Enantiopure Turbo Chirality in Tri-Propeller Targets: Design and Asymmetric Synthesis, and Computational Analysis

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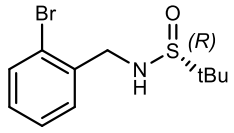
[†]These authors contributed equally to this work.

Supporting Information

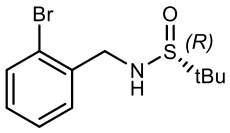
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1. Copies of ^{1}H, ^{13}C, ^{19}F and ^{31}P NMR spectra of compounds 1, 2, 4, 5 ..... S1
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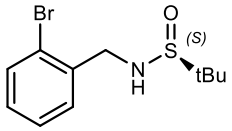
1. Copies of ^{1}H, ^{13}C, ^{19}F and ^{31}P NMR spectra of compounds 1, 2, 4, 5



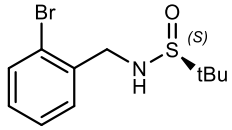
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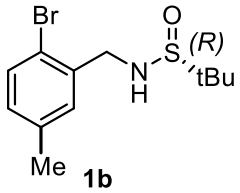
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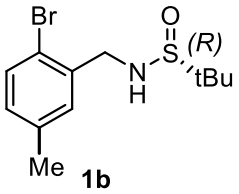
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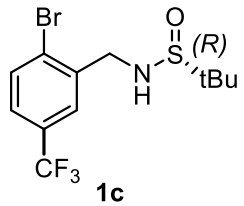
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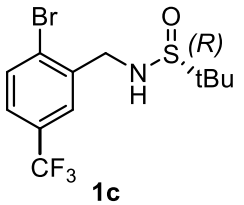
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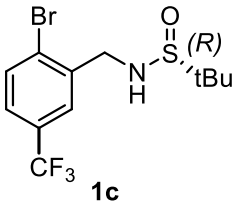
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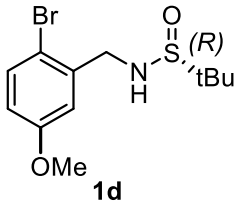
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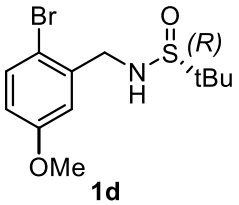
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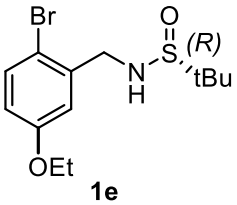
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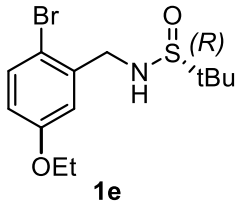
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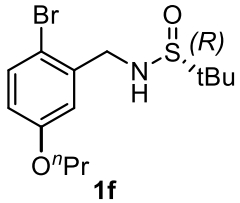
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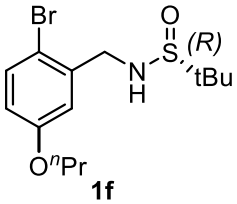
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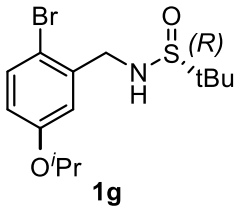
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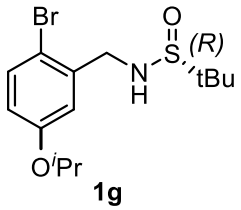
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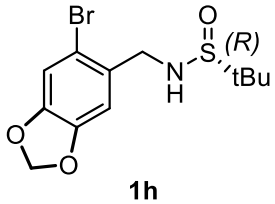
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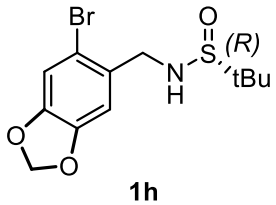
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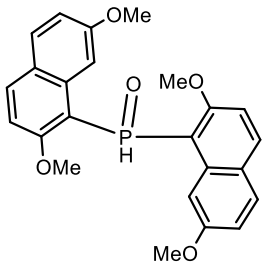
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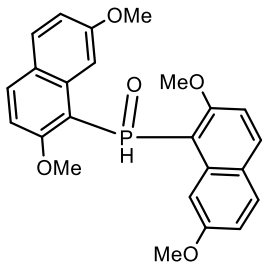
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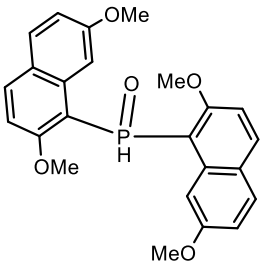
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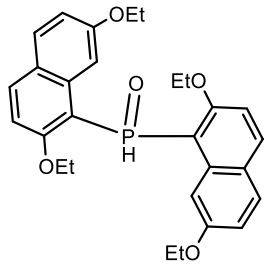
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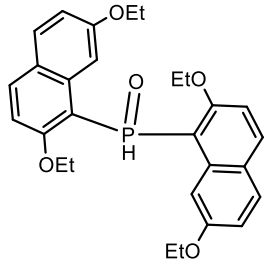
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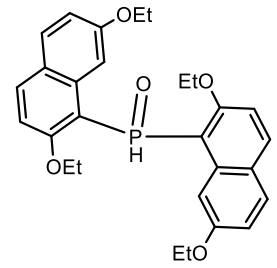
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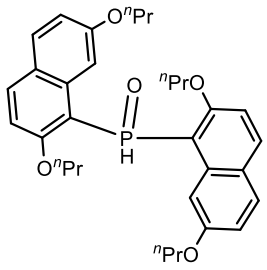
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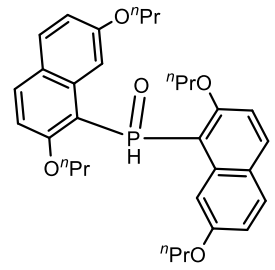
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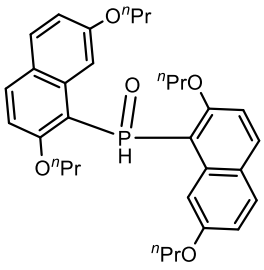
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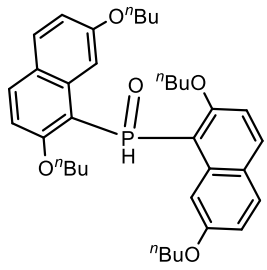
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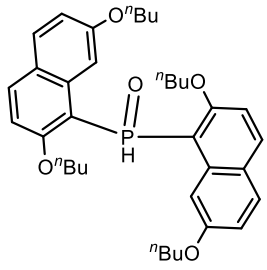
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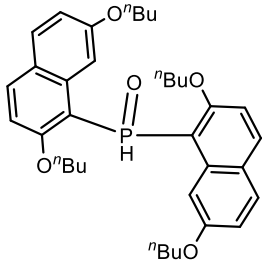
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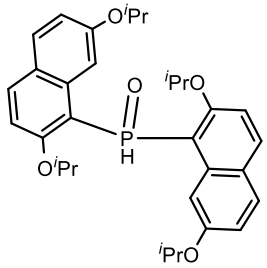
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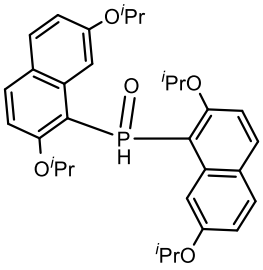
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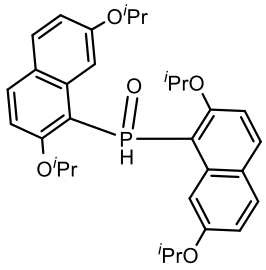
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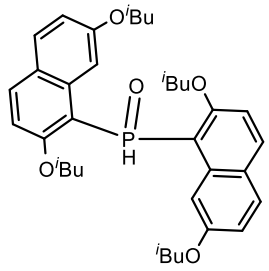
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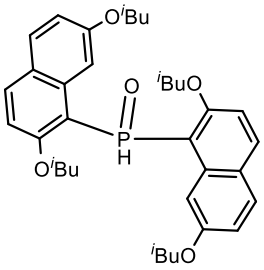
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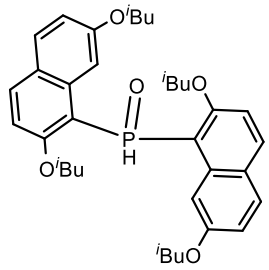
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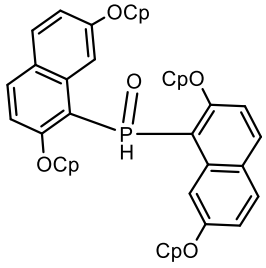
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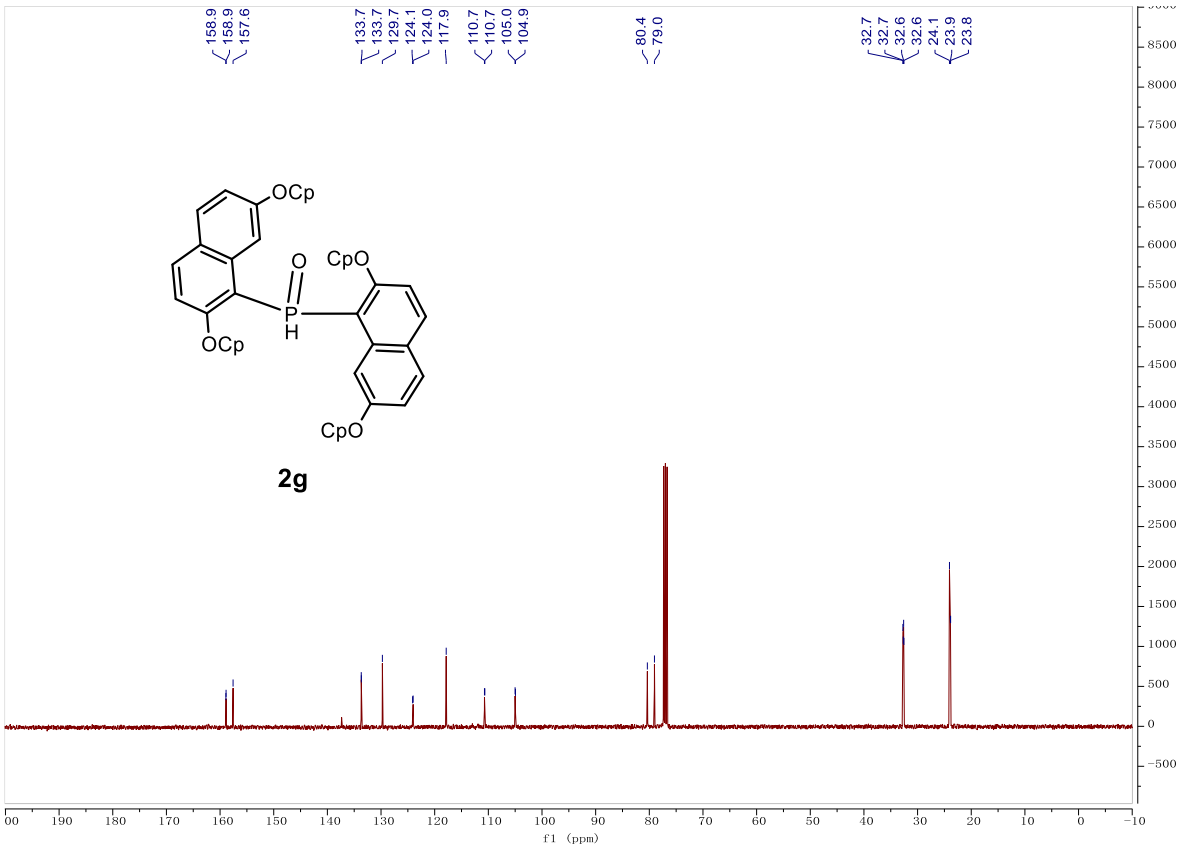
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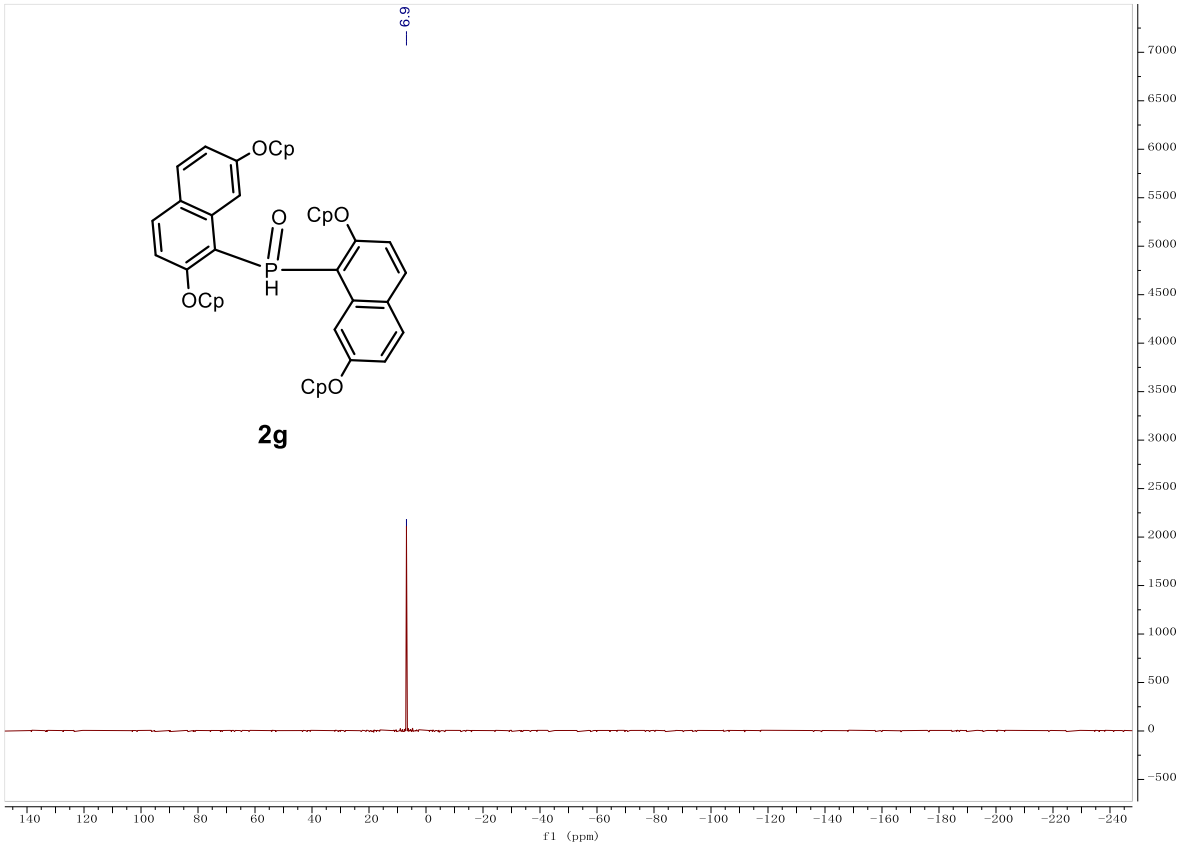


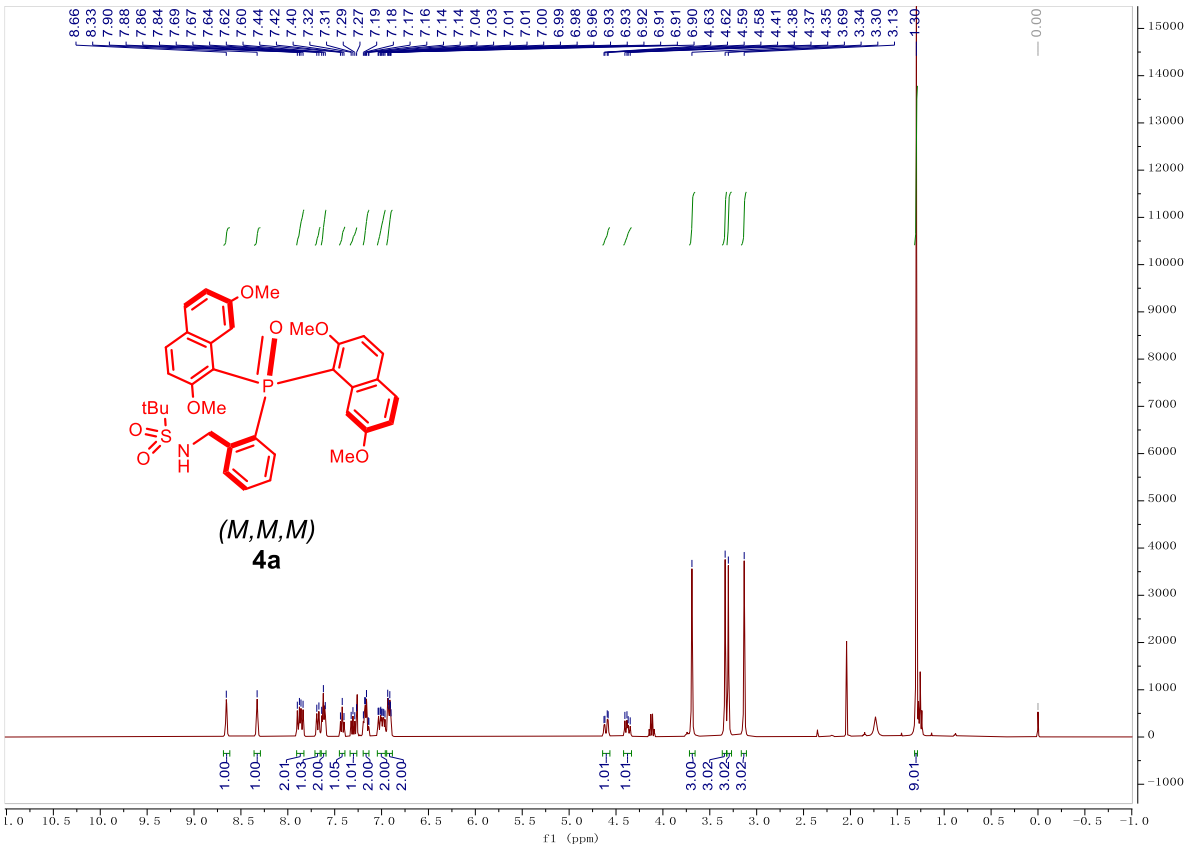
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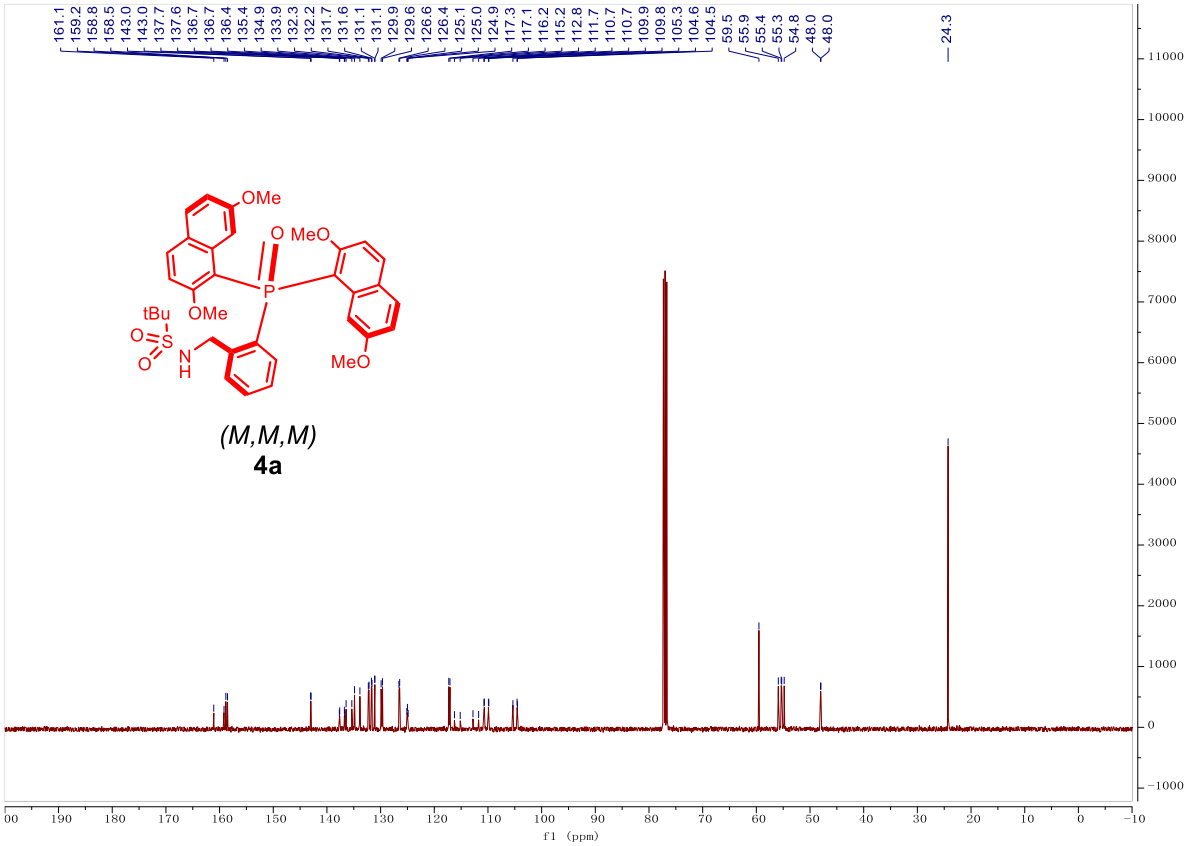


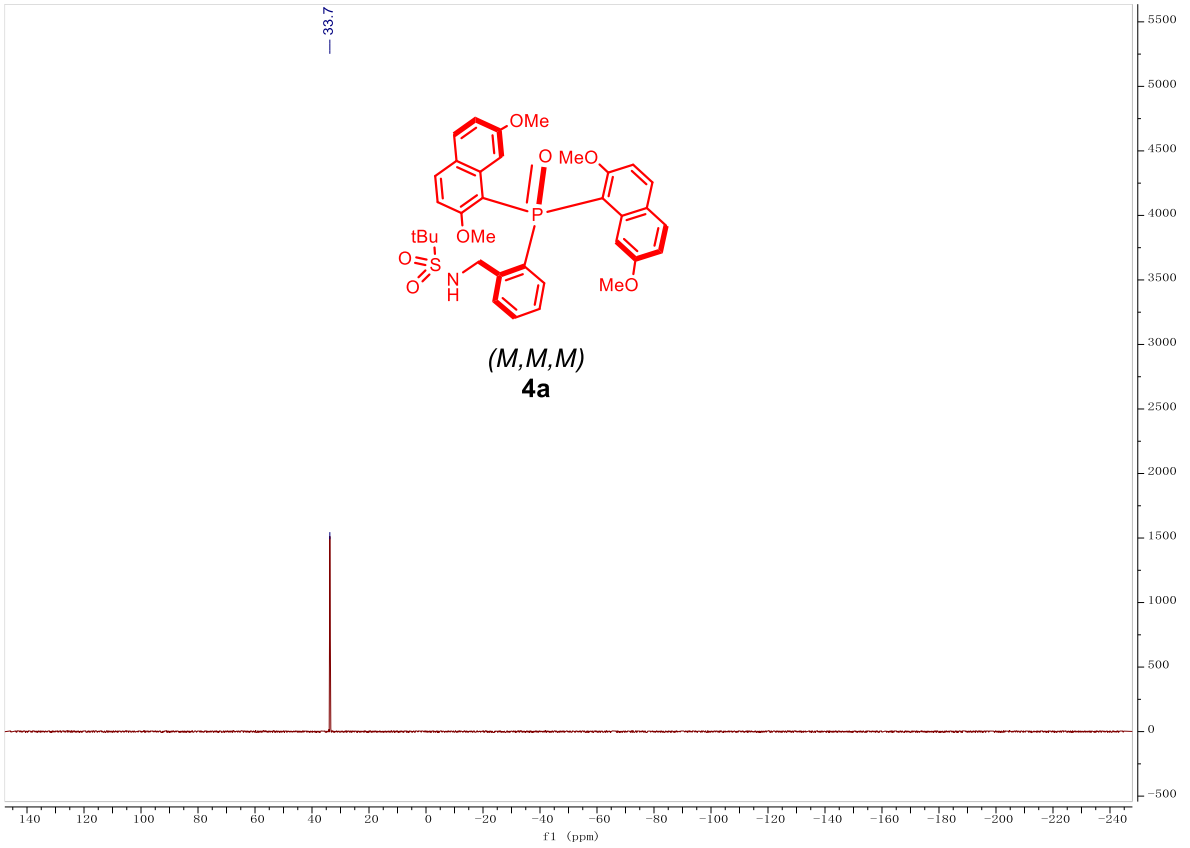
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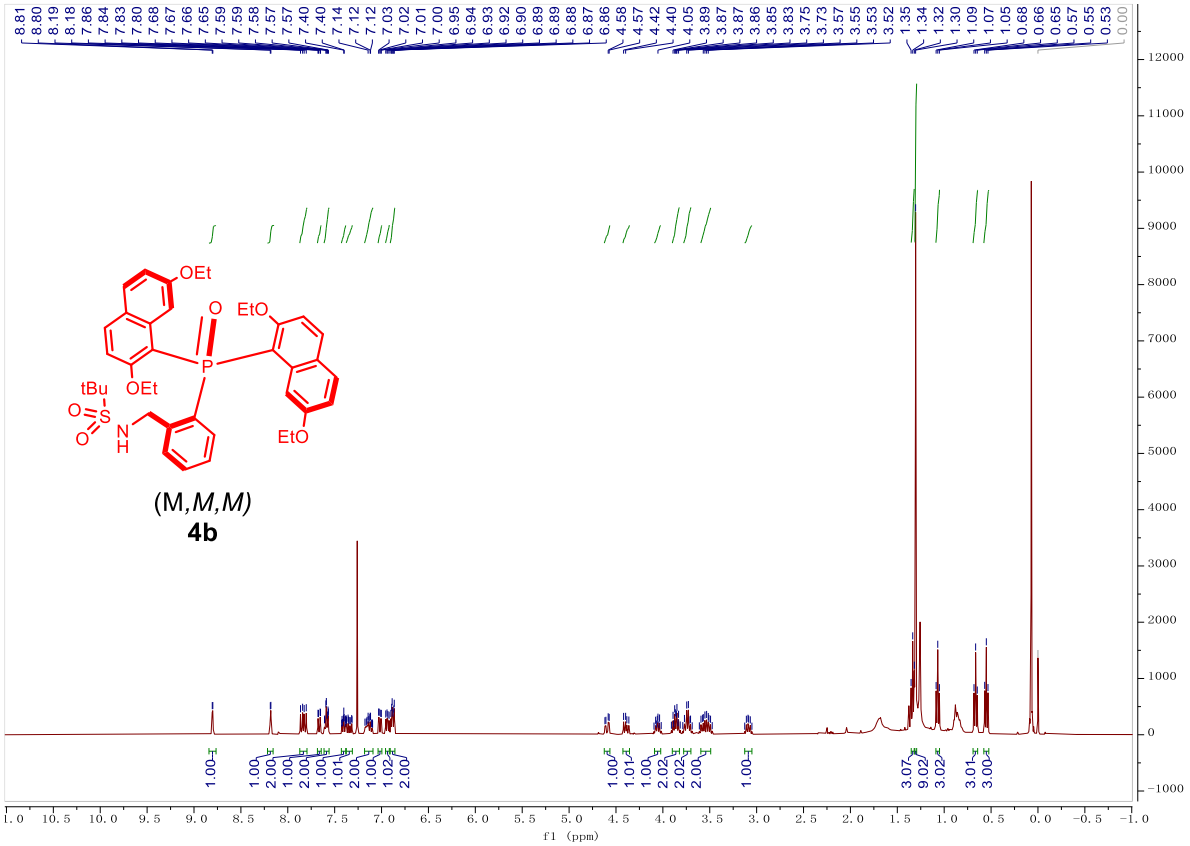

158.9
158.9
157.6
133.7
133.7
129.7
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124.0
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110.7
105.0
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80.4
79.0
32.7
32.7
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CpO
2g
f1 (ppm)

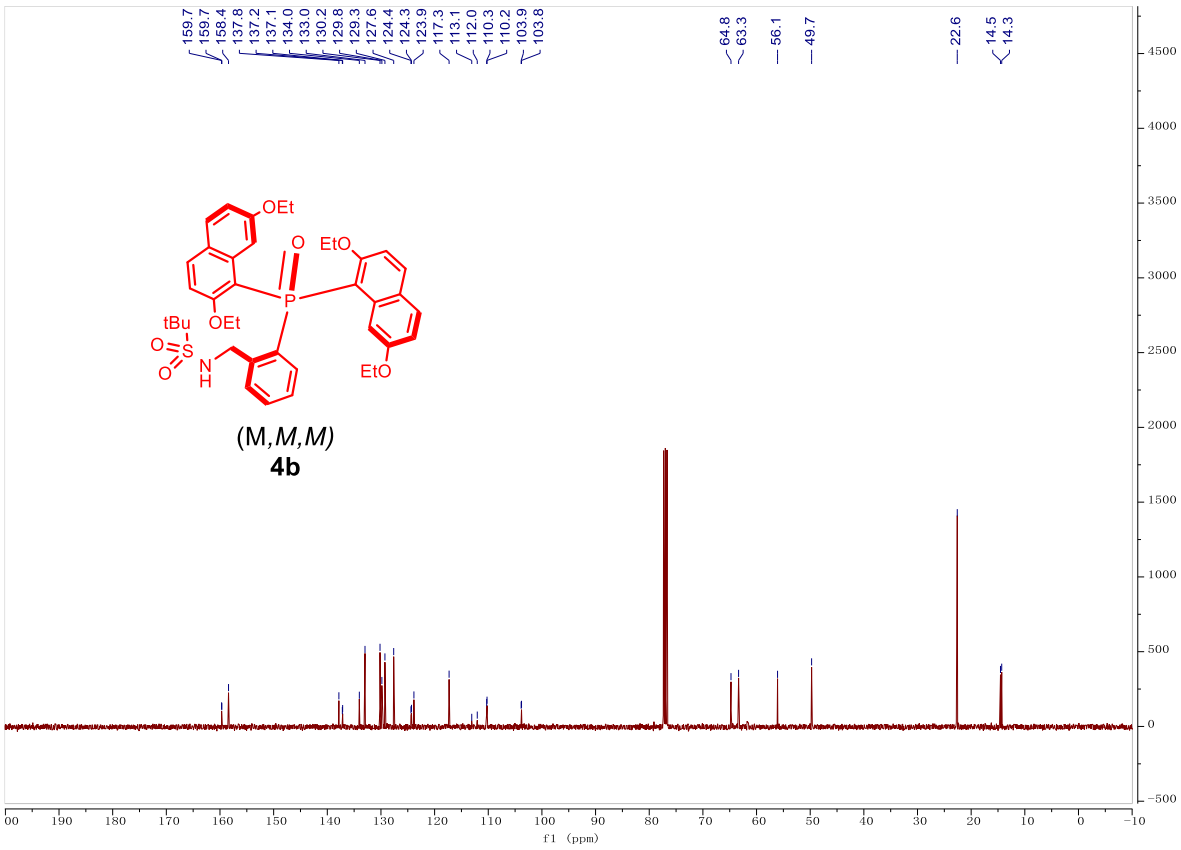

6.9
OCp
O
CpO
P
H
OCp
CpO
2g
f1 (ppm)


OMe
O MeO
P
tBu
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4a
f1 (ppm)

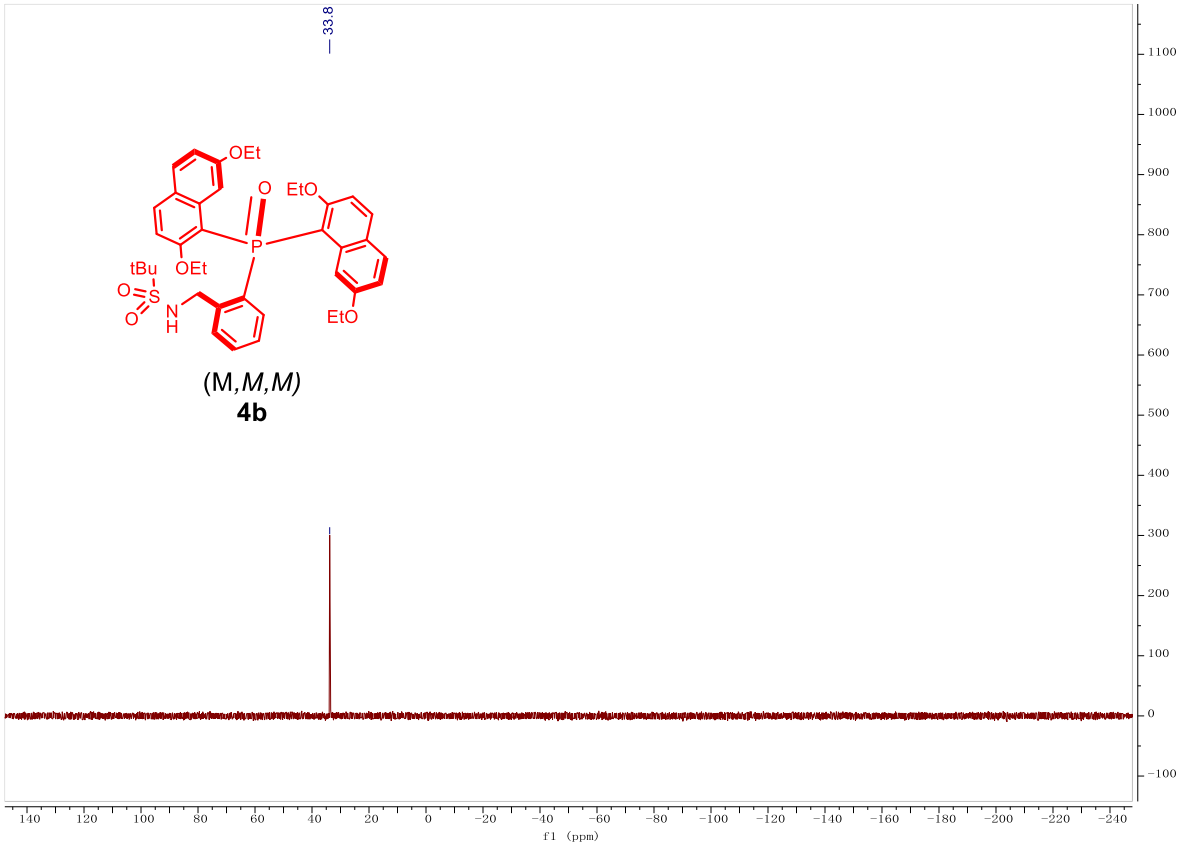

OMe
O MeO
P
tBu
OMe
O
S
O
N
H
MeO
(M,M,M)
4a
f1 (ppm)


33.7
OMe
O MeO
P
tBu OMe
O
S
O
N
H
MeO
(M,M,M)
4a
f1 (ppm)

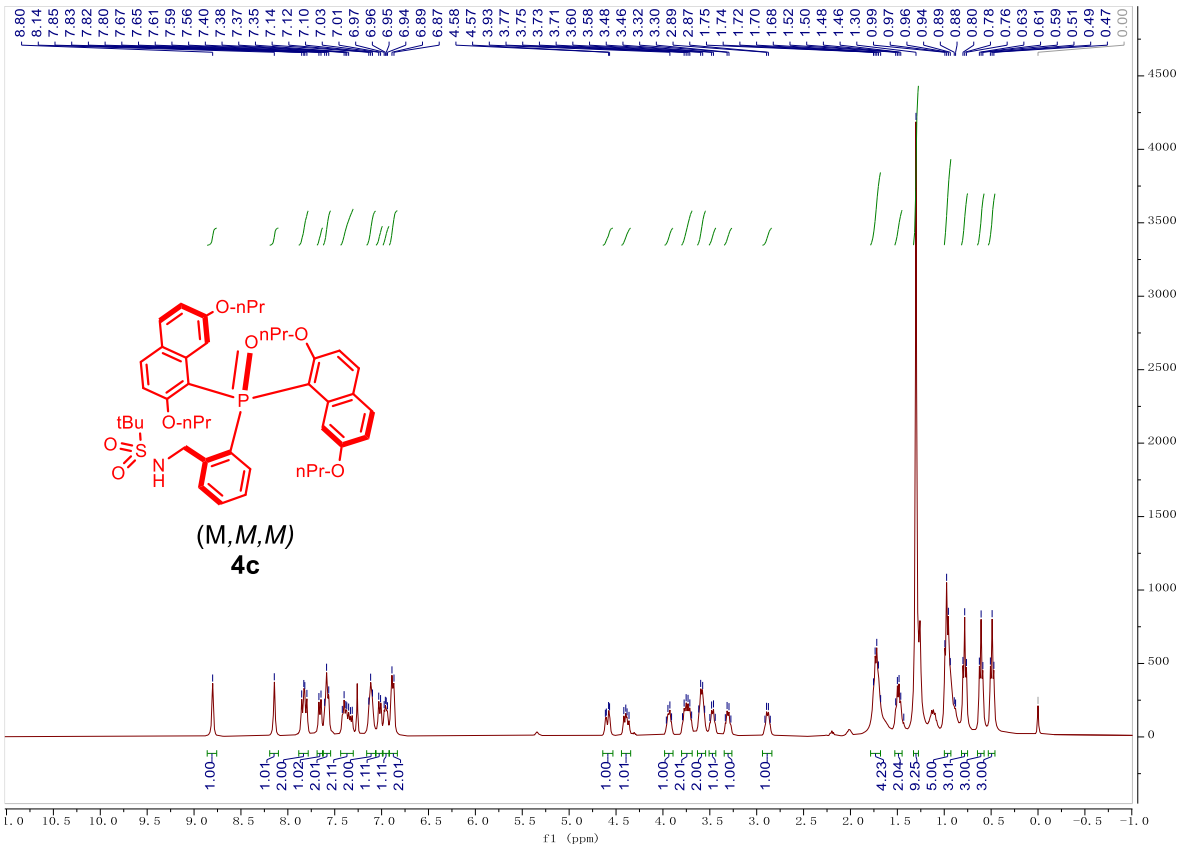

OEt
O EtO
P
tBu OEt
O
S
O
N
H
EtO
(M,M,M)
4b
f1 (ppm)

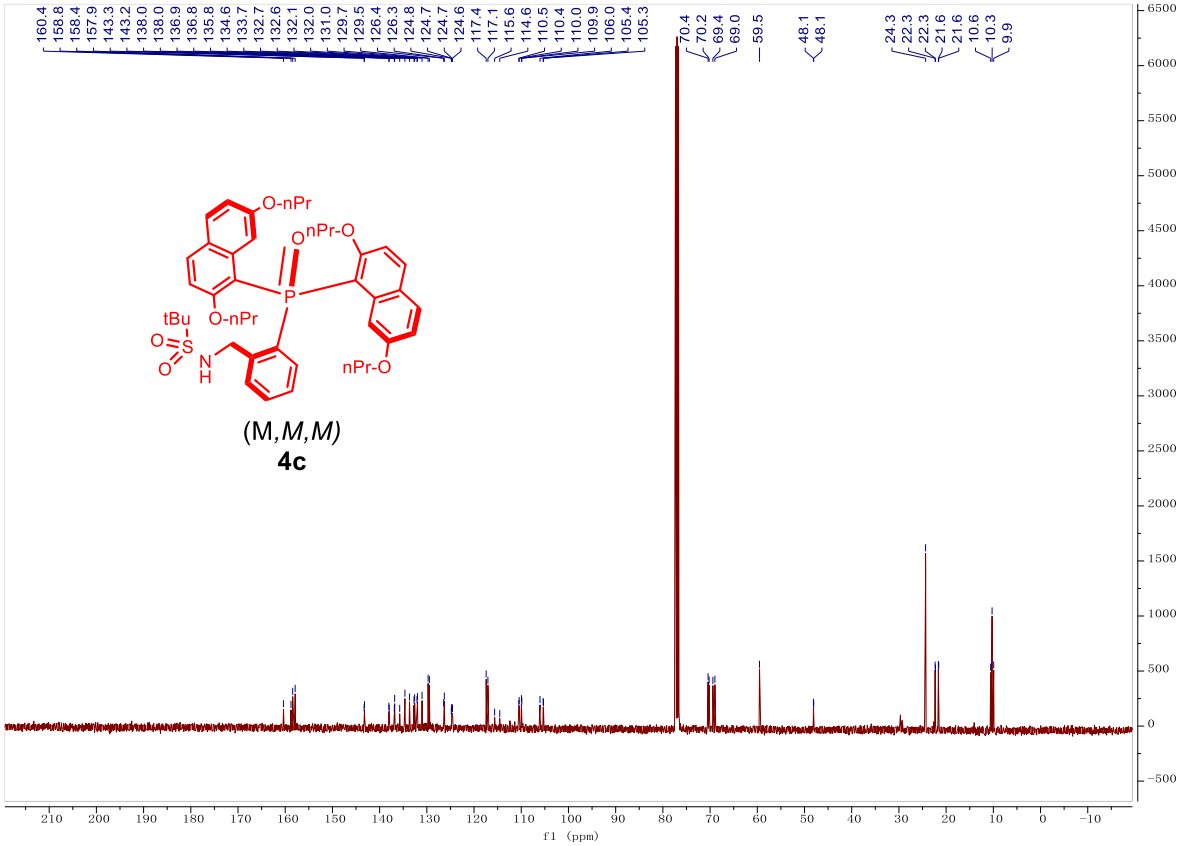

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129.3
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124.3
123.9
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113.1
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110.3
110.2
103.9
103.8
64.8
63.3
56.1
49.7
22.6
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N
H
EtO
f1 (ppm)

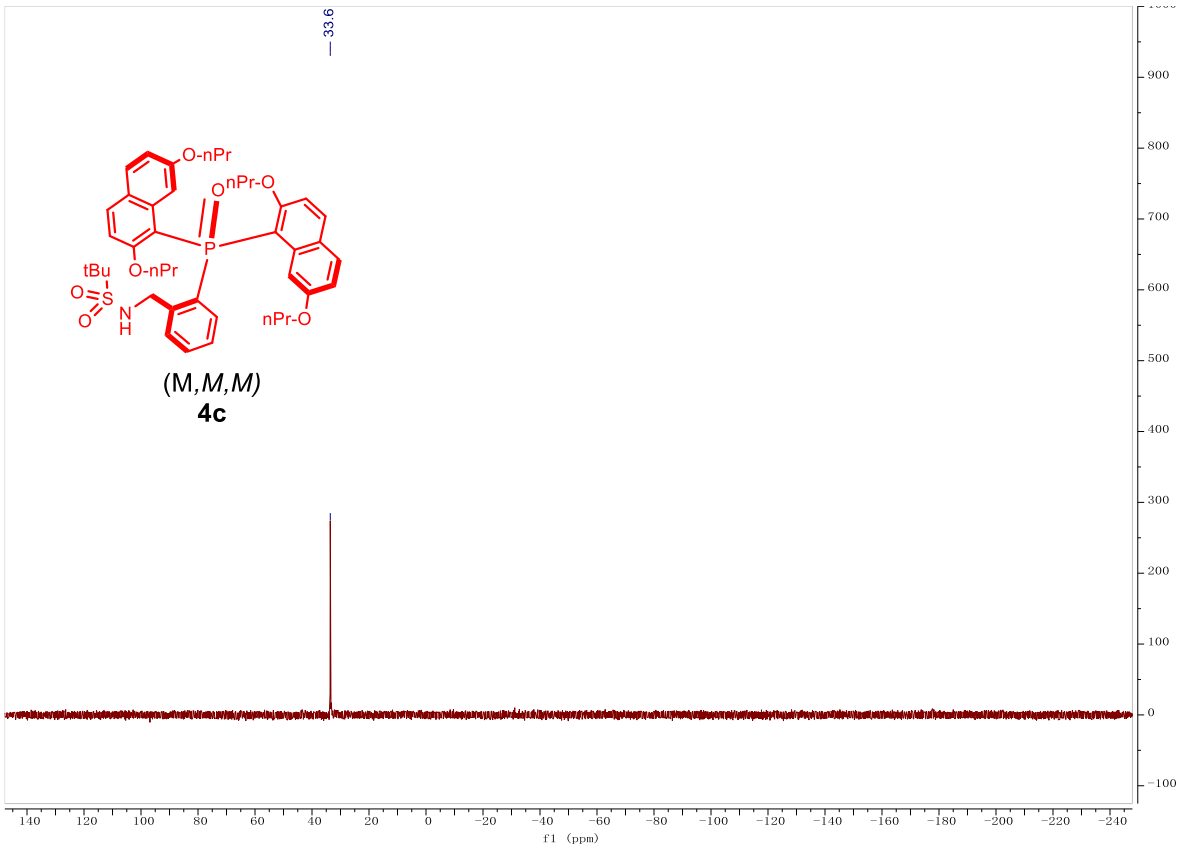
(M,*M*,*M*)
4b

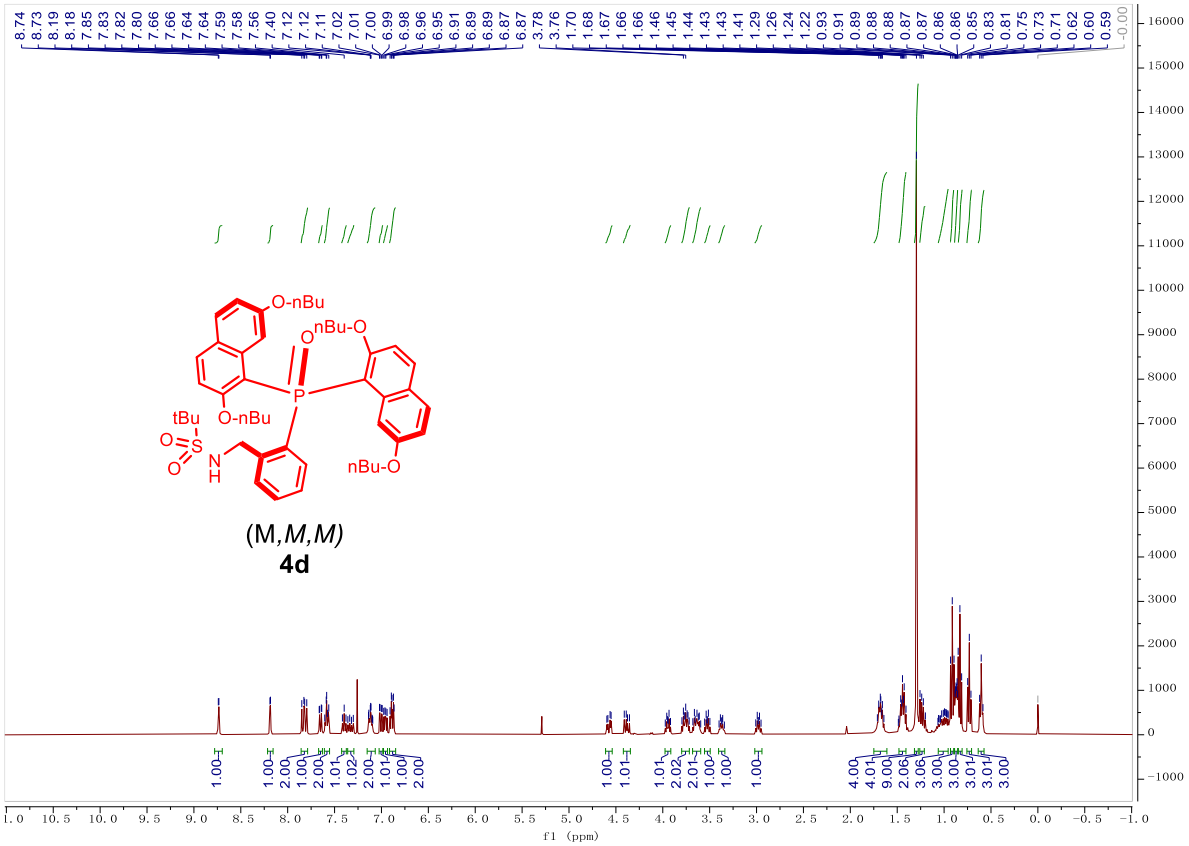

33.8
OEt
O
EtO
P
tBu
OEt
O
S
O
N
H
EtO
f1 (ppm)

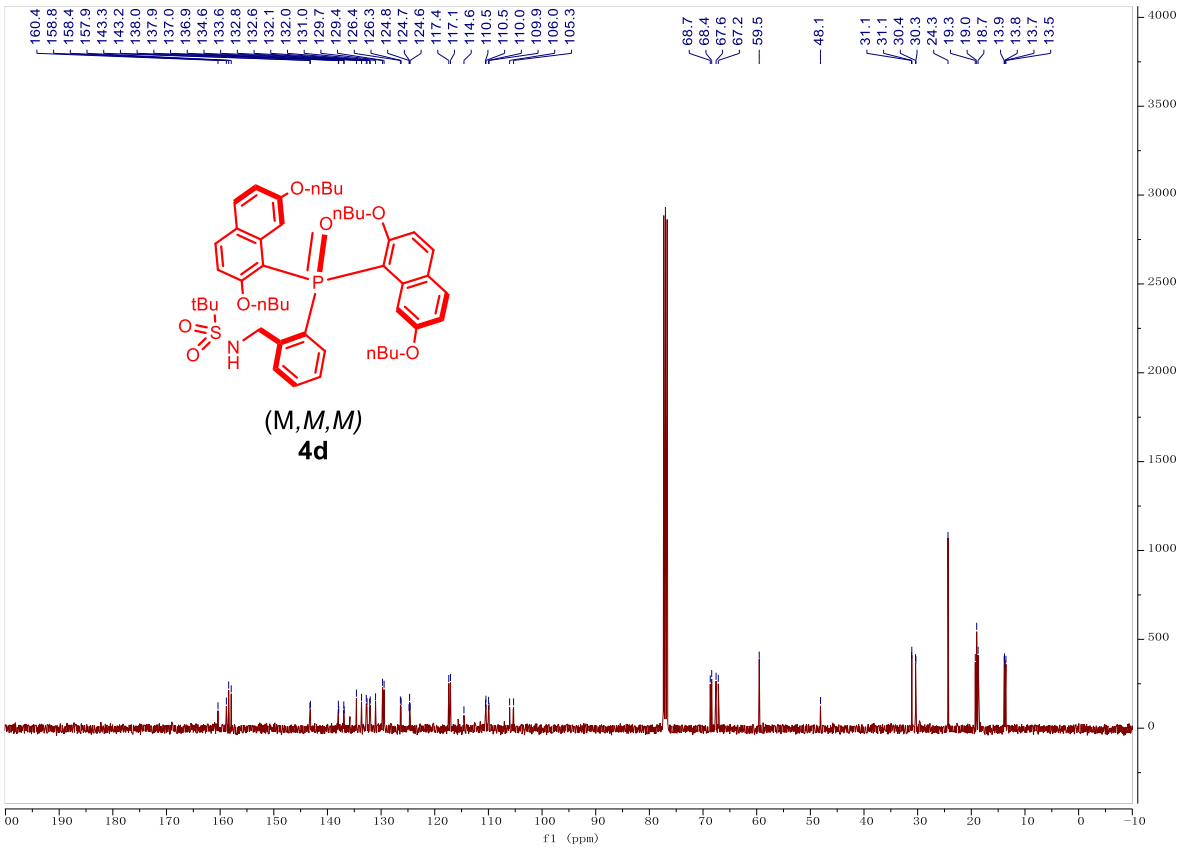
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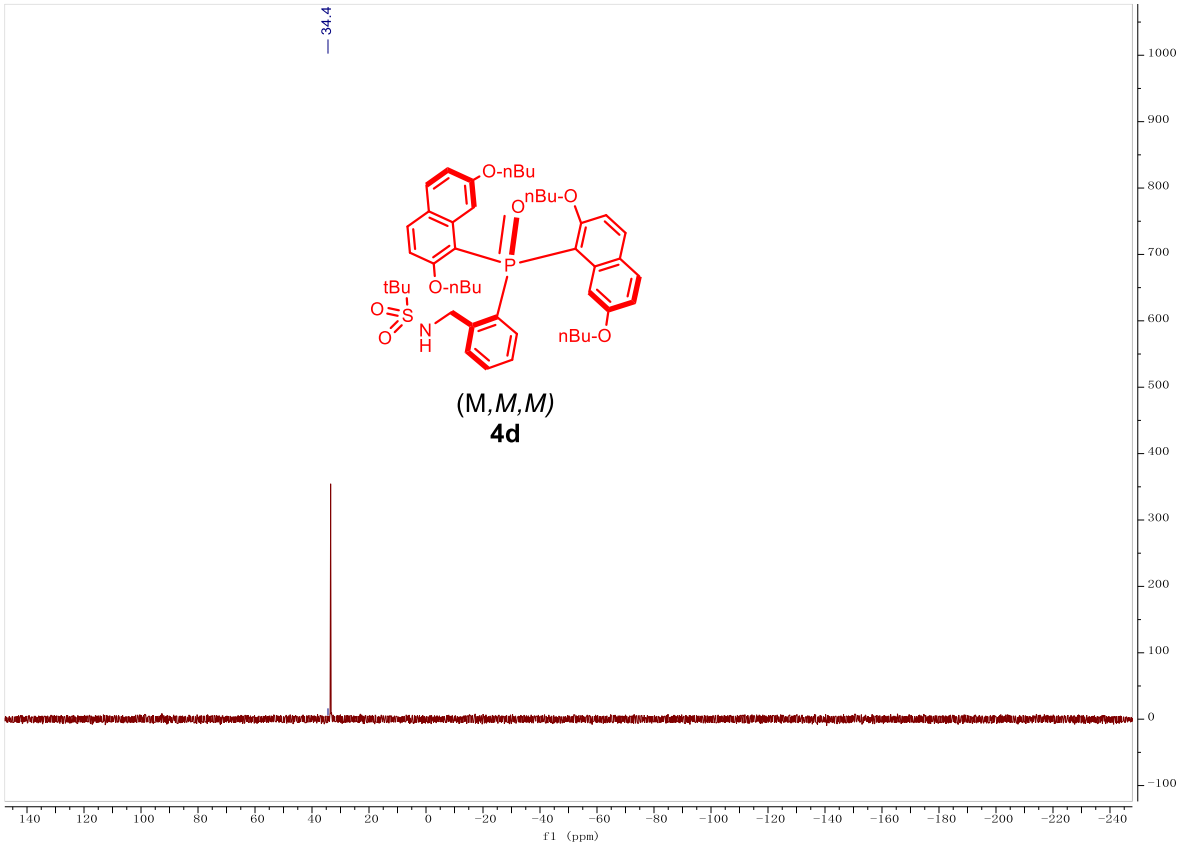

O-nPr
nPr-O
P
tBu
O-nPr
O
S
N
H
nPr-O
(M,*M*,*M*)
4c
f1 (ppm)

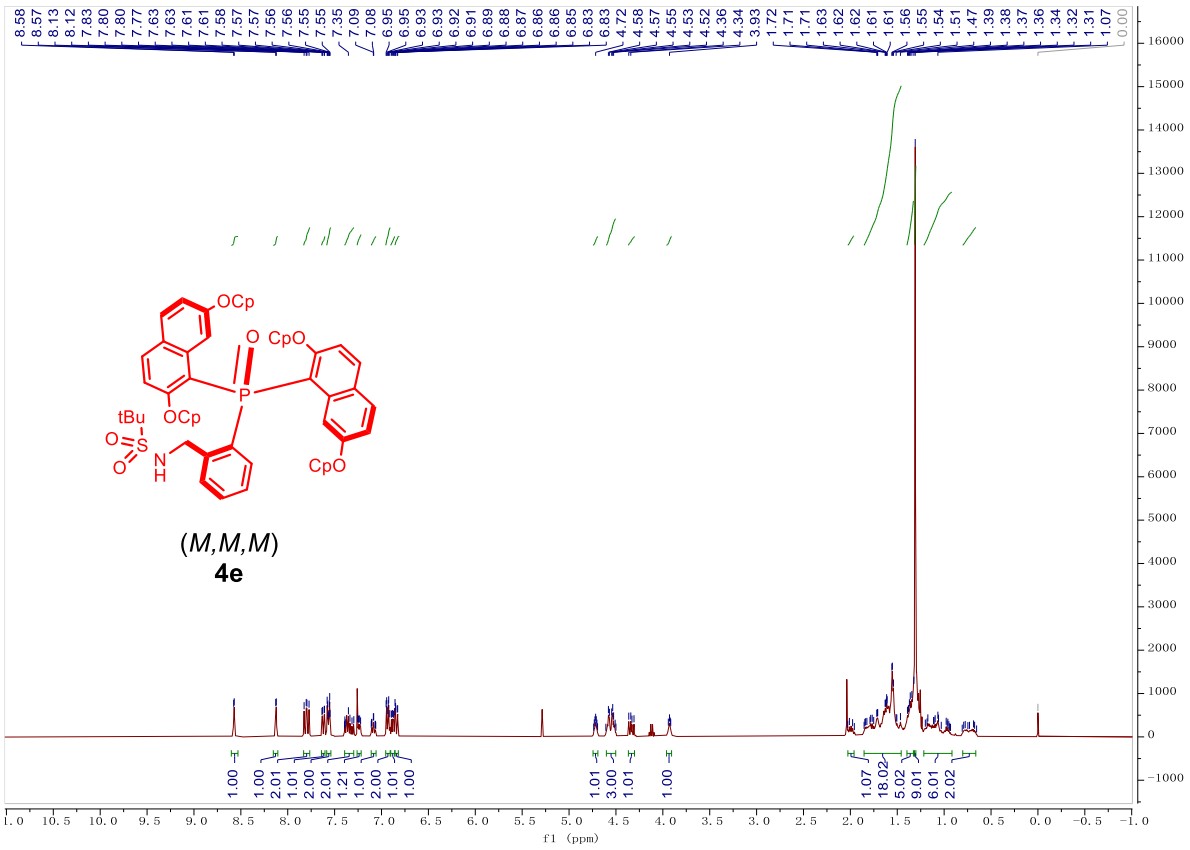

O-nPr
nPr-O
P
tBu
O-nPr
O
S
N
H
nPr-O
(M,*M*,*M*)
4c
f1 (ppm)


33.6
O-nPr
nPr-O
tBu
O-nPr
nPr-O
(M,M,M)
4c
f1 (ppm)

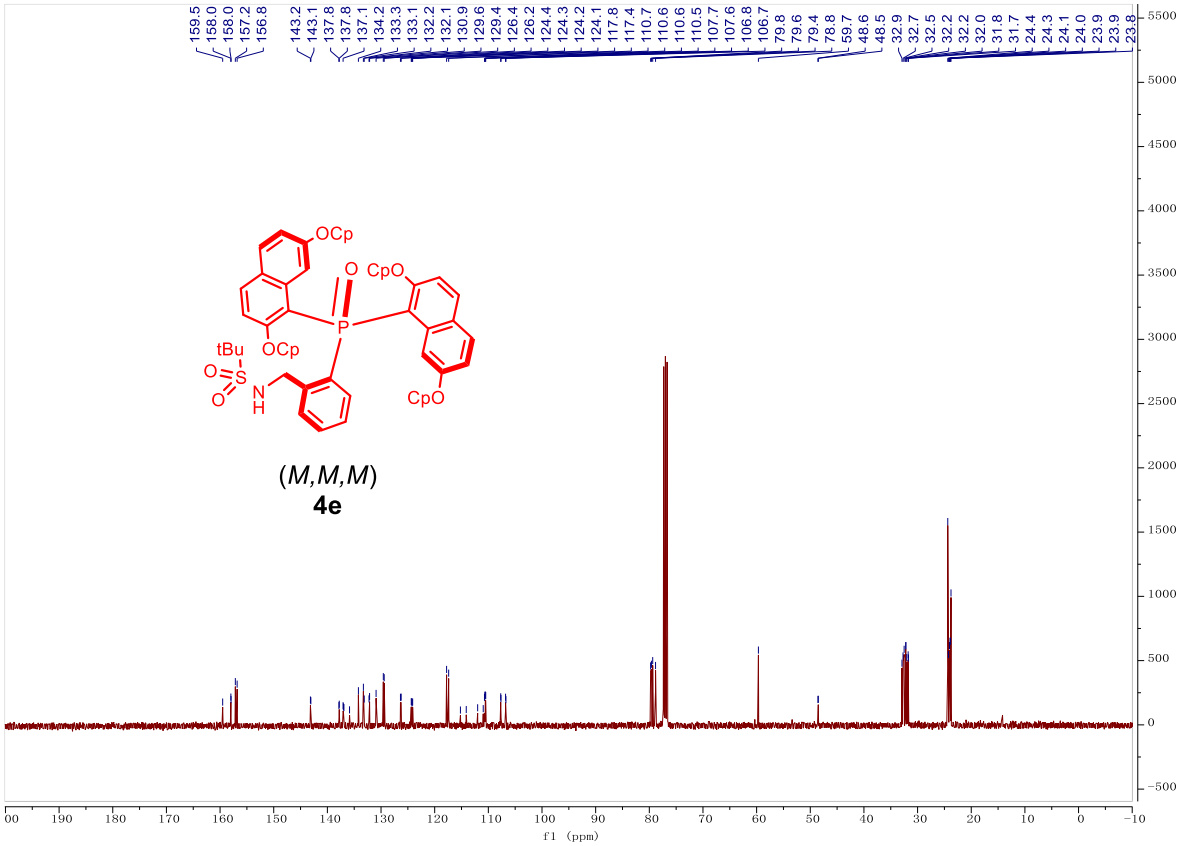

O-nBu
nBu-O
tBu
O-nBu
nBu-O
(M,M,M)
4d
f1 (ppm)


160.4
158.8
158.4
157.9
143.3
143.2
138.0
137.9
137.0
136.9
134.6
133.6
132.8
132.6
132.1
132.0
131.0
129.7
129.4
126.4
126.3
124.8
124.7
124.6
117.4
117.1
114.6
110.5
110.5
110.0
109.9
106.0
105.3
68.7
68.4
67.6
67.2
59.5
48.1
31.1
31.1
30.4
30.3
24.3
19.3
19.0
18.7
13.9
13.8
13.7
13.5
O-nBu
nBu-O
O
P
tBu
O-nBu
O
S
O
N
H
nBu-O
(M,M,M)
4d
f1 (ppm)

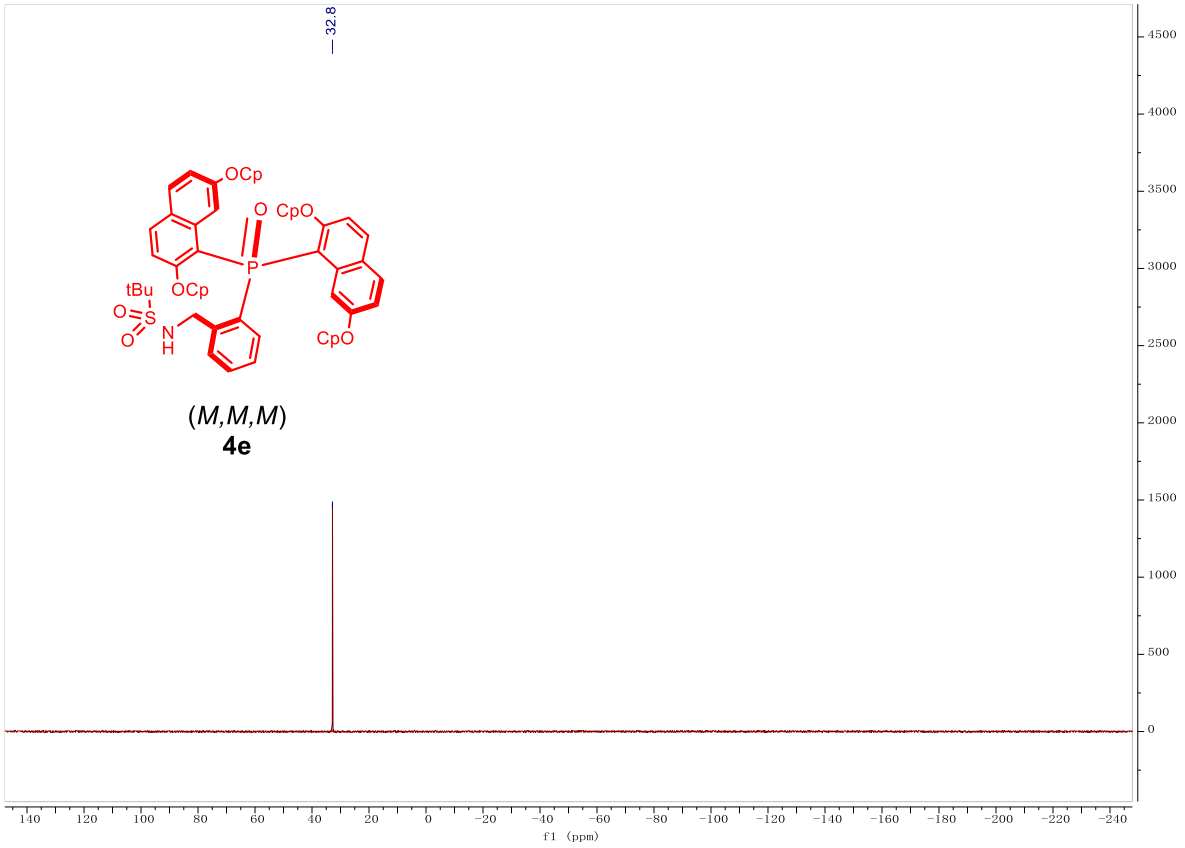

34.4
O-nBu
nBu-O
O
P
tBu
O-nBu
O
S
O
N
H
nBu-O
(M,M,M)
4d
f1 (ppm)



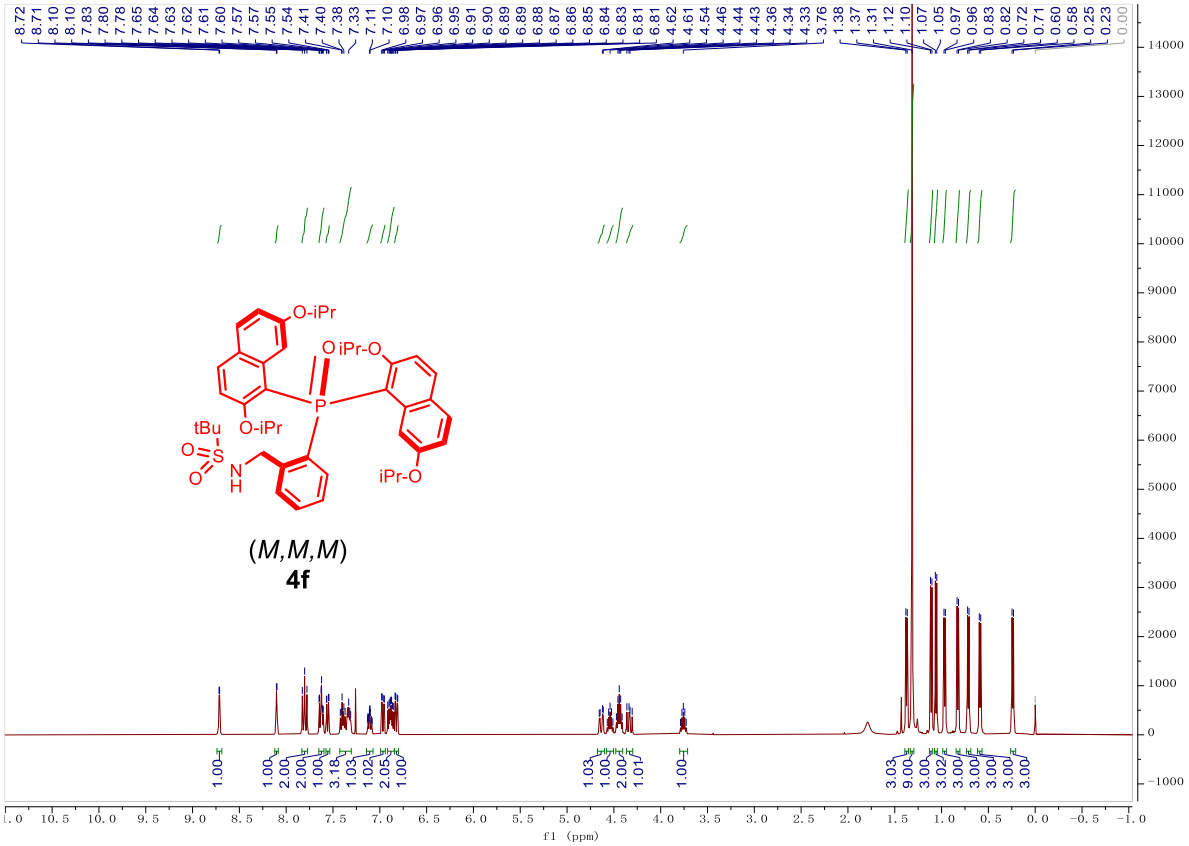
(*M*,*M*,*M*)
4e



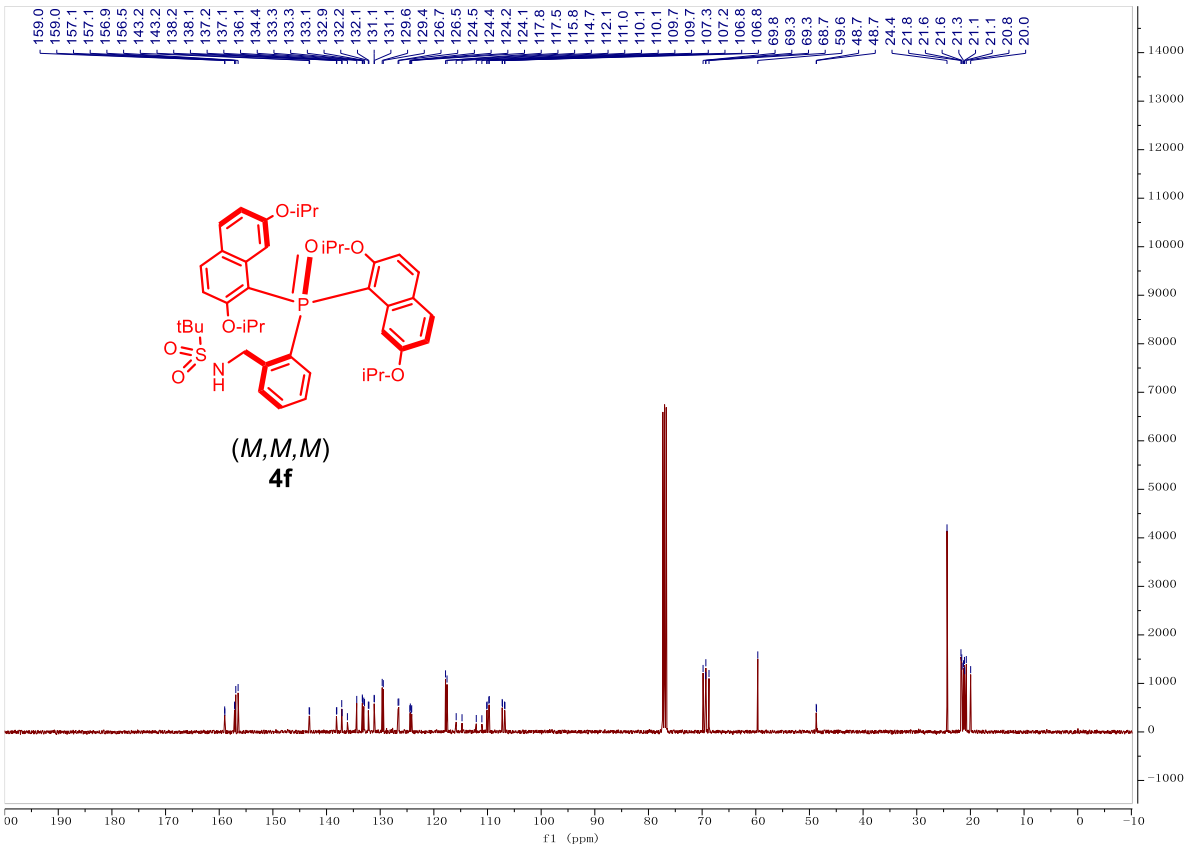
(*M*,*M*,*M*)
4e

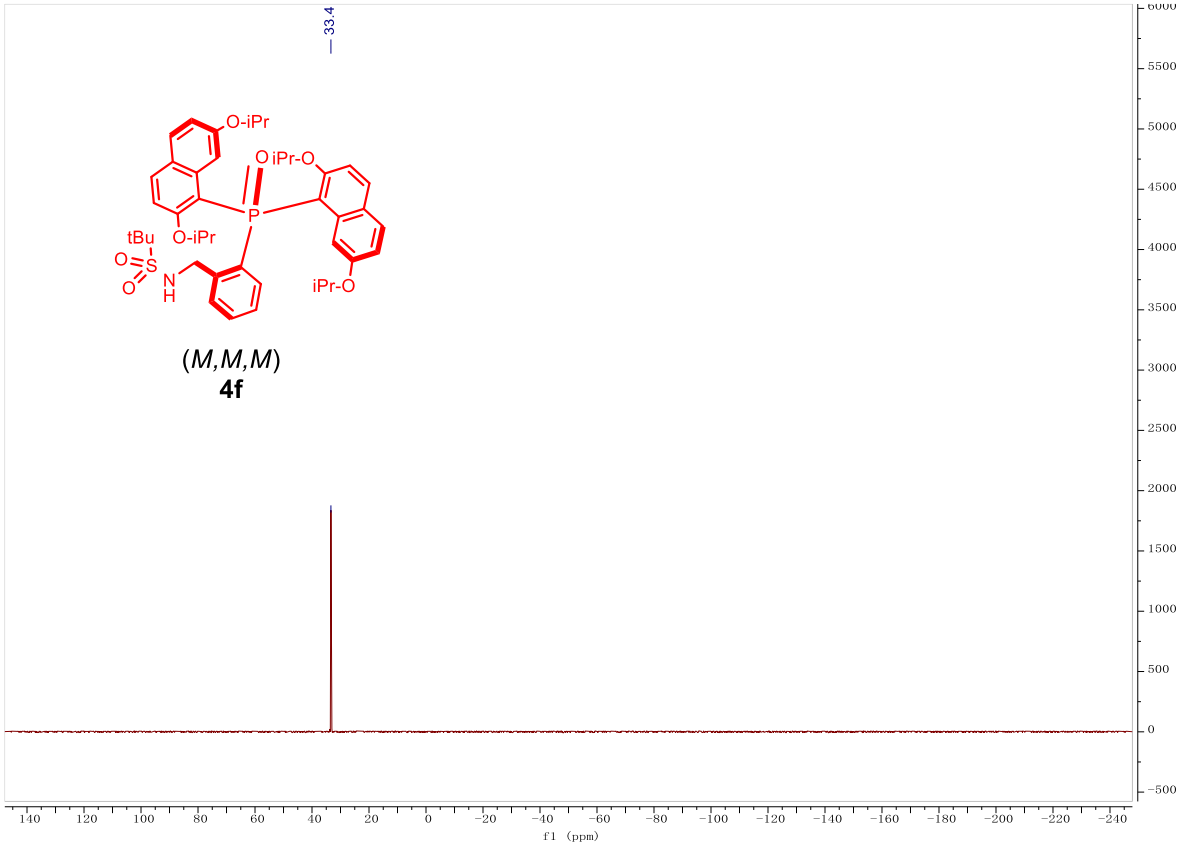

32.8
OCp
O CpO
P
tBu OCp
O
S
O
N
H
CpO
f1 (ppm)

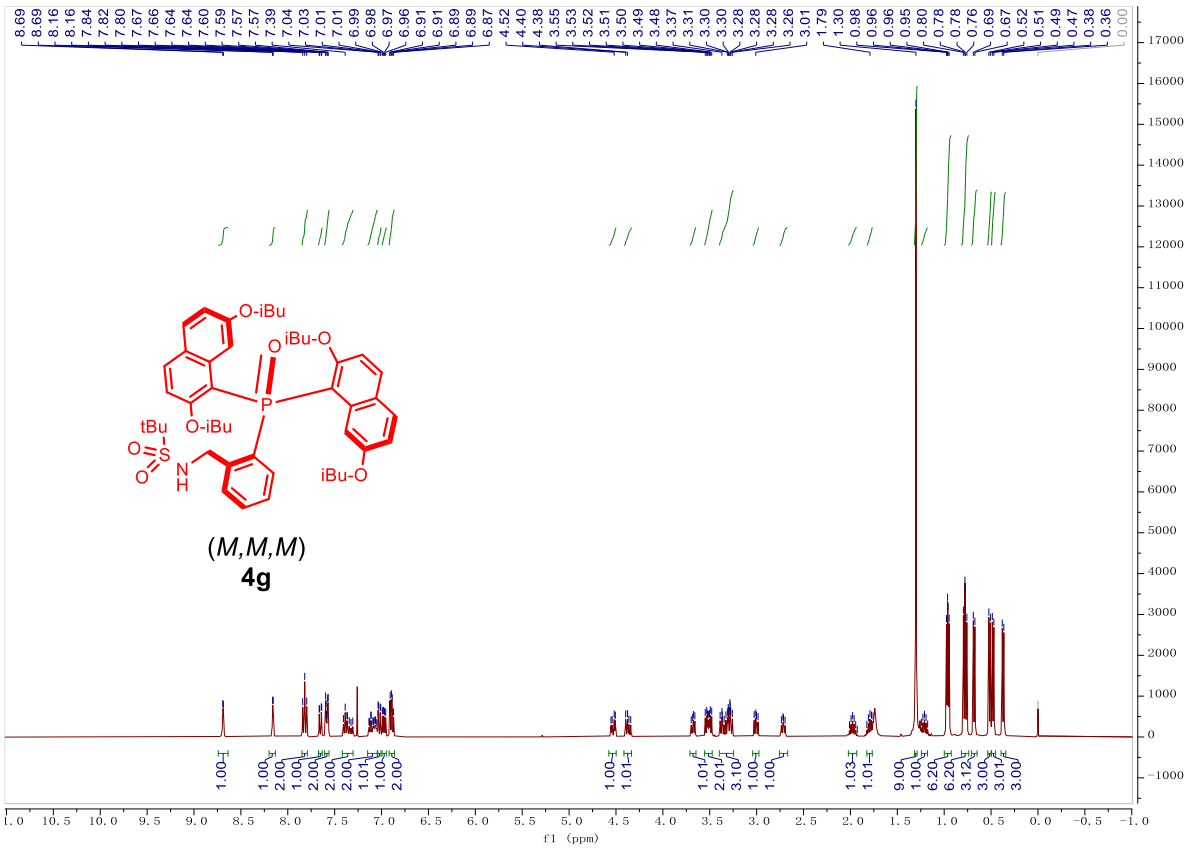
(*M*,*M*,*M*)
4e

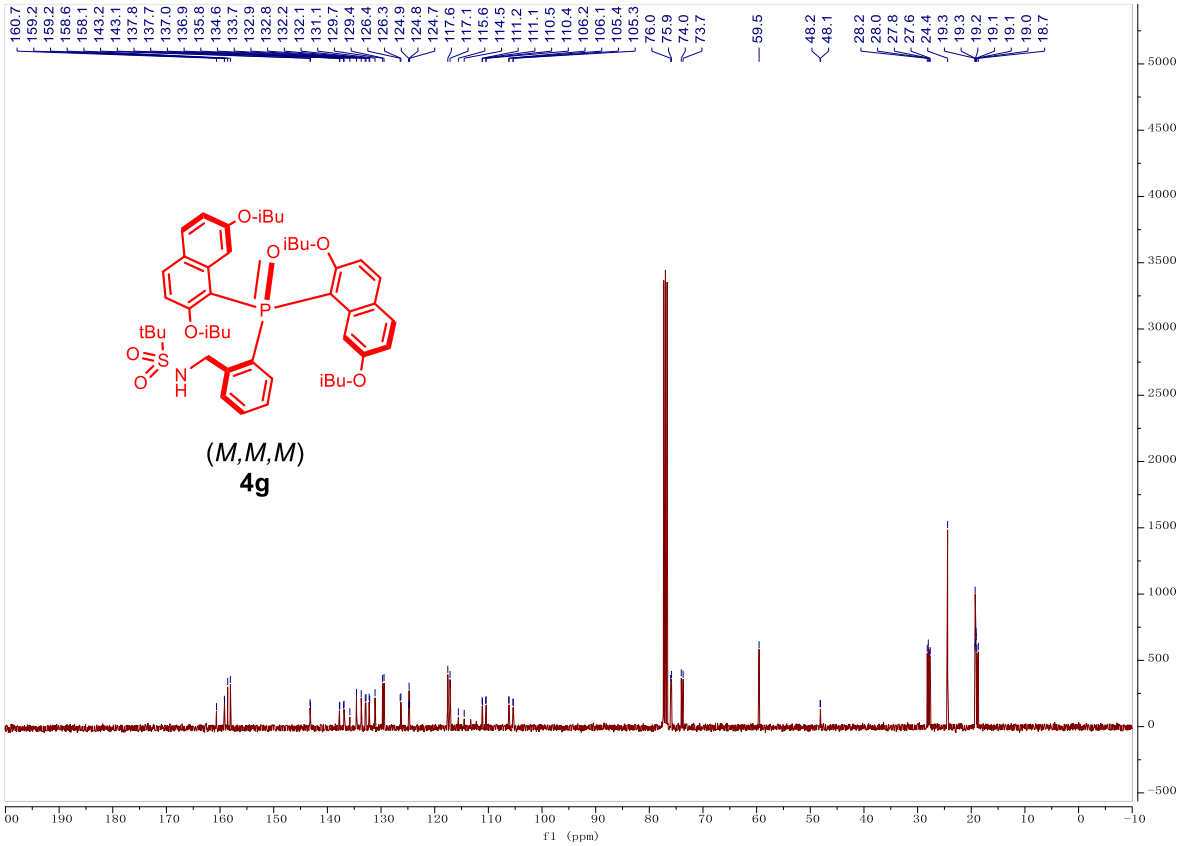

O-iPr
O iPr-O
P
tBu O-iPr
O
S
O
N
H
iPr-O
f1 (ppm)

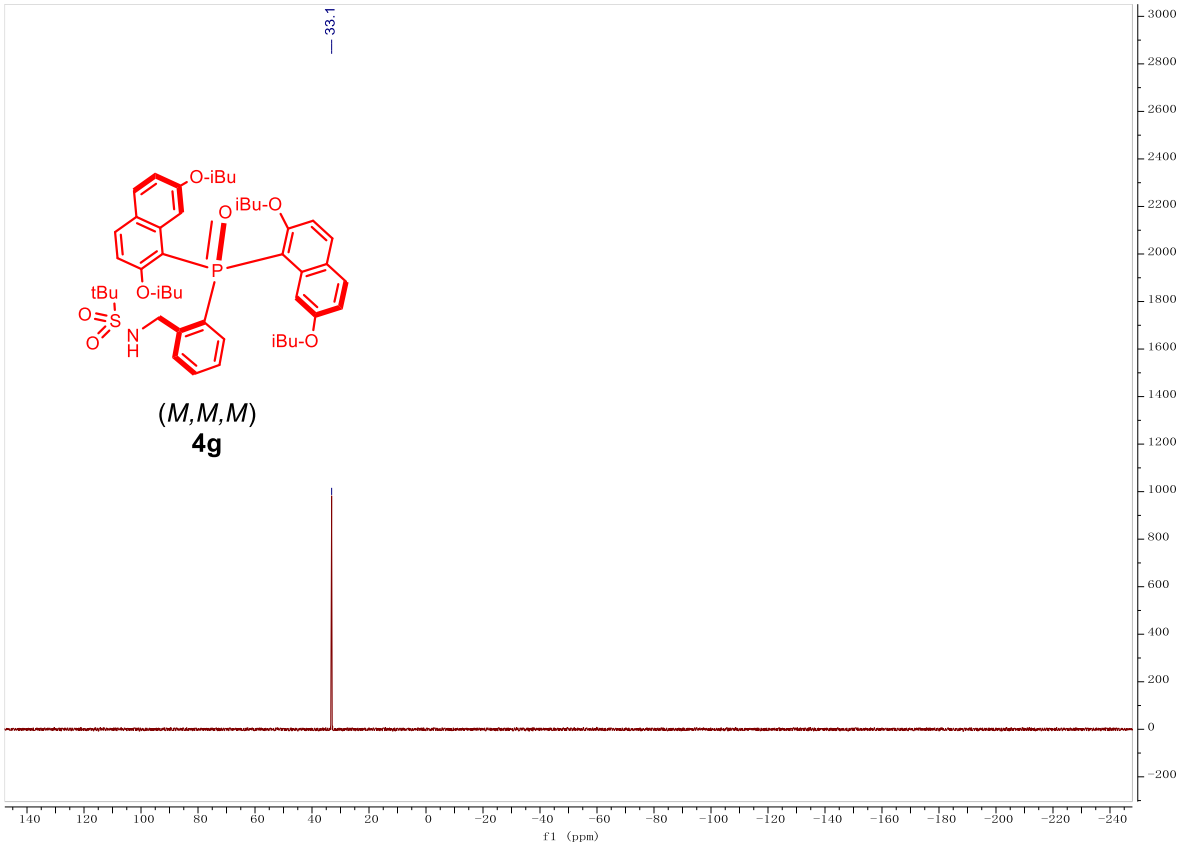
(*M*,*M*,*M*)
4f

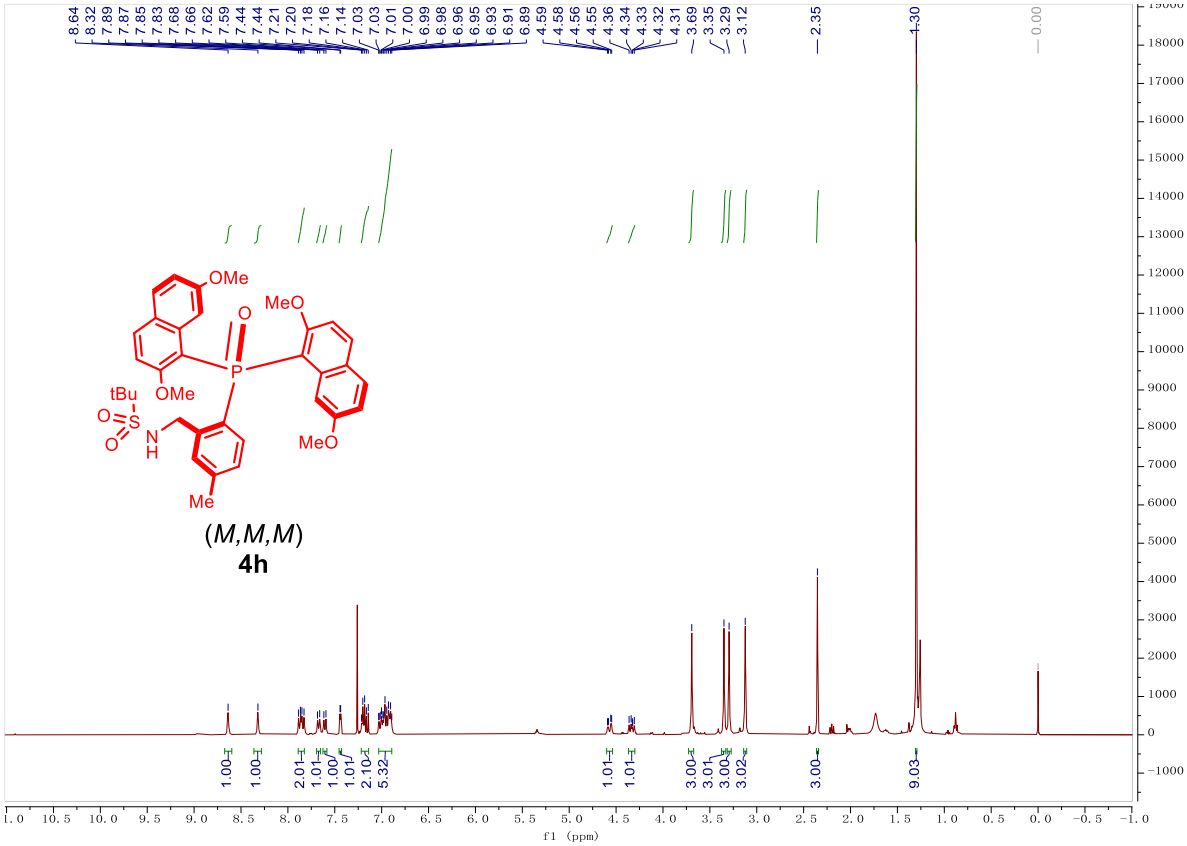

159.0
159.0
157.1
157.1
156.9
156.5
143.2
143.2
138.2
138.1
137.2
137.1
136.1
134.4
133.3
133.3
133.1
132.9
132.2
132.1
131.1
131.1
129.6
129.4
126.7
126.5
124.5
124.4
124.2
124.1
117.8
117.5
115.8
114.7
112.1
111.0
110.1
109.7
109.7
107.3
107.2
106.8
106.8
69.8
69.3
69.3
68.7
59.6
48.7
48.7
24.4
21.8
21.6
21.6
21.3
21.1
21.1
20.8
20.0
O-iPr
O iPr-O
P
tBu
O-iPr
O
S
O
N
H
iPr-O
(M,M,M)
4f
f1 (ppm)

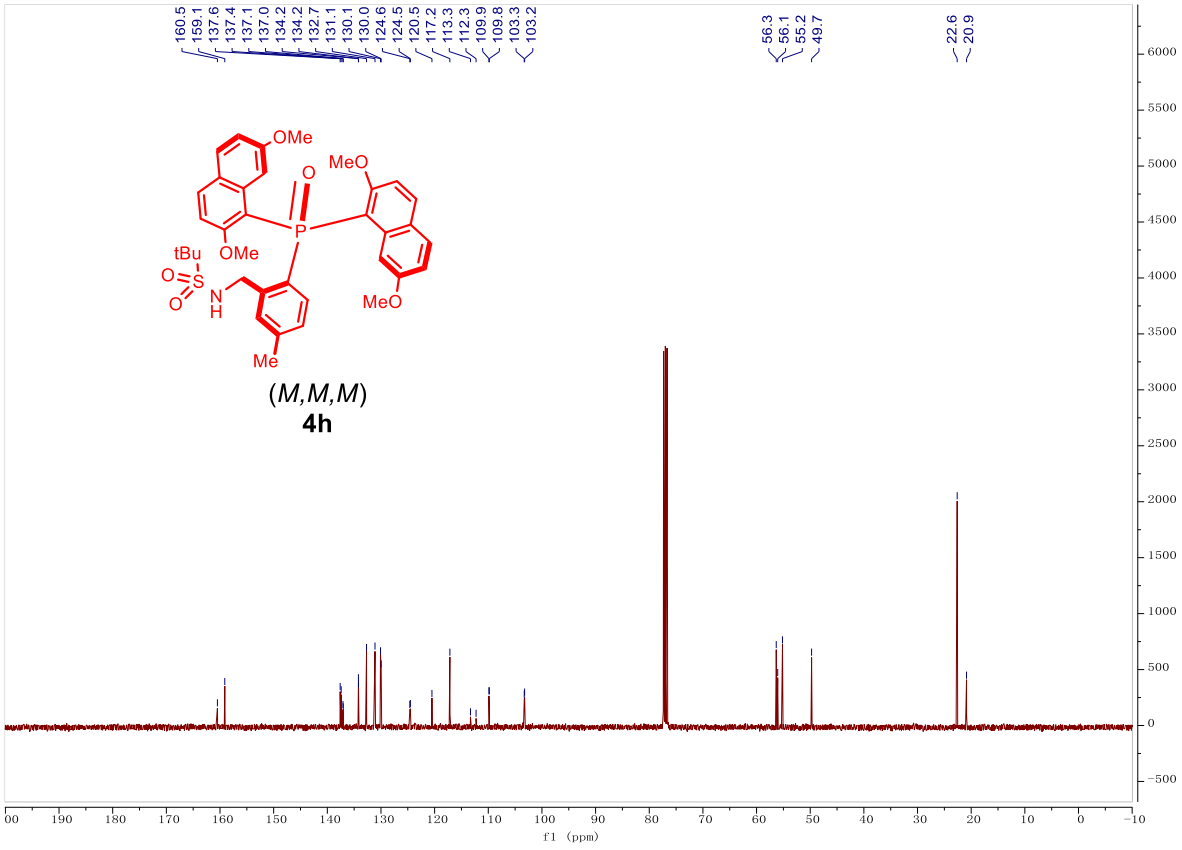

33.4
O-iPr
O iPr-O
P
tBu
O-iPr
O
S
O
N
H
iPr-O
(M,M,M)
4f
f1 (ppm)


O-iBu
iBu-O
O
P
tBu
O-iBu
O
S
O
N
H
iBu-O
(M,M,M)
4g
f1 (ppm)

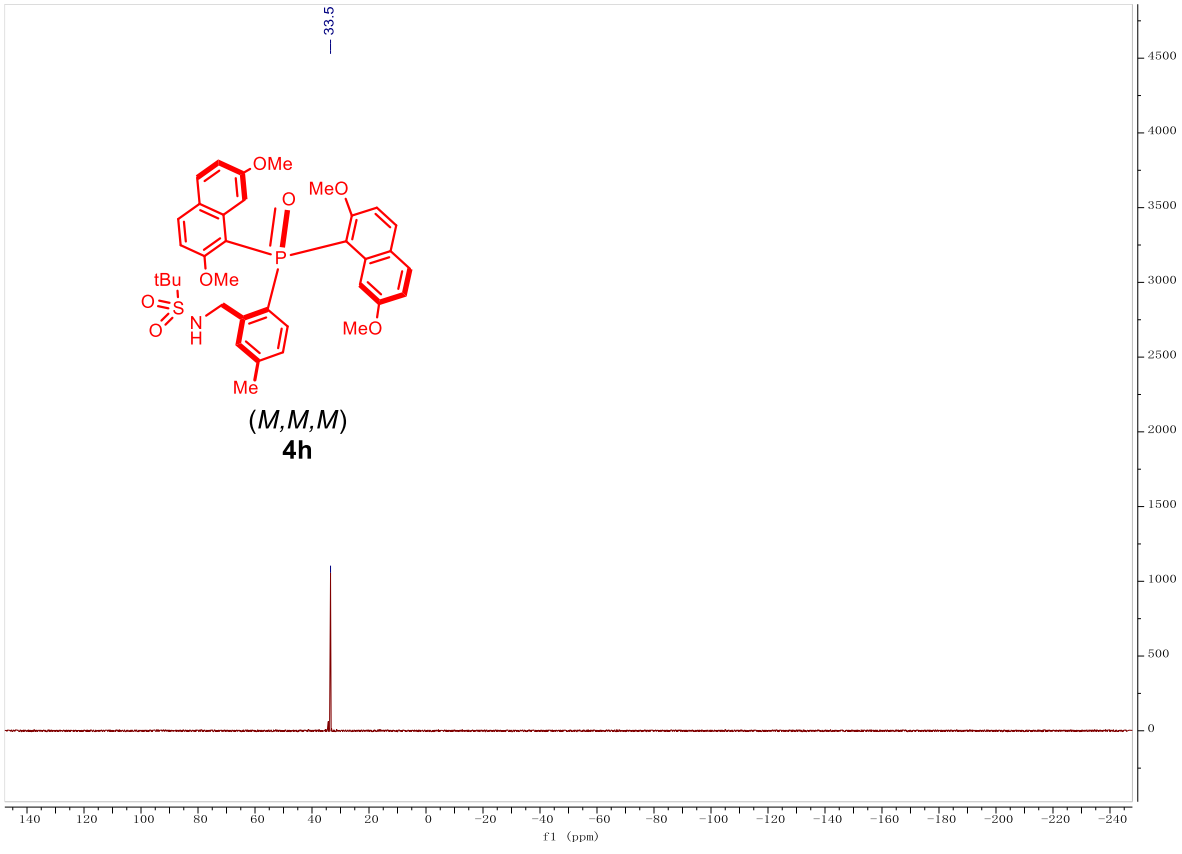

O-iBu
iBu-O
O
P
tBu
O-iBu
O
S
O
N
H
iBu-O
(M,M,M)
4g
f1 (ppm)


33.1
O-iBu
iBu-O
O
P
tBu
O-iBu
O
S
O
N
H
iBu-O
(M,M,M)
4g
f1 (ppm)

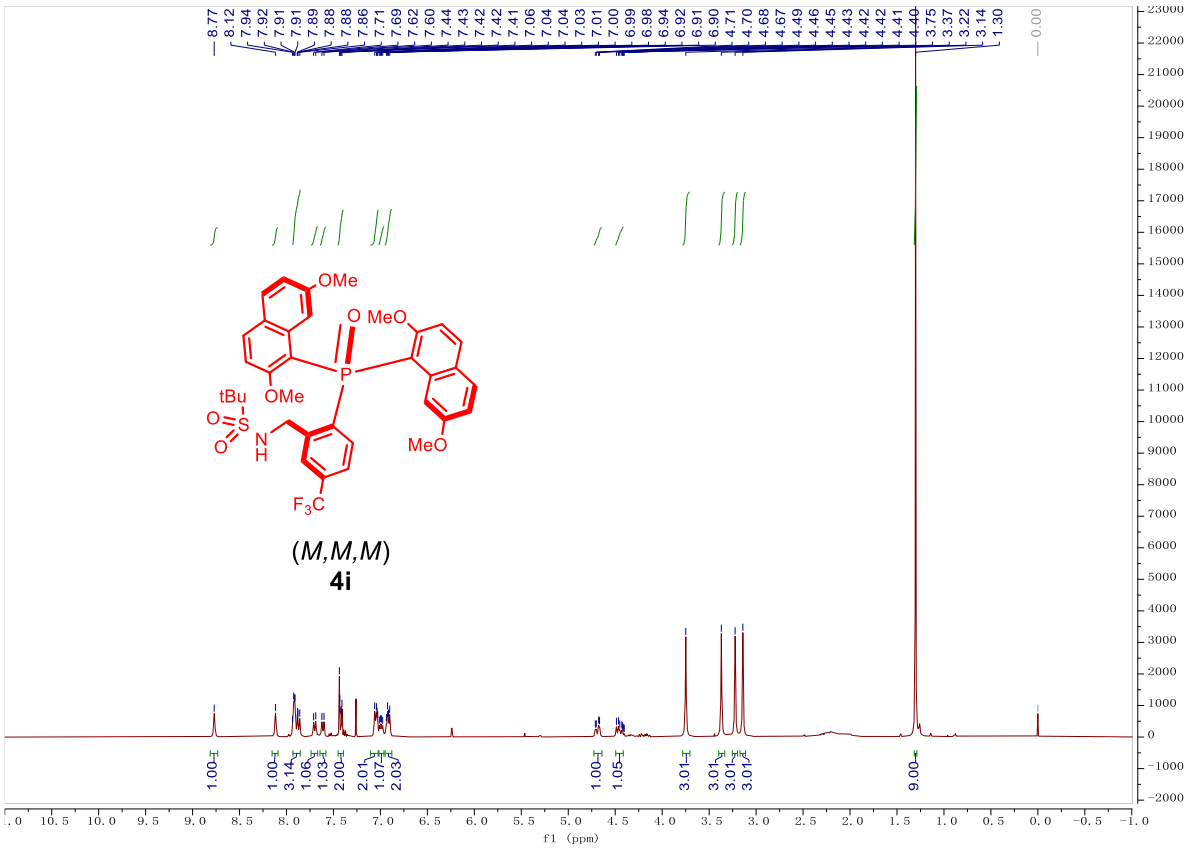

8.64
8.32
7.89
7.87
7.85
7.83
7.68
7.66
7.62
7.59
7.44
7.44
7.21
7.20
7.18
7.16
7.14
7.03
7.03
7.01
7.00
6.99
6.98
6.96
6.95
6.93
6.91
6.89
4.59
4.58
4.56
4.55
4.36
4.34
4.33
4.32
4.31
3.69
3.35
3.29
3.12
2.35
1.30
0.00
OMe
MeO
O
P
tBu
OMe
O
S
O
N
H
MeO
Me
(M,M,M)
4h
1.00
1.00
2.01
1.01
1.00
1.01
2.10
5.32
1.01
1.01
3.00
3.01
3.00
3.02
3.00
9.03
f1 (ppm)

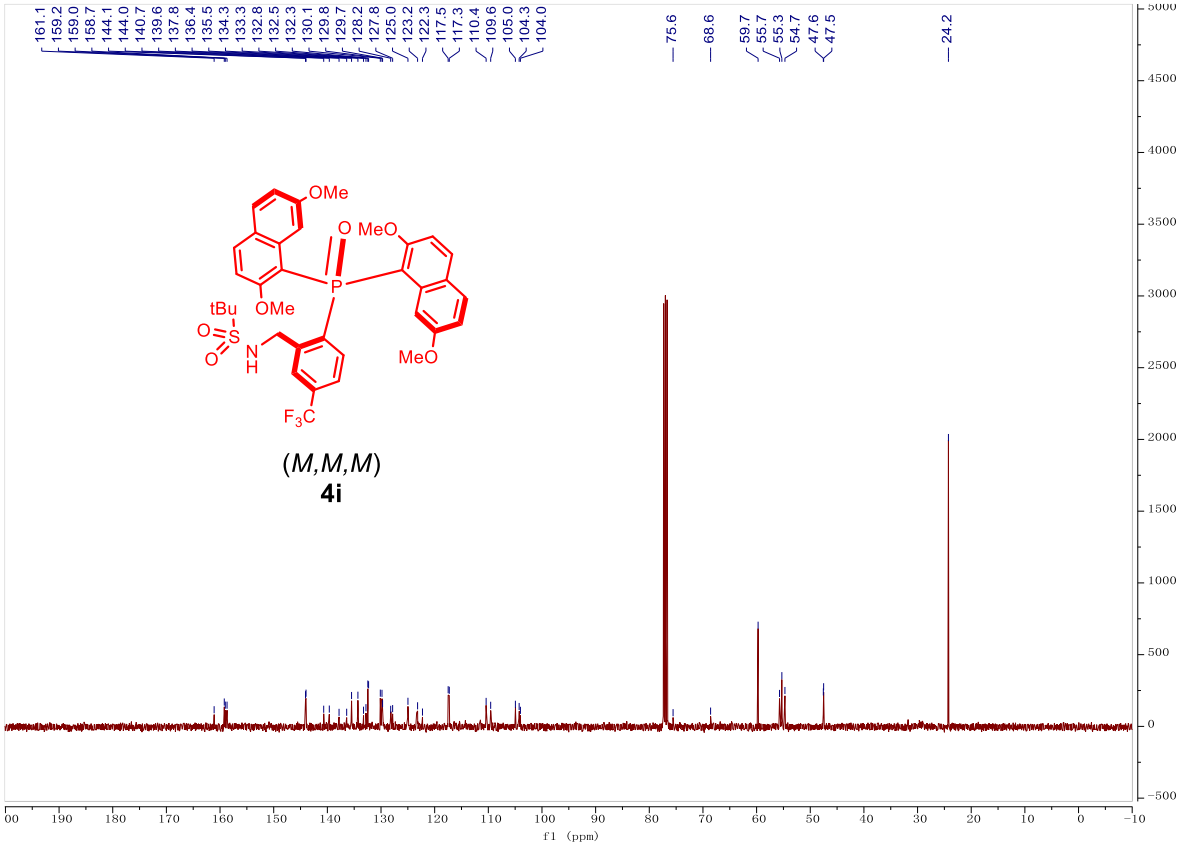

160.5
159.1
137.6
137.4
137.1
137.0
134.2
134.2
132.7
131.1
130.1
130.0
124.6
124.5
120.5
117.2
113.3
112.3
109.9
109.8
103.3
103.2
56.3
56.1
55.2
49.7
22.6
20.9
OMe
MeO
O
P
tBu
OMe
O
S
O
N
H
MeO
Me
f1 (ppm)

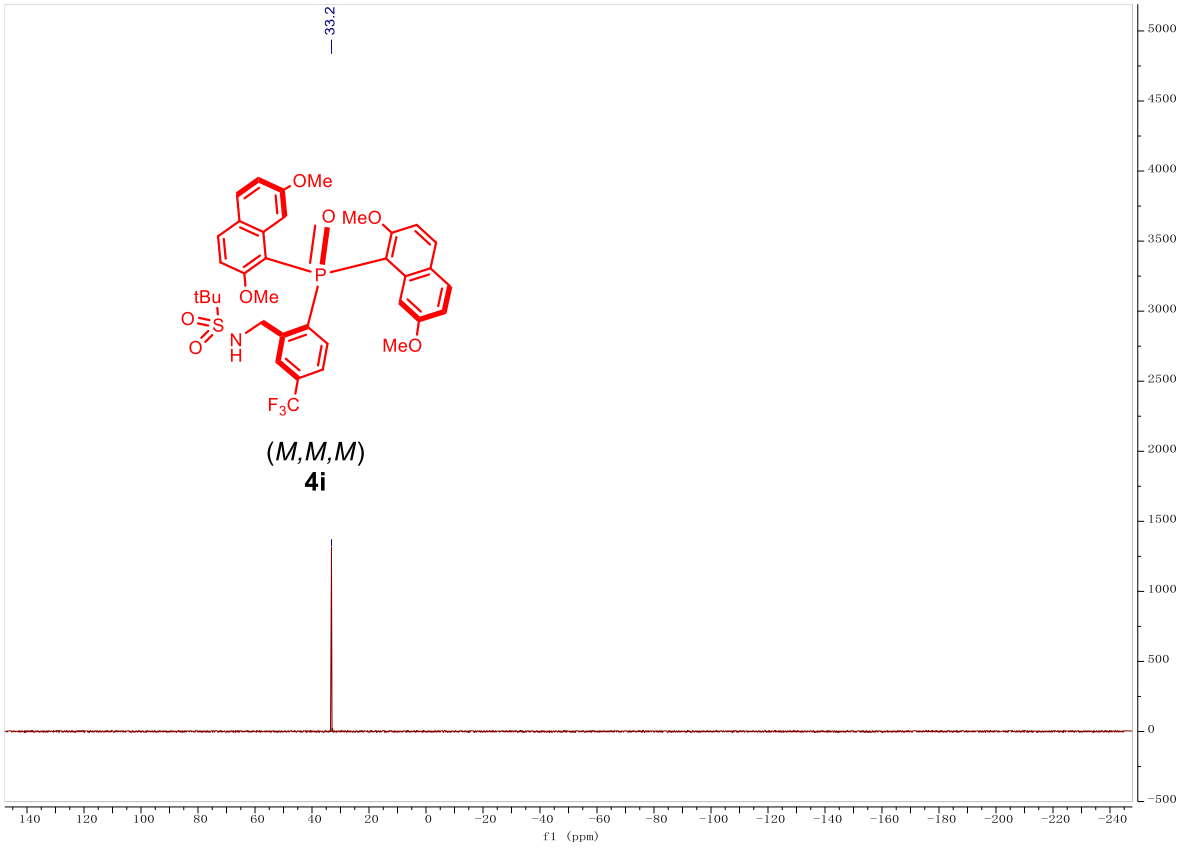
(*M*,*M*,*M*)
4h

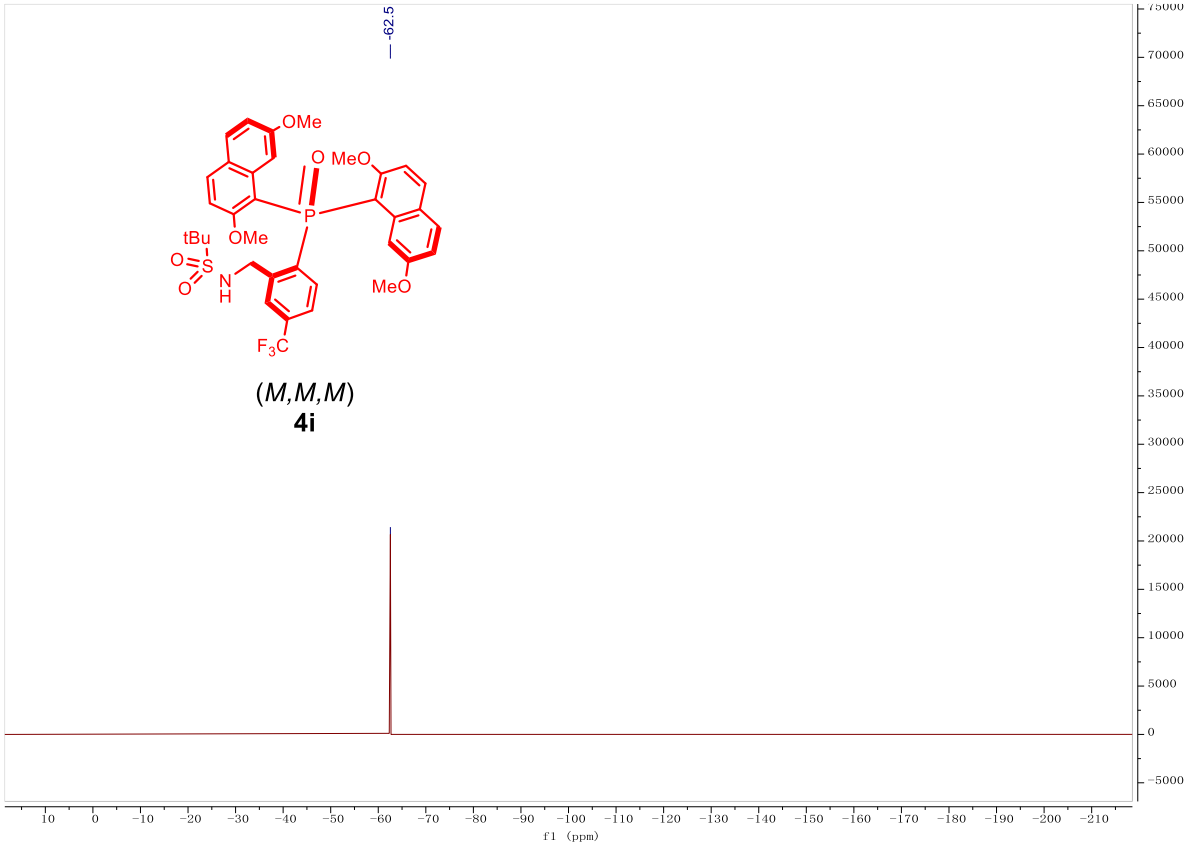

33.5
OMe
MeO
O
P
tBu
OMe
O
S
O
N
H
MeO
Me
f1 (ppm)

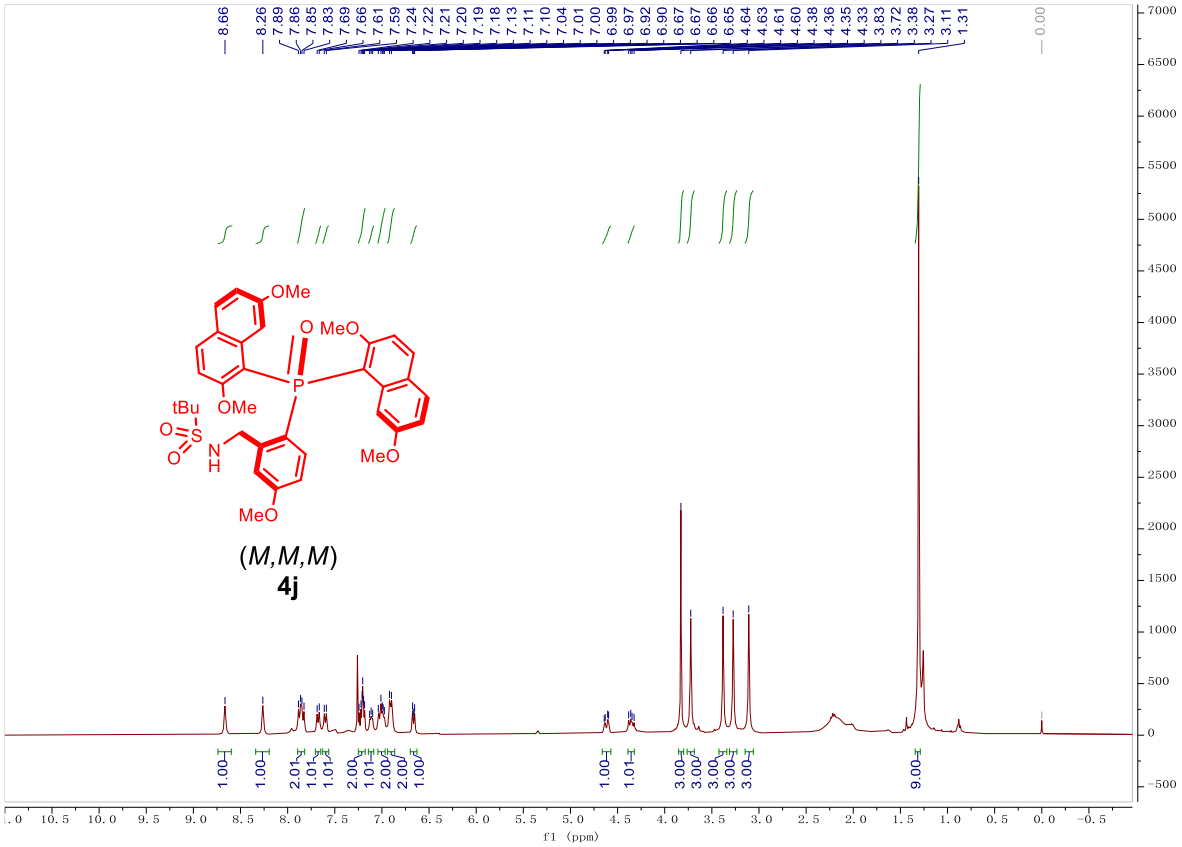
(*M*,*M*,*M*)
4h

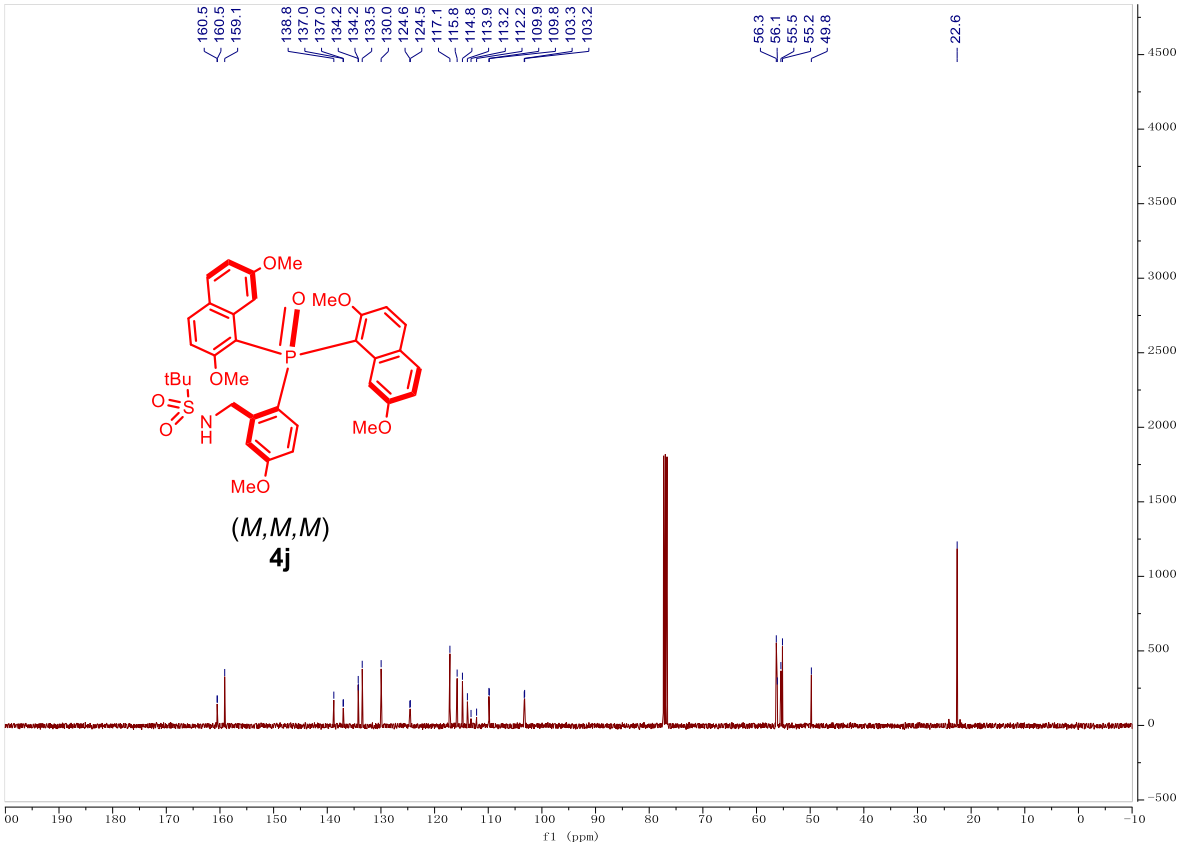

OMe
O MeO
P
tBu OMe
O
S
O
N
H
MeO
F3C
(M,M,M)
4i
f1 (ppm)

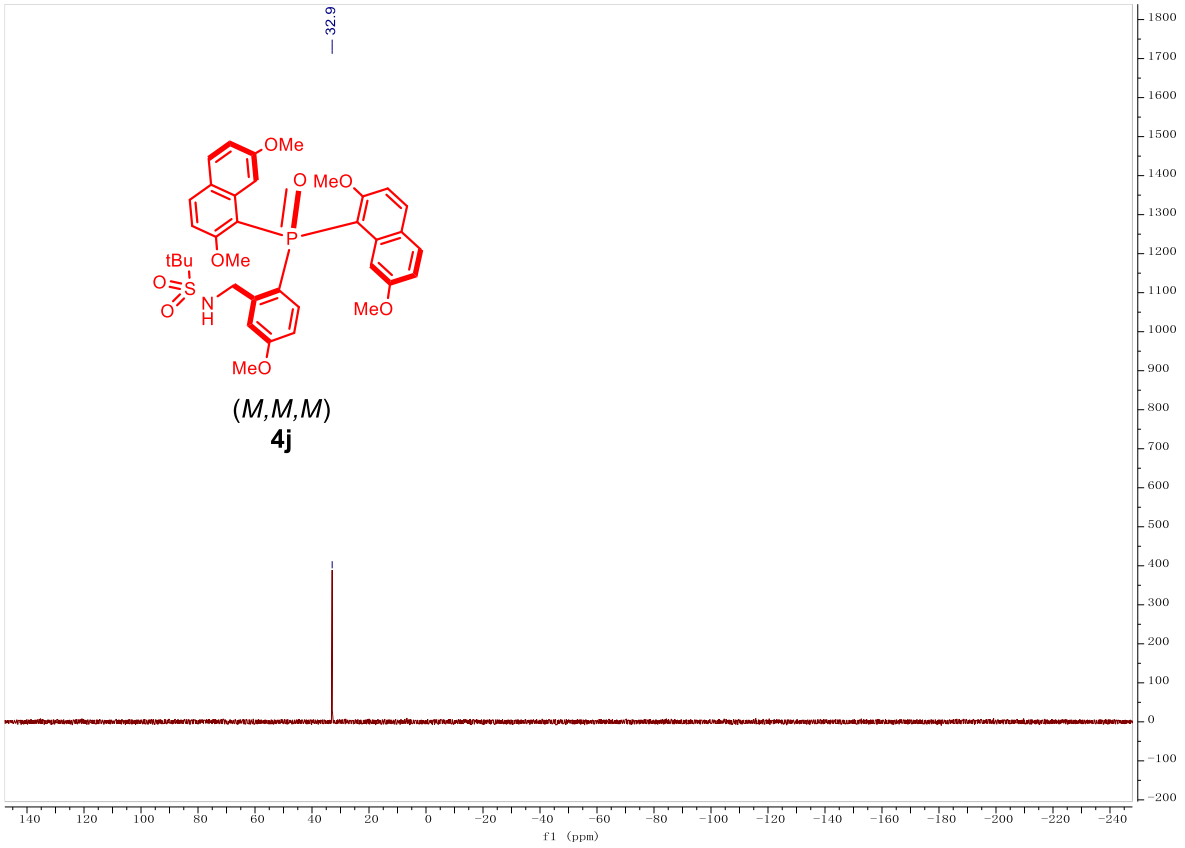

OMe
O MeO
P
tBu OMe
O
S
O
N
H
MeO
F3C
(M,M,M)
4i
f1 (ppm)


33.2
OMe
O MeO
P
tBu
OMe
O
S
O
N
H
MeO
F3C
(M,M,M)
4i
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
−500
140 120 100 80 60 40 20 0 −20 −40 −60 −80 −100 −120 −140 −160 −180 −200 −220 −240
f1 (ppm)

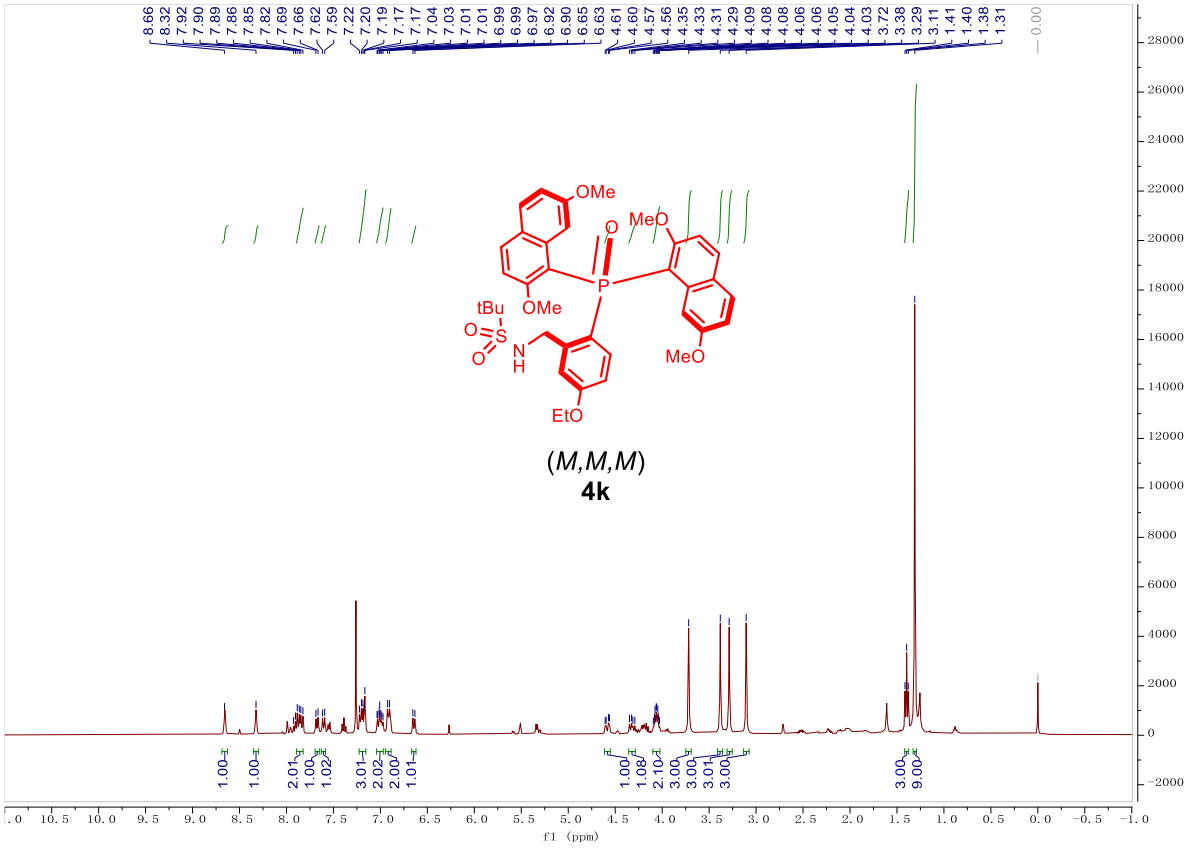

62.5
OMe
O MeO
P
tBu
OMe
O
S
O
N
H
MeO
F3C
(M,M,M)
4i
70000
65000
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
−5000
10 0 −10 −20 −30 −40 −50 −60 −70 −80 −90 −100 −110 −120 −130 −140 −150 −160 −170 −180 −190 −200 −210
f1 (ppm)


OMe
O MeO
P
tBu
OMe
O
S
O
N
H
MeO
MeO
(M,M,M)
4j
f1 (ppm)

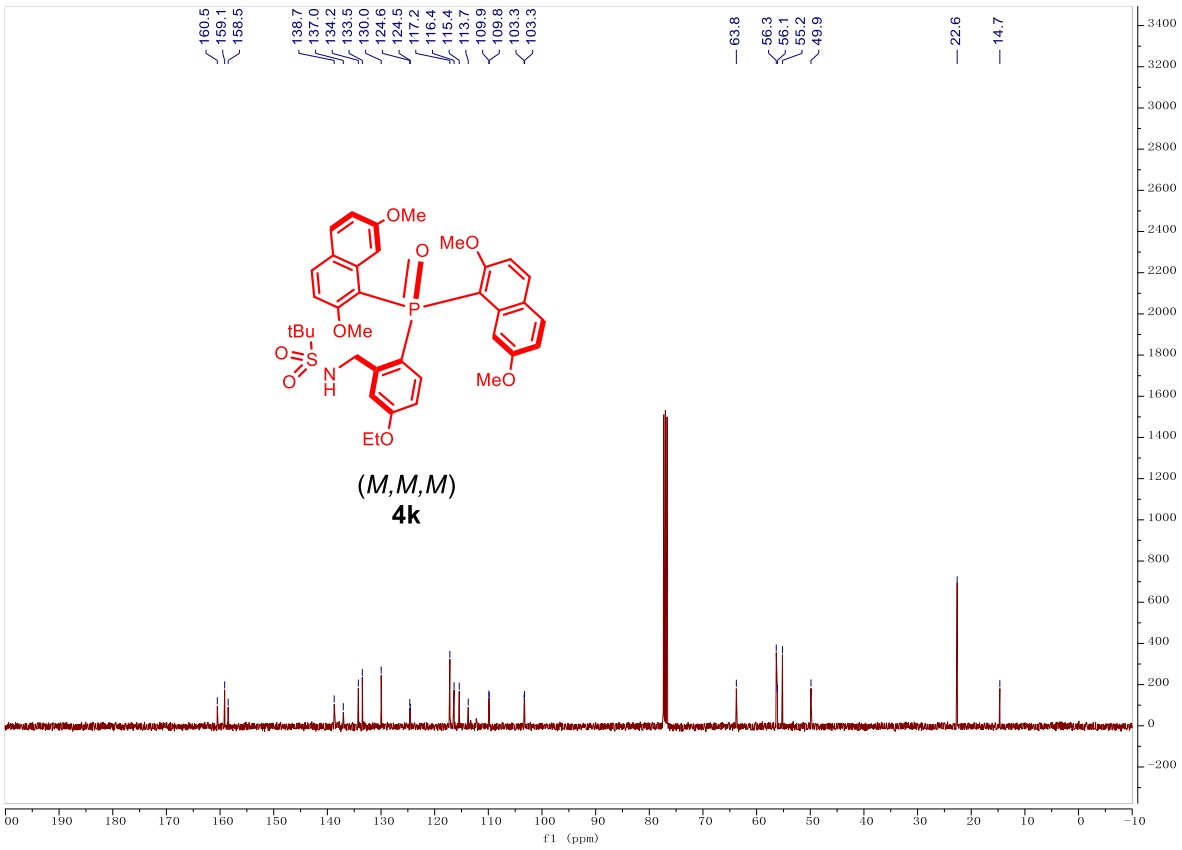

OMe
O MeO
P
tBu
OMe
O
S
O
N
H
MeO
MeO
(M,M,M)
4j
f1 (ppm)


32.9
OMe
O MeO
P
tBu
OMe
O
S
O
N
H
MeO
MeO
f1 (ppm)

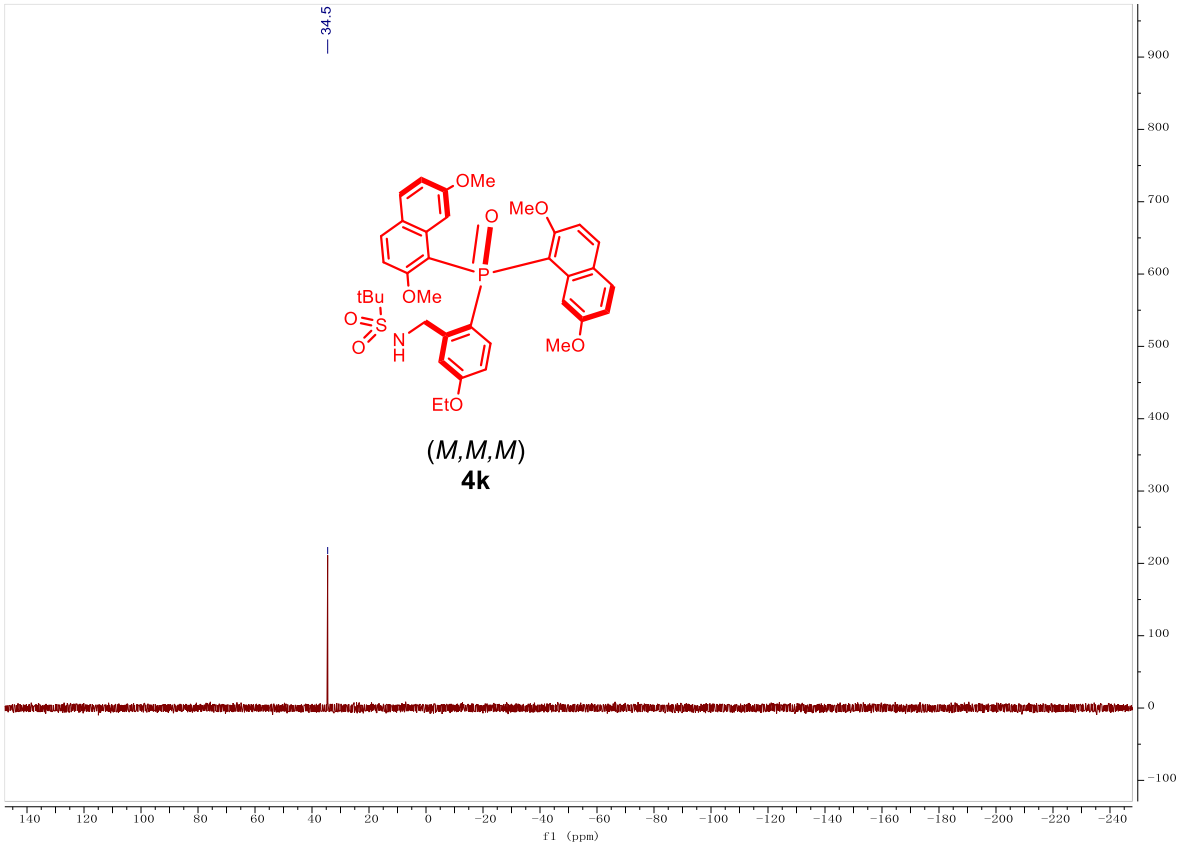
(*M*,*M*,*M*)
4j


8.66
8.32
7.92
7.90
7.89
7.86
7.85
7.82
7.69
7.66
7.62
7.59
7.22
7.20
7.19
7.17
7.17
7.04
7.03
7.01
7.01
6.99
6.99
6.97
6.92
6.90
6.65
6.63
4.61
4.60
4.57
4.56
4.35
4.33
4.31
4.29
4.09
4.08
4.08
4.06
4.06
4.05
4.04
4.03
3.72
3.38
3.29
3.11
1.41
1.40
1.38
1.31
0.00
OMe
MeO
O
P
tBu
OMe
O
S
O
N
H
MeO
EtO
1.00
1.00
2.01
1.00
1.02
3.01
2.02
2.00
1.01
1.00
1.08
2.10
3.00
3.01
3.00
3.00
9.00
f1 (ppm)

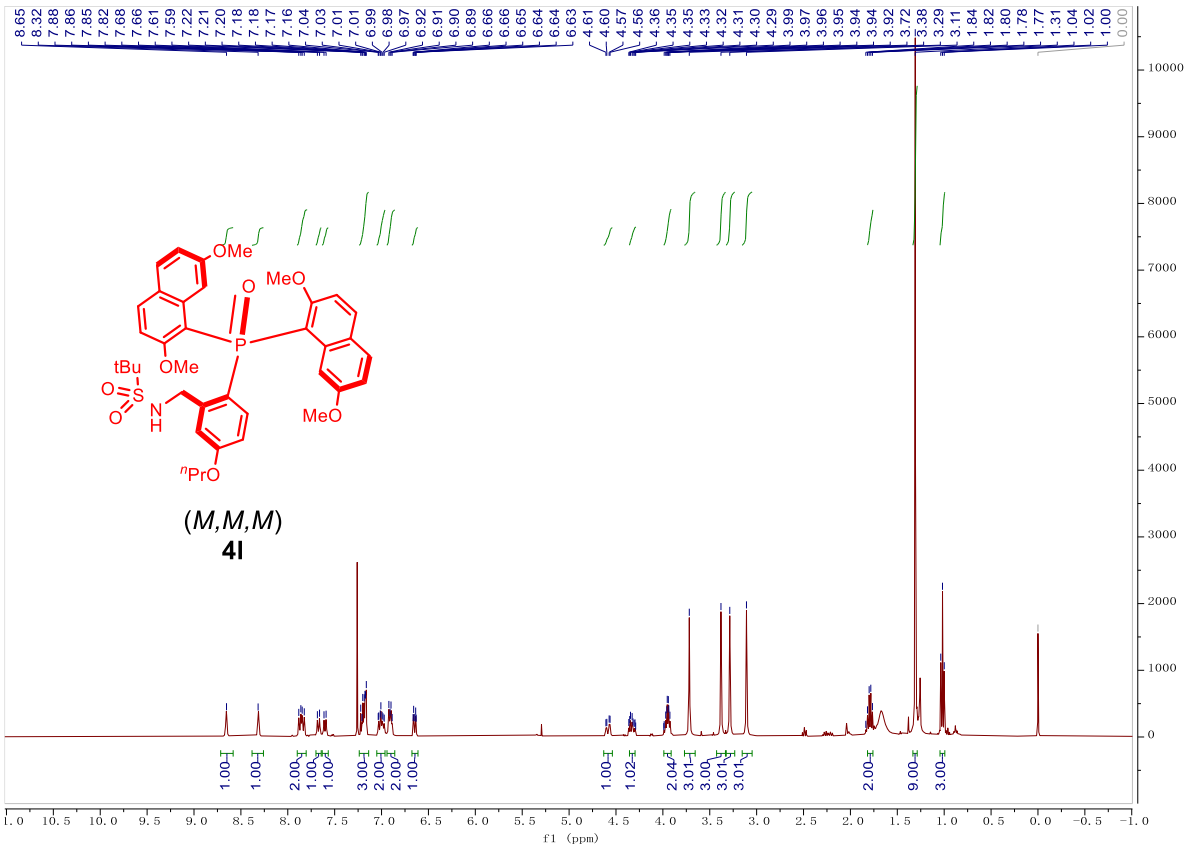
(*M*,*M*,*M*)
4k

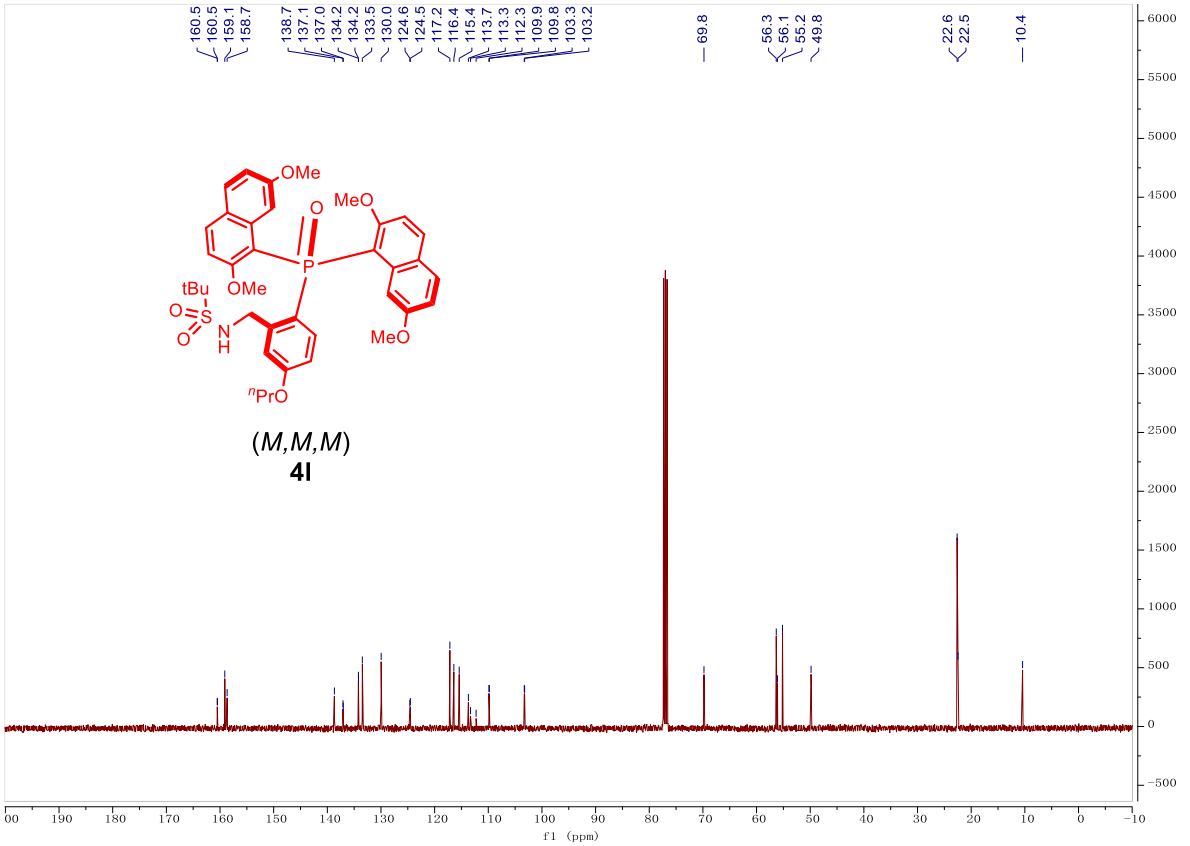

160.5
159.1
158.5
138.7
137.0
134.2
133.5
130.0
124.6
124.5
117.2
116.4
115.4
113.7
109.9
109.8
103.3
103.3
63.8
56.3
56.1
55.2
49.9
22.6
14.7
OMe
MeO
O
P
tBu
OMe
O
S
O
N
H
MeO
EtO
f1 (ppm)

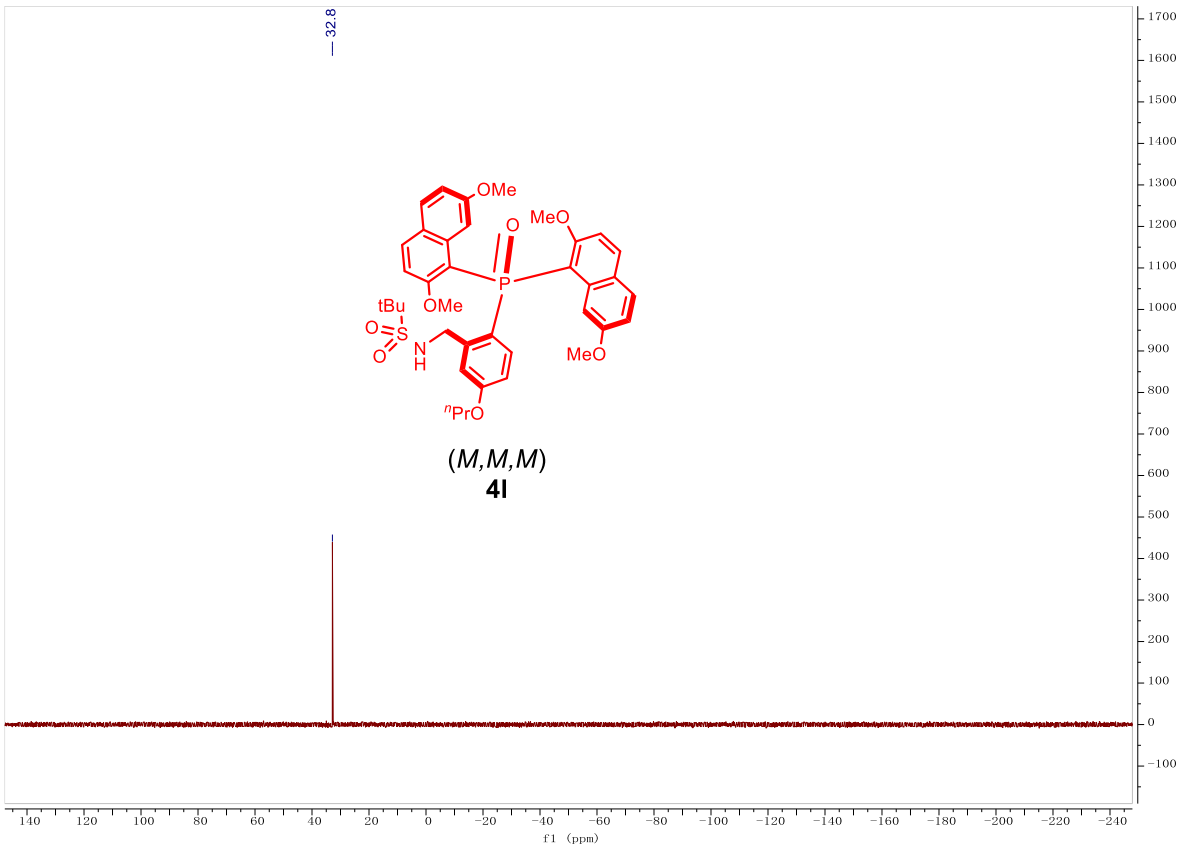
(*M*,*M*,*M*)
4k

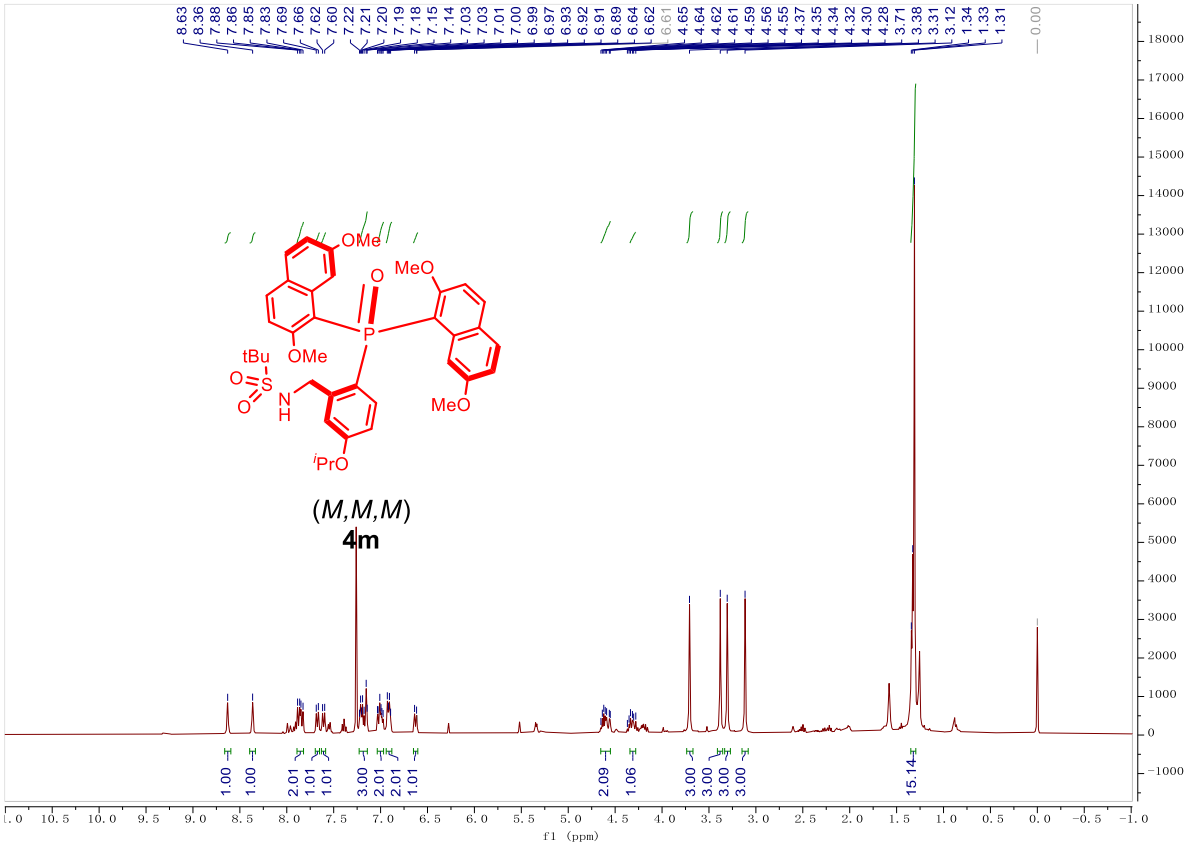

34.5
OMe
MeO
O
P
tBu
OMe
O
S
O
N
H
MeO
EtO
f1 (ppm)

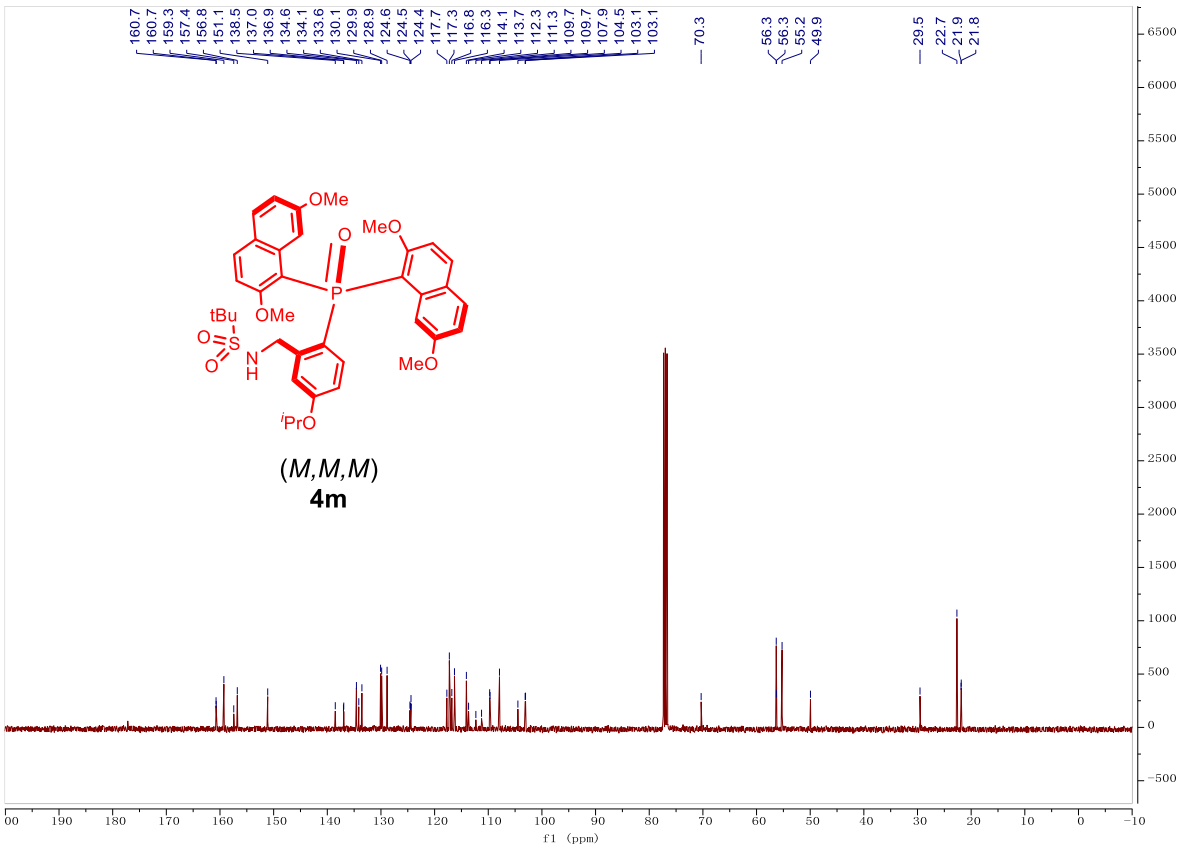
(*M*,*M*,*M*)
4k


OMe
MeO
O
P
tBu
OMe
O
S
O
N
H
MeO
nPrO
(M,M,M)
4l
f1 (ppm)

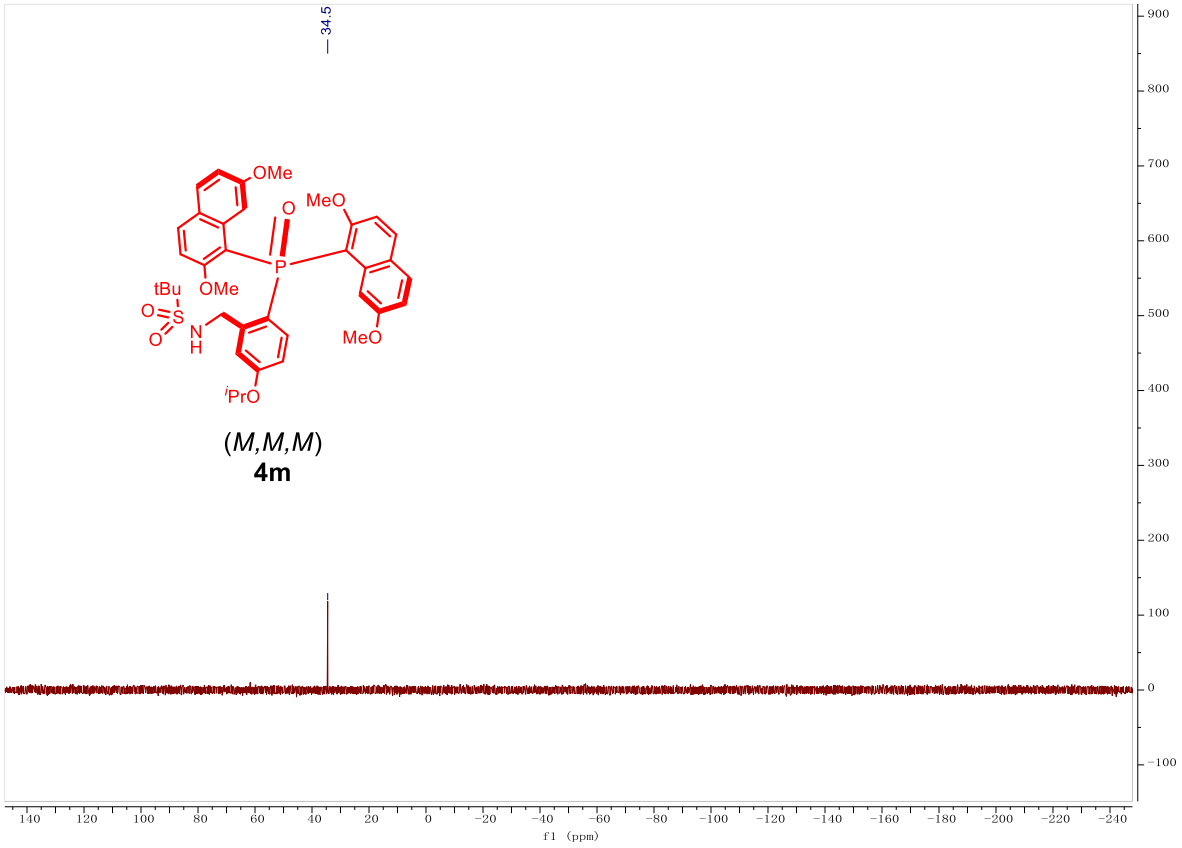

OMe
MeO
O
P
tBu
OMe
O
S
O
N
H
MeO
nPrO
(M,M,M)
4l
f1 (ppm)


32.8
OMe
MeO
O
P
tBu
OMe
O
S
O
N
H
MeO
nPrO
(M,M,M)
4l
f1 (ppm)

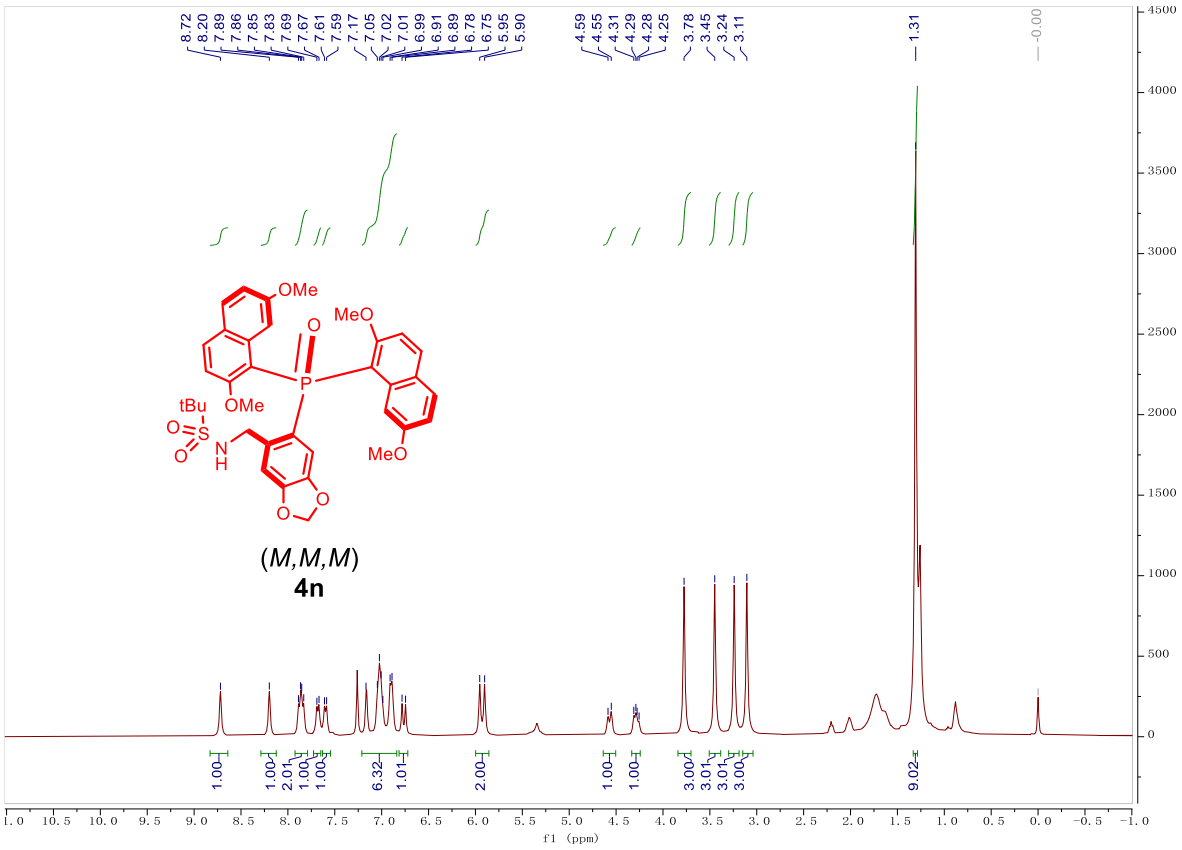

8.63
8.36
7.88
7.86
7.85
7.83
7.69
7.66
7.62
7.60
7.22
7.21
7.20
7.19
7.18
7.15
7.14
7.03
7.03
7.01
7.00
6.99
6.97
6.93
6.92
6.91
6.89
6.64
6.62
6.61
4.65
4.64
4.62
4.61
4.59
4.56
4.55
4.37
4.35
4.34
4.32
4.30
4.28
3.71
3.38
3.31
3.12
1.34
1.33
1.31
0.00
OMe
MeO
O
P
tBu
OMe
O
S
O
N
H
MeO
iPrO
(M,M,M)
4m
1.00
1.00
2.01
1.01
1.01
3.00
2.01
2.01
1.01
2.09
1.06
3.00
3.00
3.00
3.00
15.14
f1 (ppm)

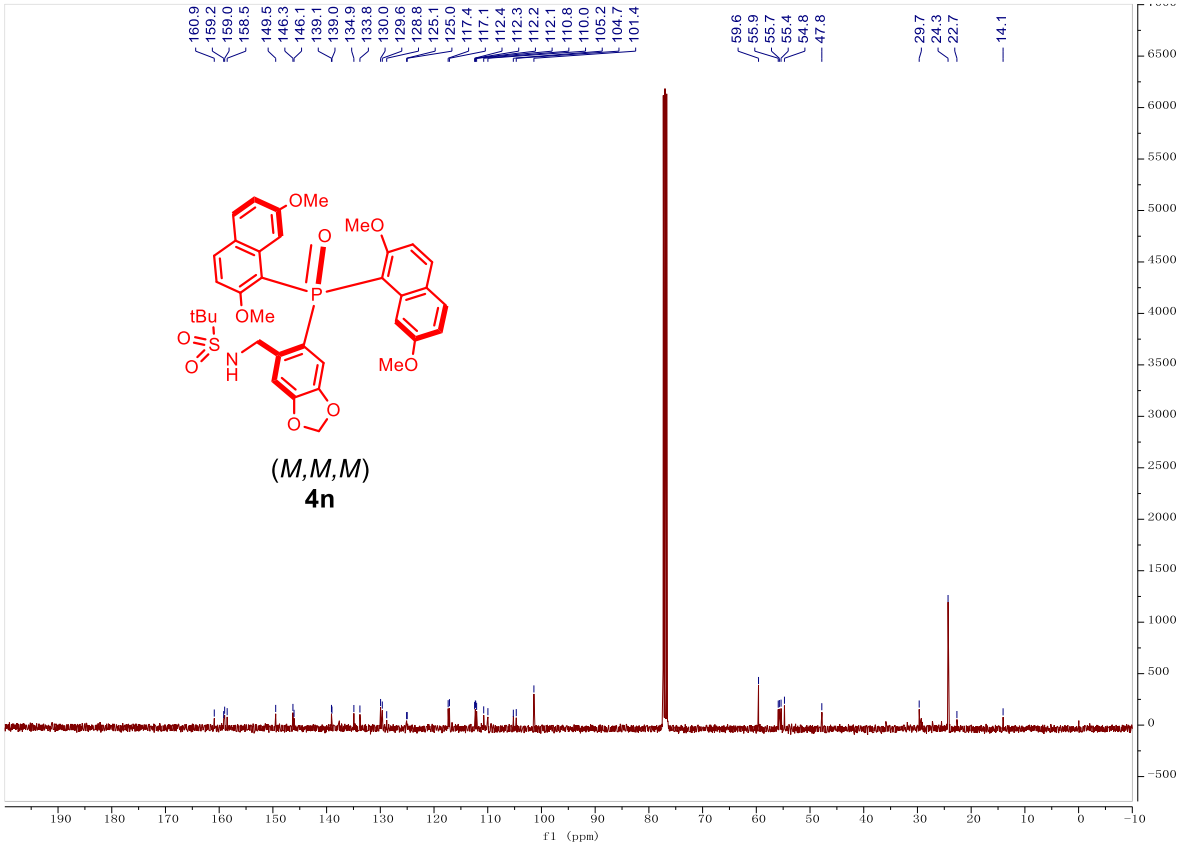

160.7
160.7
159.3
157.4
156.8
151.1
138.5
137.0
136.9
134.6
134.1
133.6
130.1
129.9
128.9
124.6
124.5
124.4
117.7
117.3
116.8
116.3
114.1
113.7
112.3
111.3
109.7
109.7
107.9
104.5
103.1
103.1
70.3
56.3
56.3
55.2
49.9
29.5
22.7
21.9
21.8
OMe
MeO
O
P
tBu
OMe
O
S
O
N
H
MeO
iPrO
f1 (ppm)

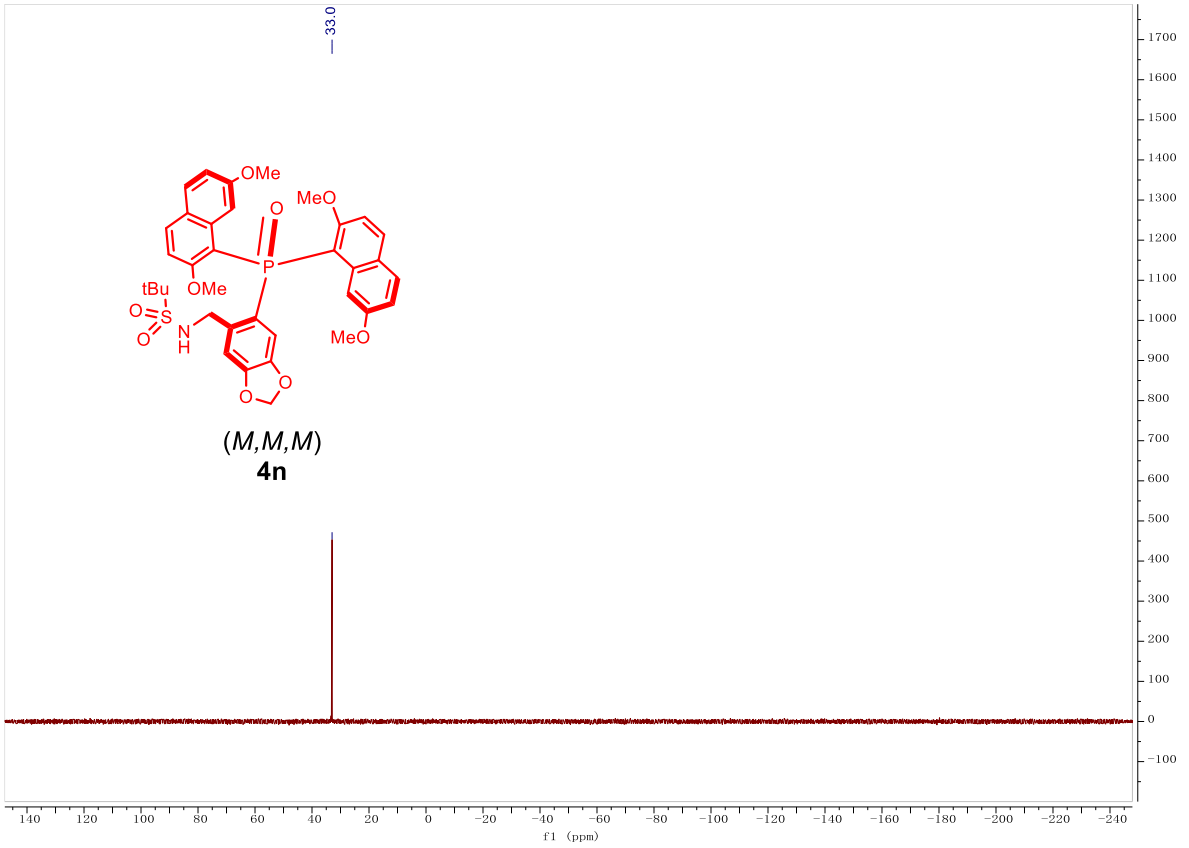
(*M*,*M*,*M*)
4m


34.5
OMe
MeO
O
P
tBu
OMe
O
S
O
N
H
MeO
iPrO
f1 (ppm)

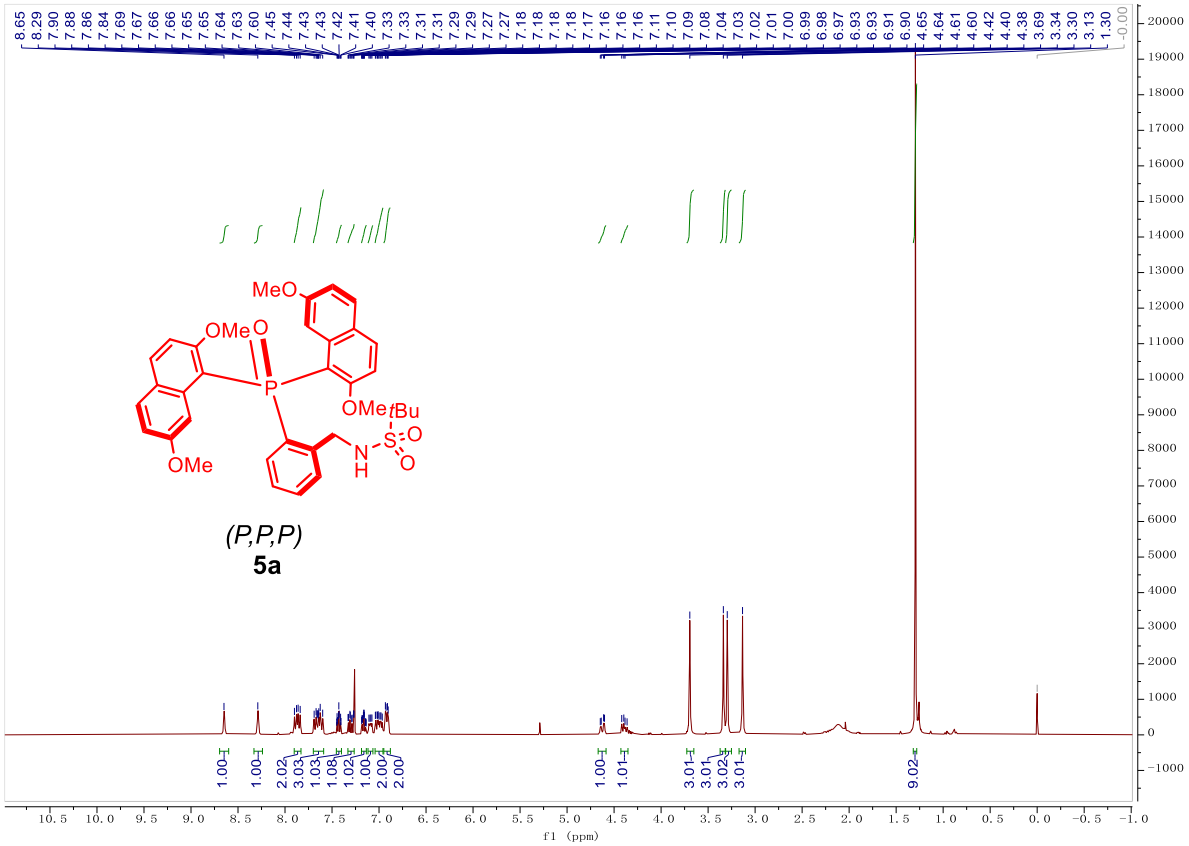
(*M*,*M*,*M*)
4m


8.72
8.20
7.89
7.86
7.85
7.83
7.69
7.67
7.61
7.59
7.17
7.05
7.02
7.01
6.99
6.91
6.89
6.78
6.75
5.95
5.90
4.59
4.55
4.31
4.29
4.28
4.25
3.78
3.45
3.24
3.11
1.31
-0.00
OMe
MeO
O
P
tBu
OMe
O
S
O
N
H
MeO
O
O
(M,M,M)
4n
1.00
1.00
2.01
1.00
1.00
6.32
1.01
2.00
1.00
1.00
3.00
3.01
3.01
3.00
9.02
f1 (ppm)

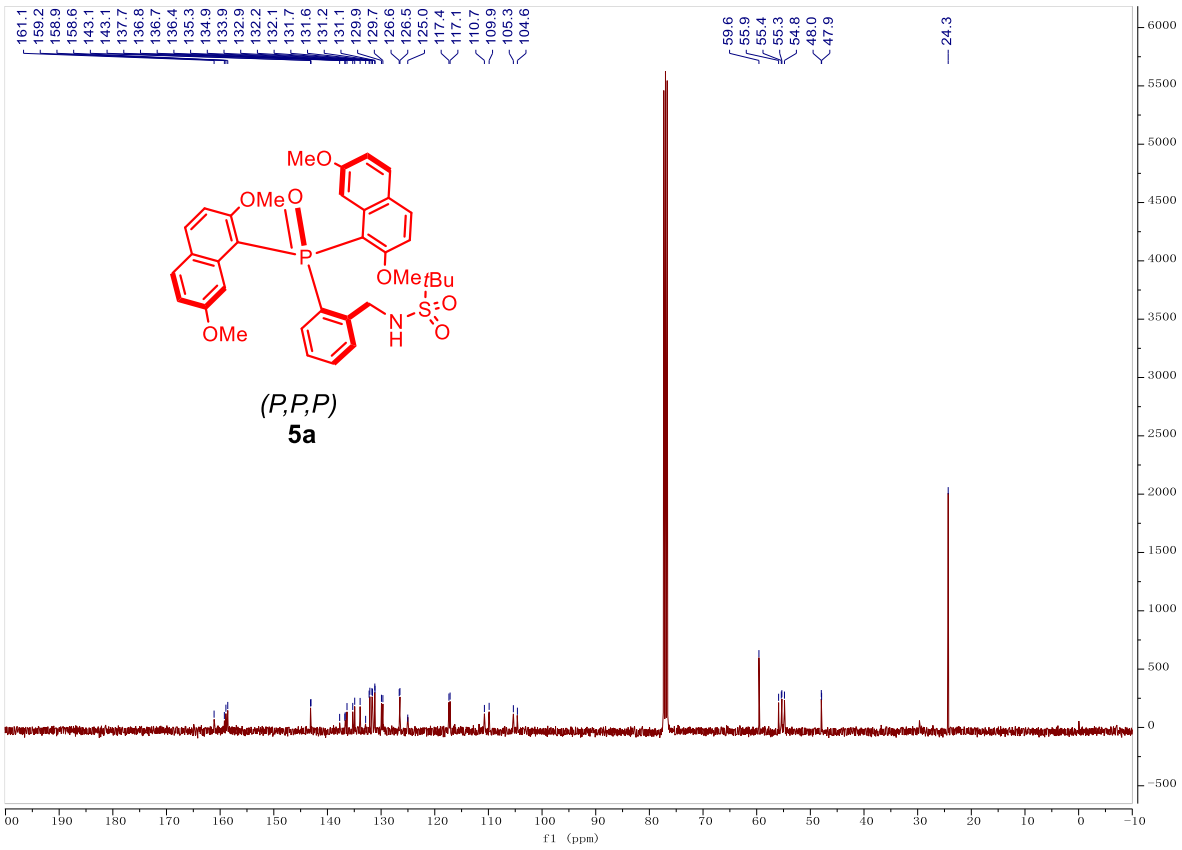

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139.1
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129.6
128.8
125.1
125.0
117.4
117.1
112.4
112.3
112.2
112.1
110.8
110.0
105.2
104.7
101.4
59.6
55.9
55.7
55.4
54.8
47.8
29.7
24.3
22.7
14.1
OMe
MeO
O
P
tBu
OMe
O
S
O
N
H
MeO
O
O
(M,M,M)
4n
f1 (ppm)


33.0
OMe
MeO
O
P
tBu
OMe
O
S
O
N
H
MeO
O
O
f1 (ppm)

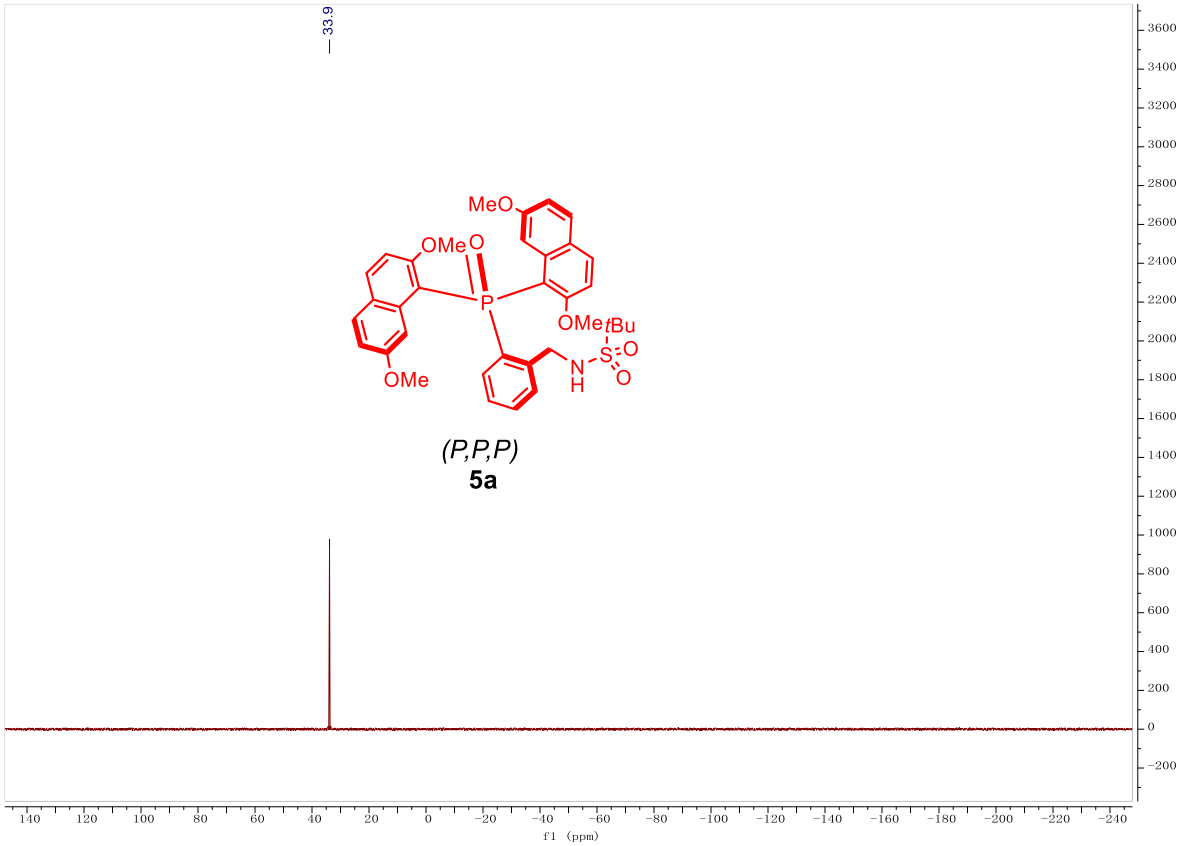
(*M*,*M*,*M*)
4n


MeO
OMe
O
P
OMe
tBu
N
H
S
O
O
OMe
f1 (ppm)

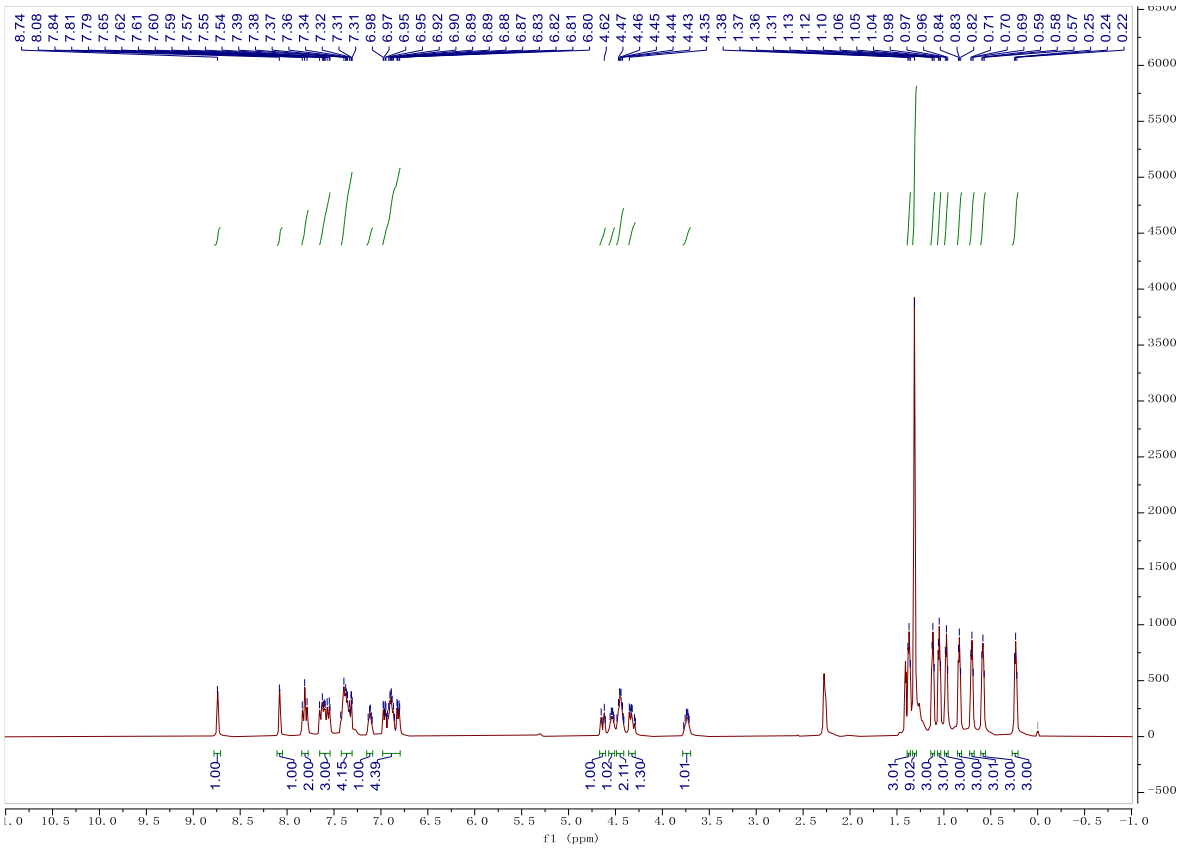
(*P*,*P*,*P*)
5a

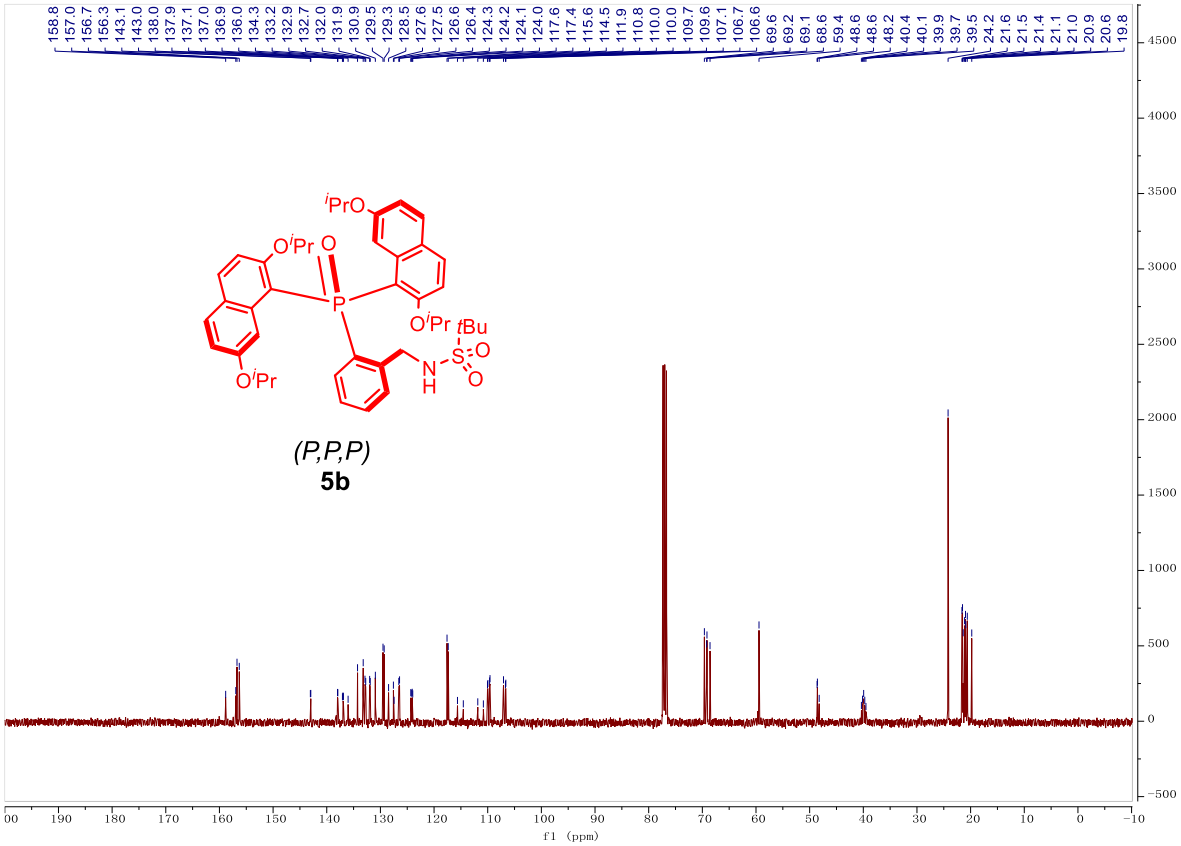

161.1
159.2
158.9
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143.1
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136.8
136.7
136.4
135.3
134.9
133.9
132.9
132.2
132.1
131.7
131.6
131.2
131.1
129.9
129.7
126.6
126.5
125.0
117.4
117.1
110.7
109.9
105.3
104.6
59.6
55.9
55.4
55.3
54.8
48.0
47.9
24.3
MeO
OMe
O
P
OMe
tBu
N
H
S
O
O
OMe
f1 (ppm)

(P,P,P)
5a

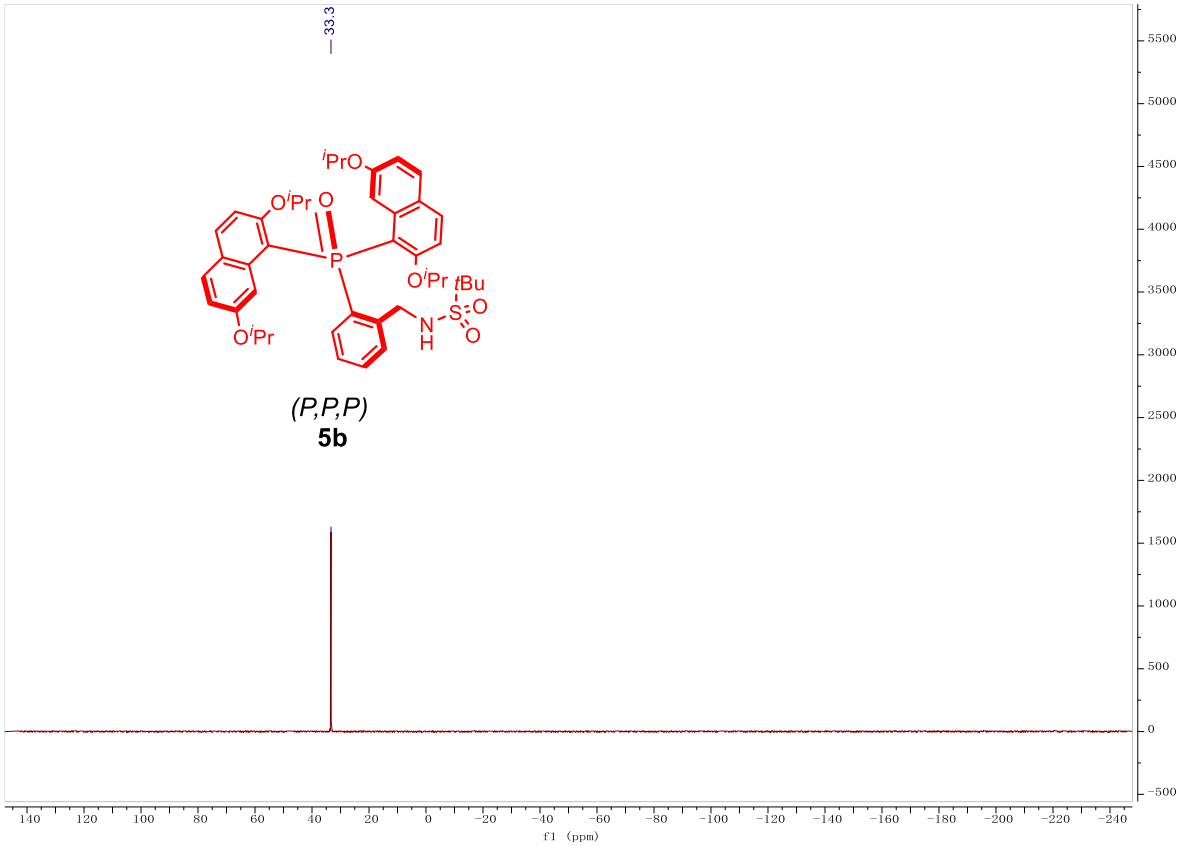

33.9
MeO
OMe
O
P
OMe
tBu
N
H
S
O
O
OMe
f1 (ppm)

(P,P,P)
5a

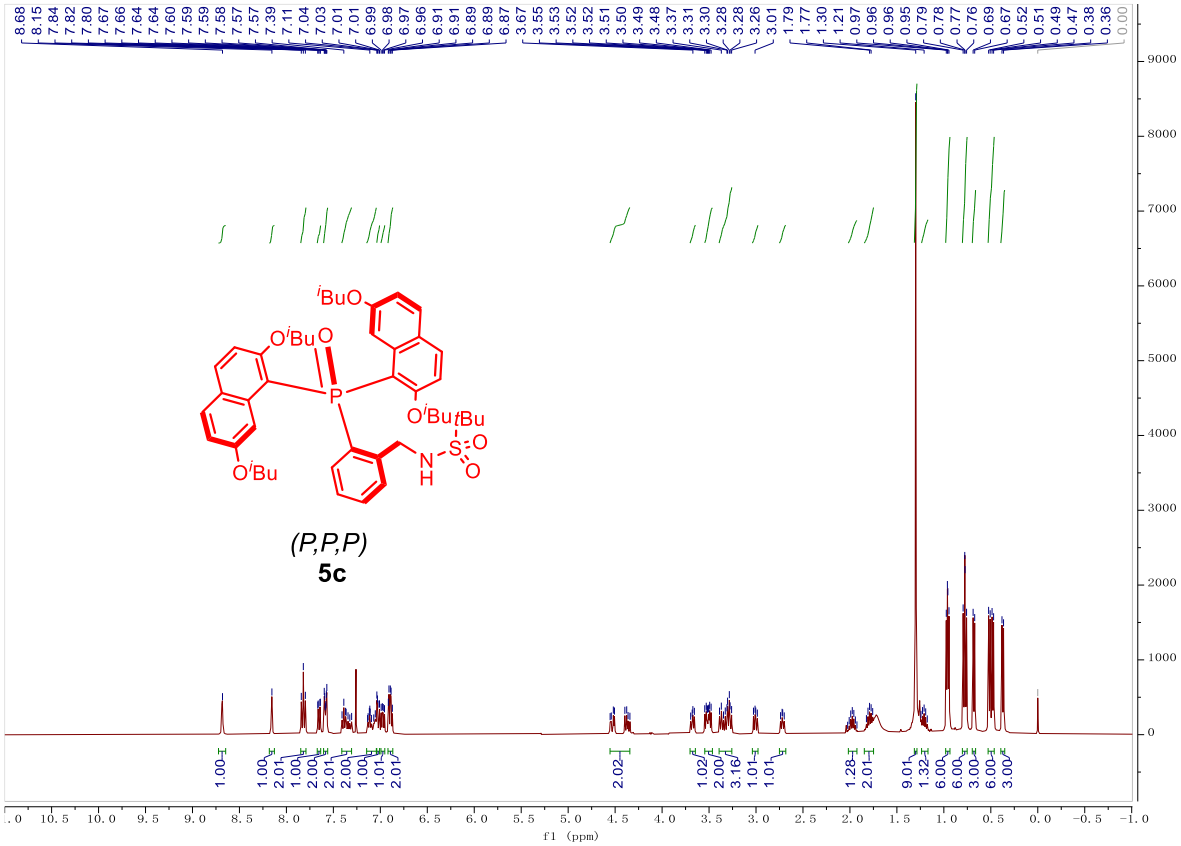




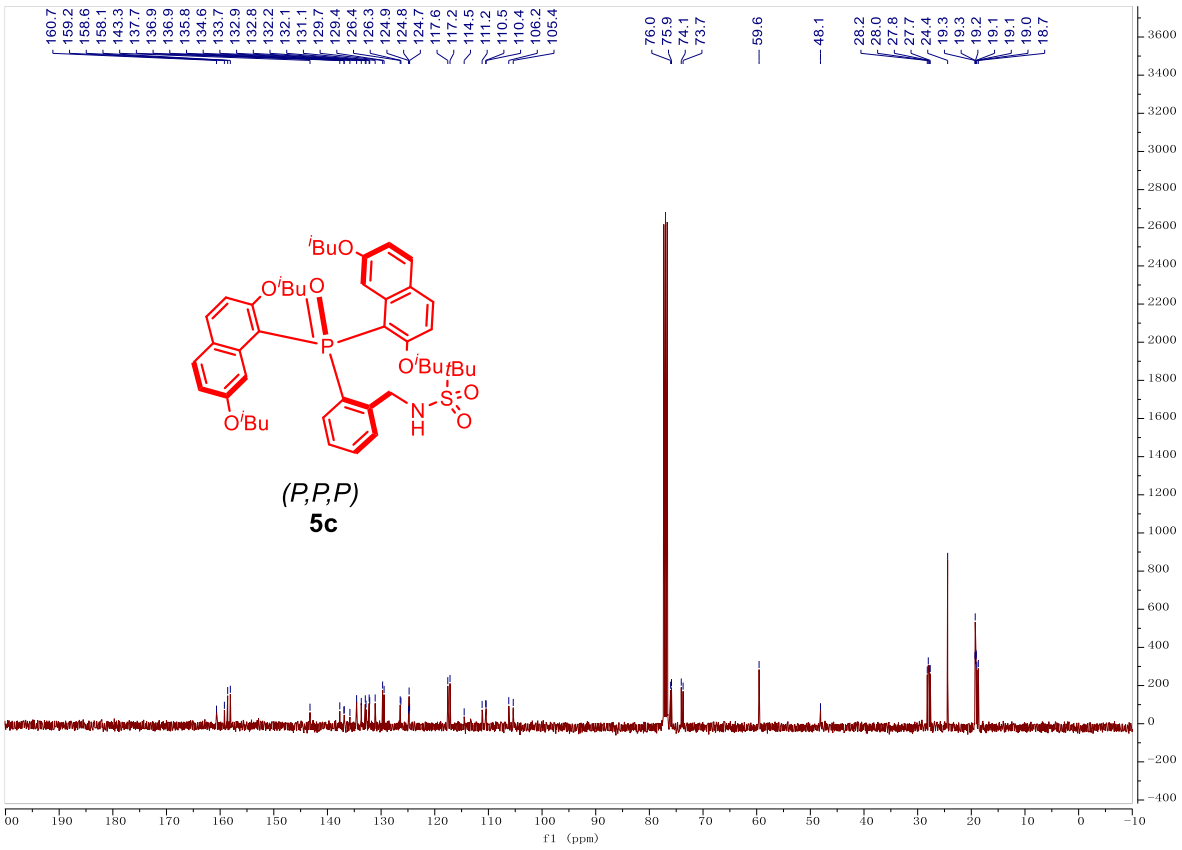
(P,P,P)
5b


33.3
iPrO
OiPr
O
P
OiPr
tBu
N
H
S
O
O
OiPr
f1 (ppm)

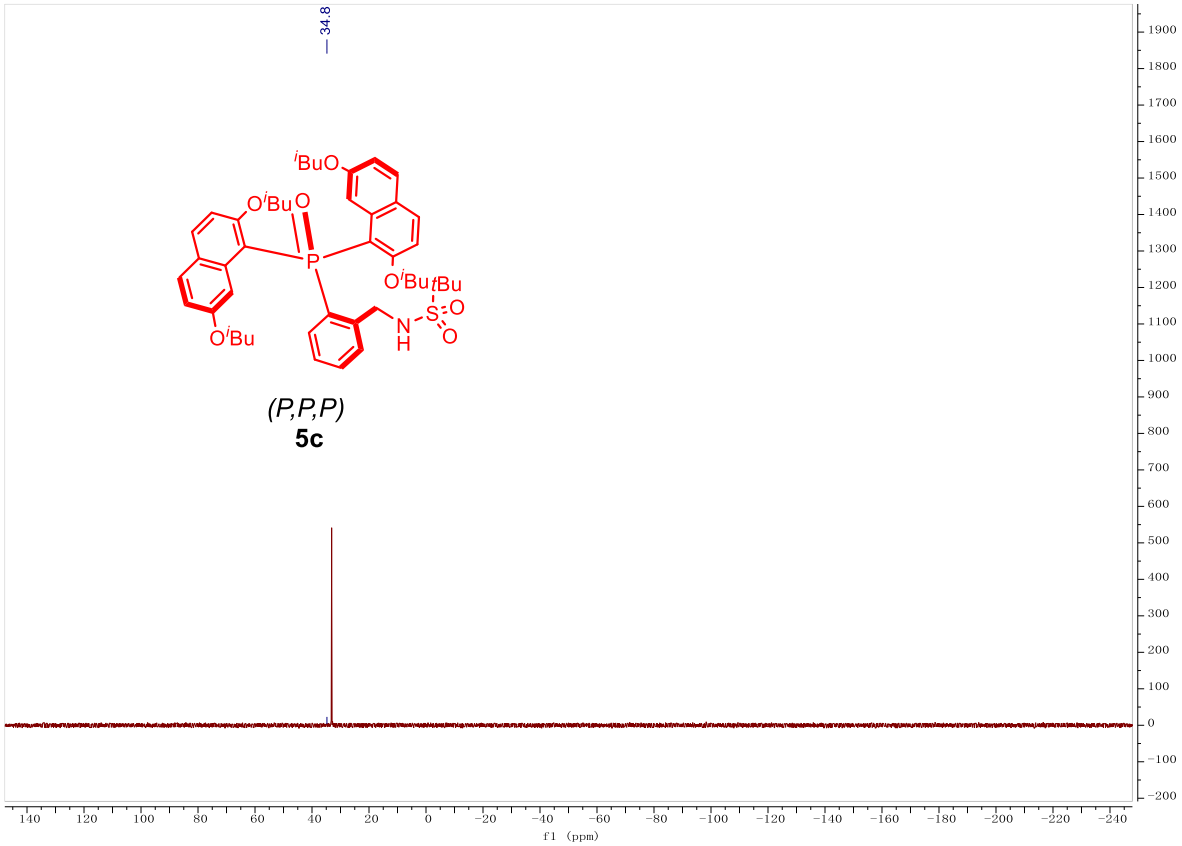
(P,P,P)
5b


iBuO
OiBu
O
P
OiBu
tBu
N
H
S
O
O
OiBu
f1 (ppm)

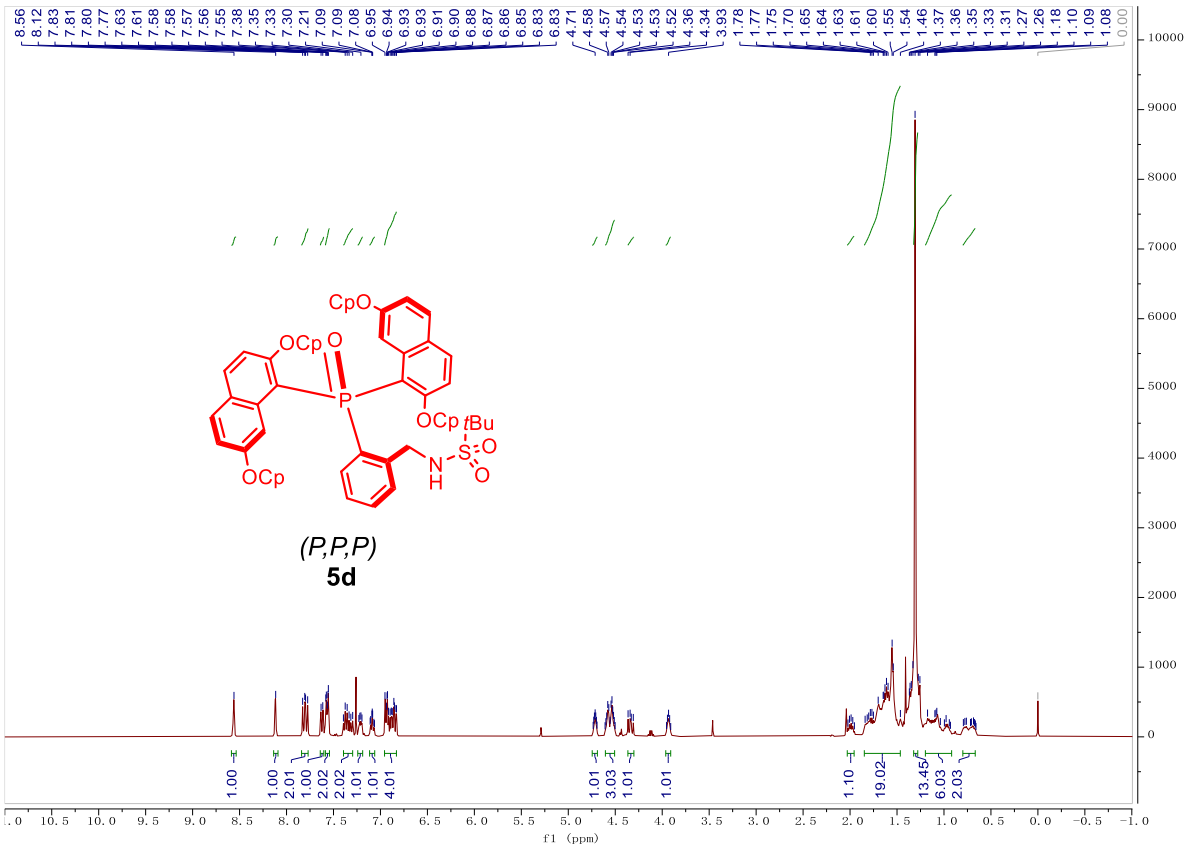
(P,P,P)
5c


160.7
159.2
158.6
158.1
143.3
137.7
136.9
136.9
135.8
134.6
133.7
132.9
132.8
132.2
132.1
131.1
129.7
129.4
126.4
126.3
124.9
124.8
124.7
117.6
117.2
114.5
111.2
110.5
110.4
106.2
105.4
76.0
75.9
74.1
73.7
59.6
48.1
28.2
28.0
27.8
27.7
24.4
19.3
19.3
19.2
19.1
19.1
19.0
18.7
iBuO
OiBu
O
P
OiBu
tBu
S
O
O
N
H
OiBu
f1 (ppm)

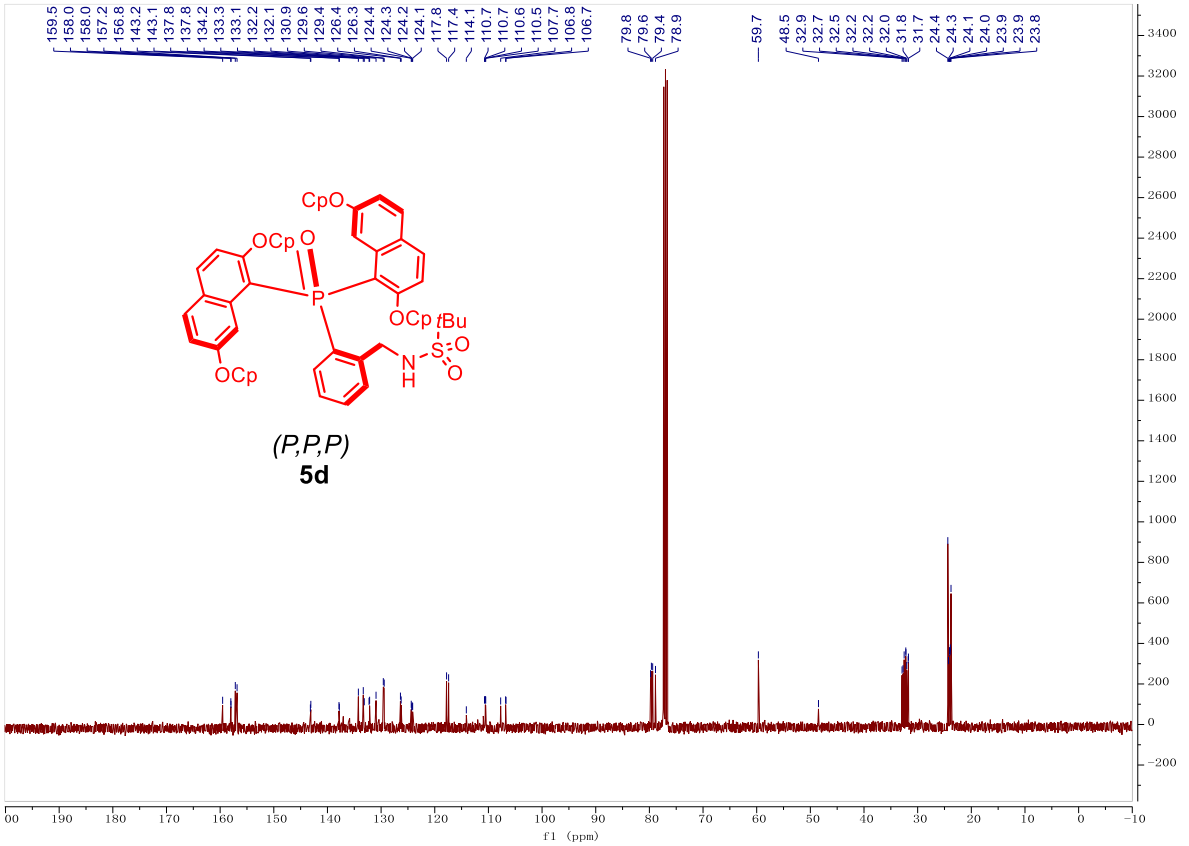
(P,P,P)
5c


34.8
iBuO
OiBu
O
P
OiBu
tBu
S
O
O
N
H
OiBu
f1 (ppm)

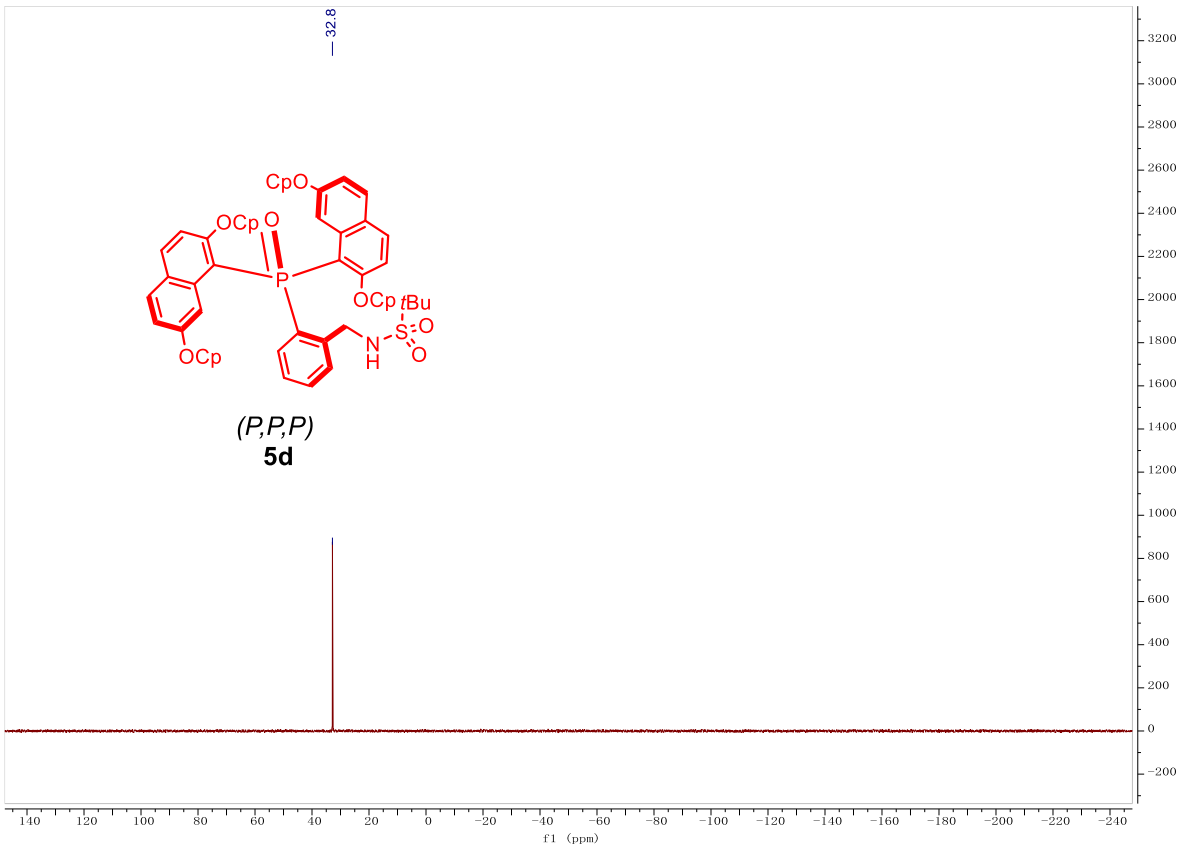
(P,P,P)
5c



(P,P,P)
5d



(P,P,P)
5d



2. X-ray Diffraction Data for 4a

Table S1. Crystal data and structure refinement for **4a**.

Identification code	240705b	
Empirical formula	C35.50 H39 Cl N O7 P S	
Formula weight	690.16	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 10.8152(10) Å	α= 90°.
	b = 18.4090(13) Å	β= 92.353(8)°.
	c = 17.7931(15) Å	γ = 90°.
Volume	3539.6(5) $Å^3$	
Z	4	
Density (calculated)	1.294 Mg/m^3	
Absorption coefficient	0.260 mm^{-1}	
F(000)	1450	
Crystal size	0.20 x 0.18 x 0.10 mm^3	

Theta range for data collection	3.44 to 25.05°.
Index ranges	-9<=h<=12, -21<=k<=21, -21<=l<=21
Reflections collected	17384
Independent reflections	10804 [R(int) = 0.0526]
Completeness to theta = 25.05°	99.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9745 and 0.9499
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10804 / 29 / 860
Goodness-of-fit on F^2	1.019
Final R indices [I>2sigma(I)]	R1 = 0.0765, wR2 = 0.1731
R indices (all data)	R1 = 0.1112, wR2 = 0.1977
Absolute structure parameter	0.03(11)
Largest diff. peak and hole	0.384 and -0.262 e.$Å^{-3}$

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 240705b. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	7766(5)	9341(3)	593(3)	56(1)
N(2)	7399(5)	6021(3)	5544(3)	58(1)
O(1)	5838(4)	8040(2)	1477(2)	53(1)
O(2)	4248(5)	6760(3)	-332(3)	64(1)
O(3)	3027(6)	8008(4)	3419(3)	98(2)
O(4)	6507(5)	7436(3)	-741(3)	69(1)
O(5)	6506(7)	5916(3)	3023(3)	89(2)
O(6)	9366(5)	10084(3)	1167(3)	91(2)
O(7)	9640(5)	9609(3)	-87(3)	70(1)
O(8)	9281(4)	7252(2)	6367(2)	52(1)
O(9)	8528(5)	7892(2)	4114(3)	70(1)
O(10)	8518(7)	9318(3)	7935(3)	92(2)
O(11)	10806(5)	8551(2)	4616(3)	62(1)
O(12)	12070(6)	7303(4)	8430(3)	103(2)
O(13)	5966(6)	5291(4)	6213(3)	100(2)
O(14)	5402(5)	5679(3)	4946(3)	73(1)
P(1)	5377(1)	7683(1)	775(1)	45(1)
P(2)	9705(2)	7624(1)	5673(1)	45(1)
S(1)	9222(2)	9505(1)	656(1)	59(1)
S(2)	5968(2)	5840(1)	5664(1)	60(1)
Cl(1)	3469(15)	4284(7)	7861(8)	136(2)
Cl(2)	1552(14)	5102(9)	7143(8)	170(3)
Cl(3)	9429(9)	5835(4)	6707(5)	136(2)
Cl(4)	8312(11)	5686(7)	8053(6)	170(3)
Cl(5)	3832(12)	4484(6)	8117(6)	136(2)
Cl(6)	5975(11)	5196(7)	7828(6)	170(3)
C(1)	7271(6)	8784(3)	61(4)	61(2)
C(2)	5935(6)	8885(3)	-120(4)	53(2)
C(3)	5014(6)	8400(3)	96(4)	46(1)
C(4)	3799(7)	8522(4)	-105(4)	60(2)
C(5)	3481(8)	9158(4)	-521(4)	77(2)
C(6)	4355(8)	9626(4)	-729(4)	74(2)
C(7)	5596(8)	9488(4)	-562(4)	68(2)
C(8)	3957(5)	7166(3)	883(3)	41(1)

C(9)	3616(6)	6696(3)	297(3)	51(2)
C(10)	2608(7)	6210(4)	342(5)	67(2)
C(11)	1991(8)	6204(4)	986(5)	78(2)
C(12)	2248(6)	6682(4)	1591(4)	66(2)
C(13)	3259(6)	7169(3)	1556(3)	47(2)
C(14)	3529(6)	7636(4)	2173(3)	57(2)
C(15)	2815(7)	7620(5)	2792(4)	65(2)
C(16)	1821(9)	7143(6)	2830(5)	89(3)
C(17)	1520(8)	6699(5)	2245(5)	80(2)
C(18)	4267(9)	6189(5)	-861(5)	90(3)
C(19)	4048(11)	8473(7)	3438(6)	124(4)
C(20)	6532(5)	7024(3)	489(3)	42(1)
C(21)	7010(7)	6984(3)	-216(4)	59(2)
C(22)	7985(7)	6493(4)	-364(5)	69(2)
C(23)	8471(7)	6066(4)	195(5)	74(2)
C(24)	8004(7)	6065(4)	906(5)	65(2)
C(25)	7005(6)	6535(3)	1063(4)	51(2)
C(26)	6491(6)	6478(3)	1794(4)	58(2)
C(27)	6970(8)	6000(4)	2325(5)	76(2)
C(28)	7980(8)	5560(4)	2161(6)	81(2)
C(29)	8443(7)	5595(4)	1481(6)	78(2)
C(30)	7030(10)	7469(6)	-1465(4)	106(3)
C(31)	5386(9)	6286(5)	3166(5)	91(3)
C(32)	10081(8)	8728(5)	1054(5)	80(2)
C(33)	9361(11)	8473(8)	1739(6)	150(6)
C(34)	11363(10)	9005(7)	1257(6)	141(5)
C(35)	10184(9)	8157(5)	479(6)	110(3)
C(36)	7766(6)	6519(3)	4944(4)	56(2)
C(37)	9101(6)	6417(3)	4776(3)	47(2)
C(38)	10028(6)	6913(3)	4991(3)	46(1)
C(39)	11232(7)	6775(3)	4839(4)	58(2)
C(40)	11525(8)	6152(4)	4439(4)	70(2)
C(41)	10669(8)	5682(4)	4220(4)	71(2)
C(42)	9449(7)	5810(3)	4353(4)	60(2)
C(43)	8528(6)	8288(3)	5376(4)	48(2)
C(44)	8042(6)	8336(3)	4639(4)	55(2)
C(45)	7065(7)	8830(4)	4462(5)	73(2)
C(46)	6610(8)	9250(4)	5005(6)	78(2)
C(47)	7039(7)	9228(3)	5747(5)	64(2)

C(48)	8055(6)	8756(3)	5935(4)	54(2)
C(49)	8564(7)	8779(3)	6685(4)	64(2)
C(50)	8105(8)	9253(4)	7206(5)	72(2)
C(51)	7081(9)	9704(5)	7005(6)	92(3)
C(52)	6580(8)	9683(4)	6292(6)	82(2)
C(53)	7967(9)	7831(5)	3388(4)	94(3)
C(54)	9613(9)	8918(5)	8141(4)	87(3)
C(55)	11128(5)	8146(3)	5842(3)	42(1)
C(56)	11447(6)	8599(3)	5265(4)	54(2)
C(57)	12506(7)	9080(4)	5386(5)	68(2)
C(58)	13149(8)	9073(4)	6021(5)	76(2)
C(59)	12882(7)	8607(4)	6604(4)	64(2)
C(60)	11857(6)	8129(3)	6530(4)	52(2)
C(61)	11583(6)	7670(4)	7144(4)	60(2)
C(62)	12290(7)	7692(5)	7802(4)	72(2)
C(63)	13338(9)	8138(6)	7857(5)	87(3)
C(64)	13617(8)	8596(5)	7282(5)	88(3)
C(65)	10792(8)	9127(4)	4088(4)	78(2)
C(66)	5176(8)	6622(5)	6042(4)	77(2)
C(67)	4999(9)	7190(6)	5439(5)	104(3)
C(68)	5950(11)	6945(7)	6688(5)	132(4)
C(69)	3929(9)	6344(6)	6300(6)	109(3)
C(70)	11012(10)	6850(7)	8420(5)	112(3)
C(71)	2300(60)	4280(20)	7170(40)	360(30)
C(72)	8380(50)	6230(20)	7272(18)	360(30)
C(73)	5330(30)	4610(30)	8450(20)	360(30)

Table S3. Bond lengths [Å] and angles [°] for 240705b.

N(1)-C(1)	1.481(8)
N(1)-S(1)	1.603(6)
N(1)-H(1)	0.9000
N(2)-C(36)	1.474(8)
N(2)-S(2)	1.606(6)
N(2)-H(2)	0.9000
O(1)-P(1)	1.480(4)
O(2)-C(9)	1.340(7)
O(2)-C(18)	1.413(9)
O(3)-C(15)	1.336(9)
O(3)-C(19)	1.397(12)
O(4)-C(21)	1.350(8)
O(4)-C(30)	1.429(9)
O(5)-C(27)	1.368(10)
O(5)-C(31)	1.423(11)
O(6)-S(1)	1.405(6)
O(7)-S(1)	1.427(5)
O(8)-P(2)	1.500(4)
O(9)-C(44)	1.362(8)
O(9)-C(53)	1.409(8)
O(10)-C(50)	1.358(9)
O(10)-C(54)	1.430(11)
O(11)-C(56)	1.325(8)
O(11)-C(65)	1.416(8)
O(12)-C(62)	1.358(9)
O(12)-C(70)	1.415(12)
O(13)-S(2)	1.407(6)
O(14)-S(2)	1.425(5)
P(1)-C(3)	1.822(6)
P(1)-C(8)	1.824(6)
P(1)-C(20)	1.827(6)
P(2)-C(38)	1.827(6)
P(2)-C(43)	1.828(6)
P(2)-C(55)	1.829(6)
S(1)-C(32)	1.833(8)
S(2)-C(66)	1.818(8)
Cl(1)-C(71)	1.720(10)

Cl(2)-C(71)	1.716(10)
Cl(3)-C(72)	1.707(10)
Cl(4)-C(72)	1.714(10)
Cl(5)-C(73)	1.721(10)
Cl(6)-C(73)	1.719(10)
C(1)-C(2)	1.479(9)
C(1)-H(1C)	0.9700
C(1)-H(1D)	0.9700
C(2)-C(7)	1.400(10)
C(2)-C(3)	1.403(9)
C(3)-C(4)	1.366(9)
C(4)-C(5)	1.419(10)
C(4)-H(4)	0.9300
C(5)-C(6)	1.342(11)
C(5)-H(5)	0.9300
C(6)-C(7)	1.386(11)
C(6)-H(6)	0.9300
C(7)-H(7)	0.9300
C(8)-C(9)	1.392(8)
C(8)-C(13)	1.442(8)
C(9)-C(10)	1.415(9)
C(10)-C(11)	1.348(10)
C(10)-H(10)	0.9300
C(11)-C(12)	1.409(10)
C(11)-H(11)	0.9300
C(12)-C(13)	1.418(9)
C(12)-C(17)	1.433(11)
C(13)-C(14)	1.415(9)
C(14)-C(15)	1.371(9)
C(14)-H(14)	0.9300
C(15)-C(16)	1.393(12)
C(16)-C(17)	1.352(12)
C(16)-H(16)	0.9300
C(17)-H(17)	0.9300
C(18)-H(18A)	0.9600
C(18)-H(18B)	0.9600
C(18)-H(18C)	0.9600
C(19)-H(19A)	0.9600
C(19)-H(19B)	0.9600

C(19)-H(19C)	0.9600
C(20)-C(21)	1.378(9)
C(20)-C(25)	1.440(8)
C(21)-C(22)	1.423(10)
C(22)-C(23)	1.356(10)
C(22)-H(22)	0.9300
C(23)-C(24)	1.382(10)
C(23)-H(23)	0.9300
C(24)-C(29)	1.408(11)
C(24)-C(25)	1.420(9)
C(25)-C(26)	1.440(9)
C(26)-C(27)	1.378(9)
C(26)-H(26)	0.9300
C(27)-C(28)	1.399(11)
C(28)-C(29)	1.329(11)
C(28)-H(28)	0.9300
C(29)-H(29)	0.9300
C(30)-H(30A)	0.9600
C(30)-H(30B)	0.9600
C(30)-H(30C)	0.9600
C(31)-H(31A)	0.9600
C(31)-H(31B)	0.9600
C(31)-H(31C)	0.9600
C(32)-C(35)	1.474(12)
C(32)-C(34)	1.507(14)
C(32)-C(33)	1.545(12)
C(33)-H(33A)	0.9600
C(33)-H(33B)	0.9600
C(33)-H(33C)	0.9600
C(34)-H(34A)	0.9600
C(34)-H(34B)	0.9600
C(34)-H(34C)	0.9600
C(35)-H(35A)	0.9600
C(35)-H(35B)	0.9600
C(35)-H(35C)	0.9600
C(36)-C(37)	1.498(9)
C(36)-H(36A)	0.9700
C(36)-H(36B)	0.9700
C(37)-C(38)	1.398(9)

C(37)-C(42)	1.407(9)
C(38)-C(39)	1.365(9)
C(39)-C(40)	1.393(10)
C(39)-H(39)	0.9300
C(40)-C(41)	1.316(11)
C(40)-H(40)	0.9300
C(41)-C(42)	1.370(10)
C(41)-H(41)	0.9300
C(42)-H(42)	0.9300
C(43)-C(44)	1.396(9)
C(43)-C(48)	1.426(9)
C(44)-C(45)	1.419(10)
C(45)-C(46)	1.346(11)
C(45)-H(45)	0.9300
C(46)-C(47)	1.382(11)
C(46)-H(46)	0.9300
C(47)-C(52)	1.389(11)
C(47)-C(48)	1.430(9)
C(48)-C(49)	1.424(9)
C(49)-C(50)	1.379(10)
C(49)-H(49)	0.9300
C(50)-C(51)	1.418(12)
C(51)-C(52)	1.359(12)
C(51)-H(51)	0.9300
C(52)-H(52)	0.9300
C(53)-H(53A)	0.9600
C(53)-H(53B)	0.9600
C(53)-H(53C)	0.9600
C(54)-H(54A)	0.9600
C(54)-H(54B)	0.9600
C(54)-H(54C)	0.9600
C(55)-C(56)	1.377(8)
C(55)-C(60)	1.430(8)
C(56)-C(57)	1.457(10)
C(57)-C(58)	1.302(10)
C(57)-H(57)	0.9300
C(58)-C(59)	1.387(11)
C(58)-H(58)	0.9300
C(59)-C(60)	1.417(10)

C(59)-C(64)	1.417(11)
C(60)-C(61)	1.422(9)
C(61)-C(62)	1.372(9)
C(61)-H(61)	0.9300
C(62)-C(63)	1.400(12)
C(63)-C(64)	1.368(12)
C(63)-H(63)	0.9300
C(64)-H(64)	0.9300
C(65)-H(65A)	0.9600
C(65)-H(65B)	0.9600
C(65)-H(65C)	0.9600
C(66)-C(67)	1.503(12)
C(66)-C(68)	1.516(12)
C(66)-C(69)	1.531(12)
C(67)-H(67A)	0.9600
C(67)-H(67B)	0.9600
C(67)-H(67C)	0.9600
C(68)-H(68A)	0.9600
C(68)-H(68B)	0.9600
C(68)-H(68C)	0.9600
C(69)-H(69A)	0.9600
C(69)-H(69B)	0.9600
C(69)-H(69C)	0.9600
C(70)-H(70A)	0.9600
C(70)-H(70B)	0.9600
C(70)-H(70C)	0.9600
C(71)-H(71A)	0.9700
C(71)-H(71B)	0.9700
C(72)-H(72A)	0.9700
C(72)-H(72B)	0.9700
C(73)-H(73A)	0.9700
C(73)-H(73B)	0.9700

C(1)-N(1)-S(1)	120.2(4)
C(1)-N(1)-H(1)	106.7
S(1)-N(1)-H(1)	107.1
C(36)-N(2)-S(2)	121.0(4)
C(36)-N(2)-H(2)	106.8
S(2)-N(2)-H(2)	106.6

C(9)-O(2)-C(18)	120.9(6)
C(15)-O(3)-C(19)	117.2(7)
C(21)-O(4)-C(30)	119.2(6)
C(27)-O(5)-C(31)	117.1(6)
C(44)-O(9)-C(53)	120.9(6)
C(50)-O(10)-C(54)	115.8(6)
C(56)-O(11)-C(65)	121.3(5)
C(62)-O(12)-C(70)	118.0(7)
O(1)-P(1)-C(3)	107.1(3)
O(1)-P(1)-C(8)	113.5(3)
C(3)-P(1)-C(8)	106.7(3)
O(1)-P(1)-C(20)	108.6(3)
C(3)-P(1)-C(20)	115.3(3)
C(8)-P(1)-C(20)	105.7(3)
O(8)-P(2)-C(38)	107.1(3)
O(8)-P(2)-C(43)	108.1(3)
C(38)-P(2)-C(43)	115.9(3)
O(8)-P(2)-C(55)	112.8(3)
C(38)-P(2)-C(55)	107.7(3)
C(43)-P(2)-C(55)	105.5(3)
O(6)-S(1)-O(7)	117.8(4)
O(6)-S(1)-N(1)	105.7(3)
O(7)-S(1)-N(1)	108.0(3)
O(6)-S(1)-C(32)	107.5(4)
O(7)-S(1)-C(32)	106.8(4)
N(1)-S(1)-C(32)	111.2(3)
O(13)-S(2)-O(14)	117.4(4)
O(13)-S(2)-N(2)	105.7(3)
O(14)-S(2)-N(2)	107.7(3)
O(13)-S(2)-C(66)	107.4(4)
O(14)-S(2)-C(66)	107.8(4)
N(2)-S(2)-C(66)	110.9(4)
C(2)-C(1)-N(1)	112.1(5)
C(2)-C(1)-H(1C)	109.2
N(1)-C(1)-H(1C)	109.2
C(2)-C(1)-H(1D)	109.2
N(1)-C(1)-H(1D)	109.2
H(1C)-C(1)-H(1D)	107.9
C(7)-C(2)-C(3)	119.1(6)

C(7)-C(2)-C(1)	116.9(6)
C(3)-C(2)-C(1)	124.0(6)
C(4)-C(3)-C(2)	120.6(6)
C(4)-C(3)-P(1)	118.2(5)
C(2)-C(3)-P(1)	120.5(5)
C(3)-C(4)-C(5)	118.8(7)
C(3)-C(4)-H(4)	120.6
C(5)-C(4)-H(4)	120.6
C(6)-C(5)-C(4)	121.0(8)
C(6)-C(5)-H(5)	119.5
C(4)-C(5)-H(5)	119.5
C(5)-C(6)-C(7)	120.7(7)
C(5)-C(6)-H(6)	119.7
C(7)-C(6)-H(6)	119.7
C(6)-C(7)-C(2)	119.6(7)
C(6)-C(7)-H(7)	120.2
C(2)-C(7)-H(7)	120.2
C(9)-C(8)-C(13)	119.6(5)
C(9)-C(8)-P(1)	116.4(4)
C(13)-C(8)-P(1)	123.8(4)
O(2)-C(9)-C(8)	116.2(6)
O(2)-C(9)-C(10)	121.6(6)
C(8)-C(9)-C(10)	122.1(6)
C(11)-C(10)-C(9)	117.5(7)
C(11)-C(10)-H(10)	121.2
C(9)-C(10)-H(10)	121.2
C(10)-C(11)-C(12)	123.7(7)
C(10)-C(11)-H(11)	118.1
C(12)-C(11)-H(11)	118.1
C(11)-C(12)-C(13)	119.3(7)
C(11)-C(12)-C(17)	122.5(7)
C(13)-C(12)-C(17)	118.2(7)
C(14)-C(13)-C(12)	119.1(6)
C(14)-C(13)-C(8)	123.3(5)
C(12)-C(13)-C(8)	117.6(6)
C(15)-C(14)-C(13)	120.4(7)
C(15)-C(14)-H(14)	119.8
C(13)-C(14)-H(14)	119.8
O(3)-C(15)-C(14)	125.2(7)

O(3)-C(15)-C(16)	113.8(7)
C(14)-C(15)-C(16)	120.9(8)
C(17)-C(16)-C(15)	120.4(8)
C(17)-C(16)-H(16)	119.8
C(15)-C(16)-H(16)	119.8
C(16)-C(17)-C(12)	121.0(7)
C(16)-C(17)-H(17)	119.5
C(12)-C(17)-H(17)	119.5
O(2)-C(18)-H(18A)	109.5
O(2)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
O(2)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
O(3)-C(19)-H(19A)	109.5
O(3)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
O(3)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(21)-C(20)-C(25)	118.4(5)
C(21)-C(20)-P(1)	125.1(5)
C(25)-C(20)-P(1)	116.4(4)
O(4)-C(21)-C(20)	116.2(6)
O(4)-C(21)-C(22)	123.0(6)
C(20)-C(21)-C(22)	120.8(7)
C(23)-C(22)-C(21)	120.0(7)
C(23)-C(22)-H(22)	120.0
C(21)-C(22)-H(22)	120.0
C(22)-C(23)-C(24)	121.8(7)
C(22)-C(23)-H(23)	119.1
C(24)-C(23)-H(23)	119.1
C(23)-C(24)-C(29)	122.8(7)
C(23)-C(24)-C(25)	119.3(7)
C(29)-C(24)-C(25)	117.9(7)
C(24)-C(25)-C(26)	117.3(6)
C(24)-C(25)-C(20)	119.6(6)
C(26)-C(25)-C(20)	123.1(6)
C(27)-C(26)-C(25)	121.2(7)

C(27)-C(26)-H(26)	119.4
C(25)-C(26)-H(26)	119.4
O(5)-C(27)-C(26)	123.6(8)
O(5)-C(27)-C(28)	116.3(7)
C(26)-C(27)-C(28)	120.1(8)
C(29)-C(28)-C(27)	119.2(7)
C(29)-C(28)-H(28)	120.4
C(27)-C(28)-H(28)	120.4
C(28)-C(29)-C(24)	124.2(7)
C(28)-C(29)-H(29)	117.9
C(24)-C(29)-H(29)	117.9
O(4)-C(30)-H(30A)	109.5
O(4)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
O(4)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
O(5)-C(31)-H(31A)	109.5
O(5)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
O(5)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(35)-C(32)-C(34)	108.2(8)
C(35)-C(32)-C(33)	112.7(9)
C(34)-C(32)-C(33)	113.7(9)
C(35)-C(32)-S(1)	109.9(6)
C(34)-C(32)-S(1)	106.0(7)
C(33)-C(32)-S(1)	106.2(6)
C(32)-C(33)-H(33A)	109.5
C(32)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(32)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(32)-C(34)-H(34A)	109.5
C(32)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(32)-C(34)-H(34C)	109.5

H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(32)-C(35)-H(35A)	109.5
C(32)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(32)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
N(2)-C(36)-C(37)	111.0(5)
N(2)-C(36)-H(36A)	109.4
C(37)-C(36)-H(36A)	109.4
N(2)-C(36)-H(36B)	109.4
C(37)-C(36)-H(36B)	109.4
H(36A)-C(36)-H(36B)	108.0
C(38)-C(37)-C(42)	117.4(6)
C(38)-C(37)-C(36)	123.4(6)
C(42)-C(37)-C(36)	119.2(5)
C(39)-C(38)-C(37)	120.3(6)
C(39)-C(38)-P(2)	118.3(5)
C(37)-C(38)-P(2)	119.6(5)
C(38)-C(39)-C(40)	119.5(7)
C(38)-C(39)-H(39)	120.2
C(40)-C(39)-H(39)	120.2
C(41)-C(40)-C(39)	121.4(8)
C(41)-C(40)-H(40)	119.3
C(39)-C(40)-H(40)	119.3
C(40)-C(41)-C(42)	120.4(7)
C(40)-C(41)-H(41)	119.8
C(42)-C(41)-H(41)	119.8
C(41)-C(42)-C(37)	120.7(6)
C(41)-C(42)-H(42)	119.6
C(37)-C(42)-H(42)	119.6
C(44)-C(43)-C(48)	119.0(6)
C(44)-C(43)-P(2)	123.0(5)
C(48)-C(43)-P(2)	117.9(5)
O(9)-C(44)-C(43)	117.7(6)
O(9)-C(44)-C(45)	122.5(7)
C(43)-C(44)-C(45)	119.7(7)
C(46)-C(45)-C(44)	120.1(7)

C(46)-C(45)-H(45)	120.0
C(44)-C(45)-H(45)	120.0
C(45)-C(46)-C(47)	123.3(7)
C(45)-C(46)-H(46)	118.3
C(47)-C(46)-H(46)	118.3
C(46)-C(47)-C(52)	122.2(7)
C(46)-C(47)-C(48)	117.8(7)
C(52)-C(47)-C(48)	119.8(8)
C(49)-C(48)-C(43)	122.5(6)
C(49)-C(48)-C(47)	117.7(6)
C(43)-C(48)-C(47)	119.9(7)
C(50)-C(49)-C(48)	120.9(7)
C(50)-C(49)-H(49)	119.5
C(48)-C(49)-H(49)	119.5
O(10)-C(50)-C(49)	125.7(8)
O(10)-C(50)-C(51)	114.3(8)
C(49)-C(50)-C(51)	119.9(8)
C(52)-C(51)-C(50)	119.8(8)
C(52)-C(51)-H(51)	120.1
C(50)-C(51)-H(51)	120.1
C(51)-C(52)-C(47)	121.9(8)
C(51)-C(52)-H(52)	119.1
C(47)-C(52)-H(52)	119.1
O(9)-C(53)-H(53A)	109.5
O(9)-C(53)-H(53B)	109.5
H(53A)-C(53)-H(53B)	109.5
O(9)-C(53)-H(53C)	109.5
H(53A)-C(53)-H(53C)	109.5
H(53B)-C(53)-H(53C)	109.5
O(10)-C(54)-H(54A)	109.5
O(10)-C(54)-H(54B)	109.5
H(54A)-C(54)-H(54B)	109.5
O(10)-C(54)-H(54C)	109.5
H(54A)-C(54)-H(54C)	109.5
H(54B)-C(54)-H(54C)	109.5
C(56)-C(55)-C(60)	120.4(6)
C(56)-C(55)-P(2)	115.5(5)
C(60)-C(55)-P(2)	124.1(4)
O(11)-C(56)-C(55)	118.1(6)

O(11)-C(56)-C(57)	123.3(6)
C(55)-C(56)-C(57)	118.5(7)
C(58)-C(57)-C(56)	120.7(7)
C(58)-C(57)-H(57)	119.6
C(56)-C(57)-H(57)	119.6
C(57)-C(58)-C(59)	122.4(7)
C(57)-C(58)-H(58)	118.8
C(59)-C(58)-H(58)	118.8
C(58)-C(59)-C(60)	120.0(7)
C(58)-C(59)-C(64)	121.3(8)
C(60)-C(59)-C(64)	118.7(7)
C(59)-C(60)-C(61)	119.0(6)
C(59)-C(60)-C(55)	117.9(6)
C(61)-C(60)-C(55)	123.1(6)
C(62)-C(61)-C(60)	120.7(7)
C(62)-C(61)-H(61)	119.6
C(60)-C(61)-H(61)	119.6
O(12)-C(62)-C(61)	125.2(8)
O(12)-C(62)-C(63)	114.9(7)
C(61)-C(62)-C(63)	119.9(8)
C(64)-C(63)-C(62)	120.8(7)
C(64)-C(63)-H(63)	119.6
C(62)-C(63)-H(63)	119.6
C(63)-C(64)-C(59)	120.7(8)
C(63)-C(64)-H(64)	119.6
C(59)-C(64)-H(64)	119.6
O(11)-C(65)-H(65A)	109.5
O(11)-C(65)-H(65B)	109.5
H(65A)-C(65)-H(65B)	109.5
O(11)-C(65)-H(65C)	109.5
H(65A)-C(65)-H(65C)	109.5
H(65B)-C(65)-H(65C)	109.5
C(67)-C(66)-C(68)	108.6(9)
C(67)-C(66)-C(69)	111.0(8)
C(68)-C(66)-C(69)	111.6(7)
C(67)-C(66)-S(2)	109.6(5)
C(68)-C(66)-S(2)	109.7(6)
C(69)-C(66)-S(2)	106.3(6)
C(66)-C(67)-H(67A)	109.5

C(66)-C(67)-H(67B)	109.5
H(67A)-C(67)-H(67B)	109.5
C(66)-C(67)-H(67C)	109.5
H(67A)-C(67)-H(67C)	109.5
H(67B)-C(67)-H(67C)	109.5
C(66)-C(68)-H(68A)	109.5
C(66)-C(68)-H(68B)	109.5
H(68A)-C(68)-H(68B)	109.5
C(66)-C(68)-H(68C)	109.5
H(68A)-C(68)-H(68C)	109.5
H(68B)-C(68)-H(68C)	109.5
C(66)-C(69)-H(69A)	109.5
C(66)-C(69)-H(69B)	109.5
H(69A)-C(69)-H(69B)	109.5
C(66)-C(69)-H(69C)	109.5
H(69A)-C(69)-H(69C)	109.5
H(69B)-C(69)-H(69C)	109.5
O(12)-C(70)-H(70A)	109.5
O(12)-C(70)-H(70B)	109.5
H(70A)-C(70)-H(70B)	109.5
O(12)-C(70)-H(70C)	109.5
H(70A)-C(70)-H(70C)	109.5
H(70B)-C(70)-H(70C)	109.5
Cl(2)-C(71)-Cl(1)	110.6(11)
Cl(2)-C(71)-H(71A)	109.5
Cl(1)-C(71)-H(71A)	109.5
Cl(2)-C(71)-H(71B)	109.5
Cl(1)-C(71)-H(71B)	109.5
H(71A)-C(71)-H(71B)	108.1
Cl(3)-C(72)-Cl(4)	106.5(9)
Cl(3)-C(72)-H(72A)	110.4
Cl(4)-C(72)-H(72A)	110.4
Cl(3)-C(72)-H(72B)	110.4
Cl(4)-C(72)-H(72B)	110.4
H(72A)-C(72)-H(72B)	108.6
Cl(6)-C(73)-Cl(5)	105.1(10)
Cl(6)-C(73)-H(73A)	110.7
Cl(5)-C(73)-H(73A)	110.7
Cl(6)-C(73)-H(73B)	110.7

Cl(5)-C(73)-H(73B)	110.7
H(73A)-C(73)-H(73B)	108.8

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 240705b. 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}
N(1)	45(4)	57(3)	68(3)	6(3)	8(3)	12(3)
N(2)	35(3)	64(4)	74(3)	3(3)	-1(3)	12(3)
O(1)	43(3)	40(2)	77(3)	-13(2)	-2(2)	3(2)
O(2)	64(3)	57(3)	72(3)	-14(2)	-1(2)	-10(2)
O(3)	94(5)	124(5)	78(4)	-21(4)	21(3)	0(4)
O(4)	76(4)	63(3)	69(3)	-1(2)	14(2)	5(2)
O(5)	109(5)	80(4)	77(4)	13(3)	-16(3)	9(4)
O(6)	75(4)	96(4)	100(4)	-32(3)	-16(3)	5(3)
O(7)	69(4)	69(3)	72(3)	10(3)	6(2)	-19(3)
O(8)	40(3)	46(2)	70(3)	6(2)	3(2)	4(2)
O(9)	74(4)	50(3)	85(3)	5(3)	-9(3)	10(2)
O(10)	112(5)	74(4)	92(4)	-13(3)	29(4)	10(4)
O(11)	67(3)	52(3)	66(3)	9(2)	4(2)	-16(2)
O(12)	96(5)	131(5)	82(4)	30(4)	-19(3)	-3(4)
O(13)	96(5)	99(4)	108(4)	33(4)	30(4)	11(4)
O(14)	67(4)	78(3)	75(3)	-13(3)	12(2)	-29(3)
P(1)	37(1)	31(1)	66(1)	-3(1)	0(1)	2(1)
P(2)	37(1)	30(1)	67(1)	3(1)	1(1)	1(1)
S(1)	52(1)	53(1)	70(1)	-2(1)	-3(1)	1(1)
S(2)	55(1)	51(1)	77(1)	2(1)	13(1)	2(1)
Cl(1)	169(6)	88(4)	148(5)	6(3)	-10(4)	-15(4)
Cl(2)	173(7)	166(6)	171(5)	25(5)	26(5)	21(5)
Cl(3)	169(6)	88(4)	148(5)	6(3)	-10(4)	-15(4)
Cl(4)	173(7)	166(6)	171(5)	25(5)	26(5)	21(5)
Cl(5)	169(6)	88(4)	148(5)	6(3)	-10(4)	-15(4)
Cl(6)	173(7)	166(6)	171(5)	25(5)	26(5)	21(5)
C(1)	49(5)	34(3)	101(5)	-14(3)	15(4)	-3(3)
C(2)	49(4)	34(3)	77(4)	0(3)	9(3)	0(3)
C(3)	36(4)	28(3)	74(4)	-6(3)	2(3)	2(3)
C(4)	50(5)	47(4)	83(5)	6(3)	-6(3)	16(3)
C(5)	78(6)	62(5)	89(5)	15(4)	-16(4)	25(5)
C(6)	73(6)	44(4)	104(6)	12(4)	8(5)	10(4)
C(7)	63(5)	44(4)	97(5)	-2(4)	-1(4)	-8(4)
C(8)	34(4)	31(3)	58(3)	-4(3)	-2(3)	-1(2)

C(9)	47(4)	42(3)	63(4)	5(3)	-3(3)	6(3)
C(10)	49(5)	59(4)	91(5)	-5(4)	-9(4)	-21(4)
C(11)	71(6)	59(5)	104(6)	12(5)	-8(5)	-19(4)
C(12)	44(4)	59(4)	94(5)	21(4)	1(4)	-8(3)
C(13)	41(4)	37(3)	63(4)	12(3)	-1(3)	-2(3)
C(14)	41(4)	59(4)	71(4)	1(4)	0(3)	1(3)
C(15)	60(5)	73(4)	63(4)	10(4)	10(3)	11(4)
C(16)	73(7)	105(7)	90(6)	28(6)	20(5)	-3(5)
C(17)	58(5)	85(6)	98(6)	23(5)	21(4)	-21(4)
C(18)	93(7)	79(6)	97(6)	-27(5)	3(5)	1(5)
C(19)	126(10)	136(9)	113(7)	-62(7)	32(7)	-23(8)
C(20)	23(3)	31(3)	71(4)	-12(3)	-1(3)	4(2)
C(21)	56(5)	35(3)	87(5)	-2(3)	12(4)	-7(3)
C(22)	53(5)	66(5)	90(5)	-15(4)	16(4)	8(4)
C(23)	58(5)	50(4)	114(7)	-17(4)	0(5)	24(4)
C(24)	52(5)	44(4)	98(6)	-15(4)	-11(4)	3(3)
C(25)	46(4)	20(3)	88(5)	1(3)	-7(3)	-2(3)
C(26)	46(4)	42(3)	83(5)	1(3)	-14(4)	1(3)
C(27)	83(6)	53(4)	89(6)	-2(4)	-38(5)	2(4)
C(28)	82(6)	47(4)	113(7)	9(5)	-26(5)	10(4)
C(29)	57(5)	44(4)	131(7)	-6(5)	-16(5)	15(4)
C(30)	121(9)	115(8)	83(5)	10(6)	26(5)	19(6)
C(31)	92(8)	89(6)	91(6)	27(5)	-5(5)	-26(6)
C(32)	53(5)	98(6)	89(5)	25(5)	2(4)	17(5)
C(33)	134(11)	190(13)	129(8)	83(9)	40(7)	85(10)
C(34)	86(8)	183(12)	150(9)	-29(9)	-57(7)	61(8)
C(35)	62(6)	77(6)	191(10)	10(7)	-2(6)	27(5)
C(36)	37(4)	35(3)	95(5)	7(3)	-6(3)	-10(3)
C(37)	39(4)	36(3)	65(4)	3(3)	-10(3)	-2(3)
C(38)	38(4)	37(3)	62(3)	1(3)	-2(3)	5(3)
C(39)	49(4)	40(3)	84(4)	3(3)	6(3)	0(3)
C(40)	71(6)	50(4)	90(5)	-6(4)	21(4)	7(4)
C(41)	80(6)	40(4)	95(5)	-13(4)	7(4)	5(4)
C(42)	49(5)	35(3)	96(5)	-2(3)	-2(4)	-9(3)
C(43)	34(4)	30(3)	79(4)	-1(3)	-1(3)	1(3)
C(44)	40(4)	41(4)	83(5)	6(3)	-2(3)	-13(3)
C(45)	61(5)	51(4)	105(6)	23(4)	-25(4)	-1(4)
C(46)	67(6)	30(4)	137(7)	-1(4)	-1(5)	15(3)
C(47)	47(5)	31(3)	112(6)	3(4)	0(4)	2(3)

C(48)	36(4)	35(3)	92(5)	4(3)	16(3)	1(3)
C(49)	71(5)	39(3)	84(5)	-1(4)	18(4)	10(3)
C(50)	76(6)	50(4)	93(6)	0(4)	27(5)	4(4)
C(51)	80(7)	67(5)	131(8)	-9(5)	38(6)	18(5)
C(52)	55(5)	48(4)	143(8)	2(5)	6(5)	14(4)
C(53)	99(7)	107(7)	76(5)	4(5)	-23(5)	6(6)
C(54)	100(8)	88(6)	75(5)	-20(5)	13(5)	-15(6)
C(55)	34(4)	35(3)	58(3)	-3(3)	0(3)	0(3)
C(56)	52(4)	35(3)	77(4)	-2(3)	16(4)	-4(3)
C(57)	58(5)	52(4)	94(6)	4(4)	16(4)	-9(4)
C(58)	55(5)	56(4)	116(7)	-16(5)	10(5)	-17(4)
C(59)	60(5)	55(4)	76(4)	-20(4)	2(4)	-5(4)
C(60)	40(4)	47(3)	69(4)	-9(3)	3(3)	-1(3)
C(61)	50(4)	53(4)	76(4)	8(4)	-4(3)	0(3)
C(62)	64(5)	80(5)	72(5)	-1(5)	-12(4)	1(5)
C(63)	76(7)	112(7)	72(5)	-19(5)	-29(5)	9(6)
C(64)	67(6)	103(7)	93(6)	-41(6)	-17(5)	-17(5)
C(65)	87(6)	70(5)	77(5)	26(4)	8(4)	-4(4)
C(66)	62(5)	94(6)	75(5)	-19(5)	9(4)	23(4)
C(67)	77(7)	91(6)	144(8)	12(6)	19(6)	28(5)
C(68)	131(10)	144(10)	121(7)	-81(8)	6(7)	-1(8)
C(69)	80(7)	119(8)	132(8)	-3(7)	39(6)	12(6)
C(70)	100(9)	128(9)	107(7)	40(6)	-5(6)	-13(7)
C(71)	510(70)	400(60)	170(30)	-10(40)	-150(40)	110(60)
C(72)	510(70)	400(60)	170(30)	-10(40)	-150(40)	110(60)
C(73)	510(70)	400(60)	170(30)	-10(40)	-150(40)	110(60)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 240705b.

	x	y	z	U(eq)
H(1)	7537	9208	1053	68
H(2)	7704	6207	5981	70
H(1C)	7720	8808	-400	73
H(1D)	7405	8306	279	73
H(4)	3192	8194	28	72
H(5)	2655	9251	-651	93
H(6)	4126	10047	-987	88
H(7)	6200	9794	-742	82
H(10)	2379	5906	-57	80
H(11)	1361	5866	1033	94
H(14)	4194	7955	2158	69
H(16)	1361	7129	3260	107
H(17)	829	6400	2268	96
H(18A)	4761	6329	-1273	134
H(18B)	3438	6087	-1045	134
H(18C)	4615	5762	-625	134
H(19A)	4104	8720	3914	186
H(19B)	3953	8824	3040	186
H(19C)	4788	8196	3374	186
H(22)	8290	6464	-845	83
H(23)	9137	5765	96	89
H(26)	5823	6770	1910	69
H(28)	8324	5248	2523	98
H(29)	9098	5288	1379	93
H(30A)	6575	7812	-1775	159
H(30B)	6987	6998	-1696	159
H(30C)	7879	7620	-1411	159
H(31A)	5154	6188	3671	137
H(31B)	4743	6122	2818	137
H(31C)	5504	6800	3105	137
H(33A)	9320	8862	2096	225
H(33B)	9778	8065	1970	225
H(33C)	8539	8333	1575	225

H(34A)	11316	9378	1632	212
H(34B)	11725	9200	817	212
H(34C)	11866	8612	1452	212
H(35A)	9376	7973	342	165
H(35B)	10693	7769	678	165
H(35C)	10552	8357	43	165
H(36A)	7630	7017	5099	67
H(36B)	7256	6428	4492	67
H(39)	11853	7095	5002	69
H(40)	12344	6067	4324	84
H(41)	10892	5259	3972	86
H(42)	8845	5493	4162	72
H(45)	6739	8863	3972	88
H(46)	5974	9572	4873	93
H(49)	9215	8472	6826	77
H(51)	6754	10012	7359	110
H(52)	5910	9982	6166	98
H(53A)	8431	7497	3096	142
H(53B)	7953	8298	3149	142
H(53C)	7136	7655	3425	142
H(54A)	9827	8999	8663	131
H(54B)	10279	9077	7841	131
H(54C)	9467	8409	8057	131
H(57)	12724	9396	5006	81
H(58)	13811	9393	6085	91
H(61)	10916	7352	7100	72
H(63)	13852	8123	8289	105
H(64)	14296	8905	7338	106
H(65A)	10281	8995	3655	117
H(65B)	11620	9219	3937	117
H(65C)	10466	9556	4313	117
H(67A)	4509	6992	5026	155
H(67B)	5791	7336	5267	155
H(67C)	4583	7603	5640	155
H(68A)	6070	6588	7077	198
H(68B)	5531	7359	6884	198
H(68C)	6739	7092	6512	198
H(69A)	4066	5984	6685	164
H(69B)	3473	6132	5881	164

H(69C)	3467	6741	6497	164
H(70A)	10289	7134	8293	168
H(70B)	10931	6636	8907	168
H(70C)	11097	6474	8053	168
H(71A)	2652	4184	6688	435
H(71B)	1720	3897	7274	435
H(72A)	7574	6256	7013	435
H(72B)	8641	6714	7413	435
H(73A)	5348	4817	8955	435
H(73B)	5776	4151	8472	435

Table S6. Torsion angles [°] for 240705b.

C(1)-N(1)-S(1)-O(6)	176.4(5)
C(1)-N(1)-S(1)-O(7)	49.5(5)
C(1)-N(1)-S(1)-C(32)	-67.3(6)
C(36)-N(2)-S(2)-O(13)	173.1(5)
C(36)-N(2)-S(2)-O(14)	46.9(6)
C(36)-N(2)-S(2)-C(66)	-70.9(6)
S(1)-N(1)-C(1)-C(2)	-159.6(5)
N(1)-C(1)-C(2)-C(7)	70.1(8)
N(1)-C(1)-C(2)-C(3)	-112.7(7)
C(7)-C(2)-C(3)-C(4)	-1.5(9)
C(1)-C(2)-C(3)-C(4)	-178.7(6)
C(7)-C(2)-C(3)-P(1)	-171.3(5)
C(1)-C(2)-C(3)-P(1)	11.5(8)
O(1)-P(1)-C(3)-C(4)	-110.6(5)
C(8)-P(1)-C(3)-C(4)	11.3(6)
C(20)-P(1)-C(3)-C(4)	128.4(5)
O(1)-P(1)-C(3)-C(2)	59.5(5)
C(8)-P(1)-C(3)-C(2)	-178.6(5)
C(20)-P(1)-C(3)-C(2)	-61.5(5)
C(2)-C(3)-C(4)-C(5)	-1.6(10)
P(1)-C(3)-C(4)-C(5)	168.5(5)
C(3)-C(4)-C(5)-C(6)	1.4(11)
C(4)-C(5)-C(6)-C(7)	2.0(12)
C(5)-C(6)-C(7)-C(2)	-5.1(11)
C(3)-C(2)-C(7)-C(6)	4.8(10)
C(1)-C(2)-C(7)-C(6)	-177.8(6)
O(1)-P(1)-C(8)-C(9)	-166.9(4)
C(3)-P(1)-C(8)-C(9)	75.4(5)
C(20)-P(1)-C(8)-C(9)	-47.9(5)
O(1)-P(1)-C(8)-C(13)	7.0(6)
C(3)-P(1)-C(8)-C(13)	-110.7(5)
C(20)-P(1)-C(8)-C(13)	126.0(5)
C(18)-O(2)-C(9)-C(8)	160.2(6)
C(18)-O(2)-C(9)-C(10)	-23.9(9)
C(13)-C(8)-C(9)-O(2)	175.2(5)
P(1)-C(8)-C(9)-O(2)	-10.6(7)
C(13)-C(8)-C(9)-C(10)	-0.7(9)

P(1)-C(8)-C(9)-C(10)	173.5(5)
O(2)-C(9)-C(10)-C(11)	-177.1(7)
C(8)-C(9)-C(10)-C(11)	-1.4(10)
C(9)-C(10)-C(11)-C(12)	4.0(12)
C(10)-C(11)-C(12)-C(13)	-4.3(12)
C(10)-C(11)-C(12)-C(17)	175.4(8)
C(11)-C(12)-C(13)-C(14)	-178.6(6)
C(17)-C(12)-C(13)-C(14)	1.7(10)
C(11)-C(12)-C(13)-C(8)	2.0(9)
C(17)-C(12)-C(13)-C(8)	-177.8(6)
C(9)-C(8)-C(13)-C(14)	-179.0(6)
P(1)-C(8)-C(13)-C(14)	7.2(8)
C(9)-C(8)-C(13)-C(12)	0.4(8)
P(1)-C(8)-C(13)-C(12)	-173.3(5)
C(12)-C(13)-C(14)-C(15)	-0.5(9)
C(8)-C(13)-C(14)-C(15)	178.9(6)
C(19)-O(3)-C(15)-C(14)	1.0(13)
C(19)-O(3)-C(15)-C(16)	176.9(9)
C(13)-C(14)-C(15)-O(3)	176.2(7)
C(13)-C(14)-C(15)-C(16)	0.5(11)
O(3)-C(15)-C(16)-C(17)	-178.0(8)
C(14)-C(15)-C(16)-C(17)	-1.9(13)
C(15)-C(16)-C(17)-C(12)	3.1(13)
C(11)-C(12)-C(17)-C(16)	177.2(8)
C(13)-C(12)-C(17)-C(16)	-3.0(12)
O(1)-P(1)-C(20)-C(21)	-128.4(5)
C(3)-P(1)-C(20)-C(21)	-8.3(6)
C(8)-P(1)-C(20)-C(21)	109.3(5)
O(1)-P(1)-C(20)-C(25)	48.7(5)
C(3)-P(1)-C(20)-C(25)	168.9(4)
C(8)-P(1)-C(20)-C(25)	-73.5(5)
C(30)-O(4)-C(21)-C(20)	174.6(7)
C(30)-O(4)-C(21)-C(22)	-5.0(10)
C(25)-C(20)-C(21)-O(4)	177.7(5)
P(1)-C(20)-C(21)-O(4)	-5.2(8)
C(25)-C(20)-C(21)-C(22)	-2.7(9)
P(1)-C(20)-C(21)-C(22)	174.4(5)
O(4)-C(21)-C(22)-C(23)	178.4(7)
C(20)-C(21)-C(22)-C(23)	-1.2(11)

C(21)-C(22)-C(23)-C(24)	3.3(12)
C(22)-C(23)-C(24)-C(29)	176.0(7)
C(22)-C(23)-C(24)-C(25)	-1.3(11)
C(23)-C(24)-C(25)-C(26)	175.7(6)
C(29)-C(24)-C(25)-C(26)	-1.8(9)
C(23)-C(24)-C(25)-C(20)	-2.6(9)
C(29)-C(24)-C(25)-C(20)	179.9(6)
C(21)-C(20)-C(25)-C(24)	4.6(8)
P(1)-C(20)-C(25)-C(24)	-172.8(5)
C(21)-C(20)-C(25)-C(26)	-173.6(6)
P(1)-C(20)-C(25)-C(26)	9.0(7)
C(24)-C(25)-C(26)-C(27)	1.5(9)
C(20)-C(25)-C(26)-C(27)	179.7(6)
C(31)-O(5)-C(27)-C(26)	7.3(11)
C(31)-O(5)-C(27)-C(28)	-172.1(7)
C(25)-C(26)-C(27)-O(5)	-179.0(6)
C(25)-C(26)-C(27)-C(28)	0.4(10)
O(5)-C(27)-C(28)-C(29)	177.3(7)
C(26)-C(27)-C(28)-C(29)	-2.1(11)
C(27)-C(28)-C(29)-C(24)	1.9(12)
C(23)-C(24)-C(29)-C(28)	-177.2(8)
C(25)-C(24)-C(29)-C(28)	0.2(11)
O(6)-S(1)-C(32)-C(35)	-168.2(6)
O(7)-S(1)-C(32)-C(35)	-40.9(7)
N(1)-S(1)-C(32)-C(35)	76.6(7)
O(6)-S(1)-C(32)-C(34)	-51.5(7)
O(7)-S(1)-C(32)-C(34)	75.7(7)
N(1)-S(1)-C(32)-C(34)	-166.8(6)
O(6)-S(1)-C(32)-C(33)	69.8(8)
O(7)-S(1)-C(32)-C(33)	-163.0(7)
N(1)-S(1)-C(32)-C(33)	-45.5(8)
S(2)-N(2)-C(36)-C(37)	-161.4(5)
N(2)-C(36)-C(37)-C(38)	-106.6(6)
N(2)-C(36)-C(37)-C(42)	76.2(7)
C(42)-C(37)-C(38)-C(39)	-4.8(9)
C(36)-C(37)-C(38)-C(39)	178.0(6)
C(42)-C(37)-C(38)-P(2)	-169.4(5)
C(36)-C(37)-C(38)-P(2)	13.4(8)
O(8)-P(2)-C(38)-C(39)	-108.4(5)

C(43)-P(2)-C(38)-C(39)	130.9(5)
C(55)-P(2)-C(38)-C(39)	13.2(6)
O(8)-P(2)-C(38)-C(37)	56.5(5)
C(43)-P(2)-C(38)-C(37)	-64.1(5)
C(55)-P(2)-C(38)-C(37)	178.1(5)
C(37)-C(38)-C(39)-C(40)	2.8(9)
P(2)-C(38)-C(39)-C(40)	167.7(5)
C(38)-C(39)-C(40)-C(41)	-1.8(11)
C(39)-C(40)-C(41)-C(42)	2.8(12)
C(40)-C(41)-C(42)-C(37)	-4.9(11)
C(38)-C(37)-C(42)-C(41)	5.8(9)
C(36)-C(37)-C(42)-C(41)	-176.9(6)
O(8)-P(2)-C(43)-C(44)	-130.4(5)
C(38)-P(2)-C(43)-C(44)	-10.3(6)
C(55)-P(2)-C(43)-C(44)	108.7(5)
O(8)-P(2)-C(43)-C(48)	46.8(5)
C(38)-P(2)-C(43)-C(48)	166.9(4)
C(55)-P(2)-C(43)-C(48)	-74.1(5)
C(53)-O(9)-C(44)-C(43)	170.5(6)
C(53)-O(9)-C(44)-C(45)	-8.8(10)
C(48)-C(43)-C(44)-O(9)	178.8(5)
P(2)-C(43)-C(44)-O(9)	-4.0(8)
C(48)-C(43)-C(44)-C(45)	-1.8(9)
P(2)-C(43)-C(44)-C(45)	175.3(5)
O(9)-C(44)-C(45)-C(46)	179.3(7)
C(43)-C(44)-C(45)-C(46)	0.0(10)
C(44)-C(45)-C(46)-C(47)	-0.5(12)
C(45)-C(46)-C(47)-C(52)	178.0(7)
C(45)-C(46)-C(47)-C(48)	2.8(11)
C(44)-C(43)-C(48)-C(49)	-175.2(6)
P(2)-C(43)-C(48)-C(49)	7.5(8)
C(44)-C(43)-C(48)-C(47)	4.2(9)
P(2)-C(43)-C(48)-C(47)	-173.1(5)
C(46)-C(47)-C(48)-C(49)	174.7(6)
C(52)-C(47)-C(48)-C(49)	-0.6(10)
C(46)-C(47)-C(48)-C(43)	-4.6(10)
C(52)-C(47)-C(48)-C(43)	-180.0(6)
C(43)-C(48)-C(49)-C(50)	178.2(6)
C(47)-C(48)-C(49)-C(50)	-1.2(10)

C(54)-O(10)-C(50)-C(49)	7.8(11)
C(54)-O(10)-C(50)-C(51)	-174.9(7)
C(48)-C(49)-C(50)-O(10)	179.7(7)
C(48)-C(49)-C(50)-C(51)	2.5(11)
O(10)-C(50)-C(51)-C(52)	-179.5(8)
C(49)-C(50)-C(51)-C(52)	-2.0(12)
C(50)-C(51)-C(52)-C(47)	0.2(13)
C(46)-C(47)-C(52)-C(51)	-174.0(8)
C(48)-C(47)-C(52)-C(51)	1.1(12)
O(8)-P(2)-C(55)-C(56)	-169.1(4)
C(38)-P(2)-C(55)-C(56)	72.9(5)
C(43)-P(2)-C(55)-C(56)	-51.4(5)
O(8)-P(2)-C(55)-C(60)	7.9(6)
C(38)-P(2)-C(55)-C(60)	-110.0(5)
C(43)-P(2)-C(55)-C(60)	125.7(5)
C(65)-O(11)-C(56)-C(55)	159.7(6)
C(65)-O(11)-C(56)-C(57)	-23.3(10)
C(60)-C(55)-C(56)-O(11)	174.4(5)
P(2)-C(55)-C(56)-O(11)	-8.4(7)
C(60)-C(55)-C(56)-C(57)	-2.7(9)
P(2)-C(55)-C(56)-C(57)	174.5(5)
O(11)-C(56)-C(57)-C(58)	-175.8(7)
C(55)-C(56)-C(57)-C(58)	1.2(10)
C(56)-C(57)-C(58)-C(59)	1.1(12)
C(57)-C(58)-C(59)-C(60)	-1.9(11)
C(57)-C(58)-C(59)-C(64)	178.3(8)
C(58)-C(59)-C(60)-C(61)	-178.3(6)
C(64)-C(59)-C(60)-C(61)	1.5(10)
C(58)-C(59)-C(60)-C(55)	0.3(10)
C(64)-C(59)-C(60)-C(55)	-179.9(6)
C(56)-C(55)-C(60)-C(59)	1.9(9)
P(2)-C(55)-C(60)-C(59)	-175.0(5)
C(56)-C(55)-C(60)-C(61)	-179.5(6)
P(2)-C(55)-C(60)-C(61)	3.6(9)
C(59)-C(60)-C(61)-C(62)	0.6(10)
C(55)-C(60)-C(61)-C(62)	-177.9(7)
C(70)-O(12)-C(62)-C(61)	-1.7(13)
C(70)-O(12)-C(62)-C(63)	178.8(8)
C(60)-C(61)-C(62)-O(12)	176.7(7)

C(60)-C(61)-C(62)-C(63)	-3.8(11)
O(12)-C(62)-C(63)-C(64)	-175.4(8)
C(61)-C(62)-C(63)-C(64)	5.0(13)
C(62)-C(63)-C(64)-C(59)	-2.9(14)
C(58)-C(59)-C(64)-C(63)	179.4(8)
C(60)-C(59)-C(64)-C(63)	-0.4(12)
O(13)-S(2)-C(66)-C(67)	-172.4(7)
O(14)-S(2)-C(66)-C(67)	-45.0(7)
N(2)-S(2)-C(66)-C(67)	72.7(7)
O(13)-S(2)-C(66)-C(68)	68.5(8)
O(14)-S(2)-C(66)-C(68)	-164.2(6)
N(2)-S(2)-C(66)-C(68)	-46.5(7)
O(13)-S(2)-C(66)-C(69)	-52.4(7)
O(14)-S(2)-C(66)-C(69)	75.0(6)
N(2)-S(2)-C(66)-C(69)	-167.3(6)

Symmetry transformations used to generate equivalent atoms:

Table S7. Hydrogen bonds for 240705b [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(72)-H(72A)...S(2)	0.97	3.00	3.86(6)	147.6
C(72)-H(72A)...N(2)	0.97	2.65	3.23(5)	119.1
C(68)-H(68A)...Cl(6)	0.96	2.89	3.805(18)	159.0
C(65)-H(65C)...Cl(3)#1	0.96	2.98	3.453(11)	112.0
C(61)-H(61)...O(8)	0.93	2.16	2.901(8)	135.8
C(54)-H(54A)...O(7)#2	0.96	2.51	3.400(9)	154.6
C(53)-H(53B)...Cl(1)#3	0.96	2.94	3.772(16)	145.3
C(49)-H(49)...O(8)	0.93	2.39	2.977(7)	120.9
C(34)-H(34A)...Cl(4)#1	0.96	2.50	3.344(18)	146.3
C(33)-H(33A)...Cl(2)#3	0.96	2.83	3.75(2)	160.5
C(31)-H(31A)...O(14)	0.96	2.46	3.358(9)	155.9
C(30)-H(30B)...Cl(4)#4	0.96	2.85	3.678(16)	144.7
C(26)-H(26)...O(1)	0.93	2.46	3.008(7)	117.6
C(22)-H(22)...Cl(4)#4	0.93	2.43	3.216(13)	142.3
C(19)-H(19B)...Cl(6)#3	0.96	2.96	3.890(18)	162.3
C(18)-H(18A)...Cl(6)#4	0.96	2.97	3.542(14)	119.7
C(14)-H(14)...O(1)	0.93	2.20	2.929(8)	134.8
N(2)-H(2)...Cl(3)	0.90	2.33	2.974(11)	128.7
N(2)-H(2)...O(8)	0.90	2.64	3.344(7)	135.4
N(1)-H(1)...Cl(5)#3	0.90	2.19	2.941(13)	140.2
N(1)-H(1)...Cl(1)#3	0.90	2.26	3.109(18)	157.2

Symmetry transformations used to generate equivalent atoms:

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

#4 x,y,z-1