
4*a*,8*a*-Azaboranaphthalene-4-yl Phosphine Ligands: Synthesis and Electron Modulation in Suzuki-Miyaura Coupling Reactions

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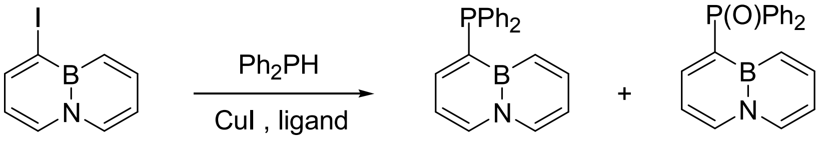
Supporting Information (SI)

Contents

EXPERIMENTAL SECTION

General Procedures. All chemicals were purchased at high purity (AR or HPLC grade) from Sigma-Aldrich and Titan (Shanghai) and were used without further purification, unless otherwise specified. All manipulations involving air- and moisture-sensitive compounds were performed under an inert atmosphere of nitrogen or argon using standard Schlenk-line techniques and an MBraun Labstar-MB10 glovebox. All solvents were dried and distilled prior to use (Et_2O/THF from Na/benzophenone; toluene from Na; pentane/hexane from Na/K alloy; CH_2Cl_2 from CaH_2). For flash chromatography, silica gel (40-60 μm) was used. The deuterated NMR solvents were purchased from the Cambridge Isotope Laboratories. $CDCl_3$ were distilled from CaH_2 and degassed prior to use. All $^1H/^{13}C$ NMR spectra were recorded in δ units relative to deuterated solvent as an internal reference using a Bruker ARX400 spectrometer. The chemical shift values (δ) are reported in ppm, while the coupling constants (J) are in hertz (Hz). The ^{11}B, ^{31}P and ^{19}F NMR spectra were calibrated by using $BF_3 \cdot Et_2O$, 85% H_3PO_4 and $CFCl_3$ as the reference standard respectively, all with the chemical shift value set at 0.00 ppm. Signal multiplicities are represented by s (singlet), d (doublet), t (triplet), m (multiplet), and bd (broad doublet). The high resolution mass spectra (HRMS) were measured on a Bruker micrOTOF II ESI-TOF mass spectrometer. The GC analysis was performed on a Varian 3900 GC system. The X-ray diffraction experiments were carried out at the X-ray facility center, Department of Chemistry, Xiamen University, People's Republic of China.



2 **3** **4**

General Procedure for Table 2. In a nitrogen-filled glovebox, a Schlenk bomb flask equipped with a Teflon magnetic stirrer was loaded with CuI (2.9 mg, 0.015 mmol), ligand (0.030 mmol) and toluene (0.5 mL). The colorless mixture was stirred for 10 min. at rt, and was further treated with diarylphosphine (0.36 mmol, 1.2 equiv.) and Cs_2CO_3 (0.60 mmol). The whole mixture was stirred 20 min and 4-iodo-ABN **2** (76 mg, 0.30 mmol), and additional toluene (1.0 mL) were added respectively into the mixture. The whole apparatus was sealed with a Teflon plug valve and taken out of the glovebox. The flask was heated in an oil bath with stirring at 100 °C for 12 h. After the reaction, the mixture was washed with brine and extracted with diethyl ether (3 x 4 mL). The organic layers were combined and dried over anhydrous $MgSO_4$. After solvent removal, the crude product containing **3** or **4** was purified by flash chromatography (ethyl acetate/hexane = 1/10) to afford colorless crystalline solid **3** or **4**. **3**: ^1H NMR (400 MHz, $CDCl_3$): δ 7.76 (t, J = 7.1 Hz, 2H), 7.57 (dd, J = 11.0, 6.5 Hz, 1H), 7.42–7.30 (m, 11H), 7.11 (dd, J = 11.0, 6.5 Hz, 1H), 6.70 (dt, J = 6.8, 1.4 Hz, 1H), 6.64 (dt, J = 6.8, 1.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 141.4 (d, J_{PC} = 2 Hz), 138.6, 138.2 (d, J =

5 Hz), 134.6, 134.4 (d, *J* = 12 Hz), 133.9, 132.5, 128.4 (d, *J* = 18 Hz), 114.7, 114.3 (d, *J* = 5 Hz). ^{11}B NMR (128 MHz, $CDCl_3$): δ 29.9. ^{31}P NMR (162 MHz, $CDCl_3$): δ −7.6. HRMS (ESI-TOF) *m/z*: calcd. for $C_{20}H_{18}{}^{11}BN^{31}P$ [M+H], 314.1268; found, 314.1264.

Entry 1: Follow the general procedure with ligand **L1** (2.6 mg, 0.030 mmol) to afford the product **3** (17.8 mg, 19%) and **4** (13.8 mg, 14%).

Entry 2: Follow the general procedure with ligand **L2** (11.4 mg, 0.030 mmol) to afford the product **3** (23.4 mg, 25%).

Entry 3: Follow the general procedure with ligand **L3** (5.4 mg, 0.030 mmol) to afford the product **3** (44 mg, 47%) and **4** (10 mg, 10%).

Entry 4: Follow the general procedure with ligand **L4** (11.3 mg, 0.030 mmol) to afford the product **3** (80 mg, 85%).

Entry 5: Follow the general procedure with ligand **L5** (8.0 mg, 0.030 mmol) to afford the ptoduct **3** (72 mg, 77%) and **4** (9.0 mg, 9%).

General Procedure for Synthesis in Table 1. In a nitrogen-filled glovebox, a Schlenk bomb flask equipped with a Teflon magnetic stirrer was loaded with CuX (0.015 mmol), diarylphosphine (0.36 mmol, 1.2 equiv.), base (0.60 mmol) and toluene (0.5 mL). The colorless mixture was stirred for 10 min at rt. 4-Iodo-ABN **2** (76 mg, 0.30 mmol), and additional toluene (1.0 mL) were added respectively into the above mixture. The whole apparatus was sealed with a Teflon plug valve and taken out of the glovebox. The flask was heated in an oil bath with stirring at 100 °C for 12 h. After the reaction, the mixture was washed with brine and extracted with diethyl ether (3 x 4 mL). The organic layers were combined and dried over anhydrous $MgSO_4$. After solvent removal, the crude product containing **3** or **4** was purified by flash chromatography (ethyl acetate/hexane = 1/10) to afford colorless crystalline solid **3** or **4**.

Entry 1: Follow the general procedure with CuCl and Cs_2CO_3 to afford no product of **3** and **4**.

Entry 2: Follow the general procedure with CuBr and Cs_2CO_3 to afford the product **3** (25 mg, 27%) and **4** (19 mg, 19%).

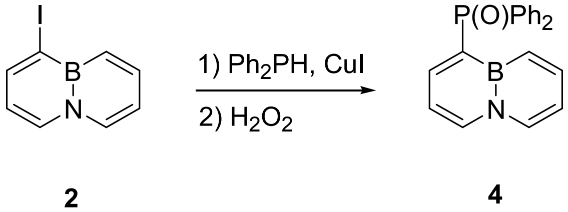
Entry 3: Follow the general procedure with CuI and Cs_2CO_3 to afford the product **3** (47 mg, 50%) and **4** (22 mg, 22%).

Entry 4: Follow the general procedure with CuI and K_2CO_3 to afford the product **3** (42 mg, 45%) and **4** (25 mg, 25%).

Entry 5: Follow the general procedure with CuI and K_3PO_4 to afford the product **3** (36 mg, 38%) and **4** (21 mg, 21%).

Entry 6: Follow the general procedure with CuI and NaOMe to afford the product **3** (21 mg, 22%) and **4** (trace).

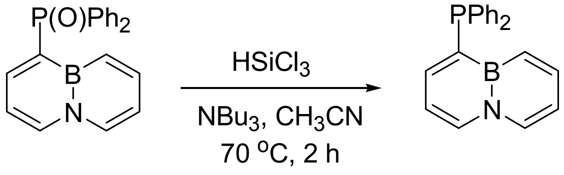
Entry 7: Follow the general procedure with CuI and NEt_3 to afford no product of **3** and **4**.



2 **4**

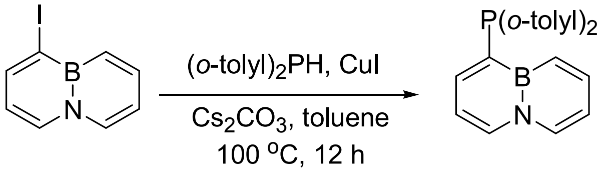
(4*a*,8*a*-Azaboranaphthalene-4-yl)diphenylphosphine oxide (4). In a nitrogen-filled glovebox, a Schlenk bomb flask equipped with a Teflon magnetic stirrer was loaded with CuI

(2.9 mg, 0.015 mmol), toluene (0.5 mL), and Ph_2PH (0.36 mmol). The colorless mixture was stirred for 5 min at rt. Iodo-ABN **2** (76 mg, 0.30 mmol), Cs_2CO_3 (0.6 mmol) and toluene (1.0 mL) were added respectively to the above mixture. The septa-sealed Schlenk flask was taken out of the glovebox and heated with stirring at 100 °C for 12 h. After the reaction, the suspension was treated with brine (2 mL) and extracted with Et_2O (3 x 4 mL). H_2O_2 (30% in H_2O, 1.8 mL) was added slowly into the mixture solution at −10 °C with stirring. The mixture was kept stirring 1 h at 0 °C and 3 h at rt. After brine-washing and $MgSO_4$-drying, the volatiles were removed by vacuum and the residue was purified by flash chromatography (ethyl acetate/hexane = 3/1) to give the product as white solid (80 mg, 81%). ^1H NMR (400 MHz, $CDCl_3$): δ 7.98 (d, J = 7.0 Hz, 1H), 7.84–7.78 (m, 2H), 7.74 (dd, J = 11.0, 7.0 Hz, 4H), 7.57–7.47 (m, 3H), 7.47–7.40 (m, 4H), 7.26 (d, J = 11.0 Hz, 1H), 6.78 (dt, J = 7.0, 3.0 Hz, 1H), 6.74 (t, J = 7.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 145.6 (d, J = 4.0 Hz), 139.1, 138.5, 134.9, 133.8 (d, J = 6.0 Hz), 132.3 (d, J = 10 Hz), 131.5 (d, J = 3.0 Hz), 128.3 (d, J = 12 Hz), 115.4, 113.1 (d, J = 20 Hz). ^{11}B NMR (128 MHz, $CDCl_3$): δ 29.0. ^{31}P NMR (162 MHz, $CDCl_3$): δ 32.8. HRMS (ESI-TOF) *m/z*: calcd. for $C_{20}H_{18}{}^{11}BN^{31}PO$ [M+H], 330.1217; found, 330.1223.



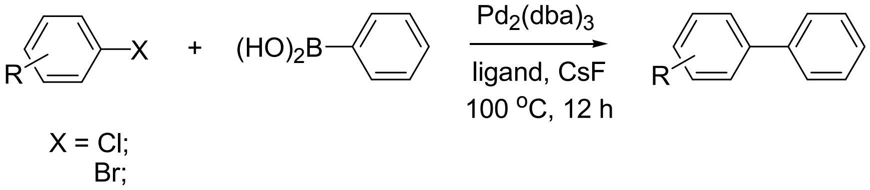
4 **3**

Alternative Synthesis of 3: Tributylamine (0.80 g, 4.3 mmol) was added into a solution of **4** (98.7 mg, 0.30 mmol) in CH_3CN (3mL) at 70 °C. $HSiCl_3$ (0.25 g, 1.8 mmol) was added dropwise via a syringe in 10 min and the mixture was stirred at 70 °C for 2 h. After the reaction, the mixture was treated with 1.0 mL of 25% NaOH solution and the organic layer was further treated with 0.5 mL of 25% NaOH solution under N_2. Volatiles were removed by vacuum and O_2-free methanol was added to facilitate the precipitation of **3**.The crude solid was carefully washed with O_2-free cold CH_3OH (3 x 0.5 mL) and dried under vacuum to afford the product **3** as white solid (41.2 mg, 44%).



2 **5**

(4*a*,8*a*-Azaboranaphthalene-4-yl)di(o-tolyl)phosphane (5). In a nitrogen-filled glovebox, a Schlenk bomb flask equipped with a Teflon magnetic stirrer was loaded with CuI (2.9 mg, 0.015 mmol), di(*o*-tolyl)phosphine (0.36 mmol) and toluene (0.5 mL). The colorless mixture was stirred for 5 min at rt. In the glovebox, 4-iodo-ABN **2** (76 mg, 0.30 mmol), Cs_2CO_3 (0.60 mmol) and additional toluene (1.0 mL) were added respectively to the mixture. The whole apparatus was sealed with a Teflon plug valve and taken out of the glovebox. The flask was heated in an oil bath with stirring at 100 °C for 12 h. After the reaction, the volatiles were removed under vacuum and the residue was extracted with CH_2Cl_2 (4 mL). The mixture was filtrated and the solution was saturated by adding pentane to afford colorless crystals as the crude product, which can be recrystallized at −35 °C to give the product **5** (51 mg, 50%). ^1H NMR (400 MHz, $CDCl_3$): δ 7.77 (d, *J* = 7.0 Hz, 1H), 7.72 (d, *J* = 7.0 Hz, 1H), 7.55 (bd, *J* = 7.0 Hz, 1H), 7.36 (dd, *J* = 11, 6.5 Hz, 1H), 7.24 (t, *J* = 7.5 Hz, 2H), 7.16–7.05 (m, 5H), 7.01 (t, *J* = 7.4 Hz, 2H), 6.62 (t, *J* = 6.5 Hz, 1H), 6.54 (t, *J* = 6.5 Hz, 1H), 2.35 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 144.5(b), 142.8 (d, *J* = 18 Hz), 138.6, 136.1, 134.0, 132.1(b), 130.8 (d, *J* = 5.0 Hz), 129.5, 126.0 (d, *J* = 5.0 Hz), 114.9, 114.1 (d, *J* = 12 Hz), 23.0. ^{11}B NMR (128 MHz, $CDCl_3$): δ 30.1. ^{31}P NMR (162 MHz, $CDCl_3$): δ −11.5. HRMS (ESI-TOF) *m/z*: calcd. for $C_{22}H_{22}{}^{11}B N {}^{31}P$ [M+H], 342.1581; found, 342.1566.



General Procedures for Catalyst Evaluation in Table 3. An oven-dried Schlenk flask sealed with a rubber septa was charged with $Pd_2(dba)_3$ (13.7 mg, 0.015 mmol, 3 mol%), phosphine ligand (5 mol%), $PhB(OH)_2$ (91.5 mg, 0.75 mmol, 1.5 equiv.), and CsF (228 mg, 1.5 mmol, 3.0 equiv.). The apparatus was subject to the evacuate–refill cycle with nitrogen three times. A solution of aryl halide (0.5 mmol) in 2 mL of toluene was added into the flask via a syringe and the mixture was heated with magnetic stirring at 100 °C for 12 h. After the reaction, the volatiles were removed by vacuum and the residue was extracted by Et_2O (2 x 5 mL). The extract solution was concentrated and further purified by flash chromatography.

1,1′-Biphenyl (CAS Registry Number: 92-52-4). ^1H NMR (400 MHz, $CDCl_3$): δ 7.60 (d, *J* = 7.3 Hz, 4H), 7.45 (t, *J* = 7.6 Hz, 4H), 7.35 (t, *J* = 7.3 Hz, 2H)

Entry 1: Follow the general coupling procedure with PhBr (0.50 mmol) and ligand **L6**. The product was isolated by flash chromatography (hexane) as white solid (68 mg, 88%).

Entry 2: Follow the general coupling procedure with PhBr (0.50 mmol) and ligand **L7**. The product was isolated by flash chromatography (hexane) as white solid (71 mg, 92%).

Entry 3: Follow the general coupling procedure with PhBr (0.50 mmol) and ligand **3**. The product was isolated by flash chromatography (hexane) as white solid (71 mg, 92%).

Entry 4: Follow the general coupling procedure with PhBr (0.50 mmol) without using phosphine ligand. The product was isolated by flash chromatography (hexane) as white solid (47 mg, 61%).

Entry 17: Follow the general coupling procedure with PhCl (0.50 mmol) and ligand **3**. The product was isolated by flash chromatography (hexane) as white solid (9 mg, 12%).

2-Methyl-1,1′-biphenyl (CAS Registry Number: 643-58-3). ^1H NMR (400 MHz, $CDCl_3$): δ 7.40–7.36 (m, 2H), 7.32–7.28 (m, 3H), 7.24–7.19 (m, 4H), 2.24 (s, 3H).

Entry 6: Follow the general coupling procedure with 1-bromo-2-methylbenzene (0.50 mmol) and ligand **L7**. The product was isolated by flash chromatography (hexane) as colorless oil (65 mg, 78%).

Entry 13: Follow the general coupling procedure with 1-bromo-2-methylbenzene (0.50 mmol) and ligand **3**. The product was isolated by flash chromatography (hexane) as colorless oil (73 mg, 87%).

4-Trifluoromethyl-1,1′-biphenyl (CAS Registry Number: 398-36-7). ^1H NMR (400 MHz,

$CDCl_3$): δ 7.70 (s, 4H), 7.61 (d, *J* = 7.1 Hz, 2H), 7.49 (t, *J* = 7.6 Hz, 2H), 7.44–7.40 (m, 1H). ^{19}F NMR (377 MHz, $CDCl_3$): δ –62.3.

Entry 7: Follow the general coupling procedure with 1-chloro-4-(trifluoromethyl)-benzene (0.50 mmol) and ligand **L7**. The product was isolated by flash chromatography (CH_2Cl_2/hexane = 1/10) as white solid (9 mg, 8%).

Entry 14: Follow the general coupling procedure with 1-chloro-4-(trifluoromethyl)-benzene (0.50 mmol) and ligand **3**. The product was isolated by flash chromatography (CH_2Cl_2/hexane = 1/10) as white solid (69 mg, 62%).

4-Nitro-1,1′-biphenyl (CAS Registry Number: 92-93-3). ^1H NMR (400 MHz, $CDCl_3$): δ 8.31 (d, *J* = 8.8 Hz, 2H), 7.75 (d, *J* = 8.8 Hz, 2H), 7.63 (d, *J* = 7.1 Hz, 2H), 7.52–7.43 (m, 3H).

Entry 8: Follow the general coupling procedure with 1-chloro-4-nitrobenzene (0.50 mmol) and ligand **L6**. The product was isolated by flash chromatography (CH_2Cl_2/hexane = 1/10) as white solid (12 mg, 12%).

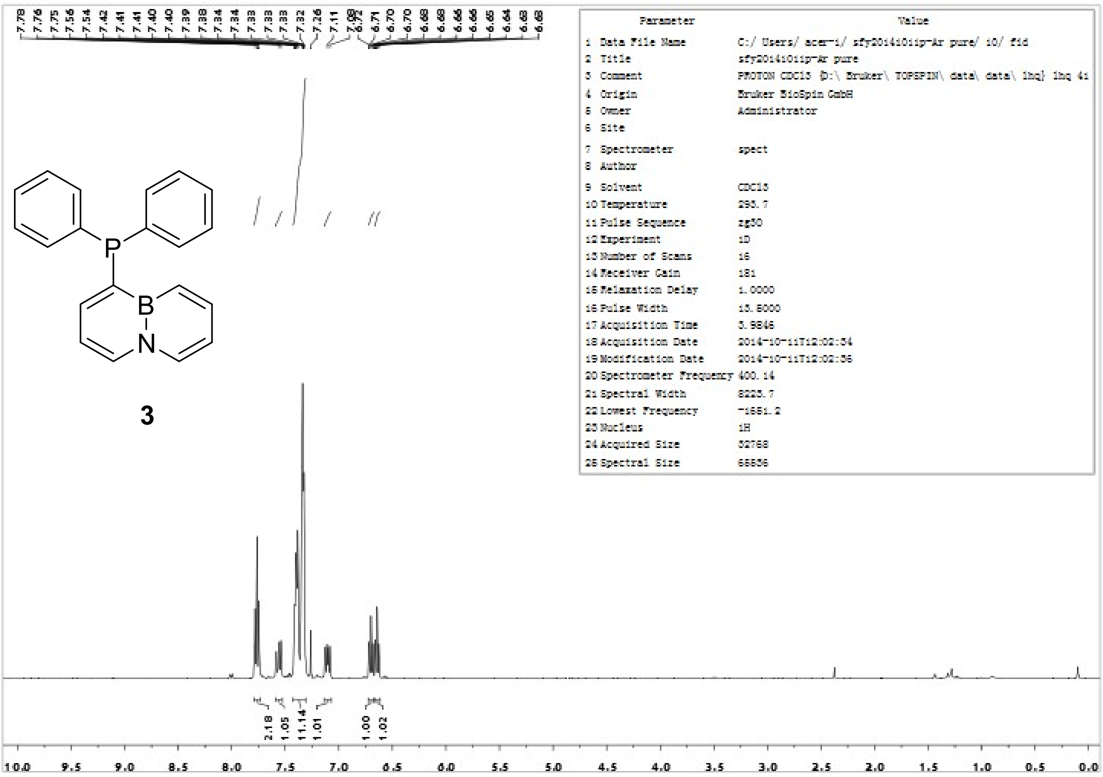
Entry 11: Follow the general coupling procedure with 1-chloro-4- nitrobenzene (0.50 mmol) and ligand **L7**. The product was isolated by flash chromatography (CH_2Cl_2/hexane = 1/10) as white solid (21 mg, 21%).

Entry 15: Follow the general coupling procedure with 1-chloro-4- nitrobenzene (0.50 mmol) and ligand **3**. The product was isolated by flash chromatography (CH_2Cl_2/hexane = 1/10) as white solid (54 mg, 54%).

4-Chloro-1,1′-biphenyl (CAS Registry Number: 2501-61-9). ^1H NMR (400 MHz, $CDCl_3$): δ 7.57–7.51 (m, 4H), 7.47–7.35 (m, 5H).

Entry 16: Follow the general coupling procedure with 1,4-dichlorobenzene (0.50 mmol) and ligand **3**. The product was isolated by flash chromatography (hexane) as white solid (22 mg, 23%).

Single Crystal X-Ray Crystallography. The single crystals of **3** were immersed in FOMBLIN oil (HVAC 140/13, Sigma-Aldrich), mounted on a glass fiber, and examined on an Oxford Gemini CCD 1K detector diffractometer equipped with a Cryostream N_2 cooling device using graphite-monochromated Mo Kα radiation (λ= 0.71073 Å) at 173 K. The determination of crystal class and unit cell was carried out by the SMART program package. The raw frame data were processed using SAINT and SADABS to yield the reflection data file. The structures were solved using SHELXTL program. Refinement was performed on F^2 anistropically for all the non-hydrogen atoms by full-matrix least-squares methods. Analytical scattering factors for neutral atoms were used throughout the analysis.



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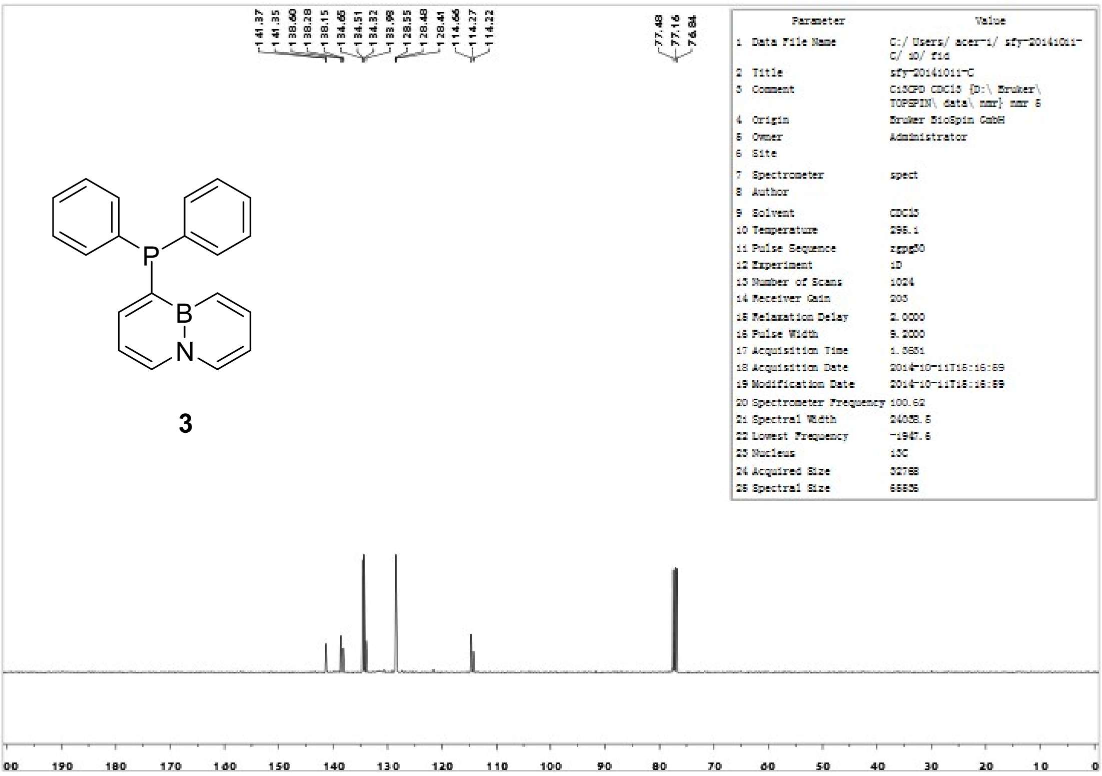

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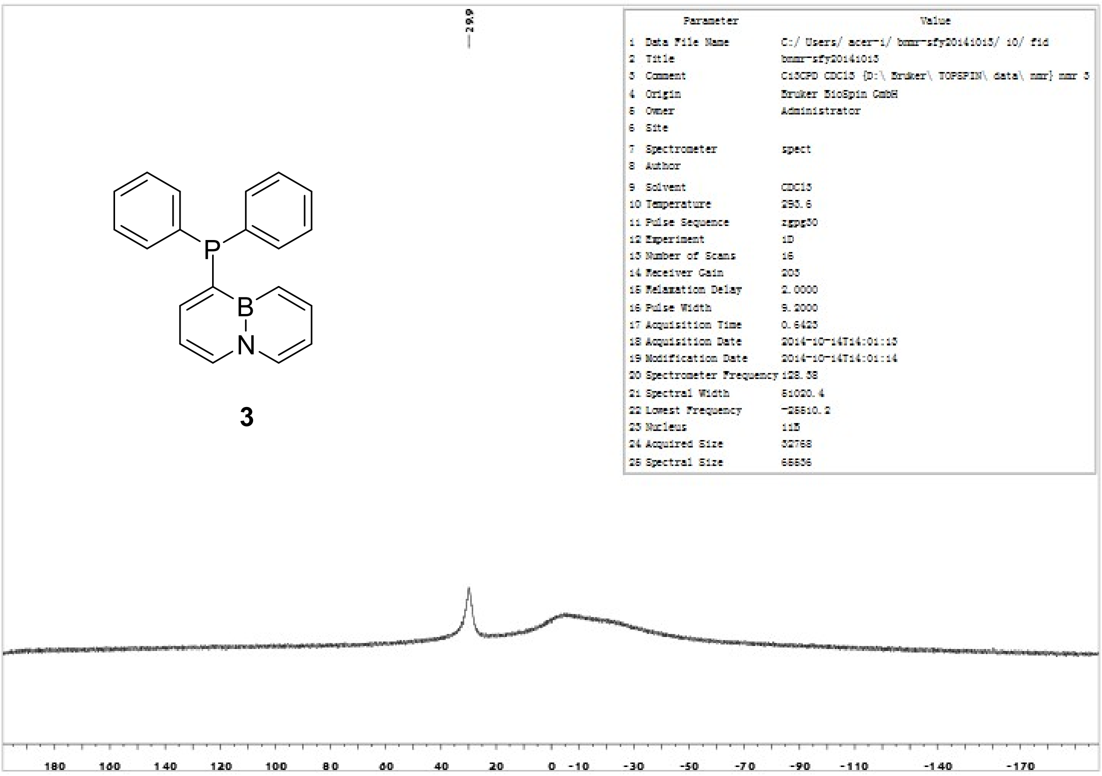

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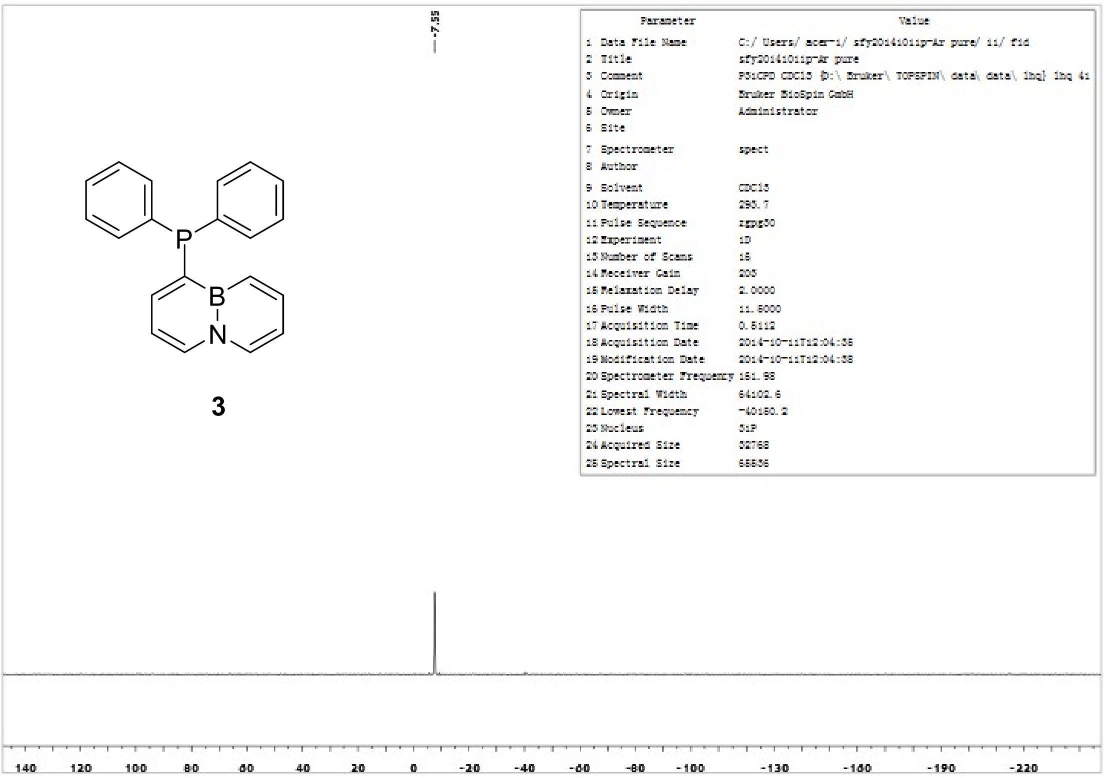

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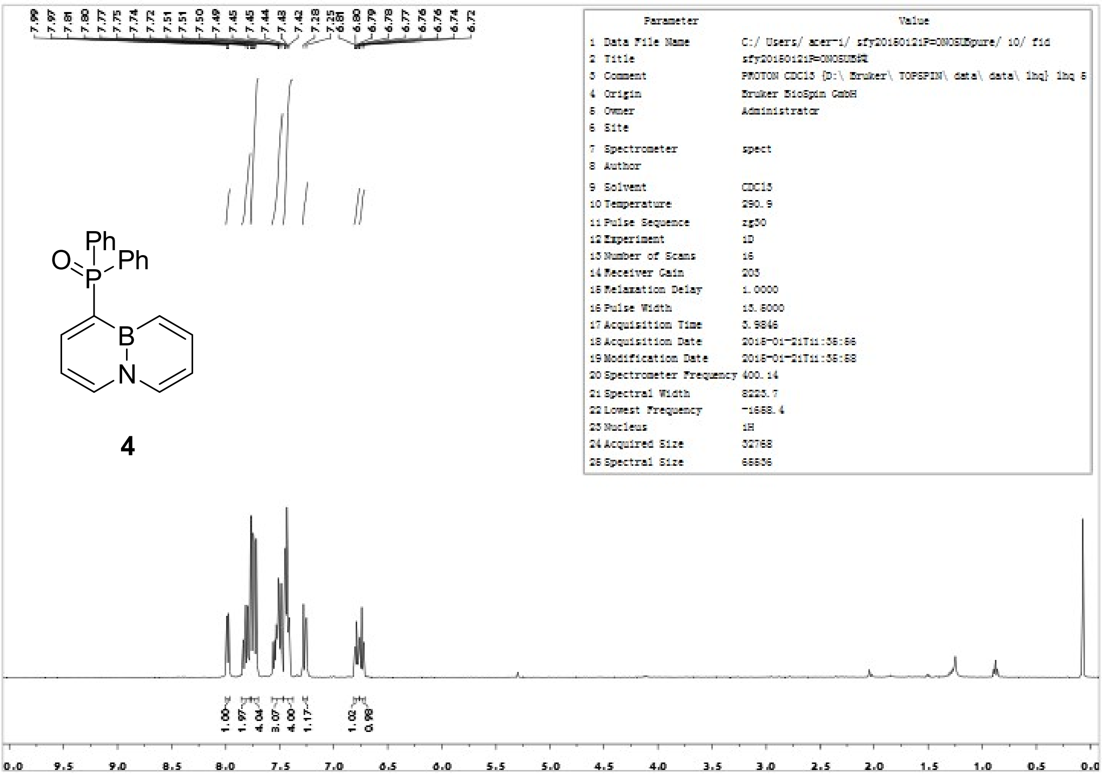

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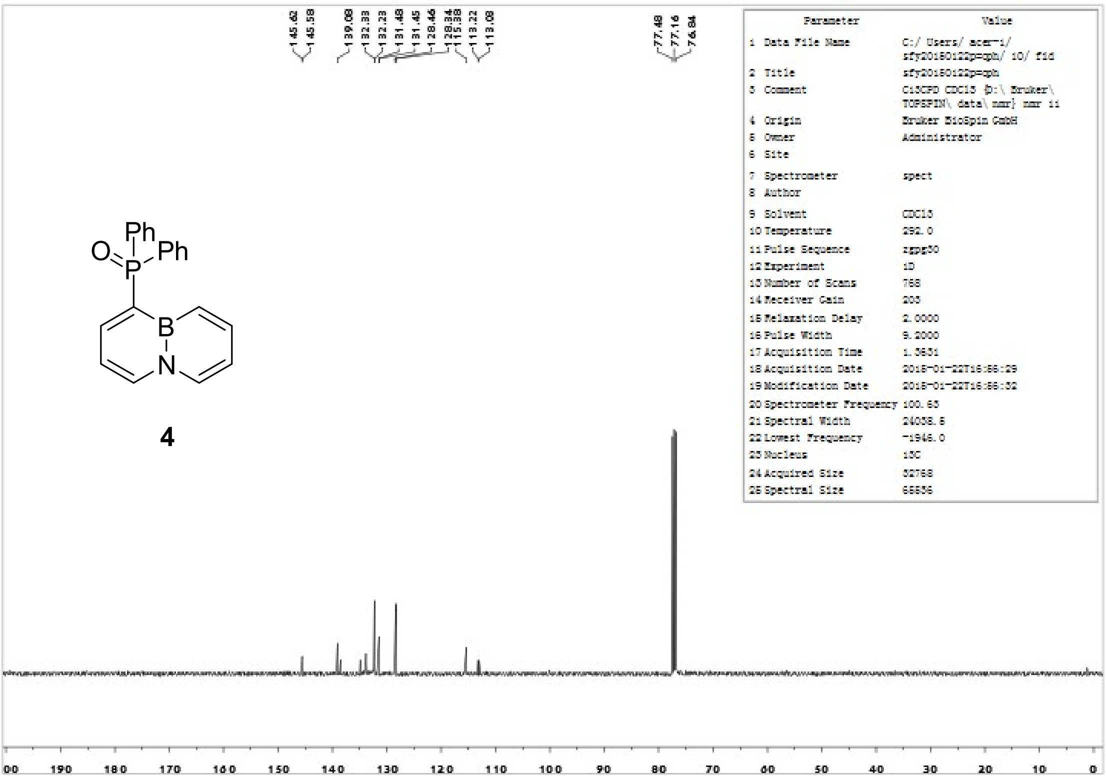

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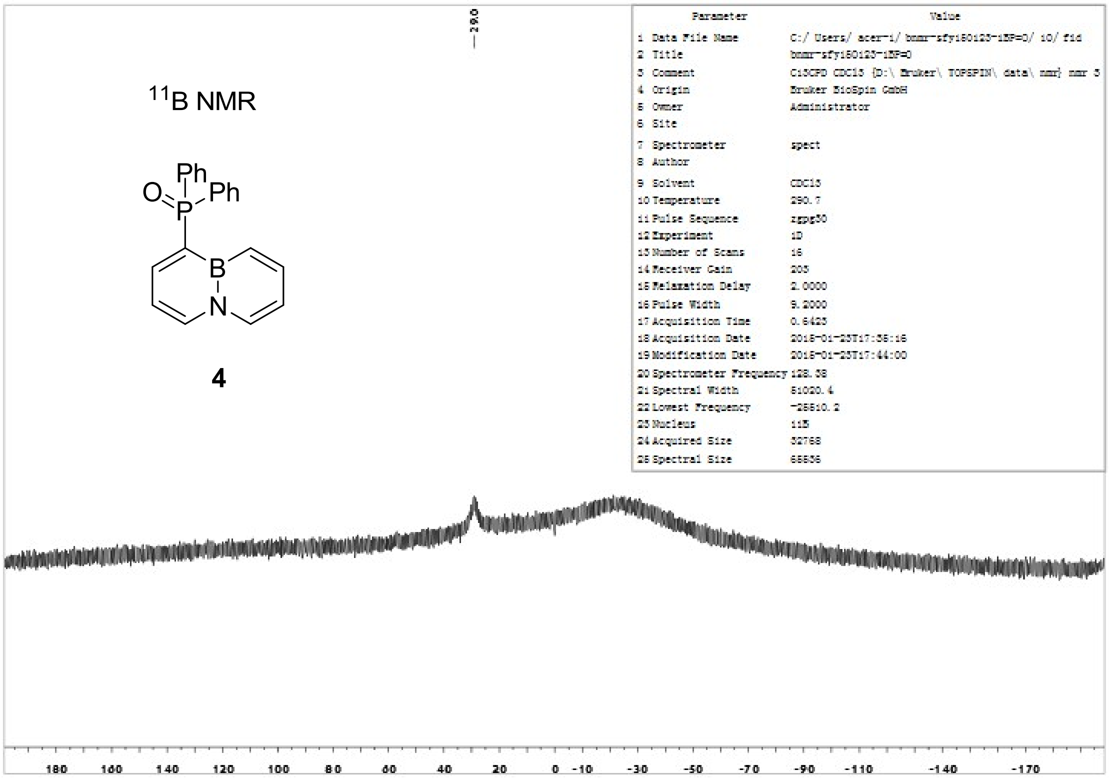

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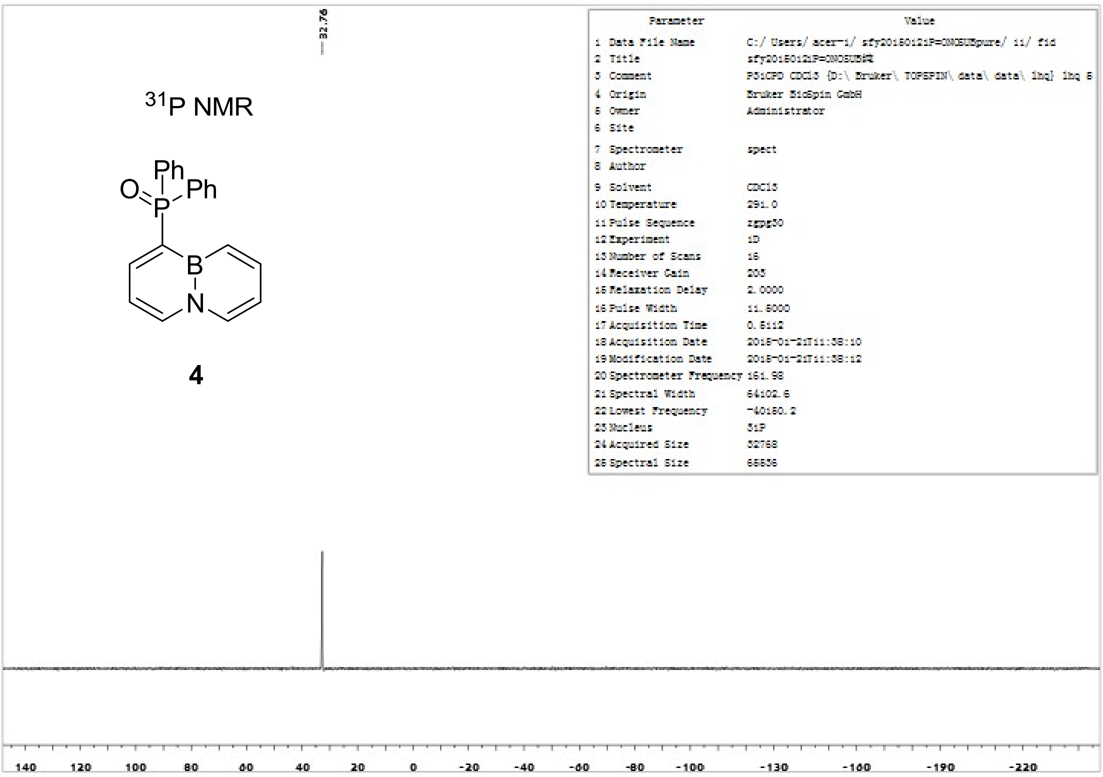
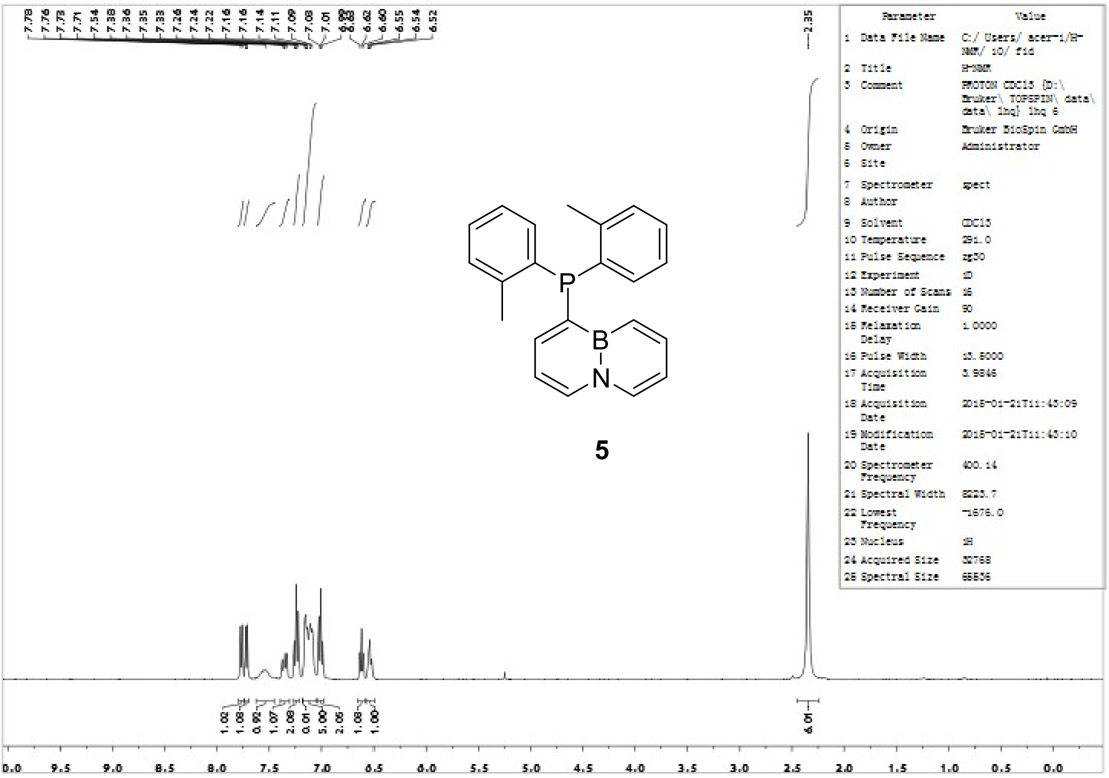
3 Comment	C13CPD CDCl3 {D:\ Bruker\ TOPSPIN\ data\ nmr} nmr 3
4 Origin	Bruker BioSpin GmbH
5 Owner	Administrator
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	290.7
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	16
14 Receiver Gain	203
15 Relaxation Delay	2.0000
16 Pulse Width	9.2000
17 Acquisition Time	0.6423
18 Acquisition Date	2015-01-23T17:35:16
19 Modification Date	2015-01-23T17:44:00
20 Spectrometer Frequency	128.38
21 Spectral Width	51020.4
22 Lowest Frequency	-25510.2
23 Nucleus	11B
24 Acquired Size	32768
25 Spectral Size	65536



4

Parameter	Value
1 Data File Name	C:/ Users/ acer~1/ sfy20150121P=ONOSUBpure/ 11/ fid
2 Title	sfy20150121P=ONOSUB纯
3 Comment	P31CPD CDCl3 {D:\ Bruker\ TOPSPIN\ data\ data\ lhq} lhq 5
4 Origin	Bruker BioSpin GmbH
5 Owner	Administrator
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	291.0
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	16
14 Receiver Gain	203
15 Relaxation Delay	2.0000
16 Pulse Width	11.5000
17 Acquisition Time	0.5112
18 Acquisition Date	2015-01-21T11:38:10
19 Modification Date	2015-01-21T11:38:12
20 Spectrometer Frequency	161.98
21 Spectral Width	64102.6
22 Lowest Frequency	-40150.2
23 Nucleus	31P
24 Acquired Size	32768
25 Spectral Size	65536



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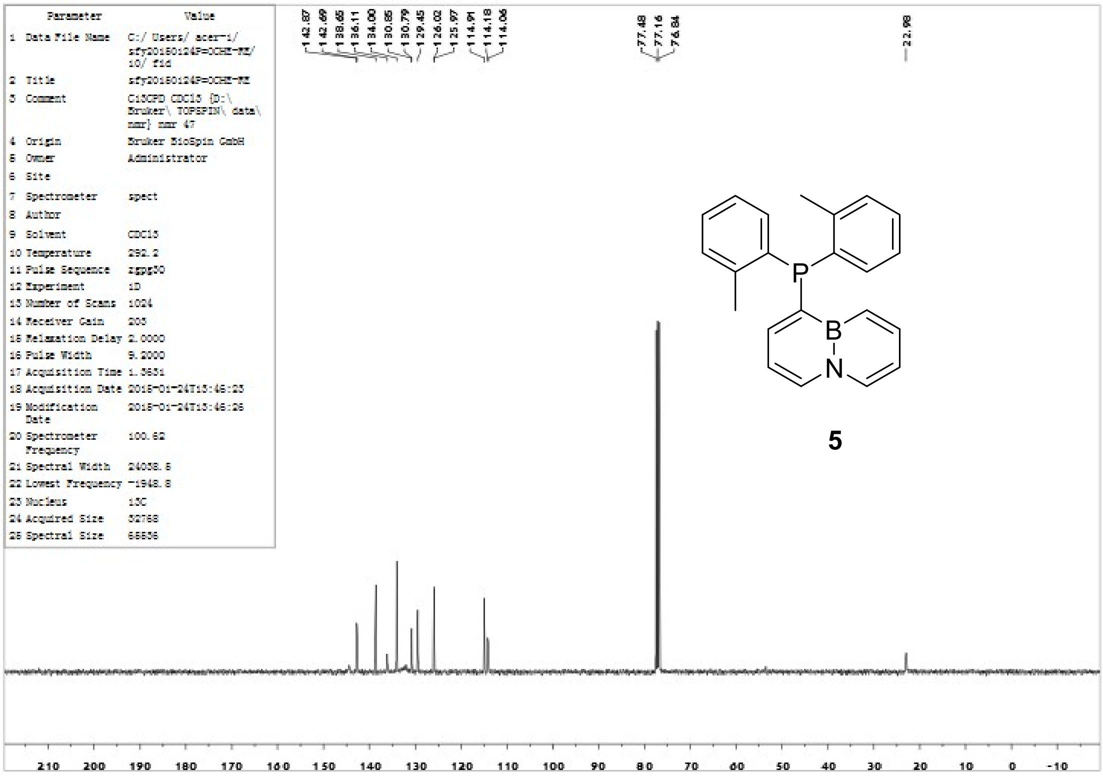
1 Data File Name	C:/ Users/ acer~1/H-NMR/ 10/ fid
2 Title	H-NMR
3 Comment	PROTON CDCl3 {D:\ Bruker\ TOPSPIN\ data\ data\ lhq} lhq 6
4 Origin	Bruker BioSpin GmbH
5 Owner	Administrator
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	291.0
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	16
14 Receiver Gain	90
15 Relaxation Delay	1.0000
16 Pulse Width	13.5000
17 Acquisition Time	3.9846
18 Acquisition Date	2015-01-21T11:43:09
19 Modification Date	2015-01-21T11:43:10
20 Spectrometer Frequency	400.14
21 Spectral Width	8223.7
22 Lowest Frequency	-1676.0
23 Nucleus	1H
24 Acquired Size	32768
25 Spectral Size	65536



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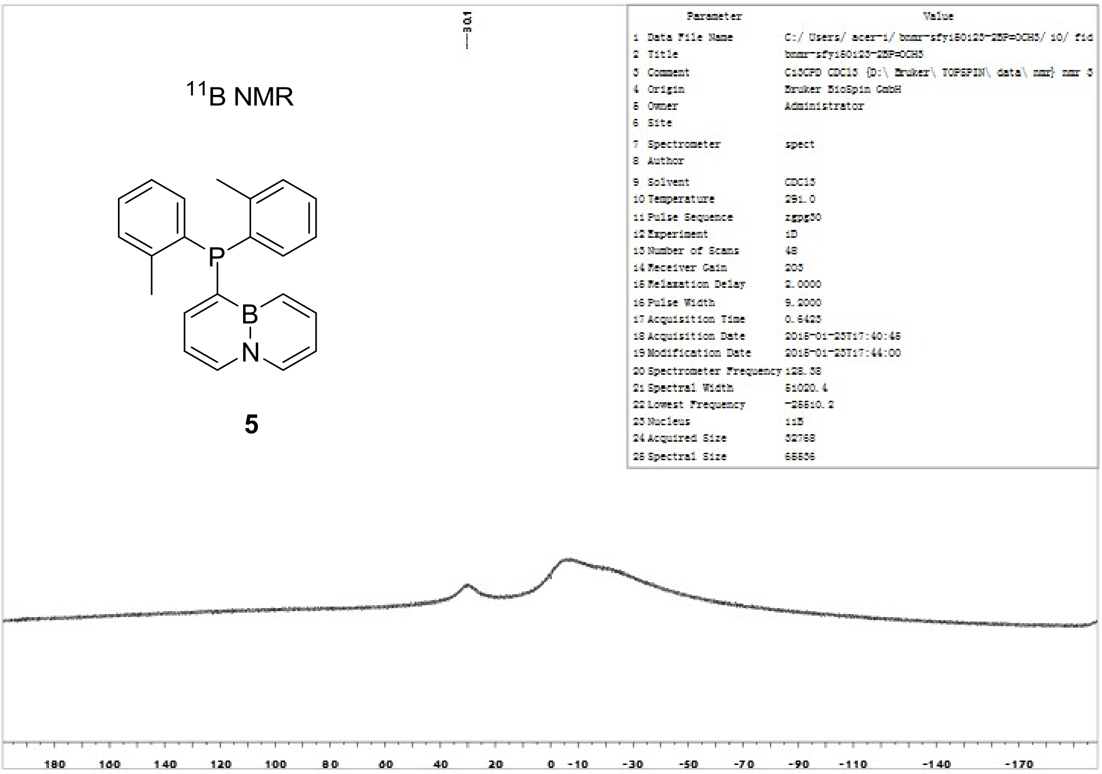
1 Data File Name	C:/ Users/ acer~1/ sfy20150124P=CCHE-WZ/ 10/ fid
2 Title	sfy20150124P=CCHE-WZ
3 Comment	C13CPD CDCl3 {D:\ Bruker\ TOPSPIN\ data\ nmr} nmr 47
4 Origin	Bruker BioSpin GmbH
5 Owner	Administrator
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	292.2
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	1024
14 Receiver Gain	203
15 Relaxation Delay	2.0000
16 Pulse Width	9.2000
17 Acquisition Time	1.3631
18 Acquisition Date	2015-01-24T13:46:23
19 Modification Date	2015-01-24T13:46:26
20 Spectrometer Frequency	100.62
21 Spectral Width	24038.5
22 Lowest Frequency	-1948.8
23 Nucleus	13C
24 Acquired Size	32768
25 Spectral Size	65536



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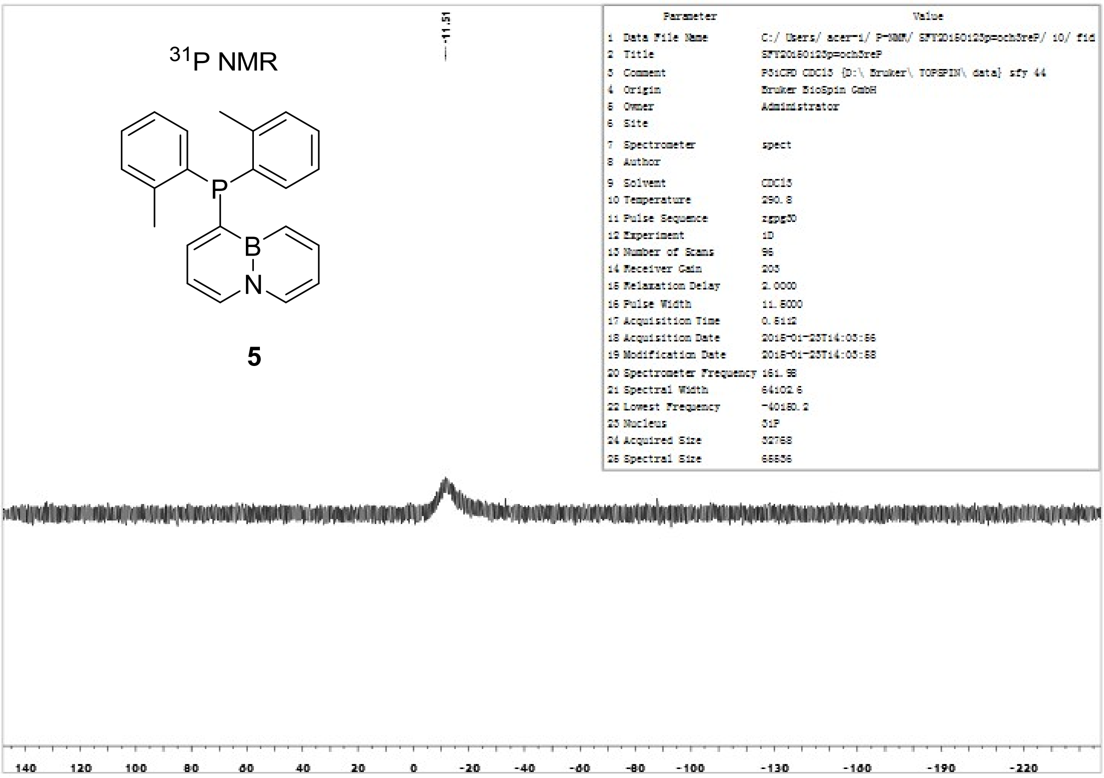
1 Data File Name	C:/ Users/ acer~1/ bnmr-sfy180123-2BP=OCH3/ 10/ fid
2 Title	bnmr-sfy180123-2BP=OCH3
3 Comment	C13CPD CDCl3 {D:\ Bruker\ TOPSPIN\ data\ nmr} nmr 3
4 Origin	Bruker BioSpin GmbH
5 Owner	Administrator
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	291.0
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	48
14 Receiver Gain	203
15 Relaxation Delay	2.0000
16 Pulse Width	9.2000
17 Acquisition Time	0.6423
18 Acquisition Date	2018-01-23T17:40:45
19 Modification Date	2018-01-23T17:44:00
20 Spectrometer Frequency	128.38
21 Spectral Width	51020.4
22 Lowest Frequency	-25510.2
23 Nucleus	11B
24 Acquired Size	32768
25 Spectral Size	65536



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Parameter	Value
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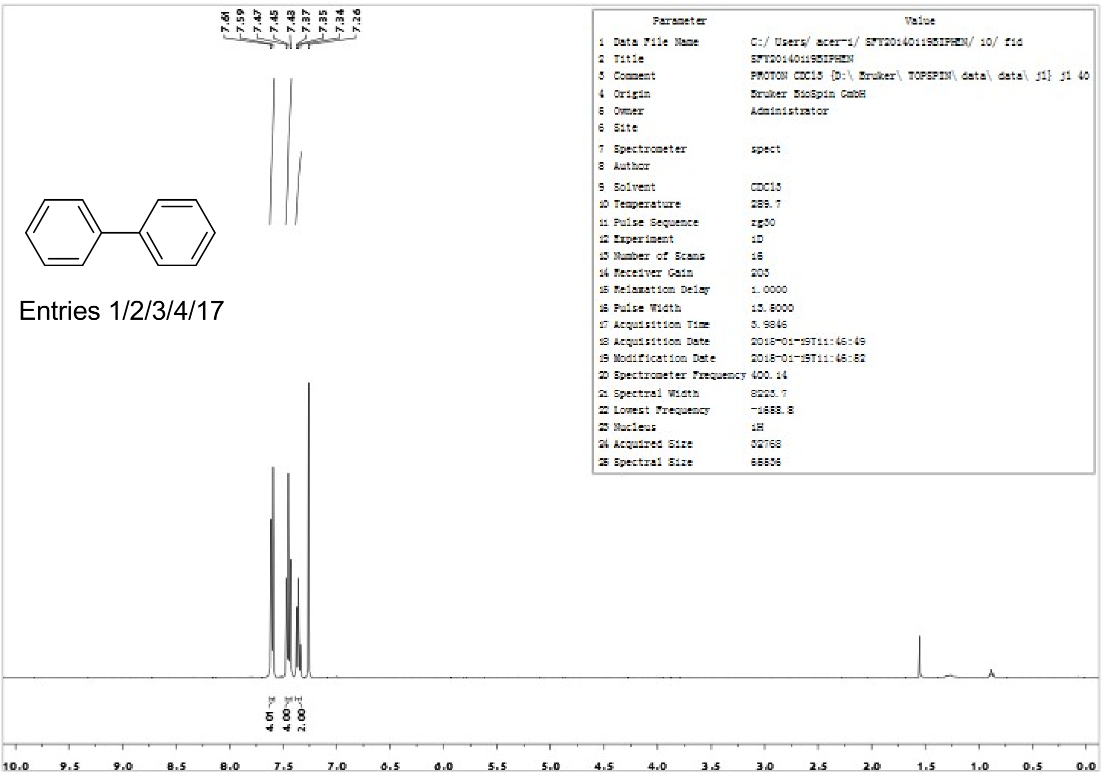
3 Comment	P31CPD CDCl3 {D:\ Bruker\ TOPSPIN\ data} sfy 44
4 Origin	Bruker BioSpin GmbH
5 Owner	Administrator
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	290.8
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	96
14 Receiver Gain	203
15 Relaxation Delay	2.0000
16 Pulse Width	11.8000
17 Acquisition Time	0.5112
18 Acquisition Date	2018-01-23T14:05:56
19 Modification Date	2018-01-23T14:05:58
20 Spectrometer Frequency	161.98
21 Spectral Width	64102.6
22 Lowest Frequency	-40180.2
23 Nucleus	31P
24 Acquired Size	32768
25 Spectral Size	65536



Entries 1/2/3/4/17

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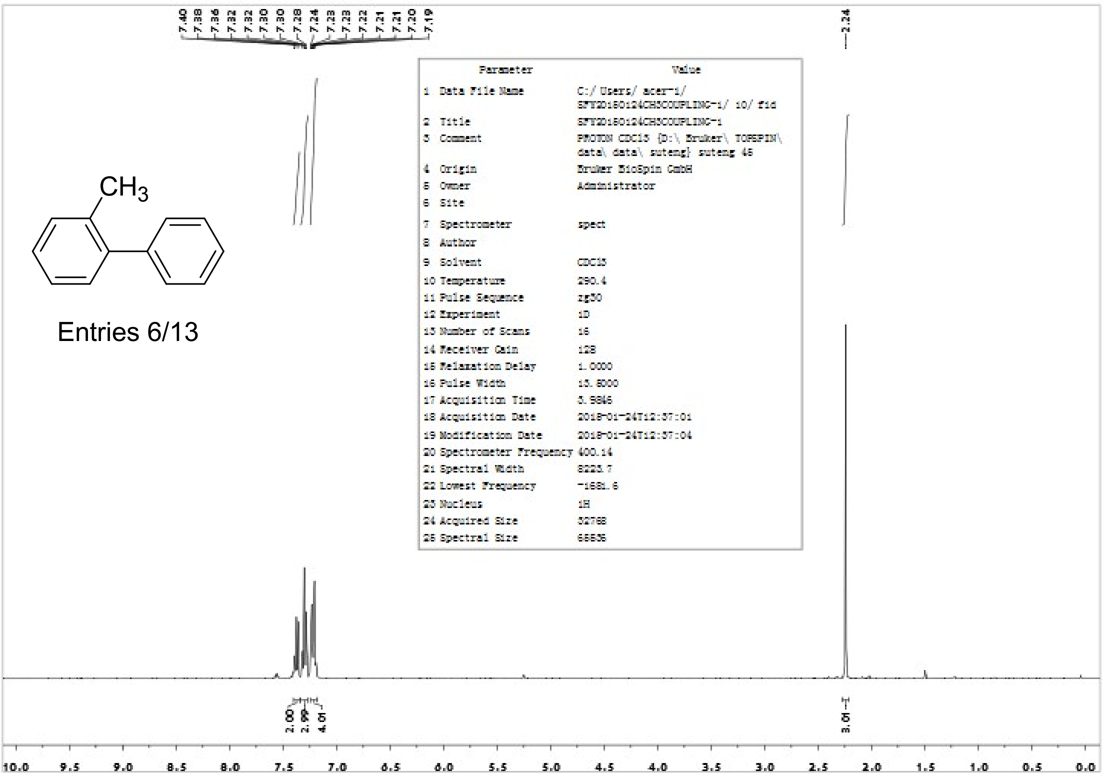
2 Title	SFY20140119BIPHEN
3 Comment	PROTON CDCl3 {D:\ Bruker\ TOPSPIN\ data\ data\ j1} j1 40
4 Origin	Bruker BioSpin GmbH
5 Owner	Administrator
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	289.7
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	16
14 Receiver Gain	203
15 Relaxation Delay	1.0000
16 Pulse Width	13.8000
17 Acquisition Time	3.9846
18 Acquisition Date	2018-01-19T11:46:49
19 Modification Date	2018-01-19T11:46:52
20 Spectrometer Frequency	400.14
21 Spectral Width	8223.7
22 Lowest Frequency	-1658.8
23 Nucleus	1H
24 Acquired Size	32768
25 Spectral Size	65536



Entries 6/13

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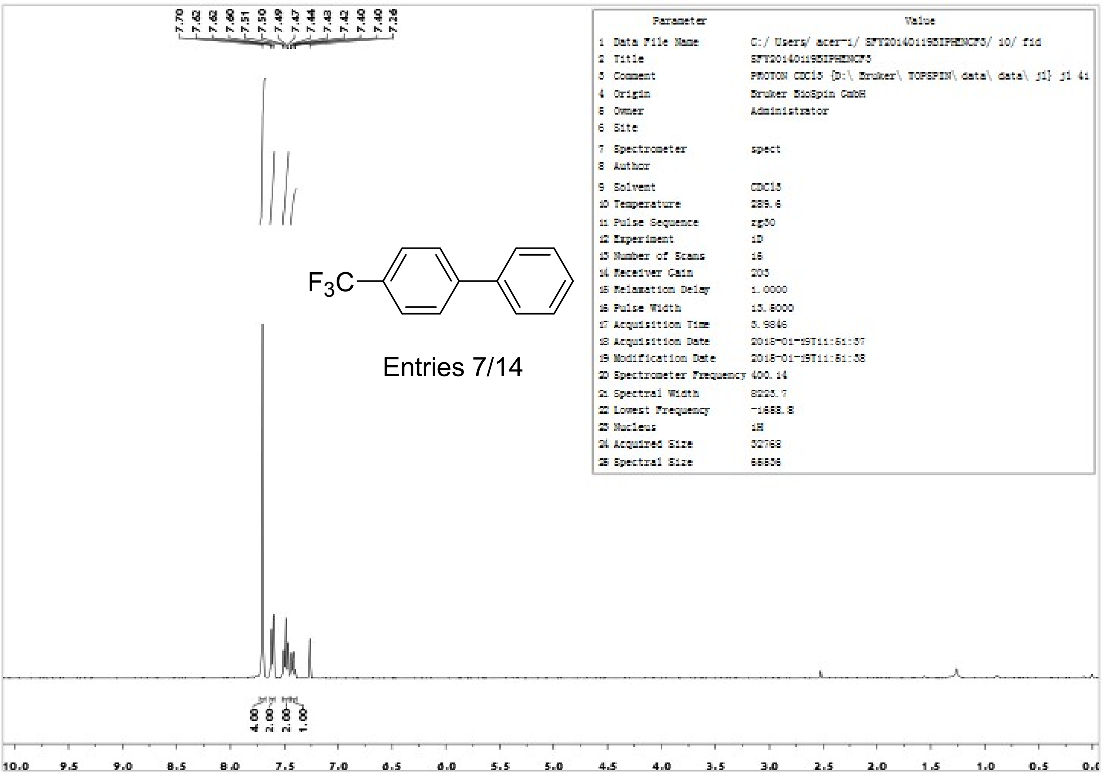
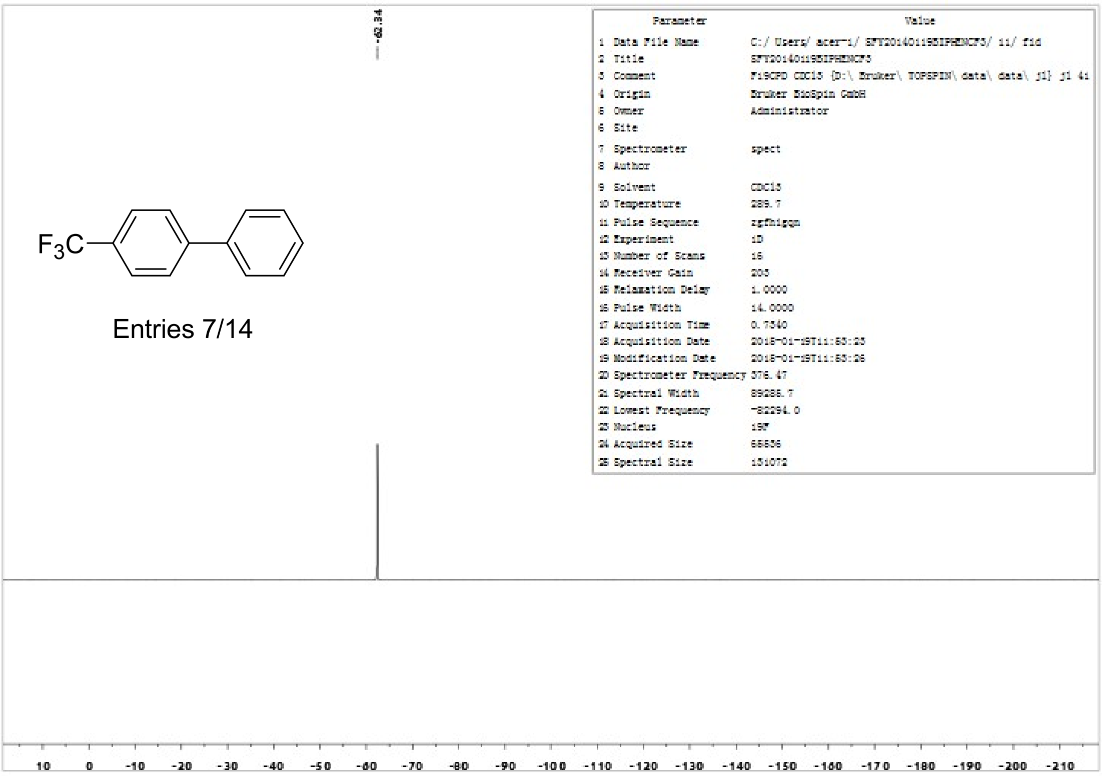
1 Data File Name	C:/ Users/ acer~1/ SFY20180124CH3COUPLING~1/ 10/ fid
2 Title	SFY20180124CH3COUPLING~1
3 Comment	PROTON CDCl3 {D:\ Bruker\ TOPSPIN\ data\ data\ suteng} suteng 45
4 Origin	Bruker BioSpin GmbH
5 Owner	Administrator
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	290.4
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	16
14 Receiver Gain	128
15 Relaxation Delay	1.0000
16 Pulse Width	13.8000
17 Acquisition Time	3.9846
18 Acquisition Date	2018-01-24T12:37:01
19 Modification Date	2018-01-24T12:37:04
20 Spectrometer Frequency	400.14
21 Spectral Width	8223.7
22 Lowest Frequency	-1681.6
23 Nucleus	1H
24 Acquired Size	32768
25 Spectral Size	65536



Parameter	Value
1 Data File Name	C:/ Users/ acer~1/ SFY20140119BIPHENCF3/ 10/ fid
2 Title	SFY20140119BIPHENCF3
3 Comment	PROTON CDCl3 {D:\ Bruker\ TOPSPIN\ data\ data\ j1} j1 4:
4 Origin	Bruker BioSpin GmbH
5 Owner	Administrator
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	289.6
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	16
14 Receiver Gain	203
15 Relaxation Delay	1.0000
16 Pulse Width	13.8000
17 Acquisition Time	3.9846
18 Acquisition Date	2015-01-19T11:51:37
19 Modification Date	2015-01-19T11:51:38
20 Spectrometer Frequency	400.14
21 Spectral Width	8223.7
22 Lowest Frequency	-1668.8
23 Nucleus	1H
24 Acquired Size	32768
25 Spectral Size	65536



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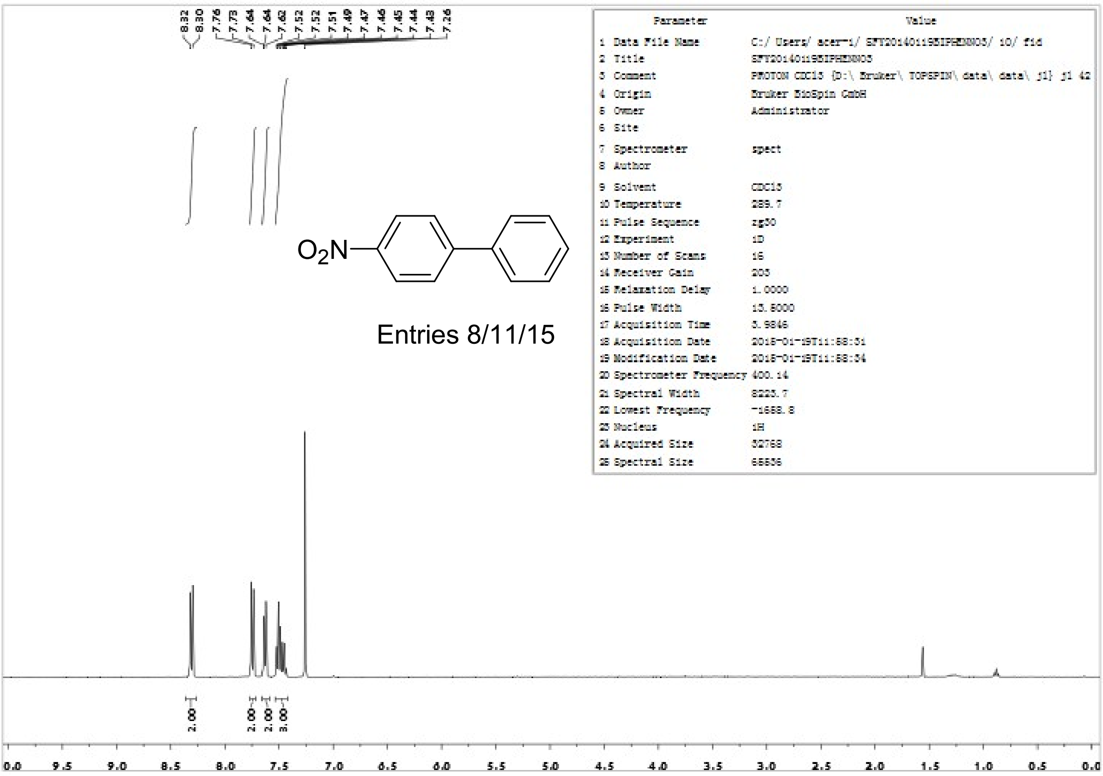
1 Data File Name	C:/ Users/ acer~1/ SFY20140119BIPHENCF3/ 11/ fid
2 Title	SFY20140119BIPHENCF3
3 Comment	F19CPD CDCl3 {D:\ Bruker\ TOPSPIN\ data\ data\ j1} j1 4:
4 Origin	Bruker BioSpin GmbH
5 Owner	Administrator
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	289.7
11 Pulse Sequence	zgfhigqn
12 Experiment	1D
13 Number of Scans	16
14 Receiver Gain	203
15 Relaxation Delay	1.0000
16 Pulse Width	14.0000
17 Acquisition Time	0.7340
18 Acquisition Date	2015-01-19T11:53:23
19 Modification Date	2015-01-19T11:53:26
20 Spectrometer Frequency	376.47
21 Spectral Width	89285.7
22 Lowest Frequency	-82294.0
23 Nucleus	19F
24 Acquired Size	65536
25 Spectral Size	131072



Entries 8/11/15

Parameter	Value
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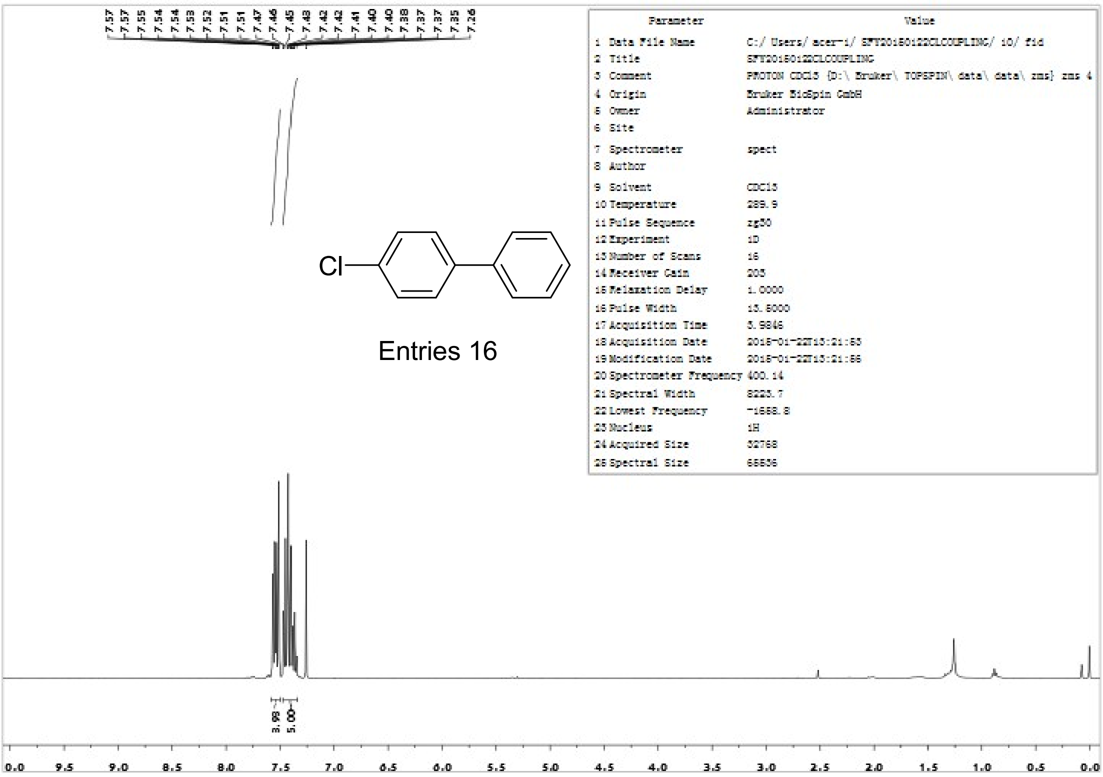
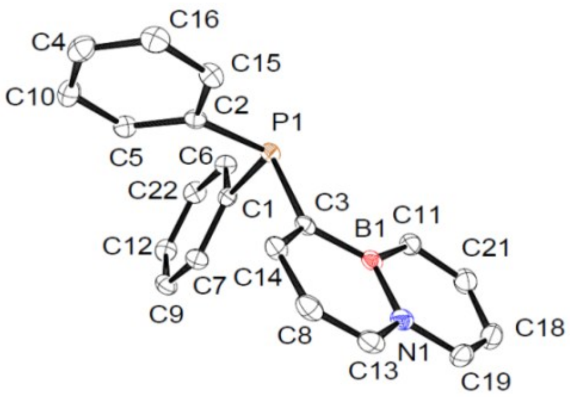
2 Title	SFY20140119BIPHENNO3
3 Comment	PROTON CDCl3 {D:\ Bruker\ TOPSPIN\ data\ data\ j1} j1 42
4 Origin	Bruker BioSpin GmbH
5 Owner	Administrator
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	299.7
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	16
14 Receiver Gain	203
15 Relaxation Delay	1.0000
16 Pulse Width	13.8000
17 Acquisition Time	3.9846
18 Acquisition Date	2015-01-19T11:58:31
19 Modification Date	2015-01-19T11:58:34
20 Spectrometer Frequency	400.14
21 Spectral Width	8223.7
22 Lowest Frequency	-1658.8
23 Nucleus	1H
24 Acquired Size	32768
25 Spectral Size	65536



Entries 16

Parameter	Value
1 Data File Name	C:/ Users/ acer~1/ SFY20150122CLCOUPLING/ 10/ fid
2 Title	SFY20150122CLCOUPLING
3 Comment	PROTON CDCl3 {D:\ Bruker\ TOPSPIN\ data\ data\ zms} zms 4
4 Origin	Bruker BioSpin GmbH
5 Owner	Administrator
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	299.9
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	16
14 Receiver Gain	203
15 Relaxation Delay	1.0000
16 Pulse Width	13.8000
17 Acquisition Time	3.9846
18 Acquisition Date	2015-01-22T13:21:53
19 Modification Date	2015-01-22T13:21:56
20 Spectrometer Frequency	400.14
21 Spectral Width	8223.7
22 Lowest Frequency	-1658.8
23 Nucleus	1H
24 Acquired Size	32768
25 Spectral Size	65536

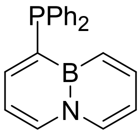


ORTEP Drawing of **3**. Thermal ellipsoids are shown at 30% probability; hydrogen atoms are omitted for clarity.

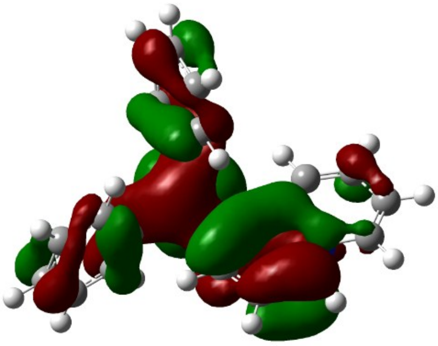
Table 1. Crystal Data and Structure Refinement for **3**

Identification code	**3**
Empirical formula	C20H17BNP
Formula weight	313.13
Temperature	173(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, *P* -1
Unit cell dimensions	a = 8.5406(9)Å alpha = 107.624(8)deg.
	b = 10.3138(9)Å beta = 90.711(8) deg.
	c = 10.8658(9)Å gamma = 113.671(9) deg.
Volume	825.56(13) A^3
Z	2
Calculated density	1.260 Mg/m^3
Absorption coefficient	0.164 mm^-1
F(000)	328
Crystal size	0.30 x 0.30 x 0.30 mm
Theta range for data collection	3.50 to 26.50 deg.
Limiting indices	-10<=h<=8, -12<=k<=12, -13<=l<=13
Reflections collected / unique	5762 / 3413 [R(int) = 0.0385]
Completeness to theta = 26.50	99.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9525 and 0.9525
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3413 / 0 / 208
Goodness-of-fit on F^2	1.083
Final R indices [I>2sigma(I)]	R1 = 0.0468, wR2 = 0.1027
R indices (all data)	R1 = 0.0575, wR2 = 0.1109
Largest diff. peak and hole	0.263 and -0.297 e.A^-3

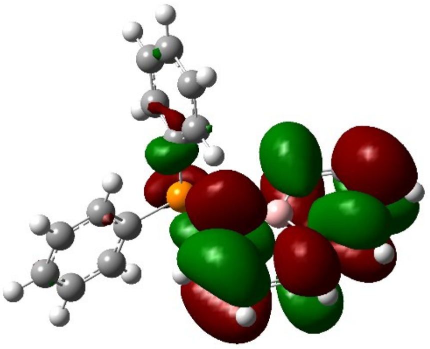
DFT Calculation



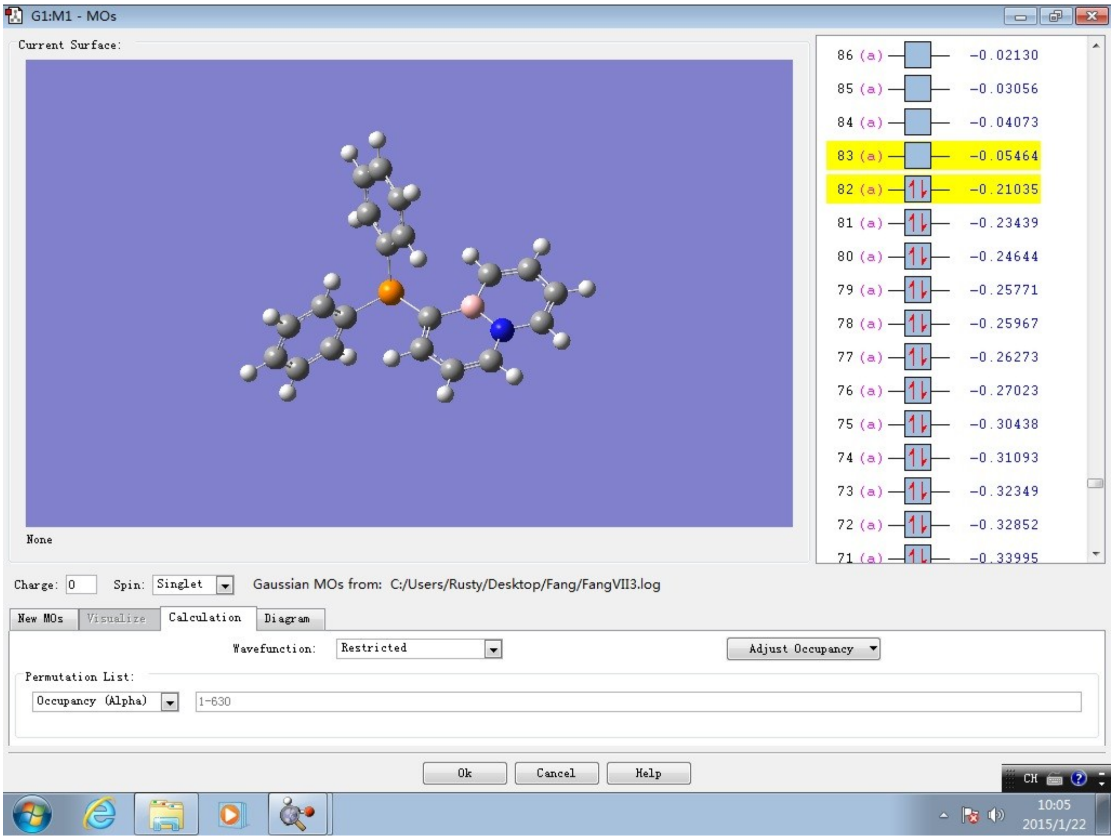
3



HOMO: –5.72 eV



LUMO: –1.49 eV



```
86 (a)  -0.02130
85 (a)  -0.03056
84 (a)  -0.04073
83 (a)  -0.05464
82 (a)  -0.21035
81 (a)  -0.23439
80 (a)  -0.24644
79 (a)  -0.25771
78 (a)  -0.25967
77 (a)  -0.26273
76 (a)  -0.27023
75 (a)  -0.30438
74 (a)  -0.31093
73 (a)  -0.32349
72 (a)  -0.32852
71 (a)  -0.33995
```

Charge: 0 Spin: Singlet Gaussian MOs from: C:/Users/Rusty/Desktop/Fang/FangVII3.log

Wavefunction: Restricted

Permutation List:

Occupancy (Alpha) 1-630

Filename = C:/Users/Rusty/Desktop/Fang/3.log

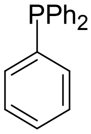
Sketch 5
File Name = 3
File Type = .log
Calculation Type = FOPT
Calculation Method = RB3LYP
Basis Set = 6-311++G(d,p)
Charge = 0
Spin = Singlet
E(RB3LYP) = –1193.60065081 a.u.
RMS Gradient Norm = 0.00000890 a.u.
Imaginary Freq =
Dipole Moment = 2.4655 Debye
Point Group = C1
Job CPU time: 3 days 19 hours 53 minutes 11.0 seconds

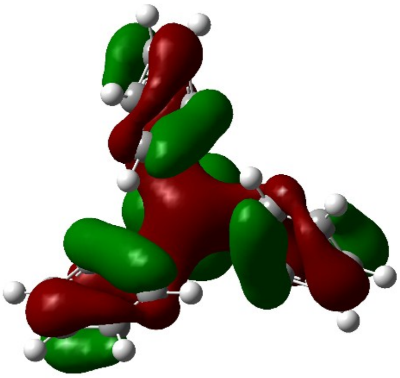
Table of Atom Coordinates of **3**

2.7302	0.6267	-1.2199	C	0	0	0	0	0	0	0	0	0	0	0	0
4.0826	0.8138	-1.2915	C	0	0	0	0	0	0	0	0	0	0	0	0
4.9780	-0.0017	-0.5342	C	0	0	0	0	0	0	0	0	0	0	0	0
4.5182	-0.9919	0.2753	C	0	0	0	0	0	0	0	0	0	0	0	0
4.5127	1.5834	-1.9269	H	0	0	0	0	0	0	0	0	0	0	0	0
6.0476	0.1558	-0.5987	H	0	0	0	0	0	0	0	0	0	0	0	0
5.1879	-1.6216	0.8497	H	0	0	0	0	0	0	0	0	0	0	0	0
3.1674	-1.2573	0.4122	N	0	0	0	0	0	0	0	0	0	0	0	0
2.1636	-0.4614	-0.3217	B	0	0	0	0	0	0	0	0	0	0	0	0
0.6945	-0.8401	-0.0838	C	0	0	0	0	0	0	0	0	0	0	0	0
0.4263	-1.8965	0.7512	C	0	0	0	0	0	0	0	0	0	0	0	0
1.4697	-2.6150	1.4104	C	0	0	0	0	0	0	0	0	0	0	0	0
2.7784	-2.2932	1.2417	C	0	0	0	0	0	0	0	0	0	0	0	0
-0.6166	0.0311	-1.0451	P	0	0	0	0	0	0	0	0	0	0	0	0
-2.1819	-0.8082	-0.5049	C	0	0	0	0	0	0	0	0	0	0	0	0
-2.9399	-0.4365	0.6129	C	0	0	0	0	0	0	0	0	0	0	0	0
-4.1135	-1.1181	0.9340	C	0	0	0	0	0	0	0	0	0	0	0	0
-4.5446	-2.1854	0.1477	C	0	0	0	0	0	0	0	0	0	0	0	0
-3.8003	-2.5638	-0.9689	C	0	0	0	0	0	0	0	0	0	0	0	0
-2.6348	-1.8739	-1.2961	C	0	0	0	0	0	0	0	0	0	0	0	0
-0.3320	3.2160	1.6420	C	0	0	0	0	0	0	0	0	0	0	0	0
-0.9915	4.2304	0.9508	C	0	0	0	0	0	0	0	0	0	0	0	0
-1.5223	3.9716	-0.3127	C	0	0	0	0	0	0	0	0	0	0	0	0
-1.3877	2.7066	-0.8800	C	0	0	0	0	0	0	0	0	0	0	0	0
-0.7380	1.6733	-0.1892	C	0	0	0	0	0	0	0	0	0	0	0	0

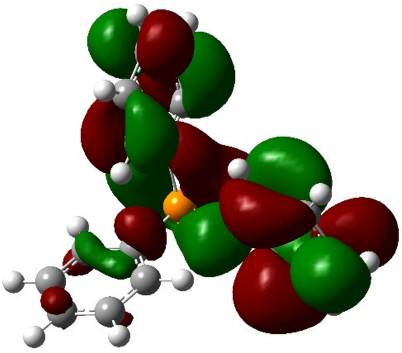
```
-0.2081     1.9464     1.0778 C    0  0  0  0  0  0  0  0  0  0  0  0
-0.5931    -2.2216     0.9375 H    0  0  0  0  0  0  0  0  0  0  0  0
 1.2217    -3.4385     2.0690 H    0  0  0  0  0  0  0  0  0  0  0  0
 3.5745    -2.8321     1.7422 H    0  0  0  0  0  0  0  0  0  0  0  0
-2.6178     0.3920     1.2327 H    0  0  0  0  0  0  0  0  0  0  0  0
-4.6912    -0.8138     1.8003 H    0  0  0  0  0  0  0  0  0  0  0  0
-5.4578    -2.7135     0.3989 H    0  0  0  0  0  0  0  0  0  0  0  0
-4.1326    -3.3875    -1.5913 H    0  0  0  0  0  0  0  0  0  0  0  0
-2.0706    -2.1612    -2.1778 H    0  0  0  0  0  0  0  0  0  0  0  0
0.0866      3.4111     2.6236 H    0  0  0  0  0  0  0  0  0  0  0  0
-1.0868     5.2171     1.3904 H    0  0  0  0  0  0  0  0  0  0  0  0
-2.0314     4.7569    -0.8608 H    0  0  0  0  0  0  0  0  0  0  0  0
-1.7877     2.5178    -1.8713 H    0  0  0  0  0  0  0  0  0  0  0  0
0.3058      1.1652     1.6255 H    0  0  0  0  0  0  0  0  0  0  0  0
2.0919      1.2693    -1.8186 H    0  0  0  0  0  0  0  0  0  0  0  0
1   2   2   0   0   0   0
1   9   1   0   0   0   0
1   40   1   0   0   0   0
 2   3   4   0   0   0   0
 2   5   1   0   0   0   0
 3   4   2   0   0   0   0
 3   6   1   0   0   0   0
 4   7   1   0   0   0   0
 4   8   1   0   0   0   0
 8   9   1   0   0   0   0
 8   13   1   0   0   0   0
 9   10   1   0   0   0   0
10   11   2   0   0   0   0
10   14   1   0   0   0   0
11   12   4   0   0   0   0
11   27   1   0   0   0   0
12   13   2   0   0   0   0
12   28   1   0   0   0   0
13   29   1   0   0   0   0
14   15   1   0   0   0   0
14   25   1   0   0   0   0
15   16   4   0   0   0   0
15   20   4   0   0   0   0
16   17   4   0   0   0   0
16   30   1   0   0   0   0
17   18   4   0   0   0   0
17   31   1   0   0   0   0
18   19   4   0   0   0   0
18   32   1   0   0   0   0
```

19	20	4	0	0	0	0
19	33	1	0	0	0	0
20	34	1	0	0	0	0
21	22	4	0	0	0	0
21	26	4	0	0	0	0
21	35	1	0	0	0	0
22	23	4	0	0	0	0
22	36	1	0	0	0	0
23	24	4	0	0	0	0
23	37	1	0	0	0	0
24	25	4	0	0	0	0
24	38	1	0	0	0	0
25	26	4	0	0	0	0
26	39	1	0	0	0	0

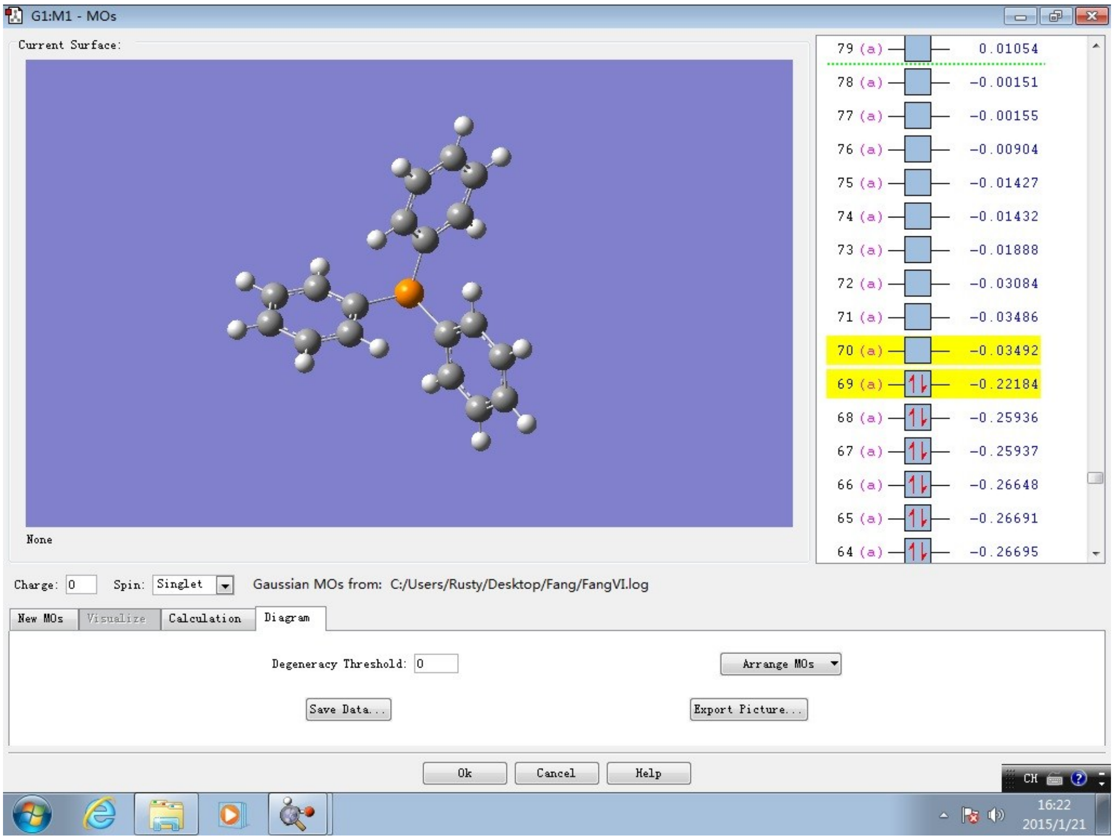




HOMO: –6.04 eV



LUMO: –0.95 eV



Current Surface:

None

Charge: 0 Spin: Singlet Gaussian MOs from: C:/Users/Rusty/Desktop/Fang/FangVI.log

Degeneracy Threshold: 0

79 (a)	0.01054
78 (a)	–0.00151
77 (a)	–0.00155
76 (a)	–0.00904
75 (a)	–0.01427
74 (a)	–0.01432
73 (a)	–0.01888
72 (a)	–0.03084
71 (a)	–0.03486
70 (a)	–0.03492
69 (a)	–0.22184
68 (a)	–0.25936
67 (a)	–0.25937
66 (a)	–0.26648
65 (a)	–0.26691
64 (a)	–0.26695

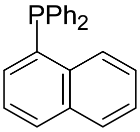
Filename = C:/Users/Rusty/Desktop/Fang/PPh3.log

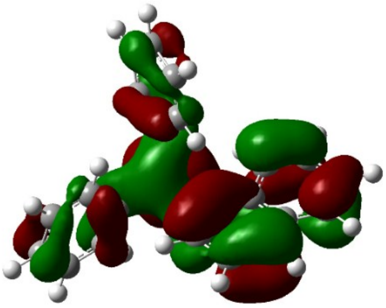
Fang VI
File Name = PPh3
File Type = .log
Calculation Type = FOPT
Calculation Method = RB3LYP
Basis Set = 6-311++G(d,p)
Charge = 0
Spin = Singlet
E(RB3LYP) = –1036.49883599 a.u.
RMS Gradient Norm = 0.00003731 a.u.
Imaginary Freq =
Dipole Moment = 1.3670 Debye
Point Group = C1
Job CPU time: 7 days 5 hours 32 minutes 13.9 seconds

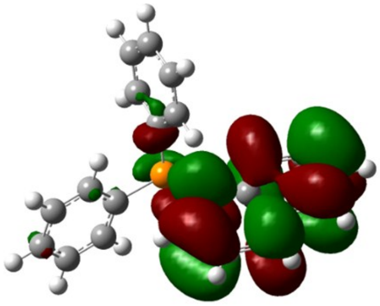
Table of Atom Coordinates of PPh_3

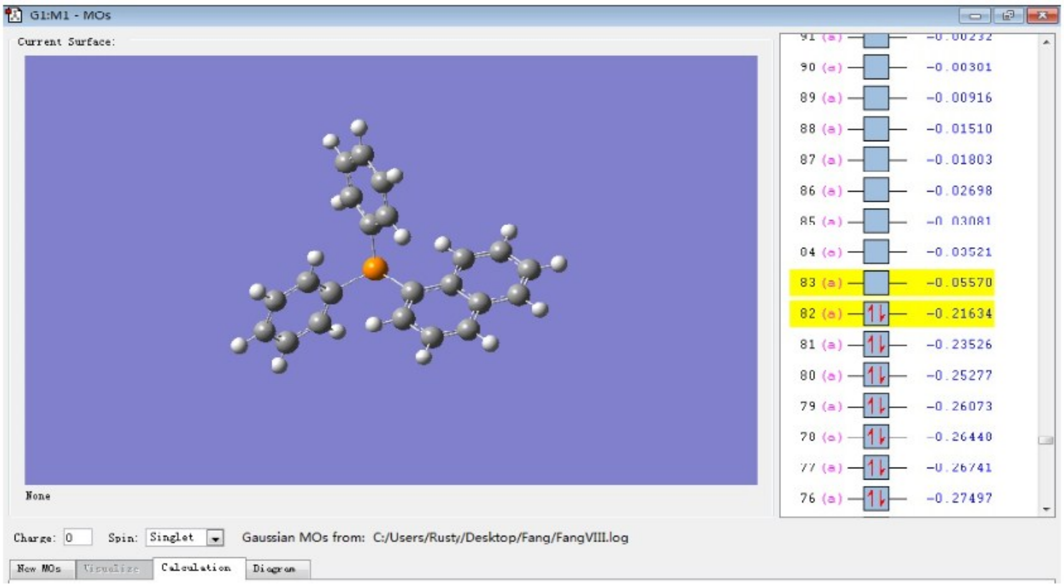
2.0872	-3.4547	-0.4622 C	0	0	0	0	0	0	0	0	0	0	0	0
1.2446	-2.4834	-0.9970 C	0	0	0	0	0	0	0	0	0	0	0	0
1.1454	-1.2140	-0.4081 C	0	0	0	0	0	0	0	0	0	0	0	0
1.9322	-0.9340	0.7158 C	0	0	0	0	0	0	0	0	0	0	0	0
2.7859	-1.9026	1.2438 C	0	0	0	0	0	0	0	0	0	0	0	0
2.8629	-3.1655	0.6602 C	0	0	0	0	0	0	0	0	0	0	0	0
-0.0006	-0.0005	-1.2174 P	0	0	0	0	0	0	0	0	0	0	0	0
0.4776	1.5985	-0.4081 C	0	0	0	0	0	0	0	0	0	0	0	0
-0.1528	2.1368	0.7203 C	0	0	0	0	0	0	0	0	0	0	0	0
0.2611	3.3598	1.2487 C	0	0	0	0	0	0	0	0	0	0	0	0
1.3124	4.0601	0.6609 C	0	0	0	0	0	0	0	0	0	0	0	0
1.9449	3.5361	-0.4662 C	0	0	0	0	0	0	0	0	0	0	0	0
1.5235	2.3213	-1.0010 C	0	0	0	0	0	0	0	0	0	0	0	0
-3.0414	-1.4555	1.2478 C	0	0	0	0	0	0	0	0	0	0	0	0
-4.1735	-0.8933	0.6615 C	0	0	0	0	0	0	0	0	0	0	0	0
-4.0359	-0.0815	-0.4642 C	0	0	0	0	0	0	0	0	0	0	0	0
-2.7733	0.1603	-0.9997 C	0	0	0	0	0	0	0	0	0	0	0	0
-1.6245	-0.3857	-0.4080 C	0	0	0	0	0	0	0	0	0	0	0	0
-1.7755	-1.2021	0.7194 C	0	0	0	0	0	0	0	0	0	0	0	0
2.1468	-4.4321	-0.9283 H	0	0	0	0	0	0	0	0	0	0	0	0
0.6584	-2.7112	-1.8817 H	0	0	0	0	0	0	0	0	0	0	0	0
1.8822	0.0434	1.1806 H	0	0	0	0	0	0	0	0	0	0	0	0
3.3903	-1.6683	2.1135 H	0	0	0	0	0	0	0	0	0	0	0	0
3.5269	-3.9172	1.0722 H	0	0	0	0	0	0	0	0	0	0	0	0
-0.9712	1.6031	1.1887 H	0	0	0	0	0	0	0	0	0	0	0	0
-0.2398	3.7636	2.1220 H	0	0	0	0	0	0	0	0	0	0	0	0
1.6323	5.0108	1.0728 H	0	0	0	0	0	0	0	0	0	0	0	0
2.7586	4.0782	-0.9355 H	0	0	0	0	0	0	0	0	0	0	0	0

```
2.0094      1.9297     -1.8892 H    0   0   0   0   0   0   0   0   0   0   0   0
-3.1407     -2.0914      2.1209 H    0   0   0   0   0   0   0   0   0   0   0   0
-5.1565     -1.0905      1.0745 H    0   0   0   0   0   0   0   0   0   0   0   0
-4.9121      0.3540     -0.9320 H    0   0   0   0   0   0   0   0   0   0   0   0
-2.6774      0.7773     -1.8876 H    0   0   0   0   0   0   0   0   0   0   0   0
-0.9041     -1.6452      1.1866 H    0   0   0   0   0   0   0   0   0   0   0   0
1   2   4   0   0   0   0
1   6   4   0   0   0   0
1   20   1   0   0   0   0
2   3   4   0   0   0   0
2 21   1   0   0   0   0
3   4   4   0   0   0   0
3   7   1   0   0   0   0
4   5   4   0   0   0   0
4   22   1   0   0   0   0
5   6   4   0   0   0   0
5   23   1   0   0   0   0
6   24   1   0   0   0   0
7   8   1   0   0   0   0
7   18   1   0   0   0   0
8   9   4   0   0   0   0
8   13   4   0   0   0   0
9   10   4   0   0   0   0
9   25   1   0   0   0   0
10   11   4   0   0   0   0
10   26   1   0   0   0   0
11   12   4   0   0   0   0
11   27   1   0   0   0   0
12   13   4   0   0   0   0
12   28   1   0   0   0   0
13   29   1   0   0   0   0
14   15   4   0   0   0   0
14   19   4   0   0   0   0
14   30   1   0   0   0   0
15   16   4   0   0   0   0
15   31   1   0   0   0   0
16   17   4   0   0   0   0
16   32   1   0   0   0   0
17   18   4   0   0   0   0
17   33   1   0   0   0   0
18   19   4   0   0   0   0
19   34   1   0   0   0   0
```




HOMO: –5.89 eV


LUMO: –1.52 eV



```
91 (a)  -0.00232
90 (a)  -0.00301
89 (a)  -0.00916
88 (a)  -0.01510
87 (a)  -0.01803
86 (a)  -0.02698
85 (a)  -0.03081
84 (a)  -0.03521
83 (a)  -0.05570
82 (a)  -0.21634
81 (a)  -0.23526
80 (a)  -0.25277
79 (a)  -0.26073
78 (a)  -0.26440
77 (a)  -0.26741
76 (a)  -0.27497
```

Charge: 0 Spin: Singlet Gaussian MOs from: C:/Users/Rusty/Desktop/Fang/FangVIII.log

Filename = C:/Users/Rusty/Desktop/Fang/FangVIII.log
Sketch 5
File Name = FangVIII
File Type = .log
Calculation Type = FOPT
Calculation Method = RB3LYP
Basis Set = 6-311++G(d,p)
Charge = 0
Spin = Singlet
E(RB3LYP) = -1190.17397118 a.u.
RMS Gradient Norm = 0.00000880 a.u.
Imaginary Freq =
Dipole Moment = 1.2714 Debye
Point Group = C1
Job cpu time: 3 days 10 hours 11 minutes 23.1 seconds.

Table of Atom Coordinates of (1-Naphthyl)diphenylphosphine

```
***************************************************************************
      2.5603     0.4154    -1.2509 C   0  0  0  0  0  0  0  0  0  0  0  0
      3.8939     0.6783    -1.4599 C   0  0  0  0  0  0  0  0  0  0  0  0
      4.8840     0.0068    -0.7088 C   0  0  0  0  0  0  0  0  0  0  0  0
      4.5140    -0.9226     0.2323 C   0  0  0  0  0  0  0  0  0  0  0  0
      4.1884     1.4040    -2.2097 H   0  0  0  0  0  0  0  0  0  0  0  0
      5.9322     0.2236    -0.8810 H   0  0  0  0  0  0  0  0  0  0  0  0
      5.2667    -1.4485     0.8107 H   0  0  0  0  0  0  0  0  0  0  0  0
      3.1462    -1.2189     0.4710 C   0  0  0  0  0  0  0  0  0  0  0  0
      2.1362    -0.5327    -0.2808 C   0  0  0  0  0  0  0  0  0  0  0  0
      0.7518    -0.8233    -0.0207 C   0  0  0  0  0  0  0  0  0  0  0  0
      0.4347    -1.7751     0.9287 C   0  0  0  0  0  0  0  0  0  0  0  0
      1.4357    -2.4589     1.6563 C   0  0  0  0  0  0  0  0  0  0  0  0
      2.7612    -2.1841     1.4375 C   0  0  0  0  0  0  0  0  0  0  0  0
     -0.5488     0.0338    -1.0381 P   0  0  0  0  0  0  0  0  0  0  0  0
     -2.1014    -0.8353    -0.5200 C   0  0  0  0  0  0  0  0  0  0  0  0
     -2.9192    -0.4312     0.5425 C   0  0  0  0  0  0  0  0  0  0  0  0
     -4.0892    -1.1290     0.8417 C   0  0  0  0  0  0  0  0  0  0  0  0
     -4.4556    -2.2426     0.0882 C   0  0  0  0  0  0  0  0  0  0  0  0
     -3.6515    -2.6517    -0.9750 C   0  0  0  0  0  0  0  0  0  0  0  0
     -2.4904    -1.9463    -1.2825 C   0  0  0  0  0  0  0  0  0  0  0  0
     -0.3041     3.2401     1.6252 C   0  0  0  0  0  0  0  0  0  0  0  0
     -1.0118     4.2286     0.9444 C   0  0  0  0  0  0  0  0  0  0  0  0
     -1.5631     3.9458    -0.3051 C   0  0  0  0  0  0  0  0  0  0  0  0
     -1.4019     2.6824    -0.8686 C   0  0  0  0  0  0  0  0  0  0  0  0
     -0.7061     1.6741    -0.1854 C   0  0  0  0  0  0  0  0  0  0  0  0
     -0.1538     1.9709     1.0664 C   0  0  0  0  0  0  0  0  0  0  0  0
     -0.6029    -2.0101     1.1303 H   0  0  0  0  0  0  0  0  0  0  0  0
      1.1434    -3.1985     2.3936 H   0  0  0  0  0  0  0  0  0  0  0  0
      3.5335    -2.7007     1.9981 H   0  0  0  0  0  0  0  0  0  0  0  0
     -2.6451     0.4325     1.1367 H   0  0  0  0  0  0  0  0  0  0  0  0
     -4.7139    -0.8010     1.6656 H   0  0  0  0  0  0  0  0  0  0  0  0
     -5.3657    -2.7837     0.3225 H   0  0  0  0  0  0  0  0  0  0  0  0
     -3.9340    -3.5117    -1.5723 H   0  0  0  0  0  0  0  0  0  0  0  0
     -1.8799    -2.2583    -2.1239 H   0  0  0  0  0  0  0  0  0  0  0  0
      0.1321     3.4546     2.5949 H   0  0  0  0  0  0  0  0  0  0  0  0
     -1.1282     5.2144     1.3808 H   0  0  0  0  0  0  0  0  0  0  0  0
     -2.1094     4.7113    -0.8453 H   0  0  0  0  0  0  0  0  0  0  0  0
     -1.8189     2.4758    -1.8493 H   0  0  0  0  0  0  0  0  0  0  0  0
      0.3979     1.2109     1.6069 H   0  0  0  0  0  0  0  0  0  0  0  0
      1.8172     0.9341    -1.8444 H   0  0  0  0  0  0  0  0  0  0  0  0
  1  2  2  0  0  0  0
  1  9  4  0  0  0  0
```

```
  1   40   1   0   0   0   0
  2   3   4   0   0   0   0
  2   5   1   0   0   0   0
  3   4   2   0   0   0   0
  3   6   1   0   0   0   0
  4   7   1   0   0   0   0
  4   8   4   0   0   0   0
  8   9   4   0   0   0   0
  8   13   4   0   0   0   0
  9   10   4   0   0   0   0
 10   11   2   0   0   0   0
 10   14   1   0   0   0   0
 11   12   4   0   0   0   0
 11   27   1   0   0   0   0
 12   13   2   0   0   0   0
 12   28   1   0   0   0   0
 13   29   1   0   0   0   0
 14   15   1   0   0   0   0
 14   25   1   0   0   0   0
 15   16   4   0   0   0   0
 15   20   4   0   0   0   0
 16   17   4   0   0   0   0
 16   30   1   0   0   0   0
 17   18   4   0   0   0   0
 17   31   1   0   0   0   0
 18   19   4   0   0   0   0
 18   32   1   0   0   0   0
 19   20   4   0   0   0   0
 19   33   1   0   0   0   0
 20   34   1   0   0   0   0
 21   22   4   0   0   0   0
 21   26   4   0   0   0   0
 21   35   1   0   0   0   0
 22   23   4   0   0   0   0
 22   36   1   0   0   0   0
 23   24   4   0   0   0   0
 23   37   1   0   0   0   0
 24   25   4   0   0   0   0
 24   38   1   0   0   0   0
 25   26   4   0   0   0   0
 26   39   1   0   0   0   0
****************************************************************************
```