) δ: 75.6 ppm; HRMS (ESI): *m*/*z*: calcd for $C_{12}H_{23}NaPS$ ([*M*+Na]$^+$): 253.1156; found: 253.1151.

(1*S*,2*R*,3a*S*,7a*S*)-2-(*tert*-butyl)-1-(di-tert-butylphosphino)octahydro-1*H*-isophosphindole 2-sulfide (7). At -78 ˚C, to a solution of **6** (0.7 g, 3 mmol), TMEDA (0.55 mL,3.6mmol), HMPA (0.62 mL, 3.6 mmol) in THF (35 mL) was addeddropwise*t*BuLi (2.1 mL, 1.7 M in pentane, 3.6 mmol). The reactionmixture was stirred at -78 ˚Cfor 1 h, followed by slow addition ofa solution of P*t*Bu_2Cl (0.59 mL, 3.1 mmol) in 10 mL of THF at thesame temperature in 10 min. The resulting mixture was stirred at -78 ˚Cfor another 10 min, then allowed to slowly warm to rt andstirred overnight before quenching with NH_4Cl (aq). The organiclayer was extracted with ether (3×15 mL) and washed with brine(10 mL), dried over Na_2SO_4, and concentrated under reducedpressure. The residue was purified by flash column chromatographyon silica gel (hexenes/EtOAc, 90:10) to afford **7** as a white solid (0.56g, 52%).$[\alpha]^{24}_D$ = -37.8(c = 1.0, $CHCl_3$)^{1}H NMR (400 MHz, $CDCl_3$) δ: 2.54 (ddd, *J* =22.1, 11.6, 1.5 Hz, 1H), 2.17-2.14(m, 1H), 1.98-1.94 (m, 2H), 1.83-1.69 (m, 5H), 1.42-1.38 (m, 10H), 1.24-1.18 (m, 23H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 54.0 (q, *J* = 63.5, 39.3 Hz), 48.5 (t, *J* = 4.4 Hz), 42.2 (d, *J* = 6.2 Hz), 37.0 (d, *J* = 1.1 Hz), 36.6 (d, *J* = 1.2 Hz), 36.1 (d, *J* = 3.2 Hz), 35.6 (d, *J* = 3.5 Hz), 35.5 (d, *J* = 6.4 Hz), 35.1 (d, *J* = 6.5 Hz), 34.5 (d, *J* = 14.1 Hz), 33.6 (d, *J* = 15.5 Hz), 33.0 (d, *J* = 7.2 Hz), 32.8(d, *J* = 16.1 Hz), 30.5 (d, *J* = 15.2 Hz), 26.4 (d, *J* = 1.9 Hz), 25.8 (d, *J* = 1.0 Hz); ^{31}P NMR (162 MHz, $CDCl_3$) δ: 80.1(d, *J* = 103.6 Hz), 33.4 (d, *J* = 103.6 Hz); HRMS (ESI): *m*/*z*: calcd for $C_{20}H_{40}P_2S$ ($[M+H]^+$): 375.2404; found: 375.2411.

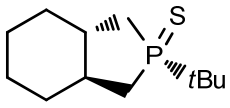
(1*S*,2*R*,3a*S*,7a*S*)-2-(*tert*-butyl)-1-(2,2,4,4-tetramethylpentan-3-yl)octahydro-1*H*-isophosphindole (8).To a solution of **7** (0.36 g, 1mmol) in anhydrous degassed toluene (10 mL) was added Si_2Cl_6 (0.86 mL, 5.0mmol) dropwise. The mixture was stirred at 70 ˚C for 10h.The solution was cooled to r.t. and added degassed aqueous NaOH solution (20 mL, 30 % w/w) in an ice bath. The resulting mixture was then stirred at 50 ˚C until the aqueous layer became clear. The aqueous layer was washed twice with degassed toluene (15 mL). The combined organic layer was dried over Na_2SO_4 and concentrated in vacuum. The residue was purified by passing through a basic alumina plug with a mixture of Et_2O (10 mL) and hexanes (50 mL) as eluent under N_2. Concentration the

resulted solution in vacuum afforded **8** as colorless oil (0.29g, 91%).^{1}H NMR (400 MHz, $CDCl_3$) δ: 2.16-2.14 (m, 1H), 1.99-1.94 (m, 2H), 1.87-1.82 (m, 2H), 1.81-1.67(m, 5H), 1.36-1.28 (m, 13H), 1.25-1.1.09 (m, 13H), 1.08-0.97 (m, 14H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 52.4, 49.7, 49.5, 44. (d, J = 2.4 Hz), 34.3 (d, J = 2.5 Hz), 34.2, 33.7, 33.3, 31.9 (m), 31.5 (m), 30.5, 30.4 (d, J = 2.2 Hz), 30.3, 30.0, 29.7 (m), 29.4, 28.2 (m), 27.6, 27.5, 25.6 (d, J = 2.0 Hz),24.9; ^{31}P NMR (162 MHz, $CDCl_3$) δ: 36.3 (br s), 10.1(br s);HRMS (ESI): *m*/*z*: calcd for $C_{20}H_{40}P_2$ ($[M+H]^+$):343.2684; found: 343.2682.

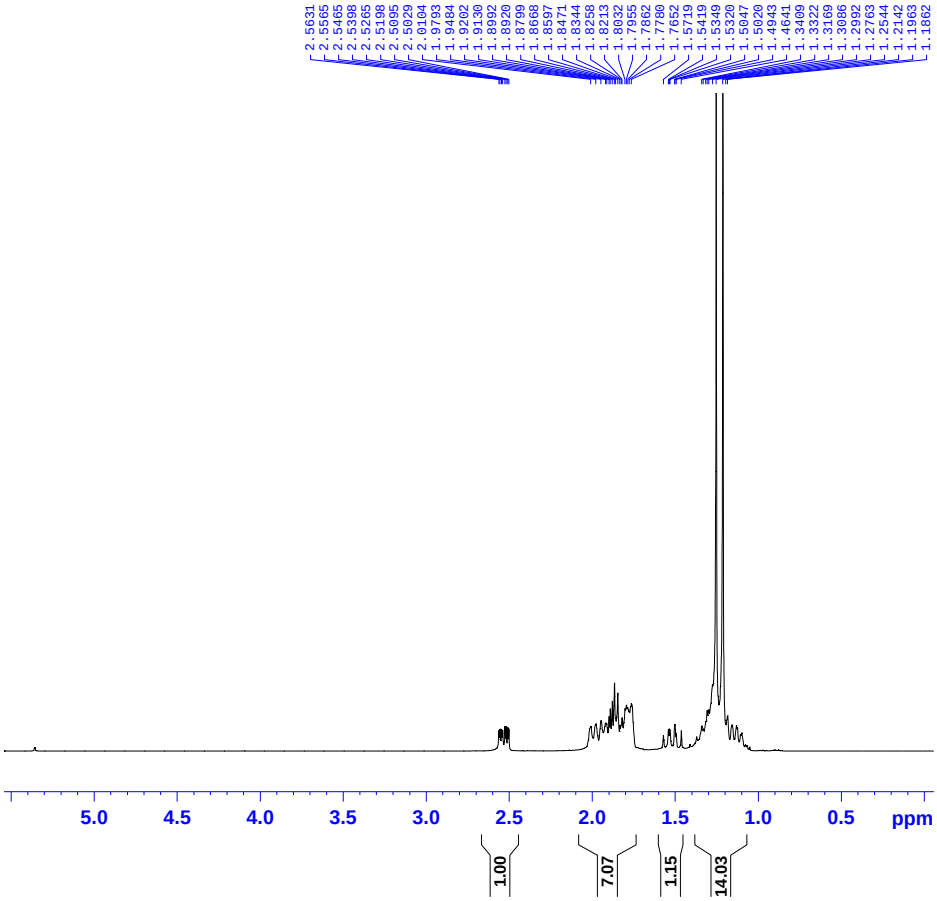
Preparation of Rh[(8)(NBD)]BF_4. To a solution of $[Rh(nbd)_2]BF_4$ (37.4 mg, 0.1 mmol) in degassed MeOH (1 mL) at 0˚C was added a solution of **8** (37.6 mg, 0.11mmol) in THF (1 mL). The resulting red solution was allowed to warm to r.t. and stirred for 20 min. The solution was concentrated to about 1 mL and then was added degassed Et_2O (12 mL) under vigorous stirring. The resulting precipitate was filtered, further washed with ether (2×5 mL) twice, and dried under vacuum to afford red solid (43.6 mg, 70%).^{1}H NMR (400 MHz, $CDCl_3$) δ: 5.65 (m, 4H), 4.23 (br s, 2H), 2.45-2.40 (m, 2H), 2.20-1.95 (m, 6H), 1.93-0.96 (m, 34H); ^{31}P NMR (162 MHz, $CDCl_3$) δ:20.1 (dd J= 128.7, 51.7Hz), -1.8 (dd J = 128.9, 52.1Hz) ;*m/z* (ESI-MS) 625.1 $[M+H]^+$.

General procedure for asymmetric hydrogenation:(Procedure with a s/c ratio of 1000) In a glovebox filled with nitrogen,Rh[(**8**)(NBD)]BF_4 complex (6.3 mg, 0.01 mmol) was dissolved in 10 mLdeoxygenatedMeOH. 0.1 mL of this solution was added to 1ml methanol solution dissolving0.1 mmolsubstrate. The resulting solution was then transferred into an autoclave and charged with 50 psi of hydrogen. The hydrogenation was performed at room temperature for 12 h. After carefully releasing the pressure in hood, the reaction mixture was passed through a short silica-gel plug to remove the catalyst. Enantiomeric excess were determined with the resulting solution by chiral GC or HPLC. For the hydrogenation of dehydroamino acids, the enantiomeric excesses were measured after conversion into their corresponding methyl esters by treatment with $TMSCHN_2$ (TMS = trimethylsilyl).The *ee* values of **10a-m** were determined according to reference [2], The*ee* values of hydrogenation products of **11a-e** were determined according to reference [3].

^{1}H NMR (400 MHz CD_2Cl_2)



(*S*, *S*)-**6**

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FIDRES             0.125483 Hz
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RG                        32
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DE                     6.50 usec
TE                    299.4 K
D1                 1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
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PL1                   -2.00 dB
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SFO1           400.1324710 MHz
SI                     32768
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WDW                       EM
SSB                        0
LB                    0.30 Hz
GB                         0
PC                     1.00
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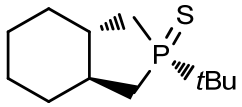
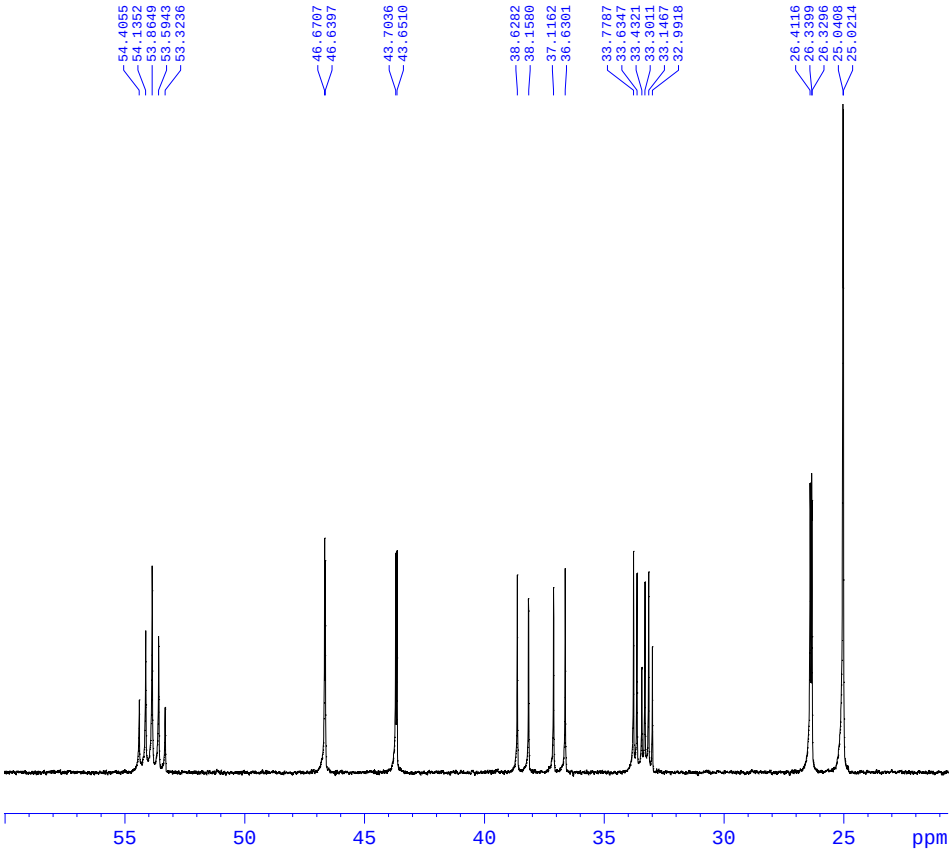
^{13}C NMR (100 MHz CD_2Cl_2)



(*S, S*)-**6**

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TE                301.2 K
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D11           0.03000000 sec
TD0                   1

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PL12               18.23 dB
PL13               19.00 dB
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PL12W         0.29563907 W
PL13W         0.24760634 W
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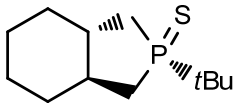
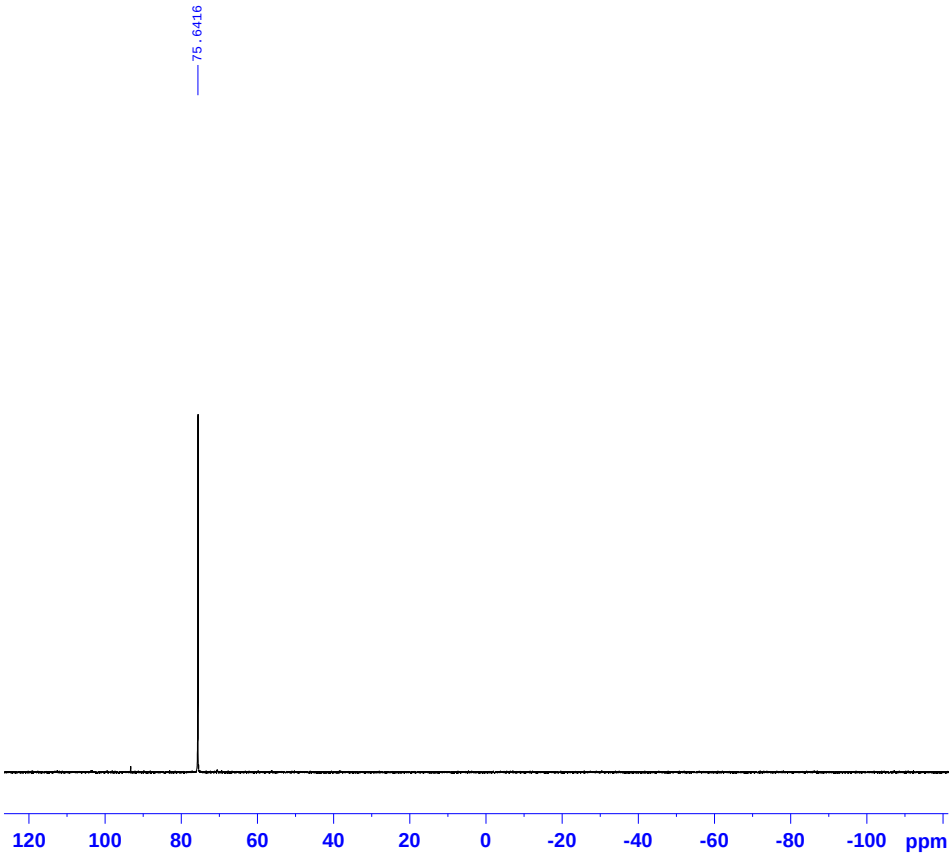
^{31}P NMR (162 MHz CD_2Cl_2)



(*S, S*)-**6**

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D1             2.00000000 sec
D11            0.03000000 sec
TD0                      1

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PL12                 18.23 dB
PL13                 19.00 dB
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PL12W          0.29563907 W
PL13W          0.24760634 W
SFO2         400.1316005 MHz
SI                   32768
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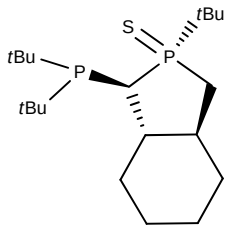
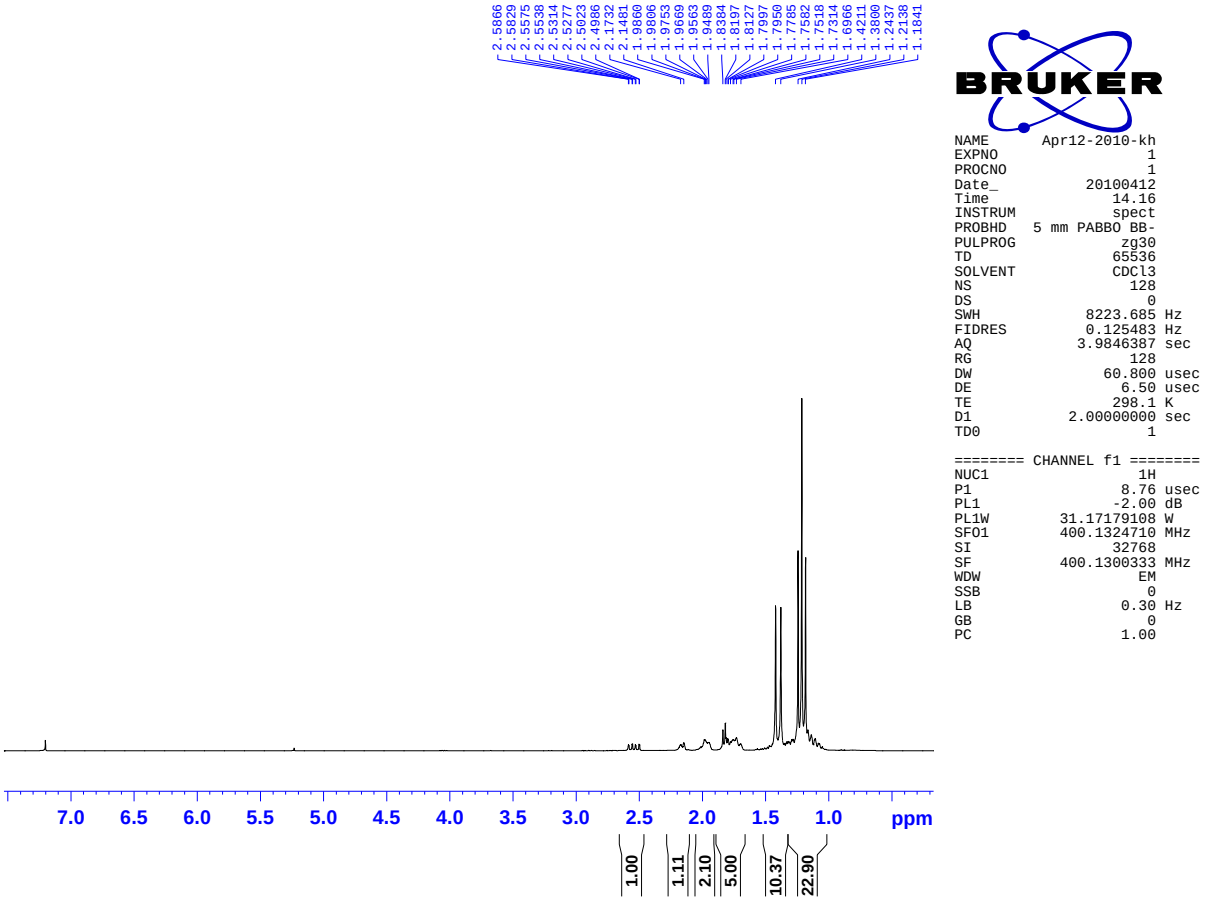
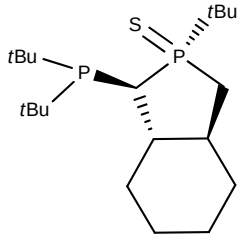
^{1}H NMR (400 MHz $CDCl_3$)



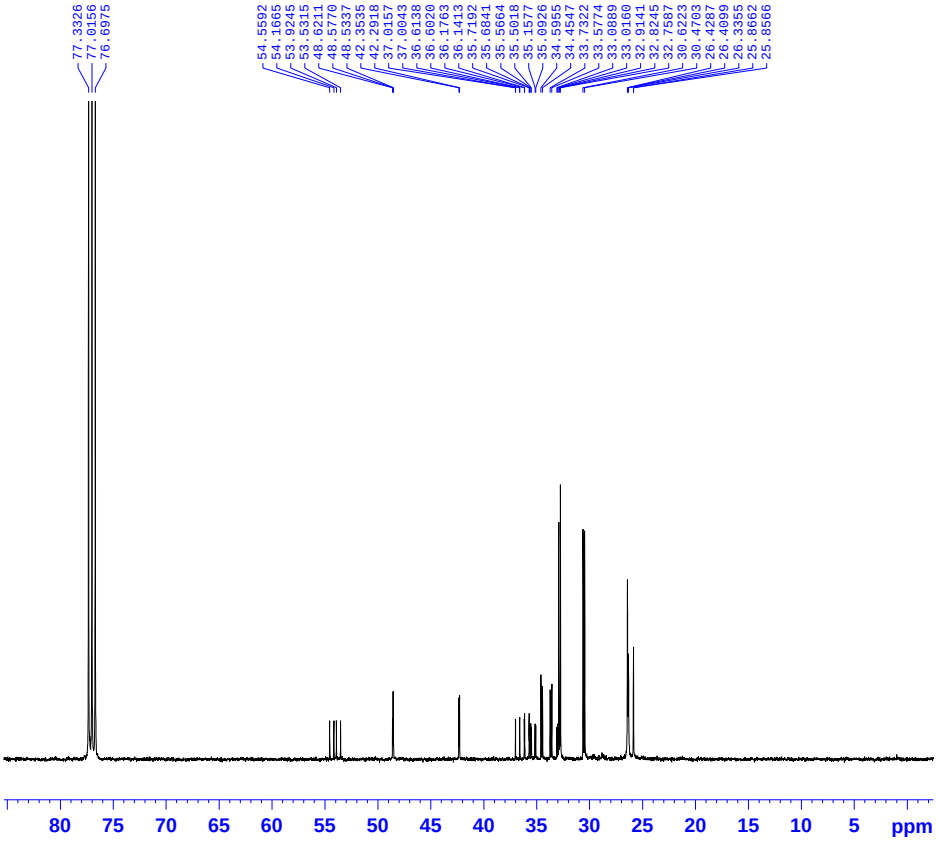
(1*S*,2*R*,3a*S*,7a*S*)-**7**



^{13}C NMR (100 MHz $CDCl_3$)



(1*S*,2*R*,3a*S*,7a*S*)-**7**



BRUKER

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FIDRES          0.366798 Hz
AQ              1.3631988 sec
RG                  2050
DW                20.800 usec
DE                 6.50 usec
TE                301.9 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                   8.50 usec
PL1                  1.00 dB
PL1W         75.02186584 W
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2               90.00 usec
PL2                 -2.00 dB
PL12                18.23 dB
PL13                19.00 dB
PL2W         31.17179108 W
PL12W         0.29563907 W
PL13W         0.24760634 W
SFO2        400.1316005 MHz
SI                 32768
SF          100.6127690 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
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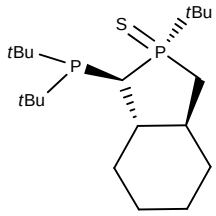
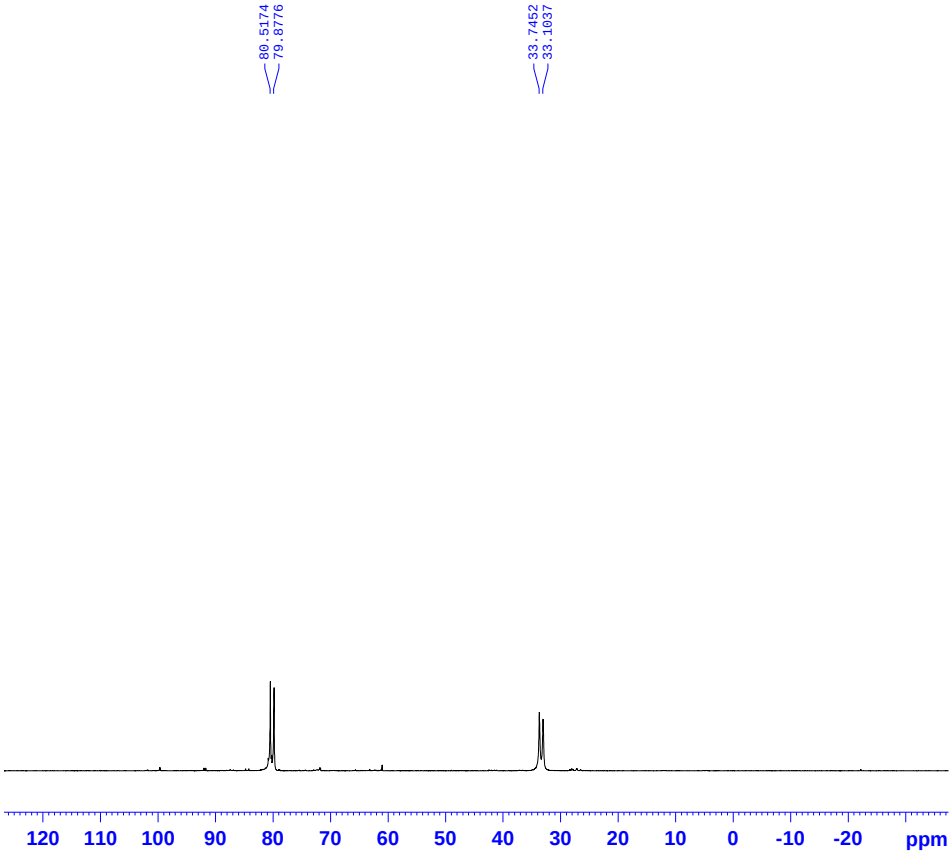
^{31}P NMR (162 MHz $CDCl_3$)



(1*S*,2*R*,3a*S*,7a*S*)-**7**

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FIDRES        0.978127 Hz
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DE               6.50 usec
TE               303.2 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                31P
P1                8.50 usec
PL1               4.00 dB
PL1W       37.79999924 W
SFO1      161.9755930 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            90.00 usec
PL2              -2.00 dB
PL12             18.23 dB
PL13             19.00 dB
PL2W       31.17179108 W
PL12W       0.29563907 W
PL13W       0.24760634 W
SFO2       400.1316005 MHz
SI               32768
SF        161.9755930 MHz
WDW                 EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
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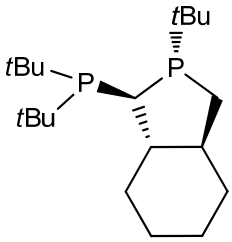
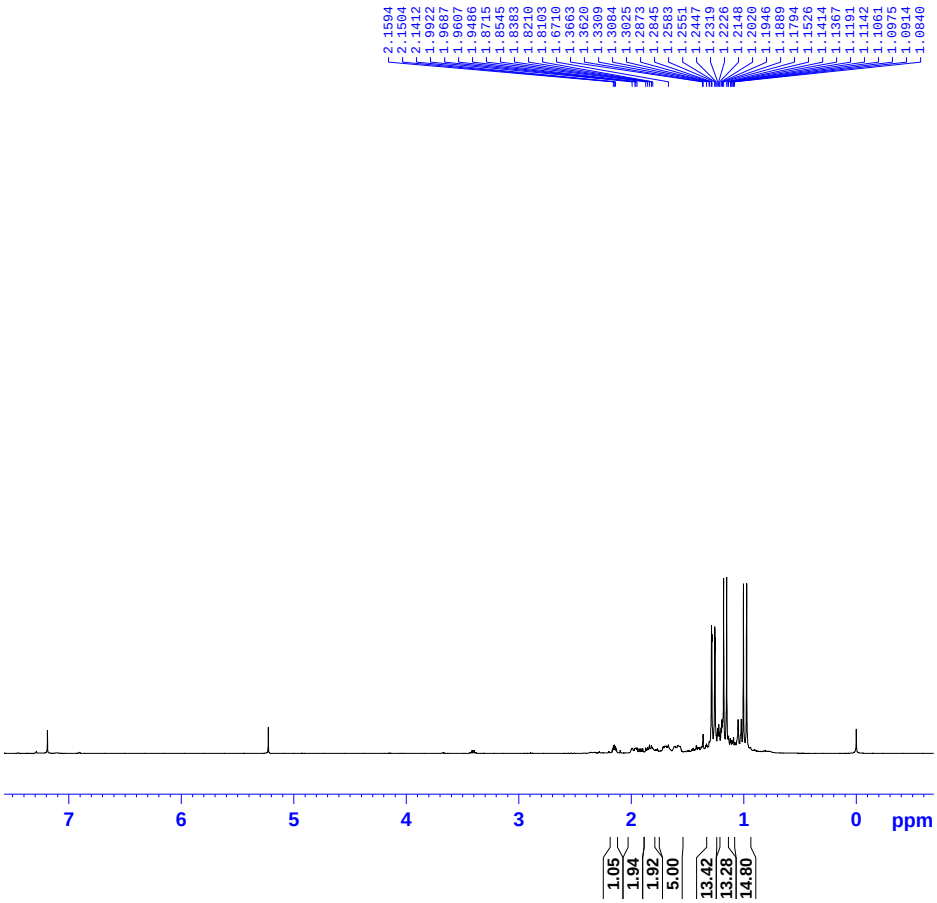
^{1}H NMR (400 MHz $CDCl_3$)



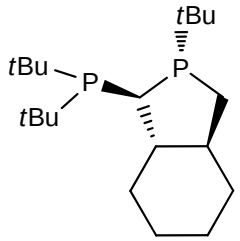
(1*R*,2*S*,3a*S*,7a*S*)-**8**



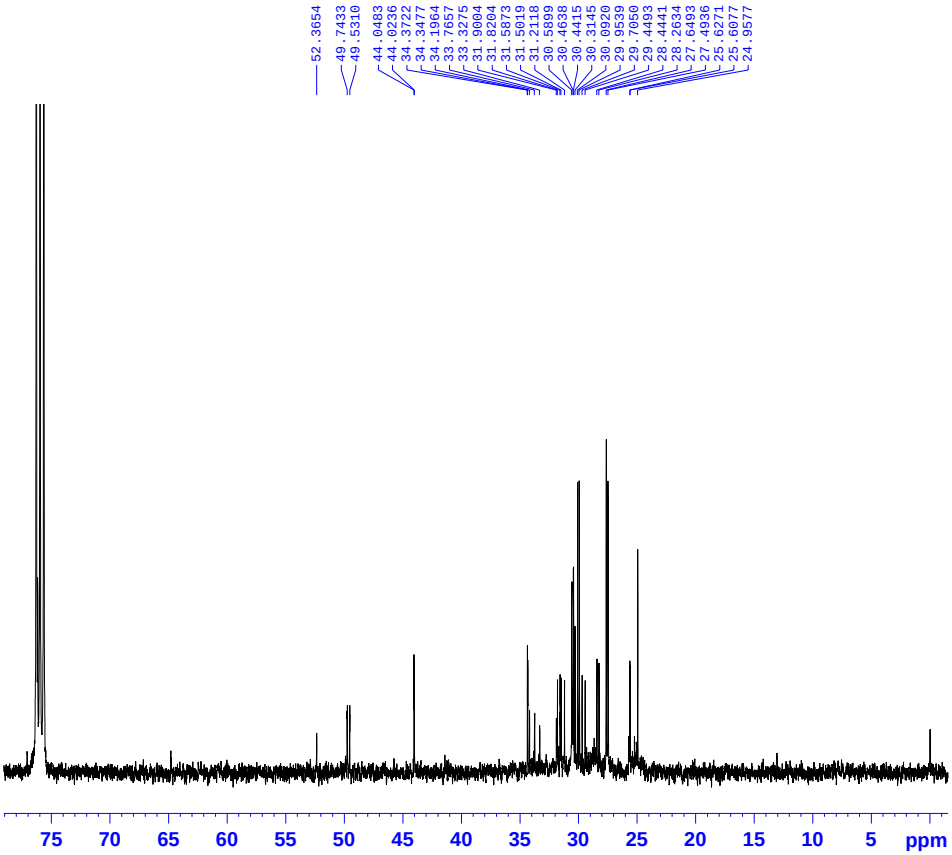
BRUKER

NAME	Jul13-2010-kh
EXPNO	2
PROCNO	1
Date_	20100713
Time	1.05
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	128
DS	0
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	362
DW	60.800 usec
DE	6.50 usec
TE	301.8 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	8.76 usec
PL1	-2.00 dB
PL1W	31.17179108 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300374 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

^{13}C NMR (100 MHz $CDCl_3$)



(1*R*,2*S*,3a*S*,7a*S*)-**8**



BRUKER

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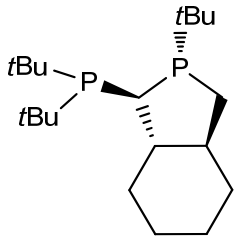
NAME          Jul13-2010-kh
EXPNO                    3
PROCNO                   1
Date_             20100713
Time                 8.30
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    7000
DS                       2
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631988 sec
RG                    2050
DW                  20.800 usec
DE                   6.50 usec
TE                  302.7 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                      1

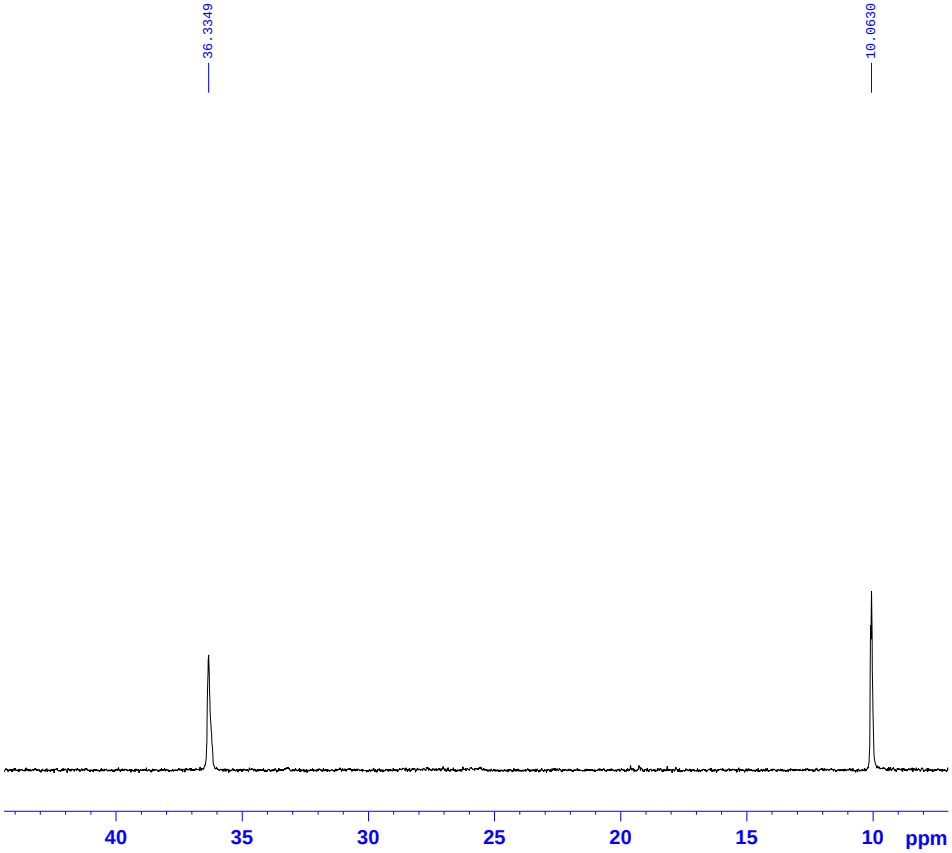
======== CHANNEL f1 ========
NUC1                   13C
P1                    8.50 usec
PL1                   1.00 dB
PL1W           75.02186584 W
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                   1H
PCPD2                90.00 usec
PL2                  -2.00 dB
PL12                 18.23 dB
PL13                 19.00 dB
PL2W           31.17179108 W
PL12W           0.29563907 W
PL13W           0.24760634 W
SFO2          400.1316005 MHz
SI                    32768
SF            100.6128693 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

^{31}P NMR (162 MHz $CDCl_3$)



(1*R*,2*S*,3a*S*,7a*S*)-**8**

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NAME          Jul13-2010-kh
EXPNO                    1
PROCNO                   1
Date_             20100713
Time                  0.57
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     160
DS                       4
SWH              64102.563 Hz
FIDRES           0.978127 Hz
AQ               0.5112308 sec
RG                    2050
DW                   7.800 usec
DE                    6.50 usec
TE                   302.3 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   31P
P1                    8.50 usec
PL1                   4.00 dB
PL1W           37.79999924 W
SFO1           161.9755930 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2                90.00 usec
PL2                  -2.00 dB
PL12                 18.23 dB
PL13                 19.00 dB
PL2W           31.17179108 W
PL12W           0.29563907 W
PL13W           0.24760634 W
SFO2           400.1316005 MHz
SI                    32768
SF             161.9755930 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```
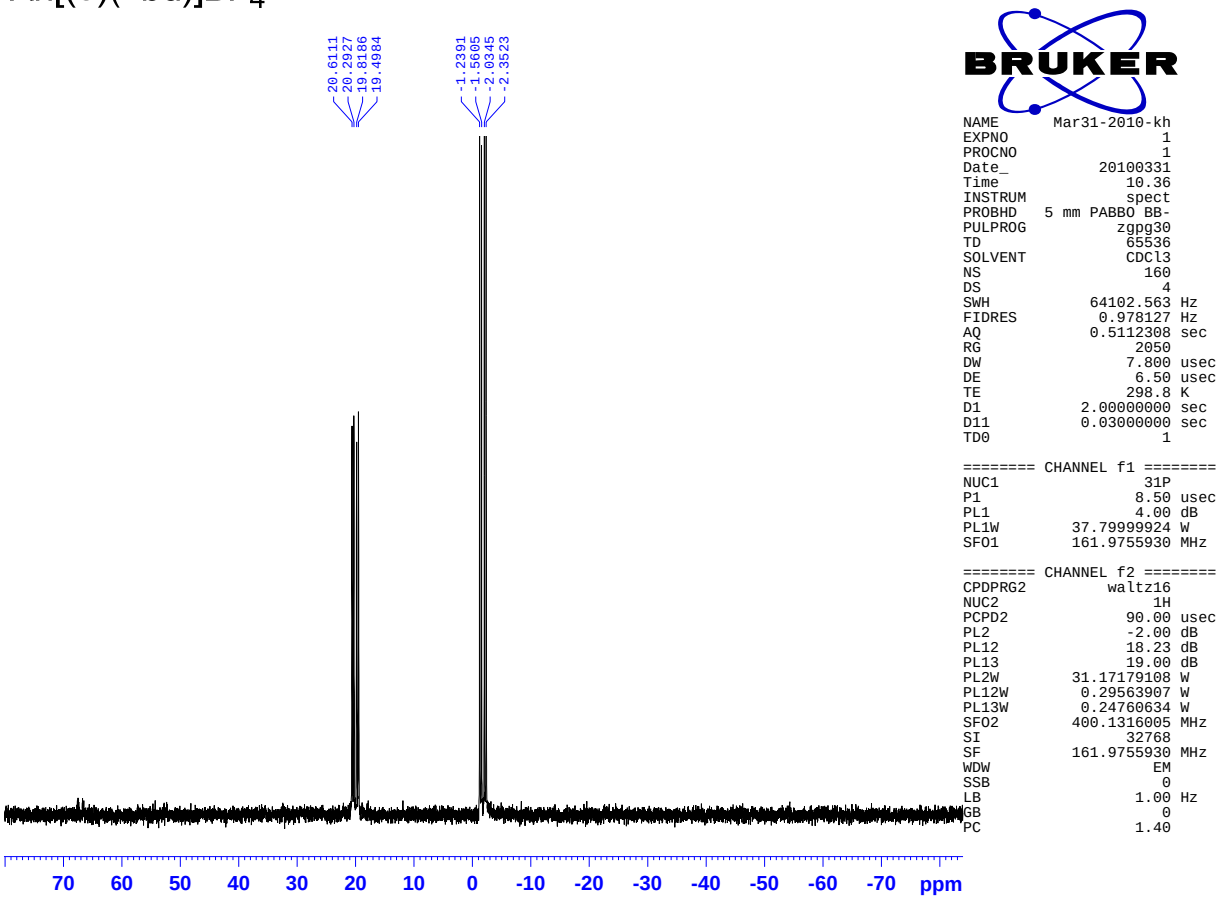

^{31}P NMR (162 MHz $CDCl_3$)

Rh[(**8**)(nbd)]BF_4



Reference:

[1]a) L. Ma, D. Du, J. Xu, *J. Org. Chem.***2005**, *70*, 10155–10158 ; b) A. Berkessel, K. Glaubitz, J. Lex, *Eur. J. Org. Chem.***2002**, 2948–2952.

[2] a) G.Zhu, P.Cao, Q.Jiang, X.Zhang, *J. Am. Chem. Soc.* **1997**,*119*, 1799-1800; b) W. Tang, X. Zhang, *Angew. Chem.***2002**, *114*, 1682-1684; *Angew. Chem. Int. Ed.* **2002**, *41*, 1612-1614; c) W. Zhang, X, Zhang, *J. Org. Chem.* **2007**,*72*, 1020-1023.

[3] a) Y.-G. Zhou, W. Tang, W.-B. Wang, W. Li, X. Zhang *J. Am. Chem. Soc.* **2002**, *124*,4952-4953; b) W. Tang, X. Zhang, *Org. Lett.***2002**, *4*, 4159-4161

Table 1.Crystal data and structure refinement for p_s_1a.

Identification code	p_s_1a	
Empirical formula	C21 H41 Cl3 P2 S	
Formula weight	493.89	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 8.4109(5) Å	α= 90°.
	b = 15.8263(10) Å	β= 90°.
	c = 39.840(3) Å	γ = 90°.
Volume	5303.3(6) $Å^3$	
Z	8	
Density (calculated)	1.237 Mg/m^3	
Absorption coefficient	0.551 mm^{-1}	
F(000)	2112	
Crystal size	0.42 x 0.18 x 0.10 mm^3	
Theta range for data collection	2.74 to 30.54°.	
Index ranges	-12<=h<=12, -22<=k<=22, -56<=l<=56	
Reflections collected	58982	
Independent reflections	16069 [R(int) = 0.0418]	
Completeness to theta = 30.54°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.947 and 0.801	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	16069 / 363 / 577	
Goodness-of-fit on F^2	1.006	
Final R indices [I>2sigma(I)]	R1 = 0.0593, wR2 = 0.1296	
R indices (all data)	R1 = 0.0651, wR2 = 0.1324	
Absolute structure parameter	0.09(6)	
Largest diff. peak and hole	0.704 and -0.447 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for p_s_1a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
P(1)	10288(1)	-727(1)	970(1)	15(1)
P(2)	10898(1)	1074(1)	694(1)	15(1)
S(1)	12562(1)	-896(1)	884(1)	22(1)
C(1)	9497(3)	384(2)	951(1)	15(1)
C(2)	8946(3)	578(2)	1318(1)	17(1)
C(3)	7611(3)	1224(2)	1360(1)	22(1)
C(4)	7200(4)	1338(2)	1732(1)	29(1)
C(5)	6760(4)	507(2)	1903(1)	29(1)
C(6)	8041(4)	-159(2)	1849(1)	24(1)
C(7)	8402(3)	-263(2)	1476(1)	17(1)
C(8)	9695(4)	-916(2)	1402(1)	20(1)
C(9)	9481(3)	1740(2)	433(1)	20(1)
C(10)	10434(5)	2444(2)	257(1)	33(1)
C(11)	8018(4)	2134(2)	600(1)	28(1)
C(12)	8905(4)	1135(2)	158(1)	25(1)
C(13)	12093(3)	1762(2)	993(1)	20(1)
C(14)	11188(4)	2443(2)	1189(1)	28(1)
C(15)	12974(3)	1174(2)	1238(1)	26(1)
C(16)	13398(4)	2197(2)	784(1)	29(1)
C(17)	9057(4)	-1424(2)	698(1)	21(1)
C(18)	9476(4)	-2347(2)	789(1)	27(1)
C(19)	7274(4)	-1282(2)	749(1)	25(1)
C(20)	9512(5)	-1268(2)	329(1)	29(1)
P(3)	5175(1)	6891(1)	1549(1)	15(1)
S(2)	7306(1)	7260(1)	1685(1)	23(1)
C(21)	4761(3)	5728(2)	1522(1)	15(1)
C(22)	4431(3)	5571(2)	1143(1)	15(1)
C(23)	3363(4)	4814(2)	1063(1)	21(1)
C(24)	3106(4)	4729(2)	684(1)	27(1)
C(25)	2482(4)	5546(2)	524(1)	28(1)
C(26)	3523(4)	6300(2)	613(1)	20(1)

C(27)	3689(3)	6370(2)	995(1)	17(1)
C(28)	4694(4)	7115(2)	1113(1)	18(1)
P(4A)	6032(5)	5102(3)	1808(1)	18(1)
C(29A)	7596(8)	4537(4)	1547(2)	27(1)
C(30A)	7144(12)	3966(6)	1255(2)	27(1)
C(31A)	8651(8)	5262(5)	1403(2)	37(2)
C(32A)	8624(9)	4029(5)	1795(2)	40(2)
C(33A)	4676(9)	4270(4)	2010(2)	23(1)
C(34A)	4507(10)	3410(4)	1828(2)	36(2)
C(35A)	3018(7)	4625(4)	2068(2)	31(1)
C(36A)	5423(9)	4099(4)	2360(2)	39(1)
P(4B)	6368(7)	5109(5)	1765(2)	18(1)
C(29B)	7862(10)	4690(6)	1451(2)	21(2)
C(30B)	7334(18)	4043(9)	1191(3)	27(1)
C(31B)	8584(10)	5444(5)	1262(2)	24(2)
C(32B)	9246(11)	4309(6)	1660(2)	35(2)
C(33B)	5212(11)	4224(6)	1964(2)	22(2)
C(34B)	4117(12)	3652(6)	1752(2)	28(2)
C(35B)	4181(11)	4626(6)	2233(2)	35(2)
C(36B)	6423(12)	3656(6)	2154(2)	40(2)
C(37)	3631(4)	7388(2)	1820(1)	20(1)
C(38)	3869(4)	8352(2)	1807(1)	27(1)
C(39)	1931(3)	7177(2)	1702(1)	24(1)
C(40)	3889(4)	7078(2)	2180(1)	24(1)
Cl(1)	10036(1)	4606(1)	-173(1)	35(1)
Cl(2)	9078(1)	6313(1)	-21(1)	43(1)
Cl(3)	7588(2)	4906(1)	316(1)	65(1)
C(41)	8430(4)	5260(2)	-63(1)	29(1)
Cl(4)	10070(1)	5852(1)	2406(1)	40(1)
Cl(5)	9123(2)	7557(1)	2561(1)	55(1)
Cl(6)	7276(2)	6154(1)	2814(1)	60(1)
C(42)	8436(4)	6528(3)	2479(1)	33(1)

Table 3. Bond lengths [Å] and angles [°] for p_s_1a.

P(1)-C(8)	1.815(3)	C(11)-H(11A)	0.9800
P(1)-C(17)	1.863(3)	C(11)-H(11B)	0.9800
P(1)-C(1)	1.882(3)	C(11)-H(11C)	0.9800
P(1)-S(1)	1.9623(10)	C(12)-H(12A)	0.9800
P(2)-C(13)	1.901(3)	C(12)-H(12B)	0.9800
P(2)-C(9)	1.901(3)	C(12)-H(12C)	0.9800
P(2)-C(1)	1.903(3)	C(13)-C(14)	1.532(4)
C(1)-C(2)	1.565(4)	C(13)-C(16)	1.539(4)
C(1)-H(1)	1.0000	C(13)-C(15)	1.539(4)
C(2)-C(3)	1.527(4)	C(14)-H(14A)	0.9800
C(2)-C(7)	1.542(4)	C(14)-H(14B)	0.9800
C(2)-H(2)	1.0000	C(14)-H(14C)	0.9800
C(3)-C(4)	1.534(4)	C(15)-H(15A)	0.9800
C(3)-H(3A)	0.9900	C(15)-H(15B)	0.9800
C(3)-H(3B)	0.9900	C(15)-H(15C)	0.9800
C(4)-C(5)	1.526(5)	C(16)-H(16A)	0.9800
C(4)-H(4A)	0.9900	C(16)-H(16B)	0.9800
C(4)-H(4B)	0.9900	C(16)-H(16C)	0.9800
C(5)-C(6)	1.522(4)	C(17)-C(19)	1.530(4)
C(5)-H(5A)	0.9900	C(17)-C(20)	1.537(4)
C(5)-H(5B)	0.9900	C(17)-C(18)	1.547(4)
C(6)-C(7)	1.524(4)	C(18)-H(18A)	0.9800
C(6)-H(6A)	0.9900	C(18)-H(18B)	0.9800
C(6)-H(6B)	0.9900	C(18)-H(18C)	0.9800
C(7)-C(8)	1.529(4)	C(19)-H(19A)	0.9800
C(7)-H(7)	1.0000	C(19)-H(19B)	0.9800
C(8)-H(8A)	0.9900	C(19)-H(19C)	0.9800
C(8)-H(8B)	0.9900	C(20)-H(20A)	0.9800
C(9)-C(11)	1.532(4)	C(20)-H(20B)	0.9800
C(9)-C(12)	1.534(4)	C(20)-H(20C)	0.9800
C(9)-C(10)	1.542(4)	P(3)-C(28)	1.817(3)
C(10)-H(10A)	0.9800	P(3)-C(37)	1.864(3)
C(10)-H(10B)	0.9800	P(3)-C(21)	1.875(3)
C(10)-H(10C)	0.9800	P(3)-S(2)	1.9622(10)

C(21)-C(22)	1.556(4)	C(32A)-H(32C)	0.9800
C(21)-P(4A)	1.850(6)	C(33A)-C(35A)	1.521(9)
C(21)-P(4B)	1.930(8)	C(33A)-C(34A)	1.548(8)
C(21)-H(21)	1.0000	C(33A)-C(36A)	1.550(8)
C(22)-C(27)	1.528(4)	C(34A)-H(34A)	0.9800
C(22)-C(23)	1.532(4)	C(34A)-H(34B)	0.9800
C(22)-H(22)	1.0000	C(34A)-H(34C)	0.9800
C(23)-C(24)	1.534(4)	C(35A)-H(35A)	0.9800
C(23)-H(23A)	0.9900	C(35A)-H(35B)	0.9800
C(23)-H(23B)	0.9900	C(35A)-H(35C)	0.9800
C(24)-C(25)	1.533(5)	C(36A)-H(36A)	0.9800
C(24)-H(24A)	0.9900	C(36A)-H(36B)	0.9800
C(24)-H(24B)	0.9900	C(36A)-H(36C)	0.9800
C(25)-C(26)	1.523(4)	P(4B)-C(33B)	1.881(9)
C(25)-H(25A)	0.9900	P(4B)-C(29B)	1.893(9)
C(25)-H(25B)	0.9900	C(29B)-C(30B)	1.523(11)
C(26)-C(27)	1.530(4)	C(29B)-C(31B)	1.535(11)
C(26)-H(26A)	0.9900	C(29B)-C(32B)	1.553(10)
C(26)-H(26B)	0.9900	C(30B)-H(30D)	0.9800
C(27)-C(28)	1.526(4)	C(30B)-H(30E)	0.9800
C(27)-H(27)	1.0000	C(30B)-H(30F)	0.9800
C(28)-H(28A)	0.9900	C(31B)-H(31D)	0.9800
C(28)-H(28B)	0.9900	C(31B)-H(31E)	0.9800
P(4A)-C(29A)	1.901(7)	C(31B)-H(31F)	0.9800
P(4A)-C(33A)	1.919(7)	C(32B)-H(32D)	0.9800
C(29A)-C(30A)	1.523(8)	C(32B)-H(32E)	0.9800
C(29A)-C(32A)	1.540(9)	C(32B)-H(32F)	0.9800
C(29A)-C(31A)	1.560(10)	C(33B)-C(35B)	1.517(11)
C(30A)-H(30A)	0.9800	C(33B)-C(34B)	1.544(10)
C(30A)-H(30B)	0.9800	C(33B)-C(36B)	1.555(11)
C(30A)-H(30C)	0.9800	C(34B)-H(34D)	0.9800
C(31A)-H(31A)	0.9800	C(34B)-H(34E)	0.9800
C(31A)-H(31B)	0.9800	C(34B)-H(34F)	0.9800
C(31A)-H(31C)	0.9800	C(35B)-H(35D)	0.9800
C(32A)-H(32A)	0.9800	C(35B)-H(35E)	0.9800
C(32A)-H(32B)	0.9800	C(35B)-H(35F)	0.9800

C(36B)-H(36D)	0.9800	C(40)-H(40A)	0.9800
C(36B)-H(36E)	0.9800	C(40)-H(40B)	0.9800
C(36B)-H(36F)	0.9800	C(40)-H(40C)	0.9800
C(37)-C(40)	1.531(4)	Cl(1)-C(41)	1.757(3)
C(37)-C(38)	1.541(4)	Cl(2)-C(41)	1.762(4)
C(37)-C(39)	1.541(4)	Cl(3)-C(41)	1.760(4)
C(38)-H(38A)	0.9800	C(41)-H(41)	1.0000
C(38)-H(38B)	0.9800	Cl(4)-C(42)	1.766(4)
C(38)-H(38C)	0.9800	Cl(5)-C(42)	1.759(4)
C(39)-H(39A)	0.9800	Cl(6)-C(42)	1.754(4)
C(39)-H(39B)	0.9800	C(42)-H(42)	1.0000
C(39)-H(39C)	0.9800		

C(8)-P(1)-C(17)	107.57(13)	C(4)-C(3)-H(3A)	109.5
C(8)-P(1)-C(1)	95.52(12)	C(2)-C(3)-H(3B)	109.5
C(17)-P(1)-C(1)	109.43(13)	C(4)-C(3)-H(3B)	109.5
C(8)-P(1)-S(1)	114.35(10)	H(3A)-C(3)-H(3B)	108.1
C(17)-P(1)-S(1)	111.01(10)	C(5)-C(4)-C(3)	112.6(3)
C(1)-P(1)-S(1)	117.70(9)	C(5)-C(4)-H(4A)	109.1
C(13)-P(2)-C(9)	110.85(13)	C(3)-C(4)-H(4A)	109.1
C(13)-P(2)-C(1)	108.70(13)	C(5)-C(4)-H(4B)	109.1
C(9)-P(2)-C(1)	102.91(12)	C(3)-C(4)-H(4B)	109.1
C(2)-C(1)-P(1)	104.41(17)	H(4A)-C(4)-H(4B)	107.8
C(2)-C(1)-P(2)	124.93(18)	C(6)-C(5)-C(4)	111.2(3)
P(1)-C(1)-P(2)	109.83(13)	C(6)-C(5)-H(5A)	109.4
C(2)-C(1)-H(1)	105.4	C(4)-C(5)-H(5A)	109.4
P(1)-C(1)-H(1)	105.4	C(6)-C(5)-H(5B)	109.4
P(2)-C(1)-H(1)	105.4	C(4)-C(5)-H(5B)	109.4
C(3)-C(2)-C(7)	108.3(2)	H(5A)-C(5)-H(5B)	108.0
C(3)-C(2)-C(1)	116.8(2)	C(5)-C(6)-C(7)	110.7(3)
C(7)-C(2)-C(1)	107.5(2)	C(5)-C(6)-H(6A)	109.5
C(3)-C(2)-H(2)	108.0	C(7)-C(6)-H(6A)	109.5
C(7)-C(2)-H(2)	108.0	C(5)-C(6)-H(6B)	109.5
C(1)-C(2)-H(2)	108.0	C(7)-C(6)-H(6B)	109.5
C(2)-C(3)-C(4)	110.5(2)	H(6A)-C(6)-H(6B)	108.1
C(2)-C(3)-H(3A)	109.5	C(6)-C(7)-C(8)	113.8(2)

C(6)-C(7)-C(2)	111.4(2)	C(14)-C(13)-C(15)	110.0(3)
C(8)-C(7)-C(2)	107.1(2)	C(16)-C(13)-C(15)	105.6(2)
C(6)-C(7)-H(7)	108.2	C(14)-C(13)-P(2)	117.3(2)
C(8)-C(7)-H(7)	108.2	C(16)-C(13)-P(2)	107.2(2)
C(2)-C(7)-H(7)	108.2	C(15)-C(13)-P(2)	107.68(19)
C(7)-C(8)-P(1)	105.49(19)	C(13)-C(14)-H(14A)	109.5
C(7)-C(8)-H(8A)	110.6	C(13)-C(14)-H(14B)	109.5
P(1)-C(8)-H(8A)	110.6	H(14A)-C(14)-H(14B)	109.5
C(7)-C(8)-H(8B)	110.6	C(13)-C(14)-H(14C)	109.5
P(1)-C(8)-H(8B)	110.6	H(14A)-C(14)-H(14C)	109.5
H(8A)-C(8)-H(8B)	108.8	H(14B)-C(14)-H(14C)	109.5
C(11)-C(9)-C(12)	108.1(3)	C(13)-C(15)-H(15A)	109.5
C(11)-C(9)-C(10)	108.7(3)	C(13)-C(15)-H(15B)	109.5
C(12)-C(9)-C(10)	106.8(3)	H(15A)-C(15)-H(15B)	109.5
C(11)-C(9)-P(2)	119.5(2)	C(13)-C(15)-H(15C)	109.5
C(12)-C(9)-P(2)	104.06(19)	H(15A)-C(15)-H(15C)	109.5
C(10)-C(9)-P(2)	108.9(2)	H(15B)-C(15)-H(15C)	109.5
C(9)-C(10)-H(10A)	109.5	C(13)-C(16)-H(16A)	109.5
C(9)-C(10)-H(10B)	109.5	C(13)-C(16)-H(16B)	109.5
H(10A)-C(10)-H(10B)	109.5	H(16A)-C(16)-H(16B)	109.5
C(9)-C(10)-H(10C)	109.5	C(13)-C(16)-H(16C)	109.5
H(10A)-C(10)-H(10C)	109.5	H(16A)-C(16)-H(16C)	109.5
H(10B)-C(10)-H(10C)	109.5	H(16B)-C(16)-H(16C)	109.5
C(9)-C(11)-H(11A)	109.5	C(19)-C(17)-C(20)	110.3(3)
C(9)-C(11)-H(11B)	109.5	C(19)-C(17)-C(18)	109.3(3)
H(11A)-C(11)-H(11B)	109.5	C(20)-C(17)-C(18)	108.6(2)
C(9)-C(11)-H(11C)	109.5	C(19)-C(17)-P(1)	112.4(2)
H(11A)-C(11)-H(11C)	109.5	C(20)-C(17)-P(1)	108.9(2)
H(11B)-C(11)-H(11C)	109.5	C(18)-C(17)-P(1)	107.2(2)
C(9)-C(12)-H(12A)	109.5	C(17)-C(18)-H(18A)	109.5
C(9)-C(12)-H(12B)	109.5	C(17)-C(18)-H(18B)	109.5
H(12A)-C(12)-H(12B)	109.5	H(18A)-C(18)-H(18B)	109.5
C(9)-C(12)-H(12C)	109.5	C(17)-C(18)-H(18C)	109.5
H(12A)-C(12)-H(12C)	109.5	H(18A)-C(18)-H(18C)	109.5
H(12B)-C(12)-H(12C)	109.5	H(18B)-C(18)-H(18C)	109.5
C(14)-C(13)-C(16)	108.4(2)	C(17)-C(19)-H(19A)	109.5

C(17)-C(19)-H(19B)	109.5	C(22)-C(23)-H(23B)	109.5
H(19A)-C(19)-H(19B)	109.5	C(24)-C(23)-H(23B)	109.5
C(17)-C(19)-H(19C)	109.5	H(23A)-C(23)-H(23B)	108.1
H(19A)-C(19)-H(19C)	109.5	C(25)-C(24)-C(23)	112.6(2)
H(19B)-C(19)-H(19C)	109.5	C(25)-C(24)-H(24A)	109.1
C(17)-C(20)-H(20A)	109.5	C(23)-C(24)-H(24A)	109.1
C(17)-C(20)-H(20B)	109.5	C(25)-C(24)-H(24B)	109.1
H(20A)-C(20)-H(20B)	109.5	C(23)-C(24)-H(24B)	109.1
C(17)-C(20)-H(20C)	109.5	H(24A)-C(24)-H(24B)	107.8
H(20A)-C(20)-H(20C)	109.5	C(26)-C(25)-C(24)	111.6(3)
H(20B)-C(20)-H(20C)	109.5	C(26)-C(25)-H(25A)	109.3
C(28)-P(3)-C(37)	108.45(13)	C(24)-C(25)-H(25A)	109.3
C(28)-P(3)-C(21)	95.47(12)	C(26)-C(25)-H(25B)	109.3
C(37)-P(3)-C(21)	108.55(13)	C(24)-C(25)-H(25B)	109.3
C(28)-P(3)-S(2)	114.13(10)	H(25A)-C(25)-H(25B)	108.0
C(37)-P(3)-S(2)	110.54(10)	C(25)-C(26)-C(27)	109.9(2)
C(21)-P(3)-S(2)	118.52(9)	C(25)-C(26)-H(26A)	109.7
C(22)-C(21)-P(4A)	128.0(2)	C(27)-C(26)-H(26A)	109.7
C(22)-C(21)-P(3)	104.20(17)	C(25)-C(26)-H(26B)	109.7
P(4A)-C(21)-P(3)	112.5(2)	C(27)-C(26)-H(26B)	109.7
C(22)-C(21)-P(4B)	122.0(3)	H(26A)-C(26)-H(26B)	108.2
P(4A)-C(21)-P(4B)	9.8(2)	C(28)-C(27)-C(22)	107.0(2)
P(3)-C(21)-P(4B)	109.9(3)	C(28)-C(27)-C(26)	114.5(2)
C(22)-C(21)-H(21)	103.0	C(22)-C(27)-C(26)	111.2(2)
P(4A)-C(21)-H(21)	103.0	C(28)-C(27)-H(27)	108.0
P(3)-C(21)-H(21)	103.0	C(22)-C(27)-H(27)	108.0
P(4B)-C(21)-H(21)	112.7	C(26)-C(27)-H(27)	108.0
C(27)-C(22)-C(23)	109.1(2)	C(27)-C(28)-P(3)	105.59(18)
C(27)-C(22)-C(21)	108.4(2)	C(27)-C(28)-H(28A)	110.6
C(23)-C(22)-C(21)	115.5(2)	P(3)-C(28)-H(28A)	110.6
C(27)-C(22)-H(22)	107.8	C(27)-C(28)-H(28B)	110.6
C(23)-C(22)-H(22)	107.8	P(3)-C(28)-H(28B)	110.6
C(21)-C(22)-H(22)	107.8	H(28A)-C(28)-H(28B)	108.8
C(22)-C(23)-C(24)	110.8(2)	C(21)-P(4A)-C(29A)	108.4(3)
C(22)-C(23)-H(23A)	109.5	C(21)-P(4A)-C(33A)	106.5(3)
C(24)-C(23)-H(23A)	109.5	C(29A)-P(4A)-C(33A)	108.6(4)

C(30A)-C(29A)-C(32A)	108.7(6)	C(29B)-C(30B)-H(30F)	109.5
C(30A)-C(29A)-C(31A)	107.2(6)	H(30D)-C(30B)-H(30F)	109.5
C(32A)-C(29A)-C(31A)	107.6(6)	H(30E)-C(30B)-H(30F)	109.5
C(30A)-C(29A)-P(4A)	121.6(6)	C(29B)-C(31B)-H(31D)	109.5
C(32A)-C(29A)-P(4A)	106.5(5)	C(29B)-C(31B)-H(31E)	109.5
C(31A)-C(29A)-P(4A)	104.5(4)	H(31D)-C(31B)-H(31E)	109.5
C(35A)-C(33A)-C(34A)	108.2(6)	C(29B)-C(31B)-H(31F)	109.5
C(35A)-C(33A)-C(36A)	107.5(5)	H(31D)-C(31B)-H(31F)	109.5
C(34A)-C(33A)-C(36A)	107.8(5)	H(31E)-C(31B)-H(31F)	109.5
C(35A)-C(33A)-P(4A)	110.7(4)	C(29B)-C(32B)-H(32D)	109.5
C(34A)-C(33A)-P(4A)	117.4(5)	C(29B)-C(32B)-H(32E)	109.5
C(36A)-C(33A)-P(4A)	104.8(5)	H(32D)-C(32B)-H(32E)	109.5
C(33A)-C(35A)-H(35A)	109.5	C(29B)-C(32B)-H(32F)	109.5
C(33A)-C(35A)-H(35B)	109.5	H(32D)-C(32B)-H(32F)	109.5
H(35A)-C(35A)-H(35B)	109.5	H(32E)-C(32B)-H(32F)	109.5
C(33A)-C(35A)-H(35C)	109.5	C(35B)-C(33B)-C(34B)	107.0(8)
H(35A)-C(35A)-H(35C)	109.5	C(35B)-C(33B)-C(36B)	105.9(7)
H(35B)-C(35A)-H(35C)	109.5	C(34B)-C(33B)-C(36B)	108.5(8)
C(33A)-C(36A)-H(36A)	109.5	C(35B)-C(33B)-P(4B)	106.4(6)
C(33A)-C(36A)-H(36B)	109.5	C(34B)-C(33B)-P(4B)	120.8(6)
H(36A)-C(36A)-H(36B)	109.5	C(36B)-C(33B)-P(4B)	107.3(6)
C(33A)-C(36A)-H(36C)	109.5	C(33B)-C(34B)-H(34D)	109.5
H(36A)-C(36A)-H(36C)	109.5	C(33B)-C(34B)-H(34E)	109.5
H(36B)-C(36A)-H(36C)	109.5	H(34D)-C(34B)-H(34E)	109.5
C(33B)-P(4B)-C(29B)	111.2(5)	C(33B)-C(34B)-H(34F)	109.5
C(33B)-P(4B)-C(21)	103.2(4)	H(34D)-C(34B)-H(34F)	109.5
C(29B)-P(4B)-C(21)	108.1(4)	H(34E)-C(34B)-H(34F)	109.5
C(30B)-C(29B)-C(31B)	107.7(8)	C(33B)-C(35B)-H(35D)	109.5
C(30B)-C(29B)-C(32B)	108.8(8)	C(33B)-C(35B)-H(35E)	109.5
C(31B)-C(29B)-C(32B)	105.5(7)	H(35D)-C(35B)-H(35E)	109.5
C(30B)-C(29B)-P(4B)	119.5(8)	C(33B)-C(35B)-H(35F)	109.5
C(31B)-C(29B)-P(4B)	108.3(6)	H(35D)-C(35B)-H(35F)	109.5
C(32B)-C(29B)-P(4B)	106.2(6)	H(35E)-C(35B)-H(35F)	109.5
C(29B)-C(30B)-H(30D)	109.5	C(33B)-C(36B)-H(36D)	109.5
C(29B)-C(30B)-H(30E)	109.5	C(33B)-C(36B)-H(36E)	109.5
H(30D)-C(30B)-H(30E)	109.5	H(36D)-C(36B)-H(36E)	109.5

C(33B)-C(36B)-H(36F)	109.5	H(39B)-C(39)-H(39C)	109.5
H(36D)-C(36B)-H(36F)	109.5	C(37)-C(40)-H(40A)	109.5
H(36E)-C(36B)-H(36F)	109.5	C(37)-C(40)-H(40B)	109.5
C(40)-C(37)-C(38)	109.3(2)	H(40A)-C(40)-H(40B)	109.5
C(40)-C(37)-C(39)	110.3(3)	C(37)-C(40)-H(40C)	109.5
C(38)-C(37)-C(39)	109.0(2)	H(40A)-C(40)-H(40C)	109.5
C(40)-C(37)-P(3)	108.0(2)	H(40B)-C(40)-H(40C)	109.5
C(38)-C(37)-P(3)	107.9(2)	Cl(1)-C(41)-Cl(3)	109.7(2)
C(39)-C(37)-P(3)	112.22(19)	Cl(1)-C(41)-Cl(2)	110.07(18)
C(37)-C(38)-H(38A)	109.5	Cl(3)-C(41)-Cl(2)	110.14(19)
C(37)-C(38)-H(38B)	109.5	Cl(1)-C(41)-H(41)	109.0
H(38A)-C(38)-H(38B)	109.5	Cl(3)-C(41)-H(41)	109.0
C(37)-C(38)-H(38C)	109.5	Cl(2)-C(41)-H(41)	109.0
H(38A)-C(38)-H(38C)	109.5	Cl(6)-C(42)-Cl(5)	110.7(2)
H(38B)-C(38)-H(38C)	109.5	Cl(6)-C(42)-Cl(4)	110.7(2)
C(37)-C(39)-H(39A)	109.5	Cl(5)-C(42)-Cl(4)	109.6(2)
C(37)-C(39)-H(39B)	109.5	Cl(6)-C(42)-H(42)	108.6
H(39A)-C(39)-H(39B)	109.5	Cl(5)-C(42)-H(42)	108.6
C(37)-C(39)-H(39C)	109.5	Cl(4)-C(42)-H(42)	108.6
H(39A)-C(39)-H(39C)	109.5		

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for p_s_1a. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
P(1)	15(1)	14(1)	17(1)	2(1)	1(1)	3(1)
P(2)	13(1)	14(1)	20(1)	1(1)	0(1)	-2(1)
S(1)	17(1)	22(1)	26(1)	4(1)	4(1)	8(1)
C(1)	11(1)	13(1)	20(1)	2(1)	0(1)	1(1)
C(2)	12(1)	20(1)	19(1)	-1(1)	2(1)	-1(1)
C(3)	15(1)	19(1)	31(1)	-2(1)	3(1)	3(1)
C(4)	22(1)	27(2)	36(2)	-8(1)	11(1)	2(1)
C(5)	24(2)	31(2)	32(2)	-6(1)	10(1)	0(1)
C(6)	25(1)	30(2)	18(1)	-1(1)	5(1)	-1(1)
C(7)	14(1)	15(1)	22(1)	0(1)	3(1)	-2(1)
C(8)	23(1)	16(1)	19(1)	1(1)	1(1)	2(1)
C(9)	21(1)	14(1)	26(1)	6(1)	-3(1)	-1(1)
C(10)	40(2)	22(2)	36(2)	12(1)	-2(1)	-9(1)
C(11)	24(2)	25(2)	34(2)	2(1)	-3(1)	11(1)
C(12)	27(2)	25(1)	24(1)	2(1)	-9(1)	4(1)
C(13)	12(1)	19(1)	28(1)	-5(1)	0(1)	-3(1)
C(14)	15(1)	27(2)	43(2)	-18(1)	0(1)	-2(1)
C(15)	12(1)	33(2)	32(2)	-3(1)	-7(1)	-1(1)
C(16)	17(1)	26(2)	46(2)	-4(1)	3(1)	-6(1)
C(17)	25(1)	18(1)	20(1)	-2(1)	0(1)	-1(1)
C(18)	41(2)	17(1)	24(1)	-2(1)	1(1)	1(1)
C(19)	23(1)	19(1)	34(2)	-1(1)	-6(1)	-6(1)
C(20)	45(2)	23(1)	18(1)	0(1)	2(1)	-4(1)
P(3)	15(1)	13(1)	17(1)	0(1)	-1(1)	-1(1)
S(2)	18(1)	23(1)	29(1)	3(1)	-5(1)	-8(1)
C(21)	14(1)	15(1)	15(1)	0(1)	0(1)	-1(1)
C(22)	13(1)	15(1)	19(1)	-2(1)	-1(1)	-1(1)
C(23)	18(1)	20(1)	25(1)	-4(1)	-2(1)	-4(1)
C(24)	30(2)	26(2)	25(1)	-12(1)	-4(1)	-6(1)
C(25)	26(2)	40(2)	19(1)	-3(1)	-7(1)	-3(1)
C(26)	23(1)	22(1)	16(1)	-1(1)	-1(1)	3(1)

C(27)	13(1)	19(1)	18(1)	-1(1)	0(1)	2(1)
C(28)	20(1)	18(1)	18(1)	3(1)	-1(1)	0(1)
P(4A)	17(2)	16(1)	21(1)	-3(1)	-5(1)	7(1)
C(29A)	21(2)	26(2)	33(3)	-11(2)	-5(2)	4(2)
C(30A)	24(2)	28(2)	28(3)	-5(2)	5(2)	4(2)
C(31A)	21(2)	43(3)	47(3)	-9(3)	5(3)	3(2)
C(32A)	31(3)	37(3)	52(3)	-10(2)	-12(2)	11(2)
C(33A)	25(3)	19(2)	24(2)	5(2)	-4(2)	1(2)
C(34A)	38(3)	28(3)	42(3)	-2(2)	-1(3)	0(2)
C(35A)	31(2)	28(2)	33(3)	8(2)	11(2)	-3(2)
C(36A)	51(3)	30(3)	34(3)	11(2)	-10(2)	5(2)
P(4B)	17(2)	16(1)	21(1)	-3(1)	-5(1)	7(1)
C(29B)	15(3)	26(3)	21(3)	1(2)	1(2)	7(2)
C(30B)	24(2)	28(2)	28(3)	-5(2)	5(2)	4(2)
C(31B)	13(3)	27(3)	32(3)	-3(3)	4(3)	-2(2)
C(32B)	30(3)	40(3)	34(3)	-4(3)	-7(3)	17(3)
C(33B)	26(3)	20(3)	22(3)	5(2)	2(2)	-2(3)
C(34B)	30(3)	26(3)	29(3)	2(3)	-1(3)	-7(3)
C(35B)	38(3)	36(3)	32(3)	5(3)	6(3)	-5(3)
C(36B)	46(4)	36(3)	39(4)	10(3)	-3(3)	1(3)
C(37)	20(1)	18(1)	20(1)	-3(1)	-2(1)	6(1)
C(38)	36(2)	15(1)	29(2)	-1(1)	-4(1)	4(1)
C(39)	19(1)	26(1)	25(1)	-3(1)	-1(1)	3(1)
C(40)	32(2)	23(1)	19(1)	-3(1)	-3(1)	6(1)
Cl(1)	23(1)	29(1)	52(1)	-4(1)	-5(1)	3(1)
Cl(2)	50(1)	35(1)	42(1)	-14(1)	-17(1)	10(1)
Cl(3)	44(1)	120(1)	31(1)	6(1)	6(1)	-23(1)
C(41)	22(1)	38(2)	27(2)	-3(1)	-1(1)	4(1)
Cl(4)	30(1)	53(1)	36(1)	2(1)	0(1)	7(1)
Cl(5)	52(1)	55(1)	57(1)	-16(1)	6(1)	-1(1)
Cl(6)	46(1)	96(1)	38(1)	12(1)	18(1)	-4(1)
C(42)	25(2)	48(2)	25(2)	3(1)	1(1)	2(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for p_s_1a.

	x	y	z	U(eq)
H(1)	8497	348	816	18
H(2)	9890	785	1446	20
H(3A)	6657	1030	1236	26
H(3B)	7947	1772	1264	26
H(4A)	8123	1590	1849	34
H(4B)	6298	1736	1752	34
H(5A)	6619	604	2146	35
H(5B)	5739	299	1811	35
H(6A)	7679	-705	1942	29
H(6B)	9021	10	1969	29
H(7)	7404	-446	1361	20
H(8A)	9274	-1496	1429	23
H(8B)	10609	-841	1556	23
H(10A)	11440	2212	174	49
H(10B)	10653	2899	417	49
H(10C)	9815	2667	68	49
H(11A)	8357	2502	785	42
H(11B)	7331	1686	688	42
H(11C)	7429	2468	434	42
H(12A)	8218	1441	1	38
H(12B)	8306	670	260	38
H(12C)	9824	906	37	38
H(14A)	11934	2758	1331	42
H(14B)	10379	2175	1330	42
H(14C)	10674	2832	1031	42
H(15A)	13652	1511	1386	39
H(15B)	13633	776	1110	39
H(15C)	12199	859	1372	39
H(16A)	12918	2633	642	44
H(16B)	13930	1776	643	44

H(16C)	14176	2457	935	44
H(18A)	8950	-2732	631	41
H(18B)	9114	-2469	1018	41
H(18C)	10630	-2426	776	41
H(19A)	6676	-1673	605	38
H(19B)	7003	-699	689	38
H(19C)	7000	-1384	984	38
H(20A)	10626	-1426	294	43
H(20B)	9368	-668	276	43
H(20C)	8831	-1610	183	43
H(21)	3683	5676	1626	18
H(22)	5476	5478	1029	19
H(23A)	2323	4886	1176	25
H(23B)	3861	4291	1151	25
H(24A)	4125	4573	576	32
H(24B)	2338	4268	641	32
H(25A)	2452	5479	277	34
H(25B)	1383	5651	602	34
H(26A)	3041	6824	523	25
H(26B)	4587	6232	510	25
H(27)	2600	6434	1092	20
H(28A)	4089	7649	1095	22
H(28B)	5675	7163	977	22
H(30A)	6481	3501	1337	41
H(30B)	8109	3737	1151	41
H(30C)	6549	4293	1088	41
H(31A)	9051	5611	1587	55
H(31B)	8015	5611	1250	55
H(31C)	9549	5018	1279	55
H(32A)	8046	3520	1865	60
H(32B)	8859	4377	1992	60
H(32C)	9621	3865	1685	60
H(34A)	3973	3495	1612	54
H(34B)	3878	3024	1967	54
H(34C)	5564	3168	1790	54
H(35A)	3097	5165	2187	46

H(35B)	2394	4226	2201	46
H(35C)	2495	4715	1851	46
H(36A)	5636	4638	2472	58
H(36B)	6421	3787	2332	58
H(36C)	4684	3764	2495	58
H(30D)	6941	3536	1305	41
H(30E)	8237	3893	1047	41
H(30F)	6483	4284	1052	41
H(31D)	9004	5852	1424	36
H(31E)	7761	5714	1125	36
H(31F)	9446	5245	1117	36
H(32D)	8983	3727	1723	52
H(32E)	9405	4647	1863	52
H(32F)	10222	4312	1526	52
H(34D)	3227	3986	1665	42
H(34E)	3707	3192	1892	42
H(34F)	4723	3415	1564	42
H(35D)	4662	5160	2305	53
H(35E)	4097	4243	2425	53
H(35F)	3119	4736	2142	53
H(36D)	7044	3329	1991	61
H(36E)	5850	3269	2303	61
H(36F)	7140	4012	2287	61
H(38A)	3699	8553	1577	40
H(38B)	4953	8492	1878	40
H(38C)	3105	8627	1957	40
H(39A)	1160	7429	1857	35
H(39B)	1788	6562	1699	35
H(39C)	1763	7404	1476	35
H(40A)	4941	7257	2258	37
H(40B)	3823	6460	2186	37
H(40C)	3070	7318	2327	37
H(41)	7608	5231	-244	35
H(42)	7762	6542	2272	39

Table 6.Torsion angles [°] for p_s_1a.

C(8)-P(1)-C(1)-C(2)	6.10(19)	C(13)-P(2)-C(9)-C(10)	54.0(3)
C(17)-P(1)-C(1)-C(2)	116.94(18)	C(1)-P(2)-C(9)-C(10)	170.0(2)
S(1)-P(1)-C(1)-C(2)	-115.14(15)	C(9)-P(2)-C(13)-C(14)	45.1(3)
C(8)-P(1)-C(1)-P(2)	142.24(15)	C(1)-P(2)-C(13)-C(14)	-67.3(3)
C(17)-P(1)-C(1)-P(2)	-106.92(15)	C(9)-P(2)-C(13)-C(16)	-77.0(2)
S(1)-P(1)-C(1)-P(2)	21.01(16)	C(1)-P(2)-C(13)-C(16)	170.61(19)
C(13)-P(2)-C(1)-C(2)	21.2(2)	C(9)-P(2)-C(13)-C(15)	169.82(19)
C(9)-P(2)-C(1)-C(2)	-96.4(2)	C(1)-P(2)-C(13)-C(15)	57.4(2)
C(13)-P(2)-C(1)-P(1)	-103.91(15)	C(8)-P(1)-C(17)-C(19)	56.5(2)
C(9)-P(2)-C(1)-P(1)	138.50(14)	C(1)-P(1)-C(17)-C(19)	-46.1(2)
P(1)-C(1)-C(2)-C(3)	-152.7(2)	S(1)-P(1)-C(17)-C(19)	-177.66(18)
P(2)-C(1)-C(2)-C(3)	79.9(3)	C(8)-P(1)-C(17)-C(20)	179.1(2)
P(1)-C(1)-C(2)-C(7)	-30.8(2)	C(1)-P(1)-C(17)-C(20)	76.4(2)
P(2)-C(1)-C(2)-C(7)	-158.14(19)	S(1)-P(1)-C(17)-C(20)	-55.1(2)
C(7)-C(2)-C(3)-C(4)	58.0(3)	C(8)-P(1)-C(17)-C(18)	-63.6(2)
C(1)-C(2)-C(3)-C(4)	179.5(2)	C(1)-P(1)-C(17)-C(18)	-166.2(2)
C(2)-C(3)-C(4)-C(5)	-55.9(3)	S(1)-P(1)-C(17)-C(18)	62.2(2)
C(3)-C(4)-C(5)-C(6)	53.1(4)	C(28)-P(3)-C(21)-C(22)	6.19(19)
C(4)-C(5)-C(6)-C(7)	-53.6(4)	C(37)-P(3)-C(21)-C(22)	117.76(18)
C(5)-C(6)-C(7)-C(8)	179.3(2)	S(2)-P(3)-C(21)-C(22)	-115.11(15)
C(5)-C(6)-C(7)-C(2)	58.3(3)	C(28)-P(3)-C(21)-P(4A)	148.59(19)
C(3)-C(2)-C(7)-C(6)	-60.2(3)	C(37)-P(3)-C(21)-P(4A)	-99.84(19)
C(1)-C(2)-C(7)-C(6)	172.8(2)	S(2)-P(3)-C(21)-P(4A)	27.3(2)
C(3)-C(2)-C(7)-C(8)	174.9(2)	C(28)-P(3)-C(21)-P(4B)	138.5(2)
C(1)-C(2)-C(7)-C(8)	47.8(3)	C(37)-P(3)-C(21)-P(4B)	-109.9(2)
C(6)-C(7)-C(8)-P(1)	-165.0(2)	S(2)-P(3)-C(21)-P(4B)	17.2(2)
C(2)-C(7)-C(8)-P(1)	-41.6(2)	P(4A)-C(21)-C(22)-C(27)	-165.1(3)
C(17)-P(1)-C(8)-C(7)	-92.3(2)	P(3)-C(21)-C(22)-C(27)	-30.7(2)
C(1)-P(1)-C(8)-C(7)	20.1(2)	P(4B)-C(21)-C(22)-C(27)	-155.6(3)
S(1)-P(1)-C(8)-C(7)	143.90(16)	P(4A)-C(21)-C(22)-C(23)	72.1(3)
C(13)-P(2)-C(9)-C(11)	-71.7(3)	P(3)-C(21)-C(22)-C(23)	-153.5(2)
C(1)-P(2)-C(9)-C(11)	44.4(3)	P(4B)-C(21)-C(22)-C(23)	81.6(3)
C(13)-P(2)-C(9)-C(12)	167.65(19)	C(27)-C(22)-C(23)-C(24)	56.8(3)
C(1)-P(2)-C(9)-C(12)	-76.3(2)	C(21)-C(22)-C(23)-C(24)	179.3(2)

C(22)-C(23)-C(24)-C(25)	-53.8(3)
C(23)-C(24)-C(25)-C(26)	52.7(4)
C(24)-C(25)-C(26)-C(27)	-54.5(3)
C(23)-C(22)-C(27)-C(28)	173.8(2)
C(21)-C(22)-C(27)-C(28)	47.2(3)
C(23)-C(22)-C(27)-C(26)	-60.5(3)
C(21)-C(22)-C(27)-C(26)	172.9(2)
C(25)-C(26)-C(27)-C(28)	-179.2(2)
C(25)-C(26)-C(27)-C(22)	59.4(3)
C(22)-C(27)-C(28)-P(3)	-40.5(2)
C(26)-C(27)-C(28)-P(3)	-164.2(2)
C(37)-P(3)-C(28)-C(27)	-92.2(2)
C(21)-P(3)-C(28)-C(27)	19.5(2)
S(2)-P(3)-C(28)-C(27)	144.10(15)
C(22)-C(21)-P(4A)-C(29A)	25.3(4)
P(3)-C(21)-P(4A)-C(29A)	-106.1(3)
P(4B)-C(21)-P(4A)-C(29A)	-30(2)
C(22)-C(21)-P(4A)-C(33A)	-91.3(3)
P(3)-C(21)-P(4A)-C(33A)	137.3(3)
P(4B)-C(21)-P(4A)-C(33A)	-147(2)
C(21)-P(4A)-C(29A)-C(30A)	-55.1(7)
C(33A)-P(4A)-C(29A)-C(30A)	60.2(7)
C(21)-P(4A)-C(29A)-C(32A)	179.8(4)
C(33A)-P(4A)-C(29A)-C(32A)	-65.0(5)
C(21)-P(4A)-C(29A)-C(31A)	66.2(5)
C(33A)-P(4A)-C(29A)-C(31A)	-178.6(5)
C(21)-P(4A)-C(33A)-C(35A)	-34.9(5)
C(29A)-P(4A)-C(33A)-C(35A)	-151.4(5)
C(21)-P(4A)-C(33A)-C(34A)	89.9(6)
C(29A)-P(4A)-C(33A)-C(34A)	-26.6(7)
C(21)-P(4A)-C(33A)-C(36A)	-150.6(4)
C(29A)-P(4A)-C(33A)-C(36A)	93.0(5)
C(22)-C(21)-P(4B)-C(33B)	-95.4(4)
P(4A)-C(21)-P(4B)-C(33B)	35(2)
P(3)-C(21)-P(4B)-C(33B)	142.3(4)
C(22)-C(21)-P(4B)-C(29B)	22.4(5)
P(4A)-C(21)-P(4B)-C(29B)	152(3)
P(3)-C(21)-P(4B)-C(29B)	-99.8(4)
C(33B)-P(4B)-C(29B)-C(30B)	48.2(10)
C(21)-P(4B)-C(29B)-C(30B)	-64.4(9)
C(33B)-P(4B)-C(29B)-C(31B)	171.9(6)
C(21)-P(4B)-C(29B)-C(31B)	59.3(7)
C(33B)-P(4B)-C(29B)-C(32B)	-75.2(8)
C(21)-P(4B)-C(29B)-C(32B)	172.2(6)
C(29B)-P(4B)-C(33B)-C(35B)	174.6(6)
C(21)-P(4B)-C(33B)-C(35B)	-69.7(7)
C(29B)-P(4B)-C(33B)-C(34B)	-63.5(9)
C(21)-P(4B)-C(33B)-C(34B)	52.3(9)
C(29B)-P(4B)-C(33B)-C(36B)	61.6(8)
C(21)-P(4B)-C(33B)-C(36B)	177.3(6)
C(28)-P(3)-C(37)-C(40)	170.9(2)
C(21)-P(3)-C(37)-C(40)	68.3(2)
S(2)-P(3)-C(37)-C(40)	-63.2(2)
C(28)-P(3)-C(37)-C(38)	-70.9(2)
C(21)-P(3)-C(37)-C(38)	-173.53(19)
S(2)-P(3)-C(37)-C(38)	54.9(2)
C(28)-P(3)-C(37)-C(39)	49.1(2)
C(21)-P(3)-C(37)-C(39)	-53.5(2)
S(2)-P(3)-C(37)-C(39)	174.96(19)

Table 7. Hydrogen bonds for p_s_1a [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(12)-H(12B)...Cl(1)#1	0.98	2.81	3.459(3)	124.7
C(18)-H(18A)...Cl(2)#2	0.98	3.01	3.876(3)	148.1
C(12)-H(12C)...Cl(3)#3	0.98	3.01	3.984(4)	176.3
C(35A)-H(35A)...Cl(4)#4	0.98	2.90	3.427(6)	114.4
C(32B)-H(32E)...Cl(4)	0.98	2.94	3.911(9)	171.6
C(6)-H(6B)...Cl(4)#5	0.99	2.93	3.727(3)	138.8
C(35A)-H(35B)...Cl(5)#6	0.98	3.08	4.019(6)	160.4
C(36A)-H(36A)...Cl(6)	0.98	3.09	4.036(7)	163.9

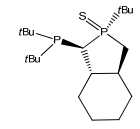
Symmetry transformations used to generate equivalent atoms:

#1 x-1/2,-y+1/2,-z #2 x,y-1,z #3 x+1/2,-y+1/2,-z

#4 x-1,y,z #5 -x+2,y-1/2,-z+1/2 #6 -x+1,y-1/2,-z+1/2

HRMS (ESI)

report



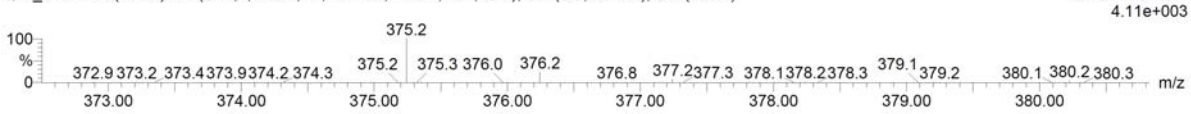
(1*S*,2*R*,3a*S*,7a*S*)-**7**

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 150.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
18 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-120 H: 0-250 P: 0-3 S: 1-1

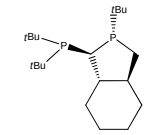
Guohua Hou, HKX-1 University of Illnois, SCS, Mass Spectrometry Lab Q-tof UE521
Qtof_30677 53 (3.793) AM (Cen,3, 80.00, Ar,15000.0,716.46,0.70,LS 3); Sm (SG, 2x3.00); Cm (52:54) 1: TOF MS ES+
4.11e+003



Minimum:				-1.5		
Maximum:		5.0	10.0	150.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
375.2411	375.2404	0.7	1.9	1.5	0.2	C20 H41 P2 S

Elemental Composition Report **Page 1**

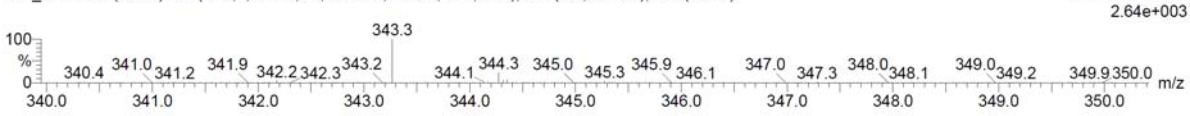
Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 150.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3



(1*R*,2*S*,3a*S*,7a*S*)-**8**

Monoisotopic Mass, Even Electron Ions
18 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-120 H: 0-250 P: 0-3

Guohua Hou, HKX-2 University of Illnois, SCS, Mass Spectrometry Lab Q-tof UE521
Qtof_30678 51 (3.650) AM (Cen,3, 80.00, Ar,15000.0,716.46,0.70,LS 3); Sm (SG, 2x3.00); Cm (51:54) 1: TOF MS ES+
2.64e+003



Minimum:				-1.5		
Maximum:		5.0	10.0	150.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
343.2682	343.2684	-0.2	-0.6	1.5	0.2	C20 H41 P2