Supporting Information

for

Synthetic and mechanistic studies of the multicomponent reaction of 2-(phenylethynyl)benzaldehyde, primary amine and diphenylphosphine oxide

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Experimental section

Materials and instrumentation

All starting materials were purchased from commercial sources and were used without further purification.

The reactions under conventional heating were carried out in an oil bath.

High-performance liquid chromatography-mass spectrometry (HPLC-MS) measurements were performed with an Agilent 1200 liquid chromatography system coupled with a 6130-quadrupole mass spectrometer equipped with an ESI ion source (Agilent Technologies, Palo Alto, CA, USA). Analysis was performed at 40 °C on a Gemini C18 column (150 mm × 4.6 mm, 3 μm; Phenomenex, Torrance, CA, USA) with a mobile phase flow rate of 0.6 mL/min. Composition of eluent A was 0.1% $(NH_4)(HCOO)$ in water; eluent B was 0.1% $(NH_4)(HCOO)$ and 8% water in acetonitrile, 0–3 min 5% B, 3–13 min gradient, 13–20 min 100% B. The injection volume was 2 μL. The chromatographic profile was registered at 254 nm. The MSD operating parameters were as follows: positive ionization mode, scan spectra from m/z 120 to 1000, drying gas temperature 300 °C, nitrogen flow rate 12 L/min, nebulizer pressure 60 psi, capillary voltage 4000 V.

High resolution mass spectrometric measurements were performed using a Sciex 5600+ Q-TOF mass spectrometer in positive electrospray mode.

The ^{1}H, ^{13}C and ^{31}P NMR spectra were taken in $CDCl_3$ solution on a Bruker AV-300 spectrometer operating at 300, 75.5 and 121.5 MHz, respectively. The chemical shifts (δ) are reported in parts per million (ppm) and downfield relative to 85% H_3PO_4, as well as TMS, the coupling constants (*J*) are reported in Hz.

General procedure for the synthesis of α-amino(2-alkynylphenyl)methylphosphine oxides (7a and 7b)

To the mixture of 1.0 mmol (0.21 g) of 2-(phenylethynyl)benzaldehyde, 1.0 mmol of primary amine (butylamine: 0.10 mL or aniline: 0.09 mL), and 1.0 mmol (0.20 g) of diphenylphosphine oxide were added 2 mL of solvent (ethanol, toluene, ethyl acetate or acetonitrile). The reaction mixture was stirred at 25 °C for 10–240 min on a magnetic stirrer. At the end of the reaction, the solvent was removed in vacuum and the reaction mixtures were analyzed by ^{31}P NMR spectroscopy and HPLC-MS. The α-amino(2-alkynylphenyl)methylphosphine oxides were obtained by column chromatography using silica gel as the absorbent and hexane:ethyl acetate (6:4) as the eluent.

General procedure for the catalyst screening of the three-component reaction

To the mixture of 1.0 mmol (0.21 g) of 2-(phenylethynyl)benzaldehyde, 1.0 mmol (0.09 mL) of aniline and 1.0 mmol (0.20 g) of diphenylphosphine oxide were added in the presence of 0.05 mmol catalyst (copper(I) chloride: 0.005 g, copper(II) chloride: 0.007 g, cerium(III) chloride heptahydrate: 0.019 g, zirconium(IV) chloride: 0.012 g, bis(benzonitrile)palladium(II) chloride: 0.016 g, silver(I) acetate: 0.009 g, mercury(II) acetate: 0.016 g, copper(II) acetate monohydrate: 0.010 g, cobalt(II) acetate tetrahydrate: 0.012 g, silver trifluoromethanesulfonate: 0.013 g, zinc(II) trifluoromethanesulfonate: 0.017 g, scandium(III) trifluoromethanesulfonate: 0.025 g or yttrium(III) trifluoromethanesulfonate: 0.027 g). The reaction mixtures were stirred in 2 mL of acetonitrile in a Schlenk tube at 70 °C for 18 h on a magnetic stirrer. At given intervals, the reaction composition was analyzed by TLC and HPLC.

General procedure for the synthesis of (2,3-diphenyl-1,2-dihydroisoquinolin-1-yl)diphenylphosphine oxide (8)

To the mixture of 1.0 mmol (0.21 g) of 2-(phenylethynyl)benzaldehyde, 1.0 mmol (0.09 mL) of aniline, 1.0 mmol (0.20 g) of diphenylphosphine oxide, and 0.05 mmol (0.012 g) of zirconium(IV) chloride were added 2 mL of acetonitrile. The reaction mixture was stirred in a Schlenk tube at 70–100 °C for 0.5–1 h on a magnetic stirrer. The solvent was removed in vacuum and the reaction mixtures were analysed by ^{31}P NMR spectroscopy and HPLC-MS. The (2,3-diphenyl-1,2-dihydroisoquinolin-1-yl)diphenylphosphine oxide was obtained by column chromatography using silica gel as the absorbent and hexane:ethyl acetate (6:4) as the eluent.

General procedure for the synthesis of (3-benzyl-2-phenyl-2*H*-isoindol-1-yl)diphenylphosphine oxide (9)

To the mixture of 1.0 mmol (0.21 g) of 2-(phenylethynyl)benzaldehyde, 1.0 mmol (0.09 mL) of aniline, 1.0 mmol (0.20 g) of diphenylphosphine oxide and 0.05 mmol (0.012 g) of 0.05 mmol (0.005 g) of silver(I) acetate were added 2 mL of acetonitrile. The reaction mixture was stirred in a Schlenk tube at 70–90 °C for 0.5–5 h on magnetic stirrer. The solvent was removed in vacuum and the reaction mixtures were analyzed by ^{31}P NMR spectroscopy and HPLC-MS. The (3-benzyl-2-phenyl-2*H*-isoindol-1-yl)diphenylphosphine oxide was obtained by column chromatography using silica gel as the absorbent and hexane:ethyl acetate (6:4) as the eluent.

General procedure for ring closure reactions of diphenyl((phenylamino)(2-(phenylethynyl) phenyl)methyl)phosphine oxide (7b)

To the reaction mixture of 1.0 mmol (0.48 g) of diphenyl((phenylamino)(2-(phenylethynyl) phenyl)methyl)phosphine oxide (**7b**) and 0.05 mmol of catalyst (bis(benzonitrile)palladium(II) dichloride: 0.016 g, silver trifluoromethanesulfonate: 0.013 g, silver(I) acetate: 0.009 g, copper(I) chloride: 0.005 g or copper(II) chloride: 0.007 g) were added 2 mL of acetonitrile. The reaction mixtures were stirred in a Schlenk tube at 70 °C for 40 h on magnetic stirrer. At given intervals, the reaction composition was analyzed by TLC and HPLC.

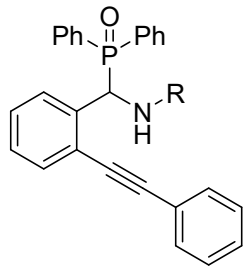
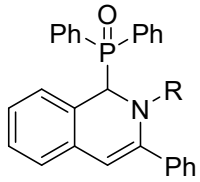
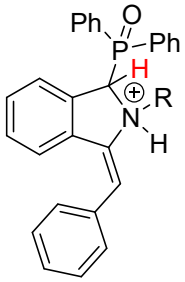
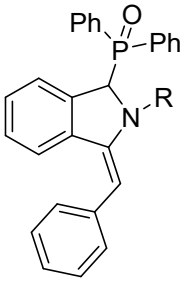
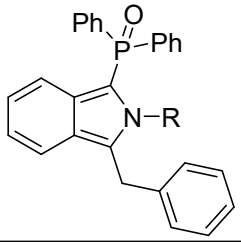
General procedure for ring rearrangement of (1,2-dihydroisoquinolin-1-yl)phosphine oxide (8)

The mixture of 1.0 mmol (0.48 g) of (1,2-dihydroisoquinolin-1-yl)phosphine oxide (**8**) and 0.05 mmol of catalyst (triethylamine: 0.007 mL, silver(I) acetate: 0.009 g, copper(I) chloride: 0.005 g or copper(II) chloride: 0.007 g) were reacted in 2 mL of acetonitrile. The reaction mixtures were stirred in a Schlenk tube at 80 °C for 40 h on a magnetic stirrer. At given intervals, the reaction composition was analyzed by TLC and HPLC.

Computational details

All DFT calculations were carried out with the Gaussian 16 suite of programs.[1] In our previous studies, we showed that the functional ωB97X-D describes properly similar systems, therefore geometry optimizations were performed at the ωB97X-D/6-311+G** level of theory.[2] Harmonic vibrational analysis was obtained at the same level to check the nature of the stationary points obtained. Gibbs free energies (at 298 °K) were calculated using frequency calculations. In order to save computation time, butyl substituents were replaced by ethyl substituents.

Table S1. The relative energy of the computed transition states and intermediates starting from aniline of ethylamin

	E[kcal/mol]	E[kcal/mol]
	starting from aniline R=Ph	starting from ethylamine R=Et
	0.0	0.0
TS-1	61.5	69.1
	-34.6	-37.2
TS-2	44.4	41.1
	43.6	36.6
TS-3	55.5	51.1
	1.4	-31.1
	-29.9	-32.0

((Butylamino)(2-(phenylethynyl)phenyl)methyl)diphenylphosphine oxide (7a)

Yield: 86% (0.39 g), yellow solid; Mp: 142–143 °C; ^{31}P NMR ($CDCl_3$) δ 31.6; ^{13}C NMR ($CDCl_3$) δ 13.9, 20.2, 31.7, 47.4 (d, J_{CP} = 13.1 Hz), 58.8 (d, $^1J_{CP}$ = 80.1 Hz), 87.8, 93.9, 123.0, 123.8 (d, $^3J_{CP}$ = 6.9 Hz), 127.4 (d, $^3J_{CP}$ = 2.4 Hz), 127.7, 127.8, 128.1 (d, J_{CP} = 4.0 Hz), 128.4 (d, J_{CP} = 2.4 Hz), 128.5 (d, J_{CP} = 4.1 Hz), 128.6, 128.9 (d, J_{CP} = 2.7 Hz), 131.3, 131.41 (d, J_{CP} = 4.0), 131.45 (d, J_{CP} = 4.6 Hz), 131.7 (d, $^2J_{CP}$ = 2.6 Hz), 131.8 (d, $^2J_{CP}$ = 2.2 Hz), 131.9 (d, J_{CP} = 9.2 Hz), 132.2 (d, J_{CP} = 9.0 Hz), 138.6; ^{1}H NMR ($CDCl_3$) δ 0.80 (t, 3H, J_{HH} = 7.4 Hz), 1.23 (p, 2H, J_{HH} = 7.3 Hz), 1.42 (dt, 2H, J_{HH} = 7.4 Hz, J_{HH} = 15.3 Hz), 2.49 (ddd, 2H, J_{HH} = 6.0 Hz, J_{HH} = 7.7 Hz, J_{HH} = 11.7 Hz), 2.59 (dt, 1H, J_{HH} = 7.2 Hz, J_{HH} = 11.5 Hz), 5.37 (d, 1H, $^2J_{HP}$ = 9.4 Hz), 7.18 (q, 2H, J_{HH} = 7.2 Hz), 7.31 (dd, 2H, J_{HH} = 6.7 Hz, J_{HH} = 14.0 Hz), 7.35 (d, 2H, J_{HH} = 5.8 Hz), 7.38–7.41 (m, 2H), 7.47 (dd, 2H, J_{HH} = 2.2 Hz, J_{HH} = 4.8 Hz), 7.50 (d, 2H, J_{HH} = 4.5 Hz), 7.52–7.59 (m, 2H), 7.73 (dt, 4H, J_{HH} = 7.7 Hz, J_{HH} = 10.1 Hz), 7.97 (s, 1H); $[M+H]^+_{found}$ = 464.2065; $C_{31}H_{31}NOP$ requires 464.2069.

Diphenyl((phenylamino)(2-(phenylethynyl)phenyl)methyl)phosphine oxide (7b)

Yield: 96% (0.46 g), white solid; Mp: 175–176 °C; ^{31}P NMR ($CDCl_3$) δ 33.6; ^{13}C NMR ($CDCl_3$) δ 53.8 (d, $^1J_{CP}$ = 74.9 Hz), 87.6 (d, J_{CP} = 1.7 Hz), 94.9, 113.6, 118.1, 122.9, 123.1 (d, $^3J_{CP}$ = 5.5 Hz), 127.6 (d, $^3J_{CP}$ = 4.2 Hz), 127.6 (d, $^3J_{CP}$ = 12.2 Hz), 128.0 (d, J_{CP} = 3.9 Hz), 128.67, 128.69, 128.9 (d, $^3J_{CP}$ = 11.8 Hz), 129.1 (d, J_{CP} = 2.8 Hz), 129.3, 129.7 (d, $^1J_{CP}$ = 100.4 Hz), 130.9 (d, $^1J_{CP}$ = 97.0 Hz), 131.3, 131.5 (d, $^2J_{CP}$ = 8.7 Hz), 131.5 (d, $^3J_{CP}$ = 1.8 Hz), 131.8, (d, $^2J_{CP}$ = 9.6 Hz) 131.9 (d, J_{CP} = 3.1 Hz), 132.3 (d, J_{CP} = 2.8 Hz) 137.9 (d, J_{CP} = 1.2 Hz), 146.1 (d, $^2J_{CP}$ = 11.1 Hz); ^{1}H NMR ($CDCl_3$) δ 5.51 (t, 1H, $^2J_{HP}$ = 8.9 Hz), 6.05 (dd, 1H, J_{HH} = 9.2 Hz, J_{HH} = 10.9 Hz), 6.65 (t, 1H, J_{HH} = 7.3 Hz), 6.71 (d, 2H, J_{HH} = 7.8 Hz), 7.05–7.17 (m, 5H), 7.19 (d, 1H, J_{HH} =7.6 Hz), 7.28–7.36 (m, 4H), 7.37–7.42 (m, 3H), 7.43–7.50 (m, 4H), 7.54 (ddd, 1H, J_{HH} =1.5 Hz, J_{HH} = 5.2 Hz, J_{HH} = 7.5 Hz), 7.75 (dt, 1H, J_{HH} = 1.7 Hz, J_{HH} = 7.9 Hz), 7.97 (ddd, 2H, J_{HH} = 1.5 Hz, J_{HH} = 6.8 Hz, J_{HH} = 11.2 Hz); $[M+H]^+_{found}$ = 484.1838; $C_{33}H_{27}NOP$ requires 484.1752.

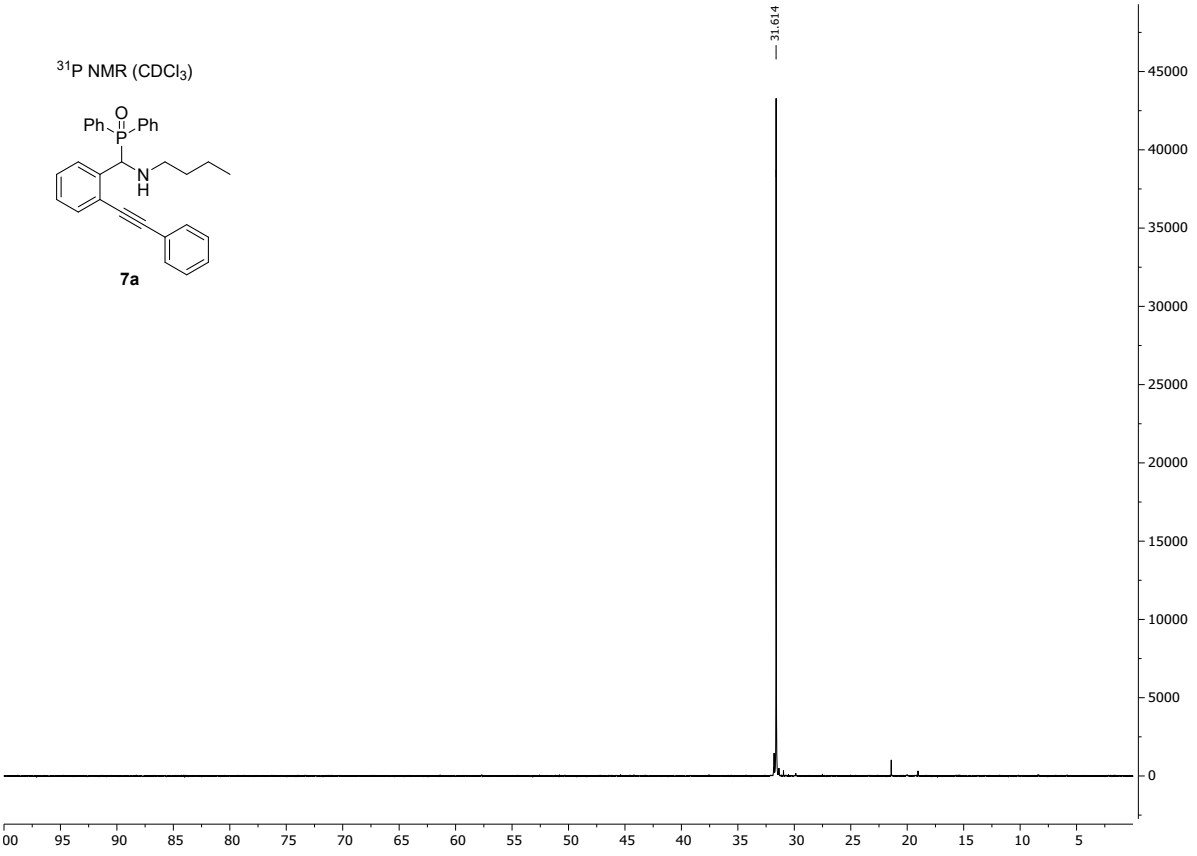
(2,3-Diphenyl-1,2-dihydroisoquinolin-1-yl)diphenylphosphine oxide (8)

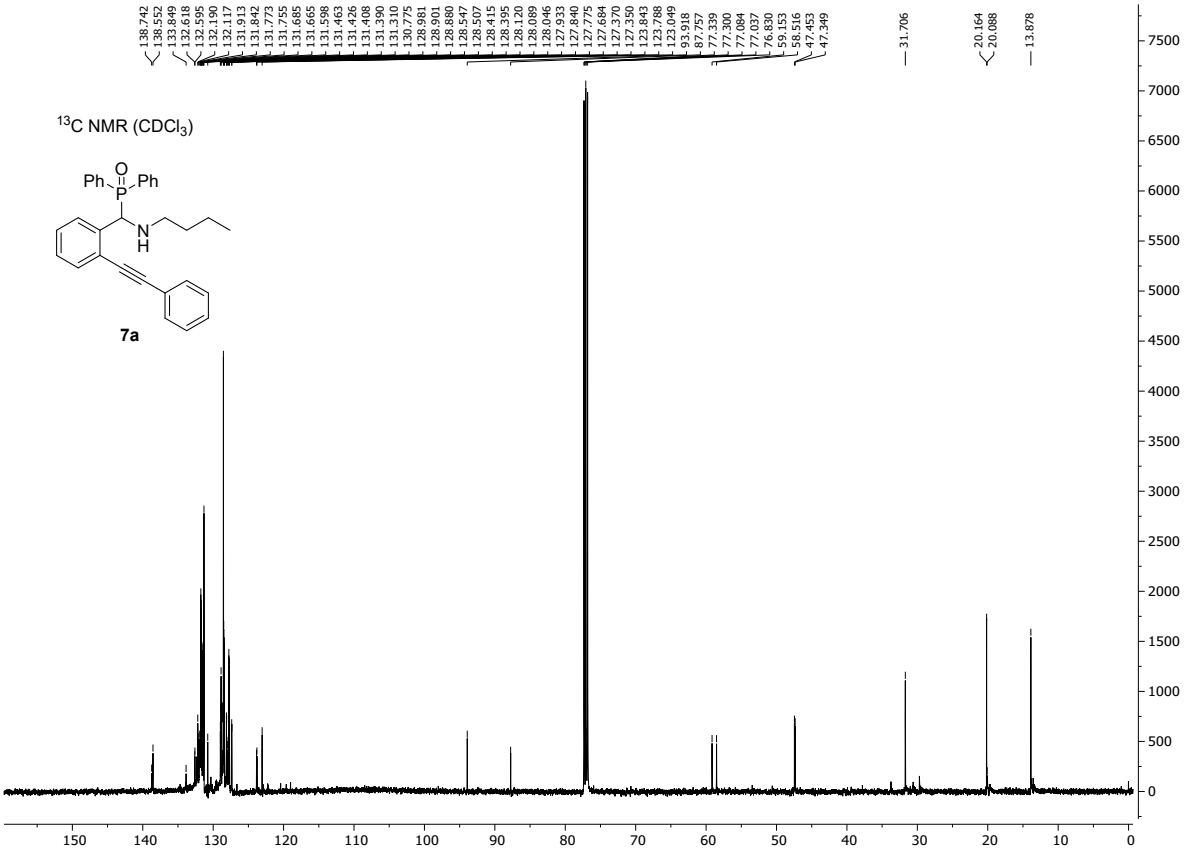
Yield: 91% (0.44 g), white solid; Mp: 235–236 °C; ^{31}P NMR ($CDCl_3$) δ 24.7; ^{13}C NMR ($CDCl_3$) δ 69.5 (d, $^{1}J_{CP}$ = 78.6 Hz), 112.3, 122.8, 123.5 (d, J_{CP} = 1.5 Hz), 124.7 (d, J_{CP} = 2.3 Hz), 125.2 (d, J_{CP} = 6.1), 126.1 (d, J_{CP} = 2.2 Hz), 127.1 (d, J_{CP} = 4.3 Hz), 127.5 (d, J_{CP} = 11.2 Hz), 127.88, 127.9, 128.0, 128.3 (d, J_{CP} = 2.9 Hz), 128.5 (d, J_{CP} = 11.1 Hz), 128.6, 129.1, 131.5, 131.8 (d, J_{CP} = 2.9 Hz), 131.9 (d, J_{CP} = 8.7 Hz), 132.0 (d, J_{CP} = 2.9 Hz), 132.2, 132.8 (d, J_{CP} = 8.6 Hz), 134.4 (d, J_{CP} = 2.9 Hz), 137.1, 142.6, 148.2 (d, J_{CP} = 4.8 Hz); ^{1}H NMR ($CDCl_3$) δ 5.87 (s, 1H), 5.98 (d, 1H, J_{HP} = 13.5 Hz), 6.55 (d, 1H, J_{HH} = 7.5 Hz), 6.91 (t, 1H, J_{HH} = 7.3 Hz), 6.97 (t, 1H, J_{HH} = 7.5 Hz), 7.05 (d, 1H, J_{HH} = 7.6 Hz), 7.13 (d, 2H, J_{HH} = 7.8 Hz), 7.19 (dq, 5H, J_{HH} = 2.9 Hz J_{HH} = 6.9 Hz), 7.24 (t, 3H, J_{HH} = 7.3 Hz), 7.38 (dt, 1H, J_{HH} = 4.4 Hz, J_{HH} = 7.6 Hz), 7.45–7.52 (m, 2H), 7.54 (d, 2H, J_{HH} = 6.9 Hz), 7.58 (t, 1H, J_{HH} = 7.0 Hz), 7.88–7.93 (m, 2H); $[M+H]^{+}_{found}$ = 484.1795; $C_{33}H_{26}NOP$ requires 484.1752.

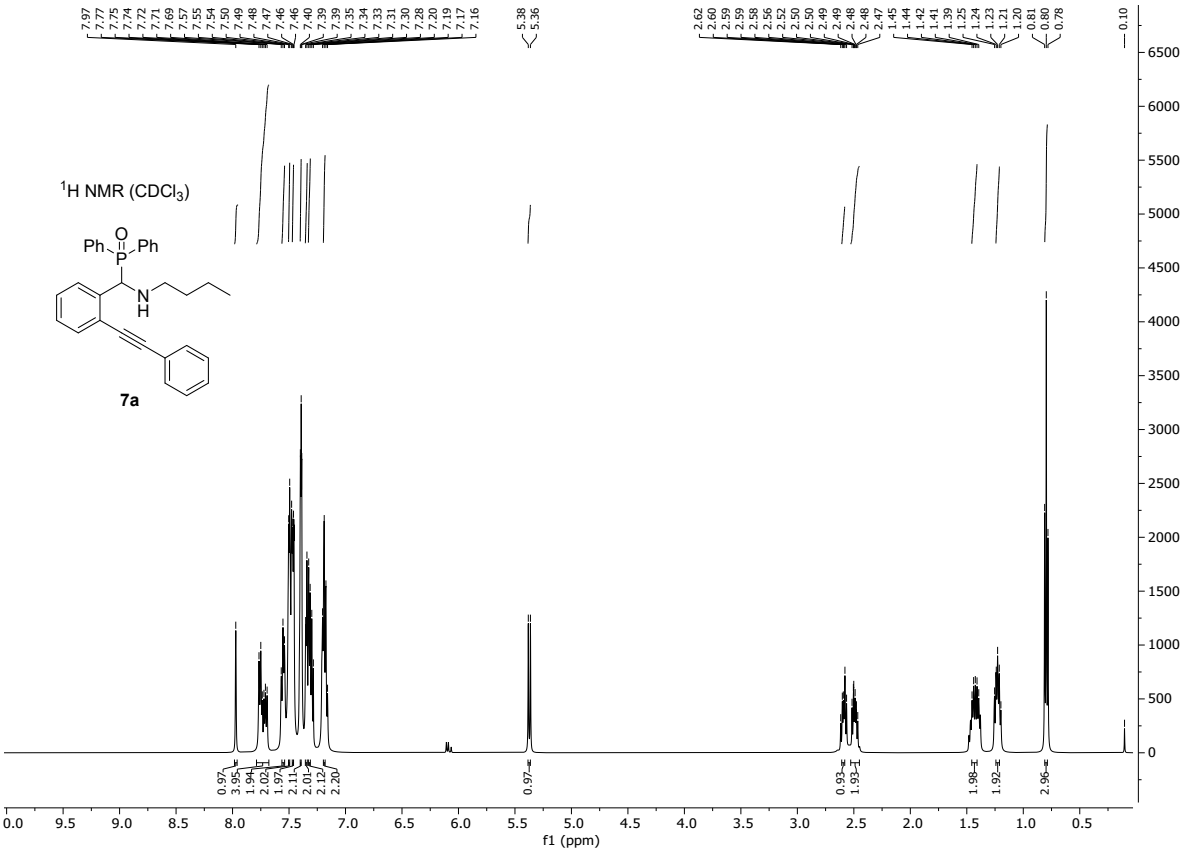
(3-Benzyl-2-phenyl-2*H*-isoindol-1-yl)diphenylphosphine oxide (9)

Yield: 93% (0.44 g), white solid; Mp: 235–236 °C; ^{31}P NMR ($CDCl_3$) δ 13.9; ^{13}C NMR ($CDCl_3$) δ 21.2, 118.9, 120.2, 121.1, 124.0, 126.2 (d, J_{CP} = 11.2 Hz), 126.5, 126.8, 127.6, 128.1, 128.3, 128.7 (d, J_{CP} = 11.6 Hz), 129.1, 129.6 0 (d, J_{CP} = 9.0 Hz), 130.0 (d, J_{CP} = 8.6 Hz), 130.4, 131.0, 131.6, 132.2, 132.8, 133.0, 133.2, 133.4, 134.1, 136.6, 137.2, 137.6, 137.7, 137.8, 138.7; ^{1}H NMR ($CDCl_3$) δ 4.11 (s, 1H), 6.79–6.83 (m, 1H), 6.84–6.87 (m, 1H), 6.90 (ddd, 1H, J_{HH} = 1.1 Hz, J_{HH} = 6.6 Hz, J_{HH} = 8.8 Hz), 6.96 (s, 1H), 7.00 (d, 2H, J_{HH} = 7.5 Hz), 7.06 (s, 1H), 7.13 (dd, 2H, J_{HH} = 1.9 Hz, J_{HH} = 5.1 Hz), 7.22 (d, 2H, J_{HH} = 1.7 Hz), 7.23–7.25 (m, 2H), 7.29 (t, 2H, J_{HH} = 7.4 Hz), 7.49 (dd, 2H, J_{HH} = 7.2 Hz, J_{HH} = 8.5 Hz), 7.54–7.58 (m, 3H), 7.60–7.64 (m, 1H), 7.68 (d, 2H, J_{HH} = 6.8 Hz); $[M+H]^{+}_{found}$ = 484.1867; $C_{33}H_{27}NOP$ requires 484.1752.

^{31}P NMR, ^{13}C NMR and ^{1}H NMR spectra



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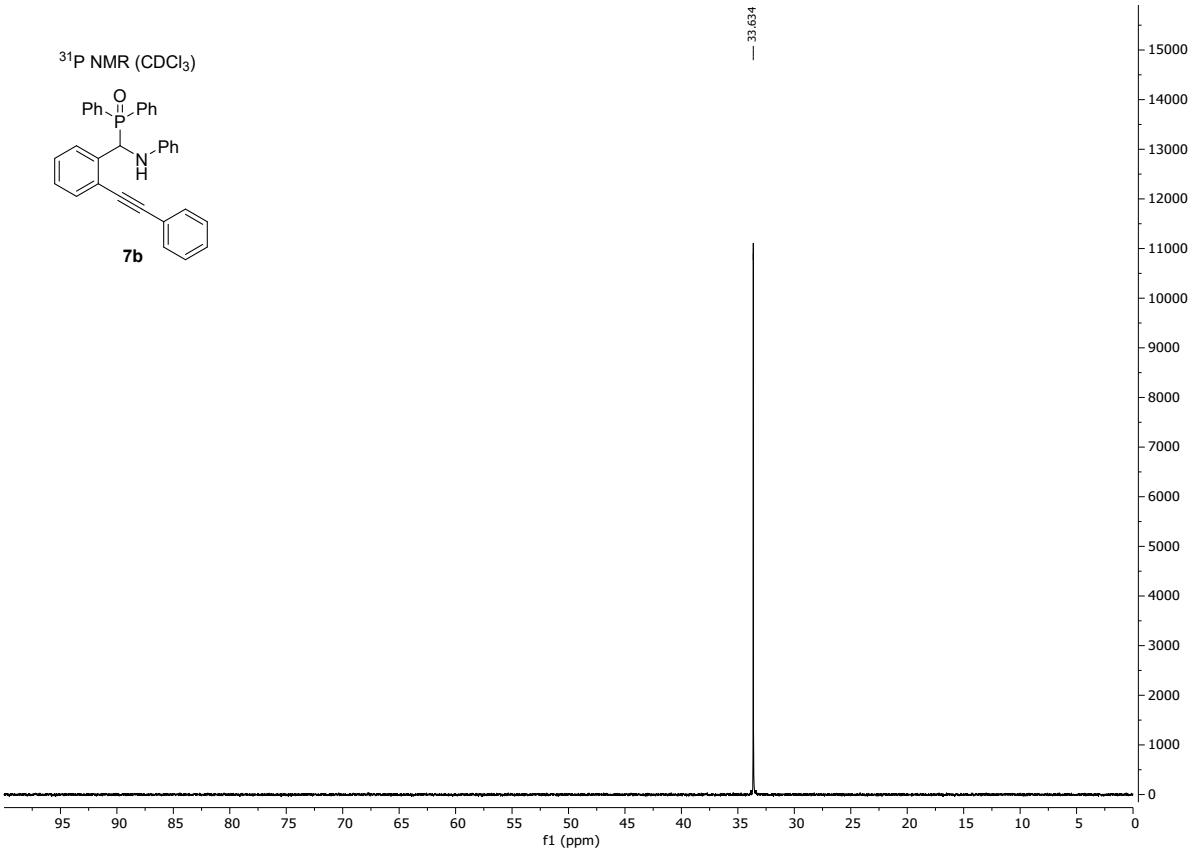
O
P
Ph
N
H
7a
f1 (ppm)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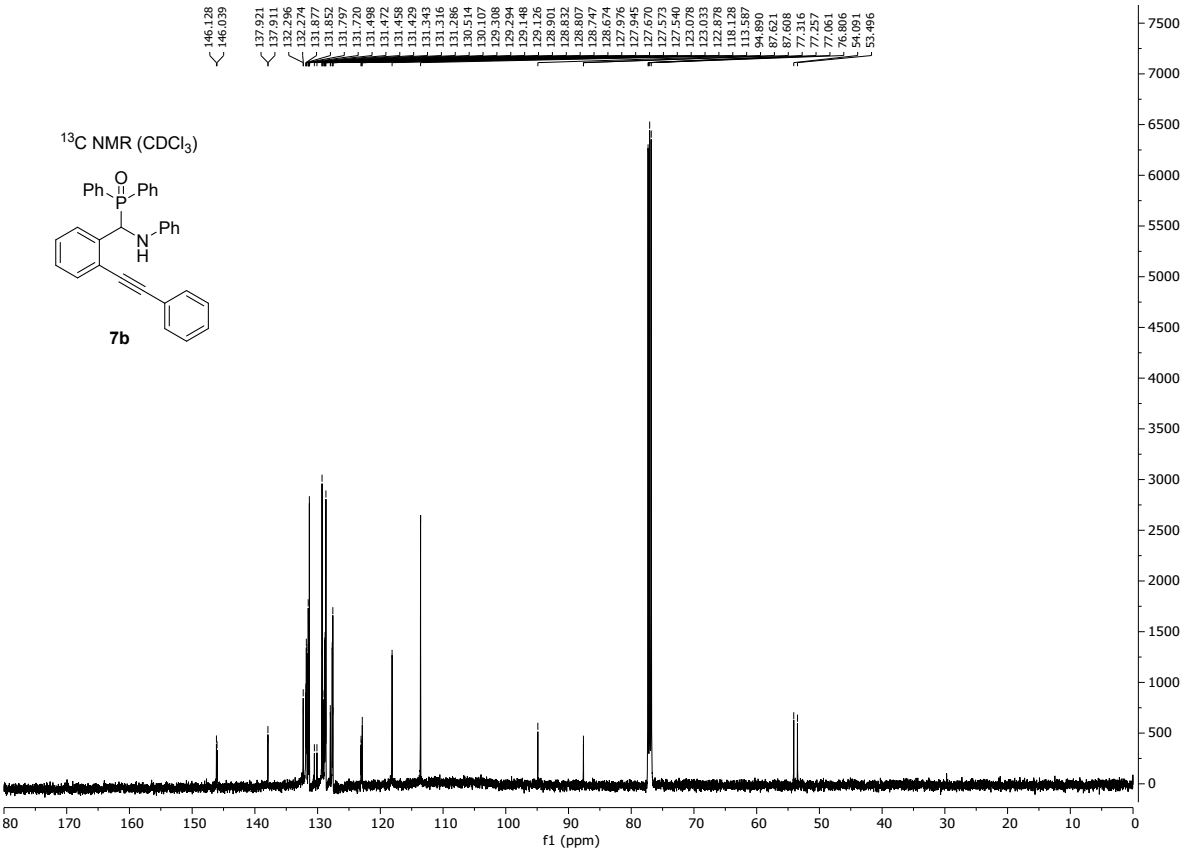
7b
33.634
f1 (ppm)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7b
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146.039
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137.911
132.296
132.274
131.877
131.852
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131.720
131.498
131.472
131.458
131.429
131.343
131.316
131.286
130.514
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129.308
129.294
129.148
129.126
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127.945
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127.573
127.540
123.078
123.033
122.878
118.128
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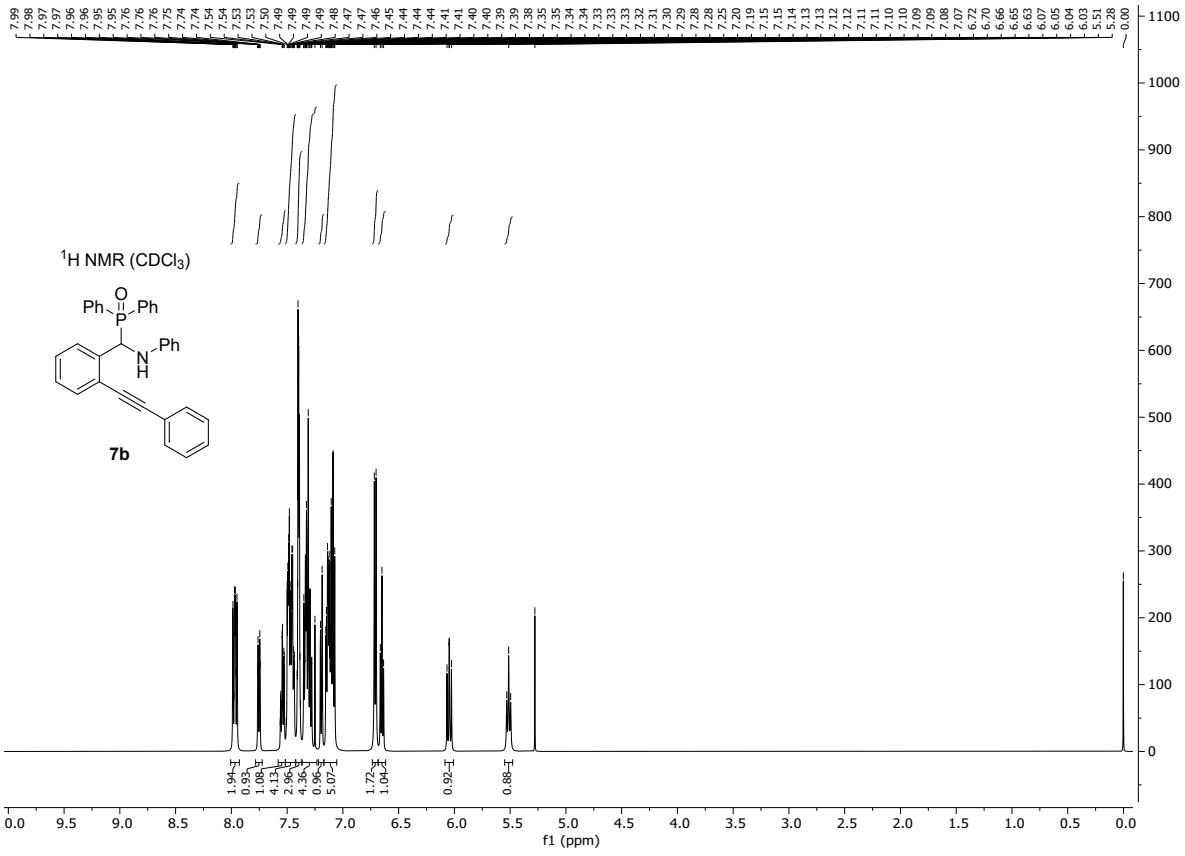
53.496
f1 (ppm)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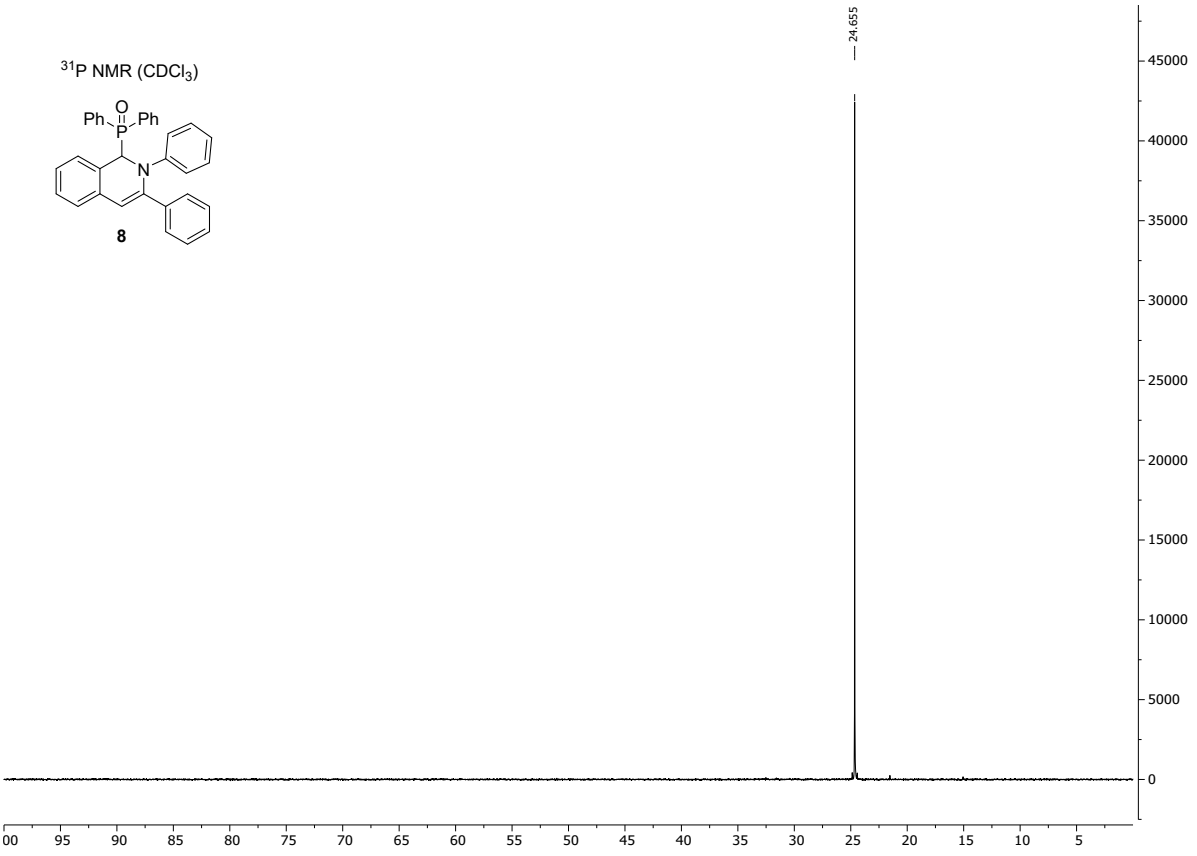
Ph
O
P
Ph
N
H
Ph
7b
f1 (ppm)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P
Ph
N
8
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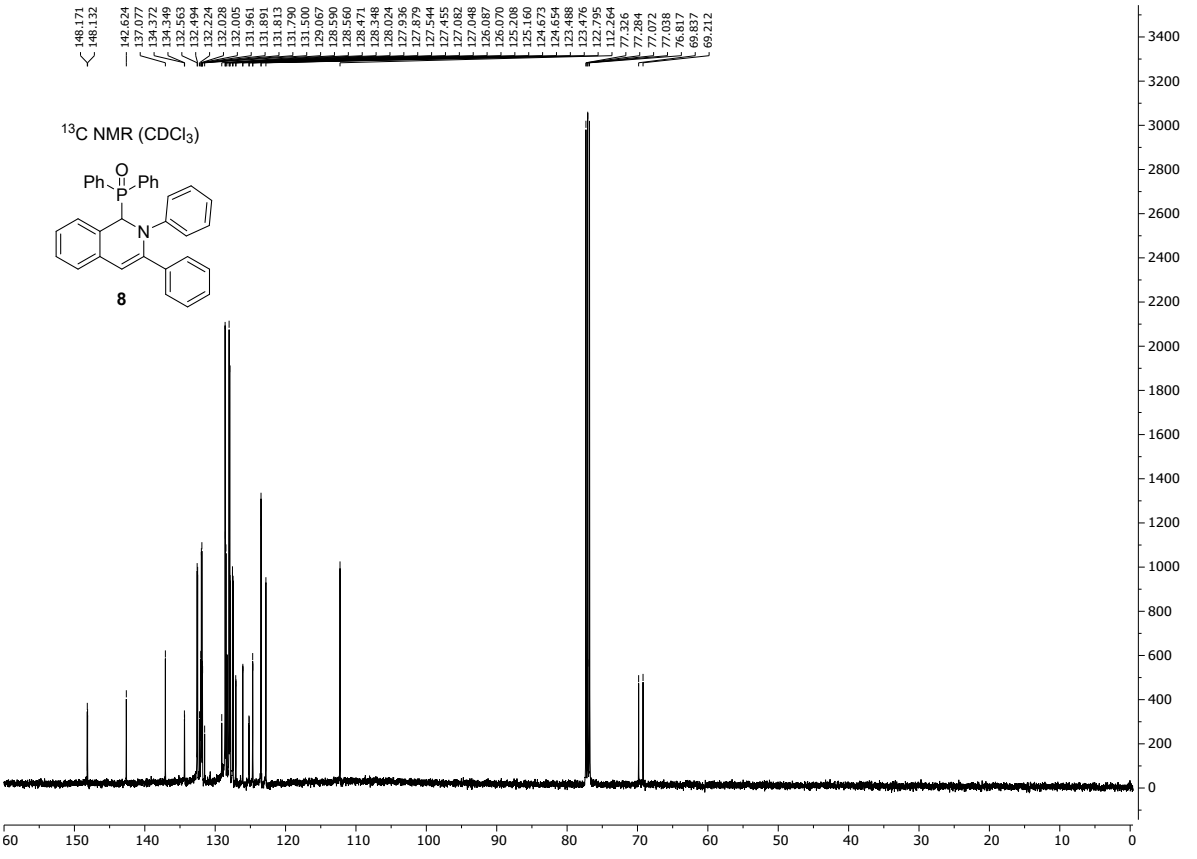
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128.024
127.936
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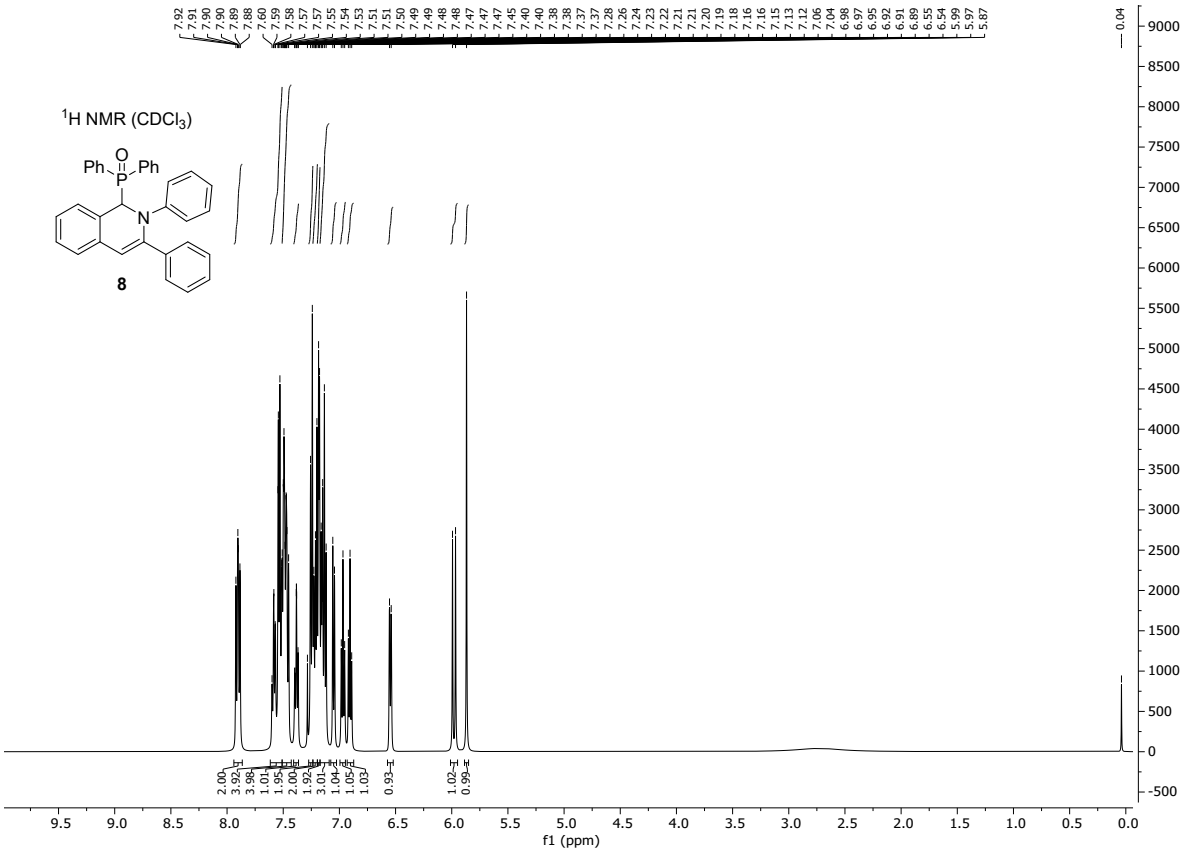
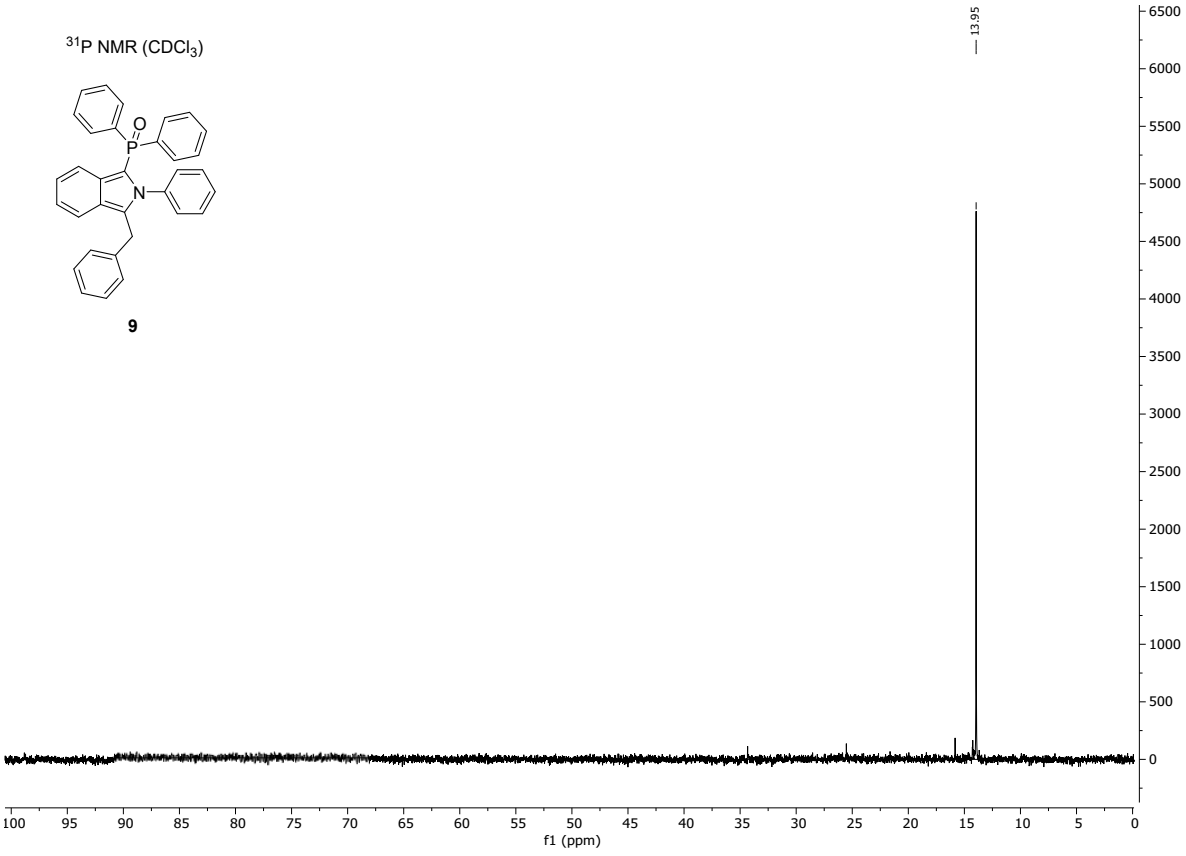
127.544
127.455
127.082
127.048
126.087
126.070
125.208
125.160
124.673
124.654
123.488
123.476
122.795
112.264
77.326
77.284
77.072
77.038
76.817
69.837
69.212
^{13}C NMR ($CDCl_3$)
Ph
O
P
Ph
N
8


^{1}H NMR ($CDCl_3$)
Ph
O
P
Ph
N
8
f1 (ppm)

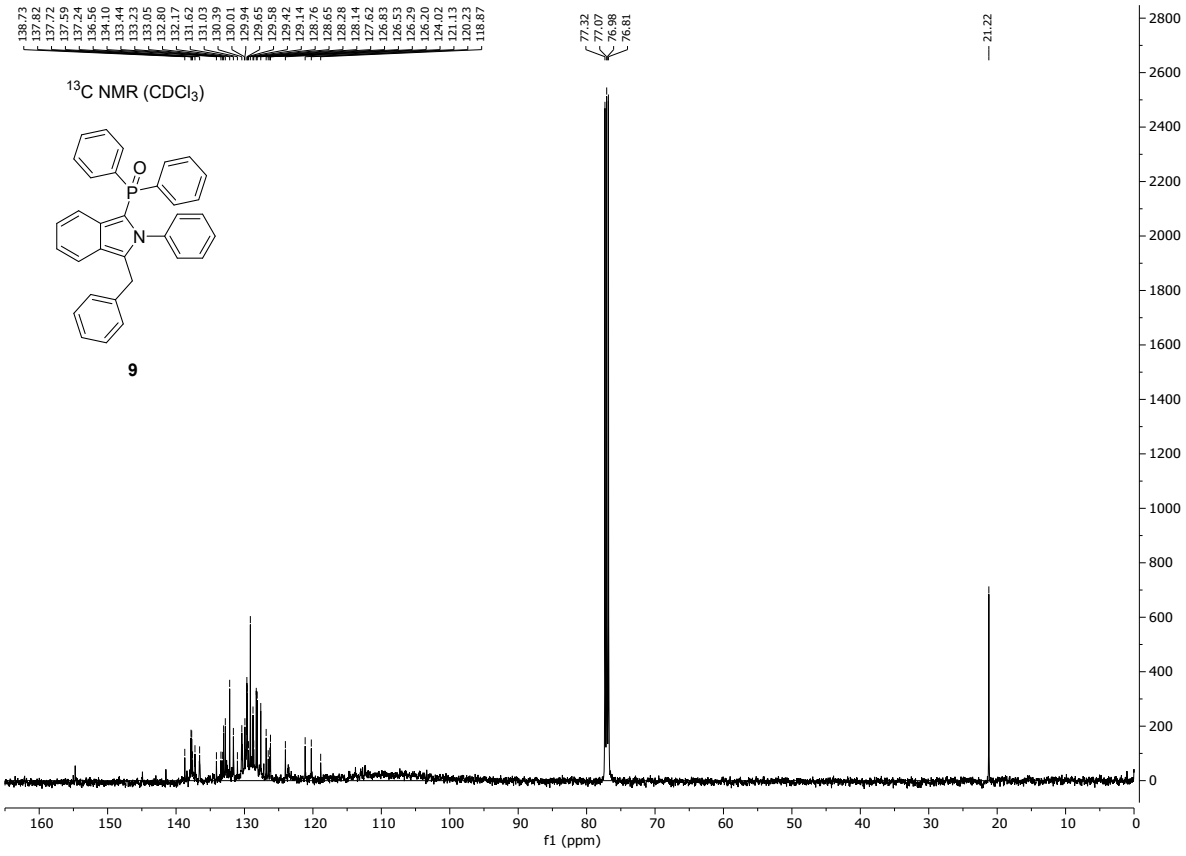
^{31}P NMR ($CDCl_3$)

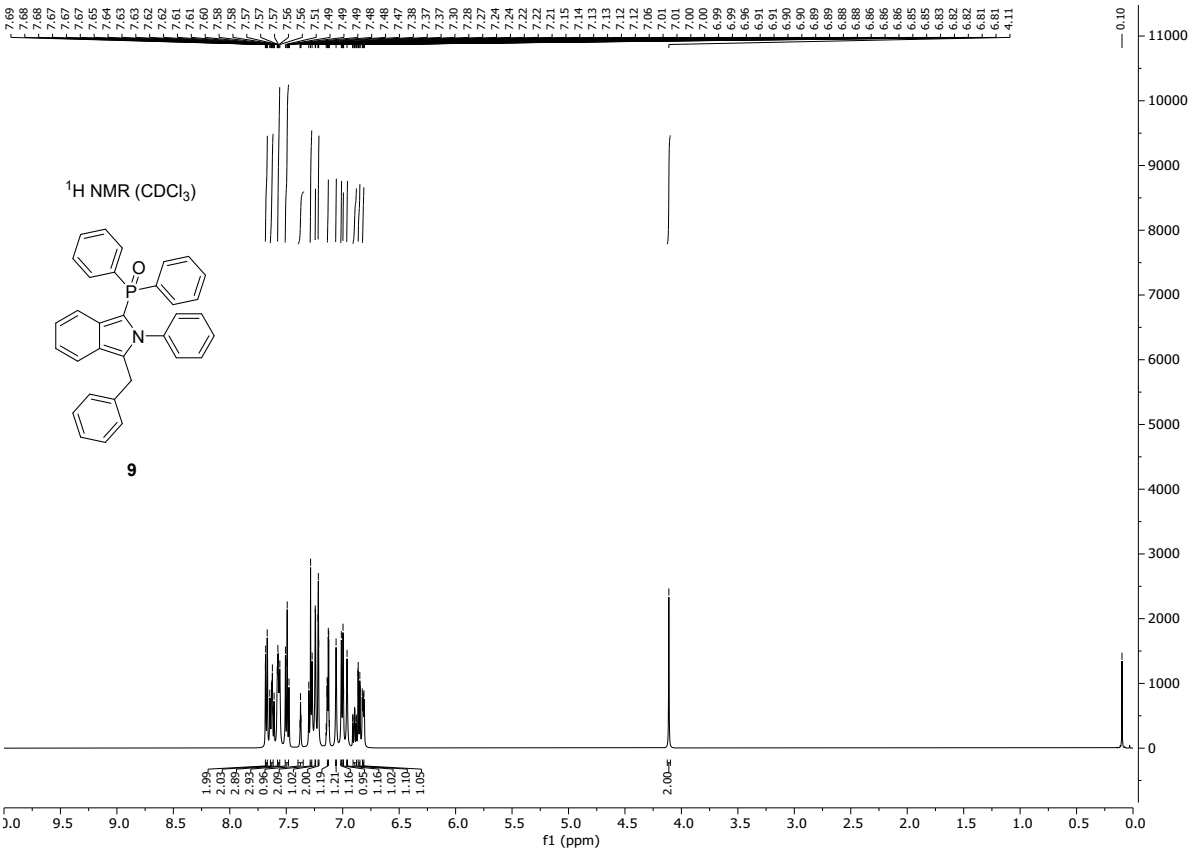
9



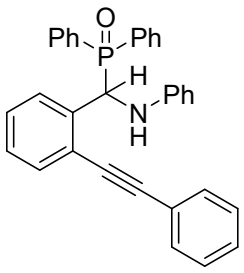
^{13}C NMR ($CDCl_3$)

9




^{1}H NMR ($CDCl_3$)
9
f1 (ppm)

XYZ coordinates and total energies of the investigated systems



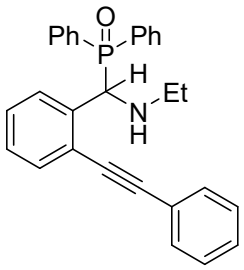
62

E(ωB97X-D/6-311+G**) = -1744.350029

C	-3.462165	-1.591065	-0.863260
C	-2.161892	-2.104456	-0.829499
C	-1.975780	-3.465902	-0.588578
C	-3.067437	-4.293490	-0.352523
C	-4.353622	-3.770567	-0.362926
C	-4.549467	-2.418526	-0.623912
P	-0.767883	-1.020542	-1.276557
C	-0.880671	0.569363	-0.296964
N	-1.939595	1.343746	-0.918942
C	-2.006063	2.732311	-0.712283
C	-1.261913	3.400950	0.261497
C	-1.403872	4.775915	0.426195
C	-2.272559	5.506024	-0.370727
C	-3.009835	4.841300	-1.348096
C	-2.884143	3.473143	-1.514714
C	0.751512	-1.814174	-0.690057
C	1.863769	-1.730804	-1.526474
C	3.090588	-2.225206	-1.101996
C	3.206141	-2.809800	0.152518
C	2.095402	-2.906367	0.984768
C	0.869438	-2.408778	0.568081
O	-0.745304	-0.653192	-2.728842
C	-1.043361	0.384551	1.195184
C	0.079254	0.405969	2.046368

C	-0.088467	0.210429	3.422431
C	-1.349636	0.007271	3.957179
C	-2.461173	0.012679	3.121505
C	-2.303792	0.204212	1.756836
C	1.388344	0.629043	1.521981
C	2.478446	0.769860	1.028407
C	3.741222	0.855159	0.369663
C	4.910038	0.425622	1.006340
C	6.120466	0.446332	0.328742
C	6.179573	0.896524	-0.986237
C	5.021459	1.333066	-1.621586
C	3.807901	1.314894	-0.950456
H	-3.170709	0.233445	1.110069
H	-3.453959	-0.126857	3.533569
H	-1.467022	-0.140431	5.024533
H	0.785695	0.229426	4.062432
H	4.856004	0.066149	2.027193
H	7.021640	0.108772	0.828154
H	7.126633	0.910387	-1.513668
H	5.063154	1.687553	-2.645199
H	2.901169	1.644029	-1.444634
H	-0.978859	-3.890142	-0.590801
H	-2.909818	-5.349504	-0.165155
H	-5.204324	-4.416734	-0.177308
H	-5.552578	-2.007985	-0.646098
H	-3.622331	-0.539623	-1.071980
H	0.012677	-2.465906	1.230495
H	2.186762	-3.359792	1.965159
H	4.166600	-3.186506	0.486232
H	3.958942	-2.139253	-1.744967
H	1.756842	-1.269911	-2.502538
H	-3.468826	2.960198	-2.272081
H	-3.692082	5.394057	-1.984725
H	-2.375095	6.576426	-0.237423

H	-0.817267	5.275811	1.189272
H	-0.570019	2.864524	0.897126
H	-2.007329	1.115969	-1.905610
H	0.105703	1.020451	-0.484797



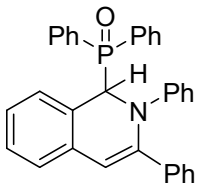
58

E(ωB97X-D/6-311+G**) = -1591.943768

C	3.901270	0.327010	-1.311205
C	3.745233	0.609749	0.050802
C	4.810641	0.373513	0.925555
C	6.005738	-0.142686	0.445435
C	6.153004	-0.426721	-0.908321
C	5.098710	-0.188294	-1.784309
C	2.489020	1.078151	0.538890
C	1.391492	1.395706	0.921636
C	0.063892	1.679610	1.364198
C	-1.037874	1.501693	0.505115
C	-2.313178	1.778911	0.990571
C	-2.509030	2.207147	2.294808
C	-1.419918	2.375418	3.144053
C	-0.141798	2.116884	2.678710
C	-0.839927	1.020572	-0.913619
N	-1.680758	1.690944	-1.901183
C	-1.169479	2.993937	-2.338307
P	-1.061617	-0.817955	-1.148554
O	-0.844087	-1.128292	-2.598247
C	-2.704366	-1.313512	-0.536755
C	-3.831900	-0.587138	-0.931750

C	-5.100860	-1.008353	-0.560566
C	-5.259884	-2.163859	0.197004
C	-4.145974	-2.901729	0.575689
C	-2.873250	-2.481266	0.207701
C	0.168669	-1.569212	-0.048068
C	1.318565	-2.079926	-0.647621
C	2.356437	-2.564397	0.138618
C	2.244145	-2.546053	1.522763
C	1.091016	-2.051943	2.124793
C	0.053926	-1.563265	1.343852
H	-3.156157	1.674076	0.320607
H	-3.512785	2.414694	2.647911
H	-1.566393	2.713644	4.163439
H	0.717827	2.250281	3.324814
H	4.687566	0.588135	1.980568
H	6.825688	-0.325395	1.130835
H	7.087631	-0.831036	-1.280180
H	5.208676	-0.407507	-2.840310
H	3.072230	0.501144	-1.987366
H	-2.012677	-3.071244	0.500733
H	-4.265015	-3.809819	1.155723
H	-6.252348	-2.492185	0.485232
H	-5.968538	-0.434897	-0.866802
H	-3.710970	0.314702	-1.521622
H	-0.834220	-1.161091	1.819093
H	1.003882	-2.037234	3.205255
H	3.059074	-2.914528	2.135956
H	3.258976	-2.939561	-0.330146
H	1.391702	-2.082545	-1.729880
H	-1.711261	1.088203	-2.719169
H	0.227761	1.133981	-1.165063
H	-1.704171	3.242631	-3.259519
C	-1.378934	4.113757	-1.327161
H	-0.098534	2.930536	-2.594966

H	-1.095349	5.070677	-1.773752
H	-2.427740	4.167074	-1.025172
H	-0.774896	3.974097	-0.428714



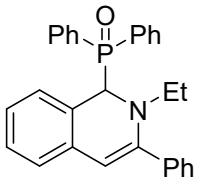
62

E(ωB97X-D/6-311+G**) = -1744.397678

N	0.704166	0.610158	-0.462410
C	1.460072	1.101860	0.620169
C	2.784568	0.477943	0.845382
C	-0.741048	0.734326	-0.335001
P	-1.483000	-0.508137	0.873083
C	-0.413254	-1.978950	0.808965
C	1.265232	0.613879	-1.763339
C	-1.146973	2.110077	0.119225
C	-0.310337	2.722158	1.060523
C	-0.685437	3.956157	1.592680
C	-1.863231	4.567743	1.186776
C	-2.680751	3.957866	0.240256
C	-2.319814	2.726405	-0.293733
O	-1.652410	-0.014306	2.271531
C	-3.085187	-0.924937	0.106704
H	-0.046270	4.437419	2.325724
H	-2.146289	5.525245	1.609425
H	-3.601841	4.435491	-0.073292
H	-2.962180	2.233753	-1.017248
C	-0.287323	-2.813478	-0.300620
C	0.594531	-3.885817	-0.271047
C	1.345167	-4.137358	0.873282
C	1.209529	-3.318704	1.987213
C	0.334768	-2.239752	1.956226

H	-0.886861	-2.647737	-1.188301
H	0.690382	-4.529676	-1.137966
H	2.032002	-4.976209	0.895723
H	1.792926	-3.512342	2.879881
H	0.222076	-1.587186	2.814693
C	-4.186999	-0.956138	0.960668
C	-5.448754	-1.257260	0.462297
C	-5.618811	-1.524022	-0.890847
C	-4.525889	-1.485186	-1.750259
C	-3.264468	-1.183466	-1.253961
H	-4.039173	-0.729719	2.010961
H	-6.301239	-1.277821	1.131662
H	-6.604088	-1.756298	-1.279346
H	-4.657046	-1.683939	-2.807877
H	-2.427930	-1.144075	-1.944520
C	2.298254	1.489871	-2.098137
C	2.855358	1.461579	-3.369393
C	2.379688	0.579415	-4.331679
C	1.342327	-0.286516	-4.004981
C	0.796130	-0.278443	-2.729686
H	2.660056	2.196033	-1.360605
H	3.659776	2.147163	-3.611292
H	2.812500	0.565507	-5.325034
H	0.966064	-0.987306	-4.742105
H	0.019276	-0.988516	-2.473011
C	3.810801	1.185435	1.476945
C	5.041648	0.589556	1.712786
C	5.273284	-0.720093	1.305860
C	4.264952	-1.425013	0.659353
C	3.032428	-0.831573	0.427737
H	3.650437	2.217702	1.767813
H	5.826808	1.153694	2.203732
H	6.237140	-1.183749	1.483867
H	4.434574	-2.445485	0.334206

H	2.250621	-1.389394	-0.072741
C	0.937130	2.058217	1.412005
H	1.449863	2.353551	2.318585
H	-1.182026	0.524594	-1.308777



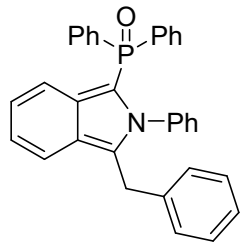
58

E(ωB97X-D/6-311+G**) =-1591.994744

C	-1.029429	2.356771	-0.648478
C	-1.593833	1.365545	0.066362
N	-0.827980	0.622682	0.991807
C	0.599484	0.611403	0.721495
C	1.156656	1.972497	0.401325
C	0.327617	2.805485	-0.361897
C	0.817083	4.044802	-0.775701
C	2.099261	4.447091	-0.426989
C	2.909173	3.620176	0.345068
C	2.433986	2.380937	0.759674
C	-1.203414	0.809677	2.398961
C	-3.008328	0.951103	-0.070880
C	-4.003039	1.868541	-0.419137
C	-5.320072	1.458893	-0.575706
C	-5.667620	0.127441	-0.372508
C	-4.688088	-0.789554	-0.008273
C	-3.370196	-0.381890	0.144780
P	1.025730	-0.536919	-0.702143
C	2.737177	-1.037656	-0.313922
C	3.676864	-0.857511	-1.327323
C	5.011251	-1.179334	-1.107818
C	5.414250	-1.679833	0.123865
C	4.481845	-1.857935	1.141123

C	3.149170	-1.535328	0.923739
C	-0.077988	-1.970475	-0.509672
C	-0.206499	-2.705677	0.668091
C	-1.132980	-3.735667	0.750801
C	-1.936519	-4.038179	-0.345248
C	-1.808629	-3.311417	-1.521778
C	-0.882931	-2.277298	-1.604702
O	0.932318	0.047461	-2.072710
H	0.185045	4.695878	-1.370834
H	2.469641	5.410965	-0.757914
H	3.911371	3.934219	0.613271
H	3.067859	1.719094	1.342118
H	0.399844	-2.472303	1.535128
H	-1.232065	-4.300548	1.671014
H	-2.662089	-4.841357	-0.278289
H	-2.436367	-3.541286	-2.375052
H	-0.782689	-1.686358	-2.508240
H	3.345737	-0.454624	-2.278173
H	5.737308	-1.034463	-1.899737
H	6.455553	-1.929088	0.295123
H	4.794072	-2.245773	2.104195
H	2.438907	-1.674477	1.732090
H	-3.744277	2.913533	-0.549435
H	-6.080278	2.183719	-0.845084
H	-6.697345	-0.190851	-0.491236
H	-4.947634	-1.830362	0.151729
H	-2.604012	-1.097250	0.418521
H	-1.585145	2.845433	-1.439245
H	1.106566	0.193149	1.593681
C	-0.969607	-0.427978	3.252128
H	-0.671433	1.675890	2.819572
H	-2.266394	1.057067	2.415050
H	-1.287204	-0.237137	4.280414
H	-1.538314	-1.274043	2.860587

H	0.086865	-0.711495	3.287639



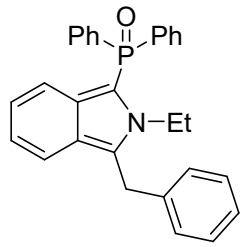
62

E(ωB97X-D/6-311+G**) = -1744.405116

N	0.512967	0.269508	-0.987627
C	1.758341	0.604899	-1.428297
C	2.768983	-0.416983	-1.835001
C	-0.199633	1.391384	-0.595897
P	-1.738419	1.442637	0.324635
C	-1.321027	0.842216	1.995593
C	0.010363	-1.072671	-1.035863
C	0.651268	2.486220	-0.782204
C	1.884274	1.985763	-1.309921
C	2.959505	2.871111	-1.589771
C	2.787194	4.200818	-1.339862
C	1.557900	4.700660	-0.811026
C	0.503994	3.879543	-0.532652
O	-2.329472	2.814729	0.311190
C	-2.870441	0.202154	-0.383601
H	3.895086	2.495703	-1.991301
H	3.592145	4.897875	-1.544831
H	1.465380	5.765936	-0.629885
H	-0.431620	4.255317	-0.137596
C	-2.347457	0.668184	2.927258
C	-2.056641	0.255000	4.219712
C	-0.737248	0.019147	4.595204
C	0.289885	0.208112	3.679338
C	-0.000630	0.622571	2.384409
H	-3.375981	0.860346	2.639388

H	-2.858466	0.120450	4.936886
H	-0.511238	-0.303811	5.605415
H	1.320122	0.037104	3.970989
H	0.806237	0.781295	1.676774
C	-3.108734	-1.051835	0.174490
C	-3.988376	-1.933577	-0.441703
C	-4.631204	-1.569095	-1.617814
C	-4.401151	-0.315710	-2.176748
C	-3.528896	0.569567	-1.559227
H	-2.597006	-1.352455	1.080924
H	-4.163948	-2.909948	-0.004452
H	-5.315785	-2.259563	-2.098290
H	-4.909358	-0.024906	-3.089314
H	-3.360785	1.555967	-1.978660
C	-0.666433	-1.492367	-2.174709
C	-1.138189	-2.794537	-2.246919
C	-0.927257	-3.670474	-1.186632
C	-0.246595	-3.242825	-0.054107
C	0.227237	-1.938906	0.025560
H	-0.831441	-0.789176	-2.982466
H	-1.679769	-3.121813	-3.126483
H	-1.297982	-4.687684	-1.244081
H	-0.075833	-3.923873	0.771370
H	0.771992	-1.598905	0.897119
H	3.589239	0.103681	-2.337887
C	3.310147	-1.207397	-0.655325
H	2.344352	-1.109705	-2.567842
C	3.463724	-2.588173	-0.737461
C	3.917194	-3.319017	0.354911
C	4.223750	-2.673701	1.546575
C	4.081613	-1.292421	1.634891
C	3.628453	-0.565586	0.541509
H	3.200802	-3.101458	-1.657164
H	4.021227	-4.395628	0.276839

H	4.571638	-3.242321	2.401640
H	4.324238	-0.779129	2.559053
H	3.504574	0.510316	0.619923



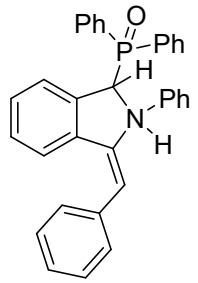
58

E(ωB97X-D/6-311+G**) = -1592.002992

C	-2.494976	1.870715	2.175592
C	-1.456993	1.141194	1.589360
C	-0.157012	1.642750	1.635203
C	0.099804	2.869588	2.237299
C	-0.938707	3.596114	2.805474
C	-2.236477	3.093108	2.779136
P	-1.857300	-0.478743	0.852780
C	-0.323021	-1.141002	0.205072
N	0.499960	-0.583524	-0.757544
C	1.665088	-1.276596	-0.860393
C	1.621256	-2.319841	0.061718
C	0.365376	-2.236756	0.741867
C	0.056165	-3.173915	1.766579
C	0.981715	-4.130889	2.069405
C	2.236206	-4.210161	1.392969
C	2.561988	-3.325864	0.406308
C	0.161178	0.538380	-1.630409
C	2.807383	-0.821603	-1.708830
C	3.459207	0.452245	-1.191880
C	3.948624	1.407837	-2.079735
C	4.540158	2.576656	-1.612663
C	4.648576	2.804421	-0.246383
C	4.164790	1.854922	0.647525

C	3.573653	0.688629	0.178290
C	-2.939436	-0.112796	-0.572655
C	-3.538472	-1.214353	-1.188567
C	-4.347786	-1.038977	-2.302224
C	-4.570090	0.238768	-2.806965
C	-3.990514	1.339854	-2.189062
C	-3.179668	1.165413	-1.072840
O	-2.506131	-1.427629	1.806296
H	3.517169	-3.389295	-0.104736
H	2.936376	-4.989191	1.673595
H	0.763811	-4.854638	2.847212
H	-0.894835	-3.110297	2.279816
H	-2.732520	2.031344	-0.596189
H	-4.171111	2.337462	-2.573371
H	-5.200855	0.375560	-3.678283
H	-4.807319	-1.898831	-2.776247
H	-3.368189	-2.207661	-0.786743
H	0.663128	1.075210	1.208933
H	1.113962	3.252153	2.263034
H	-0.738136	4.551945	3.276641
H	-3.046057	3.652758	3.233734
H	-3.504862	1.473528	2.165400
H	3.192355	-0.046463	0.880348
H	4.249004	2.021353	1.715954
H	5.106600	3.716162	0.120022
H	4.912050	3.311528	-2.318030
H	3.860405	1.239675	-3.149166
H	1.067485	1.126705	-1.783065
C	-0.431197	0.087523	-2.959014
H	-0.535451	1.183986	-1.099402
H	-0.676512	0.960876	-3.567858
H	0.276003	-0.533096	-3.514295
H	-1.345258	-0.487473	-2.802253
H	2.501237	-0.673412	-2.749265

H	3.549418	-1.625231	-1.726113



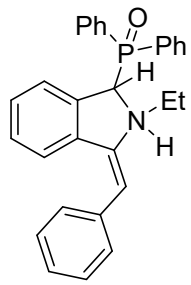
62

E(ωB97X-D/6-311+G**) = -1744.2793309

C	3.710198	-1.787605	-0.471523
C	2.635730	-1.388312	-1.264509
C	1.969148	-2.343895	-2.038244
C	2.334982	-3.680865	-1.977241
C	3.384843	-4.075270	-1.153898
C	4.079117	-3.126459	-0.414406
P	2.086149	0.343201	-1.388816
C	2.794508	1.278324	-0.001429
C	3.260064	2.556324	-0.318412
C	3.811944	3.363563	0.667553
C	3.912941	2.896294	1.972327
C	3.468390	1.617626	2.289224
C	2.911466	0.809716	1.307938
C	0.228383	0.210836	-1.260632
C	-0.561819	1.492137	-1.092831
C	-1.839985	1.218680	-0.607050
C	-2.765658	2.248098	-0.455212
C	-2.388957	3.543771	-0.786996
C	-1.113752	3.809599	-1.280079
C	-0.192684	2.779590	-1.447833
C	-2.117492	-0.179061	-0.310214
C	-2.997185	-1.071957	-0.092215
C	-4.427628	-0.928904	0.025008
C	-5.274713	-1.103951	-1.081523

C	-6.648501	-0.950510	-0.957110
C	-7.222581	-0.634070	0.270051
C	-6.394605	-0.475315	1.377085
C	-5.019612	-0.623935	1.262852
N	-0.424914	-0.748638	-0.335394
C	0.067574	-0.902449	1.014250
C	0.680390	-2.095507	1.374899
C	1.114113	-2.280394	2.682647
C	0.926259	-1.279126	3.626806
C	0.298492	-0.093295	3.259618
C	-0.135806	0.100460	1.957214
O	2.368604	1.006207	-2.697522
H	-3.760021	2.026176	-0.084768
H	-3.098394	4.354594	-0.665460
H	-0.837377	4.823320	-1.545825
H	0.784087	2.975729	-1.873045
H	4.263471	-1.057986	0.106667
H	4.912780	-3.426941	0.209772
H	3.670062	-5.119876	-1.102361
H	1.806646	-4.413007	-2.576824
H	1.168566	-2.047503	-2.708661
H	2.578062	-0.185344	1.571527
H	3.551578	1.244461	3.303565
H	4.345037	3.526049	2.742074
H	4.168015	4.355334	0.414016
H	3.198540	2.899285	-1.344990
H	-4.841537	-1.358160	-2.042808
H	-7.278352	-1.083279	-1.830913
H	-8.296457	-0.520767	0.363715
H	-6.824200	-0.235091	2.344455
H	-4.384919	-0.506556	2.134877
H	0.001954	-0.164479	-2.267712
H	-0.515056	-1.666432	-0.758609
H	-0.628619	1.022359	1.678948

H	0.141341	0.689176	3.992583
H	1.258146	-1.425763	4.648171
H	1.593527	-3.212020	2.959132
H	0.831064	-2.875323	0.635976



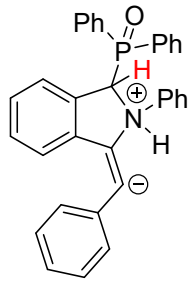
58

E(ωB97X-D/6-311+G**) = -1591.878289

C	-2.290691	2.772903	-0.734263
C	-2.974770	1.570489	-0.554205
C	-4.324937	1.608240	-0.192244
C	-4.964009	2.821647	0.017309
C	-4.264481	4.013491	-0.138160
C	-2.929652	3.988326	-0.520370
P	-2.244379	-0.053983	-0.934718
O	-2.663317	-0.619205	-2.252521
C	-2.699571	-1.148980	0.445521
C	-2.644202	-2.521153	0.192232
C	-2.926552	-3.430697	1.202840
C	-3.285753	-2.977862	2.466553
C	-3.373137	-1.613005	2.716897
C	-3.080872	-0.701971	1.711621
C	-0.393457	0.205332	-0.992104
N	0.342397	0.871184	0.096023
C	2.080964	0.312017	-0.132992
C	1.750558	-0.895200	-0.870787
C	0.441573	-1.022709	-1.333710
C	0.068056	-2.117103	-2.103007
C	1.005771	-3.111180	-2.362708

C	2.307664	-2.999713	-1.880750
C	2.690172	-1.888140	-1.143502
C	-0.007250	0.671742	1.516613
C	2.958616	1.060949	0.378536
C	4.390313	1.045656	0.495888
C	5.018319	0.423671	1.588854
C	6.401447	0.403060	1.698530
C	7.201268	1.007786	0.734030
C	6.590282	1.638410	-0.345212
C	5.208083	1.665177	-0.464204
H	3.705436	-1.774588	-0.780353
H	3.031223	-3.778882	-2.092539
H	0.720757	-3.971504	-2.957480
H	-0.931564	-2.174078	-2.517077
H	-4.880646	0.683655	-0.078876
H	-6.010694	2.837189	0.298195
H	-4.763253	4.961550	0.027574
H	-2.384781	4.914538	-0.660947
H	-1.259355	2.783795	-1.065984
H	-3.152576	0.359014	1.921111
H	-3.669190	-1.256733	3.696911
H	-3.507085	-3.688447	3.254922
H	-2.870643	-4.493852	1.000177
H	-2.384326	-2.872735	-0.798562
H	4.745025	2.165135	-1.307832
H	7.197350	2.118935	-1.105685
H	8.281188	0.993023	0.824909
H	6.859164	-0.089667	2.550321
H	4.406482	-0.044790	2.352534
H	-0.322808	0.874727	-1.860387
H	0.439578	1.864080	-0.074138
H	0.668560	1.344085	2.053024
H	-1.029078	1.019143	1.691354
C	0.201122	-0.748281	2.020497

H	-0.176724	-0.814065	3.043108
H	-0.327540	-1.491880	1.424875
H	1.261705	-0.999968	2.023403



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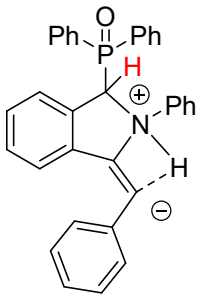
E(ωB97X-D/6-311+G**) = -1744.280485

C	4.200829	-1.439144	-0.855589
C	2.814635	-1.477399	-1.031518
C	2.167686	-2.713764	-1.020885
C	2.881348	-3.884063	-0.793678
C	4.254316	-3.831148	-0.591070
C	4.914454	-2.608002	-0.632528
P	1.958120	0.079948	-1.424881
O	2.148668	0.552564	-2.828023
C	0.141423	-0.278082	-1.229624
N	-0.416284	-0.834182	0.053807
C	-1.965634	-0.545196	-0.016880
C	-2.013347	0.653143	-0.855348
C	-0.817738	0.855554	-1.547688
C	-3.087396	1.516610	-1.051698
C	-2.938391	2.573165	-1.942782
C	-1.748970	2.756901	-2.644466
C	-0.677111	1.886455	-2.463079
C	0.155091	-0.376161	1.320606
C	-0.073352	0.919269	1.767601
C	0.420334	1.295975	3.005401
C	1.122367	0.387754	3.792976
C	1.336404	-0.904137	3.336712

C	0.850314	-1.291280	2.091990
C	-2.746222	-1.440244	0.538737
C	-4.184439	-1.233488	0.501666
C	-4.845246	-0.568993	1.548939
C	-6.215857	-0.353965	1.507186
C	-6.974284	-0.805326	0.430857
C	-6.335442	-1.484260	-0.602212
C	-4.964981	-1.702355	-0.567786
C	2.498097	1.309047	-0.202370
C	3.163848	0.994062	0.982039
C	3.560239	2.002916	1.848374
C	3.282882	3.330470	1.546868
C	2.619524	3.651407	0.368069
C	2.238859	2.646922	-0.510804
H	-4.018600	1.353305	-0.522581
H	-3.765250	3.256453	-2.101464
H	-1.658932	3.575005	-3.349810
H	0.235114	1.989112	-3.038860
H	4.726187	-0.491289	-0.896635
H	5.988645	-2.564189	-0.495351
H	4.811978	-4.743800	-0.414775
H	2.364014	-4.836356	-0.785750
H	1.104008	-2.792424	-1.215361
H	3.358578	-0.037586	1.245741
H	4.074932	1.747687	2.767404
H	3.587525	4.116607	2.228762
H	2.407868	4.686278	0.125322
H	1.749013	2.900472	-1.442729
H	-0.633291	1.619662	1.162130
H	0.251686	2.306177	3.358381
H	1.495729	0.688928	4.764898
H	1.871813	-1.620861	3.948101
H	1.006305	-2.303264	1.734354
H	-4.480182	-2.234950	-1.379351

H	-6.911217	-1.849400	-1.446803
H	-8.045230	-0.639810	0.402788
H	-6.697836	0.169929	2.326704
H	-4.265183	-0.218297	2.396422
H	-0.023912	-1.061641	-1.981092
H	-0.386367	-1.852052	0.062203



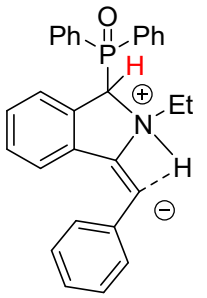
58

E(ωB97X-D/6-311+G**) = -1744.261535

C	3.800946	-1.995555	-1.224338
C	2.430430	-1.767307	-1.068840
C	1.595963	-2.831825	-0.731296
C	2.125964	-4.101157	-0.528519
C	3.490753	-4.315943	-0.668278
C	4.328114	-3.262222	-1.021081
P	1.828800	-0.092015	-1.436853
O	2.030571	0.330988	-2.855875
C	0.001399	-0.119598	-1.119641
N	-0.569441	-0.487722	0.213668
C	-1.991333	0.018016	0.135972
C	-1.935660	1.215073	-0.700429
C	-0.760158	1.160509	-1.466384
C	-2.854506	2.236440	-0.893411
C	-2.580009	3.206642	-1.854495
C	-1.421203	3.142030	-2.620461
C	-0.504420	2.104458	-2.445151
C	0.138571	-0.084381	1.416140
C	0.198776	1.247343	1.816939

C	0.833374	1.570090	3.005705
C	1.396359	0.573487	3.797664
C	1.325038	-0.751961	3.394836
C	0.692925	-1.083754	2.201045
C	-2.741084	-1.045572	0.437010
C	-4.199339	-1.046483	0.445090
C	-4.902943	-2.094965	-0.162137
C	-6.290398	-2.100440	-0.191159
C	-7.010176	-1.077664	0.419128
C	-6.327702	-0.046634	1.055620
C	-4.939107	-0.027976	1.064244
C	2.660702	1.022760	-0.269505
C	3.379763	0.576371	0.838182
C	4.012059	1.489246	1.671388
C	3.923428	2.850563	1.409292
C	3.210377	3.301347	0.303754
C	2.589311	2.391488	-0.540040
H	-3.767591	2.270140	-0.312028
H	-3.283572	4.016368	-2.012443
H	-1.230295	3.899169	-3.372390
H	0.378487	2.020977	-3.067972
H	4.454990	-1.178321	-1.510137
H	5.392086	-3.429222	-1.142962
H	3.902585	-5.306386	-0.510819
H	1.468217	-4.921890	-0.266484
H	0.527309	-2.689560	-0.625289
H	3.435226	-0.481324	1.064736
H	4.565752	1.134539	2.533017
H	4.414064	3.561815	2.064549
H	3.146581	4.362475	0.091645
H	2.055438	2.740959	-1.415622
H	-0.241041	2.023624	1.203870
H	0.891124	2.607380	3.313802
H	1.887343	0.833435	4.728492

H	1.752830	-1.535061	4.010133
H	0.622306	-2.116709	1.882448
H	-4.408937	0.769036	1.575778
H	-6.880096	0.747354	1.547096
H	-8.094295	-1.090475	0.408257
H	-6.814961	-2.913581	-0.681423
H	-4.342540	-2.904160	-0.617844
H	-0.346478	-0.897456	-1.815478
H	-1.232290	-1.491290	0.390117



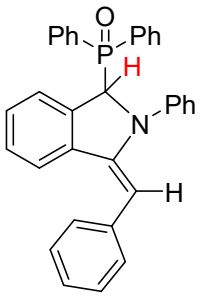
58

E(ωB97X-D/6-311+G**) = -1591.862394

C	-2.756716	-2.406021	-0.031904
C	-2.775127	-1.035193	0.234047
C	-3.375282	-0.570578	1.404359
C	-3.916678	-1.467756	2.315665
C	-3.867671	-2.833311	2.060143
C	-3.294652	-3.301026	0.882867
P	-2.014489	0.064164	-0.998835
C	-0.169354	0.117046	-0.787623
N	0.503305	0.580265	0.460255
C	1.900348	0.049402	0.333790
C	1.788176	-1.200386	-0.414786
C	0.566203	-1.185761	-1.105406
C	0.247205	-2.186735	-2.006669
C	1.147111	-3.239271	-2.175011
C	2.351580	-3.265221	-1.479932
C	2.689317	-2.238942	-0.601769

C	-0.113277	0.302255	1.778628
C	2.684470	1.112680	0.541610
C	4.142195	1.092650	0.492805
C	4.833428	2.107815	-0.181635
C	6.218600	2.094440	-0.265411
C	6.950473	1.086021	0.354337
C	6.282282	0.088536	1.056005
C	4.895009	0.089105	1.120602
C	-2.643306	1.727949	-0.625092
C	-3.998244	1.946279	-0.893182
C	-4.564518	3.191053	-0.663108
C	-3.782219	4.230932	-0.169578
C	-2.433339	4.024545	0.086809
C	-1.862660	2.776761	-0.141432
O	-2.294228	-0.393986	-2.393223
H	3.638691	-2.242640	-0.080576
H	3.041575	-4.087661	-1.631969
H	0.908139	-4.038440	-2.867417
H	-0.669327	-2.133502	-2.582407
H	-4.604669	1.139550	-1.291594
H	-5.615252	3.352849	-0.874200
H	-4.224675	5.204622	0.008054
H	-1.818474	4.834889	0.460891
H	-0.807116	2.638688	0.056958
H	-3.425999	0.493881	1.607006
H	-4.381017	-1.099737	3.223407
H	-4.287158	-3.533133	2.774169
H	-3.269319	-4.364261	0.674182
H	-2.323822	-2.768193	-0.956398
H	4.377409	-0.682170	1.682205
H	6.844676	-0.693925	1.554574
H	8.033351	1.084105	0.299824
H	6.732439	2.881583	-0.806769
H	4.264277	2.905813	-0.646089

H	0.111530	0.845666	-1.563366
H	1.198884	1.588624	0.515378
H	0.469151	0.906438	2.480634
H	-1.125126	0.709273	1.766385
C	-0.098403	-1.151870	2.222989
H	-0.611145	-1.230938	3.184520
H	-0.605152	-1.810283	1.517879
H	0.926453	-1.505922	2.348536



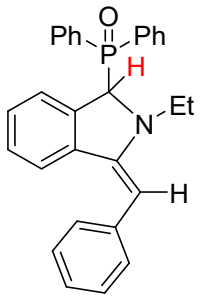
62

E(ωB97X-D/6-311+G**) = -1744.395484

C	-3.185402	-0.682703	1.679859
C	-3.000898	-0.730209	0.299750
C	-3.867343	-0.017931	-0.533238
C	-4.880499	0.757642	0.007946
C	-5.047532	0.816109	1.387812
C	-4.207124	0.089878	2.221001
P	-1.684398	-1.701967	-0.490609
O	-2.165734	-2.819054	-1.360539
C	-0.694086	-0.474809	-1.498139
N	-0.292336	0.708540	-0.757164
C	1.100895	0.790453	-0.577491
C	1.659670	-0.372621	-1.298852
C	0.615913	-1.096802	-1.872069
C	2.976152	-0.762529	-1.535035
C	3.210907	-1.890008	-2.311124
C	2.156327	-2.624885	-2.851145
C	0.841613	-2.231362	-2.636524

C	-1.162786	1.820419	-0.613109
C	-1.525240	2.273373	0.652589
C	-2.405518	3.337450	0.787036
C	-2.936279	3.952903	-0.341090
C	-2.570390	3.508098	-1.605751
C	-1.678826	2.451630	-1.742123
C	1.711691	1.784362	0.091531
C	3.141823	1.850140	0.447382
C	3.756198	0.820847	1.168857
C	5.094158	0.902407	1.531951
C	5.842886	2.025733	1.197164
C	5.239620	3.066493	0.499807
C	3.902596	2.979760	0.131882
C	-0.531911	-2.242575	0.806173
C	0.081063	-1.370478	1.709142
C	1.026309	-1.848757	2.605697
C	1.364100	-3.198509	2.607110
C	0.756216	-4.069416	1.711354
C	-0.187524	-3.593226	0.808982
H	3.806709	-0.201064	-1.130803
H	4.232414	-2.200574	-2.499647
H	2.363544	-3.505849	-3.448041
H	0.008048	-2.793991	-3.040417
H	-2.533648	-1.245815	2.337513
H	-4.344474	0.123122	3.295955
H	-5.837622	1.425639	1.812102
H	-5.536749	1.320615	-0.645370
H	-3.745739	-0.063039	-1.610360
H	-0.165003	-0.315947	1.703525
H	1.500779	-1.165999	3.301737
H	2.103764	-3.570314	3.307606
H	1.020676	-5.120687	1.709875
H	-0.660894	-4.256613	0.093341
H	-1.131008	1.773052	1.528839

H	-2.691826	3.674320	1.776728
H	-3.632541	4.776896	-0.234379
H	-2.973336	3.989053	-2.490013
H	-1.380422	2.110410	-2.727507
H	3.438454	3.791785	-0.418379
H	5.813527	3.948738	0.237892
H	6.886448	2.092511	1.483563
H	5.551676	0.089472	2.085531
H	3.171915	-0.053659	1.436887
H	-1.308030	-0.241148	-2.376109
H	1.100873	2.615992	0.429524



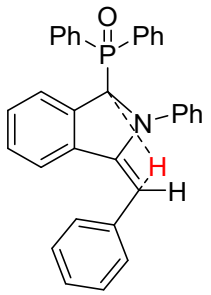
58

E(ωB97X-D/6-311+G**) = -1591.993333

C	2.961240	-1.236083	1.419951
C	3.229260	-0.737800	0.145091
C	4.236436	-1.318490	-0.627110
C	4.951554	-2.404462	-0.137063
C	4.668359	-2.909924	1.126703
C	3.678559	-2.321046	1.906717
P	2.281968	0.603645	-0.636021
O	3.068298	1.329217	-1.682530
C	1.656832	1.692871	0.676409
C	2.188705	2.981469	0.709944
C	1.745753	3.893213	1.660235
C	0.762711	3.526529	2.571174
C	0.220446	2.246443	2.532791
C	0.664640	1.328625	1.590739

C	0.787881	-0.219494	-1.396669
N	0.111848	-1.164420	-0.522230
C	-1.232233	-0.809693	-0.319431
C	-1.433546	0.478189	-1.013636
C	-0.261906	0.807980	-1.691187
C	-0.141836	1.984727	-2.416134
C	-1.232008	2.844554	-2.452855
C	-2.400661	2.537360	-1.756490
C	-2.511908	1.360262	-1.028540
C	0.506877	-2.565857	-0.585241
C	-0.130031	-3.324540	-1.747581
C	-2.091147	-1.541275	0.415353
C	-3.536786	-1.289112	0.582897
C	-4.087276	-1.142999	1.859556
C	-5.449821	-0.931498	2.031118
C	-6.291795	-0.866426	0.926512
C	-5.760749	-1.025495	-0.348907
C	-4.399347	-1.243512	-0.516741
H	-3.419580	1.143276	-0.482425
H	-3.234269	3.230236	-1.777117
H	-1.167561	3.770160	-3.013578
H	0.789430	2.230394	-2.913558
H	2.196350	-0.779886	2.036591
H	3.467673	-2.705278	2.898331
H	5.226361	-3.757339	1.509255
H	5.733676	-2.852079	-0.739720
H	4.458778	-0.904455	-1.604874
H	0.220693	0.340651	1.558048
H	-0.557485	1.962698	3.232454
H	0.412109	4.240921	3.307834
H	2.163349	4.893402	1.682797
H	2.938568	3.260811	-0.022110
H	-1.706531	-2.419966	0.924592
H	-3.988738	-1.374191	-1.512339

H	-6.410281	-0.988355	-1.216672
H	-7.354918	-0.700172	1.059056
H	-5.854878	-0.813388	3.030263
H	-3.433268	-1.184664	2.724712
H	1.174101	-0.698730	-2.307003
H	0.266107	-3.045322	0.366910
H	1.594480	-2.598105	-0.663602
H	0.213731	-4.361840	-1.756241
H	-1.218949	-3.322696	-1.666450
H	0.142992	-2.870654	-2.704622



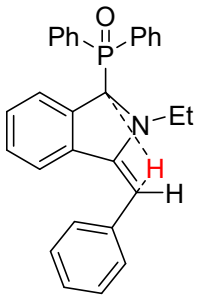
62

E(ωB97X-D/6-311+G**) = -1744.262203

C	1.003124	-1.492050	-2.587026
C	1.973260	-0.761315	-1.896463
C	3.288487	-1.220030	-1.874046
C	3.621281	-2.417655	-2.497584
C	2.646825	-3.154283	-3.158265
C	1.337318	-2.685370	-3.209962
P	1.506854	0.854085	-1.205775
C	2.709204	1.306686	0.086031
C	2.990162	2.671233	0.176586
C	3.858751	3.142203	1.152704
C	4.457433	2.253867	2.038171
C	4.189474	0.892711	1.945068
C	3.317843	0.417643	0.974307
C	-0.116756	0.639775	-0.339718
N	-0.219221	0.250633	1.033180

C	-1.615795	0.330922	1.205455
C	-2.020806	1.566999	0.571482
C	-1.086801	1.738228	-0.461465
C	-1.276450	2.749400	-1.414189
C	-2.392804	3.554947	-1.286287
C	-3.332250	3.363818	-0.259050
C	-3.166327	2.353317	0.667859
C	0.473383	-0.863016	1.587846
C	0.815257	-1.996792	0.856765
C	1.538286	-3.018211	1.462209
C	1.902923	-2.923167	2.799396
C	1.529458	-1.803535	3.537193
C	0.820635	-0.775282	2.933977
C	-2.211731	-0.855420	0.714832
C	-3.663474	-0.974527	0.405152
C	-4.199147	-0.380425	-0.737694
C	-5.550770	-0.507049	-1.030528
C	-6.384722	-1.227787	-0.182979
C	-5.858581	-1.828875	0.955016
C	-4.504640	-1.707755	1.242366
O	1.412959	1.897859	-2.272533
H	-1.291732	-0.518119	-0.519951
H	-3.898474	2.173374	1.445967
H	-4.198501	4.013248	-0.201047
H	-2.546518	4.358842	-1.997951
H	-0.551917	2.897649	-2.203431
H	4.059422	-0.647018	-1.372450
H	4.645559	-2.771646	-2.469432
H	2.907761	-4.088768	-3.642396
H	0.576833	-3.249772	-3.737484
H	-0.019855	-1.132320	-2.622603
H	3.118626	-0.645510	0.917109
H	4.657458	0.195320	2.630528
H	5.137237	2.621478	2.798973

H	4.071007	4.203250	1.217785
H	2.529816	3.351787	-0.531244
H	0.554622	0.119910	3.482969
H	1.806537	-1.723031	4.582166
H	2.470637	-3.719378	3.267315
H	1.811549	-3.891465	0.880848
H	0.523058	-2.082910	-0.179166
H	-4.094292	-2.179764	2.129473
H	-6.502368	-2.396091	1.618026
H	-7.440360	-1.324689	-0.410815
H	-5.953138	-0.040644	-1.922754
H	-3.549807	0.186819	-1.396330
H	-1.747412	-1.794358	1.007587



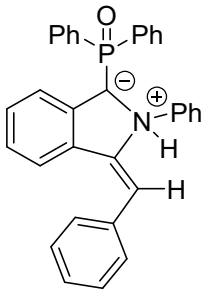
58

E(ωB97X-D/6-311+G**) = -1591.864789

C	-2.751863	-1.464487	1.258960
C	-2.904417	-1.113080	-0.082255
C	-4.047899	-1.510940	-0.777978
C	-5.039720	-2.235085	-0.130093
C	-4.891072	-2.571961	1.211419
C	-3.746620	-2.191932	1.902426
P	-1.671544	-0.142239	-1.003050
C	-2.184010	1.596244	-0.842662
C	-1.392086	2.557068	-1.475341
C	-1.726511	3.901140	-1.390789
C	-2.856640	4.293726	-0.679576
C	-3.655941	3.340083	-0.061356

C	-3.322326	1.992616	-0.143692
C	-0.067466	-0.279251	-0.134123
N	0.175967	0.072917	1.233186
C	1.562332	-0.174723	1.270380
C	1.749671	-1.457086	0.610719
C	0.720322	-1.498320	-0.340691
C	2.780223	-2.392961	0.606671
C	2.720728	-3.410102	-0.326812
C	1.680650	-3.464904	-1.269670
C	0.679822	-2.510531	-1.304187
C	2.270192	0.914962	0.734372
C	3.683536	0.828736	0.275331
C	4.706869	1.381940	1.044945
C	6.029595	1.300651	0.627465
C	6.342131	0.675238	-0.574398
C	5.326722	0.133753	-1.354663
C	4.006001	0.209002	-0.931918
C	-0.353078	1.326906	1.753525
C	0.064730	1.554694	3.197161
O	-1.523343	-0.565260	-2.428676
H	1.075463	0.669359	-0.461291
H	3.597468	-2.323982	1.314721
H	3.491410	-4.172542	-0.342514
H	1.663070	-4.275191	-1.990295
H	-0.106364	-2.533260	-2.048671
H	-3.946349	1.251922	0.344794
H	-4.542044	3.643571	0.484601
H	-3.117120	5.344271	-0.613505
H	-1.107572	4.643515	-1.881803
H	-0.515055	2.246849	-2.033317
H	-1.849627	-1.191057	1.795323
H	-3.622333	-2.469696	2.942966
H	-5.664348	-3.140765	1.715780
H	-5.925668	-2.543058	-0.673699

H	-4.146880	-1.260566	-1.828885
H	4.464488	1.872390	1.982633
H	6.816122	1.728647	1.239017
H	7.373381	0.614236	-0.903726
H	5.562440	-0.350137	-2.295781
H	3.214022	-0.218281	-1.538080
H	1.974294	1.914162	1.044697
H	-0.076070	2.175340	1.112758
H	-1.440537	1.257568	1.705229
H	-0.396481	2.471582	3.570477
H	-0.258577	0.722375	3.826326
H	1.147432	1.651059	3.299577



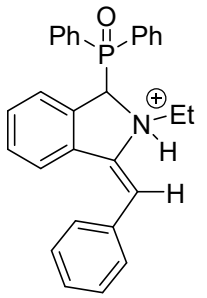
62

E(ωB97X-D/6-311+G**) = -1744.316418

C	-3.539217	-1.767459	-1.579281
C	-2.299015	-1.802519	-0.937643
C	-1.226504	-2.432669	-1.575484
C	-1.381427	-2.991076	-2.840049
C	-2.615216	-2.932320	-3.475917
C	-3.695493	-2.327857	-2.840121
P	-2.041174	-1.149177	0.760833
O	-2.423762	-2.114527	1.837688
C	-0.349598	-0.676571	0.874639
N	0.269624	0.130651	-0.232106
C	1.773264	-0.043593	-0.095570
C	1.945392	-1.174963	0.791441
C	0.694479	-1.514355	1.360057

C	3.102897	-1.898508	1.090656
C	3.027374	-2.955211	1.977396
C	1.793060	-3.281723	2.563395
C	0.636647	-2.588029	2.273094
C	-0.162156	1.530424	-0.325980
C	-0.292565	2.278522	0.831058
C	-0.705920	3.596867	0.724296
C	-0.978670	4.151848	-0.523296
C	-0.840828	3.386051	-1.672231
C	-0.430908	2.060617	-1.575337
C	2.581145	0.797427	-0.749374
C	4.052729	0.834554	-0.649976
C	4.696022	0.888042	0.589313
C	6.079908	0.961320	0.664311
C	6.844371	0.990292	-0.497444
C	6.213876	0.953867	-1.735593
C	4.828543	0.882920	-1.810489
C	-3.053849	0.374207	0.838997
C	-3.379863	1.179450	-0.251049
C	-4.075009	2.368513	-0.066087
C	-4.455081	2.760158	1.211542
C	-4.144989	1.956056	2.303550
C	-3.450161	0.768337	2.118327
H	4.046751	-1.640886	0.626969
H	3.913707	-3.530332	2.216180
H	1.743121	-4.112301	3.260201
H	-0.314842	-2.860510	2.711092
H	-4.388936	-1.306857	-1.087262
H	-4.663874	-2.298211	-3.327120
H	-2.739916	-3.367950	-4.461023
H	-0.542445	-3.481838	-3.320503
H	-0.272632	-2.525203	-1.061018
H	-3.087024	0.888174	-1.253187
H	-4.316550	2.989480	-0.921562

H	-4.997680	3.688034	1.356280
H	-4.450072	2.252420	3.301058
H	-3.212081	0.129272	2.961979
H	-0.111205	1.806697	1.788695
H	-0.831425	4.190528	1.621705
H	-1.310023	5.181133	-0.595946
H	-1.060817	3.810921	-2.644410
H	-0.336322	1.445757	-2.465652
H	4.340432	0.855331	-2.779469
H	6.801604	0.981477	-2.646351
H	7.925274	1.047421	-0.437521
H	6.562990	1.001015	1.634180
H	4.102574	0.868047	1.496593
H	2.135835	1.542146	-1.401099
H	0.024471	-0.310168	-1.128979



58

E(ωB97X-D/6-311+G**) = -1591.932044

C	-2.788023	-1.472662	-1.435556
C	-3.141919	-1.038996	-0.157482
C	-4.294425	-1.536596	0.447745
C	-5.092771	-2.454687	-0.225493
C	-4.741441	-2.877608	-1.501868
C	-3.587359	-2.387757	-2.106256
P	-2.165828	0.180553	0.777892
O	-2.659325	0.301272	2.193061
C	-2.383713	1.803126	-0.058422
C	-3.022363	2.822713	0.645470

C	-3.186363	4.077114	0.067087
C	-2.711784	4.320916	-1.216470
C	-2.073798	3.307946	-1.926270
C	-1.910771	2.054224	-1.349090
C	-0.504560	-0.197961	0.416296
N	0.505859	0.887041	0.550889
C	1.825122	0.281575	0.189932
C	1.617852	-1.152950	0.193706
C	0.227197	-1.407547	0.340789
C	-0.212511	-2.746779	0.352023
C	0.706049	-3.760631	0.168993
C	2.070672	-3.499819	-0.022404
C	2.525812	-2.193353	-0.008351
C	0.547397	1.538647	1.921300
C	0.813427	0.547023	3.032017
C	2.833198	1.119186	-0.086207
C	4.237073	0.742489	-0.337227
C	4.955855	-0.016751	0.589109
C	6.285910	-0.342607	0.358503
C	6.921017	0.093343	-0.798915
C	6.219979	0.863715	-1.719993
C	4.890368	1.190488	-1.487870
H	3.577906	-1.985700	-0.153112
H	2.766292	-4.316799	-0.169711
H	0.359861	-4.789096	0.177578
H	-1.259712	-2.978569	0.499271
H	-4.545378	-1.201487	1.448294
H	-5.987393	-2.842308	0.248898
H	-5.363289	-3.595483	-2.025535
H	-3.305391	-2.727983	-3.096332
H	-1.869783	-1.115654	-1.888683
H	-1.417849	1.260387	-1.903038
H	-1.708155	3.493931	-2.930122
H	-2.840004	5.299273	-1.666294

H	-3.685397	4.865449	0.619689
H	-3.381596	2.612384	1.647421
H	4.345973	1.789410	-2.210684
H	6.709824	1.210542	-2.622931
H	7.959298	-0.160647	-0.979428
H	6.828792	-0.933614	1.087573
H	4.464018	-0.349382	1.496900
H	2.613695	2.184352	-0.128604
H	0.290457	1.631740	-0.114585
H	1.322301	2.307431	1.865732
H	-0.424606	2.017292	2.053659
H	0.814173	1.088499	3.979918
H	0.024255	-0.204113	3.071548
H	1.781929	0.057590	2.912926

TS-2

62

E(ωB97X-D/6-311+G**) = -1744.2793

C	3.710198	-1.787605	-0.471523
C	2.635730	-1.388312	-1.264509
C	1.969148	-2.343895	-2.038244
C	2.334982	-3.680865	-1.977241
C	3.384843	-4.075270	-1.153898
C	4.079117	-3.126459	-0.414406
P	2.086149	0.343201	-1.388816
C	2.794508	1.278324	-0.001429
C	3.260064	2.556324	-0.318412
C	3.811944	3.363563	0.667553
C	3.912941	2.896294	1.972327
C	3.468390	1.617626	2.289224
C	2.911466	0.809716	1.307938
C	0.228383	0.210836	-1.260632
C	-0.561819	1.492137	-1.092831
C	-1.839985	1.218680	-0.607050

C	-2.765658	2.248098	-0.455212
C	-2.388957	3.543771	-0.786996
C	-1.113752	3.809599	-1.280079
C	-0.192684	2.779590	-1.447833
C	-2.117492	-0.179061	-0.310214
C	-2.997185	-1.071957	-0.092215
C	-4.427628	-0.928904	0.025008
C	-5.274713	-1.103951	-1.081523
C	-6.648501	-0.950510	-0.957110
C	-7.222581	-0.634070	0.270051
C	-6.394605	-0.475315	1.377085
C	-5.019612	-0.623935	1.262852
N	-0.424914	-0.748638	-0.335394
C	0.067574	-0.902449	1.014250
C	0.680390	-2.095507	1.374899
C	1.114113	-2.280394	2.682647
C	0.926259	-1.279126	3.626806
C	0.298492	-0.093295	3.259618
C	-0.135806	0.100460	1.957214
O	2.368604	1.006207	-2.697522
H	-3.760021	2.026176	-0.084768
H	-3.098394	4.354594	-0.665460
H	-0.837377	4.823320	-1.545825
H	0.784087	2.975729	-1.873045
H	4.263471	-1.057986	0.106667
H	4.912780	-3.426941	0.209772
H	3.670062	-5.119876	-1.102361
H	1.806646	-4.413007	-2.576824
H	1.168566	-2.047503	-2.708661
H	2.578062	-0.185344	1.571527
H	3.551578	1.244461	3.303565
H	4.345037	3.526049	2.742074
H	4.168015	4.355334	0.414016
H	3.198540	2.899285	-1.344990

H	-4.841537	-1.358160	-2.042808
H	-7.278352	-1.083279	-1.830913
H	-8.296457	-0.520767	0.363715
H	-6.824200	-0.235091	2.344455
H	-4.384919	-0.506556	2.134877
H	0.001954	-0.164479	-2.267712
H	-0.515056	-1.666432	-0.758609
H	-0.628619	1.022359	1.678948
H	0.141341	0.689176	3.992583
H	1.258146	-1.425763	4.648171
H	1.593527	-3.212020	2.959132
H	0.831064	-2.875323	0.635976

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TS-1 in the presence of CuCl E(ωB97X-D/6-311+G**) = -3845.138929

C	2.092152	0.966721	-2.270754
C	2.408566	0.836422	-0.914903
C	3.676841	1.216529	-0.462710
C	4.612257	1.719326	-1.356154
C	4.289096	1.856119	-2.701533
C	3.029769	1.477891	-3.156395
C	1.415099	0.369074	0.042707
Cu	2.367630	-1.991427	0.720867
Cl	3.547392	-3.752883	0.532769
C	1.161433	-0.496270	0.966032
C	0.011730	-0.493425	1.878370
C	-1.138420	0.254219	1.590081
C	-2.232353	0.211850	2.451767
C	-2.201541	-0.572621	3.597630
C	-1.061016	-1.310701	3.894376
C	0.031942	-1.268677	3.040729
C	-1.243033	1.059539	0.326085
N	0.010619	1.714294	-0.082860
C	0.397072	2.933474	0.567159

C	1.165942	3.838860	-0.161478
C	1.637935	4.992964	0.446288
C	1.342751	5.256122	1.779556
C	0.568624	4.354487	2.498320
C	0.094357	3.191801	1.900891
P	-1.803765	0.073562	-1.185742
O	-1.294378	0.827656	-2.383167
C	-1.159582	-1.612780	-1.096630
C	-0.296677	-1.981353	-2.129661
C	0.359710	-3.202984	-2.088602
C	0.158147	-4.065365	-1.018274
C	-0.725626	-3.717024	-0.003541
C	-1.384362	-2.496463	-0.037865
C	-3.615088	0.086898	-1.079551
C	-4.271251	0.952324	-1.957332
C	-5.656317	1.055719	-1.925029
C	-6.390374	0.300310	-1.018908
C	-5.740130	-0.566005	-0.146702
C	-4.356466	-0.677270	-0.176687
H	0.919548	-1.854662	3.254245
H	-1.024121	-1.922295	4.789124
H	-3.060197	-0.599161	4.257295
H	-3.117341	0.797186	2.218195
H	-3.686902	1.527683	-2.665976
H	-6.161429	1.724931	-2.611908
H	-7.471254	0.381246	-0.995095
H	-6.311671	-1.162518	0.554995
H	-3.868985	-1.362346	0.504364
H	-2.024787	-2.228850	0.792946
H	-0.874924	-4.382498	0.838401
H	0.713348	-4.992809	-0.958140
H	1.054558	-3.469699	-2.875510
H	-0.127844	-1.295459	-2.951615
H	1.406365	3.631738	-1.199215

H	2.239994	5.688495	-0.127176
H	1.713921	6.156969	2.253637
H	0.332982	4.547609	3.537857
H	-0.486717	2.489142	2.483976
H	3.914154	1.110788	0.589212
H	5.593360	2.009650	-0.999711
H	5.019339	2.254789	-3.396796
H	2.776394	1.577135	-4.205764
H	1.105768	0.686242	-2.624952
H	-2.020715	1.823507	0.443542
H	-0.048546	1.857891	-1.095046

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TS-2 in the presence of CuCl E(ωB97X-D/6-311+G**) = -3845.138929

C	2.092152	0.966721	-2.270754
C	2.408566	0.836422	-0.914903
C	3.676841	1.216529	-0.462710
C	4.612257	1.719326	-1.356154
C	4.289096	1.856119	-2.701533
C	3.029769	1.477891	-3.156395
C	1.415099	0.369074	0.042707
Cu	2.367630	-1.991427	0.720867
Cl	3.547392	-3.752883	0.532769
C	1.161433	-0.496270	0.966032
C	0.011730	-0.493425	1.878370
C	-1.138420	0.254219	1.590081
C	-2.232353	0.211850	2.451767
C	-2.201541	-0.572621	3.597630
C	-1.061016	-1.310701	3.894376
C	0.031942	-1.268677	3.040729
C	-1.243033	1.059539	0.326085
N	0.010619	1.714294	-0.082860
C	0.397072	2.933474	0.567159
C	1.165942	3.838860	-0.161478

C	1.637935	4.992964	0.446288
C	1.342751	5.256122	1.779556
C	0.568624	4.354487	2.498320
C	0.094357	3.191801	1.900891
P	-1.803765	0.073562	-1.185742
O	-1.294378	0.827656	-2.383167
C	-1.159582	-1.612780	-1.096630
C	-0.296677	-1.981353	-2.129661
C	0.359710	-3.202984	-2.088602
C	0.158147	-4.065365	-1.018274
C	-0.725626	-3.717024	-0.003541
C	-1.384362	-2.496463	-0.037865
C	-3.615088	0.086898	-1.079551
C	-4.271251	0.952324	-1.957332
C	-5.656317	1.055719	-1.925029
C	-6.390374	0.300310	-1.018908
C	-5.740130	-0.566005	-0.146702
C	-4.356466	-0.677270	-0.176687
H	0.919548	-1.854662	3.254245
H	-1.024121	-1.922295	4.789124
H	-3.060197	-0.599161	4.257295
H	-3.117341	0.797186	2.218195
H	-3.686902	1.527683	-2.665976
H	-6.161429	1.724931	-2.611908
H	-7.471254	0.381246	-0.995095
H	-6.311671	-1.162518	0.554995
H	-3.868985	-1.362346	0.504364
H	-2.024787	-2.228850	0.792946
H	-0.874924	-4.382498	0.838401
H	0.713348	-4.992809	-0.958140
H	1.054558	-3.469699	-2.875510
H	-0.127844	-1.295459	-2.951615
H	1.406365	3.631738	-1.199215
H	2.239994	5.688495	-0.127176

H	1.713921	6.156969	2.253637
H	0.332982	4.547609	3.537857
H	-0.486717	2.489142	2.483976
H	3.914154	1.110788	0.589212
H	5.593360	2.009650	-0.999711
H	5.019339	2.254789	-3.396796
H	2.776394	1.577135	-4.205764
H	1.105768	0.686242	-2.624952
H	-2.020715	1.823507	0.443542
H	-0.048546	1.857891	-1.095046

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