Reductive Openings of Acetals; Explanation of Regioselectivity in Borane Reductions by Mechanistic Studies

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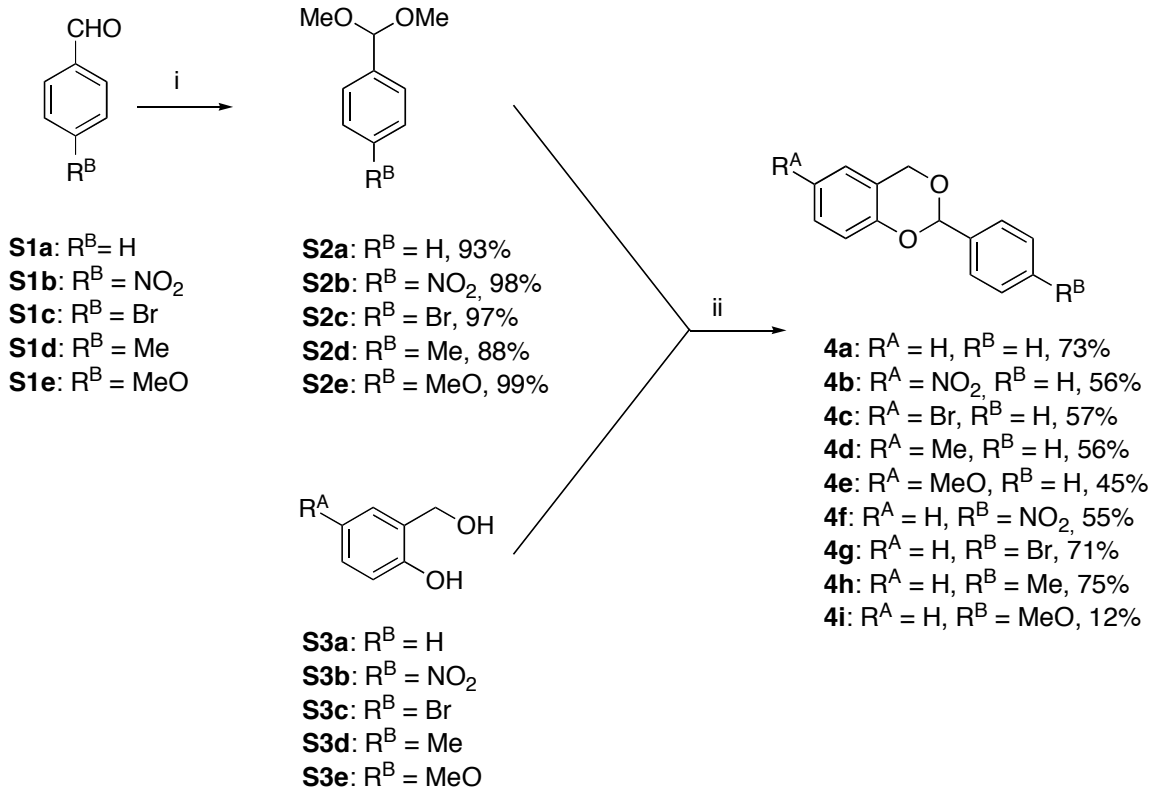
1) Synthesis and reductive openings of compounds 4a-i

To build a collection of substituted 2-phenyl-1,3-benzodioxines we initiated a study to optimize the synthesis. Benzylidene acetals are commonly synthesized by trans acetalization, using the corresponding dimethyl acetal, rather than the more straightforward condensation of the aldehyde. Today, a range of methods are available for the important formation of dialkyl acetals from the corresponding aldehyde using either alcohols (MeOH or EtOH) and catalytic amount of acid (HBr,[1a] Ce^{3+},[1b] or $TiCl_4$[1c]) or trialkyl orthoformates ($(MeO)_3CH$ or $(EtO)_3CH$)) and a suitable catalyst (*p*TSA,[2a] HCl,[2b] decaborane ($B_{10}H_{14}$),[2c] $HClO_4/SiO_2$,[2d] $ZrCl_4$,[2e] $Sc(NTf_2)_3$,[2f] $InCl_3$,[2g] $LiBF_4$,[2h] Amberlyst-15,[2i] NBS,[2j,k] or DDQ[2l]). Unfortunately the majority of these methods suffer from long reaction times (usually 12-48h), the use of expensive and/or not commercially available reagents or the necessity of subsequent purification steps to remove the catalyst.

We reasoned that a combination of a resin bound acid (Amberlite IR-120 H^+) and microwave heating would enhance the reaction rates and also facilitate the reaction work-up. The optimized reaction conditions turned out to be 15 minutes reaction time with trimethyl orthoformate at 110 °C in MeOH. Traces of unreacted aldehyde were easily removed by washing with aq. $NaHSO_3$, which gave the pure dimethyl acetals **S2a-e** in 88-99% yield without the need for further purification (Scheme S1).



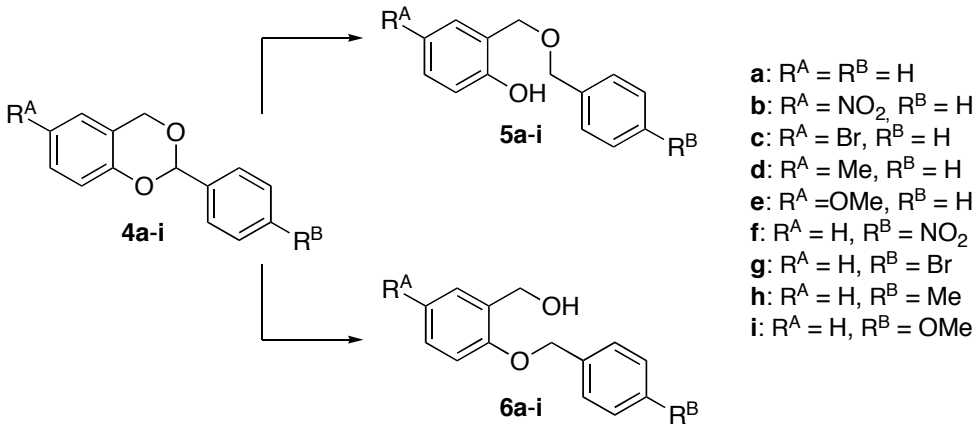
Scheme S1 i) $(MeO)_3CH$, Amberlite IR-120 H^+, 110°C, 15 min. ii) 2-hydroxybenzyl alcohols, MeCN, *p*TSA, r.t. 3 h. (Anisaldehyde, Amberlite IR-120 H^+, MeCN gave **4i** in 68%.)

We have earlier shown that mixed phenolic-benzylic acetals can be formed by treatment of a suitable dimethyl acetal with substituted salicylic alcohols. Thus, treatment of salicylic alcohol with dimethyl acetals **S2a**-**S2d** gave 2-phenyl-4*H*-benzo[1,3]dioxine (**4a**), 2-(4-nitrophenyl)-4*H*-benzo[1,3]dioxine (**4f**), 2-(4-bromophenyl)-4*H*-benzo[1,3]dioxine (**4g**), and 2-(4-methylphenyl)-4*H*-benzo[1,3]dioxine (**4h**) in 55-75% yield. Despite prolonged reaction times, the yield of 2-(4-methoxyphenyl)-4*H*-benzo[1,3]dioxine (**4i**) turned out a disappointing 12%. Several conditions were tested (Amberlite IR-120 H^+ in MeCN, camphor sulfonic acid in MeCN, $ZnBr_2$ in DMSO, and TMSOTf in CH_2Cl_2) without success. However, the use of anisaldehyde with Amberlite IR-120 H^+ in MeCN gave **4i** in 68% yield.

The time for the reactions to reach equilibrium (as judged by TLC) varied from about 3 h for **S2d** and **S2a** up to almost 8 h for compound **S2b** (carrying a strongly electron withdrawing nitro group). This observation reflects the importance of the stabilization of the intermediate oxonium cation.

Treatment of compound **S2a** with different salicylic alcohols (i.e. 4-nitro-, 4-bromo-, 4-methyl-, and 4-methoxy-) gave 6-nitro-2-phenyl-4*H*-benzo[1,3]dioxine (**4b**), 6-bromo-2-phenyl-4*H*-benzo[1,3]dioxine (**4c**), 6-methyl-2-phenyl-4*H*-benzo[1,3]dioxine (**4d**), and 6-methoxy-2-phenyl-4*H*-benzo[1,3]dioxine (**4e**) in moderate yields (45-57%). We have earlier observed low to moderate yields in the formation of anthracenylidene acetals from substituted salicylic alcohols (compared to the unsubstituted compound).[3] Interestingly the yields are low for both electron donating and withdrawing groups. The time for completion did not vary much and most reactions were finished after 3-5 h with no obvious, substituent dependent, trend. The reaction times were not shortened by the use of microwave heating.

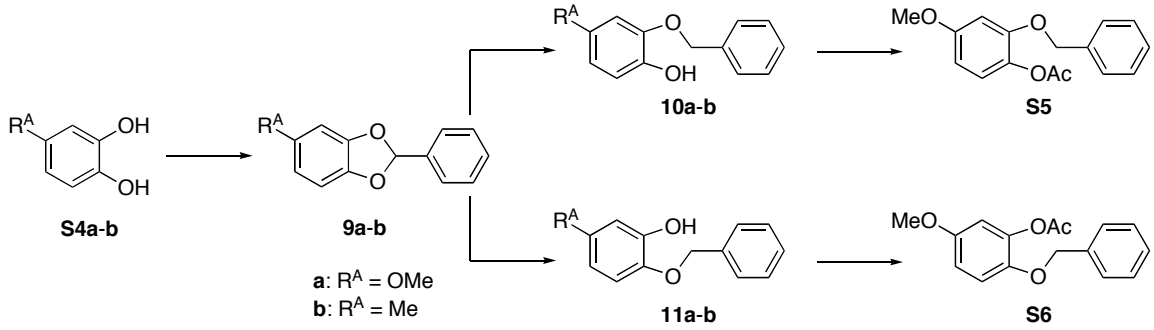
Compounds **4a**-**i** were then opened using the following conditions: BH_3•NMe_3, $AlCl_3$, THF, 0 °C). In all cases the double benzylic ether (compounds **5a**-**i**) were isolated as the single product.



a: $R^A = R^B = H$
b: $R^A = NO_2$, $R^B = H$
c: $R^A = Br$, $R^B = H$
d: $R^A = Me$, $R^B = H$
e: $R^A = OMe$, $R^B = H$
f: $R^A = H$, $R^B = NO_2$
g: $R^A = H$, $R^B = Br$
h: $R^A = H$, $R^B = Me$
i: $R^A = H$, $R^B = OMe$

Scheme S2. BH_3•NMe_3, $AlCl_3$, THF, 0°C

2) Synthesis and reductive openings of compounds 9a-b



Scheme S3. Synthesis and opening of catechols.

5-Methoxy-2-phenyl-benzo[1,3]dioxole (**9a**) and 5-methyl-2-phenyl-benzo[1,3]dioxole (**9b**) was synthesized from benzal bromide under basic conditions in DMF. The low yields in these reactions have been observed.[4]

The reductive opening of these acetals were slower compared to the corresponding benzylic-phenolic acetals and the reactions were performed in refluxing THF. The product distribution of 2-benzyloxy-4/5-methyl-phenol (**10b**, **11b**) was easily determined based on the known **11b**.[5] However the assignment of 2-benzyloxy-4/5-methoxy-phenol (**10a**, **10a**) was not possible due to overlapping signals in NMR and the product was acetylated. The signals for the 2-benzyloxy-4/5-methoxy-phenyl acetates (**S5**, **S6**) were separated and assigned.

3) General experimental details and data for compounds

^{1}H-NMR spectra were assigned using 2D-methods (COSY). Chemical shifts are given in ppm downfield from the signal for Me_4Si, with reference to residual $CHCl_3$ or DMSO. ^{11}B-NMR was calibrated on BF_3•OEt_2 (0 ppm) in glass capillary before and after the followed reaction. Reactions were monitored by TLC using alumina plates coated with silica gel and visualized using either UV light or by charring with *para*-anisaldehyde. Preparative chromatography was performed with silica gel (35-70 μm, 60 Å). THF was distilled from sodium, acetonitrile was distilled from CaH_2 and other reaction solvents were dried on Al_2O_3. Known and commercially available compounds were in agreement with previously published data (e.g. NMR).

Table S1: Data for compounds

Compound	Data
1	Commercially available
2	Commercially available
3	Ref: 6
4a	Ref: 7, 8
4b	Commercially available
4c	Ref. 9
4d	Commercially available
4e	New compound
4f	Ref: 8
4g	Ref: 8, 9
4h	New compound
4i	Ref: 8
5a	Ref: 10
5b	Ref: 11
5c	New compound
5d	New compound
5e	New compound
5f	New compound
5g	New compound
5h	New compound
5i	New compound
9a	New compound
9b	New compound
10a	Ref: 12
10b	New compound
11a	Ref: 12
11b	Ref: 5
S1a	Commercially available
S1b	Commercially available
S1c	Commercially available
S1d	Commercially available
S1e	Commercially available

S2a	Commercially available
S2b	Ref: 13
S2c	Commercially available
S2d	Ref: 14
S2e	Commercially available
S3a	Commercially available
S3b	Commercially available
S3c	Commercially available
S3d	Commercially available
S3e	Commercially available
S4a	Commercially available
S4b	Commercially available
S5	New compound
S6	New compound

4) Experimental part

Representative procedure for formation of dimethyl acetals (S2a-S2e). To a solution of **S1e** (500 mg, 3.67 mmol) and trimethyl orthoformate (0.645 mL, 5.88 mmol) in MeOH (4 mL) was added Amberlite IR-120 H^+ (15 mg). The mixture was heated to 110 °C for 15 min in a microwave reactor, filtered and diluted with EtOAc. The filtrate was washed with $NaHSO_3$ (sat. aq.) twice. The water fractions were then extracted once with EtOAc and the combined organic fractions were dried ($MgSO_4$) and concentrated to give **S2e** as a colorless oil (663 mg, 99%).

Representative experimental procedure for formation of phenyl-1,3-benzodioxines (4a-i). To a solution of **S2a** (478 mg, 3.14 mmol) and 2-hydroxybenzyl alcohol (300 mg, 2.42 mmol) in MeCN (12 mL) was added *p*TSA (15 mg). The mixture was stirred at r.t. for 180 min and was then diluted with CH_2Cl_2 and washed with $NaHCO_3$ (sat. aq.) twice. The combined water phases were washed with CH_2Cl_2 and the combined organic phases were dried ($MgSO_4$). The residue was chromatographed (SiO_2, heptane/toulene 1:3) to give **4a** as a white solid (374 mg, 73%).

6-Bromo-2-phenyl-*4H*-benzo[d][1,3]dioxine (4c): ^{1}H-NMR ($CDCl_3$): δ 7.42-7.60 (m, 5H, H-2′-H-6′), 7.30 (dd, 1H, *J* 8.7, 2.4 Hz, H-7), 7.16-7.17 (m, 1H, H-5), 6.84 (d, 1H, *J* 8.7 Hz, H-8), 5.97 (s, 1H, H-2), 5.15, 4.97 (ABq, 1H each, *J* 14.8 Hz, H-4). ^{13}C-NMR ($CDCl_3$): δ 152.3, 136.7, 131.2, 129.8, 128.7, 127.9, 126.5, 122.9, 119.0, 113.7, 99.4, 66.4. HRMS calcd. for $C_{14}H_{11}O_2Br$ (M+): 289.9942; found: 289.9946.

6-Methoxy-2-phenyl-*4H*-benzo[d][1,3]dioxine (4e): ^{1}H-NMR ($CDCl_3$): δ 7.41-7.62 (m, 5H, H-2′-H-6′), 6.90 (d, 1H, *J* 8.9 Hz, H-8), 6.77 (dd, 1H, *J* 8.9, 3.0 Hz, H-7), 6.57 (d, 1H, *J* 2.9 Hz, H-5), 5.94 (s, 1H, H-2), 5.19, 4.98 (ABq, 1H each, *J* 14.7 Hz, H-4), 3.78 (s, 3H, OMe). ^{13}C-NMR ($CDCl_3$): δ 154.3, 147.2, 137.3, 129.6, 128.6, 126.5, 121.5, 117.9, 114.3, 109.6, 99.2, 67.0, 55.9. HRMS calcd. for $C_{15}H_{14}O_3Na$ (M+Na): 265.0841; found: 265.0842.

2-*p*-Tolyl-*4H*-benzo[d][1,3]dioxine (4h): ^{1}H-NMR ($CDCl_3$): δ 7.50 (d, 2H, *J* 8.0 Hz, H-2′, H-6′), 7.25 (d, 2H, *J* 8.0 Hz, H-3′, H-5′), 7.18-7.22 (m, 1H, H-5), 6.95-7.04 (m, 3H, H-6-H-8), 5.98 (s, 1H, H-2), 5.21, 5.00 (ABq, 1H each, *J* 14.4 Hz, H-4), 2.39 (s, 3H, Me).^{13}C-NMR ($CDCl_3$): δ 139.5, 134.4, 129.3, 128.2, 126.4, 125.0, 121.4, 121.1, 117.2, 99.3, 67.0, 21.5. HRMS calcd. for $C_{15}H_{14}O_2Na$ (M+Na): 249.0891; found: 249.0900.

2-Benzyloxymethyl-phenol (5a). To a solution of **4a** (31 mg, 0.15 mmol) and borane trimethyl amine complex (65 mg, 0.87 mmol) in THF (3 mL) was added $AlCl_3$ (136 mg, 1.0 mmol) dissolved in THF (1.5 mL) drop wise at 0 °C. The mixture was stirred at 0 °C for 60 min, sample was taken at 5, 10, 20, 40, 60 min for initial rate and Hammett study. Samples were quenched in $NaHCO_3$ (aq. sat.) in micro vials and extracted with ether. First reaction was stirred at 0 °C for 360 min and chromatographed (SiO_2, heptane/EtOAc 8:1) to give **5a** as a white solid.

2-Benzyloxymethyl-4-nitro-phenol (5b). Synthesized according to the same procedure as for **5a**: **4b** (38 mg, 0.15 mmol), borane trimethyl amine complex (65 mg, 0.87 mmol), THF (3 mL), $AlCl_3$ (136 mg, 1.0 mmol in 1.5 mL THF), 0 °C 60 min. First reaction was stirred at 0 °C for 380 min to give **5b** as a white solid.

2-Benzyloxymethyl-4-bromo-phenol (5c). Synthesized according to the same procedure as for **5a**: **4c** (43 mg, 0.15 mmol), borane trimethyl amine complex (65 mg, 0.87 mmol), THF (3 mL), $AlCl_3$ (136 mg, 1.0 mmol in 1.5 mL THF), 0 °C 60 min. First reaction was stirred at 0 °C for 1350 min to give **5c** as a white solid. ^{1}H-NMR ($CDCl_3$): δ 7.57 (s, 1H), 7.31-7.43 (m, 6H), 7.15 (d, 1H, *J* 2.4 Hz), 6.80 (d, 1H, *J* 8.8 Hz), 4.70 (s, 2H), 4.61 (s, 2H). ^{13}C-NMR ($CDCl_3$): δ 155.4, 136.4, 132.2, 130.8, 128.7, 128.4, 128.2, 124.1, 118.5, 111.7, 72.7, 70.8. HRMS calcd. for $C_{14}H_{13}O_2BrNa$ (M+Na): 314.9997; found: 314.0001.

2-Benzyloxymethyl-4-methyl-phenol (5d). Synthesized according to the same procedure as for **5a**: **4d** (33 mg, 0.15 mmol), borane trimethyl amine complex (65 mg, 0.87 mmol), THF (3 mL), $AlCl_3$ (136 mg, 1.0 mmol in 1.5 mL THF), 0 °C 60 min. First reaction was stirred at 0 °C for 380 min to give **5d** as a white solid. ^{1}H-NMR ($CDCl_3$): δ 7.32-7.42 (m, 5H), 7.30 (s, 1H), 7.04 (dd, 1H, *J* 8.0, 2.0 Hz), 6.81-6.84 (m, 2H), 4.72 (s, 2H), 4.60 (s, 2H), 2.27 (s, 3H). ^{13}C-NMR ($CDCl_3$): δ 153.9, 136.9, 130.0, 129.0, 128.8, 128.6, 128.2, 128.1, 121.7, 116.3, 72.4, 71.5, 20.4. HRMS calcd. for $C_{15}H_{16}O_2Na$ (M+Na): 251.1048; found: 251.1051.

2-Benzyloxymethyl-4-methoxy-phenol (5e). Synthesized according to the same procedure as for **5a**: **4e** (35 mg, 0.15 mmol), borane trimethyl amine complex (65 mg, 0.87 mmol), THF (3 mL), $AlCl_3$ (136 mg, 1.0 mmol in 1.5 mL THF), 0 °C 60 min. First reaction was stirred at 0 °C for 400 min to give **5e** as a white solid. ^{1}H-NMR ($CDCl_3$): δ 7.32-7.42 (m, 5H), 7.09 (s, 1H), 6.86 (d, 1H, *J* 8.8 Hz), 6.80 (dd, 1H. *J* 8.8, 3.0 Hz), 6.61 (d, 1H, *J* 2.9 Hz), 4.72 (s, 2H), 4.61 (s, 2H), 3.76 (s, 3H). ^{13}C-NMR ($CDCl_3$): δ 153.0, 150.0, 136.8, 128.6, 128.2, 122.8, 117.1, 114.5, 113.9, 72.4, 71.3, 55.8. HRMS calcd. for $C_{15}H_{16}O_3Na$ (M+Na): 267.0997; found: 267.1000.

2-(4-Nitro-benzyloxymethyl)-phenol (5f). Synthesized according to the same procedure as for **5a**: **4f** (38 mg, 0.15 mmol), borane trimethyl amine complex (65 mg, 0.87 mmol), THF (3 mL), $AlCl_3$ (136 mg, 1.0 mmol in 1.5 mL THF), 0 °C 60 min. First reaction was stirred at 0 °C for 1320 min to give **5f** as a white solid. ^{1}H-NMR ($CDCl_3$): δ 8.25 (ddd, 2H, *J* 9.1, 2.3, 2.0 Hz), 7.53 (ddd, 2H, *J* 9.1, 2.9, 2.3 Hz), 7.25-7.29 (m, 1H), 7.07 (dd, 1H, *J* 7.5, 1.3 Hz), 7.00 (s, 1H), 6.88-6.94 (m, 2H), 4.81 (s, 2H), 4.70 (s, 2H). ^{13}C-NMR ($CDCl_3$): δ 156.0, 144.5, 130.1, 128.8, 128.3, 124.0, 120.4, 116.8, 71.9, 71.1. HRMS calcd. for $C_{14}H_{13}O_4NNa$ (M+Na): 282.0742; found: 282.0744.

2-(4-Bromo-benzyloxymethyl)-phenol (5g). Synthesized according to the same procedure as for **5a**: **4g** (43 mg, 0.15 mmol), borane trimethyl amine complex (65 mg, 0.87 mmol), THF (3 mL), $AlCl_3$ (136 mg, 1.0 mmol in 1.5 mL THF), 0 °C 60 min. First reaction was stirred at 0 °C for 1390 min to give **5g** as a white solid. ^{1}H-NMR ($CDCl_3$): δ 7.51 (dt, 2H, *J* 8.8, 1.6 Hz), 7.33 (s, 1H), 7.22-7.26 (m, 3H), 7.03 (dd, 1H, *J* 7.5, 1.3 Hz), 6.92 (dd, 1H, *J* 8.0, 1.2 Hz), 6.87 (dt, 1H, *J* 7.6, 1.2 Hz), 4.75 (s, 2H), 4.55 (s, 2H). ^{13}C-

NMR ($CDCl_3$): δ 156.2, 135.8, 131.8, 129.72, 129.70, 128.4, 122.2, 121.8, 120.0, 116.6, 71.54, 71.48. HRMS calcd. for $C_{14}H_{13}O_2BrNa$ (M+Na): 314.9997; found: 315.0001.

2-(4-Methyl-benzyloxymethyl)-phenol (5h). Synthesized according to the same procedure as for **5a**: **4h** (34 mg, 0.15 mmol), borane trimethyl amine complex (65 mg, 0.87 mmol), THF (3 mL), $AlCl_3$ (136 mg, 1.0 mmol in 1.5 mL THF), 0 °C 60 min. First reaction was stirred at 0 °C for 360 min to give **5h** as a white solid. ^{1}H-NMR ($CDCl_3$): δ 7.57 (s, 1H), 7.19-7.26 (m, 5H), 7.02 (dd, 1H, *J* 7.4, 1.1 Hz), 6.92 (d, 1H, *J* 8.1 Hz), 6.86 (dt, 1H, *J* 7.4, 1.0 Hz), 4.74 (s, 2H), 4.57 (s, 2H), 2.37 (s, 3H). ^{13}C-NMR ($CDCl_3$): δ 156.3, 138.1, 133.7, 129.5, 129.3, 128.3, 128.2, 122.1, 119.9, 116.5, 72.3, 71.3, 21.2. HRMS calcd. for $C_{15}H_{16}O_2Na$ (M+Na): 251.1058; found: 251.1060.

2-(4-Methoxy-benzyloxymethyl)-phenol (5i). Synthesized according to the same procedure as for **5a**: **4i** (35 mg, 0.15 mmol), borane trimethyl amine complex (65 mg, 0.87 mmol), THF (3 mL), $AlCl_3$ (136 mg, 1.0 mmol in 1.5 mL THF), 0 °C 60 min. First reaction was stirred at 0 °C for 360 min to give **5i** as a white solid. ^{1}H-NMR ($CDCl_3$): δ 7.59 (s, 1H), 7.29 (dt, 2H, *J* 9.5, 2.9 Hz), 7.24 (dt, 1H, *J* 7.8, 1.5 Hz), 7.03 (dd, 1H, *J* 7.5, 1.3 Hz), 6.90-6.94 (m, 3H), 6.87 (dt, 1H, *J* 7.4, 1.2 Hz), 4.74 (s, 2H), 4.54 (s, 2H), 3.83 (s, 3H). ^{13}C-NMR ($CDCl_3$): δ 159.6, 156.3, 129.9, 129.5, 128.8, 128.3, 122.1, 119.9, 116.5, 114.0, 72.1, 71.1, 55.3. HRMS calcd. for $C_{15}H_{16}O_3Na$ (M+Na): 267.0997; found: 267.1000.

5-Methoxy-2-phenyl-benzo[1,3]dioxole (9a): 4-Methoxy catechol (210 mg, 1.50 mmol) and K_3PO_4 (954 mg, 4.49 mmol) was dissolved in DMF (5 mL). Benzal bromide (0.270 mL, 1.99 mmol) was added, stirred at r.t. under N_2 for 18 hours. The mixture was diluted with water and extracted two times with EtOAc, dried with $MgSO_4$ and concentrated. The residue was chromatographed (heptane/toluene 1:1) to give **9a** as an amorphous solid (84 mg, 24%). ^{1}H-NMR ($CDCl_3$): δ 7.56-7.59 (m, 2H, H-1′, H-5′), 7.43-7.46 (m, 3H, H-2′, H-3′, H-4′), 6.93 (s, 1H, H-2), 6.7 (d, 1H, *J* 8.4 Hz, H-7), 6.52 (d, 1H, *J* 2.4 Hz, H-4), 6.35 (dd, 1H, *J* 8.4, 2.4 Hz, H-6), 3.76 (s, 3H, OMe). ^{13}C-NMR ($CDCl_3$): δ 155.4, 148.6, 142.0, 136.3, 130.4, 128.8, 126.5, 110.6, 108.0, 104.9, 97.5, 56.2. HRMS calcd. for $C_{14}H_{13}O_3$ (M+H): 229.0865; found: 229.0862.

5-Methyl-2-phenyl-benzo[1,3]dioxole (9b): 4-Methyl catechol (219 mg, 1.76 mmol) and K_3PO_4 (599 mg, 2.82 mmol) was dissolved in DMF (5 mL). Benzal bromide (0.310 mL, 2.29 mmol) was added, stirred at r.t. under N_2 for 18 hours. The mixture was diluted with water and extracted two times with EtOAc, dried with $MgSO_4$ and concentrated. The residue was chromatographed (heptane/toluene 2:1) to give **9b** as an amorphous solid (74 mg, 20%). ^{1}H-NMR ($CDCl_3$): δ 7.45-7.58 (m, 2H, H-1′, H-5′), 7.42-7.45 (m, 3H, H-2′, H-3′, H-4′), 6.92 (s, 1H, H-2), 6.74 (d, 1H, *J* 7.9 Hz, H-7), 6.69 (bs, 1H, H-4), 6.64 (ddd, 1H, *J* 7.9, 1.6, 0.8 Hz, H-6), 2.29 (s, 3H, Me). ^{13}C-NMR ($CDCl_3$): δ 147.8, 145.6, 136.5, 131.7, 130.3, 128.8, 126.5, 121.7, 110.1, 109.6, 108.1, 21.4. HRMS calcd. for $C_{14}H_{12}O_2Na$ (M+Na): 235.0735; found: 235.0736.

2-Benzyloxy-4/5-methoxy-phenol (10a/11a): Compound **9a** (12 mg, 0.05 mmol) and BH_3•NMe_3 (24 mg, 0.33 mmol) was dissolved in THF (2 mL) and cooled to 0°C under

N_2. After 10 min $AlCl_3$ (53 mg, 0.40 mmol) dissolved in THF (1.0 mL) was added. After 20 min the mixture was heated to reflux and after an additional 1.5 h the mixture was diluted with ether and washed once with $NaHCO_3$ (sat, aq), water phase extracted once with ether. The combined organic phase was dried with $MgSO_4$ and concentrated. The residue was chromatographed (heptane/EtOAc 5:1) to give **10a** and **11a** as an inseparable mixture as an colorless oil (7 mg, 58%). NMR gave the distribution **10a**/**11a** 36:64. HRMS calcd. for $C_{14}H_{15}O_3$ (M+H): 231.1021; found: 231.1030.[12]

2-Benzyloxy-4/5-methoxy-phenol (10a/11a): Compound **9a** (39 mg, 0.17 mmol) and BH_3•THF (1.03 mL, 1 M) was dissolved in THF (4.5 mL) and cooled to 0°C under N_2. After 10 min $AlCl_3$ (162 mg, 1.21 mmol) dissolved in THF (2.0 mL) was added. After 20 min the mixture was heated to reflux and after an additional 1.5 h the mixture was diluted with ether and washed once with $NaHCO_3$ (sat, aq), water phase extracted once with ether. The combined organic phase was dried with $MgSO_4$ and concentrated. The residue was chromatographed (heptane/EtOAc 5:1) to give **10a** and **11a** as an inseparable mixture as an colorless oil (18 mg, 45%). NMR gave the distribution **10a**/**11a** 65:35.

2-Benzyloxy-4/5-methyl-phenol (10b/11b): Compound **9b** (49 mg, 0.23 mmol) and BH_3•NMe_3 (104 mg, 1.43 mmol) was dissolved in THF (6 mL) and cooled to 0°C under N_2. After 10 min $AlCl_3$ (218 mg, 1.63 mmol) dissolved in THF (3.0 mL) was added. After 20 min the mixture was heated to reflux and after an additional 1.5 h the mixture was diluted with ether and washed once with $NaHCO_3$ (sat, aq), water phase extracted once with ether. The combined organic phase was dried with $MgSO_4$ and concentrated. The residue was chromatographed (heptane/EtOAc 5:1) to give **10b** and **11b** as an inseparable mixture as an colorless oil (30 mg, 61%). NMR gave the distribution **10b**/**11b** 47:53. **11b** was in agreement with published data.[5] HRMS calcd. for $C_{14}H_{14}O_2Na$ (M+Na): 237.0891; found: 237.0883.

2-Benzyloxy-4/5-methyl-phenol (10b/11b): Compound **9b** (45 mg, 0.21 mmol) and BH_3•THF (1.27 mL, 1 M) was dissolved in THF (4.5 mL) and cooled to 0°C under N_2. After 10 min $AlCl_3$ (201 mg, 1.50 mmol) dissolved in THF (3.0 mL) was added. After 20 min the mixture was heated to reflux and after an additional 1.5 h the mixture was diluted with ether and washed once with $NaHCO_3$ (sat, aq), water phase extracted once with ether. The combined organic phase was dried with $MgSO_4$ and concentrated. The residue was chromatographed (heptane/EtOAc 5:1) to give **10b** and **11b** as an inseparable mixture as an colorless oil (29 mg, 64%). NMR gave the distribution **10b**/**11b** 53:47.

2-Benzyloxy-4/5-methoxy-phenyl acetate (S5/S6): The mixture **10a**:**11a** (7 mg, 0.03 mmol) was dissolved in pyridine (0.500 mL) and Ac_2O (0.400 mL) was added. The mixture was stirred at r.t under N_2 for 2.5 h and then co-concentrated from toluene to give a mixture of **S5** and **S6** (9 mg, quant).

5) Electrostatic potential for compounds 1 and 4a-i

The electrostatic potential for compounds **4a-i** and **1** were calculated using density functional theory at the B3LYP/6-31G* level and default settings in Spartan '02 for Macintosh.[15] Results in kcal/mol.

Table S1. Electron densities for compounds **4a-i** (kcal/mol)

Compound	Phenolic oxygen	Benzylic oxygen
4a	-32.8359	-34.7195
4b	-22.7444	-26.3747
4c	-28.6462	-31.3332
4d	-33.5266	-35.6560
4e	-34.4963	-35.8430
4f	-23.9499	-25.7651
4g	-28.3918	-30.7140
4h	-33.7781	-35.3578
4i	-34.2345	-35.8558

Table S2. Electron densities for compounds **1** (kcal/mol)

Compound	O-4	O-6
1	-32.9040	-36.5412

6) Calculations of complexes

The energies for compounds **7-8**, **12-17** and **S7** (Figure S1) were calculated using density functional theory at the B3LYP/6-31G** level and default settings in Jaguar.[16] The data are presented in Table S3. The energy differences in the three series were calculated and the distribution between the two different compounds was calculated using the Equation S1 at T = 273 K

$$\frac{N_i}{N_j} = e^{-\frac{(E_i - E_j)}{RT}}$$

Equation S1. Boltzmann distribution

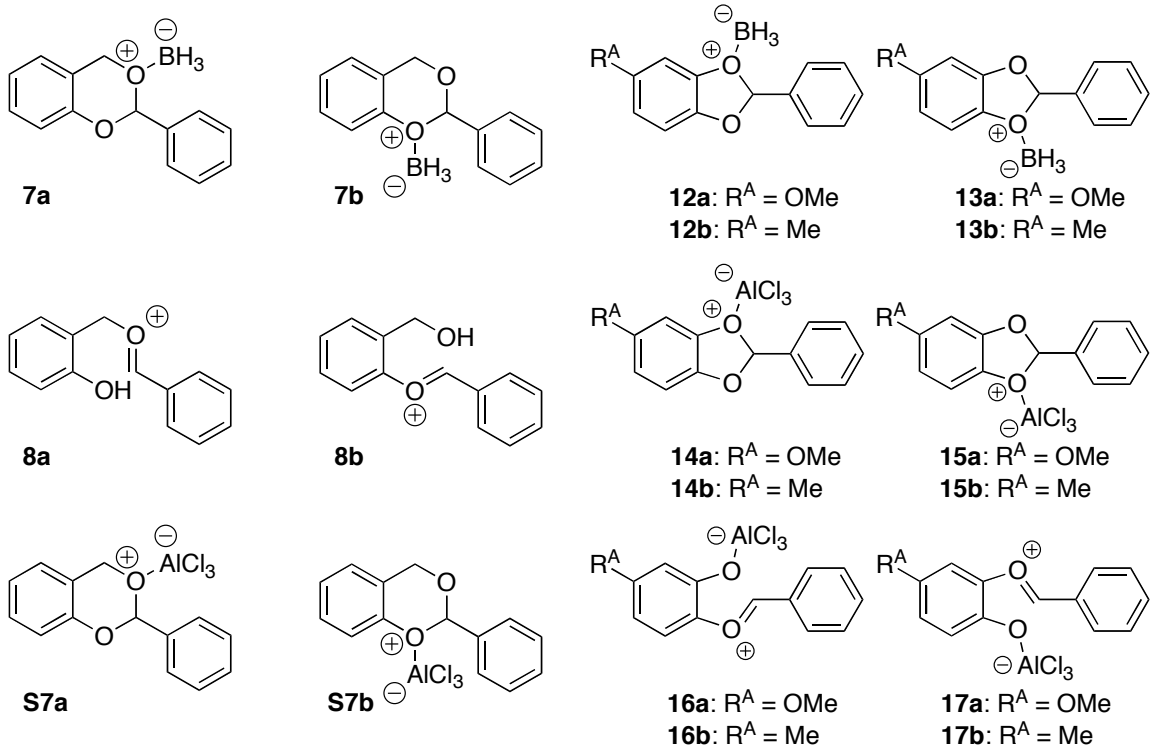


Figure S1. Calculated complexes.

Table S3. Boltzmann distributions of **X6-X7**, **XS4** and **Y7-Y12** complexes

Compound	E_i (Hartrees)	E_j (Hartrees)	E_i-E_j (J/mol)	N_i/N_j	N_i (%)	N_j (%)
7	-717.805985(**a**)	-717.795623(**b**)	-27209	161735	100	0
8	-691.535612(**a**)	-691.517865(**b**)	-37516	15199764	100	0
S7	-2314.440589(**a**)	-2314.432388(**b**)	-21521	13182	100	0
12a/13a	-793.007560(**13**)	-793.006895(**12**)	-1746.20	1.86	65	35
12b/13b	-717.803074(**13**)	-717.802922(**12**)	-399.13	1.15	54	46
14a/15a	-2389.643084(**15**)	-2389.642189(**14**)	-2350.16	2.31	70	30
14b/15b	-2314.439264(**15**)	-2314.439164(**14**)	-262.59	1.10	52	48
16a/17a	-2389.648326(**16**)	-2314.644316(**17**)	-10529.75	42.47	98	2
16b/17b	-2314.443969(**16**)	-2314.442638(**17**)	-3495.04	3.47	78	22

7) Hammett plots

General procedure. **4a** (0.146 mmol) and BH_3•NMe_3 (0.874 mmol) was dissolved in 3 mL of THF. $AlCl_3$ (1.019 mmol) was dissolved in 1.5 mL of THF carefully at 0 °C and the solution was then added to the mixture stirring at 0 °C. At 5, 10, 20, 40 and 60 min of reaction time samples of 0.450 mL were taken and quenched with 0.500 mL $NaHCO_3$ (aq. sat.) in micro vials. The samples were extracted twice with 0.450 mL diethyl ether and concentrated in vacuum. The residues were dissolved in $CDCl_3$ and analyzed by ^{1}H-NMR. All reactions were run in triplicate. For compound **4f** the samples were taken at 120, 240, 360, 870 and 1458 min due to slow reaction rate and for compound **4i** samples were taken at 2, 4, 6, 8 and 10 min due to the fast reaction rate.

The molar concentration of product was determined from NMR peak ratios plotted versus time. Linear regression over the linear part of the curves (determined by f-values) gave the reaction rates.

Initial rate constants for compounds 4a-i

Compound	k_1	k_2	k_3	k_{avg}	$\log(k_{avg}/k_{X1F\ avg})$
4a	0.657	0.644	0.553	0.621	0.000
4b	0.028	0.028	0.031	0.029	-1.330
4c	0.109	0.110	0.115	0.111	-0.747
4d	1.085	0.859	0.704	0.883	0.153
4e	1.245	1.202	0.747	1.053	0.230
4f	0.003	0.003	0.002	0.002	-2.435
4g	0.092	0.092	0.067	0.072	-0.934
4h	1.433	1.304	1.048	1.538	0.394
4i	8.416	8.419	8.248	8.361	1.129

Sigma values for substituents in Hammett relations[17]

Substituent	σ_{para}	σ_{meta}	σ^+
-H	0	0	0
$-NO_2$	0.81	0.71	0.79[b]
-Br	0.26	0.37	0.15
$-CH_3$	-0.14	-0.06	-0.31
$-OCH_3$	-0.12	0.10	-0.78

Hammett regression information

Compounds	σ	Linear equation	R^2
4f-g, 4a$_{ref}$	+	y = -2.3185x - 0.4385	0.959
	para	y = -3.3629x + 0.1758	0.938
4b-e, 4a$_{ref}$	+	y = -1.0695x - 0.371	0.842
	para	y = -1.6698x - 0.0684	0.955
	meta	y = -2.0495x + 0.1202	0.927

Compound 4a

	1			2			3			Average
Time (min)	Prod.	Start.	% Prod.	Prod.	Start.	% Prod.	Prod.	Start.	% Prod.	% Prod.
0	0	1	0.0	0	1	0.0	0	1	0.0	0.0
5	0.08	1.09	3.5	0.07	1.09	3.1	0.06	1.09	2.7	3.1
10	0.15	1.09	6.4	0.15	1.08	6.5	0.13	1.08	5.7	6.2
20	0.28	1.09	11.4	0.28	1.09	11.4	0.27	1.09	11.0	11.3
40	0.58	1.1	20.9	0.56	1.09	20.4	0.58	1.08	21.2	20.8
60	0.87	1.08	28.7	0.83	1.08	27.8	0.9	1.09	29.2	28.6

Statistics	1	2	3	Average
Data points	3 points	3 points	4 points	3 points
k	6.566E-01	6.439E-01	5.535E-01	6.206E-01
Std dev.	0.02	0.01	0.00	0.00
r^2	1.00	1.00	1.00	1.00
f	1308	7043	15824	1673741
SSreg	53.89	51.83	160.82	48.14

Compound 4b

	1			2			3			Average
Time (min)	Prod.	Start.	% Prod.	Prod.	Start.	% Prod.	Prod.	Start.	% Prod.	% Prod.
0	0.00	1.00	0.000	0.00	1.00	0.000	0.00	1.00	0.000	0.00
5	0.00	1.08	0.000	0.00	1.07	0.000	0.00	1.08	0.000	0.00
10	0.01	1.08	0.461	0.01	1.08	0.461	0.01	1.09	0.457	0.46
20	0.01	1.07	0.465	0.01	1.07	0.465	0.01	1.07	0.465	0.47
40	0.02	1.07	0.926	0.02	1.07	0.926	0.03	1.09	1.357	1.07
60	0.04	1.07	1.835	0.04	1.08	1.818	0.04	1.08	1.818	1.82

Statistics	1	2	3	Average
Data points	6 points	6 points	6 points	6 points
k	2.813E-02	2.795E-02	3.096E-02	2.902E-02
Std dev.	0.00	0.00	0.00	0.00
r^2	0.97	0.97	0.98	0.98
f	184	189	323	309
SSreg	4.53	4.47	5.49	4.82

Compound 4c

	1			2			3			Average
Time (min)	Prod.	Start.	% Prod.	Prod.	Start.	% Prod.	Prod.	Start.	% Prod.	% Prod.
0	0.00	1.00	0.00	0.00	1.00	0.00	0.00	1.00	0.00	0.00
5	0.02	1.10	0.90	0.02	1.10	0.90	0.01	1.09	0.46	0.75
10	0.03	1.09	1.36	0.03	1.09	1.36	0.03	1.08	1.37	1.36
20	0.05	1.09	2.24	0.05	1.09	2.24	0.06	1.09	2.68	2.39
40	0.10	1.09	4.39	0.10	1.09	4.39	0.10	1.08	4.42	4.40
60	0.15	1.10	6.38	0.15	1.08	6.49	0.16	1.08	6.90	6.59

Statistics	1	2	3	Average
Data points	6 points	6 points	6 points	6 points
k	1.085E-01	1.097E-01	1.153E-01	1.112E-01
Std dev.	0.00	0.00	0.00	0.00
r^2	1.00	1.00	1.00	1.00
f	1491	1703	1616	2587
SSreg	67.43	68.88	76.17	70.78

Compound 4d

	1			2			3			Average
Time (min)	Prod.	Start.	% Prod.	Prod.	Start.	% Prod.	Prod.	Start.	% Prod.	% Prod.
0	0.00	1.00	0.0	0.00	1.00	0.0	0.00	1.00	0.0	0.0
5	0.14	1.14	5.8	0.11	1.14	4.6	0.09	1.16	3.7	4.7
10	0.27	1.13	10.7	0.21	1.14	8.4	0.17	1.14	6.9	8.7
20	0.57	1.15	19.9	0.42	1.16	15.3	0.32	1.16	12.1	15.8
40	1.25	1.17	34.8	0.87	1.17	27.1	0.67	1.17	22.3	28.1
60	2.03	1.19	46.0	1.38	1.18	36.9	1.04	1.22	29.9	37.6

Statistics	1	2	3	Average
Data points	3 points	3 points	3 points	3 points
k	1.085E+00	8.588E-01	7.045E-01	8.828E-01
Std dev.	0.03	0.02	0.01	0.02
r^2	1.00	1.00	1.00	1.00
f	1824	1550	2208	1812
SSreg	147.20	92.19	62.04	97.42

Compound 4e

	1			2			3			Average
Time (min)	Prod.	Start.	% Prod.	Prod.	Start.	% Prod.	Prod.	Start.	% Prod.	% Prod.
0	0.00	1.00	0.00	0.00	1.00	0.00	0.00	1.00	0.00	0.0
5	0.15	1.11	6.33	0.18	1.08	7.69	0.09	1.09	3.96	6.0
10	0.30	1.06	12.40	0.32	1.07	13.01	0.17	1.07	7.36	10.9
20	0.83	1.16	26.35	0.65	1.08	23.13	0.31	1.08	12.55	20.7
40	1.53	1.08	41.46	1.31	1.08	37.75	0.60	1.08	21.74	33.7
60	2.76	1.10	55.65	2.09	1.08	49.18	0.88	1.07	29.14	44.7

Statistics	1	2	3	Average
Data points	3 points	4 points	3 points	4 points
k	1.245E+00	1.202E+00	7.473E-01	1.053E+00
Std dev.	0.01	0.05	0.02	0.02
r^2	1.00	0.99	1.00	1.00
f	28322	492	2147	2095
SSreg	193.72	758.83	69.81	581.93

Compound 4f

	1			2			3			Average
Time (min)	Prod.	Start.	% Prod.	Prod.	Start.	% Prod.	Prod.	Start.	% Prod.	% Prod.
0	0	1	0	0	1	0	0	1	0	0.0
120	0	1.08	0	0	1.09	0	0	1.1	0	0.0
240	0.01	1.08	0.46083	0.01	1.09	0.45662	0.01	1.09	0.45662	0.5
360	0.02	1.1	0.9009	0.02	1.1	0.9009	0.01	1.09	0.45662	0.8
870	0.05	1.1	2.22222	0.05	1.09	2.24215	0.03	1.08	1.36986	1.9
1458	0.09	1.09	3.96476	0.09	1.08	4	0.05	1.09	2.24215	3.4

Statistics	1	2	3	Average
Data points	6 points	6 points	6 points	6 points
k	2.642E-03	2.664E-03	1.535E-03	2.280E-03
Std dev.	0.00	0.00	0.00	0.00
r^2	0.99	0.99	0.99	0.99
f	710	692	697	844
SSreg	21.53	21.89	7.27	16.04

Compound 4g

	1			2			3			Average
Time (min)	Prod.	Start.	% Prod.	Prod.	Start.	% Prod.	Prod.	Start.	% Prod.	% Prod.
0	0	1	0	0	1	0	0	1	0	0.0
5	0.01	1.09	0.45662	0.01	1.08	0.46083	0.01	1.08	0.46083	0.5
10	0.02	1.08	0.91743	0.02	1.08	0.91743	0.01	1.05	0.47393	0.8
20	0.03	1.1	1.34529	0.03	1.08	1.36986	0.03	1.08	1.36986	1.4
40	0.07	1.08	3.13901	0.07	1.08	3.13901	0.06	1.08	2.7027	3.0
60	0.1	1.08	4.42478	0.1	1.08	4.42478	0.09	1.08	4	4.3

Statistics	1	2	3	Average
Data points	3 points	3 points	6 points	6 points
k	9.166E-02	9.183E-02	6.682E-02	7.231E-02
Std dev.	0.00	0.00	0.00	0.00
r^2	1.00	1.00	1.00	1.00
f	598418	589698	2286	4649
SSreg	1.05	1.05	25.56	29.93

Compound 4h

	1			2			3			Average
Time (min)	Prod.	Start.	% Prod.	Prod.	Start.	% Prod.	Prod.	Start.	% Prod.	% Prod.
0	0.00	1.00	0.00	0.00	1.00	0.00	0.00	1.00	0.00	0.0
5	0.19	1.07	8.15	0.17	1.08	7.30	0.29	1.08	11.84	9.1
10	0.35	1.09	13.83	0.31	1.07	12.65	0.46	1.08	17.56	14.7
20	0.67	1.09	23.51	0.59	1.09	21.30	0.86	1.08	28.48	24.4
40	1.33	1.08	38.11	1.16	1.07	35.15	1.76	1.08	44.90	39.4
60	2.13	1.09	49.42	1.77	1.09	44.81	2.82	1.08	56.63	50.3

Statistics	1	2	3	Average
Data points	3 points	3 points	6 points	3 points
k	1.433E+00	1.304E+00	1.048E+00	1.538E+00
Std dev.	0.07	0.05	0.08	0.10
r^2	1.00	1.00	0.97	0.99
f	419	565	159	240
SSreg	256.65	212.58	6283.60	295.81

Compound 4i

	1			2			3			Average
Time (min)	Prod.	Start.	% Prod.	Prod.	Start.	% Prod.	Prod.	Start.	% Prod.	% Prod.
0	0.00	1.00	0.00	0.00	1.00	0.00	0.00	1.00	0.00	0.0
2	1.08	1.09	33.13	1.04	1.09	32.30	1.00	1.08	31.65	32.4
4	1.99	1.09	47.72	2.01	1.11	47.52	1.87	1.09	46.17	47.1
6	2.95	1.08	57.73	3.02	1.10	57.85	2.83	1.09	56.49	57.4
8	4.20	1.10	65.63	4.21	1.13	65.07	3.92	1.09	64.26	65.0
10	5.64	1.08	72.31	5.89	1.09	72.99	5.63	1.13	71.36	72.2

Statistics	1	2	3	Average
Data points	6 points	6 points	6 points	6 points
k	8.416E+00	8.419E+00	8.248E+00	8.361E+00
Std dev.	0.77	0.75	0.73	0.75
r^2	0.96	0.96	0.96	0.96
f	118	127	129	125
SSreg	15583.76	15594.07	14966.56	15380.06

8) Rate determination for 4

General procedure. Equivalents of **4a**, BH_3•NMe_3 and $AlCl_3$ was varied according to Table S4. **4a** and BH_3•NMe_3 was dissolved in 3 mL of THF. $AlCl_3$ was dissolved in 1.5 mL of THF carefully at 0 °C and the solution was then added to the mixture at 0 °C. At 5, 10, 20, 40 and 60 min of reaction time samples of 0.450 mL were taken and quenched with 0.500 mL $NaHCO_3$ (aq. sat.) in micro vials. The samples were extracted twice with 0.450 mL diethyl ether and concentrated in vacuum. The residues were dissolved in $CDCl_3$ and analyzed by ^{1}H-NMR. All reactions were run in at least duplicate.

The molar concentration of product was determined from NMR peak ratios plotted versus time. Linear regression over the linear part of the curves (determined by f-values) gave the reaction rates, which were plotted versus the starting concentration of the three different components respectively.

Table S4. Starting concentrations and linear regressions for the three different components.

	Entry	[**4a**]	[BH_3•NMe_3]	[$AlCl_3$]	Linear regression slope (k)	Avg. Regression slope (k_{avg})
4a	1a	0.0163	0.1953	0.2287	1.89E-06	2.07E-06
	1b	0.0165	0.1937	0.2263	1.64E-06	
	1c	0.0171	0.2065	0.2295	2.68E-06	
	2a	0.0243	0.1940	0.2272	3.46E-06	2.62E-06
	2b	0.0246	0.1931	0.2273	3.06E-06	
	2c	0.0240	0.2004	0.2290	1.70E-06	
	2d	0.0245	0.1962	0.2327	2.26E-06	
Norm.	3a	0.0326	0.1968	0.2285	3.56E-06	3.54E-06
	3b	0.0328	0.1864	0.2298	3.52E-06	
4a	4a	0.0388	0.1943	0.2267	5.24E-06	4.33E-06
	4b	0.0391	0.1940	0.2273	4.65E-06	
	4c	0.0420	0.2044	0.2450	3.10E-06	
	5a	0.0489	0.1965	0.2267	5.69E-06	4.84E-06
	5b	0.0487	0.1953	0.2277	4.74E-06	
	5c	0.0489	0.2172	0.2362	4.27E-06	
	5d	0.0487	0.2132	0.2350	4.65E-06	
	6a	0.0650	0.1977	0.2288	5.73E-06	6.43E-06
	6b	0.0646	0.2026	0.2278	6.00E-06	
	6c	0.0681	0.2023	0.2372	7.55E-06	
BH_3•NMe_3	7a	0.0322	0.0347	0.2263	2.39E-06	2.36E-06
	7b	0.0327	0.0347	0.2268	2.34E-06	
	8a	0.0328	0.0981	0.2268	2.95E-06	2.84E-06
	8b	0.0322	0.0978	0.2272	2.72E-06	
	9a	0.0326	0.2909	0.2390	4.72E-06	5.19E-06
	9b	0.0346	0.2940	0.2443	5.29E-06	
	9c	0.0333	0.3010	0.2333	5.56E-06	
	10a	0.0326	0.3890	0.2267	4.24E-06	3.98E-06
	10b	0.0327	0.3878	0.2277	3.62E-06	
	10c	0.0347	0.3939	0.2400	4.08E-06	
$AlCl_3$	11a	0.0325	0.1947	0.0327	1.24E-07	1.00E-07
	11b	0.0324	0.1953	0.0325	7.69E-08	
	12a	0.0324	0.1965	0.1140	9.73E-07	9.08E-07
	12b	0.0325	0.1965	0.1142	8.43E-07	
	13a	0.0325	0.2023	0.3300	5.47E-06	5.56E-06
	13b	0.0326	0.2011	0.3228	5.65E-06	
	14a	0.0324	0.1959	0.4540	9.58E-06	9.63E-06
	14b	0.0324	0.1953	0.4661	9.67E-06	

Entry:	1a			
Reaction time (s)	Product	Starting material	Product (%)	Conc. prod
0	0	1	0.0	0.00E+00
300	0.1	1.11	4.3	7.04E-04
600	0.17	1.11	7.1	1.16E-03
1200	0.35	1.11	13.6	2.22E-03
2400	0.6	1.1	21.4	3.50E-03
3600	1.15	1.11	34.1	5.57E-03
Entry:	1b			
Reaction time (s)	Product	Starting material	Product (%)	Conc. prod
0	0	1	0.0	0.00E+00
300	0.04	1.08	1.8	3.01E-04
600	0.1	1.11	4.3	7.13E-04
1200	0.25	1.1	10.2	1.69E-03
2400	0.75	1.1	25.4	4.21E-03
3600	1.21	1.1	35.5	5.87E-03
Entry:	1c			
Reaction time (s)	Product	Starting material	Product (%)	Conc. prod
0	0	1	0.0	0.00E+00
300	0.11	1.1	4.8	8.13E-04
600	0.23	1.11	9.4	1.60E-03
1200	0.4	1.1	15.4	2.63E-03
2400	0.78	1.08	26.5	4.53E-03
3600	1.2	1.1	35.3	6.02E-03

Statistics for reactions 1a-c			
Parameter	a	b	c
Data points	4 points	6 points	3 points
k	1.893E-06	1.639E-06	2.678E-06
Std dev.	6.149E-08	5.045E-08	1.095E-08
r^2	9.968E-01	9.953E-01	1.000E+00
f	9.478E+02	1.055E+03	5.986E+04
SSreg	6.772E-06	5.533E-05	3.227E-06

Entry:	2a			
Reaction time (s)	Product	Starting material	Product (%)	Conc. prod
0	0	1	0.0	0.00E+00
300	0.12	1.1	5.2	1.26E-03
600	0.22	1.12	8.9	2.17E-03
1200	0.44	1.1	16.7	4.05E-03
2400	0.86	1.11	27.9	6.78E-03
3600	1.32	1.1	37.5	9.11E-03

Entry:	2b			
Reaction time (s)	Product	Starting material	Product (%)	Conc. prod
0	0	1	0.0	0.00E+00
300	0.09	1.1	3.9	9.67E-04
600	0.18	1.1	7.6	1.86E-03
1200	0.38	1.09	14.8	3.65E-03
2400	0.8	1.12	26.3	6.48E-03
3600	1.21	1.11	35.3	8.68E-03
Entry:	2c			
Reaction time (s)	Product	Starting material	Product (%)	Conc. prod
0	0	1	0.0	0.00E+00
300	0.08	1.09	3.5	8.49E-04
600	0.12	1.08	5.3	1.26E-03
1200	0.23	1.09	9.5	2.29E-03
2400	0.46	1.1	17.3	4.15E-03
3600	0.72	1.1	24.7	5.91E-03
Reaction number:	2d			
Reaction time (s)	Product	Starting material	Product (%)	Conc. prod
0	0	1	0.0	0.00E+00
300	0.07	1.08	3.1	7.69E-04
600	0.13	1.09	5.6	1.38E-03
1200	0.27	1.1	10.9	2.68E-03
2400	0.53	1.1	19.4	4.76E-03
3600	0.82	1.09	27.3	6.70E-03
Statistics for reactions 2 a-d				
Parameter	a	b	c	d
Data points	4 points	4 points	6 points	4 points
K	3.460E-06	3.063E-06	1.698E-06	2.260E-06
Std dev.	1.093E-07	2.445E-08	5.235E-08	4.191E-08
r^2	9.970E-01	9.998E-01	9.953E-01	9.990E-01
F	1.002E+03	1.569E+04	1.052E+03	2.909E+03
Ssreg	2.262E-05	1.773E-05	5.941E-05	9.655E-06

Reaction 3

Entry:	3a			
Reaction time (s)	Product	Starting material	Product (%)	Conc. prod
0	0	1	0.0	0.00E+00
300	0.08	1.09	3.5	1.15E-03
600	0.15	1.09	6.4	2.10E-03
1200	0.28	1.09	11.4	3.71E-03
2400	0.58	1.1	20.9	6.79E-03
3600	0.87	1.08	28.7	9.35E-03

Entry:	3b			
Reaction time (s)	Product	Starting material	Product (%)	Conc. prod
0	0	1	0.0	0.00E+00
300	0.07	1.09	3.1	1.02E-03
600	0.15	1.08	6.5	2.13E-03
1200	0.28	1.09	11.4	3.73E-03
2400	0.56	1.09	20.4	6.70E-03
3600	0.83	1.08	27.8	9.10E-03

Statistics for reactions 3a-b		
Parameter	a	b
Data points	3 points	3 points
K	3.564E-06	3.517E-06
Std dev.	9.853E-08	4.191E-08
r^2	9.985E-01	9.997E-01
F	1.308E+03	7.043E+03
Ssreg	5.714E-06	5.567E-06

Entry:	4a			
Reaction time (s)	Product	Starting material	Product (%)	Conc. prod
0	0	1	0.0	0.00E+00
300	0.1	1.1	4.3	1.69E-03
600	0.19	1.1	7.9	3.09E-03
1200	0.37	1.1	14.4	5.59E-03
2400	0.71	1.11	24.2	9.41E-03
3600	1.1	1.11	33.1	1.29E-02
Entry:	4b			
Reaction time (s)	Product	Starting material	Product (%)	Conc. prod
0	0	1	0.0	0.00E+00
300	0.1	1.09	4.4	1.71E-03
600	0.17	1.1	7.2	2.80E-03
1200	0.36	1.1	14.1	5.49E-03
2400	0.74	1.1	25.2	9.83E-03
3600	1.12	1.1	33.7	1.32E-02
Entry:	4c			
Reaction time (s)	Product	Starting material	Product (%)	Conc. prod
0	0	1	0.0	0.00E+00
300	0.05	1.09	2.2	9.41E-04
600	0.1	1.08	4.4	1.86E-03
1200	0.19	1.08	8.1	3.39E-03
2400	0.35	1.09	13.8	5.81E-03
3600	0.5	1.08	18.8	7.89E-03

Statistics for reactions 4a-c			
Parameter	a	b	c
Data points	3 points	4 points	3 points
K	5.243E-06	4.648E-06	3.105E-06
Std dev.	1.366E-07	1.386E-07	1.178E-08
r^2	9.986E-01	9.973E-01	1.000E+00
F	1.474E+03	1.125E+03	6.944E+04
Ssreg	1.237E-05	4.083E-05	4.337E-06

Entry:	5a			
Reaction time (s)	Product	Starting material	Product (%)	Conc. prod
0	0	1	0.0	0.00E+00
300	0.1	1.09	4.4	2.14E-03
600	0.18	1.11	7.5	3.67E-03
1200	0.34	1.09	13.5	6.60E-03
2400	0.64	1.09	22.7	1.11E-02
3600	0.95	1.1	30.2	1.47E-02
Entry:	5b			
Reaction time (s)	Product	Starting material	Product (%)	Conc. prod
0	0	1	0.0	0.00E+00
300	0.06	1.09	2.7	1.30E-03
600	0.14	1.09	6.0	2.94E-03
1200	0.29	1.1	11.6	5.67E-03
2400	0.59	1.1	21.1	1.03E-02
3600	0.87	1.09	28.5	1.39E-02
Entry:	5c			
Reaction time (s)	Product	Starting material	Product (%)	Conc. prod
0	0	1	0.0	0.00E+00
300	0.06	1.08	2.7	1.32E-03
600	0.12	1.09	5.2	2.54E-03
1200	0.24	1.09	9.9	4.83E-03
2400	0.43	1.08	16.6	8.08E-03
3600	0.63	1.09	22.4	1.09E-02
Entry:	5d			
Reaction time (s)	Product	Starting material	Product (%)	Conc. prod
0	0	1	0.0	0.00E+00
300	0.01	1.08	0.5	2.24E-04
600	0.13	1.09	5.6	2.74E-03
1200	0.29	1.08	11.8	5.76E-03
2400	0.72	1.08	25.0	1.22E-02
3600	1.08	1.09	33.1	1.61E-02

Statistics for reactions 5a-d				
Parameter	a	b	c	d
Data points	4 points	4 points	3 points	6 points
K	5.693E-06	4.740E-06	4.268E-06	4.653E-06
Std dev.	2.334E-07	6.375E-08	4.849E-08	1.649E-07
r^2	9.950E-01	9.995E-01	9.997E-01	9.938E-01
F	5.950E+02	5.528E+03	7.748E+03	7.962E+02
Ssreg	6.126E-05	4.246E-05	8.197E-06	4.463E-04

Reaction 6

Entry:	6a			
Reaction time (s)	Product	Starting material	Product (%)	Conc. prod
0	0	1	0.0	0.00E+00
300	0.06	1.08	2.7	1.76E-03
600	0.12	1.08	5.3	3.42E-03
1200	0.22	1.09	9.2	5.96E-03
2400	0.4	1.09	15.5	1.01E-02
3600	0.57	1.09	20.7	1.35E-02
Entry:	6b			
Reaction time (s)	Product	Starting material	Product (%)	Conc. prod
0	0	1	0.0	0.00E+00
300	0.06	1.09	2.7	1.73E-03
600	0.13	1.09	5.6	3.64E-03
1200	0.21	1.08	8.9	5.72E-03
2400	0.41	1.09	15.8	1.02E-02
3600	0.58	1.08	21.2	1.37E-02
Entry:	6c			
Reaction time (s)	Product	Starting material	Product (%)	Conc. prod
0	0	1	0.0	0.00E+00
300	0.08	1.09	3.5	2.41E-03
600	0.16	1.08	6.9	4.46E-03
1200	0.29	1.09	11.7	7.58E-03
2400	0.51	1.08	19.1	1.23E-02
3600	0.72	1.09	24.8	1.60E-02

Statistics for reactions 6a-c			
Parameter	a	b	c
Data points	3 points	3 points	3 points
K	5.734E-06	6.001E-06	7.546E-06
Std dev.	4.360E-08	8.240E-08	1.711E-07
r^2	9.999E-01	9.996E-01	9.990E-01
F	1.730E+04	5.304E+03	1.946E+03
SSreg	1.480E-05	1.621E-05	2.563E-05

Entry:	7a			
Reaction time (s)	Product	Starting material	Product (%)	Conc. prod
0	0	1	0.0	0.00E+00
300	0.04	1.12	1.8	5.66E-04
600	0.09	1.1	3.9	1.27E-03
1200	0.23	1.1	9.5	3.05E-03
2400	0.49	1.1	18.2	5.87E-03
3600	0.79	1.11	26.2	8.46E-03
Entry:	7b			
Reaction time (s)	Product	Starting material	Product (%)	Conc. prod
0	0	1	0.0	0.00E+00
300	0.03	1.1	1.3	4.39E-04
600	0.1	1.1	4.3	1.42E-03
1200	0.23	1.1	9.5	3.09E-03
2400	0.46	1.1	17.3	5.65E-03
3600	0.75	1.1	25.4	8.31E-03

Statistics for reactions 7a-b		
Parameter	a	b
Data points	6 points	6 points
K	2.385E-06	2.336E-06
Std dev.	3.453E-08	3.998E-08
r^2	9.990E-01	9.985E-01
F	4.771E+03	3.414E+03
Ssreg	1.173E-04	1.125E-04

Entry:	8a			
Reaction time (s)	Product	Starting material	Product (%)	Conc. prod
0	0	1	0.0	0.00E+00
300	0.05	1.1	2.2	7.28E-04
600	0.12	1.1	5.2	1.70E-03
1200	0.26	1.1	10.6	3.46E-03
2400	0.61	1.09	21.9	7.17E-03
3600	0.96	1.09	30.6	1.00E-02
Entry:	8b			
Reaction time (s)	Product	Starting material	Product (%)	Conc. prod
0	0	1	0.0	0.00E+00
300	0.04	1.09	1.8	5.81E-04
600	0.1	1.1	4.3	1.40E-03
1200	0.23	1.1	9.5	3.05E-03
2400	0.56	1.1	20.3	6.54E-03
3600	0.98	1.1	30.8	9.94E-03

Statistics for reactions 8a-b		
Parameter	a	b
Data points	5 points	6 points
K	2.953E-06	2.725E-06
Std dev.	3.757E-08	4.109E-08
r^2	9.994E-01	9.989E-01
F	6.176E+03	4.398E+03
Ssreg	6.670E-05	1.530E-04

Entry:	9a			
Reaction time (s)	Product	Starting material	Product (%)	Conc. prod
0	0	1	0.0	0.00E+00
300	0.11	1.09	4.8	1.56E-03
600	0.2	1.08	8.5	2.76E-03
1200	0.38	1.09	14.8	4.83E-03
2400	0.74	1.09	25.3	8.25E-03
3600	1.07	1.09	32.9	1.07E-02
Entry:	9b			
Reaction time (s)	Product	Starting material	Product (%)	Conc. prod
0	0	1	0.0	0.00E+00
300	0.11	1.1	4.8	1.65E-03
600	0.22	1.1	9.1	3.14E-03
1200	0.42	1.1	16.0	5.54E-03
2400	0.79	1.1	26.4	9.13E-03
3600	1.14	1.08	34.5	1.19E-02
Entry:	9c			
Reaction time (s)	Product	Starting material	Product (%)	Conc. prod
0	0	1	0.0	0.00E+00
300	0.12	1.09	5.2	1.74E-03
600	0.24	1.09	9.9	3.30E-03
1200	0.45	1.1	17.0	5.65E-03
2400	0.86	1.09	28.3	9.42E-03
3600	1.29	1.1	37.0	1.23E-02

Statistics for reactions 9a-c			
Parameter	a	b	c
Data points	3 points	3 points	3 points
K	4.722E-06	5.285E-06	5.561E-06
Std dev.	1.738E-07	7.051E-08	8.121E-08
r^2	9.973E-01	9.996E-01	9.996E-01
F	7.380E+02	5.618E+03	4.688E+03
Ssreg	1.003E-05	1.257E-05	1.392E-05

Entry:	10a			
Reaction time (s)	Product	Starting material	Product (%)	Conc. prod
0	0	1	0.0	0.00E+00
300	0.08	1.1	3.5	1.14E-03
600	0.19	1.11	7.9	2.57E-03
1200	0.41	1.1	15.7	5.12E-03
2400	0.78	1.1	26.2	8.52E-03
3600	1.31	1.09	37.5	1.22E-02
Entry:	10b			
Reaction time (s)	Product	Starting material	Product (%)	Conc. prod
0	0	1	0.0	0.00E+00
300	0.09	1.1	3.9	1.28E-03
600	0.16	1.11	6.7	2.20E-03
1200	0.36	1.12	13.8	4.52E-03
2400	0.79	1.11	26.2	8.57E-03
3600	1.29	1.08	37.4	1.22E-02
Entry:	10c			
Reaction time (s)	Product	Starting material	Product (%)	Conc. prod
0	0	1	0.0	0.00E+00
300	0.09	1.09	4.0	1.37E-03
600	0.16	1.09	6.8	2.37E-03
1200	0.3	1.09	12.1	4.19E-03
2400	0.54	1.09	19.9	6.88E-03
3600	0.8	1.09	26.8	9.30E-03

Statistics for reactions 10a-c			
Parameter	a	b	c
Data points	4 points	5 points	3 points
K	4.244E-06	3.622E-06	4.076E-06
Std dev.	5.635E-08	5.266E-08	1.784E-07
r^2	9.995E-01	9.992E-01	9.962E-01
F	5.673E+03	4.731E+03	5.220E+02
Ssreg	3.404E-05	1.004E-04	7.475E-06

Entry:	11a			
Reaction time (s)	Product	Starting material	Product (%)	Conc. prod
0	0	1	0.0	0.00E+00
300	0.0022	1.1	0.1	3.24E-05
600	0.0052	1.1	0.2	7.65E-05
1200	0.006	1.1	0.3	8.83E-05
2400	0.0148	1.1	0.7	2.17E-04
3600	0.0172	1.09	0.8	2.54E-04

Entry:	11b			
Reaction time (s)	Product	Starting material	Product (%)	Conc. prod
0	0	1	0.0	0.00E+00
300	0.0018	1.1	0.1	2.64E-05
600	0.005	1.1	0.2	7.34E-05
1200	0.0078	1.09	0.4	1.15E-04
2400	0.0116	1.1	0.5	1.70E-04
3600	0.0188	1.1	0.8	2.74E-04

Statistics for reactions 11a-b		
Parameter	a	b
Data points	3 points	6 points
K	1.237E-07	7.688E-08
Std dev.	5.509E-09	3.832E-09
r^2	9.960E-01	9.877E-01
F	5.039E+02	4.026E+02
Ssreg	6.882E-09	1.218E-07

Entry:	12a			
Reaction time (s)	Product	Starting material	Product (%)	Conc. prod
0	0	1	0.0	0.00E+00
300	0.02	1.09	0.9	2.94E-04
600	0.04	1.09	1.8	5.83E-04
1200	0.09	1.09	4.0	1.28E-03
2400	0.16	1.08	6.9	2.23E-03
3600	0.22	1.09	9.2	2.97E-03
Entry:	12b			
Reaction time (s)	Product	Starting material	Product (%)	Conc. prod
0	0	1	0.0	0.00E+00
300	0.01	1.1	0.5	1.47E-04
600	0.03	1.1	1.3	4.37E-04
1200	0.12	1.1	5.2	1.68E-03
2400	0.13	1.08	5.7	1.84E-03
3600	0.22	1.1	9.1	2.95E-03

Statistics for reactions 12a-b		
Parameter	a	b
Data points	3 points	6 points
K	9.733E-07	8.426E-07
Std dev.	2.498E-09	6.972E-08
r^2	1.000E+00	9.669E-01
F	1.518E+05	1.460E+02
Ssreg	4.263E-07	1.463E-05

Entry:	13a			
Reaction time (s)	Product	Starting material	Product (%)	Conc. prod
0	0	1	0.0	0.00E+00
300	0.14	1.09	6.0	1.96E-03
600	0.26	1.09	10.7	3.46E-03
1200	0.54	1.1	19.7	6.40E-03
2400	1.13	1.09	34.1	1.11E-02
3600	1.72	1.09	44.1	1.43E-02
Entry:	13b			
Reaction time (s)	Product	Starting material	Product (%)	Conc. prod
0	0	1	0.0	0.00E+00
300	0.09	1.09	4.0	1.29E-03
600	0.26	1.09	10.7	3.47E-03
1200	0.58	1.09	21.0	6.84E-03
2400	1.24	1.1	36.0	1.17E-02
3600	1.86	1.11	45.6	1.48E-02

Statistics for reactions 13a-b		
Parameter	a	b
Data points	4 points	4 points
K	5.470E-06	5.651E-06
Std dev.	1.680E-07	1.749E-07
r^2	9.972E-01	9.971E-01
F	1.060E+03	1.044E+03
Ssreg	5.656E-05	6.036E-05

Entry:	14a			
Reaction time (s)	Product	Starting material	Product (%)	Conc. prod
0	0	1	0.0	0.00E+00
300	0.25	1.1	10.2	3.30E-03
600	0.45	1.09	17.1	5.54E-03
1200	0.87	1.09	28.5	9.23E-03
2400	1.84	1.1	45.5	1.47E-02
3600	2.84	1.1	56.3	1.82E-02
Entry:	14b			
Reaction time (s)	Product	Starting material	Product (%)	Conc. prod
0	0	1	0.0	0.00E+00
300	0.25	1.1	10.2	3.33E-03
600	0.45	1.09	17.1	5.59E-03
1200	0.9	1.09	29.2	9.55E-03
2400	1.63	1.09	42.8	1.40E-02
3600	2.86	1.09	56.7	1.85E-02

Statistics for reactions 14a-b		
Parameter	a	b
Data points	3 points	3 points
K	9.582E-06	9.675E-06
Std dev.	5.030E-07	5.079E-07
r^2	9.945E-01	9.945E-01
F	3.629E+02	3.629E+02
Ssreg	4.132E-05	4.212E-05

9) Experimental detail for reaction rate of 1

Borane tetrahydrofuran-complex: 1 was dissolved in THF to give a stock solution of 100 mg/mL. $AlCl_3$ was dissolved in THF to give a stock solution of 145 mg/mL.

2 eq of $AlCl_3$
A stock solution of **1** (0.250 mL, 0.054 mmol), BH_3•THF (0.215 mL, 1 M) and THF (0.435 mL) was stirred at r.t. under N_2 for 15 min. Then, a stock solution of $AlCl_3$ (0.100 mL, 0.109 mmol) was added. Samples (0.050 mL) were taken at 35, 70, 105, 140 and 180 min and quenched in micro vials with $NaHCO_3$ (0.250 mL, sat. aq.) and extracted with ether (0.100 mL). Analyzed by quantitative TLC.[18]

4 eq of $AlCl_3$
A stock solution of **1** (0.250 mL, 0.054 mmol), BH_3•THF (0.215 mL, 1 M) and THF (0.335 mL) was stirred at r.t. under N_2 for 15 min. Then, a stock solution of $AlCl_3$ (0.200 mL, 0.217 mmol) was added. Samples (0.050 mL) were taken at 24, 48, 72, 96 and 120 min and quenched in micro vials with $NaHCO_3$ (0.250 mL, sat. aq.) and extracted with ether (0.100 mL). Analyzed by quantitative TLC.[18]

6 eq of $AlCl_3$
A Stock solution of **1** (0.250 mL, 0.054 mmol), BH_3•THF (0.215 mL, 1 M) and THF (0.235 mL) was stirred at r.t. under N_2 for 15 min. Then, a stock solution of $AlCl_3$ (0.300 mL, 0.326 mmol) was added. Samples (0.050 mL) were taken at 12, 24, 36, 48 and 60 min and quenched in micro vials with $NaHCO_3$ (0.250 mL, sat. aq.) and extracted with ether (0.100 mL). Analyzed by quantitative TLC.[18]

8 eq of $AlCl_3$
A stock solution of **1** (0.250 mL, 0.054 mmol), BH_3•THF (0.215 mL, 1 M) and THF (0.135 mL) was stirred at r.t. under N_2 for 15 min. Then, a stock solution of $AlCl_3$ (0.400 mL, 0.435 mmol) was added. Samples (0.050 mL) were taken at 9, 18, 27, 36 and 45 min and quenched in micro vials with $NaHCO_3$ (0.250 mL, sat. aq.) and extracted with ether (0.100 mL). Analyzed by quantitative TLC.[18]

Borane trimethylamine: 1 was dissolved in THF to give a stock solution of 100 mg/mL. BH_3•NMe_3 was dissolved in THF to give a stock solution of 64 mg/mL. $AlCl_3$ was dissolved in THF to give a stock solution of 145 mg/mL.

2 eq of $AlCl_3$
A stock solution of **1** (0.250 mL, 0.054 mmol), a stock solution of BH_3•NMe_3 (0.250 mL, 0.219 mmol) and THF (0.400 mL) was stirred at 0 °C under N_2 for 15 min. Then, a stock solution of $AlCl_3$ (0.100 mL, 0.109 mmol) was added. Samples (0.050 mL) were taken at 15, 30, 45, 60 and 75 min and quenched in micro vials with $NaHCO_3$ (0.250 mL, sat. aq.) and extracted with ether (0.100 mL). Analyzed by quantitative TLC.[18]

4 eq of $AlCl_3$

A stock solution of **1** (0.250 mL, 0.054 mmol), a stock solution of BH_3•NMe_3 (0.250 mL, 0.219 mmol) and THF (0.300 mL) was stirred at 0 °C under N_2 for 15 min. Then, a stock solution of $AlCl_3$ (0.200 mL, 0.217 mmol) was added. Samples (0.050 mL) were taken at 5, 10, 15, 20 and 30 min and quenched in micro vials with $NaHCO_3$ (0.250 mL, sat. aq.) and extracted with ether (0.100 mL). Analyzed by quantitative TLC.[18]

6 eq of $AlCl_3$

A stock solution of **1** (0.250 mL, 0.054 mmol), a stock solution of BH_3•NMe_3 (0.250 mL, 0.219 mmol) and THF (0.200 mL) was stirred at 0 °C under N_2 for 15 min. Then, a stock solution of $AlCl_3$ (0.300 mL, 0.326 mmol) was added. Samples (0.050 mL) were taken at 4, 8, 12, 16 and 20 min and quenched in micro vials with $NaHCO_3$ (0.250 mL, sat. aq.) and extracted with ether (0.100 mL). Analyzed by quantitative TLC.[18]

8 eq of $AlCl_3$

A stock solution of **1** (0.250 mL, 0.054 mmol), a stock solution of BH_3•NMe_3 (0.250 mL, 0.219 mmol) and THF (0.100 mL) was stirred at 0 °C under N_2 for 15 min. Then, a stock solution of $AlCl_3$ (0.400 mL, 0.435 mmol) was added. Samples (0.050 mL) were taken at 4, 8, 12, 16 and 20 min and quenched in micro vials with $NaHCO_3$ (0.250 mL, sat. aq.) and extracted with ether (0.100 mL). Analyzed by quantitative TLC.[18]

10) Quantitative TLC study of reaction kinetics of 1

To maximize the precision in the quantitative TLC study, ratios of **2** and **3** versus **1** were used. Known amounts were weighted and calibration curves were plotted (Figures S1 and S2). The molar concentration of product was determined from quantitative TLC, ratios plotted versus time. Linear regression over the linear part of the curves (determined by f-values) gave the reaction rates. To confirm the TLC-data some points were checked with NMR and was in agreement with quantitative TLC.

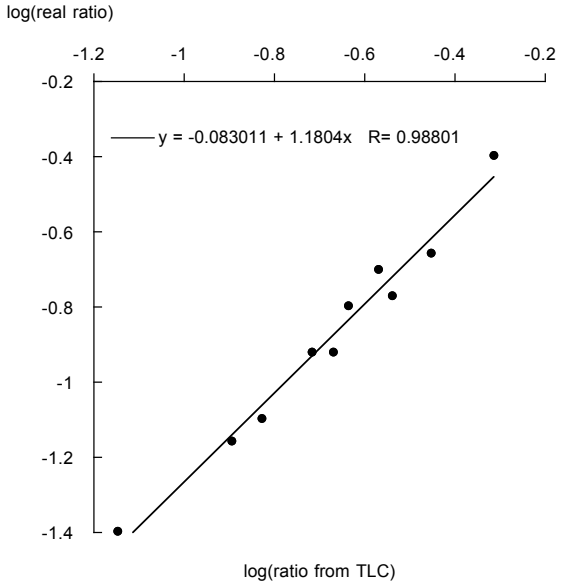


Figure S2: Calibration curve for the ratio of **2**:**1** (reaction using BH_3•THF)

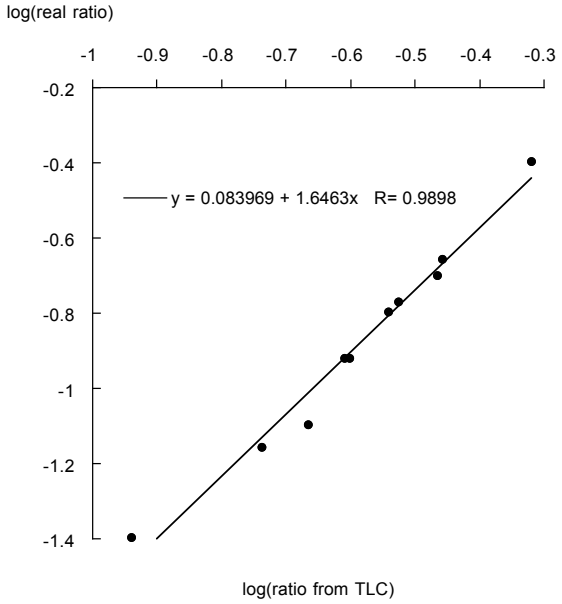


Figure S3: Calibration curve for the ratio of **3**:**1** (reaction using BH_3•NMe_3)

$[\mathbf{1}]_0$ =0.054 mol L^{-1}, $[AlCl_3]_0$ = 0.1085 mol L^{-1}, $[BH_3 \bullet THF]_0$ = 0.215 mol L^{-1}

	Experiment 1		Experiment 2	
Time (s)	Ratio (TLC)	[**2**]	Ratio (TLC)	[**2**]
0	0	0.0000	0	0.0000
2100	0.0241	0.0013	0.0380	0.0021
4200	0.0453	0.0024	0.0692	0.0037
6300	0.0752	0.0041	0.0970	0.0052
8400	0.0903	0.0049	0.1091	0.0059
10800	0.0984	0.0053	0.1469	0.0079

$[\mathbf{1}]_0$ =0.054 mol L^{-1}, $[AlCl_3]_0$ = 0.217 mol L^{-1}, $[BH_3 \bullet THF]_0$ = 0.215 mol L^{-1}

	Experiment 1		Experiment 2	
Time (s)	Ratio (TLC)	[**2**]	Ratio (TLC)	[**2**]
0	0	0.0000	0	0.0000
1440	0.0562	0.0030	0.0635	0.0034
2880	0.1070	0.0058	0.1142	0.0062
4320	0.1532	0.0083	0.1572	0.0085
5700	0.1845	0.0100	0.1968	0.0106
7200	0.2370	0.0128	0.2276	0.0123

$[\mathbf{1}]_0$ =0.054 mol L^{-1}, $[AlCl_3]_0$ = 0.3255 mol L^{-1}, $[BH_3 \bullet THF]_0$ = 0.215 mol L^{-1}

	Experiment 1		Experiment 2	
Time (s)	Ratio (TLC)	[**2**]	Ratio (TLC)	[**2**]
0	0	0.0000	0	0.0000
720	0.0383	0.0021	0.0624	0.0034
1440	0.0779	0.0042	0.0945	0.0051
2160	0.1060	0.0057	0.1312	0.0071
2880	0.1306	0.0071	0.1594	0.0086
3600	0.1524	0.0082	0.1950	0.0105

$[\mathbf{1}]_0$ =0.054 mol L^{-1}, $[AlCl_3]_0$ = 0.435 mol L^{-1}, $[BH_3 \bullet THF]_0$ = 0.215 mol L^{-1}

	Experiment 1		Experiment 2	
Time (s)	Ratio (TLC)	[**2**]	Ratio (TLC)	[**2**]
0	0	0.0000	0	0.0000
540	0.0445	0.0024	0.0776	0.0042
1080	0.0769	0.0042	0.0949	0.0051
1620	0.1148	0.0062	0.1246	0.0067
2160	0.1427	0.0077	0.1522	0.0082
2700	0.1661	0.0090	0.1767	0.0095

$[\mathbf{1}]_0$ =0.054 mol L^{-1}, $[AlCl_3]_0$ = 0.1085 mol L^{-1}, $[BH_3{\bullet}NMe_3]_0$ = 0.217 mol L^{-1}

	Experiment 1		Experiment 2	
Time (s)	Ratio (TLC)	[**3**]	Ratio (TLC)	[**3**]
0	0	0.0000	0	0.0000
900	0.0067	0.0004	0.0079	0.0004
1800	0.0316	0.0017	0.0582	0.0031
2700	0.0695	0.0038	0.0734	0.0040
3600	0.1275	0.0069	0.1103	0.0060
4500	0.0739	0.0040	0.1152	0.0062

$[\mathbf{1}]_0$ =0.054 mol L^{-1}, $[AlCl_3]_0$ = 0.217 mol L^{-1}, $[BH_3{\bullet}NMe_3]_0$ = 0.217 mol L^{-1}

	Experiment 1		Experiment 2	
Time (s)	Ratio (TLC)	[**3**]	Ratio (TLC)	[**3**]
0	0	0.0000	0	0.0000
300	0.0079	0.0004	0.0055	0.0003
600	0.0386	0.0021	0.0469	0.0025
900	0.0792	0.0043	0.1078	0.0058
1200	0.0693	0.0037	0.1430	0.0077
1800	0.1567	0.0085	0.1885	0.0102

$[\mathbf{1}]_0$ =0.054 mol L^{-1}, $[AlCl_3]_0$ = 0.3255 mol L^{-1}, $[BH_3{\bullet}NMe_3]_0$ = 0.217 mol L^{-1}

	Experiment 1		Experiment 2	
Time (s)	Ratio (TLC)	[**3**]	Ratio (TLC)	[**3**]
0	0	0.0000	0	0.0000
240	0.0223	0.0012	0.0409	0.0022
480	0.0608	0.0033	0.0903	0.0049
720	0.1124	0.0061	0.1513	0.0082
960	0.1580	0.0085	0.1642	0.0089
1200	0.1458	0.0079	0.1546	0.0083

$[\mathbf{1}]_0$ =0.054 mol L^{-1}, $[AlCl_3]_0$ = 0.435 mol L^{-1}, $[BH_3{\bullet}NMe_3]_0$ = 0.217 mol L^{-1}

	Experiment 1		Experiment 2	
Time (s)	Ratio (TLC)	[**3**]	Ratio (TLC)	[**3**]
0	0	0.0000	0	0.0000
240	0.1091	0.0059	0.1027	0.0055
480	0.1955	0.0106	0.2478	0.0134
720	0.3029	0.0164	0.2388	0.0129
960	0.3719	0.0201	0.2760	0.0149
1200	0.3709	0.0200	0.3535	0.0191

Results: BH_3•THF

$[\mathbf{1}]_0$ (mol L^{-1})	$[AlCl_3]_0$ (mol L^{-1})	$[BH_3•THF]_0$ (mol L^{-1})	$dP/dt * 10^6$
0.054	0.1085	0.215	0.90714
0.054	0.1085	0.215	0.58976
0.054	0.217	0.215	2.0265
0.054	0.217	0.215	2.1895
0.054	0.3255	0.215	3.0786
0.054	0.3255	0.215	2.9117
0.054	0.435	0.215	3.8776
0.054	0.435	0.215	3.8786

Results BH_3•NMe_3

$[\mathbf{1}]_0$ (mol L^{-1})	$[AlCl_3]_0$ (mol L^{-1})	$[BH_3•THF]_0$ (mol L^{-1})	$dP/dt * 10^6$
0.054	0.1085	0.217	1.4850
0.054	0.1085	0.217	1.5767
0.054	0.217	0.217	4.1998
0.054	0.217	0.217	5.7979
0.054	0.3255	0.217	9.9643
0.054	0.3255	0.217	8.3471
0.054	0.435	0.217	22.643
0.054	0.435	0.217	26.925

11) Computational data

Computational data for 1

		Standard Nuclear Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	C	-2.298629	-2.156016	0.091147
2	C	-2.105862	-0.736222	-0.474102
3	C	-0.639782	-0.467787	-0.866738
4	C	0.252720	-0.855438	0.313734
5	C	-0.051221	-2.277063	0.794844
6	O	-1.417001	-2.395927	1.185211
7	O	1.633942	-0.794294	-0.043891
8	C	0.859960	-2.581474	1.979620
9	H	-2.369201	-0.039749	0.333411
10	H	-0.381727	-1.080260	-1.741482
11	H	0.056895	-0.150129	1.139044
12	H	0.178637	-2.977384	-0.017303
13	H	0.605385	-1.925466	2.827820
14	H	0.771912	-3.621276	2.304970
15	C	-3.555613	0.715801	-1.748144
16	O	-2.996309	-0.590860	-1.567322
17	C	0.613916	1.359121	-1.872625
18	O	-0.560124	0.914580	-1.194985
19	C	2.464726	-1.086050	1.074752
20	H	2.250041	-0.348124	1.867775
21	O	2.215535	-2.389572	1.575324
22	C	3.073914	4.013459	0.495816
23	C	1.750044	3.775417	0.864948
24	C	0.953947	2.910134	0.112345
25	C	1.474545	2.266838	-1.014083
26	C	2.804007	2.508369	-1.377582
27	C	3.598923	3.376416	-0.630518
28	H	3.693960	4.687255	1.081999
29	H	1.333309	4.265349	1.741847
30	H	-0.076194	2.722126	0.397800
31	H	3.225895	2.003776	-2.244686
32	H	4.632263	3.546995	-0.921683
33	C	-6.247953	1.880710	1.428691
34	C	-5.212206	2.731432	1.045768
35	C	-4.338494	2.352467	0.023903
36	C	-4.493906	1.126981	-0.631108
37	C	-5.537552	0.278146	-0.237166
38	C	-6.407936	0.650720	0.784750
39	H	-6.926160	2.170656	2.227295
40	H	-5.077158	3.686497	1.547279
41	H	-3.523895	3.013355	-0.265255
42	H	-5.656438	-0.680677	-0.735968
43	H	-7.213598	-0.016643	1.080966
44	H	-2.762099	1.458602	-1.872311
45	H	-4.103734	0.636821	-2.693904
46	H	1.205064	0.506706	-2.224403
47	H	0.271087	1.912783	-2.758636
48	O	-2.114841	-3.071836	-0.950254
49	C	-2.540301	-4.391589	-0.638606
50	H	-2.375462	-4.992796	-1.535357
51	H	-1.970059	-4.815988	0.196884
52	H	-3.610076	-4.409231	-0.383508
53	H	-3.305747	-2.248608	0.518248
54	C	6.567190	-0.891963	-0.204918
55	C	5.704434	-1.847547	-0.748645
56	C	4.377923	-1.909460	-0.330026
57	C	3.903143	-1.013826	0.634527
58	C	4.765950	-0.059067	1.173540
59	C	6.096900	0.001564	0.756319
60	H	7.603163	-0.845761	-0.531336
61	H	6.068518	-2.544866	-1.498840
62	H	3.701320	-2.651105	-0.743243
63	H	4.396347	0.644052	1.916154
64	H	6.763763	0.746923	1.181899

Energy is –1536.330870 Hartrees

Computational data for 4a

		Standard Nuclear Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	H	4.067959	-1.774622	0.223639
2	C	3.621959	-0.787354	0.118275
3	C	2.471999	1.742496	-0.121343
4	C	2.230069	-0.672460	0.065599
5	C	4.437988	0.340469	0.051923
6	C	3.855885	1.606989	-0.062243
7	C	1.664532	0.602859	-0.064440
8	C	1.307636	-1.865400	0.167480
9	O	0.305107	0.782332	-0.125170
10	H	1.996903	2.714164	-0.213853
11	H	1.330102	-2.468473	-0.756089
12	O	-0.032899	-1.457752	0.445669
13	H	1.594593	-2.520291	0.996335
14	C	-0.440500	-0.411284	-0.398791
15	H	-0.254232	-0.686794	-1.450437
16	C	-1.897493	-0.117204	0.162333
17	C	-4.603673	0.416531	0.293830
18	C	-2.329476	0.285154	1.106638
19	C	-2.824020	-0.250357	-1.197413
20	C	-4.176134	0.015867	-0.971611
21	C	-3.677902	0.550835	1.332681
22	H	-1.604053	0.387902	1.907462
23	H	-2.489260	-0.562155	-2.184156
24	H	-4.891437	-0.088881	-1.782806
25	H	-4.009324	0.864056	2.319170
26	H	-5.655270	0.625237	0.472355
27	H	4.482977	2.493200	-0.108196
28	H	5.517963	0.234938	0.097824

Energy is -691.151804358 Hartrees

Computational data for 4b

		Standard Nuclear Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	H	3.644432	-1.777129	-0.312924
2	C	3.169878	-0.819010	-0.131061
3	C	2.030565	1.684535	0.389303

4	C	1.786635	-0.681462	-0.169883
5	C	3.965491	0.287217	0.159949
6	C	3.408343	1.539975	0.429560
7	C	1.220820	0.582139	0.079422
8	C	0.860030	-1.845449	-0.435828
9	N	5.419018	0.127736	0.197540
10	H	4.058827	2.374398	0.659679
11	O	-0.122268	0.782975	0.042042
12	H	1.556740	2.640450	0.585837
13	H	0.873734	-2.134997	-1.499366
14	O	-0.474209	-1.528574	-0.036638
15	H	1.146846	-2.721409	0.153017
16	C	-0.890425	-0.292765	-0.546530
17	H	-0.717431	-0.250446	-1.633895
18	C	-2.338435	-0.064975	-0.213258
19	C	-5.030504	0.344355	0.410397
20	C	-2.762673	-0.105872	1.119700
21	C	-3.263945	0.181823	-1.228541
22	C	-4.609878	0.386244	-0.918384
23	C	-4.105130	0.098038	1.428981
24	H	-2.038642	-0.299715	1.904888
25	H	-2.933347	0.215131	-2.264201
26	H	-5.325521	0.577528	-1.713053
27	H	-4.432493	0.064990	2.464518
28	H	-6.077345	0.503800	0.654510
29	O	6.098583	1.119320	0.469936
30	O	5.882303	-0.988848	-0.045717

Energy is -895.655667929 Hartrees

Computational data for 4c

		Standard Nuclear Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	H	4.044119	-1.753907	-0.329045
2	C	3.590931	-0.790093	-0.115504
3	C	2.441258	1.688107	0.467651
4	C	2.200142	-0.656580	-0.129086
5	C	4.390335	0.308322	0.185296
6	C	3.825444	1.548613	0.486680
7	C	1.631943	0.593179	0.151143
8	C	1.280680	-1.823615	-0.410401
9	Br	6.298265	0.112535	0.197010
10	H	4.457034	2.396147	0.728456
11	O	0.276595	0.784709	0.139058
12	H	1.971120	2.640631	0.690379
13	H	1.314037	-2.110221	-1.474905
14	O	-0.061416	-1.519676	-0.031167
15	H	1.563919	-2.700843	0.179334
16	C	-0.465343	-0.261513	-0.507828
17	H	-0.265426	-0.188753	-1.589781
18	C	-1.924684	-0.055345	-0.207023
19	C	-4.636701	0.310573	0.361775
20	C	-2.373430	-0.083841	1.118113
21	C	-2.836791	0.156603	-1.242087
22	C	-4.192187	0.339154	-0.959662
23	C	-3.725228	0.098377	1.400382
24	H	-1.659052	-0.248179	1.918597
25	H	-2.488027	0.180891	-2.272185
26	H	-4.896442	0.504625	-1.770288
27	H	-4.070397	0.075950	2.430629
28	H	-5.690697	0.454151	0.584459

Energy is -3264.432422547 Hartrees

Computational data for 4d

		Standard Nuclear Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	H	3.415829	-1.811342	0.217692
2	C	2.984131	-0.817815	0.102640
3	C	1.860694	1.712230	-0.152876
4	C	1.593256	-0.690153	0.056667
5	C	3.831695	0.290082	0.020159
6	C	3.241893	1.558127	-0.099500
7	C	1.036880	0.586075	-0.082619
8	C	0.663034	-1.874804	0.179238
9	C	5.334825	0.130198	0.043385
10	H	3.876673	2.439784	-0.153148
11	O	-0.322483	0.778257	-0.133903
12	H	1.401997	2.691787	-0.246225
13	H	0.677844	-2.490915	-0.735959
14	O	-0.673820	-1.454186	0.456828
15	H	0.948588	-2.520310	1.015971
16	C	-1.075879	-0.411444	-0.396120
17	H	-0.894370	-0.698487	-1.445722
18	C	-2.530727	-0.107281	-0.157965
19	C	-5.233893	0.438501	0.303632
20	C	-2.953736	0.326863	1.103342
21	C	-3.464721	-0.265629	-1.182954
22	C	-4.815240	0.006453	-0.954373
23	C	-4.300595	0.598623	1.332151
24	H	-2.222260	0.450570	1.895594
25	H	-3.136889	-0.601559	-2.164114
26	H	-5.536213	-0.118183	-1.757692
27	H	-4.625048	0.936677	2.312777
28	H	-6.284208	0.651802	0.484314
29	H	5.815728	0.946931	0.593277
30	H	5.756419	0.131429	-0.971064
31	H	5.630597	-0.812282	0.516568

Energy is -730.469332407 Hartrees

Computational data for 4e

		Standard Nuclear Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	H	3.050148	-2.186270	-0.221108
2	C	2.664007	-1.176020	-0.111971
3	C	1.733060	1.427703	0.199071
4	C	1.292451	-0.936445	-0.099434
5	C	3.578531	-0.126722	0.031277
6	C	3.106694	1.181762	0.194687
7	C	0.829287	0.378664	0.048111
8	C	0.279993	-2.052117	-0.225178
9	O	4.900922	-0.483217	0.007696

10	H	3.791856	2.012975	0.313666
11	O	-0.516527	0.669302	0.063900
12	H	1.349865	2.436386	0.318107
13	H	0.270684	-2.465391	-1.248145
14	O	-1.029355	-1.607075	0.129577
15	H	0.510081	-2.873587	0.460522
16	C	-1.339711	-0.372083	-0.469834
17	H	-1.150729	-0.428783	-1.555446
18	C	-2.777079	-0.029151	-0.183937
19	C	-5.447407	0.594875	0.362052
20	C	-3.216573	0.077928	1.140377
21	C	-3.677979	0.178262	-1.229330
22	C	-5.011914	0.490175	-0.958632
23	C	-4.547174	0.387997	1.411391
24	H	-2.510221	-0.084564	1.948246
25	H	-3.337362	0.097046	-2.258965
26	H	-5.707356	0.650718	-1.777951
27	H	-4.884634	0.469256	2.441213
28	H	-6.485186	0.837464	0.575224
29	C	5.868465	0.542481	0.147451
30	H	5.799644	1.278984	-0.665028
31	H	6.840331	0.047084	0.101681
32	H	5.773187	1.062364	1.110713

Energy is -805.672306633 Hartrees

Computational data for 4f

		Standard Nuclear Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	H	4.558039	-1.627244	-0.547788
2	C	4.085549	-0.721520	-0.172531
3	C	2.870159	1.587895	0.814600
4	C	2.691802	-0.616768	-0.204726
5	C	4.869808	0.308047	0.343596
6	C	4.255778	1.460882	0.843379
7	C	2.096543	0.552309	0.284649
8	C	1.805801	-1.725707	-0.725092
9	H	5.951145	0.210147	0.364465
10	H	4.858790	2.266006	1.253754
11	O	0.730141	0.718202	0.271727
12	H	2.369678	2.474657	1.190774
13	H	1.890908	-1.828402	-1.819789
14	O	0.437763	-1.508079	-0.366856
15	H	2.073769	-2.689129	-0.280707
16	C	0.045567	-0.182050	-0.601029
17	H	0.283961	0.105165	-1.638920
18	C	-1.432077	-0.059022	-0.325966
19	C	-4.141014	0.137602	0.193186
20	C	-1.925283	-0.371622	0.946902
21	C	-2.309648	0.352359	-1.331268
22	C	-3.676274	0.455157	-1.079482
23	C	-3.285846	-0.275490	1.215114
24	H	-1.236831	-0.689438	1.722365
25	H	-1.926739	0.595449	-2.318543
26	H	-4.376498	0.772217	-1.842178
27	H	-3.693314	-0.511622	2.190391
28	N	-5.584105	0.242730	0.468861
29	O	-5.972200	-0.046884	1.600042
30	O	-6.315373	0.614152	-0.448931

Energy is -895.652836271 Hartrees

Computational data for 4g

		Standard Nuclear Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	H	4.101776	-1.706398	0.474991
2	C	3.636133	-0.748814	0.253444
3	C	2.472176	1.724493	-0.307916
4	C	2.244866	-0.647621	0.129252
5	C	4.438137	0.384127	0.104285
6	C	3.856222	1.620872	-0.172577
7	C	1.673834	0.590703	-0.169426
8	C	1.363178	-1.847630	0.278458
9	H	5.517407	0.304052	0.208671
10	H	4.479624	2.504356	-0.282614
11	O	0.325245	0.761536	-0.317575
12	H	2.015964	2.686760	-0.523663
13	H	1.389224	-2.457852	-0.631770
14	O	0.024381	-1.451000	0.546699
15	H	1.695396	-2.465286	1.119139
16	C	-0.389994	-0.475457	-0.409035
17	H	-0.270874	-0.883146	-1.423389
18	C	-1.856594	-0.171949	-0.168656
19	C	-4.561581	0.418783	0.277273
20	C	-2.307925	0.208251	1.107133
21	C	-2.785543	-0.242734	-1.219244
22	C	-4.133969	0.049692	-0.996632
23	C	-3.654947	0.500549	1.331051
24	H	-1.599487	0.274946	1.931466
25	H	-2.465773	-0.524126	-2.220176
26	H	-4.839262	-0.011358	-1.821134
27	H	-3.981580	0.790026	2.325997
28	Br	-6.386036	0.814223	0.575946

Energy is –3264.429786 Hartrees

Computational data for 4h

		Standard Nuclear Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	H	4.775330	-1.581658	0.596121
2	C	4.292123	-0.651688	0.304047
3	C	3.047132	1.738562	-0.413800
4	C	2.898702	-0.610687	0.206719
5	C	5.062781	0.480448	0.047242
6	C	4.433128	1.677979	-0.306043
7	C	2.285380	0.593358	-0.164518
8	C	2.023295	-1.804427	0.510801
9	H	6.144079	0.433229	0.130442
10	H	5.024685	2.567537	-0.501676
11	O	0.922187	0.697514	-0.282186
12	H	2.534936	2.654126	-0.690799
13	H	2.099237	-2.565725	-0.283716
14	O	0.660095	-1.414130	0.681448

15	H	2.317297	-2.280010	1.451414
16	C	0.233933	-0.559827	-0.350219
17	H	0.463095	-1.012864	-1.329681
18	C	-1.239045	-0.295627	-0.206965
19	C	-4.001500	0.197092	0.074546
20	C	-1.741442	0.260889	0.975374
21	C	-2.120760	-0.603324	-1.241065
22	C	-3.488315	-0.359442	-1.100573
23	C	-3.103920	0.501380	1.110384
24	H	-1.057963	0.498549	1.783886
25	H	-1.741683	-1.037716	-2.162779
26	H	-4.163596	-0.605755	-1.915800
27	H	-3.482995	0.932529	2.033933
28	C	-5.477580	0.478558	0.228322
29	H	-5.677440	1.556784	0.241214
30	H	-5.866428	0.069023	1.166822
31	H	-6.054750	0.045322	-0.592893

Energy is –730.470018 Hartrees

Computational data for 4i

		Standard Nuclear Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	H	4.987423	-1.645114	0.381076
2	C	4.493870	-0.677557	0.309273
3	C	3.222037	1.799410	0.157250
4	C	3.109554	-0.632053	0.121852
5	C	5.242491	0.492805	0.419031
6	C	4.598851	1.732381	0.348676
7	C	2.483337	0.618529	0.037206
8	C	2.255854	-1.876062	0.033758
9	H	6.317085	0.439931	0.567724
10	H	5.172367	2.650797	0.440514
11	O	1.129230	0.731022	-0.152877
12	H	2.699800	2.748991	0.093553
13	H	2.416321	-2.405805	-0.920857
14	O	0.870536	-1.565106	0.185642
15	H	2.491643	-2.575787	0.841947
16	C	0.491924	-0.470951	-0.612418
17	H	0.815193	-0.639266	-1.653466
18	C	-0.995048	-0.277745	-0.531091
19	C	-3.773329	0.079952	-0.366768
20	C	-1.611785	-0.070158	0.703911
21	C	-1.785255	-0.303687	-1.684786
22	C	-3.161437	-0.126911	-1.610579
23	C	-2.991588	0.108071	0.796250
24	H	-1.005784	-0.048472	1.604308
25	H	-1.319181	-0.462525	-2.654540
26	H	-3.783367	-0.144137	-2.499778
27	H	-3.444533	0.266965	1.768114
28	O	-5.127944	0.243045	-0.393227
29	C	-5.803614	0.459266	0.836146
30	H	-6.859331	0.569601	0.581320
31	H	-5.453245	1.372945	1.334254
32	H	-5.682074	-0.392376	1.518581

Energy is -805.675013044 Hartrees

Computational data for 7a

		Standard Nuclear Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	H	4.11440	-1.68210	0.34820
2	C	3.64800	-0.72200	0.14160
3	C	2.45070	1.75100	-0.36230
4	C	2.25380	-0.61560	0.17650
5	C	4.43770	0.38970	-0.13940
6	C	3.83580	1.62800	-0.38380
7	C	1.67500	0.62430	-0.09070
8	C	1.38360	-1.79610	0.51390
9	O	0.30650	0.77580	-0.06790
10	H	1.95440	2.69630	-0.55430
11	H	1.39000	-2.56070	-0.27330
12	H	1.68680	-2.27000	1.44830
13	C	-0.43600	-0.39910	-0.26120
14	H	-0.21810	-0.84100	-1.24270
15	C	-1.88850	-0.06570	-0.10010
16	C	-4.58380	0.59840	0.16920
17	C	-2.31340	0.70180	0.98920
18	C	-2.81180	-0.49070	-1.05620
19	C	-4.15940	-0.15940	-0.92140
20	C	-3.65930	1.02900	1.12360
21	H	-1.58850	1.03690	1.72330
22	H	-2.48020	-1.09070	-1.89880
23	H	-4.87540	-0.49450	-1.66570
24	H	-3.98930	1.62030	1.97250
25	H	-5.63370	0.85560	0.27610
26	H	4.44820	2.49890	-0.59650
27	H	5.51850	0.29480	-0.16010
28	O	0.00130	-1.39180	0.73790
29	B	-0.96300	-2.78790	0.89320
30	H	-1.98760	-2.39760	1.37130
31	H	-1.03370	-3.19590	-0.24540
32	H	-0.27420	-3.45500	1.62220

Energy is –717.805985 Hartrees

Computational data for 7b

		Standard Nuclear Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	H	4.03010	-1.87880	0.11920
2	C	3.64040	-0.86870	0.01620
3	C	2.62300	1.71480	-0.24590
4	C	2.26150	-0.66330	0.12060
5	C	4.50960	0.19440	-0.20540
6	C	3.99330	1.48450	-0.33380
7	C	1.76510	0.63880	-0.01360
8	C	1.32880	-1.82200	0.36080
9	H	2.21420	2.70830	-0.35410
10	H	1.35120	-2.52500	-0.48700
11	H	1.61190	-2.37800	1.25950
12	C	-0.40780	-0.37260	-0.27260
13	H	-0.12850	-0.58130	-1.31450
14	C	-1.88210	-0.15620	-0.12280
15	C	-4.63980	0.16990	0.13790
16	C	-2.46850	-0.15650	1.14740

17	C	-2.67920	-0.00780	-1.25840
18	C	-4.05770	0.15710	-1.12880
19	C	-3.84370	0.01070	1.27490
20	H	-1.84320	-0.28310	2.02430
21	H	-2.22220	-0.00870	-2.24430
22	H	-4.67380	0.27770	-2.01460
23	H	-4.29750	0.01930	2.26140
24	H	-5.71300	0.30260	0.24120
25	H	4.65840	2.32410	-0.51100
26	H	5.57820	0.01930	-0.27740
27	O	-0.01000	-1.38300	0.58570
28	O	0.37730	0.85740	0.08060
28	B	-0.25210	2.47750	-0.15310
29	H	-1.40950	2.34980	0.09880
30	H	0.37670	3.08790	0.66830
31	H	0.01890	2.70580	-1.30510

Energy is –717.795623 Hartrees

Computational data for 8a

		Standard Nuclear Orientation (Ångstroms)		
I	Atom	X	Z	Y
1	H	1.08410	2.91070	-1.88040
2	C	0.04220	2.60340	-1.85460
3	C	-2.63070	1.80180	-1.82770
4	C	-0.26540	1.23640	-1.90550
5	C	-0.96320	3.56190	-1.78930
6	C	-2.29890	3.15450	-1.78080
7	C	-1.61760	0.84550	-1.88490
8	H	-0.71170	4.61600	-1.75520
9	H	-3.09220	3.89390	-1.73680
10	H	-3.67220	1.49040	-1.81760
11	O	-1.87970	-0.50280	-1.90410
12	H	-2.82430	-0.65330	-2.04880
13	C	0.81140	0.21580	-2.02270
14	H	1.73130	0.61770	-2.44130
15	H	0.50200	-0.68040	-2.56090
16	O	1.29160	-0.27030	-0.66220
17	C	0.52730	-1.01550	0.04270
18	C	0.91960	-1.48500	1.32070
19	C	1.59120	-2.46100	3.83260
20	C	0.00880	-2.30960	2.02670
21	C	2.17540	-1.15380	1.89110
22	C	2.50130	-1.64440	3.14180
23	C	0.34910	-2.79340	3.27970
24	H	-0.95090	-2.55800	1.58240
25	H	2.86400	-0.52180	1.34100
26	H	3.45790	-1.40070	3.59100
27	H	-0.34060	-3.42510	3.82860
28	H	1.85680	-2.84150	4.81440
29	H	-0.45040	-1.28010	-0.36980

Energy is –691.535612 Hartrees

Computational data for 8b

		Standard Nuclear Orientation (Ångstroms)		
I	Atom	X	Z	Y
1	H	-0.30960	3.91890	-0.17430
2	C	-0.90320	3.18870	-0.71470
3	C	-2.32470	1.29030	-2.19730
4	C	-0.75390	1.82390	-0.49910
5	C	-1.81020	3.60210	-1.68960
6	C	-2.52340	2.65410	-2.42370
7	C	-1.42760	0.83590	-1.22730
8	H	-1.94040	4.66110	-1.88470
9	H	-3.22350	2.97720	-3.18690
10	H	-2.87570	0.56100	-2.78400
11	O	0.14960	1.32320	0.46420
12	C	0.51470	1.92650	1.53900
13	C	1.47720	1.33500	2.38320
14	C	3.35500	0.21840	4.09270
15	C	1.84870	2.02070	3.56860
16	C	2.05950	0.07770	2.06170
17	C	2.99280	-0.46850	2.92200
18	C	2.78680	1.45770	4.41660
19	H	1.39770	2.98050	3.80420
20	H	1.75750	-0.43380	1.15200
21	H	3.44610	-1.42730	2.69530
22	H	3.08120	1.97080	5.32540
23	H	4.09040	-0.22030	4.76060
24	H	0.05880	2.88800	1.78010
25	C	-1.20580	-0.64540	-0.96590
26	H	-1.83970	-1.22260	-1.65080
27	H	-1.52230	-0.89680	0.05150
28	O	0.15830	-1.03840	-1.05020
29	H	0.42840	-1.00410	-1.97800

Energy is –691.517865 Hartrees

Computational data for 12a

		Standard Nuclear Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	C	0.27420	-0.32460	-0.16750
2	C	-0.33090	0.68780	-0.89070
3	C	-1.70350	0.87270	-0.70390
4	C	-2.43600	0.06690	0.18070
5	C	-1.81060	-0.95740	0.91810
6	C	-0.45500	-1.10870	0.70430
7	H	0.23740	1.30950	-1.57280
8	H	-2.23560	1.64400	-1.24900
9	H	-2.33660	-1.60820	1.60100
10	O	1.61250	-0.67160	-0.13170
11	C	1.69400	-1.92210	0.52790
12	H	1.62450	-2.74950	-0.18890
13	O	0.41950	-2.00800	1.32810
14	C	5.12030	-2.19750	3.08230
15	C	4.74790	-3.28650	2.29520
16	C	3.63480	-3.19280	1.46060
17	C	2.89400	-2.00970	1.41380
18	C	3.27160	-0.91600	2.20080
19	C	4.38210	-1.01240	3.03400

20	H	5.98650	-2.27010	3.73360
21	H	5.32050	-4.20810	2.33140
22	H	3.33430	-4.04140	0.85330
23	H	2.69930	0.00440	2.14960
24	H	4.67480	-0.16390	3.64510
25	B	-0.11760	-3.57640	1.71640
26	H	-0.39670	-4.03830	0.63680
27	H	0.84770	-4.04450	2.25420
28	H	-1.04570	-3.35390	2.44800
29	O	-3.76930	0.34570	0.25830
30	C	-4.57180	-0.44080	1.12730
31	H	-5.58680	-0.05350	1.02920
32	H	-4.55950	-1.49980	0.84080
33	H	-4.24910	-0.34670	2.17190

Energy is –793.006895 Hartrees

Computational data for 12b

		Standard Nuclear Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	C	0.45670	-0.29140	-0.02290
2	C	-0.08020	0.86710	-0.54670
3	C	-1.34390	1.25010	-0.06830
4	C	-2.04290	0.50850	0.89020
5	C	-1.46820	-0.67270	1.40660
6	C	-0.22960	-1.02970	0.92680
7	H	0.44980	1.44750	-1.29310
8	H	-1.79390	2.15770	-0.45970
9	H	-1.97980	-1.28470	2.14010
10	O	1.65880	-0.88660	-0.33480
11	C	1.86010	-1.94490	0.59130
12	H	2.04430	-2.87220	0.04680
13	O	0.54440	-2.14650	1.27120
14	C	4.87330	-1.12930	3.54930
15	C	4.21280	-2.35980	3.53140
16	C	3.24030	-2.61690	2.56910
17	C	2.91750	-1.63720	1.62150
18	C	3.58140	-0.40850	1.63690
19	C	4.55790	-0.15730	2.60150
20	H	5.63420	-0.93190	4.29880
21	H	4.45700	-3.12030	4.26700
22	H	2.72100	-3.57060	2.55580
23	H	3.34070	0.34030	0.89090
24	H	5.07240	0.79900	2.60940
25	B	-0.14260	-3.71840	1.13640
26	H	-0.32910	-3.82490	-0.04880
27	H	0.74270	-4.39720	1.58840
28	H	-1.12080	-3.62380	1.82570
29	C	-3.40600	0.94750	1.37340
30	H	-3.43140	1.04520	2.46440
31	H	-3.68720	1.91280	0.94460
32	H	-4.17900	0.22130	1.09660

Energy is –717.802922 Hartrees

Computational data for 13a

		Standard Nuclear Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	C	0.24570	-0.34120	-0.18190
2	C	-0.32610	0.68600	-0.89790
3	C	-1.70610	0.90530	-0.70050
4	C	-2.44620	0.11100	0.18370
5	C	-1.83190	-0.92940	0.90480
6	C	-0.48810	-1.12520	0.69660
7	H	0.23760	1.30400	-1.58530
8	H	-3.50590	0.28090	0.32210
9	H	-2.39250	-1.55530	1.58720
10	O	1.56810	-0.71770	-0.17510
11	C	1.65380	-1.95940	0.51560
12	H	1.60860	-2.79470	-0.19280
13	O	0.38460	-2.04350	1.30390
14	C	5.05960	-2.15180	3.10720
15	C	4.71610	-3.25250	2.32340
16	C	3.61060	-3.18510	1.47610
17	C	2.84830	-2.01650	1.41330
18	C	3.19650	-0.91130	2.19760
19	C	4.29960	-0.98120	3.04320
20	H	5.92010	-2.20360	3.76800
21	H	5.30540	-4.16300	2.37190
22	H	3.33270	-4.04320	0.87120
23	H	2.60790	-0.00180	2.13610
24	H	4.56930	-0.12360	3.65200
25	B	-0.16530	-3.62130	1.65050
26	H	-0.44250	-4.05140	0.55760
27	H	0.79830	-4.10750	2.17660
28	H	-1.09330	-3.40920	2.38410
29	O	-2.22670	1.92850	-1.43710
30	C	-3.61170	2.21370	-1.30960
31	H	-3.80730	3.05370	-1.97760
32	H	-4.22940	1.35880	-1.61280
33	H	-3.87230	2.49970	-0.28260

Energy is –793.007560 Hartrees

Computational data for 13b

		Standard Nuclear Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	C	0.43330	-0.36030	-0.10050
2	C	-0.10230	0.79300	-0.63660
3	C	-1.33710	1.24040	-0.12240
4	C	-1.96750	0.51530	0.89500
5	C	-1.41500	-0.65940	1.43290
6	C	-0.21000	-1.06140	0.90610
7	H	0.41090	1.32930	-1.42780
8	H	-2.91750	0.86870	1.28360
9	H	-1.91090	-1.22760	2.20960
10	O	1.60450	-0.98780	-0.46030
11	C	1.84490	-2.00970	0.49850
12	H	2.00940	-2.95540	-0.02010
13	O	0.56230	-2.18480	1.23770
14	C	4.98940	-1.07920	3.28270
15	C	4.23220	-2.24330	3.43310

16	C	3.21420	-2.53710	2.53030
17	C	2.94340	-1.65950	1.47250
18	C	3.70310	-0.49770	1.31980
19	C	4.72470	-0.21000	2.22600
20	H	5.78460	-0.85340	3.98720
21	H	4.43560	-2.92320	4.25510
22	H	2.62070	-3.43880	2.64760
23	H	3.49780	0.17140	0.49190
24	H	5.31280	0.69470	2.10390
25	B	-0.15310	-3.74750	1.15520
26	H	-0.38570	-3.87220	-0.02020
27	H	0.73990	-4.43070	1.58630
28	H	-1.10330	-3.62330	1.87850
29	C	-1.96410	2.49640	-0.68240
30	H	-2.88730	2.74980	-0.15540
31	H	-1.28480	3.35230	-0.59990
32	H	-2.20690	2.37900	-1.74480

Energy is –717.803074 Hartrees

Computational data for 14a

		Standard Nuclear Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	C	0.51880	-0.37430	-0.12620
2	C	0.01680	0.84060	-0.56090
3	C	-1.21150	1.24630	-0.03620
4	C	-1.90750	0.46180	0.89790
5	C	-1.38580	-0.76930	1.34150
6	C	-0.17610	-1.13800	0.78770
7	H	0.55220	1.44480	-1.28400
8	H	-1.65730	2.18620	-0.34090
9	H	-1.88690	-1.39610	2.06580
10	O	1.68800	-1.00760	-0.51780
11	C	1.94570	-2.01430	0.42640
12	H	2.24410	-2.93270	-0.07650
13	O	0.55470	-2.32710	1.01660
14	C	4.58470	-0.89570	3.62650
15	C	4.18600	-2.22460	3.47220
16	C	3.33380	-2.58180	2.43080
17	C	2.86800	-1.60460	1.54070
18	C	3.27770	-0.27560	1.68970
19	C	4.13330	0.07530	2.73290
20	H	5.25200	-0.61940	4.43750
21	H	4.54210	-2.98510	4.16020
22	H	3.03110	-3.61720	2.30780
23	H	2.94150	0.47640	0.98550
24	H	4.44990	1.10780	2.84440
25	Al	-0.29740	-4.08680	1.15680
26	Cl	-1.72810	-4.10230	-0.41230
27	Cl	1.36260	-5.39650	0.86420
28	Cl	-1.11360	-4.04820	3.12270
29	O	-3.08760	0.97840	1.33340
30	C	-3.88290	0.19710	2.21820
31	H	-4.78640	0.78000	2.39920
32	H	-4.15450	-0.76560	1.76870
33	H	-3.36970	0.02090	3.17170

Energy is –2389.642189 Hartrees

Computational data for 14b

		Standard Nuclear Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	C	0.54040	-0.37280	-0.08640
2	C	0.06670	0.83910	-0.54460
3	C	-1.14730	1.28690	-0.00070
4	C	-1.85580	0.56130	0.96320
5	C	-1.34700	-0.67600	1.41410
6	C	-0.16230	-1.10070	0.85870
7	H	0.60790	1.41160	-1.28900
8	H	-1.54760	2.23770	-0.33940
9	H	-1.86740	-1.26740	2.15880
10	O	1.69040	-1.03670	-0.46770
11	C	1.93260	-2.03170	0.49770
12	H	2.21520	-2.96260	0.00900
13	O	0.54620	-2.30520	1.09840
14	C	4.60630	-0.88860	3.66060
15	C	4.16080	-2.20760	3.55450
16	C	3.29810	-2.57300	2.52480
17	C	2.86940	-1.61360	1.59750
18	C	3.32560	-0.29540	1.69810
19	C	4.19130	0.06370	2.73040
20	H	5.28130	-0.60620	4.46310
21	H	4.48820	-2.95360	4.27190
22	H	2.95760	-3.60060	2.43980
23	H	3.01700	0.44140	0.96570
24	H	4.54360	1.08800	2.80470
25	Al	-0.35770	-4.05070	1.12940
26	Cl	-1.64060	-3.99410	-0.56130
27	Cl	1.29690	-5.38870	0.94580
28	Cl	-1.32730	-4.04270	3.02260
29	C	-3.16070	1.07670	1.52390
30	H	-3.14070	1.10620	2.61850
31	H	-3.37610	2.08570	1.16380
32	H	-3.99720	0.43130	1.23280

Energy is –2314.439164 Hartrees

Computational data for 15a

		Standard Nuclear Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	C	0.44040	-0.50020	-0.19230
2	C	-0.05860	0.66150	-0.73490
3	C	-1.26490	1.14930	-0.18820
4	C	-1.90510	0.48270	0.86530
5	C	-1.37090	-0.70180	1.40070
6	C	-0.20440	-1.16420	0.84000
7	H	0.43100	1.18700	-1.54510
8	H	-2.82440	0.86910	1.28490
9	H	-1.86500	-1.22700	2.20880
10	O	1.58050	-1.17540	-0.57250
11	C	1.87610	-2.10190	0.44950
12	H	2.15020	-3.05940	0.00950
13	O	0.53010	-2.34630	1.12930
14	C	4.70820	-0.71960	3.37340
15	C	4.21690	-2.02590	3.42700
16	C	3.30050	-2.46830	2.47690

17	C	2.86270	-1.59860	1.46880
18	C	3.36280	-0.29430	1.40960
19	C	4.28300	0.14180	2.36280
20	H	5.42580	-0.37800	4.11330
21	H	4.55070	-2.70310	4.20700
22	H	2.92670	-3.48700	2.51550
23	H	3.04480	0.37070	0.61490
24	H	4.66930	1.15520	2.31160
25	Al	-0.36600	-4.08990	1.25650
26	Cl	-1.63620	-4.14280	-0.44430
27	Cl	1.29750	-5.42600	1.16780
28	Cl	-1.34800	-3.97350	3.14040
29	O	-1.71930	2.29600	-0.76040
30	C	-2.94450	2.84880	-0.29600
31	H	-3.11820	3.73810	-0.90280
32	H	-3.77740	2.14830	-0.43160
33	H	-2.88090	3.13780	0.76020

Energy is –2389.643084 Hartrees

Computational data for 15b

		Standard Nuclear Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	C	0.49370	-0.44760	-0.15460
2	C	0.01890	0.74830	-0.65120
3	C	-1.15590	1.27320	-0.07440
4	C	-1.78420	0.58230	0.96790
5	C	-1.29550	-0.63650	1.46740
6	C	-0.15500	-1.11900	0.86800
7	H	0.53400	1.25940	-1.45760
8	H	-2.68250	0.99940	1.41160
9	H	-1.79090	-1.16720	2.27100
10	O	1.60630	-1.14930	-0.57410
11	C	1.89300	-2.10210	0.42350
12	H	2.13740	-3.05800	-0.03730
13	O	0.54830	-2.32600	1.11720
14	C	4.77670	-0.83330	3.34590
15	C	4.24240	-2.12240	3.39580
16	C	3.31030	-2.53010	2.44560
17	C	2.90050	-1.64160	1.44220
18	C	3.44500	-0.35520	1.38610
19	C	4.38050	0.04610	2.33930
20	H	5.50530	-0.51830	4.08710
21	H	4.55370	-2.81250	4.17380
22	H	2.90220	-3.53560	2.48160
23	H	3.14800	0.32280	0.59450
24	H	4.80070	1.04610	2.29230
25	Al	-0.38700	-4.05180	1.23970
26	Cl	-1.68870	-4.04230	-0.43720
27	Cl	1.24490	-5.42160	1.09730
28	Cl	-1.32530	-3.94350	3.14520
29	C	-1.71940	2.57630	-0.59140
30	H	-2.58750	2.89390	-0.00910
31	H	-0.97350	3.37760	-0.54900
32	H	-2.03350	2.48200	-1.63710

Energy is –2314.439264 Hartrees

Computational data for 16a

		Standard Nuclear Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	H	3.76850	1.17260	1.27030
2	C	2.92670	1.39770	0.62600
3	C	0.78750	2.02390	-1.06550
4	C	1.81890	0.54350	0.61420
5	C	2.96880	2.53550	-0.18430
6	C	1.89220	2.85770	-1.04000
7	C	0.74900	0.88900	-0.25820
8	O	4.09570	3.27760	-0.08200
9	O	-0.41970	0.13920	-0.37920
10	H	-0.05940	2.23740	-1.70920
11	O	1.70790	-0.54340	1.34570
12	C	-0.72780	-0.96340	0.21980
13	C	-1.98740	-1.57690	-0.03700
14	H	-0.00960	-1.39470	0.90960
15	C	-4.40520	-2.89960	-0.42870
16	C	-2.94590	-1.04180	-0.92860
17	C	-2.25570	-2.78030	0.65480
18	C	-3.46420	-3.43460	0.45410
19	C	-4.14580	-1.70560	-1.11810
20	H	-2.73170	-0.11770	-1.45450
21	H	-1.51010	-3.17810	1.33820
22	H	-3.67450	-4.35810	0.98310
23	H	-4.88770	-1.30300	-1.80010
24	H	-5.34950	-3.41280	-0.58410
25	H	1.91580	3.73640	-1.67030
26	C	4.22450	4.45430	-0.87300
27	H	5.19890	4.87370	-0.62190
28	H	3.44310	5.18570	-0.63490
29	H	4.19500	4.22300	-1.94450
30	Al	2.55640	-1.47590	2.64000
31	Cl	1.14280	-3.11400	2.86250
32	Cl	4.46500	-2.10420	1.89200
33	Cl	2.68520	-0.23940	4.38760

Energy is –2389.648326 Hartrees

Computational data for 16b

		Standard Nuclear Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	H	2.28580	2.70780	-2.40430
2	C	2.29650	1.67860	-2.06040
3	C	2.31180	-0.95750	-1.12950
4	C	1.25020	1.26520	-1.21320
5	C	3.32040	0.81560	-2.43970
6	C	3.32000	-0.51430	-1.96480
7	C	1.29560	-0.07520	-0.75870
8	C	4.41540	1.28160	-3.36720
9	O	0.33160	-0.63370	0.08550
10	H	2.28990	-1.97340	-0.74890
11	O	0.26110	2.04030	-0.82420
12	C	-0.68150	-0.04620	0.62890
13	C	-1.56660	-0.79160	1.45780
14	H	-0.83110	1.01130	0.43480
15	C	-3.38550	-2.10530	3.10230

16	C	-2.65200	-0.08130	2.01970
17	C	-1.40200	-2.17020	1.72730
18	C	-2.31120	-2.81650	2.54650
19	C	-3.55560	-0.74380	2.84030
20	H	-2.76710	0.97660	1.79840
21	H	-0.56700	-2.70620	1.28930
22	H	-2.19490	-3.87420	2.75950
23	H	-4.39040	-0.20380	3.27410
24	H	-4.09360	-2.62160	3.74360
25	H	4.11690	-1.19160	-2.25490
26	H	5.39080	0.89650	-3.05340
27	H	4.47170	2.37150	-3.40720
28	H	4.23730	0.91990	-4.38730
29	Al	-0.49590	3.65220	-1.13280
30	Cl	-2.09310	3.56900	0.34000
31	Cl	0.95630	5.18040	-0.73880
32	Cl	-1.23920	3.67200	-3.14440

Energy is –2314.443969 Hartrees

Computational data for 17a

		Standard Nuclear Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	H	3.95420	0.88010	1.39440
2	C	3.12730	1.18450	0.76230
3	C	1.00250	1.96800	-0.87850
4	C	1.98260	0.36830	0.73270
5	C	3.21510	2.34540	0.00510
6	C	2.15180	2.74990	-0.82470
7	C	0.93480	0.80640	-0.11300
8	O	-0.27370	0.11290	-0.25140
9	H	0.17040	2.25850	-1.50890
10	O	1.83670	-0.74620	1.42250
11	C	-0.61030	-1.00250	0.30840
12	C	-1.89500	-1.55790	0.05590
13	H	0.10650	-1.48660	0.96380
14	C	-4.36600	-2.77350	-0.33350
15	C	-2.85060	-0.95090	-0.79250
16	C	-2.19230	-2.77790	0.70600
17	C	-3.42810	-3.37890	0.50650
18	C	-4.07770	-1.56240	-0.98100
19	H	-2.61200	-0.01460	-1.28500
20	H	-1.44760	-3.22900	1.35670
21	H	-3.66250	-4.31450	1.00280
22	H	-4.81850	-1.10610	-1.62940
23	H	-5.33190	-3.24510	-0.48800
24	O	2.15080	3.87110	-1.60140
25	H	4.12130	2.93600	0.06420
26	C	3.30410	4.70230	-1.58590
27	H	3.08770	5.52460	-2.26890
28	H	4.19410	4.16610	-1.93810
29	H	3.49810	5.10700	-0.58470
30	Al	2.67400	-1.75550	2.66290
31	Cl	1.21660	-3.35930	2.84090
32	Cl	4.55510	-2.40110	1.85760
33	Cl	2.87360	-0.59540	4.45670

Energy is –2389.644316 Hartrees

Computational data for 17b

		Standard Nuclear Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	H	4.23840	1.23580	1.09060
2	C	3.35960	1.51450	0.51920
3	C	1.09980	2.23630	-0.95980
4	C	2.24290	0.65420	0.55840
5	C	3.33540	2.67870	-0.22970
6	C	2.20920	3.06870	-0.98660
7	C	1.12400	1.05980	-0.20600
8	H	4.21690	3.31460	-0.23340
9	C	2.22720	4.33960	-1.80080
10	O	-0.06560	0.32450	-0.26890
11	H	0.19920	2.47640	-1.51650
12	O	2.18860	-0.46750	1.24360
13	C	-0.32890	-0.80410	0.30060
14	C	-1.60780	-1.40250	0.12360
15	H	0.44270	-1.26800	0.90630
16	C	-4.05520	-2.70070	-0.12270
17	C	-2.63320	-0.82560	-0.66140
18	C	-1.82330	-2.63440	0.78280
19	C	-3.04800	-3.27660	0.65520
20	C	-3.84800	-1.47800	-0.77920
21	H	-2.45690	0.12020	-1.16200
22	H	-1.02550	-3.06260	1.38430
23	H	-3.21960	-4.22160	1.15920
24	H	-4.64180	-1.04490	-1.37900
25	H	-5.01210	-3.20450	-0.22130
26	H	2.92620	4.26290	-2.64200
27	H	2.54510	5.19510	-1.19520
28	H	1.23940	4.56730	-2.21000
29	Al	3.14070	-1.47030	2.40770
30	Cl	1.73890	-3.11060	2.67210
31	Cl	4.96740	-2.06270	1.45350
32	Cl	3.43980	-0.32450	4.19550

Energy is –2314.442638 Hartrees

Computational data for S7a

		Standard Nuclear Orientation (Ångstroms)		
I	Atom	X	Z	Y
1	H	4.19660	-1.56000	-0.30670
2	C	3.73780	-0.57510	-0.27420
3	C	2.56080	1.95660	-0.14770
4	C	2.34590	-0.46940	-0.18440
5	C	4.53420	0.56630	-0.30410
6	C	3.94360	1.83140	-0.23280
7	C	1.77860	0.80360	-0.13610
8	C	1.47420	-1.69450	-0.11340
9	O	0.40790	0.95980	-0.04960
10	H	2.07380	2.92430	-0.09490
11	H	1.38490	-2.21220	-1.07630
12	H	1.84140	-2.40040	0.63040
13	C	-0.33930	-0.12580	-0.47910
14	H	-0.08050	-0.40510	-1.50760
15	C	-1.79690	0.16760	-0.33390
16	C	-4.51110	0.77930	-0.16850

17	C	-2.25390	1.05620	0.64650
18	C	-2.69970	-0.40390	-1.23710
19	C	-4.05710	-0.10290	-1.14840
20	C	-3.60910	1.36020	0.72500
21	H	-1.54780	1.50570	1.33510
22	H	-2.34450	-1.08740	-2.00240
23	H	-4.75570	-0.55270	-1.84650
24	H	-3.96340	2.04780	1.48660
25	H	-5.56850	1.01750	-0.10210
26	H	4.56260	2.72300	-0.24590
27	H	5.61300	0.47080	-0.37050
28	O	0.11770	-1.32730	0.32460
29	Al	-0.94960	-2.78790	1.10300
30	Cl	-2.46030	-1.98280	2.35190
31	Cl	-1.56910	-3.82400	-0.66450
32	Cl	0.51970	-3.86680	2.23060

Energy is –2314.440589 Hartrees

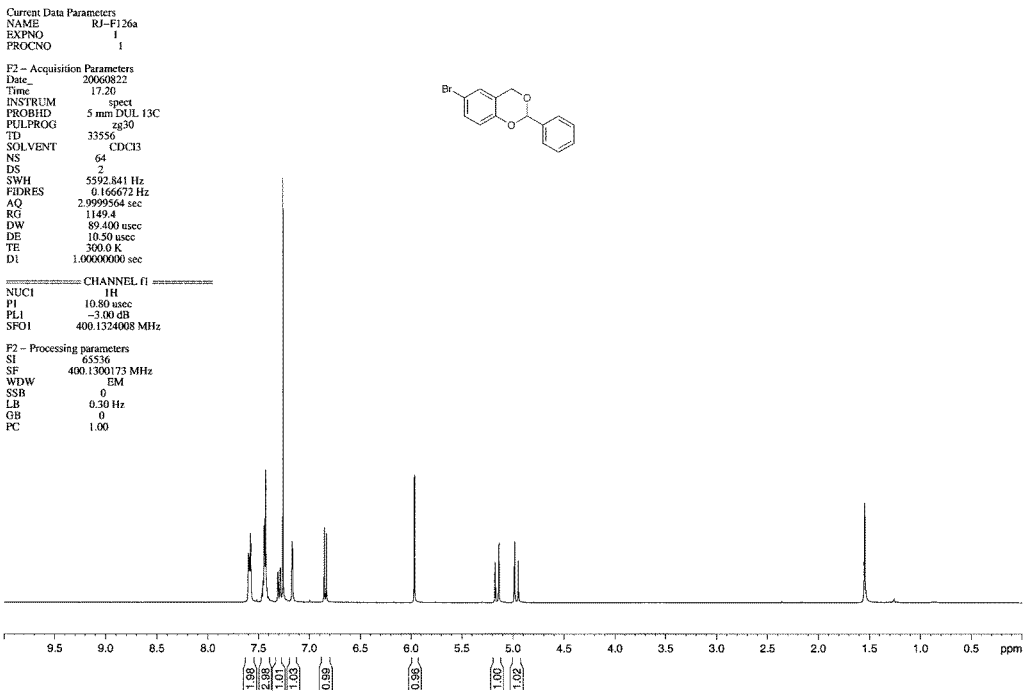
Computational data for S7b

		Standard Nuclear Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	H	4.00400	-1.79020	0.33550
2	C	3.56250	-0.93730	-0.17360
3	C	2.42340	1.23740	-1.52190
4	C	2.22240	-0.61520	0.06230
5	C	4.33180	-0.17120	-1.04600
6	C	3.76360	0.91280	-1.71900
7	C	1.69030	0.47770	-0.61980
8	C	1.36860	-1.42430	1.01260
9	H	1.95110	2.06440	-2.04060
10	H	1.52050	-2.49850	0.84380
11	H	1.62790	-1.20390	2.05250
12	C	-0.41740	-0.58800	-0.28660
13	H	0.00640	-1.11720	-1.14900
14	C	-1.89640	-0.41580	-0.42600
15	C	-4.64840	-0.18730	-0.80390
16	C	-2.77430	-0.90480	0.54420
17	C	-2.39640	0.17540	-1.59280
18	C	-3.77110	0.29750	-1.77510
19	C	-4.14910	-0.79090	0.35010
20	H	-2.37780	-1.36010	1.44370
21	H	-1.71310	0.55510	-2.34700
22	H	-4.15550	0.77090	-2.67300
23	H	-4.83100	-1.16620	1.10680
24	H	-5.72080	-0.09320	-0.94730
25	H	4.36000	1.50200	-2.40790
26	H	5.37390	-0.42600	-1.21000
27	O	-0.04190	-1.13160	0.90680
28	O	0.31460	0.76350	-0.41860
29	Al	-0.13780	2.50960	0.42500
30	Cl	-1.80110	2.24860	1.71610
31	Cl	1.64210	2.98920	1.50040
32	Cl	-0.48530	3.70020	-1.31720

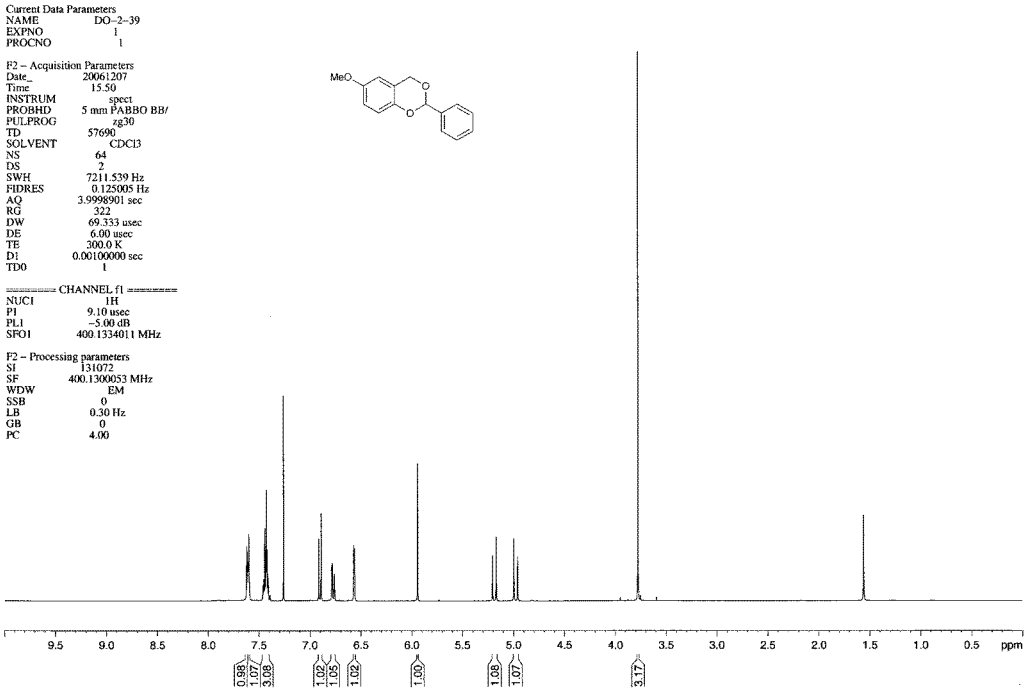
Energy is –2314.432388 Hartrees

12) ^{1}H-NMR spectra

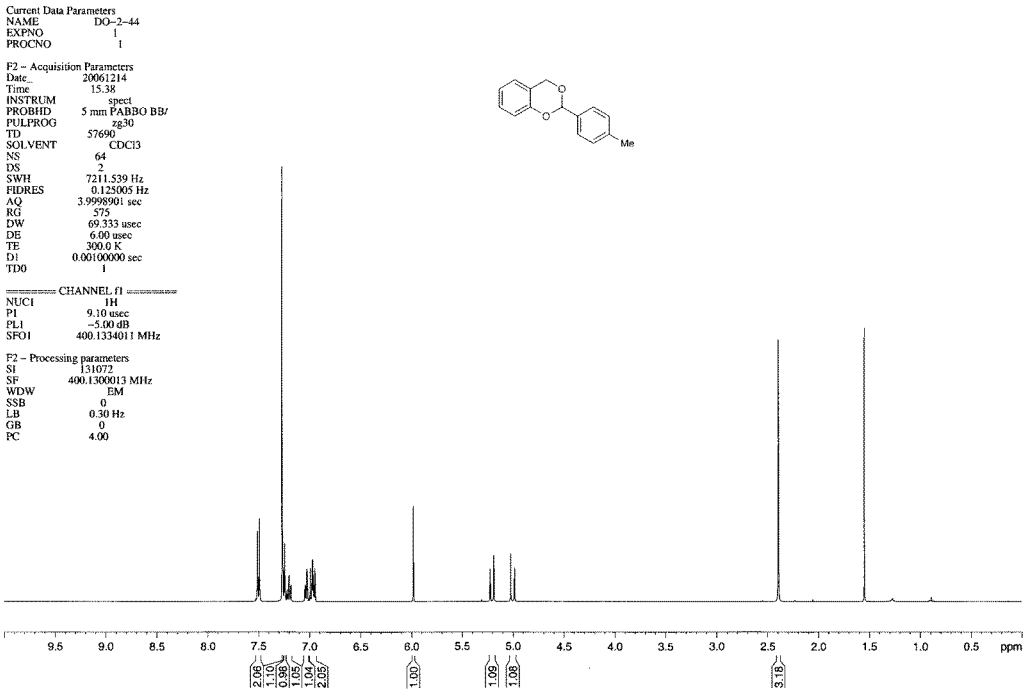
12.a) Compound 4c



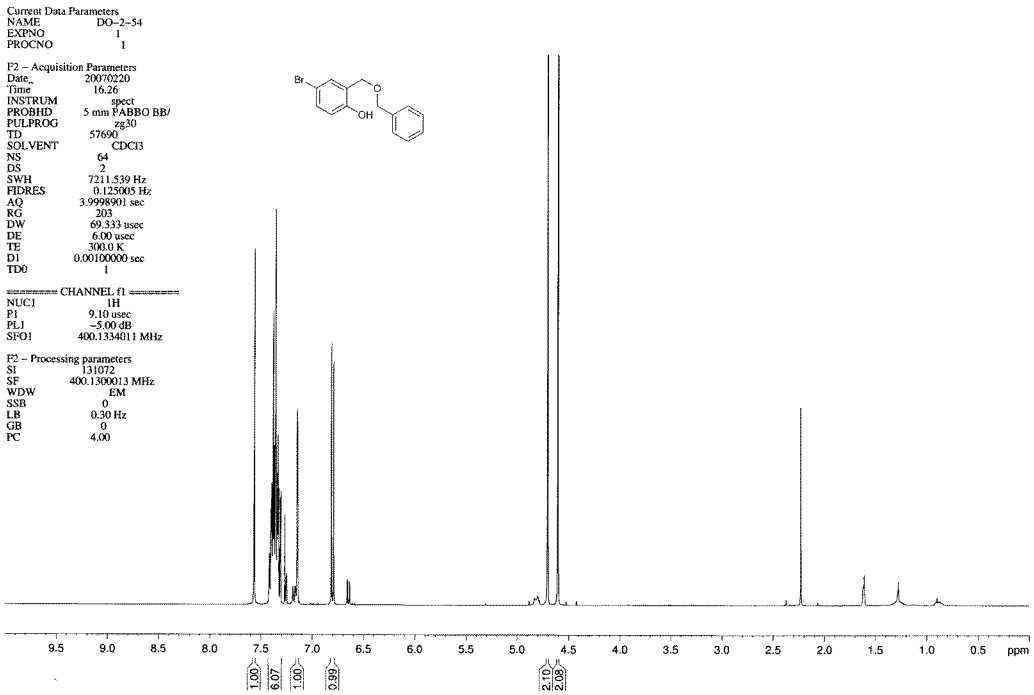
12.b) Compound 4e



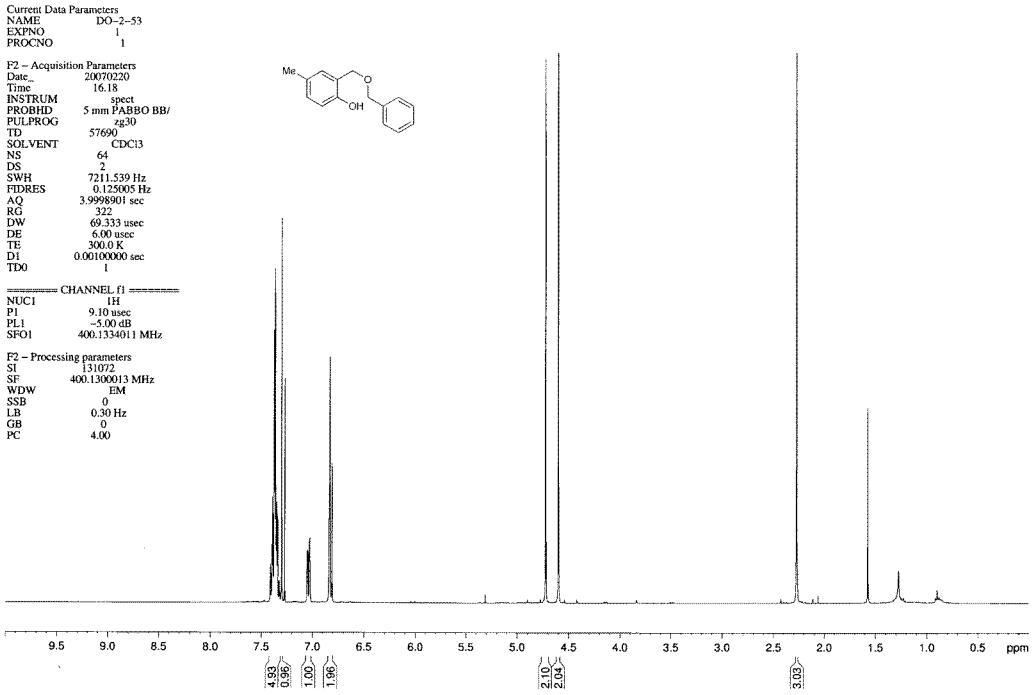
12.c) Compound 4h



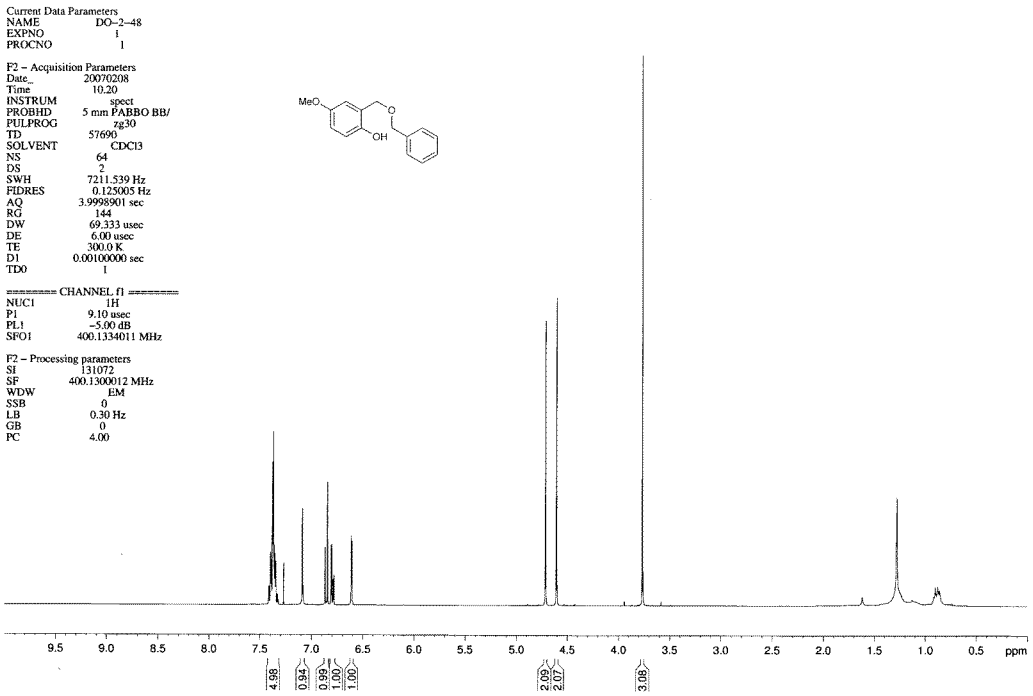
12.d) Compound 5c



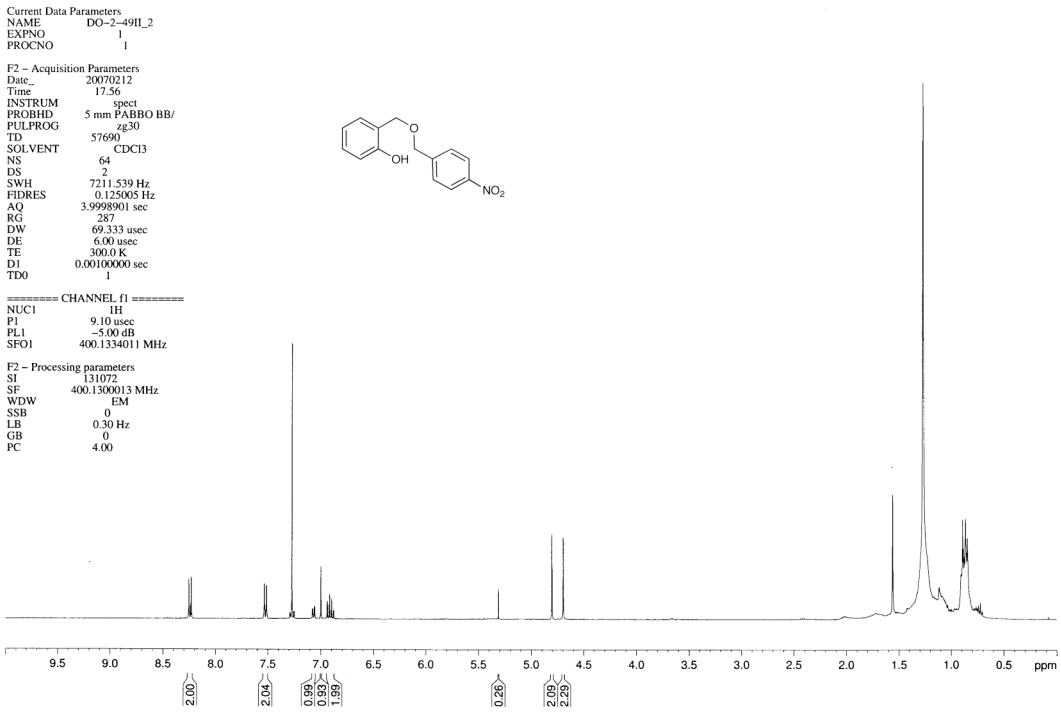
12.e) Compound 5d



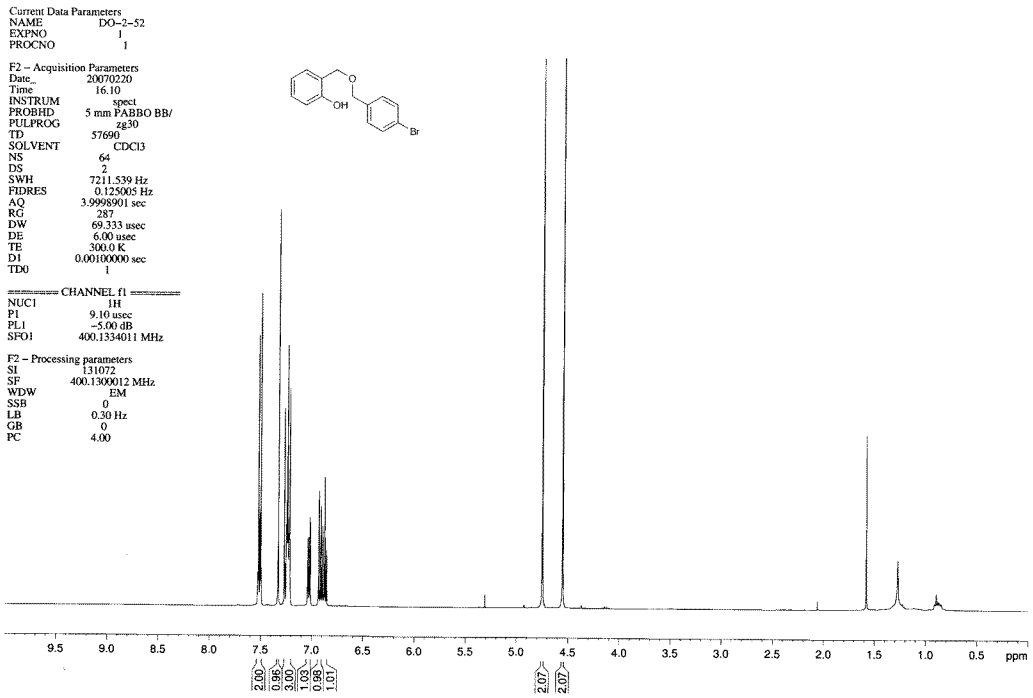
12.f) Compound 5e



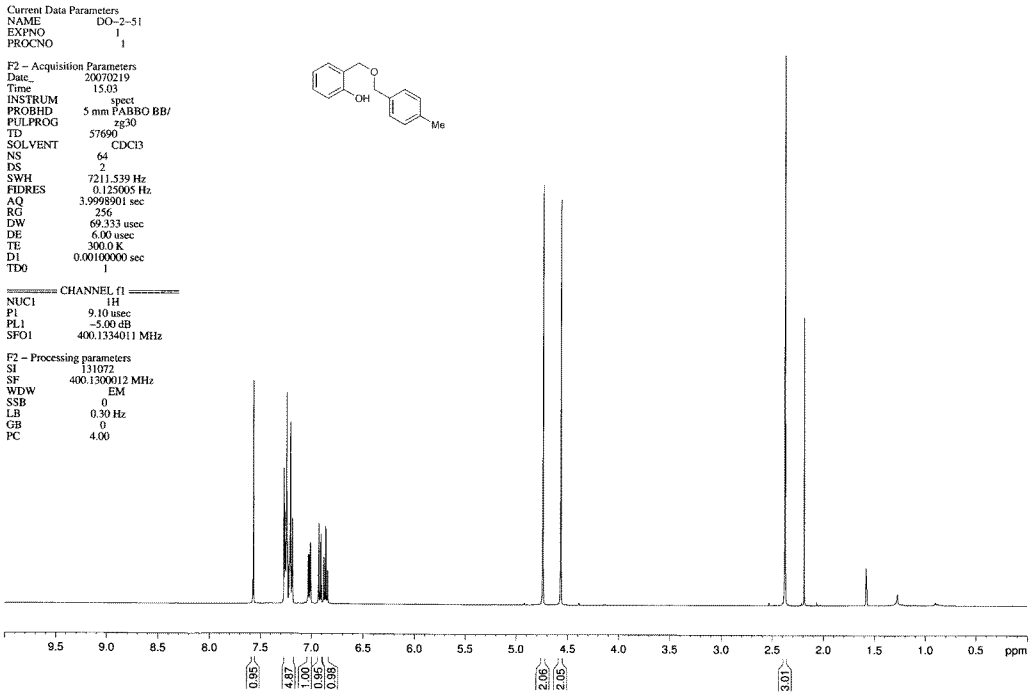
12.g) Compound 5f



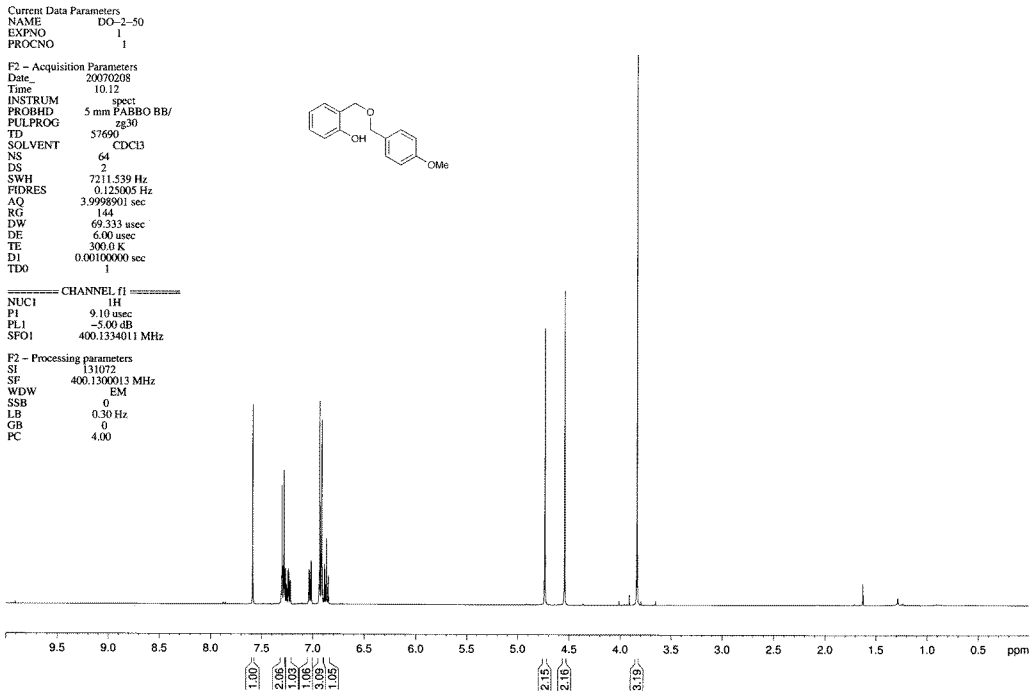
12.h) Compound 5g



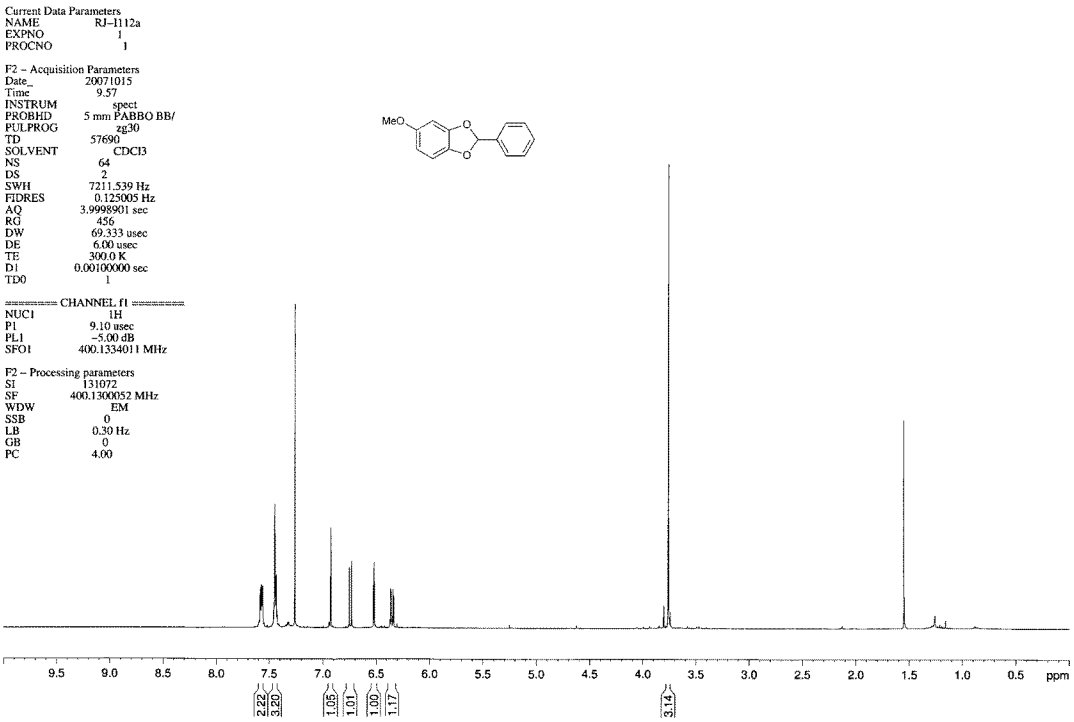
12.i) Compound 5h



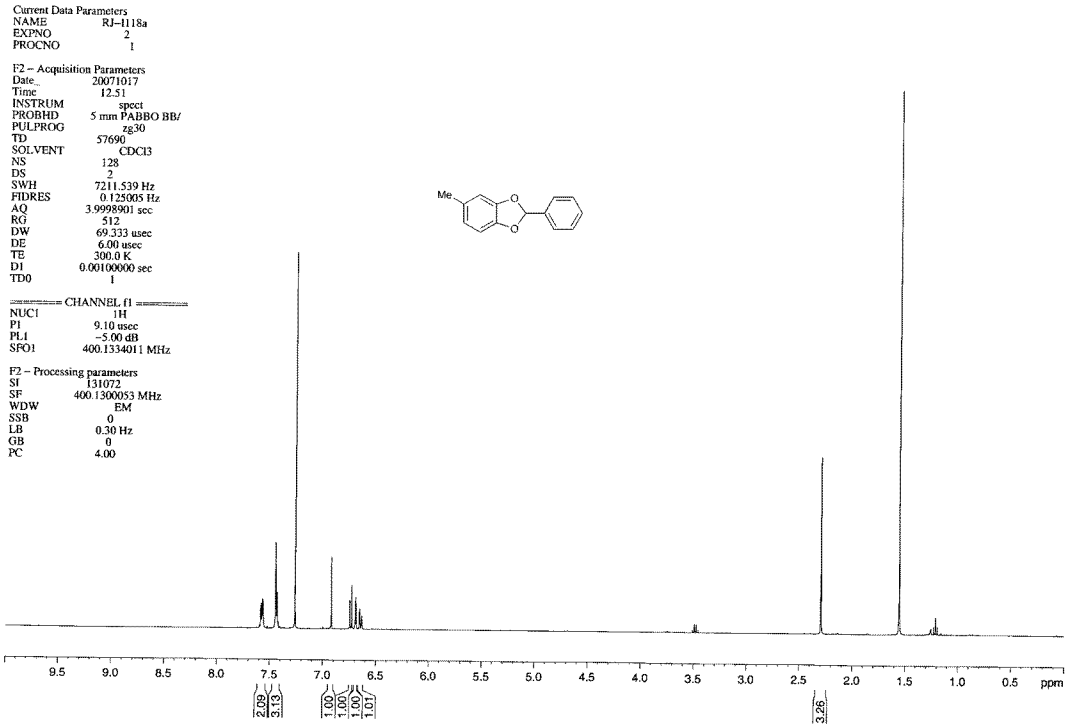
12.j) Compound 5i



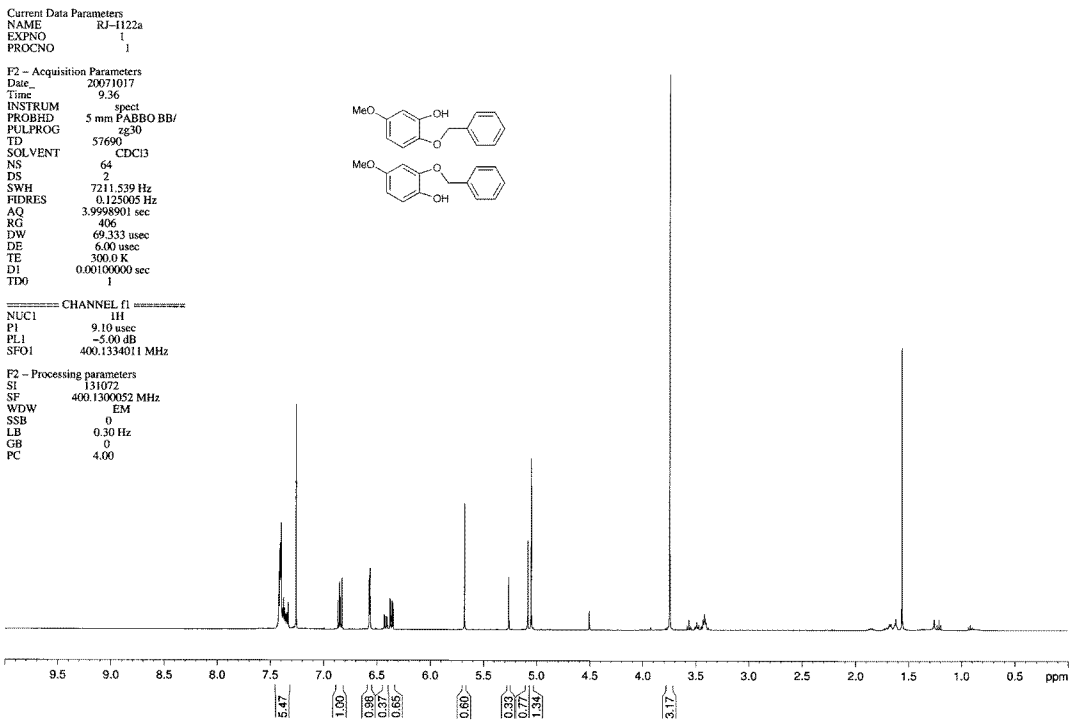
12.k) Compound 9a



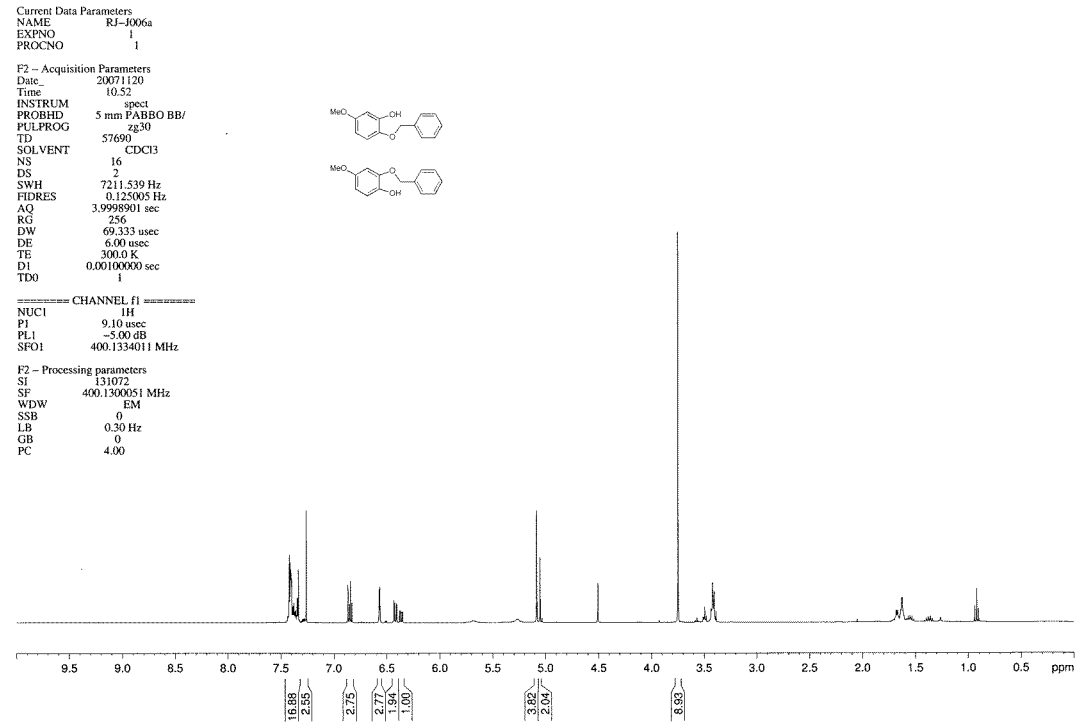
12.l) Compound 9b



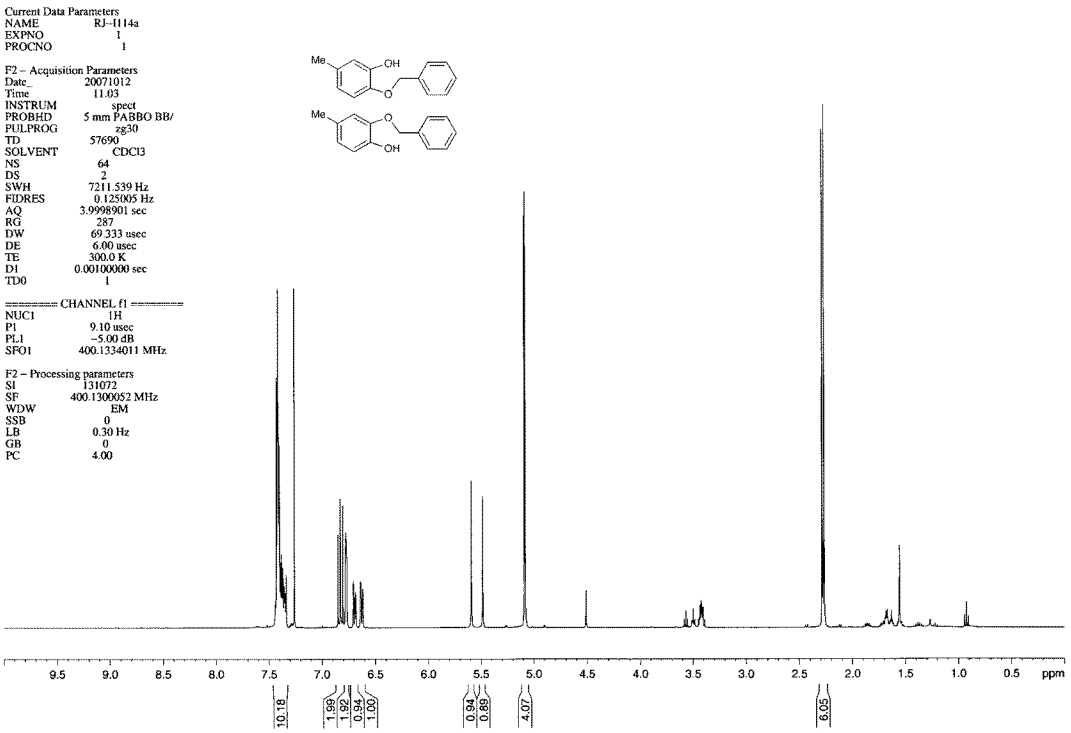
12.m) Compound 10a/11a (from $BH_3 \bullet NMe_3$)



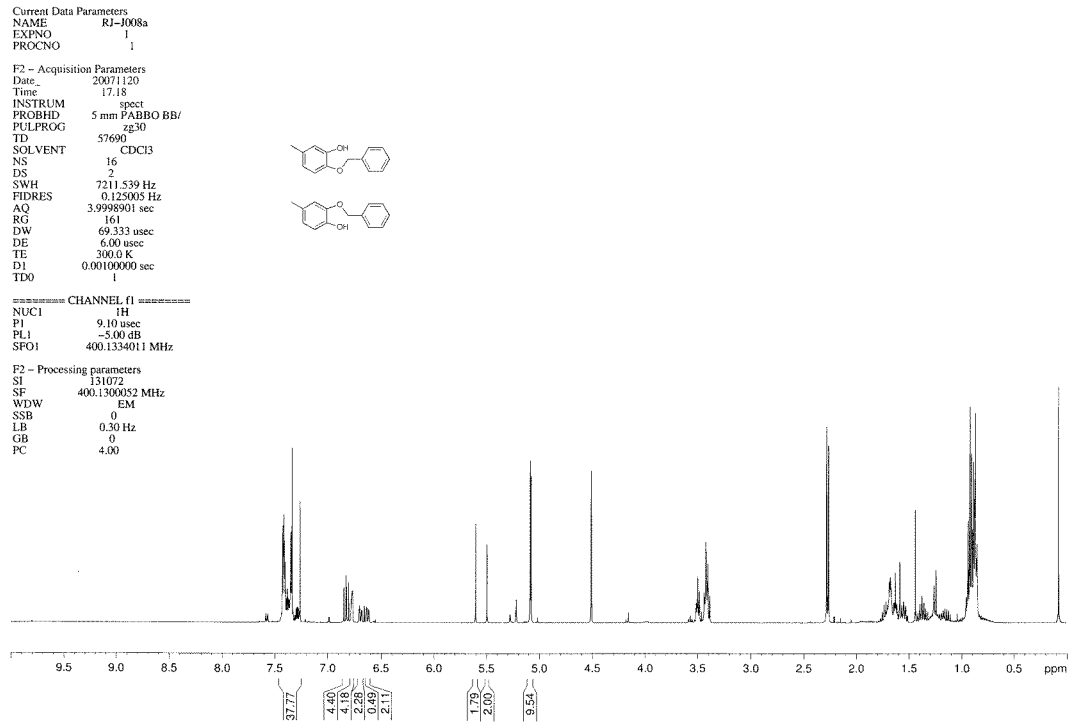
12.n) Compound 10a/11a (from $BH_3 \bullet THF$)



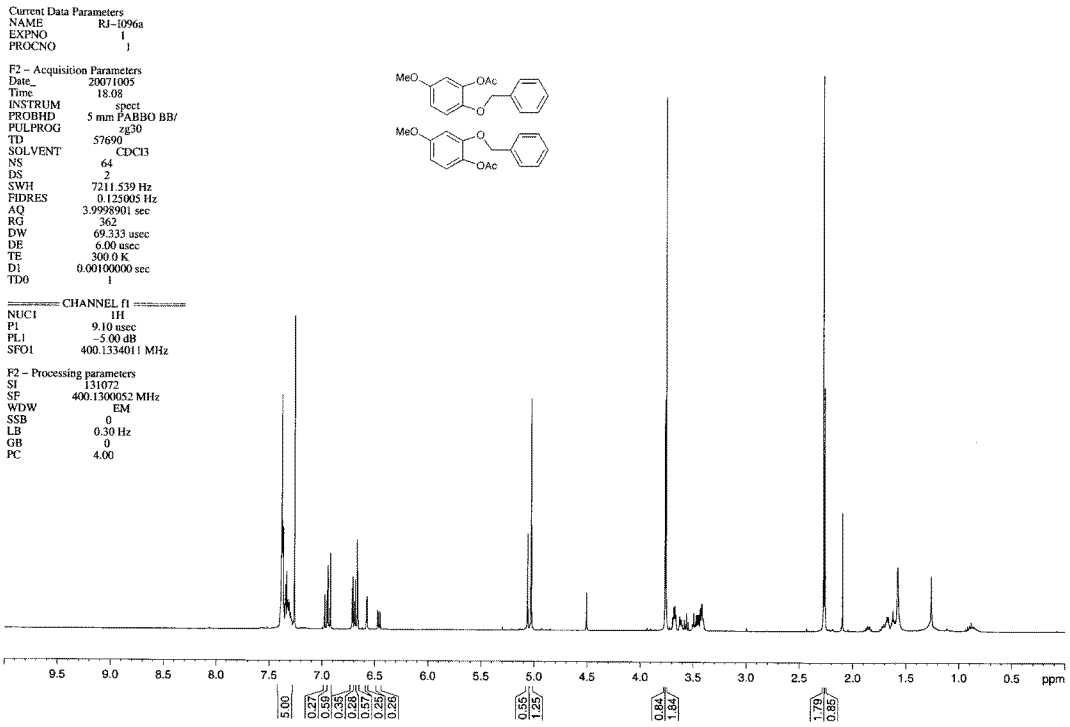
12.o) Compound 10b/11b (from $BH_3 \bullet NMe_3$)



12.p) Compound 10b/11b (from $BH_3 \bullet THF$)



12.q) Compound S5/S6



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