Enantioselective Synthesis of Multisubstituted Biaryl Skeleton by Chiral Phosphoric Acid Catalyzed Desymmetrization/Kinetic Resolution Sequence

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General experimental procedures

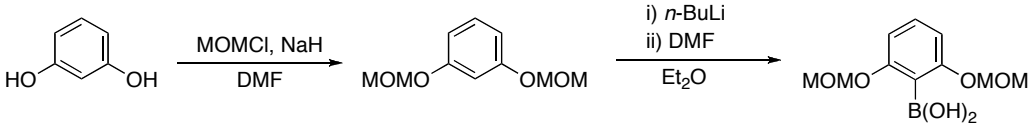
All reactions utilizing air- and moisture-sensitive reagents were performed in dried glassware under an atmosphere of dry nitrogen. Ethereal solvents (THF, Et_2O) were distilled from benzophenone ketyl. Dichloromethane and 1,2-dichloroethane were distilled over CaH_2. Benzene and toluene were distilled over CaH_2, and stored over 4A molecular sieves. *N*,*N*-Dimethylformamide (DMF) was distilled over CaH_2, and stored over 4A molecular sieves.

For thin-layer chromatography (TLC) analysis, Merck pre-coated plates (silica gel 60 F_{254}, Art 5715, 0.25 mm) were used. Column chromatography and preparative TLC (PTLC) were performed on PSQ 60B, Fuji Silysia Chemical Ltd. and Wakogel B-5F, Wako Pure Chemical Industries, respectively.

Melting point (mp) determinations were performed by using a AS ONE ATM-01 instrument and are uncorrected. ^{1}H NMR, ^{13}C NMR, ^{19}F NMR, and ^{31}P NMR were measured on a varian-400 MR (Varian Ltd., 400 MHz) spectrometer. Chemical shifts are expressed in parts per million (ppm) downfield from internal standard (tetramethylsilane for ^{1}H, C_6F_6 for ^{19}F, and H_3PO_4 for ^{31}P NMR, 0.00 ppm), and coupling constants are reported as hertz (Hz). Splitting patterns are indicated as follows: br, broad; s, singlet; d, doublet; t, triplet; q, quartet; sep, septet; m, multiplet. Infrared (IR) spectra were recorded on a FTIR-8600PC instrument (Shimadzu Co.). Elemental analysis (EA) was carried out on Flash2000 instrument (Amco Inc.).

1. Preparation of starting materials (aryl boronic acid and its coupling partners).

Scheme 1. Preparation of MOM-protected boronic acid **s3**.[1]



s1 **s2** 68% (2 steps) **s3**

To a suspension of NaH (60% oil, 1.67 g, 41.8 mmol) in DMF (30.0 mL) were successively added a solution of resorcinol (**s1**) (2.01 g, 18.3 mmol) in DMF (30.0 mL) and MOMCl (3.04 mL, 40.2 mmol) at 0 °C. After being stirred for 4 h at room temperature, the reaction was stopped by adding 1 M aqueous HCl. The crude products were extracted with EtOAc (x4) and the combined organic extracts were washed with 1 M aqueous HCl (x6), brine, dried (Na_2SO_4), and concentrated in vacuo to give crude **s2** (3.71 g). This material was used to next reaction without further purification.

To a solution of **s2** in Et_2O (72.7 mL) was added *n*-BuLi (1.60 M in hexane, 13.6 mL, 21.8 mmol) at 0 °C. After stirring for 3 h at room temperature, $B(OMe)_3$ (3.04 mL, 27.4 mmol) was added to the reaction mixture at 0 °C. After being stirred for 1 h at room temperature, the reaction was acidified by 2 M HCl at 0 °C. After being stirred for 1 h at room temperature, the resulting white precipitates were filtered off and washed by H_2O to afford analytically pure **s3** (3.01 g, 68%) as a white solid.

Mp. 115–116 °C.

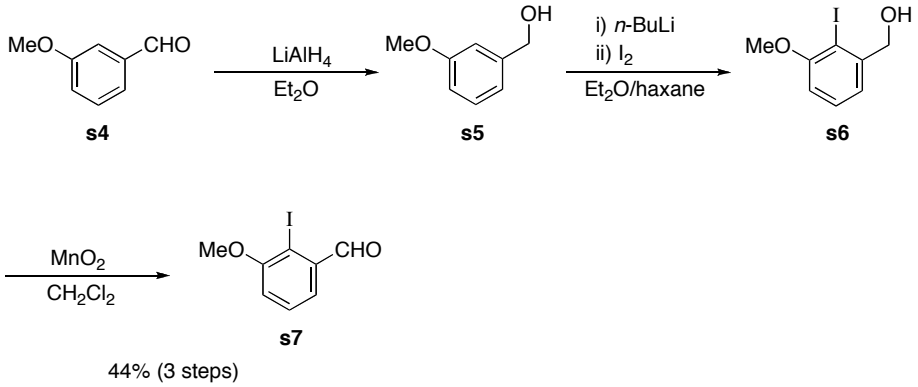
IR (KBr) 3316, 2951, 2898, 2826, 1600, 1585, 1461, 1441, 1397, 1370, 1337, 1308, 1241, 1199, 1152, 1097, 1044, 1008, 921, 893 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$) δ 3.51 (s, 6H), 5.30 (s, 4H), 6.88 (d, 1H, J = 8.0 Hz), 7.23 (brs, 2H), 7.35 (dd, 1H, J = 8.0, 8.0 Hz).

^{13}C NMR (100 MHz, $CDCl_3$) δ 56.5, 94.8, 108.2, 133.0, 163.0.

Anal. Calcd for $C_{10}H_{15}BO_6$: C, 49.62; H, 6.25. Found: C, 49.45; H, 6.55.

Scheme 2. Preparation of iodide **s7**.



Synthesis of 2-iodo-3-methoxybenzaldehyde (s7):

To a solution of *m*-anisaldehyde **s4** (4.30 g, 31.6 mmol) in Et_2O (105 mL) was added LiAlH4 (900 mg, 23.7 mmol) at 0 °C (portionwise). After being stirred for 0.5 h at 0 °C, the reaction was stopped by adding $Na_2SO_4 \bullet 10H_2O$. After being stirred for another 1 h at room temperature, the crude material was filtered through Celite® pad and the resulting filtrate was concentrated in vacuo to give crude benzyl alcohol **s5** (4.70 g). The crude material was used for the next reaction without further purification.

To a solution of benzyl alcohol **s5** in Et_2O (53.0 mL) and hexane (158 mL) was added *n*-BuLi (1.60 M in hexane, 43.4 mL, 69.4 mmol) at 0 °C, and the reaction mixture was stirred for 4 h at room temperature. After the reaction mixture was cooled to 0 °C, a solution of I_2 (12.0 g, 47.3 mmol) in THF (53.0 mL) was added and the reaction mixture was stirred for 0.5 h at room temperature. The reaction was stopped by adding 10% aqueous $Na_2S_2O_3$ at 0 °C. The crude products were extracted with EtOAc (x3) and the combined organic extracts were washed with brine, dried (Na_2SO_4), and concentrated in vacuo. The residue was purified by column chromatography (silica gel, hexane/EtOAc = 5/1) to give **s6** as a colorless oil with inseparable impurities. This material was used to next reaction without further purification.

To a solution of **s6** in CH_2Cl_2 (69.0 mL) was added MnO_2 (3.62 g, 41.6 mmol) at room temperature. After the reaction mixture was heated to reflux for 24 h, the crude material was filtered through Celite® pad and the resulting filtrate was concentrated in vacuo. The residue was purified by recrystallization (hexane/ethyl acetate) to give aldehyde **s7** (3.64 g, 44% from **s4**) as a pale yellow solid.

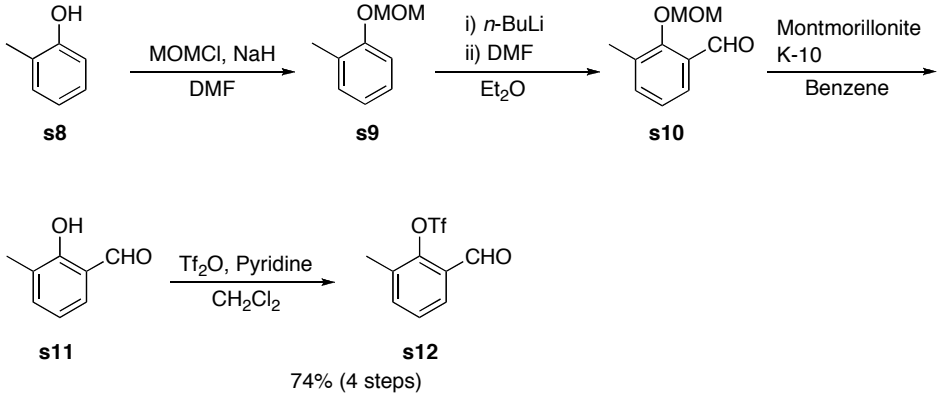
IR (KBr) 3073, 3028, 2976, 2946, 2847, 2739, 1685, 1588, 1562, 1469, 1430, 1381, 1302, 1271, 1241, 1176, 1107, 1067, 1013, 904, 789 cm^{-1}.

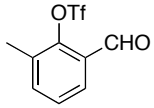
^{1}H NMR (400 MHz, $CDCl_3$) δ 3.95 (s, 3H), 7.04 (dd, 1H, *J* = 1.6, 8.0 Hz), 7.38 (dd, 1H, *J* = 8.0, 8.0 Hz), 7.48 (dd, 1H, *J* = 1.6, 8.0 Hz), 10.2 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 56.8, 93.9, 116.0, 122.3, 129.5, 136.7, 158.3, 196.5.

Anal. Calcd for $C_8H_7IO_2$: C, 36.67; H, 2.69. Found: C, 36.46; H, 2.80.

Scheme 3. General synthetic route to triflate. Preparation of **s12** is shown as a representative example.





Synthesis of 2-formyl-6-methylphenyl trifluoromethanesulfonate (s12):

To a suspension of NaH (60% oil, 1.11 g, 27.7 mmol) in DMF (30.0 mL) were successively added a solution of 2-methylphenol (**s8**) (2.00 g, 18.5 mmol) in DMF (30.0 mL) and MOMCl (1.83 mL, 24.0 mmol) at 0 °C. After being stirred for 3 h at room temperature, the reaction was stopped by adding 1 M aqueous HCl. The crude products were extracted with EtOAc(x4) and the combined organic extracts were washed with 1 M aqueous HCl (x6), brine, dried (Na_2SO_4), and concentrated in vacuo to give crude **s9** (2.80 g). This material was used to next reaction without further purification.

To a solution of **s9** in Et_2O (92.5 mL) was added *n*-BuLi (1.65 M in hexane, 20.2 mL, 33.3 mmol) at 0 °C. After stirring for 3 h at room temperature, DMF (3.63 mL, 37.0 mmol) was added to the reaction mixture at 0 °C. After being stirred for 10 min at 0 °C, the reaction was stopped by adding saturated aqueous NH_4Cl. The crude products were extracted with EtOAc (x3) and the combined organic extracts were washed with brine, dried (Na_2SO_4), and concentrated in vacuo to give crude **s10** (3.75 g).

This material was used to next reaction without further purification.

To a solution of **s10** in Benzene (185 mL) was added Montmorillonite K-10 (3.50 g) at room temperature, then heated at reflux. After heating for 24 h, the crude material was filtered through Celite® pad, and the resulting filtrate was concentrated in vacuo to give crude **s11** (2.56 g). This material was used to next reaction without further purification.

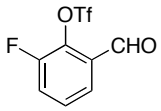
To a solution of **s11** in CH_2Cl_2 (92.4 mL) were successively added pyridine (4.49 mL, 55.5 mmol) and Tf_2O (4.66 mL, 27.7 mmol) at 0 °C. After being stirred for 2.5 h at room temperature, the reaction was stopped by adding saturated aqueous $NaHCO_3$ at 0 °C. The crude products were extracted with CH_2Cl_2 (x4) and the combined organic extracts were washed with 1 M aqueous HCl (x2), brine, dried (Na_2SO_4), and concentrated in vacuo. The residue was purified by column chromatography (silica gel, hexane/EtOAc = 8/1) to give **s12** (3.65 g, 74% from **s8**) as a pale yellow oil.

IR (neat) 2938, 2884, 2756, 1706, 1608, 1580, 1468, 1426, 1408, 1249, 1216, 1170, 1139, 1078, 954, 918, 878, 789 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$) δ 2.48 (s, 3H), 7.45 (dd, 1H, *J* = 7.6, 7.6 Hz), 7.59 (dd, 1H, *J* = 0.8, 7.6 Hz), 7.85 (dd, 1H, *J* = 0.8, 7.6 Hz), 10.24 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 16.3, 118.5 (q, *J* = 318.5 Hz), 128.2, 128.6, 129.5, 132.8, 138.1, 147.6, 186.9.

Anal. Calcd for $C_9H_7F_3O_4S$: C, 40.30; H, 2.63. Found: C, 40.55; H, 2.58.



2-Fluoro-6-formylphenyl trifluoromethanesulfonate (**s13**).

Pale yellow oil.

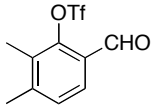
Yield: 42% (from commercially available 2-fluorophenol).

IR (neat) 3090, 2884, 2848, 2759, 1714, 1614, 1591, 1476, 1433, 1401, 1280, 1218, 1173, 1138, 1077, 1066, 1010, 961, 887 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$) δ 7.49–7.62 (m, 1H), 7.73–7.88 (m, 1H), 10.23 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 118.5 (q, *J* = 318.8 Hz), 123.1 (d, *J* = 19.3 Hz), 126.3 (d, *J* = 3.0 Hz), 129.8 (d, *J* = 7.4 Hz), 130.5, 136.7 (d, *J* = 14.1 Hz), 153.9 (d, *J* = 254.5 Hz), 185.8 (d, *J* = 2.2 Hz).

Anal. Calcd for $C_8H_4F_4O_4S$: C, 35.30; H, 1.48. Found: C, 35.55; H, 1.58.



6-Formyl-2,3-dimethylphenyl trifluoromethanesulfonate (**s14**).

Colorless oil.

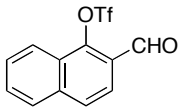
Yield: 72% (from commercially available 2,3-dimethylphenol).

IR (neat) 2982, 2891, 2755, 1696, 1611, 1565, 1455, 1426, 1407, 1253, 1213, 1178, 1136, 1054, 952, 894, 808 cm^{-1}.

^{1}H NMR (400 MHz, $CDCl_3$) δ 2.34 (s, 3H), 2.42 (s, 3H), 7.33 (d, 1H, *J* = 8.0 Hz), 7.75 (d, 1H, *J* = 8.0 Hz), 10.17 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 13.0, 20.7, 118.5 (q, *J* = 318.5 Hz), 127.4, 127.5, 129.9, 131.2, 147.2, 147.5, 186.8.

Anal. Calcd for $C_{10}H_9F_3O_4S$: C, 42.56; H, 3.21. Found: C, 42.80; H, 3.10.



2-Formylnaphthalen-1-yl trifluoromethanesulfonate (**s15**).

Pale grey solid.

Yield: 41% (from commercially available 2-naphthol).

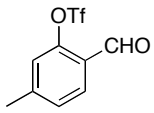
Mp. 50–51 °C.

IR (KBr) 3073, 2889, 2862, 2769, 2739, 1699, 1631, 1601, 1468, 1415, 1344, 1246, 1224, 1134, 1039, 916, 880, 807 cm^{-1}.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68–7.78 (m, 2H), 7.90–8.08 (m, 3H), 8.18–8.29 (m, 1H), 10.45 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 118.7 (q, *J* = 319.2 Hz), 122.6, 123.0, 125.9, 126.4, 128.3, 128.6, 129.1, 130.2, 137.8, 147.4, 186.6.

Anal. Calcd for $C_{12}H_7F_3O_4S$: C, 47.37; H, 2.32. Found: C, 47.15; H, 2.10.



2-Formyl-5-methylphenyl trifluoromethanesulfonate (**s16**).

Pale yellow oil.

Yield: 67% (from commercially available 3-methylphenol).

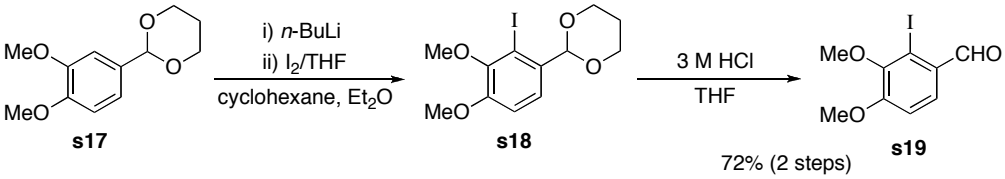
IR (neat) 2964, 2927, 2871, 2764, 1702, 1616, 1428, 1274, 1252, 1219, 1139, 1096, 1078, 963, 946, 833 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$) δ 2.49 (s, 3H), 7.21 (s, 1H), 7.35 (d, 1H, J = 8.0 Hz), 7.88 (d, 1H, J = 8.0 Hz), 10.21 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 21.8, 118.6 (q, J = 318.5 Hz), 122.8, 126.1, 129.6, 130.7, 148.0, 149.8, 186.2.

Anal. Calcd for $C_9H_7F_3O_4S$: C, 40.30; H, 2.63. Found: C, 40.50; H, 2.48.

Scheme 4. Preparation of **s19**.



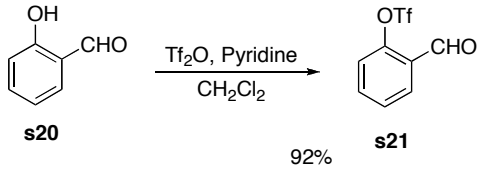
To a solution of acetal **s17**[1] (1.85 g, 8.25 mmol) in Et_2O (27.5 mL) and cyclohexane (27.5 mL) was added *n*-BuLi (1.60 M in hexane, 6.70 mL, 10.7 mmol) at 0 °C. After stirring for 6 h at room temperature, a solution of I_2 (3.14 g, 12.4 mmol) in THF (10.1 mL) was added to the reaction mixture at 0 °C. After being stirred for 30 min at 0 °C, the reaction was stopped by adding aqueous 10 % $Na_2S_2O_3$. The crude products were extracted with EtOAc (x4) and the combined organic extracts were washed with brine, dried (Na_2SO_4), and concentrated in vacuo to give crude **s18** (2.85 g). This material was used to next reaction without further purification.

To a solution of **s18** in THF (41.2 mL) was added 3 M HCl (8.25 mL, 24.8 mmol). After being stirred for 14 h at room temperature, the reaction was stopped by adding saturated aqueous $NaHCO_3$ at 0 °C. The crude products were extracted with EtOAc (x3) and the combined organic extracts were washed with brine, dried (Na_2SO_4), and concentrated in vacuo. The residue was purified by column chromatography (silica gel,

hexane/EtOAc = 8/1) to give **s19** (1.73 g, 72%) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 3.87 (s, 3H), 3.96 (s, 3H), 6.98 (d, 1H, *J* = 8.8 Hz), 7.72 (d, 1H, *J* = 8.8 Hz), 10.02 (s, 1H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 56.2, 60.4, 100.3, 118.3, 127.4, 128.9, 148.7, 157.7, 194.5.
The ^{1}H and ^{13}C NMR spectra were in complete agreement with those in the literature.[2]

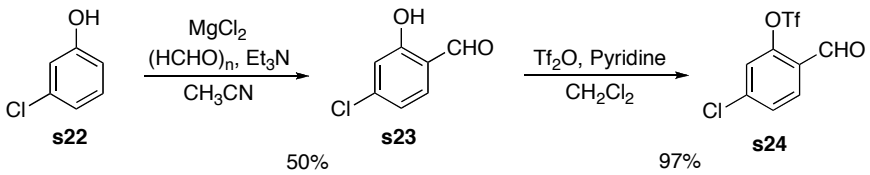
Scheme 5. Preparation of **s21**.[3]

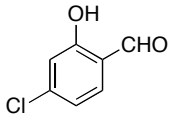


To a solution of salicylaldehyde (**s20**) (1.50 g, 12.3 mmol) in CH_2Cl_2 (123 mL) were successively added pyridine (2.98 mL, 36.8 mmol) and Tf_2O (3.09 mL, 18.4 mmol) at 0 °C. After being stirred for 3 h at room temperature, the reaction was stopped by adding saturated aqueous $NaHCO_3$ at 0 °C. The crude products were extracted with CH_2Cl_2 (x4) and the combined organic extracts were washed with 1 M aqueous HCl (x1), brine, dried (Na_2SO_4), and concentrated in vacuo. The residue was purified by column chromatography (silica gel, hexane/EtOAc = 8/1) to give **s21** (2.87 g, 92%) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 (d, 1H, *J* = 8.0 Hz), 7.57 (d, 1H, *J* = 8.0, 8.0 Hz), 7.73 (ddd, 1H, *J* = 2.0, 8.0, 8.0 Hz), 8.01 (dd, 1H, *J* = 2.0, 8.0 Hz), 10.29 (s, 1H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 118.6 (q, *J* = 319.3 Hz), 122.4, 128.5, 128.9, 130.9, 135.8, 149.8, 186.5.
The ^{1}H and ^{13}C NMR spectra were in complete agreement with those in the literature.[4]

Scheme 6. Preparation of **s24**.

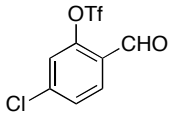




Synthesis of 4-chloro-2-hydroxybenzaldehyde (s23):[5]

To a solution of *m*-chlorophenol (**s22**) (731 mg, 5.68 mmol) in CH_3CN (28.5 mL) were successively added paraformaldehyde (1.19 g, 39.7 mmol), NEt_3 (3.0 mL, 21.3 mmol) and $MgCl_2$ (837 mg, 8.79 g). After stirring for 3 h at room temperature, DMF (3.63 mL, 37.0 mmol) was added to the reaction mixture at 0 °C. After being stirred for 4 h at reflux, the reaction was stopped by adding saturated aqueous 1 M HCl. The crude products were extracted with EtOAc (x4) and the combined organic extracts were washed with brine, dried (Na_2SO_4), and concentrated in vacuo. The residue was purified by column chromatography (silica gel, hexane/EtOAc = 20/1) to give **s23** (446 mg g, 50%) as white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.00 (d, 1H, *J* = 8.0 Hz), 7.01 (s, 1H), 7.50 (d, 1H, *J* = 8.0 Hz), 9.86 (s, 3H), 11.16 (s, 1H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 117.9, 119.2, 120.6, 134.5, 143.2, 162.2, 195.5.
The ^{1}H and ^{13}C NMR spectra were in complete agreement with those in the literature.[6]



Synthesis of 5-chloro-2-formylphenyl trifluoromethanesulfonate (s24):

To a solution of **s23** (554 mg, 3.54 mmol) in CH_2Cl_2 (14.0 mL) were successively added pyridine (0.90 mL, 11.1 mmol) and Tf_2O (5.35 mL, 5.35 mmol) at 0 °C. After being stirred for 1.5 h at 0 °C, the reaction was stopped by adding saturated aqueous $NaHCO_3$ at 0 °C. The crude products were extracted with CH_2Cl_2 (x3) and the combined organic extracts were washed with 1 M aqueous HCl (x2), brine, dried (Na_2SO_4), and concentrated in vacuo. The residue was purified by column chromatography (silica gel, hexane/EtOAc = 5/1) to **s24** (992 mg, 97%) as a white solid.

Mp. 55–57 °C.

IR (KBr) 3101, 2875, 2771, 1703, 1600, 1569, 1478, 1432, 1395, 1293, 1251, 1218, 1159, 1138, 1110, 1071, 921, 875, 822 cm^{-1}.

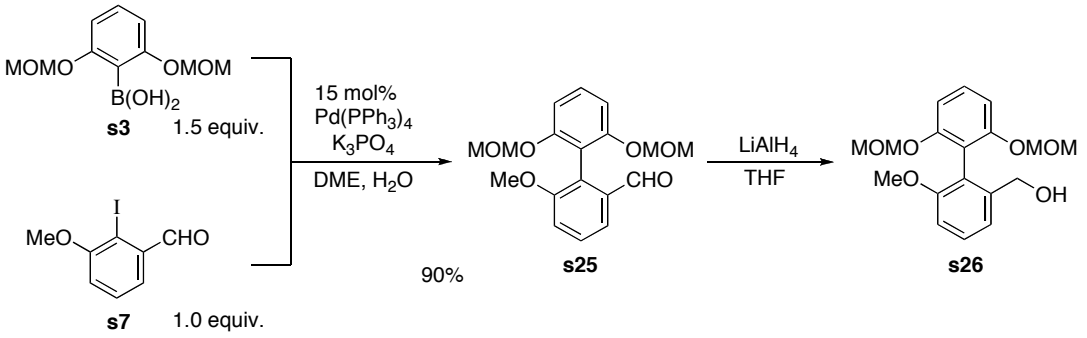
^1H NMR (400 MHz, $CDCl_3$) δ 7.44 (d, 1H, *J* = 2.0 Hz), 7.55 (d, 1H, *J* = 2.0, 8.0 Hz), 7.96 (d, 1H, *J* = 8.0 Hz), 10.23 (s, 1H).

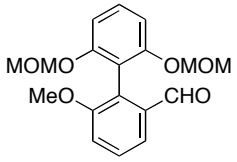
^{13}C NMR (100 MHz, $CDCl_3$) δ 118.5 (q, *J* = 319.3 Hz), 123.0, 127.0, 129.4, 131.5, 141.7, 149.7, 185.2.

Anal. Calcd for $C_8H_4ClF_3O_4S$: C, 33.29; H, 1.40. Found: C, 33.51; H, 1.22.

2. Preparation of starting materials (biphenol derivatives).

Scheme 7. General synthetic route to biphenol **2a**.[7] Preparation of **2a** is shown as a representative example.



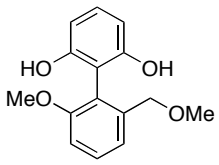


Synthesis of 6-methoxy-2',6'-bis(methoxymethoxy)biphenyl-2-carbaldehyde (s25):

The mixture of boronic acid **s3** (530 mg, 2.18 mmol), iodobenzene **s7** (438 mg, 1.67 mmol), $Pd(PPh_3)_4$ (290 mg, 0.250 mmol), K_3PO_4 (1.08 g, 5.09 mmol), DME (17.0 mL), and H_2O (5.6 mL) were heated at reflux for 4.5 h. After cooling to room temperature, the reaction was stopped by adding H_2O. The crude mixture was extracted with EtOAc (x3) and the combined organic extracts were washed with brine, dried (Na_2SO_4),

and concentrated in vacuo. The residue was purified by column chromatography (silica gel, hexane/EtOAc = 2/1) to give **s25** (500 mg, 90%) as a colorless amorphous.

IR (neat) 2959, 2828, 1689, 1591, 1466, 1402, 1306, 1261, 1247, 1202, 1181, 1153, 1100, 1044, 918, 894, 783, 741, 727, 666 cm^{-1}.
^{1}H NMR (400 MHz, $CDCl_3$) δ 3.26 (s, 6H), 3.77 (s, 3H), 5.01 (d, 2H, *J* = 6.8 Hz), 5.05 (d, 2H, *J* = 6.8 Hz), 6.92 (d, 2H, *J* = 8.4 Hz), 7.20 (d, 1H, *J* = 8.0 Hz), 7.33 (dd, 1H, *J* = 8.4, 8.4 Hz), 7.46 (dd, 1H, *J* = 8.0, 8.0 Hz), 7.64 (dd, 1H, *J* = 1.2, 8.0 Hz).
^{13}C NMR (100 MHz, $CDCl_3$) δ 55.8, 55.9, 94.6, 108.5, 113.1, 115.9, 118.6, 128.0, 128.7, 130.0, 135.4, 155.9, 157.5, 192.9.
Anal. Calcd for $C_{18}H_{20}O_6$: C, 65.05; H, 6.07. Found: C, 64.93; H, 6.08.



Synthesis of 2'-methoxy-6'-(methoxymethyl)biphenyl-2,6-diol (2a):
To a solution of **s25** (2.55 g, 7.68 mmol) in THF (38.0 mL) was added $LiAlH_4$ (219 mg, 5.75 mmol) at 0 °C. After being stirred for 0.5 h at 0 °C, the reaction was stopped by adding $Na_2SO_4 \cdot 10H_2O$. After being stirred for another 1 h at room temperature, the crude material was filtered through Celite® pad and the resulting filtrate was concentrated in vacuo to give crude benzyl alcohol **s26** (2.57 g). The crude material was used for the next reaction without further purification.
To a solution of **s26** in DMF (38.0 mL) were successively added NaH (60% oil, 590 mg, 14.7 mmol) and MeI (0.90 mL, 14.5 mmol) at 0 °C. After being stirred for 4 h at room temperature, the reaction was stopped by adding aqueous 1 M HCl at 0 °C. The crude mixture was extracted with EtOAc (x3) and the combined organic extracts were washed with brine, dried (Na_2SO_4), and concentrated in vacuo to give methyl ether **s27** (2.75 g). The crude material was used for the next reaction without further purification.
To a solution of **s27** in THF (29.0 mL) and MeOH (38.5 mL) was added aqueous 2 M HCl (19.0 mL, 38.0 mmol) at 0 °C. After being stirred for 5.5 h at 50 °C, the reaction was stopped by adding saturated aqueous $NaHCO_3$ at 0 °C. The crude mixture was extracted with EtOAc (x3) and the combined organic extracts were washed with brine,

dried (Na_2SO_4), and concentrated in vacuo. The residue was purified by column chromatography (silica gel, hexane/EtOAc = 2/1) to give **2a** (1.60 g, 96% from **s3**) as a white solid.

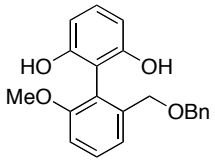
Mp. 110–111 °C.

IR (neat) 3398, 2934, 2836, 1620, 1581, 1506, 1463, 1437, 1378, 1265, 1188, 1151, 1069, 1008, 911, 787, 732, 676, 645 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$) δ 3.27 (s, 3H), 3.72 (s, 3H), 4.16 (s, 2H), 5.29 (s, 2H), 6.59 (d, 2H, *J* = 8.4 Hz), 7.00 (d, 1H, *J* = 8.0 Hz), 7.16 (dd, 1H, *J* = 8.4, 8.4 Hz), 7.18 (d, 1H, *J* = 8.0 Hz), 7.43 (dd, 1H, *J* = 8.0, 8.0 Hz).

^{13}C NMR (100 MHz, $CDCl_3$) δ 56.0, 58.5, 73.0, 108.5, 111.0, 111.5, 118.8, 122.1, 129.6, 130.6, 140.0, 154.1, 158.0.

Anal. Calcd for $C_{15}H_{16}O_4$: C, 69.22; H, 6.20. Found: C, 69.37; H, 6.09.



2'-(Benzyloxymethyl)-6'-methoxybiphenyl-2,6-diol (**2b**).

Colorless amorphous.

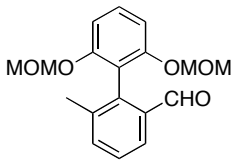
Yield: 85% (prepared from **s25**).

IR (neat) 3408, 3063, 3030, 2931, 2865, 1621, 1580, 1497, 1462, 1437, 1358, 1304, 1265, 1179, 1150, 1064, 1007, 910, 787, 733, 699 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$) δ 3.74 (s, 3H), 4.25 (s, 2H), 4.42 (s, 2H), 5.08 (s, 2H), 6.62 (d, 2H, *J* = 8.4 Hz), 7.02 (d, 1H, *J* = 8.4 Hz), 7.13–7.36 (m, 7H), 7.46 (dd, 1H, *J* = 8.0, 8.0 Hz).

^{13}C NMR (100 MHz, $CDCl_3$) δ 56.1, 70.7, 73.2, 108.6, 111.0, 111.6, 118.7, 122.6, 127.8, 128.0, 128.4, 129.7, 130.8, 137.4, 140.3, 154.1, 158.2.

Anal. Calcd for $C_{21}H_{20}O_4$: C, 78.73; H, 6.29. Found: C, 78.72; H, 6.29.



2',6'-bis(methoxymethoxy)-6-methylbiphenyl-2-carbaldehyde (**s28**).

Pale yellow solid.

Yield: 81% (prepared from **s3** and **s12**)

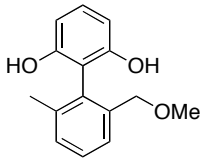
Mp. 88–89 °C.

IR (neat) 2955, 2905, 2847, 2827, 2744, 1691, 1590, 1466, 1442, 1401, 1310, 1247, 1203, 1154, 1097, 1081, 1042, 922, 897 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$) δ 2.11 (s, 3H), 3.23 (s, 6H), 5.01 (d, 2H, *J* = 6.8 Hz), 5.04 (d, 2H, *J* = 6.8 Hz), 6.91 (d, 2H, *J* = 8.0 Hz), 7.33 (dd, 1H, *J* = 8.0, 8.0 Hz), 7.39 (dd, 1H, *J* = 8.0, 8.0 Hz), 7.53 (dd, 1H, *J* = 0.8, 8.0 Hz), 7.86 (dd, 1H, *J* = 0.8, 8.0 Hz), 9.72 (d, 1H, *J* = 0.8 Hz).

^{13}C NMR (100 MHz, $CDCl_3$) δ 19.4, 55.9, 94.5, 108.3, 115.9, 124.2, 127.5, 130.0, 134.4, 135.1, 138.5, 138.5, 155.4, 193.2.

Anal. Calcd for $C_{18}H_{20}O_5$: C, 68.34; H, 6.37. Found: C, 68.72; H, 6.11.



2'-(Methoxymethyl)-6'-methylbiphenyl-2,6-diol (**2c**).

Colorless oil.

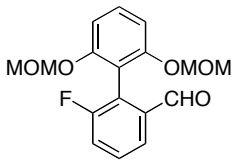
Yield: 96% (prepared from **s28**).

IR (neat) 3397, 3065, 2925, 2827, 2362, 1620, 1580, 1505, 1459, 1380, 1305, 1276, 1247, 1177, 1150, 1079, 1037, 1006, 933, 910, 889, 787, 761, 733 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$) δ 2.06 (s, 3H), 3.27 (s, 3H), 4.15 (s, 2H), 5.11 (s, 2H), 6.62 (d, 2H, *J* = 8.0 Hz), 7.19 (dd, 1H, *J* = 8.0, 8.0 Hz), 7.32–7.44 (m, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 19.7, 58.6, 73.8, 108.6, 113.9, 127.7, 129.5, 129.7, 129.9, 131.0, 138.6, 139.9, 153.5.

Anal. Calcd for $C_{15}H_{16}O_3$: C, 73.75; H, 6.60. Found: C, 73.99; H, 6.71.



6-fluoro-2',6'-bis(methoxymethoxy)biphenyl-2-carbaldehyde (**s29**).

White solid.

Yield: 50% (prepared from **s3** and **s13**).

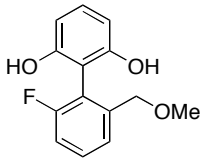
Mp. 110–112 °C.

IR (neat) 2957, 2905, 2851, 2828, 2749, 1695, 1597, 1469, 1457, 1401, 1310, 1253, 1204, 1155, 1099, 1083, 1044, 990, 957 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$) δ 3.30 (s, 6H), 5.07 (s, 4H), 6.93 (d, 2H, *J* = 8.0 Hz), 7.33–7.42 (m, 2H), 7.44–7.52 (m, 1H), 7.83 (dd, 1H, *J* = 0.8, 8.0 Hz), 9.56 (d, 1H, *J* = 0.8 Hz).

^{13}C NMR (100 MHz, $CDCl_3$) δ 56.0, 94.6, 108.1, 110.0, 120.5 (d, *J* = 23.1 Hz), 122.3 (d, *J* = 3.0 Hz), 125.7 (d, *J* = 18.6 Hz), 129.0 (d, *J* = 8.2 Hz), 130.8, 136.0 (d, J = 3.0 Hz), 155.8, 160.2 (d, *J* = 245.5 Hz), 191.6 (d, *J* = 3.8 Hz).

Anal. Calcd for $C_{17}H_{17}FO_5$: C, 63.74; H, 5.35. Found: C, 63.99; H, 5.31.



2'-Fluoro-6'-(methoxymethyl)biphenyl-2,6-diol (**2d**).

White solid.

Yield: 64% (prepared from **s29**).

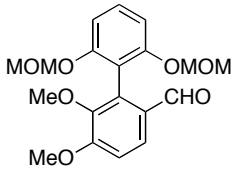
Mp. 165–166 °C.

IR (KBr) 3366, 3200, 2942, 1612, 1458, 1396, 1304, 1278, 1253, 1234, 1193, 1104, 1068, 1012, 930, 897, 882, 782, 747, 727, 670 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$) δ 3.33 (s, 3H), 4.24 (s, 2H), 5.26 (s, 2H), 6.63 (d, 2H, *J* = 8.0 Hz), 7.16–7.30 (m, 4H), 7.37 (dd, 1H, *J* = 0.8, 7.2 Hz), 7.43–7.51 (m, 1H).

^{13}C NMR (100 MHz, CD_3COCD_3) δ 58.3, 72.2 (d, *J* = 3.0 Hz), 107.8, 109.0, 114.3 (d, *J* = 22.4 Hz), 121.6 (d, *J* = 17.8 Hz), 122.9 (d, *J* = 3.0 Hz), 129.4 (d, *J* = 9.0 Hz), 130.2, 141.9 (d, *J* = 2.9 Hz), 156.8, 161.4 (d, *J* = 241.9 Hz).

Anal. Calcd for $C_{14}H_{13}FO_3$: C, 67.73; H, 5.28. Found: C, 68.03; H, 5.26.



5,6-dimethoxy-2',6'-bis(methoxymethoxy)biphenyl-2-carbaldehyde (**s30**).

White solid.

Yield: 65% (prepared from **s3** and **s19**).

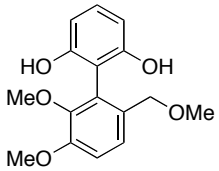
Mp. 99–100 °C.

IR (KBr) 2942, 2093, 2827, 2749, 1683, 1585, 1484, 1465, 1419, 1401, 1305, 1281, 1256, 1203, 1154, 1119, 1098, 1042, 922, 897 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$) δ 3.27 (s, 6H), 3.59 (s, 3H), 3.97 (s, 3H), 5.01 (d, 2H, *J* = 6,8 Hz), 5.08 (d, 2H, *J* = 6.8 Hz), 6.92 (d, 2H, *J* = 8.0 Hz), 7.05 (d, 1H, *J* = 8.4 Hz), 7.33 (dd, 1H, *J* = 8.0, 8.0 Hz), 7.83 (d, 1H, *J* = 8.4 Hz).

^{13}C NMR (100 MHz, $CDCl_3$) δ 55.8, 55.9, 60.3, 94.5, 108.1, 111.2, 112.8, 123.9, 128.2, 130.0, 133.2, 146.8, 155.8, 157.6, 191.3.

Anal. Calcd for $C_{19}H_{22}O_7$: C, 62.97; H, 6.12. Found: C, 63.16; H, 6.15.



2',3'-Dimethoxy-6'-(methoxymethyl)biphenyl-2,6-diol (**2e**).

White solid.

Yield: 51% (prepared from **s30**).

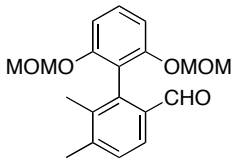
Mp. 136–137 °C.

IR (KBr) 3357, 2938, 2835, 1618, 1578, 1487, 1461, 1419, 1377, 1306, 1272, 1189, 1121, 1078, 1044, 1012, 912, 851, 811, 788, 732, 648 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$) δ 3.29 (s, 3H), 3.57 (s, 3H), 3.92 (s, 3H), 4.12 (s, 2H), 5.52 (s, 2H), 6.65 (d, 2H, *J* = 8.4 Hz), 7.03 (d, 1H, *J* = 8.4 Hz), 7.19 (dd, 1H, *J* = 8.4, 8.4 Hz), 7.28 (d, 1H, *J* = 8.4 Hz).

^{13}C NMR (100 MHz, $CDCl_3$) δ 55.9, 58.4, 60.9, 73.5, 109.4, 112.2, 112.8, 126.2, 126.6, 129.8, 130.4, 147.7, 153.6, 154.3.

Anal. Calcd for $C_{16}H_{18}O_5$: C, 66.19; H, 6.25. Found: C, 66.36; H, 6.06.



2',6'-bis(methoxymethoxy)-5,6-dimethylbiphenyl-2-carbaldehyde (**s31**).

White solid.

Yield: 67% (prepared from **s3** and **s14**).

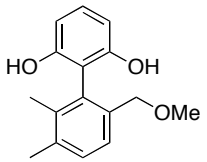
Mp. 105–106 °C.

IR (KBr) 2935, 2905, 2846, 2827, 2745, 1684, 1588, 1463, 1400, 1387, 1310, 1249, 1203, 1154, 1097, 1041, 942, 922, 897 cm^{-1}.

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.99 (s, 3H), 2.40 (s, 3H), 3.23 (s, 6H), 5.00 (d, 2H, J = 6.8 Hz), 5.03 (d, 2H, J = 6.8 Hz), 6.91 (d, 2H, J = 8.4 Hz), 7.29 (d, 1H, J = 8.0 Hz), 7.33 (dd, 1H, J = 8.4, 8.4 Hz), 7.79 (d, 1H, J = 8.0 Hz), 9.63 (d, 1H, J = 0.8 Hz).

^{13}C NMR (100 MHz, $CDCl_3$) δ 15.9, 21.3, 55.9, 94.4, 108.2, 116.4, 124.1, 129.4, 129.8, 132.6, 136.7, 138.4, 143.4, 155.5, 193.2.

Anal. Calcd for $C_{19}H_{22}O_5$: C, 69.07; H, 6.71. Found: C, 69.36; H, 6.88.



6'-(Methoxymethyl)-2',3'-dimethylbiphenyl-2,6-diol (**2f**).

White solid.

Yield: 86% (prepared from **s31**).

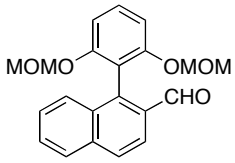
Mp. 96–97 °C.

IR (neat) 3407, 2925, 2826, 1620, 1582, 1504, 1462, 1411, 1383, 1340, 1307, 1277, 1245, 1182, 1150, 1083, 1006, 910, 821, 790, 732 cm^{-1}.

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.96 (s, 3H), 2.34 (s, 3H), 3.24 (s, 3H), 4.10 (s, 2H), 5.11 (s, 2H), 6.62 (d, 2H, *J* = 8.0 Hz), 7.18 (dd, 1H, *J* = 8.0, 8.0 Hz), 7.25 (d, 1H, *J* = 8.0 Hz), 7.29 (d, 1H, *J* = 8.0 Hz).

^{13}C NMR (100 MHz, $CDCl_3$) δ 16.1, 20.7, 58.5, 73.9, 108.6, 114.6, 127.5, 129.6, 129.7, 130.9, 136.0, 138.2, 138.4, 153.6.

Anal. Calcd for $C_{16}H_{18}O_3$: C, 74.39; H, 7.02. Found: C, 73.21; H, 6.96.



1-(2,6-Bis(methoxymethoxy)phenyl)-2-naphthaldehyde (**s32**).

Pale yellow solid.

Yield: 63% (prepared from **s3** and **s15**).

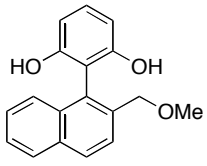
Mp. 134–136 °C.

IR (KBr) 3060, 2955, 2931, 2903, 2847, 2827, 2791, 1690, 1673, 1617, 1597, 1465, 1441, 1430, 1401, 1380, 1333, 1310, 1240, 1203, 1155, 1098, 1082, 1043, 972, 922 cm^{-1}.

^{1}H NMR (400 MHz, $CDCl_3$) δ 3.08 (s, 6H), 4.94 (s, 4H), 6.99 (d, 2H, *J* = 8.4 Hz), 7.38–7.50 (m, 2H), 7.54–7.68 (m, 2H), 7.91 (dd, 2H, *J* = 8.4, 8.4 Hz), 8.10 (d, 1H, *J* = 8.4 Hz), 9.60 (d, 1H, *J* = 0.4 Hz).

^{13}C NMR (100 MHz, $CDCl_3$) δ 55.8, 94.1, 108.2, 114.3, 121.9, 126.4, 126.8, 128.1, 128.2, 128.5, 130.5, 131.5, 132.4, 136.2, 140.1, 156.1, 193.0.

Anal. Calcd for $C_{21}H_{20}O_5$: C, 71.58; H, 5.72. Found: C, 71.70; H, 5.57.



2-(2-(Methoxymethyl)naphthalen-1-yl)benzene-1,3-diol (**2g**).

White solid.

Yield: 71% (prepared from **s32**).

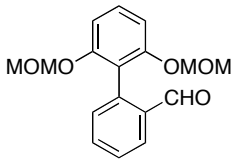
Mp. 156–158 °C.

IR (KBr) 3364, 3058, 2930, 1619, 1583, 1507, 1460, 1382, 1305, 1275, 1176, 1150, 1078, 1007, 969, 911, 818, 789, 756, 733 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$) δ 3.34 (s, 3H), 4.36 (s, 2H), 5.01 (s, 2H), 6.70 (d, 2H, *J* = 8.0 Hz), 7.28 (dd, 1H, *J* = 8.0, 8.0 Hz), 7.38–7.58 (m, 3H), 7.69 (d, 1H, *J* = 8.4 Hz), 7.91 (d, 1H, *J* = 8.4 Hz), 7.99 (d, 1H, *J* = 8.4 Hz).

^{13}C NMR (100 MHz, $CDCl_3$) δ 58.8, 73.5, 108.7, 112.3, 125.4, 126.8, 127.1, 127.2, 127.4, 128.3, 130.0, 130.2, 132.6, 133.8, 136.9, 154.3.

Anal. Calcd for $C_{18}H_{16}O_3$: C, 77.12; H, 5.75. Found: C, 77.08; H, 5.69.



2',6'-Bis(methoxymethoxy)biphenyl-2-carbaldehyde (**s33**).

White solid.

Yield: 81% (prepared from **s3** and **s21**).

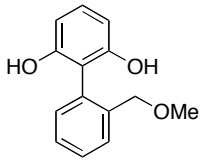
Mp. 100–102 °C.

IR (KBr) 2955, 2902, 2828, 2749, 1695, 1597, 1465, 1442, 1400, 1309, 1248, 1199, 1154, 1098, 1081, 1040, 922, 898, 828 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$) δ 3.26 (s, 6H), 5.03 (s, 4H), 6.91 (d, 2H, *J* = 8.0 Hz), 7.32 (dd, 1H, *J* = 8.0, 8.0 Hz), 7.35 (dd, 1H, *J* = 0.8, 8.0 Hz), 7.47 (dd, 1H, *J* = 8.0, 8.0 Hz), 7.63 (ddd, 1H, *J* = 1.2, 8.0, 8.0 Hz), 8.02 (dd, 1H, *J* = 1.2, 8.0 Hz), 9.82 (d, 1H, *J* = 0.8 Hz).

^{13}C NMR (100 MHz, $CDCl_3$) δ 56.1, 94.6, 108.5, 117.3, 126.5, 127.6, 130.0, 132.1, 133.2, 134.4, 138.3, 155.4, 192.7.

Anal. Calcd for $C_{17}H_{18}O_5$: C, 67.54; H, 6.00. Found: C, 67.80; H, 5.72.



2'-(Methoxymethyl)biphenyl-2,6-diol (**2i**).

White solid.

Yield: 70% (prepared from **s33**).

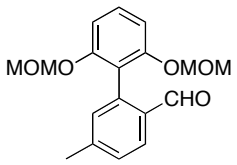
Mp. 126–128 °C.

IR (neat) 3389, 3064, 2990, 2929, 2828, 1620, 1584, 1507, 1462, 1378, 1309, 1181, 1151, 1117, 1077, 1046, 1007, 937, 910, 789, 764, 732 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$) δ 3.34 (s, 3H), 4.25 (s, 2H), 5.36 (s, 2H), 6.62 (d, 2H, *J* = 8.0 Hz), 7.18 (dd, 1H, *J* = 8.0, 8.0 Hz), 7.28–7.36 (m, 1H), 7.44–7.54 (m, 2H), 7.55–7.64 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 58.7, 73.4, 108.8, 115.4, 129.6, 129.7, 129.8, 130.8, 131.1, 131.9, 138.1, 153.9.

Anal. Calcd for $C_{14}H_{14}O_3$: C, 73.03; H, 6.13. Found: C, 73.32; H, 6.22.



2',6'-Bis(methoxymethoxy)-5-methylbiphenyl-2-carbaldehyde (**s34**).

White solid.

Yield: 86% (prepared from **s3** and **s16**).

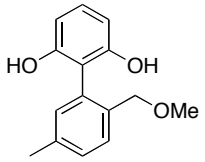
Mp. 120–122 °C.

IR (KBr) 2954, 2900, 2828, 2750, 1692, 1603, 1463, 1441, 1398, 1309, 1258, 1246, 1208, 1154, 1120, 1098, 1082, 1042, 922 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$) δ 2.44 (s, 3H), 3.27 (s, 6H), 5.03 (d, 2H, *J* = 6.8 Hz), 5.05 (d, 2H, *J* = 6.8 Hz), 6.90 (d, 2H, *J* = 8.0 Hz), 7.15 (s, 1H), 7.22–7.38 (m, 2H), 7.93 (dd, 1H, *J* = 8.0 Hz), 9.75 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 21.8, 56.0, 94.6, 108.5, 117.5, 126.6, 128.6, 129.8, 132.1, 132.6, 138.4, 144.0, 155.4, 192.3.

Anal. Calcd for $C_{18}H_{20}O_5$: C, 68.34; H, 6.37. Found: C, 68.12; H, 6.67.



2'-(Methoxymethyl)-5'-methylbiphenyl-2,6-diol (**2j**).

White solid.

Yield: 96% (prepared from **s34**).

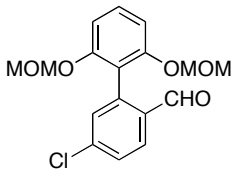
Mp. 105–107 °C.

IR (KBr) 3387, 2925, 2827, 1621, 1585, 1462, 1378, 1301, 1189, 1150, 1078, 1033, 1007, 937, 909, 825, 787, 730 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$) δ 2.39 (s, 3H), 3.32 (s, 3H), 4.20 (s, 2H), 5.44 (s, 2H), 6.61 (d, 2H, *J* = 8.0 Hz), 7.13 (s, 1H), 7.16 (dd, 1H, *J* = 8.0, 8.0 Hz), 7.28 (dd, 1H, *J* = 1.2, 7.6 Hz), 7.46 (d, 1H, *J* = 7.6 Hz).

^{13}C NMR (100 MHz, $CDCl_3$) δ 21.1, 58.6, 73.3, 108.8, 115.6, 129.6, 130.3, 131.0, 131.0, 132.4, 135.0, 139.9, 153.9.

Anal. Calcd for $C_{15}H_{16}O_3$: C, 73.75; H, 6.60. Found: C, 73.64; H, 6.88.



5-chloro-2',6'-bis(methoxymethoxy)biphenyl-2-carbaldehyde (**s35**).

White solid.

Yield: 70% (prepared from **s3** and **s24**).

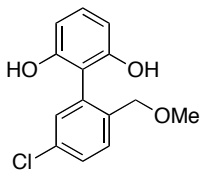
Mp. 122–124 °C.

IR (KBr) 2955, 2903, 2847, 2751, 1700, 1687, 1589, 1560, 1466, 1441, 1398, 1310, 1290, 1247, 1202, 1155, 1098, 1083, 1042, 922 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$) δ 3.29 (s, 6H), 5.06 (s, 4H), 6.91 (d, 2H, *J* = 8.0 Hz), 7.33 (dd, 1H, *J* = 8.0, 8.0 Hz), 7.36 (s, 1H), 7.45 (dd, 1H, *J* = 0.8, 8.0 Hz), 7.96 (d, 1H, *J* = 8.0 Hz), 9.74 (d, 1H, *J* = 0.8 Hz).

^{13}C NMR (100 MHz, $CDCl_3$) δ 56.2, 94.6, 108.3, 115.8, 128.0, 128.0, 130.5, 132.1, 132.8, 139.4, 139.8, 155.3, 191.4.

Anal. Calcd for $C_{17}H_{17}ClO_5$: C, 60.63; H, 5.09. Found: C, 60.83; H, 4.99.



5'-Chloro-2'-(methoxymethyl)biphenyl-2,6-diol (**2k**).

White solid.

Yield: 59% (prepared from **s35**).

Mp. 104–105 °C.

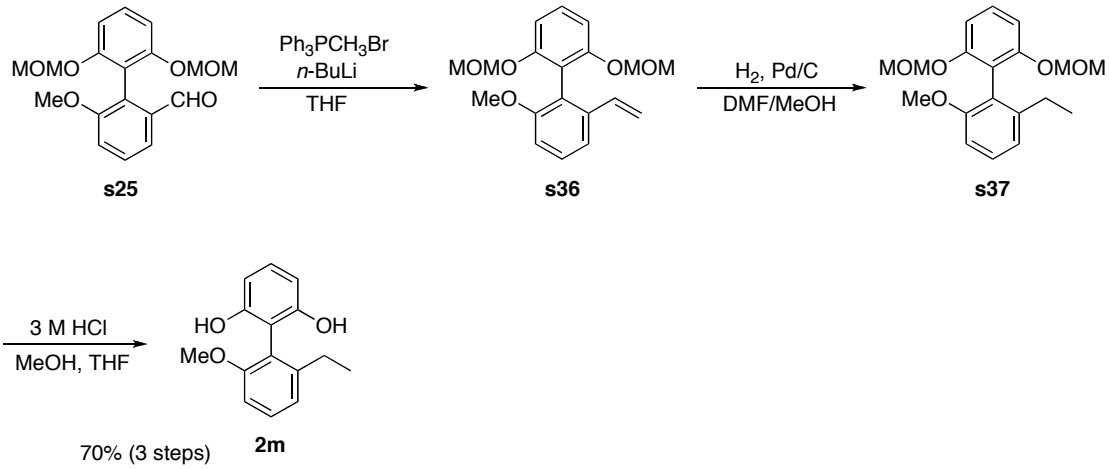
IR (KBr) 3366, 2991, 2930, 2829, 2250, 1909, 1620, 1595, 1462, 1377, 1306, 1279, 1256, 1190, 1152, 1129, 1092, 1008, 937, 909, 856, 822, 792, 735, 649 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$) δ 3.31 (s, 3H), 4.20 (s, 2H), 5.46 (s, 2H), 6.58 (d, 2H, J = 8.0 Hz), 7.16 (dd, 1H, J = 8.0, 8.0 Hz), 7.30 (d, 1H, J = 2.4 Hz), 7.44 (dd, 1H, J = 2.4, 8.4 Hz), 7.51 (d, 1H, J = 8.4 Hz).

^{13}C NMR (100 MHz, $CDCl_3$) δ 58.7, 72.7, 109.0, 114.4, 129.4, 130.1, 131.7, 131.8, 133.4, 135.1, 136.4, 153.8.

Anal. Calcd for $C_{14}H_{13}ClO_3$: C, 63.52; H, 4.95. Found: C, 63.84; H, 4.93.

Scheme 8. Preparation of **2m**.



Synthesis of 2'-Ethyl-6'-methoxybiphenyl-2,6-diol (2m):

To a suspension of Ph_3PCH_3Br (1.41 g, 3.95 mmol) in THF (10.0 mL) was *n*-BuLi (1.63 M in hexane, 2.3 mL, 3.75 mmol) at 0 °C. After stirring for 3 h at room temperature, a solution of aldehyde **s25** (870 mg, 2.62 mmol) was added to the reaction mixture at 0 °C. After being stirred at room temperature for 2 h, the reaction was stopped by adding saturated aqueous NH_4Cl at 0°C. The crude mixture was extracted with EtOAc (x3) and the combined organic extracts were washed with brine, dried (Na_2SO_4), and concentrated in vacuo. The residue was purified by column chromatography (silica gel, hexane/EtOAc = 2/1) to give **s36** (814 mg) with inseparable impurities. This material was used to next reaction without further purification.

To a solution of **s36** in MeOH (10.0 mL) and DMF (10.0 mL) was added 10% Pd/C (450 mg). After being stirred under H_2 (1 atm) at room temperature for 40 h, the reaction mixture was filtered through Celite® pad and concentrated in vacuo to give crude ester **s37** (1.33 g). The material was used for the next reaction without further purification.

To a solution of **s45** in THF (12.0 mL) and MeOH (12.0 mL) was added aqueous 2 M HCl (6.0 mL, 12.0 mmol) at 0 °C. After being stirred for 70 h at room temperature, the reaction was stopped by adding saturated aqueous $NaHCO_3$ at 0 °C. The crude mixture was extracted with EtOAc (x5) and the combined organic extracts were washed with brine, dried (Na_2SO_4), and concentrated in vacuo. The residue was purified by column chromatography (silica gel, hexane/EtOAc = 3/1) to give **2m** (548 mg, 70% from **s25**) as a white solid.

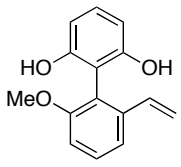
Mp. 139–141 °C.

IR (neat) 3534, 3490, 3413, 2968, 2936, 2872, 2838, 1626, 1576, 1508, 1465, 1437, 1338, 1303, 1260, 1175, 1147, 1091, 1061, 1040, 1006, 909, 886, 787, 749, 733, 648 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$) δ 1.04 (t, 3H, *J* = 7.6 Hz), 2.40 (q, 2H, *J* = 7.6 Hz), 3.74 (s, 3H), 4.62 (s, 2H), 6.59 (d, 2H, *J* = 8.0 Hz), 6.90 (d, 1H, *J* = 8.0 Hz), 7.04 (d, 1H, *J* = 8.0 Hz), 7.18 (dd, 1H, *J* = 8.0, 8.0 Hz), 7.41 (dd, 1H, *J* = 8.0, 8.0 Hz).

^{13}C NMR (100 MHz, $CDCl_3$) δ 15.0, 26.4, 55.9, 107.4, 109.1, 110.4, 116.6, 121.8, 129.5, 131.0, 147.5, 153.7, 158.4.

Anal. Calcd for $C_{15}H_{16}O_3$: C, 73.75; H, 6.60. Found: C, 73.84; H, 6.65.



2'-Methoxy-6'-vinylbiphenyl-2,6-diol (**2n**).

White solid.

Yield: (prepared from **s25**).

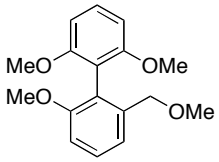
Mp. 130–131 °C.

IR (KBr) 3497, 3423, 3084, 3013, 2939, 2837, 1622, 1568, 1506, 1464, 1436, 1414, 1340, 1306, 1262, 1177, 1150, 1066, 1006, 909, 803, 787, 733, 645 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$) δ 3.77 (s, 3H), 4.66 (s, 2H), 5.24 (dd, 1H, *J* = 1.2, 11.2 Hz), 5.76 (dd, 1H, *J* = 1.2, 17.6 Hz), 6.44 (dd, 1H, *J* = 11.2, 17.6 Hz), 6.60 (d, 2H, *J* = 8.4 Hz), 6.98 (d, 1H, *J* = 8.0 Hz), 7.19 (dd, 1H, *J* = 8.4, 8.4 Hz), 7.38 (d, 1H, *J* = 8.0 Hz), 7.45 (dd, 1H, *J* = 8.0, 8.0 Hz).

^{13}C NMR (100 MHz, $CDCl_3$) δ 56.0, 107.7, 109.9, 110.7, 116.9, 117.1, 118.4, 129.8, 130.8, 133.6, 140.1, 153.8, 158.3.

Anal. Calcd for $C_{15}H_{14}O_3$: C, 74.36; H, 5.82. Found: C, 74.28; H, 6.03.



2,2',6-Trimethoxy-6'-(methoxymethyl)biphenyl (**2o**).

White solid.

Yield: 70% (from **s25**).

Mp. 136–137 °C.

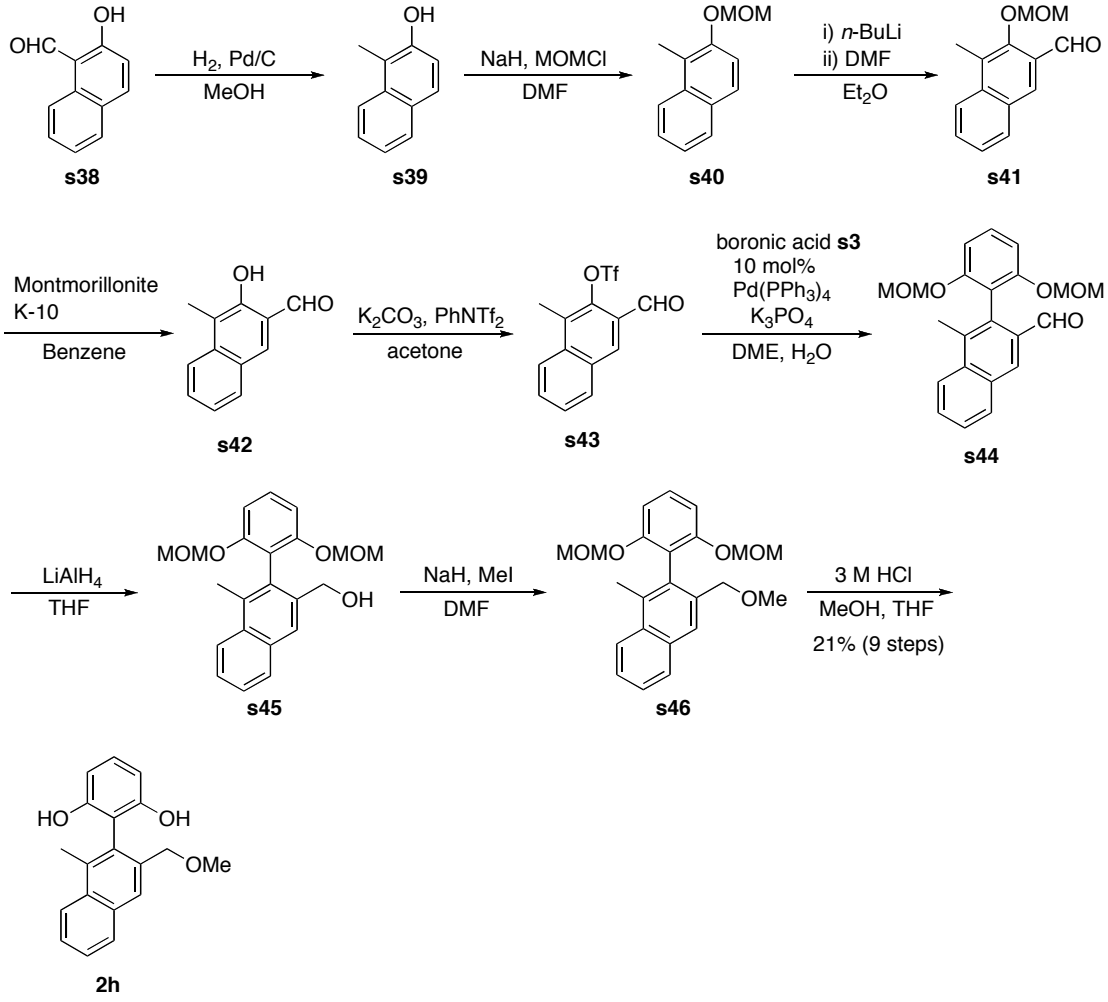
IR (neat) 3002, 2927, 2833, 1584, 1496, 1470, 1454, 1430, 1373, 1294, 1264, 1249, 1196, 1115, 1070, 1032, 1003, 904, 778, 741, 725 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$) δ 3.21 (s, 3H), 3.69 (s, 6H), 3.71 (s, 3H), 4.14 (s, 2H), 6.64 (d, 2H, *J* = 8.0 Hz), 6.90 (d, 1H, *J* = 8.0 Hz), 7.17 (d, 1H, *J* = 8.0 Hz), 7.31 (dd, 1H, *J* = 8.0, 8.0 Hz), 7.35 (dd, 1H, *J* = 8.0, 8.0 Hz).

^{13}C NMR (100 MHz, $CDCl_3$) δ 55.9, 56.1, 57.9, 71.9, 104.1, 110.0, 113.7, 119.3, 122.3, 128.3, 129.0, 138.9, 157.3, 157.9.

Anal. Calcd for $C_{17}H_{20}O_4$: C, 70.81; H, 6.99. Found: C, 70.86; H, 6.78.

Scheme 9. Preparation of **2h**.



Synthesis of 2-(3-(methoxymethyl)-1-methylnaphthalen-2-yl)benzene-1,3-diol (2h):

To a solution of aldehyde **s38** (2.00 g, 11.6 mmol) in MeOH (72.0 mL) was added 10% Pd/C (300 mg). After being stirred under H_2 (1 atm) at room temperature for 120 h, the reaction mixture was filtered through Celite® pad and concentrated in vacuo to give crude ester **s39** (2.35 g). The material was used for the next reaction without further purification.

To a suspension of NaH (60% oil, 697 mg, 17.4 mmol) in DMF (30.0 mL) were successively added a solution of **s39** in DMF (30.0 mL) and MOMCl (1.24 mL, 16.3 mmol) at 0 °C. After being stirred for 8 h at room temperature, the reaction was stopped by adding 1 M aqueous HCl. The crude products were extracted with EtOAc (x4) and the combined organic extracts were washed with 1 M aqueous HCl (x6), brine, dried (Na_2SO_4), and concentrated in vacuo to give crude **s40** (2.55 g). This material was used to next reaction without further purification.

To a solution of **s40** in Et_2O (53.0 mL) was added *n*-BuLi (1.65 M in hexane, 8.6 mL, 14.2 mmol) at 0 °C. After stirring for 3 h at room temperature, DMF (1.55 mL, 15.8 mmol) was added to the reaction mixture at 0 °C. After being stirred for 10 min at 0 °C, the reaction was stopped by adding saturated aqueous NH_4Cl. The crude products were extracted with EtOAc (x3) and the combined organic extracts were washed with brine, dried (Na_2SO_4), and concentrated in vacuo to give crude **s41** (2.70 g). This material was used to next reaction without further purification.

To a solution of **s41** in Benzene (58.0 mL) was added Montmorillonite K-10 (2.00 g) at room temperature. After being stirred for 1 h at room temperature, the crude material was filtered through Celite® pad, and the resulting filtrate was concentrated in vacuo to give crude **s42** (2.30 g). This material was used to next reaction without further purification.

To a solution of **s42** in acetone (50.0 mL) were successively added K_2CO_3 (2.40 g, 17.4 mmol) and $PhNTf_2$ (5.39 g, 15.1 mmol) at 0 °C. After being stirred for 4.5 h at room temperature, the reaction was stopped by adding $NaHCO_3$ at 0 °C. The crude products were extracted with EtOAc (x8) and the combined organic extracts were washed with brine, dried (Na_2SO_4), and concentrated in vacuo. The residue was purified by column chromatography (silica gel, hexane/EtOAc = 20/1) to give triflate **s43** (1.84 g) as a pale yellow oil with inseparable impurities. This material was used to next reaction without further purification.

The mixture of boronic acid **s3** (2.10 g, 8.68 mmol), triflate **s43**, $Pd(PPh_3)_4$ (668 mg, 0.578 mmol), K_3PO_4 (3.68 g, 17.3 mmol), DME (23.1 mL), and H_2O (5.6 mL) were heated at reflux for 3.5 h. After cooling to room temperature, the reaction was stopped by adding H_2O. The crude mixture was extracted with EtOAc (x3) and the combined organic extracts were washed with brine, dried (Na_2SO_4), and concentrated in vacuo. The residue was purified by column chromatography (silica gel, hexane/EtOAc = 3/1) to give **s44** (1.445 g) as a red solid with inseparable impurities. This material was used to next reaction without further purification.

To a solution of **s44** in THF (20.0 mL) was added $LiAlH_4$ (150 mg, 3.95 mmol) at 0 °C. After being stirred for 0.5 h at 0 °C, the reaction was stopped by adding $Na_2SO_4 \cdot 10H_2O$. After being stirred for another 1 h at room temperature, the crude material was filtered through Celite® pad and the resulting filtrate was concentrated in vacuo to give crude benzyl alcohol **s45** (1.65 g). The crude material was used for the next reaction without

further purification.

To a solution of **s45** in DMF (20.0 mL) were successively added NaH (60% oil, 315 mg, 7.88 mmol) and MeI (0.44 mL, 7.09 mmol) at 0 °C. After being stirred for 6 h at room temperature, the reaction was stopped by adding aqueous 1 M HCl at 0 °C. The crude mixture was extracted with EtOAc (x4) and the combined organic extracts were washed with 1 M aqueous HCl (x6), brine, dried (Na_2SO_4), and concentrated in vacuo to give methyl ether **s46** (1.80 g). The crude material was used for the next reaction without further purification.

To a solution of **s46** in THF (15.0 mL) and MeOH (10.0 mL) was added aqueous 3 M HCl (10.0 mL, 30.0 mmol) at 0 °C. After being stirred for 72 h at room temperature, the reaction was stopped by adding saturated aqueous $NaHCO_3$ at 0 °C. The crude mixture was extracted with EtOAc (x5) and the combined organic extracts were washed with brine, dried (Na_2SO_4), and concentrated in vacuo. The residue was purified by column chromatography (silica gel, hexane/EtOAc = 4/1) to give **2h** (700 mg, 21% from **s38**) as a white solid.

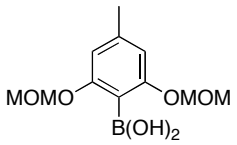
Mp. 145–146 °C.

IR (neat) 3389, 3069, 2989, 2925, 2826, 1620, 1582, 1500, 1463, 1382, 1338, 1308, 1275, 1174, 1150, 1124, 1086, 1006, 950, 910, 885, 786, 750, 732 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$) δ 2.44 (s, 3H), 3.29 (s, 3H), 4.28 (s, 2H), 4.97 (s, 2H), 6.67 (d, 2H, *J* = 8.0 Hz), 7.23 (dd, 1H, *J* = 8.0, 8.0 Hz), 7.52–7.66 (m, 2H), 7.84–7.97 (m, 2H), 8.04–8.16 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 15.6, 58.7, 74.2, 108.6, 114.5, 124.7, 126.5, 126.8, 126.9, 127.7, 128.7, 129.8, 132.8, 133.5, 135.2, 136.9, 153.8.

Anal. Calcd for $C_{19}H_{18}O_3$: C, 77.53; H, 6.16. Found: C, 77.53 ; H, 6.03.



2,6-bis(methoxymethoxy)-4-methylphenylboronic acid (**s47**) was synthesized according to the procedure of **s3**.

White solid.

Yield: 55% (from commercially available 3-methylresorcinol).

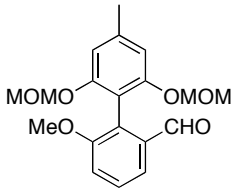
Mp. 103–104 °C.

IR (KBr) 2224, 2952, 2906, 2852, 2830, 1611, 1577, 1479, 1433, 1388, 1340, 1305, 1232, 1199, 1154, 1110, 1055, 961, 920, 906 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$) δ 2.35 (s, 3H), 3.51 (s, 6H), 5.28 (s, 4H), 6.70 (s, 2H), 7.17 (s, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 22.2, 56.6, 94.7, 109.1, 144.1, 163.1.

Anal. Calcd for $C_{11}H_{17}BO_6$: C, 51.60; H, 6.69. Found: C, 51.88; H, 6.58.



6-Methoxy-2',6'-bis(methoxymethoxy)-4'-methylbiphenyl-2-carbaldehyde (**s48**).

White amorphous.

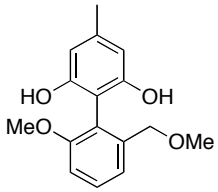
Yield: 75% (prepared from **s7** and **s47**).

IR (neat) 2955, 2907, 2831, 1697, 1686, 1610, 1593, 1579, 1468, 1439, 1391, 1304, 1263, 1244, 1210, 1152, 1111, 1048, 1011, 961, 920, 823 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$) δ 2.39 (s, 3H), 3.26 (s, 6H), 3.76 (s, 3H), 4.98 (d, 1H, J = 6.8 Hz), 5.03 (d, 1H, J = 6.8 Hz), 6.74 (s, 2H), 7.18 (dd, 1H, J = 1.2, 8.0 Hz), 7.44 (ddd, 1H, J = 0.8, 8.0, 8.0 Hz), 7.62 (dd, 1H, J = 1.2, 8.0 Hz), 9.74 (d, 1H, J = 0.8 Hz).

^{13}C NMR (100 MHz, $CDCl_3$) δ 22.1, 55.8, 55.9, 94.6, 109.4, 110.1, 115.8, 118.5, 128.1, 128.5, 135.5, 140.5, 155.7, 157.7, 193.1.

Anal. Calcd for $C_{19}H_{22}O_6$: C, 65.88; H, 6.40. Found: C, 66.13; H, 6.25.



2'-Methoxy-6'-(methoxymethyl)-4-methylbiphenyl-2,6-diol (**2l**).

White solid.

Yield: 51% (prepared from **s48**).

IR (neat) 3407, 2927, 2834, 1632, 1578, 1522, 1468, 1263, 1175, 1070, 1049, 1004, 911, 825, 798, 734 cm^{-1}.

^{1}H NMR (400 MHz, $CDCl_3$) δ 3.19 (s, 3H), 3.62 (s, 3H), 3.66 (s, 3H), 4.01 (d, 1H, *J* = 11.6 Hz), 4.16 (d, 1H, *J* = 11.6 Hz), 5.27 (s, 1H), 6.45 (s, 2H), 7.00 (d, 1H, *J* = 8.0 Hz), 7.19 (d, 1H, *J* = 8.0 Hz), 7.44 (dd, 1H, *J* = 8.0, 8.0 Hz).

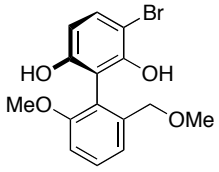
^{13}C NMR (100 MHz, $CDCl_3$) δ 21.5, 56.0, 58.6, 73.0, 108.0, 109.4, 111.5, 118.8, 122.1, 130.5, 140.1, 140.2, 153.7, 158.2.

Anal. Calcd for $C_{16}H_{18}O_4$: C, 70.06; H, 6.61. Found: C, 70.15; H, 6.56.

3. Synthesis of chiral biaryls.

General Procedure for the formation of monobrominated-biaryls.

To a suspension of biphenol **2** (0.10 mmol), chiral phosphoric acid **1** (0.01 mmol, 10 mol%) and powered MS13X (25 mg, activated) in CH_2Cl_2 (0.5 mL) and toluene (0.5 mL) was added *N*-bromophthalimide (0.11 or 0.12 mmol, 1.1–1.2 equiv.) at –20 °C. After completion of the reaction, the reaction was stopped by adding saturated aqueous $NaHCO_3$. The crude mixture was extracted with EtOAc (x3) and the combined organic extracts were washed with brine, dried (Na_2SO_4), and concentrated in vacuo. The residue was purified by preparative TLC to give monobromide **3**.



(*R*)-3-Bromo-2'-methoxy-6'-(methoxymethyl)biphenyl-2,6-diol (**3a**).

Colorless amorphous.

Yield: 88%, 97% ee.

HPLC [DAICEL CHIRALPAK® AD-H, ϕ 0.46 x 25 cm, hexane/*i*-PrOH = 5/1, 1.0 mL/min, 254 nm, retention time (min) = 14.5 (1.5%), 21.8 (98.5%)].

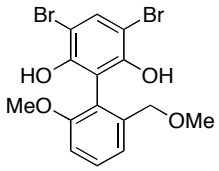
$[\alpha]_D^{27}$ –264 (c 1.00, $CHCl_3$).

IR (neat) 3490, 2933, 2835, 1613, 1596, 1578, 1469, 1439, 1378, 1307, 1265, 1176, 1120, 1070, 1031, 1009, 910, 800, 734, 690, 637 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$) δ 3.29 (s, 3H), 3.75 (s, 3H), 4.13 (d, 1H, *J* = 10.8 Hz), 4.21 (d, 1H, *J* = 10.8 Hz), 5.45 (brs, 1H), 5.52 (s, 1H), 6.58 (d, 1H, *J* = 8.4 Hz), 7.02 (dd, 1H, *J* = 0.8, 8.4 Hz), 7.19 (dd, 1H, *J* = 0.8, 8.4 Hz), 7.39 (d, 1H, *J* = 8.4 Hz), 7.46 (dd, 1H, *J* = 8.4, 8.4 Hz).

^{13}C NMR (100 MHz, $CDCl_3$) δ 56.1, 58.6, 73.1, 101.3, 110.3, 111.4, 112.3, 119.2, 121.9, 130.6, 131.9, 139.5, 150.3, 154.1, 157.8.

Anal. Calcd for $C_{15}H_{15}BrO_4$: C, 53.12; H, 4.46. Found: C, 53.26; H, 4.55.



3,5-Dibromo-2'-methoxy-6'-(methoxymethyl)biphenyl-2,6-diol (**4**).

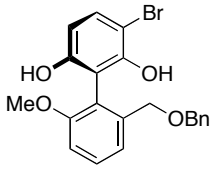
Yellow solid.

IR (neat) 3493, 2932, 2835, 1579, 1469, 1448, 1435, 1378, 1299, 1266, 1169, 1071, 1030, 909, 815, 796, 733, 686, 620 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$) δ 3.28 (s, 3H), 3.74 (s, 3H), 4.16 (s, 2H), 5.75 (s, 2H), 7.00 (dd, 1H, J = 0.8, 8.4 Hz), 7.17 (dd, 1H, J = 0.8, 8.4 Hz), 7.45 (dd, 1H, J = 8.4, 8.4 Hz), 7.66 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 56.0, 58.5, 73.0, 101.8, 111.2, 113.1, 119.3, 121.7, 130.7, 133.7, 139.0, 150.4, 157.6.

Anal. Calcd for $C_{15}H_{14}Br_2O_4$: C, 43.09; H, 3.38. Found: C, 43.26; H, 3.42.



(*R*)-2'-(Benzyloxymethyl)-3-bromo-6'-methoxybiphenyl-2,6-diol (**3b**).

Colorless amorphous.

Yield: 80%, 99% ee.

HPLC [DAICEL CHIRALPAK® AD-H, ϕ 0.46 x 25 cm, hexane/*i*-PrOH = 1/1, 1.0 mL/min, 254 nm, retention time (min) = 6.0 (0.6%), 8.9 (99.4%)].

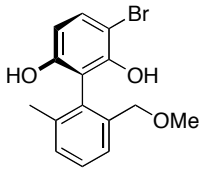
$[\alpha]_D^{26}$ +5.8 (c 1.00, $CHCl_3$), 99% ee.

IR (neat) 3493, 3064, 3031, 2932, 2865, 2838, 1614, 1596, 1579, 1469, 1456, 1439, 1356, 1305, 1266, 1175, 1121, 1063, 1029, 1009, 910, 800, 739, 699, 648, 622 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$) δ 3.74 (s, 3H), 4.21 (d, 1H, J = 10.8 Hz), 4.27 (d, 1H, J = 10.8 Hz), 4.40 (d, 1H, J = 12.0 Hz), 4.43 (d, 1H, J = 12.0 Hz), 5.29 (brs, 1H), 5.48 (s, 1H), 6.56 (d, 1H, J = 8.8 Hz), 7.00 (dd, 1H, J = 0.8, 8.4 Hz), 7.16–7.35 (m, 6H), 7.38 (d, 1H, J = 8.8 Hz), 7.45 (dd, 1H, J = 8.4, 8.4 Hz).

^{13}C NMR (100 MHz, $CDCl_3$) δ 56.1, 70.6, 73.1, 101.2, 110.1, 111.4, 112.2, 119.2, 122.3, 127.8, 128.0, 128.4, 130.7, 131.9, 137.4, 139.6, 150.2, 154.0, 157.8.

Anal. Calcd for $C_{21}H_{19}BrO_4$: C, 63.17; H, 4.80. Found: C, 63.03; H, 4.86.



(*S*)-3-Bromo-2'-(methoxymethyl)-6'-methylbiphenyl-2,6-diol (**3c**).

Colorless oil.

Yield: 90%, 95% ee.

HPLC [DAICEL CHIRALPAK® AD-H, ϕ 0.46 x 25 cm, hexane/*i*-PrOH = 5/1, 1.0 mL/min, 254 nm, retention time (min) = 6.4 (97.4%), 7.1 (2.6%)].

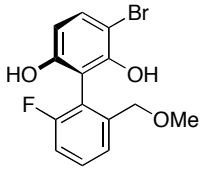
$[\alpha]_D^{26}$ –21.7 (c 0.955, $CHCl_3$).

IR (neat) 3484, 3372, 2925, 2827, 1611, 1572, 1444, 1380, 1307, 1237, 1172, 1119, 1082, 1037, 1008, 933, 909, 789, 733, 684, 623 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$) δ 2.05 (s, 3H), 3.27 (s, 3H), 4.12 (d, 1H, *J* = 10.8 Hz), 4.18 (d, 1H, *J* = 10.8 Hz), 5.38 (brs, 1H), 5.49 (s, 1H), 6.60 (d, 1H, *J* = 8.4 Hz), 7.30–7.46 (m, 4H).

^{13}C NMR (100 MHz, CD_3COCD_3) δ 19.7, 58.6, 73.8, 101.3, 110.5, 115.2, 127.4, 129.4, 130.3, 130.8, 132.0, 137.8, 139.2, 149.7, 153.7.

Anal. Calcd for $C_{16}H_{17}BrO_3$: C, 55.75; H, 4.68. Found: C, 56.03; H, 4.95.



(*R*)-3-Bromo-2'-fluoro-6'-(methoxymethyl)biphenyl-2,6-diol (**3d**).

Colorless oil.

Yield: 91%, 94% ee.

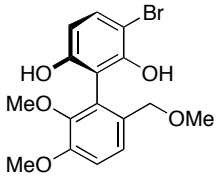
HPLC [DAICEL CHIRALPAK® AD-H, ϕ 0.46 x 25 cm, hexane/*i*-PrOH = 10/1, 1.0 mL/min, 254 nm, retention time (min) = 19.9 (96.9%), 21.8 (3.1%)].

$[\alpha]_D^{26}$ –35.0 (c 1.000, $CHCl_3$).

IR (neat) 3494, 3331, 2931, 2830, 1606, 1576, 1459, 1441, 1379, 1308, 1250, 1193, 1123, 1078, 1034, 1010, 935, 906, 795, 757, 737, 687, 635 cm^{-1}.

^{1}H NMR (400 MHz, $CDCl_3$) δ 3.30 (s, 3H), 4.18 (d, 1H, *J* = 10.8 Hz), 4.25 (d, 2H, *J* = 10.8 Hz), 5.66 (brs, 1H), 6.03 (brs, 1H), 6.56 (d, 1H, *J* = 8.8 Hz), 7.16 (dd, 1H, *J* = ^{13}C NMR (100 MHz, $CDCl_3$) δ 58.9, 72.9, 101.5, 109.9, 110.8, 115.9 (d, *J* = 22.3 Hz), 119.5 (d, *J* = 17.1 Hz), 125.2, 130.5 (d, *J* = 8.2 Hz), 132.3, 139.4, 150.4, 154.5, 160.5 (d, *J* = 246 Hz).

Anal. Calcd for $C_{14}H_{12}BrFO_3$: C, 51.40; H, 3.70. Found: C, 51.51; H, 3.70.



(*R*)-3-Bromo-2',3'-dimethoxy-6'-(methoxymethyl)biphenyl-2,6-diol (**3e**).

Colorless amorphous.

Yield: 87%, 98% ee

HPLC [DAICEL CHIRALPAK® AD-H, ϕ 0.46 x 25 cm, hexane/*i*-PrOH = 5/1, 1.0 mL/min, 254 nm, retention time (min) = 10.9 (1.0%), 18.0 (99.0%)].

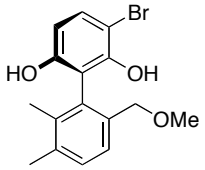
$[\alpha]_D^{26}$ –5.0 (c 0.79, $CHCl_3$).

IR (neat) 3389, 2938, 2836, 2249, 1771, 1725, 1609, 1576, 1486, 1443, 1417, 1378, 1308, 1271, 1184, 1132, 1111, 7080, 1037, 1017, 910, 865, 809, 733, 681, 647 cm^{-1}.

^{1}H NMR (400 MHz, $CDCl_3$) δ 3.27 (s, 3H), 3.59 (s, 3H), 3.91 (s, 3H), 4.08 (d, 1H, *J* = 10.4 Hz), 4.15 (d, 1H, *J* = 10.4 Hz), 5.72 (s, 1H), 5.81 (brs, 1H), 6.60 (d, 1H, *J* = 8.8 Hz), 7.02 (d, 1H, *J* = 8.4 Hz), 7.26 (d, 1H, *J* = 8.4 Hz), 7.40 (d, 1H, *J* = 8.8 Hz).

^{13}C NMR (100 MHz, $CDCl_3$) δ 55.8, 58.3, 60.8, 73.3, 101.7, 111.0, 112.8, 113.1, 126.0, 126.3, 130.0, 132.0, 147.6, 150.3, 153.3, 154.3.

Anal. Calcd for $C_{16}H_{17}BrO_5$: C, 52.05; H, 4.64. Found: C, 52.27; H, 4.52.



(*S*)-3-Bromo-6'-(methoxymethyl)-2',3'-dimethylbiphenyl-2,6-diol (**3f**).

White solid.

Yield: 76%, 96% ee.

HPLC [DAICEL CHIRALPAK® AD-H, ϕ 0.46 x 25 cm, hexane/*i*-PrOH = 5/1, 1.0 mL/min, 254 nm, retention time (min) = 6.2 (98.2%), 8.1 (1.8%)].

$[\alpha]_D^{26}$ –65.6 (c 1.00, $CHCl_3$).

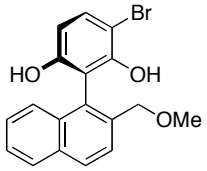
Mp. 103–104 °C.

IR (neat) 3483, 2924, 2825, 1611, 1571, 1469, 1443, 1383, 1308, 1237, 1175, 1083, 1025, 1005, 906, 845, 820, 802, 733, 671, 621 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$) δ 1.95 (s, 3H), 2.34 (s, 3H), 3.24 (s, 3H), 4.07 (d, 1H, *J* = 10.4 Hz), 4.13 (d, 1H, *J* = 10.4 Hz), 5.36 (brs, 1H), 5.49 (s, 1H), 6.59 (d, 1H, *J* = 8.8 Hz), 7.26 (d, 1H, *J* = 8.0 Hz), 7.29 (d, 1H, *J* = 8.0 Hz), 7.40 (d, 1H, *J* = 8.8 Hz).

^{13}C NMR (100 MHz, $CDCl_3$) δ 16.2, 20.7, 58.4, 73.9, 101.3, 110.4, 115.9, 127.3, 130.1, 130.9, 131.9, 135.3, 137.6, 138.1, 149.8, 153.7.

Anal. Calcd for $C_{16}H_{17}BrO_3$: C, 56.99; H, 5.08. Found: C, 56.82; H, 4.99.



(*S*)-4-Bromo-2-(2-(methoxymethyl)naphthalen-1-yl)benzene-1,3-diol (**3g**).

Colorless solid (recrystallized from hexane/CH_2Cl_2), which is subjected to X-ray crystal analysis.

Yield: 82%, 95% ee.

HPLC [DAICEL CHIRALCEL® OD-H, ϕ 0.46 x 25 cm, hexane/*i*-PrOH = 5/1, 1.0 mL/min, 254 nm, retention time (min) = 6.9 (97.7%), 9.1 (2.3%)].

$[\alpha]_D^{26}$ –37.7 (c 1.00, CHCl3).

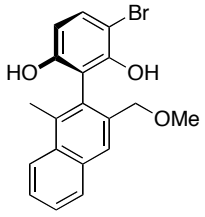
Mp. 104–105 °C.

IR (neat) 3500, 3347, 3058, 2927, 2352, 1610, 1573, 1508, 1442, 1308, 1237, 1173, 1127, 1083, 1022, 977, 908, 867, 843, 820, 754, 731, 622 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$) δ 3.32 (s, 3H), 4.32 (d, 1H, *J* = 10.8 Hz), 4.38 (d, 1H, *J* = 10.8 Hz), 5.33 (brs, 1H), 5.48 (s, 1H), 6.65 (d, 1H, *J* = 8.8 Hz), 7.34–7.58 (m, 4H), 7.68 (d, 1H, *J* = 8.8 Hz), 7.90 (d, 1H, *J* = 8.4 Hz), 7.97 (d, 1H, *J* = 8.4 Hz).

^{13}C NMR (100 MHz, $CDCl_3$) δ 58.7, 73.4, 101.3, 110.4, 113.5, 125.2, 126.6, 126.8, 127.2, 127.7, 128.3, 129.9, 132.2, 132.4, 133.7, 136.1, 150.5, 154.4.

Anal. Calcd for $C_{18}H_{15}BrO_3$: C, 60.18; H, 4.21. Found: C, 59.88; H, 4.12.



(*S*)-4-Bromo-2-(3-(methoxymethyl)-1-methylnaphthalen-2-yl)benzene-1,3-diol (**3h**).

Colorless solid (recrystallized from hexane/CH_2Cl_2), which is subjected to X-ray crystal analysis.

Yield: 90%, 95% ee.

HPLC [DAICEL CHIRALPAK® AS-H, ϕ 0.46 x 25 cm, hexane/*i*-PrOH = 10/1, 0.5 mL/min, 254 nm, retention time (min) = 28.7 (2.4%), 34.2 (97.6%)].

$[\alpha]_D^{26}$ –95.3 (c 1.00, $CHCl_3$).

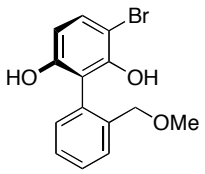
Mp. 88–89 °C.

IR (neat) 3503, 3384, 3070, 2989, 2925, 2827, 2361, 2249, 1612, 1572, 1476, 1442, 1383, 1308, 1236, 1173, 1115, 1088, 1020, 993, 909, 886, 851, 802, 750, 733, 683, 660 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$) δ 2.41 (s, 3H), 3.29 (s, 3H), 4.23 (d, 1H, *J* = 10.8 Hz), 4.29 (d, 1H, *J* = 10.8 Hz), 5.18 (brs, 1H), 5.47 (s, 1H), 6.62 (d, 1H, *J* = 8.8 Hz), 7.44 (d, 1H, *J* = 8.8 Hz), 7.50–7.66 (m, 2H), 7.84–7.97 (m, 2H), 8.03–8.15 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 15.6, 58.6, 74.1, 101.3, 110.3, 115.6, 124.7, 126.6, 126.8, 127.0, 127.3, 128.7, 132.1, 132.6, 133.5, 134.7, 136.1, 150.0, 153.8.

Anal. Calcd for $C_{19}H_{17}BrO_3$: C, 61.14; H, 4.59. Found: C, 61.02 ; H, 4.72.



(*S*)-3-Bromo-2'-(methoxymethyl)biphenyl-2,6-diol (**3i**).

White solid.

Yield: 82%, 92% ee.

HPLC [DAICEL CHIRALPAK® AD-H, ϕ 0.46 x 25 cm, hexane/*i*-PrOH = 5/1, 1.0 mL/min, 254 nm, retention time (min) = 7.2 (95.9%), 8.8 (4.1%)].

$[\alpha]_D^{26}$ –1.50 (c 1.00, $CHCl_3$).

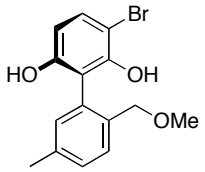
Mp. 126–128 °C.

IR (neat) 3491, 3360, 2927, 2827, 1612, 1573, 1468, 1439, 1308, 1237, 1173, 1115, 1081, 1030, 1009, 910, 801, 768, 753, 732, 698, 638 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$) δ 3.32 (s, 3H), 4.21 (d, 1H, *J* = 10.4 Hz), 4.27 (d, 1H, *J* = 10.4 Hz), 5.63 (s, 1H), 5.74 (brs, 1H), 7.21–7.31 (m, 1H), 7.38 (d, 1H, *J* = 8.8 Hz), 7.42–7.52 (m, 2H), 7.53–7.62 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 58.6, 73.3, 101.4, 110.5, 116.5, 129.3, 129.4, 130.3, 131.3, 131.5, 131.9, 137.5, 150.1, 154.0.

Anal. Calcd for $C_{14}H_{13}BrO_3$: C, 54.39; H, 4.24. Found: C, 54.47; H, 4.33.



(*S*)-3-Bromo-2'-(methoxymethyl)-5'-methylbiphenyl-2,6-diol (**3j**).

White solid.

Yield: 82%, 91% ee.

HPLC [DAICEL CHIRALPAK® AD-H, ϕ 0.46 x 25 cm, hexane/*i*-PrOH = 10/1, 1.0 mL/min, 254 nm, retention time (min) = 12.4 (95.6%), 15.7 (4.4%)].

$[\alpha]_D^{26}$ –3.7 (c 0.88, $CHCl_3$).

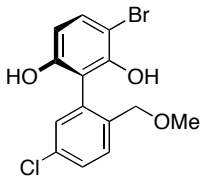
Mp. 133–134 °C.

IR (neat) 3492, 3365, 2924, 2827, 1612, 1574, 1470, 1442, 1378, 1308, 1236, 1189, 1167, 1119, 1080, 1045, 1016, 910, 826, 800, 766, 732, 696, 648 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$) δ 2.39 (s, 3H), 3.31 (s, 3H), 4.18 (d, 1H, *J* = 10.0 Hz), 4.23 (d, 1H, *J* = 10.0 Hz), 5.67 (s, 1H), 5.80 (brs, 1H), 6.58 (d, 1H, *J* = 8.8 Hz), 7.09 (brs, 1H), 7.28 (brd, 1H, *J* = 8.0 Hz), 7.38 (d, 1H, *J* = 8.8 Hz), 7.45 (d, 1H, *J* = 8.0 Hz).

^{13}C NMR (100 MHz, $CDCl_3$) δ 21.1, 58.5, 73.3, 101.4, 110.6, 116.8, 130.2, 130.5, 131.3, 131.9, 132.0, 134.4, 139.5, 150.1, 154.0.

Anal. Calcd for $C_{15}H_{15}BrO_3$: C, 55.75; H, 4.68. Found: C, 55.95; H, 4.58.



(*S*)-3-Bromo-5'-chloro-2'-(methoxymethyl)biphenyl-2,6-diol (**3k**).

White solid.

Yield: 81%, 93% ee.

HPLC [DAICEL CHIRALCEL® OD-H, ϕ 0.46 x 25 cm, hexane/*i*-PrOH = 10/1, 1.0 mL/min, 254 nm, retention time (min) = 9.6 (96.3%), 14.8 (3.7%)].

$[\alpha]_D^{26}$ –61.8 (c 0.790, $CHCl_3$).

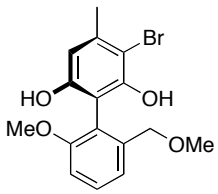
Mp. 109–110 °C.

IR (neat) 3492, 3338, 2930, 2828, 1609, 1574, 1468, 1443, 1307, 1238, 1191, 1120, 1092, 1039, 1014, 908, 863, 824, 799, 732, 668, 644 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$) δ 3.29 (s, 3H), 4.16 (d, 1H, *J* = 10.8 Hz), 4.22 (d, 1H, *J* = 10.8 Hz), 5.66 (s, 1H), 5.94 (brs, 1H), 6.53 (d, 1H, *J* = 8.8 Hz), 7.25 (d, 1H, *J* = 2.4 Hz), 7.37 (d, 1H, *J* = 8.8 Hz), 7.41 (dd, 1H, *J* = 2.4, 8.4 Hz), 7.48 (d, 1H, *J* = 8.4 Hz).

^{13}C NMR (100 MHz, $CDCl_3$) δ 58.6, 72.6, 101.5, 110.7, 115.4, 129.1, 131.2, 131.4, 132.1, 133.5, 134.6, 135.8, 149.9, 153.9.

Anal. Calcd for $C_{14}H_{12}BrClO_3$: C, 48.94; H, 3.52. Found: C, 48.71; H, 3.60.



(*R*)-3-Bromo-2'-methoxy-6'-(methoxymethyl)-4-methylbiphenyl-2,6-diol (**3l**).

White solid.

Yield: 80%, 44% ee.

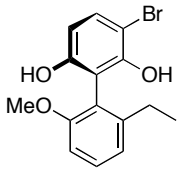
HPLC [DAICEL CHIRALPAK® AD-H, ϕ 0.46 x 25 cm, hexane/*i*-PrOH = 10/1, 1.0 mL/min, 254 nm, retention time (min) = 23.6 (27.9%), 43.3 (72.1%)].

IR (neat) 3487, 2925, 2385, 1618, 1578, 1469, 1453, 1404, 1378, 1350, 1263, 1168, 1066, 1004, 909, 836, 785 cm^{-1}.

^{1}H NMR (400 MHz, $CDCl_3$) δ 2.41 (s, 3H), 3.29 (s, 3H), 3.75 (s, 3H), 4.14 (d, 1H, *J* = 11.2 Hz), 4.56 (d, 1H, *J* = 11.2 Hz), 5.43 (brs, 1H), 5.58 (s, 1H), 6.60 (s, 1H), 7.01 (d, 1H, *J* = 8.0 Hz), 7.18 (d, 1H, *J* = 8.0 Hz), 7.44 (d, 1H, *J* = 8.0, 8.0 Hz).

^{13}C NMR (100 MHz, $CDCl_3$) δ 23.2, 56.1, 58.5, 73.0, 104.3, 109.2, 111.0, 111.2, 119.5, 121.7, 130.4, 138.7, 139.6, 150.1, 153.2, 157.9.

Anal. Calcd for $C_{16}H_{17}BrO_4$: C, 54.41; H, 4.85. Found: C, 54.28; H, 4.99.



(*R*)-3-Bromo-2'-ethyl-6'-methoxybiphenyl-2,6-diol (**3m**).

Colorless oil.

Yield: 86%, 0% ee.

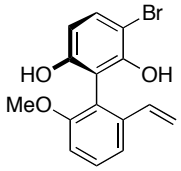
HPLC [DAICEL CHIRALPAK® AD-H, ϕ 0.46 x 25 cm, hexane/*i*-PrOH = 5/1, 1.0 mL/min, 254 nm, retention time (min) = 8.4 (50.0%), 19.3 (50.0%)].

IR (neat) 3488, 2967, 2935, 2837, 1617, 1593, 1574, 1468, 1437, 1331, 1303, 1261, 1173, 1120, 1106, 1088, 1060, 1041, 1007, 909, 887, 803, 733, 675, 623 cm^{-1}.

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.05 (t, 3H, *J* = 7.6 Hz), 2.38 (q, 2H, *J* = 7.6 Hz), 3.74 (s, 3H), 4.66 (brs, 1H), 5.26 (s, 1H), 6.55 (d, 1H, *J* = 8.8 Hz), 6.90 (d, 1H, *J* = 8.8 Hz), 7.03 (d, 1H, *J* = 8.0 Hz), 7.37 (d, 1H, *J* = 8.8 Hz), 7.41 (dd, 1H, *J* = 8.0, 8.8 Hz).

^{13}C NMR (100 MHz, $CDCl_3$) δ 14.9, 26.3, 55.9, 100.5, 108.8, 109.0, 111.8117.3, 121.6, 130.9, 131.7, 146.8, 150.0, 153.6, 157.9.

Anal. Calcd for $C_{15}H_{15}BrO_3$: C, 55.75; H, 4.68. Found: C, 55.88; H, 4.88.



(*R*)-3-Bromo-2'-methoxy-6'-vinylbiphenyl-2,6-diol (**3n**).

Colorless oil.

Yield: 84%, 2% ee.

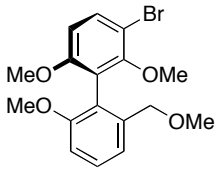
HPLC [DAICEL CHIRALPAK® AD-H, ϕ 0.46 x 25 cm, hexane/*i*-PrOH = 5/1, 1.0 mL/min, 254 nm, retention time (min) = 14.6 (51.0%), 27.1 (49.0%)].

IR (neat) 3493, 3084, 2939, 2837, 1615, 1592, 1569, 1468, 1455, 1438, 1412, 1308, 1263, 1174, 1123, 1067, 1024, 1006, 908, 805, 733 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$) δ 3.76 (s, 3H), 4.71 (brs, 1H), 5.22 (dd, 1H, *J* = 1.2, 10.8 Hz), 5.31 (s, 1H), 5.74 (dd, 1H, *J* = 1.2, 17.2 Hz), 6.40 (dd, 1H, *J* = 10.8, 17.2 Hz), 6.54 (d, 1H, *J* = 8.8 Hz), 6.96 (d, 1H, *J* = 8.0 Hz), 7.30–7.50 (m, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 56.0, 100.7, 109.0, 110.6, 111.1, 116.8, 117.5, 118.1, 130.7, 131.9, 133.6, 139.5, 150.1, 153.7, 157.9.

Anal. Calcd for $C_{15}H_{13}BrO_3$: C, 56.10; H, 4.08. Found: C, 56.10; H, 4.02.



(*R*)-3-Bromo-2,2',6-trimethoxy-6'-(methoxymethyl)biphenyl (**3o**).

Colorless amorphous.

Yield: 14%, 17% ee.

HPLC [DAICEL CHIRALCEL® OD-H, ϕ 0.46 x 25 cm, hexane/*i*-PrOH = 20/1, 0.2 mL/min, 254 nm, retention time (min) = 32.5 (58.4%), 37.4 (41.6%)].

IR (neat) 2936, 2835, 1578, 1461, 1433, 1401, 1376, 1285, 1264, 1220, 1195, 1091, 1073, 1019, 914, 802, 784, 748, 687, 634 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$) δ 3.23 (s, 3H), 3.44 (s, 3H), 3.68 (s, 3H), 3.73 (s, 3H), 4.10 (d, 1H, *J* = 12.8 Hz), 4.19 (d, 1H, *J* = 12.8 Hz), 6.66 (d, 1H, *J* = 8.8 Hz), 6.91 (d, 1H, *J* = 8.0 Hz), 7.18 (d, 1H, *J* = 8.0 Hz), 7.38 (dd, 1H, *J* = 8.0, 8.0 Hz), 7.51 (d, 1H, *J* = 8.8 Hz).

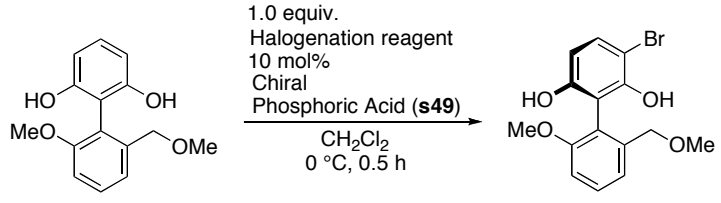
^{13}C NMR (100 MHz, $CDCl_3$) δ 55.8, 56.1, 58.2, 60.2, 72.0, 108.1, 108.3, 109.7, 119.4, 120.9, 121.4, 128.9, 132.3, 138.8, 155.2, 157.0, 157.6.

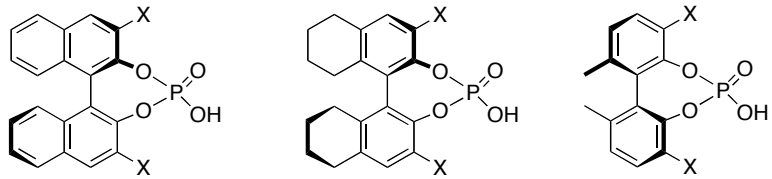
Anal. Calcd for $C_{17}H_{19}BrO_4$: C, 55.60; H, 5.21. Found: C, 55.78; H, 5.41.

4. Examination of the reaction conditions

Table 1 illustrates the screening of the catalyst and reaction conditions. Treatment of **2a** in CH_2Cl_2 with NBS (1.0 equiv) in the presence of phenyl substituted catalyst **s49a** offered **3a** in good yield, albeit with low ee (80%, 9% ee, entry 1). Although the catalysts with bulky substituent and electron withdrawing group resulted in disappointing selectivities (less than 10% ee, entries 2–5), the treatment of catalysts with polyaromatic-ring led to enhancement of the selectivities (entries 6–10). Especially, the 9-anthryl substituted catalyst **s49j** offered promising result to give **3a** in 93% with 34% ee (entry 10). The chiral scaffold of the phosphoric acids was also important, and **3a** was obtained in 96% with 48% ee when the reduced-phosphoric acid **1** (X = 9-anthryl) was employed (Entry 11). Furthermore, the use of *N*-bromophthalimide instead of NBS as a bromine source increased the selectivity to 68% ee with maintaining excellent chemical yield (entry 13). Further investigation revealed that the minute tuning of the reaction conditions (solvent, additive, and temperature) was critical for improving the enantioselectivity to excellent level (entries 14–16): treatment of **2a** in CH_2Cl_2/toluene (1/1) with **1** in the presence of MS13X at –20 °C afforded **3a** in 97% with 93% ee (entry 15).

Table 1. Examination of the reaction conditions.



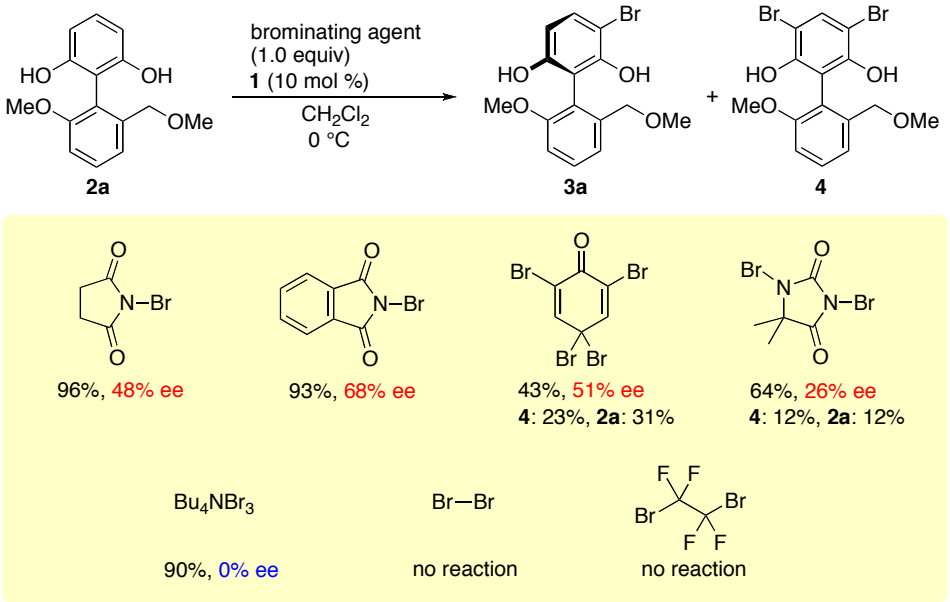


Entry	Ar	Yield (%)	Ee (%)[b]
1	Ph (**s49a**)	80	9
2	4-$(NO_2)C_6H_4$ (**s49b**)	82	6
3	4-$CF_3C_6H_4$ (**s49c**)	94	8
4	$SiPh_3$ (**s49d**)	89	2
5	2,4,6-$(i\text{-}Pr)_3C_6H_2$ (**s49e**)	79	2
6	1-naphtyl (**s49f**)	79	15
7	2-naphtyl (**s49g**)	90	23

8	9-phenanthryl (**s49h**)	89	17
9	1-pyrenyl (**s49i**)	85	14
10	9-anthryl (**s49j**)	93	34
11	[H_8]-9-anthryl (**1**)	96	48
12	(*S*)-biphenyl-9-anthryl (**s50**)	76	–23
13[c]	[H_8]-9-Anthryl (**1**)	93	68
14[c,d]	[H_8]-9-Anthryl (**1**)	90	81
15[c,d,e]	[H_8]-9-Anthryl (**1**)	97	93

[a] Unless otherwise noted, all reactions were conducted with 0.1 mmol of **2a** and 1.0 equiv. of NBS (*N*-bromosuccinimide) in the presence of 10 mol% **s49** in CH_2Cl_2 (1.0 mL) at 0 °C for 30 min. [b] DAICEL CHIRALCEL AD-H®, flow rate = 1.0 mL/min, hexane/*i*-PrOH = 10/1. [c] NBP (*N*-bromophthalimide) was employed instead of NBS. [d] Mixed solvent system (CH_2Cl_2/toluene = 1/1) was employed as the reaction solvent at -20 °C. [e] In the presence of MS13X.

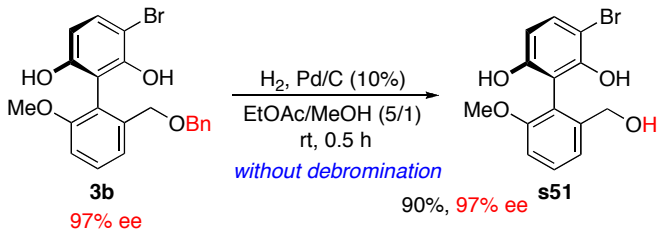
Brominating reagents were also examined which revealed that the presence of carbonyl group in the reagent was important in both reactivity and selectivity (Scheme 10). In the case of *N*-bromoimide-type reagents, the desired mono-bromide **3a** was obtained in optically active form (26–68% ee). On the other hand, no selectivity was observed by treatment of Bu_4NBr_3 (90% chemical yield), and reaction did not proceeded in the case of Br_2 and $BrCH_2CH_2Br$. These results suggest that the importance of activation of the brominating agent by hydrogen bonding, *i.e.*, the Brønsted acidic part of **1** activates the carbonyl of amide moiety.



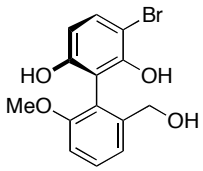
Scheme 10. Examination of the brominating reagents.

5. The removal of protecting group.

The benzyloxy group was selectively cleaved under the standard hydrogenation conditions (H_2, Pd/C, EtOAc/MeOH) without affecting bromo atom. The corresponding triol **s51** was obtained in 90% yield without losing the axial chirality.



To a solution of **3b** (9.0 mg, 97% ee) in EtOAc (1.5 mL) and MeOH (0.30 mL) was added 10% Pd/C (3.0 mg). After being stirred under H_2 (1 atm) at room temperature for 0.5 h, the reaction mixture was filtered through Celite® pad and concentrated in vacuo. The residue was purified by PTLC (hexane/EtOAc = 1/1) to give **s51** (6.3 mg, 90%, 97% ee) as a white solid.



(*R*)-3-bromo-2'-(hydroxymethyl)-6'-methoxybiphenyl-2,6-diol (**s51**).

Colorless amorphous.

Yield: 90%, 97% ee.

HPLC [DAICEL CHIRALCEL® OD-H, ϕ 0.46 x 25 cm, hexane/*i*-PrOH = 5/1, 1.0 mL/min, 254 nm, retention time (min) = 12.3 (98.7%), 15.4 (1.3%)].

$[\alpha]_D^{26}$ –43.2 (c 1.22, MeOH).

Mp. 228–230 °C.

IR (KBr) 3550, 3484, 3447, 3003, 2946, 2843, 1617, 1598, 1576, 1472, 1457, 1440, 1372, 1316, 1304, 1263, 1169, 1121, 1082, 1034, 1008, 980, 894, 803, 783 cm^{-1}.

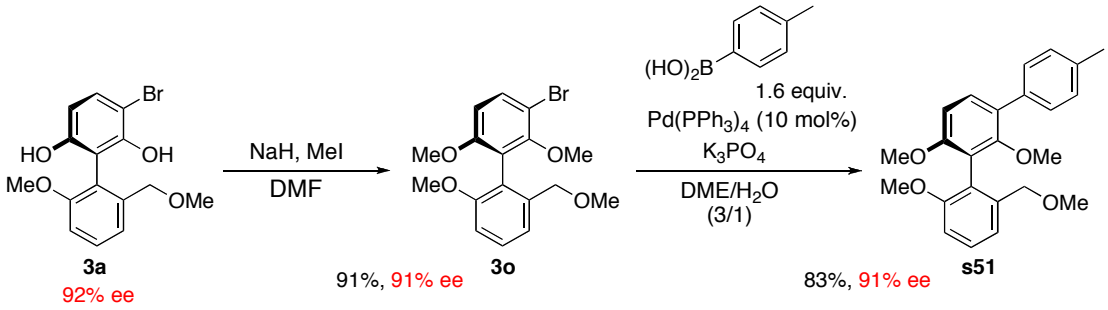
^1H NMR (400 MHz, CD_3COCD_3) δ 3.69 (s, 3H), 4.08 (brs, 1H), 4.33 (d, 1H, *J* = 13.2 Hz), 4.38 (d, 1H, *J* = 13.2 Hz), 6.47 (d, 1H, *J* = 8.8 Hz), 6.95 (d, 1H, *J* = 7.6 Hz), 7.21 (d, 1H, *J* = 7.6 Hz), 7.30 (d, 1H, *J* = 8.8 Hz), 7.35 (dd, 1H, *J* = 7.6, 7.6 Hz), 7.41 (brs, 1H), 7.93 (brs, 1H).

^{13}C NMR (100 MHz, CD_3COCD_3) δ 55.9, 62.8, 101.1, 109.9, 110.8, 114.0, 120.3, 120.5, 130.1, 132.4, 143.8, 152.7, 156.1, 158.7.

Anal. Calcd for $C_{14}H_{13}BrO_4$: C, 51.71; H, 4.03. Found: C, 51.89; H, 4.31.

6. Further transformation

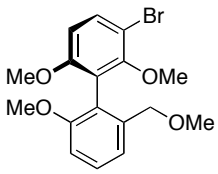
In order to demonstrate the synthetic potential of the present methodology, further transformation of the monobromide **3a** was conducted. Methylation of the two phenolic hydroxy groups followed by Suzuki coupling with *p*-tolylboronic acid gave adduct **s52** in good chemical yield (76%, 2steps). The salient feature of this transformation is that the axial chirality was completely retained through this transformation even the reaction was conducted at high temperature (more than 100 °C). This result clearly indicates the utility of the monobromides obtained by the present method as the chiral building blocks.



3a
92% ee

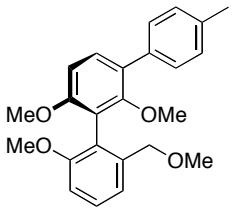
91%, 91% ee **3o**

83%, 91% ee **s51**



Synthesis of (R)-3-bromo-2,2',6-trimethoxy-6'-(methoxymethyl)biphenyl (3o):

To a solution of **3a** (19.9 mg, 0.059 mmol) in DMF (2.0 mL) were successively added NaH (60% oil, 6.8 mg, 0.17 mmol) and MeI (22 μL, 0.35 mmol) at 0 °C. After being stirred for 4 h at room temperature, the reaction was stopped by adding aqueous 1 M HCl at 0 °C. The crude mixture was extracted with EtOAc (x3) and the combined organic extracts were washed with brine, dried (Na_2SO_4), and concentrated in vacuo. The residue was purified by column chromatography (silica gel, hexane/EtOAc = 4/1) to give **3o** (19.6 mg, 91%) as a colorless amorphous.



Synthesis of (R)-3-(4-methylphenyl)-2,2',6-trimethoxy-6'-(methoxymethyl)biphenyl (s52):

The mixture of bromobiaryl **3o** (14.2 mg, 0.039 mmol), tolylboronic acid (8.3 mg, 0.061 mmol), $Pd(PPh_3)_4$ (4.8 mg, 0.0041 mmol), K_3PO_4 (25 mg, 0.118 mmol), DME (3.0 mL), and H_2O (1.0 mL) were heated at reflux for 3.5 h. After cooling to room temperature, the reaction was stopped by adding H_2O. The crude mixture was extracted with EtOAc (x3) and the combined organic extracts were washed with brine, dried (Na_2SO_4), and concentrated in vacuo. The residue was purified by column chromatography (silica gel, hexane/EtOAc = 2/1) to give **s52** (12.2 mg, 83%) as a colorless amorphous.

HPLC [DAICEL CHIRALPAK® AD-H, ϕ 0.46 x 25 cm, hexane/*i*-PrOH = 10/1, 1.0 mL/min, 254 nm, retention time (min) = 4.6 (4.7%), 6.3 (95.3%)].

$[\alpha]_D^{26}$ –20.8 (c 1.110, $CHCl_3$), 91% ee.

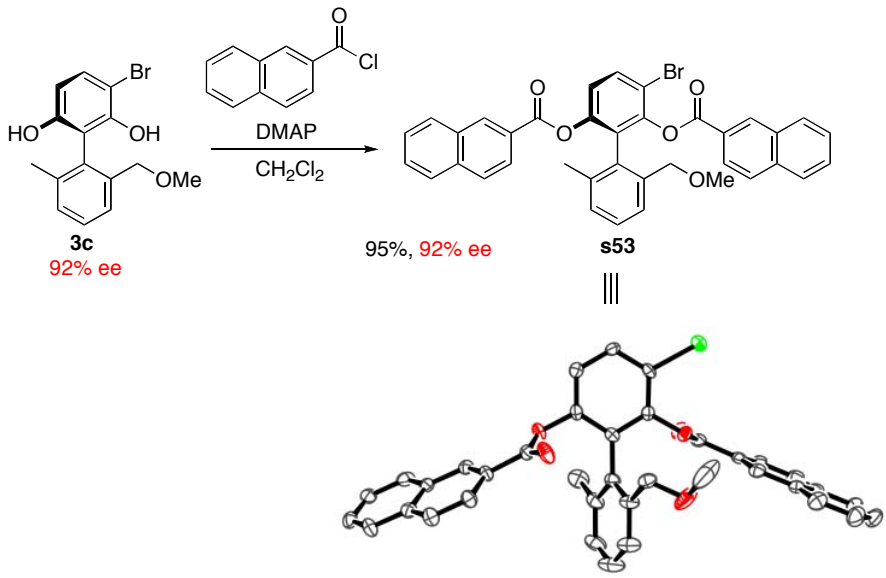
IR (neat) 2934, 2834, 1593, 1516, 1489, 1467, 1435, 1414, 1392, 1283, 1263, 1211, 1084, 1022, 912, 802, 784, 750, 695 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$) δ 2.38 (s, 3H), 3.12 (s, 3H), 3.26 (s, 3H), 3.73 (s, 3H), 3.76 (s, 3H), 4.21 (d, 1H, *J* = 12.8 Hz), 4.27 (d, 1H, *J* = 12.8 Hz), 6.81 (d, 1H, *J* = 8.8 Hz), 6.92 (d, 1H, *J* = 8.4 Hz), 7.17–7.23 (m, 2H), 7.34 (d, 1H, *J* = 8.8 Hz), 7.37 (dd, 1H, *J* = 8.0, 8.0 Hz), 7.42–7.52 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 21.2, 55.8, 55.9, 58.2, 60.0, 72.2, 106.7, 109.7, 119.1, 119.4, 122.5, 127.5, 128.4, 128.9, 128.9, 130.5, 135.9, 136.2, 138.9, 156.2, 157.2, 157.2.

Anal. Calcd for $C_{24}H_{26}O_4$: C, 76.17; H, 6.92. Found: C, 76.33; H, 7.00.

7. Determination of the absolute configuration of 3c.



All hydrogens are omitted for clarity.

Synthesis of (S)-3-bromo-2'-(methoxymethyl)-6'-methylbiphenyl-2,6-diyl di-2-naphthoate (s53):

To a solution of **3c** (21.2 mg, 0.0656 mmol) in CH_2Cl_2 (1.0 mL) were successively added DMAP (18.7 mg, 0.153 mmol) and 2-naphthoyl chloride (29.0 mg, 0.152 mmol) at 0 °C. After being stirred for 30 min at 0 °C, the reaction was stopped by adding saturated aqueous $NaHCO_3$ at 0 °C. The crude mixture was extracted with EtOAc (x3) and the combined organic extracts were washed with brine, dried (Na_2SO_4), and concentrated in vacuo. The residue was purified by preparative TLC (silica gel, hexane/EtOAc = 3/1) to give **s53** (39.2 mg, 95%) as a white solid. Recrystallization from MeOH/EtOH/benzene afforded **s53** as a colorless crystal, which was subjected to single X-ray analysis.[2]

HPLC [DAICEL CHIRALCEL® OD-H, ϕ 0.46 x 25 cm, hexane/*i*-PrOH = 20/1, 0.5 mL/min, 254 nm, retention time (min) = 29.7 (4.2%), 31.8 (95.8%)].

$[\alpha]_D^{26}$ +2.3 (c 1.000, $CHCl_3$), 92% ee.

Mp. 177–178 °C.

IR (neat) 3060, 2925, 2821, 1740, 1631, 1598, 1508, 1454, 1412, 1387, 1355, 1276, 1242, 1222, 1203, 1184, 1127, 1073, 1027, 943, 760, 732, 648 cm^{-1}.

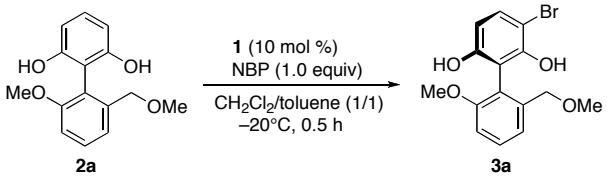
^{1}H NMR (400 MHz, $CDCl_3$) δ 2.25 (s, 3H), 3.31 (s, 3H), 4.39 (brs, 2H), 7.00–7.12 (m, 2H), 7.19–7.30 (m, 1H), 7.43 (d, 1H, J = 8.8 Hz), 7.46–7.62 (m, 4H), 7.71–7.94 (m, 9H), 8.21 (brs, 1H), 8.45 (brs, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 19.9, 58.4, 72.1, 114.4, 121.9, 124.5, 125.0, 125.1, 125.6, 126.0, 126.7, 126.8, 127.7, 127.7, 128.2, 128.3, 128.5, 128.6, 128.6, 128.8, 128.9, 129.4, 131.8, 131.9, 132.3, 132.5, 135.7, 135.8, 137.3, 137.6, 147.3, 148.7, 163.5, 164.3.

Anal. Calcd for $C_{37}H_{27}BrO_5$: C, 70.37; H, 4.31. Found: C, 70.12; H, 4.42.

8. Examination of the linear effect.

To gain further insight into the mechanism of this reaction, we examined the correlation of the selectivity of **3a** and the enantiomeric purity of catalyst **1**. We observed clear linear effect in the reaction of **2a** and NBP (1.0 equiv.) in CH_2Cl_2/toluene (v/v = 1/1) in the presence of **1** as a catalyst (Figure 1). This result clearly indicates that single molecule of catalyst is involved in the carbon-bromine bond-forming step.



2a **3a**

entry	ee% of **1**	ee% of **3a**
1	0	3
2	20	12
3	50	49
4	80	64
5	100	93

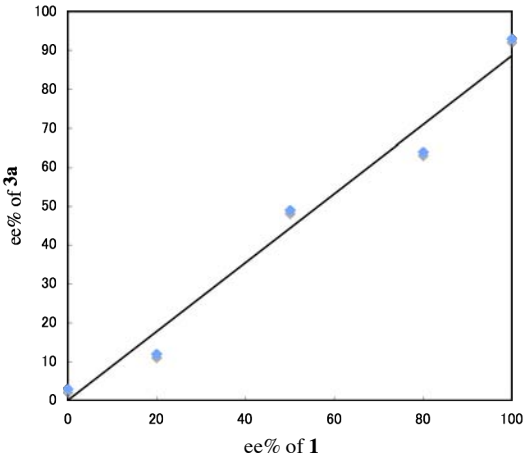
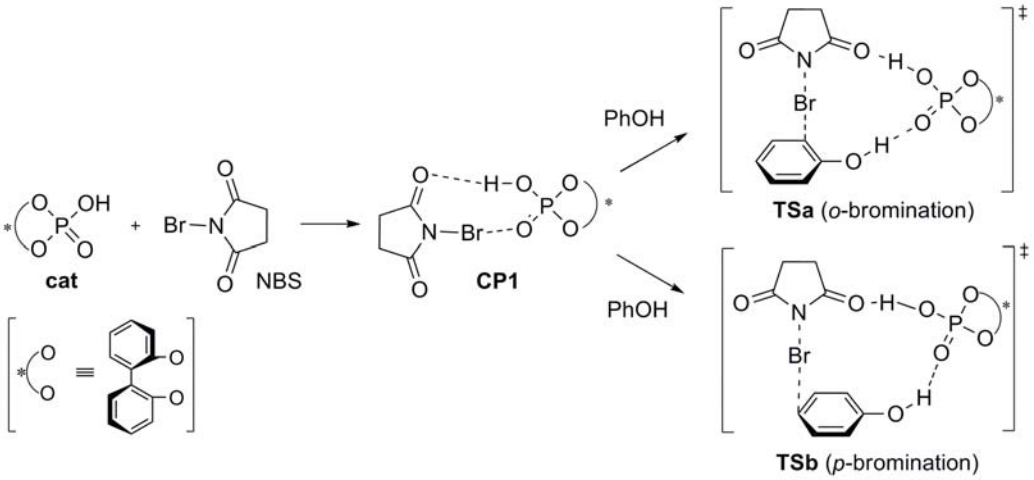


Figure 1. Examination of the linear effect in the desymmetrization reaction.

9. Preliminary Computational Studies

Focusing on the first nucleophilic attack of biaryls on brominating reagent, which is the rate-determining step, the reaction mechanism of the chiral phosphoric acid catalyzed bromination was investigated by using small models. To elucidate the substituent effects of the phosphoric acid catalyst at the 3,3'-position and biaryls on the enantioselectivity, more realistic models (biaryls, **2a**, **2l**, **2n**, NBS, and **1**) were investigated on the basis of the well-defined transition structure (as shown in the main text). All calculations were performed with the Gaussian 03 package.[8] Geometries were fully optimized and characterized by frequency calculation at the M05-2X/6-31G* level[9,10] for the small models. Natural charges were calculated by the natural population analysis at the M05-2X/6-31G* level.[11] Free energies were also computed for the gas phase. As a preliminary mechanistic study, two possible reaction pathways (*ortho*- or *para*-bromination) were firstly compared by using small models (PhOH, NBS, and biphenol-derived phosphoric acid) to reduce computational costs (Scheme 11).



Scheme 11. Two possible reaction pathways of phosphoric acid catalyzed bromination reaction

In both pathways, the biphenol-derived phosphoric acid (**cat**) coordinates to NBS and PhOH through hydrogen bonding followed by nucleophilic attack of PhOH on NBS bromine (Figure 2). Both Brønsted acidic (proton) and Lewis basic sites (phosphoryl oxygen) synergistically activate NBS and PhOH, respectively. As shown in the energy profile in Figure S1, **TSa** for the *ortho*-bromination is found to be higher in energy than **TSb** for the *para*-bromination by 8.9 kcal/mol (10.3 kcal/mol in free energy). The

phosphoric acid catalyzed bromination, therefore, would proceed predominantly at the *ortho*-position. The 3D structures and charge distributions of important stationary points are also shown in Figure S1. **CPa** is regarded as the hydrogen bonding complex. In the simultaneous activation of NBS and PhOH by the phosphoric acid, both **TSa** and **TSb** allow resonance stabilization of the phosphoric acid moiety, where two P-O bond lengths are almost same (1.50 Å, 1.51 Å) and negative charges are delocalized over the O-P-O fragment (NPA: -1.14, -1.15). The electron-withdrawing effect through protonation of NBS increases the electrophilicity of bromine to promote C-Br bond formation. The smaller charge difference of bromine in **TSa** (0.159) than **TSb** (0.139) from **CPa** (0.300) would make the C-Br bond formation easier in **TSa**. The longer lengths of PO-H and N-Br bonds in **TSb** (1.40 Å, 2.32 Å) than **TSa** (1.34 Å, 2.28 Å) indicates that the *para*-position is too far to bridge effectively both substrates through the O-P-O fragment. According to these electronic and structural disadvantages would result in the energetically disfavored **TSb**.

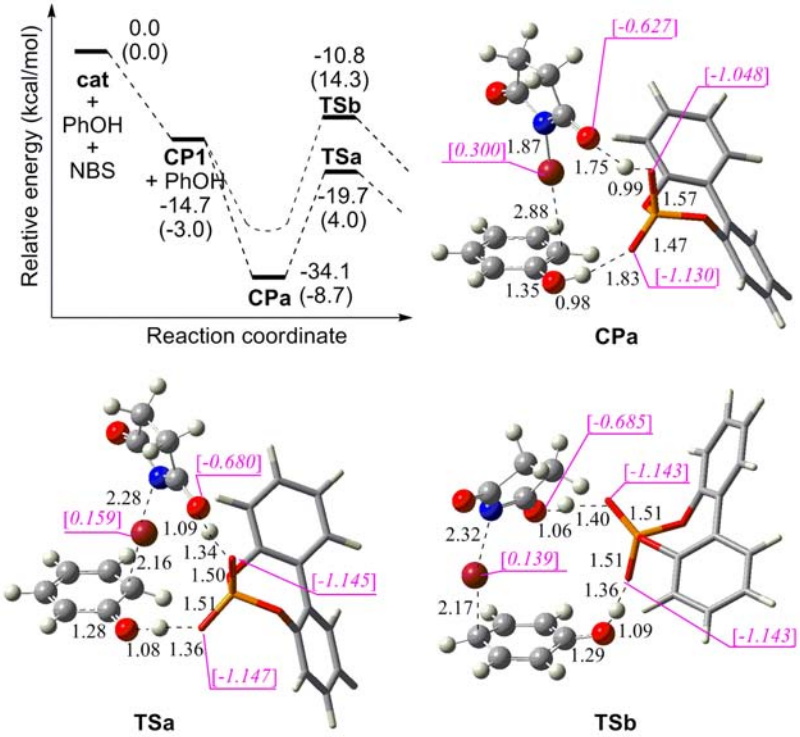


Figure 2. Energy profiles of *ortho*- and *para*-bromination and 3D structures of **CPa**, **TSa**, and **TSb** at the M05-2X/6-31G* level. The potential energy of the sum of **cat**, NBS, and PhOH is set to zero. The free energies are shown in parentheses. Bond lengths are in Å. Natural charges are shown in *italic*.

Cartesian coordinates of each structure.

Small model study

CP1 SCF Done: E(RM052X+HF-M052X) = -4036.63669541 A.U.
Sum of electronic and thermal Free Energies= -4036.413933 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.811563	0.936920	0.790561
2	6	0	-5.152982	1.634511	0.910316
3	6	0	-6.097718	0.852283	-0.013374
4	6	0	-5.259844	-0.273979	-0.603037
5	7	0	-3.972083	-0.123234	-0.074580
6	1	0	-5.455577	1.613994	1.957069
7	1	0	-6.489456	1.450634	-0.835368
8	8	0	-5.594516	-1.133782	-1.367493
9	8	0	-2.773414	1.232769	1.342125
10	1	0	-6.945979	0.410543	0.508114
11	1	0	-5.026923	2.678009	0.623402
12	35	0	-2.527661	-1.211594	-0.447330
13	1	0	-1.051401	0.354266	1.284441
14	8	0	-0.092211	0.229008	1.451784
15	15	0	0.721173	-0.659898	0.428235
16	8	0	2.073417	-0.823985	1.283589
17	8	0	1.170303	0.309591	-0.785096
18	8	0	0.108978	-1.893876	-0.095532
19	6	0	3.250906	-1.136982	0.608469
20	6	0	1.983206	1.409306	-0.533262
21	6	0	3.908398	-0.141326	-0.117784
22	6	0	3.770355	-2.414085	0.750068
23	6	0	1.430680	2.674538	-0.657924
24	6	0	3.336907	1.216869	-0.244808
25	6	0	5.133386	-0.471900	-0.704272
26	6	0	4.990023	-2.718017	0.156784
27	6	0	2.243889	3.790722	-0.501600
28	6	0	4.134171	2.354746	-0.092332
29	6	0	5.673001	-1.745125	-0.568846
30	1	0	5.402967	-3.712894	0.259464
31	6	0	3.598489	3.630207	-0.221345
32	1	0	1.819557	4.781638	-0.596765
33	1	0	3.213418	-3.141467	1.324496
34	1	0	6.619362	-1.980575	-1.037584
35	1	0	5.649053	0.279638	-1.289067
36	1	0	5.181282	2.225835	0.151812
37	1	0	4.234189	4.496403	-0.092818
38	1	0	0.376367	2.760958	-0.882812

TSa SCF Done: E(RM052X+HF-M052X) = -4344.07191400 A.U.
Sum of electronic and thermal Free Energies= -4343.751939 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.743706	-2.114033	-1.506307
2	6	0	-3.852653	-3.090954	-1.824037
3	6	0	-4.681832	-3.090030	-0.540215
4	6	0	-3.996504	-2.039066	0.338190
5	7	0	-2.842536	-1.573256	-0.314886
6	1	0	-4.394735	-2.732748	-2.700210
7	1	0	-4.665775	-4.045824	-0.016755
8	8	0	-4.367889	-1.658709	1.416753
9	8	0	-1.838345	-1.897378	-2.372289
10	1	0	-5.723327	-2.806255	-0.683850
11	1	0	-3.415160	-4.055903	-2.079166
12	35	0	-1.967203	0.437889	0.316529
13	6	0	-1.578100	2.574777	2.131083
14	6	0	-1.040856	2.321440	0.807341
15	6	0	-1.568006	3.107840	-0.299984
16	6	0	-2.701177	3.936325	-0.076724
17	6	0	-3.199597	4.074055	1.187566
18	6	0	-2.638811	3.399555	2.314823
19	1	0	-1.132655	2.035421	2.956812
20	1	0	0.003141	2.035232	0.734346
21	1	0	-3.116658	4.462952	-0.924024
22	1	0	-4.053428	4.722242	1.344300
23	1	0	-3.067367	3.547852	3.295691
24	8	0	-1.067895	3.039644	-1.479074
25	1	0	-0.214517	2.382022	-1.555809
26	6	0	4.033993	-0.367836	0.301944
27	6	0	5.223289	0.003994	0.936224
28	6	0	6.121709	0.874512	0.331750
29	6	0	5.838310	1.399761	-0.926286
30	6	0	4.662949	1.045396	-1.577781
31	6	0	3.778992	0.168063	-0.965886
32	6	0	3.083984	-1.292694	0.959660
33	6	0	3.517666	-2.432966	1.642098
34	6	0	2.612966	-3.266195	2.289732
35	6	0	1.250707	-2.973783	2.264726
36	6	0	0.793169	-1.846922	1.592122
37	6	0	1.712634	-1.028005	0.954076
38	1	0	5.425474	-0.386311	1.926164
39	1	0	7.033641	1.149845	0.845153
40	1	0	6.530036	2.083435	-1.401244
41	1	0	4.574629	-2.669404	1.643777
42	1	0	2.969683	-4.147456	2.806840
43	1	0	0.544115	-3.621848	2.766867
44	15	0	1.169562	0.171500	-1.277204
45	8	0	2.677608	-0.253682	-1.690117
46	8	0	1.259770	0.136844	0.352541
47	8	0	0.293888	-0.922998	-1.808626
48	8	0	0.908908	1.615882	-1.620959
49	1	0	-0.955346	-1.346727	-2.058522
50	1	0	4.414458	1.424515	-2.559577
51	1	0	-0.252921	-1.573089	1.552416

TSb SCF Done: E(RM052X+HF-M052X) = -4344.05767979 A.U.
Sum of electronic and thermal Free Energies= -4343.735543 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.746753	2.216451	-0.092841
2	6	0	-0.624492	2.867901	0.682519
3	6	0	-1.369712	3.459774	1.879503
4	6	0	-2.796307	2.915217	1.734890
5	7	0	-2.920543	2.281846	0.484631
6	1	0	0.105661	2.100739	0.950486
7	1	0	-1.412569	4.549053	1.854363
8	8	0	-3.676691	3.005691	2.548218
9	8	0	-1.577912	1.619270	-1.214889
10	1	0	-0.968194	3.162194	2.846419
11	1	0	-0.109394	3.595536	0.055470
12	35	0	-4.106312	0.354299	-0.035718
13	6	0	-3.711689	-1.650178	-1.843997
14	6	0	-2.422363	-2.057370	-1.728056
15	6	0	-1.971698	-2.583058	-0.474751
16	6	0	-2.915610	-2.870537	0.563523
17	6	0	-4.188751	-2.418263	0.450306
18	6	0	-4.611021	-1.649345	-0.704202
19	1	0	-4.059760	-1.202293	-2.765905
20	1	0	-1.705155	-1.939597	-2.527921
21	1	0	-2.551256	-3.365935	1.452315
22	1	0	-4.893000	-2.550303	1.261709
23	1	0	-5.673632	-1.596321	-0.905149
24	8	0	-0.727483	-2.815723	-0.241679
25	1	0	-0.073158	-2.297661	-0.937384
26	6	0	3.758423	-0.849135	0.916688
27	6	0	4.618563	-1.681505	1.638552
28	6	0	4.128481	-2.732068	2.404482
29	6	0	2.758275	-2.973154	2.455159
30	6	0	1.881409	-2.159075	1.747244
31	6	0	2.386256	-1.110915	0.991254
32	6	0	4.286225	0.275284	0.112955
33	6	0	5.287049	1.116599	0.608223
34	6	0	5.792118	2.158814	-0.159462
35	6	0	5.297973	2.381775	-1.442699
36	6	0	4.303447	1.558274	-1.957110
37	6	0	3.817140	0.517610	-1.180569
38	1	0	5.685136	-1.505113	1.573716
39	1	0	4.814366	-3.367000	2.949836
40	1	0	2.370083	-3.794700	3.043094
41	1	0	5.651389	0.954457	1.615198
42	1	0	6.562939	2.801269	0.245678
43	1	0	5.683666	3.196068	-2.042172
44	15	0	1.348264	-0.223776	-1.255668
45	8	0	1.486477	-0.252586	0.371548
46	8	0	2.886734	-0.350524	-1.736799
47	8	0	0.799548	1.134997	-1.602735
48	8	0	0.636491	-1.465589	-1.742991
49	1	0	-0.555230	1.464092	-1.443167
50	1	0	0.812845	-2.322174	1.760375
51	1	0	3.896930	1.698046	-2.949292

Realistic model study

TSr1a ONIOM: extrapolated energy = -6284.065901895045 A.U.
SCF Done: E(RM052X+HF-M052X) = -6307.32922259 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.701059	-3.350558	3.535753
2	6	0	0.210699	-3.206614	4.757181
3	6	0	0.700928	-1.761980	4.684865
4	6	0	0.055479	-1.237205	3.414772
5	7	0	-0.708868	-2.143432	2.831370
6	1	0	1.010370	-3.939159	4.662329
7	1	0	0.384022	-1.141086	5.523425
8	8	0	0.265148	-0.056375	3.031549
9	8	0	-1.315217	-4.339828	3.228013
10	1	0	1.782167	-1.664673	4.586767
11	1	0	-0.360735	-3.438427	5.655148
12	35	0	-1.921133	-1.989241	0.968659
13	6	0	-3.930300	-3.014446	-0.689070
14	6	0	-3.004505	-1.930692	-0.924203
15	6	0	-3.563774	-0.594780	-0.953228
16	6	0	-4.903965	-0.350073	-0.618546
17	6	0	-5.723003	-1.439127	-0.322261
18	6	0	-5.220827	-2.775796	-0.365088
19	1	0	-3.535329	-4.019427	-0.730463
20	1	0	-2.168061	-2.109369	-1.589766
21	1	0	-5.918755	-3.562683	-0.125376
22	8	0	-2.822184	0.415257	-1.312815
23	1	0	0.015810	0.324971	1.846924
24	8	0	-7.020485	-1.337755	-0.006007
25	1	0	-7.493733	-0.561687	-0.401724
26	6	0	-5.324135	1.076058	-0.425300
27	6	0	-4.697823	1.777550	0.612833
28	6	0	-6.255861	1.732290	-1.212632
29	6	0	-5.000204	3.107339	0.831192
30	6	0	-6.571269	3.064413	-0.971366
31	6	0	-5.938817	3.746529	0.041789
32	1	0	-4.505680	3.649285	1.608475
33	1	0	-7.302746	3.555166	-1.581910
34	1	0	-6.170340	4.777227	0.223410
35	6	0	-6.986082	1.005431	-2.309371
36	1	0	-6.343483	0.296990	-2.813645
37	1	0	-7.386696	1.702854	-3.032520
38	8	0	-8.088601	0.295410	-1.675976
39	8	0	-3.802326	1.082019	1.360892
40	6	0	-8.922158	-0.471472	-2.570098
41	1	0	-9.397377	0.180939	-3.292099
42	1	0	-9.673322	-0.948071	-1.960771
43	1	0	-8.342474	-1.224317	-3.091059
44	6	0	-2.838627	1.766213	2.195362
45	1	0	-2.263940	2.471078	1.616261
46	1	0	-2.182329	1.003555	2.567843
47	1	0	-3.332275	2.267219	3.017511
48	1	0	-1.853385	0.158789	-1.438889
49	8	0	-0.316765	-0.203540	-1.543534
50	15	0	0.539771	0.320598	-0.439607
51	8	0	1.444077	1.517263	-1.072665
52	8	0	1.657239	-0.744627	0.091144
53	8	0	-0.105295	0.847869	0.843646
54	6	0	2.534221	1.936056	-0.331445
55	6	0	2.645645	-1.094648	-0.816828
56	6	0	3.660375	1.111917	-0.314756
57	6	0	2.496043	3.155860	0.334491
58	6	0	2.653290	-2.371179	-1.368271
59	6	0	3.629702	-0.150500	-1.113700
60	6	0	4.756674	1.452770	0.499069
61	6	0	3.629447	3.511453	1.058570
62	6	0	1.325803	4.101553	0.278420
63	6	0	3.631539	-2.641064	-2.318203
64	6	0	1.729016	-3.463029	-0.901209
65	6	0	4.550844	-0.417063	-2.143969
66	6	0	4.740487	2.677079	1.176020
67	6	0	5.894124	0.446131	0.739873
68	1	0	3.625825	4.464349	1.574422
69	6	0	1.131663	4.889447	-0.859530
70	6	0	0.516177	4.271046	1.405176
71	6	0	4.546496	-1.678492	-2.747537
72	1	0	3.660949	-3.633237	-2.753321
73	6	0	2.037074	-4.142077	0.282166
74	6	0	0.643155	-3.859695	-1.682355
75	6	0	5.465886	0.699466	-2.672803
76	6	0	5.929231	3.155811	2.021279
77	1	0	6.104548	-0.108939	-0.160181
78	1	0	5.534948	-0.268375	1.476465
79	6	0	7.171766	1.111259	1.273461
80	6	0	0.108790	5.880926	-0.861150
81	6	0	1.933760	4.749351	-2.042496
82	6	0	-0.485072	5.286016	1.402490
83	6	0	0.639652	3.450981	2.579443
84	6	0	5.560952	-2.064431	-3.833587
85	6	0	1.224717	-5.235408	0.695694
86	6	0	3.159641	-3.789500	1.106605
87	6	0	-0.137202	-4.983343	-1.280534
88	6	0	0.266996	-3.171381	-2.887291
89	1	0	4.862078	1.318132	-3.331633
90	1	0	5.796027	1.331097	-1.863036
91	6	0	6.666583	0.156129	-3.461585
92	1	0	6.516544	3.846088	1.421738
93	1	0	5.555537	3.704226	2.878088
94	6	0	6.832268	2.000933	2.478126
95	1	0	7.884335	0.343567	1.554712
96	1	0	7.626960	1.715332	0.494312
97	6	0	-0.080382	6.684450	-2.033963
98	6	0	-0.666644	6.063611	0.271485
99	6	0	1.722681	5.525392	-3.122465
100	1	0	2.701178	4.005753	-2.050862
101	6	0	-1.277282	5.486239	2.582360
102	6	0	-0.129990	3.668945	3.663049
103	1	0	1.326703	2.633789	2.565376
104	1	0	5.072656	-2.701004	-4.562272
105	1	0	6.352359	-2.646216	-3.368711
106	6	0	6.181377	-0.840994	-4.524233
107	6	0	1.540076	-5.916868	1.917341
108	6	0	0.161520	-5.635026	-0.096976
109	6	0	3.432718	-4.468300	2.237845
110	1	0	3.780473	-2.975409	0.799641
111	6	0	-1.216853	-5.416197	-2.121452
112	6	0	-0.761081	-3.606813	-3.641928
113	1	0	0.796593	-2.281953	-3.151292
114	1	0	7.358765	-0.340417	-2.787991
115	1	0	7.193303	0.982239	-3.926428
116	1	0	6.320686	1.409005	3.230276
117	1	0	7.735137	2.400262	2.926665
118	6	0	0.693159	6.515224	-3.121601
119	1	0	-0.857517	7.423890	-2.019915
120	1	0	-1.422752	6.825704	0.273044
121	1	0	2.326426	5.403379	-3.999680
122	1	0	-2.011260	6.268932	2.571154
123	6	0	-1.099179	4.719109	3.673897
124	1	0	-0.034120	3.034696	4.521346
125	1	0	5.441633	-0.360892	-5.156577
126	1	0	7.003256	-1.158541	-5.156234
127	6	0	2.605475	-5.555065	2.657062
128	1	0	0.901140	-6.720468	2.225621
129	1	0	-0.441651	-6.465565	0.215262
130	1	0	4.280172	-4.197842	2.836587
131	1	0	-1.777106	-6.280394	-1.819677
132	6	0	-1.511263	-4.762750	-3.261257
133	1	0	-1.033726	-3.079029	-4.534018
134	1	0	0.545191	7.117776	-3.995614
135	1	0	-1.689054	4.878877	4.554915
136	1	0	2.844231	-6.078346	3.561896
137	1	0	-2.314332	-5.095173	-3.888781

TSr2a ONIOM: extrapolated energy = -6284.062395903982 A.U.
SCF Done: E(RM052X+HF-M052X) = -6307.31261287 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.344984	0.470250	4.682783
2	6	0	-1.566706	0.878213	5.938459
3	6	0	-0.130460	1.040539	5.442323
4	6	0	-0.234291	0.712888	3.961966
5	7	0	-1.470492	0.375660	3.610223
6	1	0	-1.687211	0.097894	6.689556
7	1	0	0.267562	2.048955	5.553713
8	8	0	0.761348	0.787098	3.205227
9	8	0	-3.538451	0.276370	4.632570
10	1	0	0.579728	0.353291	5.903096
11	1	0	-1.999647	1.794091	6.339300
12	35	0	-2.134595	-0.716021	1.740764
13	6	0	-3.602722	-2.771384	0.475650
14	6	0	-2.799660	-1.697850	-0.064808
15	6	0	-3.513704	-0.567882	-0.638580
16	6	0	-4.883298	-0.388636	-0.422168
17	6	0	-5.544985	-1.361852	0.346381
18	6	0	-4.926888	-2.600979	0.685415
19	1	0	-3.085805	-3.666948	0.787831
20	1	0	-1.867068	-1.958802	-0.550448
21	1	0	-5.543509	-3.328983	1.188616
22	8	0	-2.845697	0.335437	-1.307396
23	1	0	0.510949	0.848235	1.927091
24	8	0	-6.785531	-1.191856	0.817519
25	1	0	-6.933109	-0.252486	1.099294
26	6	0	-5.597714	0.828623	-0.938489
27	6	0	-6.279538	1.647890	-0.048345
28	6	0	-5.655141	1.145463	-2.296946
29	6	0	-6.967185	2.766470	-0.459424
30	6	0	-6.346169	2.271509	-2.713636
31	6	0	-6.991948	3.083441	-1.802457
32	1	0	-7.484640	3.357040	0.267787
33	1	0	-6.385694	2.477813	-3.759909
34	1	0	-7.526732	3.948428	-2.140419
35	6	0	-4.971156	0.290442	-3.341777
36	1	0	-5.094862	-0.760983	-3.104908
37	1	0	-3.914870	0.518217	-3.348219
38	8	0	-5.549627	0.583156	-4.623204

39	8	0	-6.327952	1.267749	1.295263
40	6	0	-4.899271	-0.060404	-5.725307
41	1	0	-3.853476	0.223500	-5.787854
42	1	0	-5.411945	0.260098	-6.619369
43	1	0	-4.961959	-1.141304	-5.645319
44	6	0	-5.285627	1.792942	2.191067
45	1	0	-4.359259	1.894251	1.646260
46	1	0	-5.156024	1.086838	2.992683
47	1	0	-5.605880	2.752961	2.567212
48	1	0	-1.846722	0.154376	-1.309870
49	8	0	-0.326754	-0.205185	-1.299553
50	15	0	0.717957	0.218739	-0.322248
51	8	0	1.890452	0.973259	-1.156532
52	8	0	1.494892	-1.042402	0.361965
53	8	0	0.330926	1.113217	0.856481
54	6	0	3.001472	1.314125	-0.397089
55	6	0	2.449414	-1.710210	-0.389988
56	6	0	3.892378	0.292946	-0.071551
57	6	0	3.197974	2.632859	-0.001794
58	6	0	2.205165	-3.011104	-0.815633
59	6	0	3.655471	-1.058316	-0.662432
60	6	0	4.959012	0.559234	0.806438
61	6	0	4.314751	2.885679	0.787659
62	6	0	2.300824	3.765331	-0.424249
63	6	0	3.188139	-3.620034	-1.589392
64	6	0	0.982462	-3.810840	-0.448368
65	6	0	4.591882	-1.662647	-1.521691
66	6	0	5.172535	1.875949	1.225952
67	6	0	5.797126	-0.591918	1.385874
68	1	0	4.497932	3.907552	1.098192
69	6	0	2.373040	4.242316	-1.737514
70	6	0	1.485179	4.399112	0.517450
71	6	0	4.354315	-2.963588	-1.977802
72	1	0	3.015907	-4.636960	-1.921676
73	6	0	0.947510	-4.477778	0.779365
74	6	0	-0.035249	-4.000147	-1.387262
75	6	0	5.793312	-0.860961	-2.050340
76	6	0	6.355398	2.259928	2.126046
77	1	0	5.949848	-1.358860	0.642747
78	1	0	5.212772	-1.037057	2.187093
79	6	0	7.141729	-0.115593	1.955607
80	6	0	1.609715	5.384693	-2.112040
81	6	0	3.201514	3.632286	-2.739465
82	6	0	0.746466	5.557683	0.136319
83	6	0	1.347792	3.929597	1.869876
84	6	0	5.359943	-3.714549	-2.861840
85	6	0	-0.119174	-5.380449	1.059301
86	6	0	1.961456	-4.301394	1.781028
87	6	0	-1.086596	-4.922365	-1.107384
88	6	0	-0.071669	-3.293107	-2.638200
89	1	0	5.421062	-0.224026	-2.848707
90	1	0	6.179912	-0.209706	-1.283143
91	6	0	6.907461	-1.759397	-2.607769
92	1	0	7.143138	2.666443	1.497484
93	1	0	6.042132	3.044242	2.805152
94	6	0	6.912050	1.063812	2.912167
95	1	0	7.623266	-0.938093	2.473035
96	1	0	7.796983	0.195719	1.147509
97	6	0	1.689541	5.866013	-3.460437
98	6	0	0.822108	6.019212	-1.165963
99	6	0	3.249487	4.118036	-3.994635
100	1	0	3.780481	2.775991	-2.468980
101	6	0	-0.056485	6.228676	1.117952
102	6	0	0.584370	4.593728	2.757880
103	1	0	1.829281	3.019822	2.152252
104	1	0	4.817118	-4.332075	-3.567920
105	1	0	5.942030	-4.377129	-2.227035
106	6	0	6.315441	-2.768040	-3.602813
107	6	0	-0.137166	-6.066725	2.318703
108	6	0	-1.100472	-5.594965	0.104466
109	6	0	1.903783	-4.963096	2.952366
110	1	0	2.762554	-3.623518	1.578117
111	6	0	-2.105667	-5.134756	-2.094573
112	6	0	-1.055005	-3.515431	-3.531357
113	1	0	0.681530	-2.560554	-2.831119
114	1	0	7.393200	-2.293429	-1.796511
115	1	0	7.656078	-1.141478	-3.091127
116	1	0	6.206665	0.769945	3.682676
117	1	0	7.838029	1.348229	3.399472
118	6	0	2.476098	5.258781	-4.367517
119	1	0	1.103603	6.724632	-3.725700
120	1	0	0.260809	6.889616	-1.448350
121	1	0	3.870772	3.647434	-4.730559
122	1	0	-0.598191	7.103658	0.814902
123	6	0	-0.126478	5.774001	2.381526
124	1	0	0.489355	4.227701	3.760921
125	1	0	5.776863	-2.234504	-4.379260
126	1	0	7.101176	-3.343970	-4.078789
127	6	0	0.832736	-5.866537	3.229476
128	1	0	-0.945043	-6.744953	2.514280
129	1	0	-1.883563	-6.302403	0.304436
130	1	0	2.664975	-4.815993	3.692356
131	1	0	-2.882659	-5.841712	-1.876862
132	6	0	-2.088689	-4.463392	-3.260824
133	1	0	-1.075508	-2.970233	-4.453555
134	1	0	2.530519	5.622943	-5.374119
135	1	0	-0.724912	6.281825	3.111760
136	1	0	0.812565	-6.381970	4.168942
137	1	0	-2.854158	-4.626381	-3.993136

TSr3a ONIOM: extrapolated energy = -6284.064362401254 A.U.
SCF Done: E(RM052X+HF-M052X) = -6307.31890039 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.411833	-0.775767	-3.645937
2	6	0	0.416010	-1.950549	-4.601861
3	6	0	1.906695	-2.241358	-4.774021
4	6	0	2.587987	-1.175185	-3.910491
5	7	0	1.623134	-0.363239	-3.330001
6	1	0	-0.138403	-2.768938	-4.143329
7	1	0	2.264330	-2.149095	-5.799160
8	8	0	3.782992	-1.056539	-3.754042
9	8	0	-0.686280	-0.294479	-3.238918
10	1	0	2.189361	-3.224433	-4.400289
11	1	0	-0.095533	-1.666487	-5.522142
12	35	0	2.118697	1.204071	-1.698987
13	6	0	2.991643	3.694301	-0.693693
14	6	0	2.380557	2.524340	-0.081187
15	6	0	3.255370	1.682339	0.731566
16	6	0	4.642880	1.799306	0.630241
17	6	0	5.170411	2.821272	-0.155269
18	6	0	4.331898	3.825713	-0.741350
19	1	0	2.335304	4.398557	-1.187489
20	1	0	1.369150	2.625467	0.297124
21	1	0	4.826887	4.629136	-1.264541
22	8	0	2.741696	0.746290	1.469792
23	1	0	-0.720044	0.397823	-2.313664
24	8	0	6.473937	2.913682	-0.433083
25	1	0	6.870971	2.008989	-0.589114
26	6	0	5.520554	0.932870	1.478277
27	6	0	5.617288	1.262064	2.831452
28	6	0	6.229841	-0.151635	0.991618
29	6	0	6.423326	0.517641	3.671419
30	6	0	7.047801	-0.890525	1.837619
31	6	0	7.140510	-0.554705	3.170228
32	1	0	6.505426	0.766662	4.707888
33	1	0	7.607986	-1.716791	1.447703
34	1	0	7.773335	-1.120062	3.825281
35	6	0	6.130630	-0.519789	-0.467773
36	1	0	6.625434	-1.463264	-0.655998
37	1	0	5.098664	-0.593765	-0.781726
38	8	0	6.784863	0.525525	-1.229819
39	8	0	4.881220	2.333345	3.246261
40	6	0	6.660933	0.390152	-2.672185
41	1	0	5.644016	0.150502	-2.949087
42	1	0	6.956836	1.338794	-3.092881
43	1	0	7.324731	-0.389713	-3.023005
44	6	0	4.820960	2.707916	4.632233
45	1	0	5.793102	3.011069	5.000222
46	1	0	4.141799	3.543060	4.672574
47	1	0	4.439340	1.897899	5.240826
48	1	0	1.746107	0.645149	1.326995
49	8	0	-0.969891	1.065834	-1.268530
50	15	0	-0.952556	0.381497	0.087994
51	8	0	-1.274623	-1.182233	-0.295591
52	8	0	-2.276209	0.827835	0.931168
53	8	0	0.192897	0.537072	1.031271
54	6	0	-1.902715	-2.005374	0.613040
55	6	0	-3.481993	0.627916	0.287118
56	6	0	-3.236421	-1.754514	0.945640
57	6	0	-1.212309	-3.101394	1.122219
58	6	0	-4.170529	1.714524	-0.242877
59	6	0	-3.974282	-0.674764	0.220259
60	6	0	-3.844352	-2.511880	1.966447
61	6	0	-1.867781	-3.891510	2.058037
62	6	0	0.170744	-3.464770	0.652688
63	6	0	-5.357523	1.439607	-0.911302
64	6	0	-3.709934	3.138456	-0.070681
65	6	0	-5.128305	-0.935951	-0.544138
66	6	0	-3.150589	-3.593185	2.519182
67	6	0	-5.202864	-2.081839	2.545666
68	1	0	-1.344245	-4.751080	2.460399
69	6	0	0.319556	-4.218021	-0.515923
70	6	0	1.285024	-3.112318	1.414262
71	6	0	-5.826478	0.138811	-1.103367
72	1	0	-5.916796	2.271126	-1.324134
73	6	0	-3.922850	3.780258	1.153930
74	6	0	-3.170491	3.838945	-1.152534
75	6	0	-5.542743	-2.382896	-0.858691
76	6	0	-3.773933	-4.501856	3.588549
77	1	0	-5.842287	-1.701634	1.765261
78	1	0	-5.008882	-1.256729	3.226320
79	6	0	-5.904172	-3.209526	3.317235
80	6	0	1.619013	-4.638013	-0.920280
81	6	0	-0.796423	-4.598118	-1.336110
82	6	0	2.581941	-3.538891	1.002175
83	6	0	1.181974	-2.315706	2.605475
84	6	0	-7.129235	-0.058672	-1.891914
85	6	0	-3.593935	5.159197	1.291271

86	6	0	-4.474474	3.104992	2.294932
87	6	0	-2.865615	5.224760	-1.009938
88	6	0	-2.899852	3.216215	-2.419501
89	1	0	-4.895084	-2.730261	-1.659718
90	1	0	-5.361650	-3.020530	-0.008048
91	6	0	-7.004693	-2.495325	-1.316130
92	1	0	-4.144897	-5.399053	3.100192
93	1	0	-3.002632	-4.805653	4.286835
94	6	0	-4.933398	-3.826083	4.334754
95	1	0	-6.779053	-2.809872	3.818279
96	1	0	-6.240577	-3.977251	2.626679
97	6	0	1.756977	-5.421166	-2.114232
98	6	0	2.718162	-4.292810	-0.150480
99	6	0	-0.623489	-5.333175	-2.453091
100	1	0	-1.774073	-4.283248	-1.039080
101	6	0	3.718301	-3.166995	1.793938
102	6	0	2.277198	-1.986883	3.314566
103	1	0	0.217268	-1.962871	2.899847
104	1	0	-7.164458	0.661348	-2.701220
105	1	0	-7.964404	0.152550	-1.229411
106	6	0	-7.277129	-1.485316	-2.440341
107	6	0	-3.819035	5.807107	2.550657
108	6	0	-3.081587	5.850332	0.205510
109	6	0	-4.670344	3.751419	3.460131
110	1	0	-4.723114	2.069920	2.201098
111	6	0	-2.347473	5.943470	-2.138805
112	6	0	-2.412266	3.928992	-3.452108
113	1	0	-3.054881	2.164473	-2.509447
114	1	0	-7.670101	-2.295932	-0.481346
115	1	0	-7.196719	-3.506875	-1.657104
116	1	0	-4.548624	-3.045789	4.983431
117	1	0	-5.440653	-4.555546	4.956467
118	6	0	0.681383	-5.757072	-2.852487
119	1	0	2.741361	-5.739950	-2.398848
120	1	0	3.695608	-4.615703	-0.455417
121	1	0	-1.468414	-5.613438	-3.050614
122	1	0	4.689266	-3.488020	1.470172
123	6	0	3.574188	-2.420459	2.903068
124	1	0	2.187671	-1.372190	4.187344
125	1	0	-6.568444	-1.644525	-3.246635
126	1	0	-8.275131	-1.619006	-2.843010
127	6	0	-4.335516	5.132930	3.594387
128	1	0	-3.564441	6.845797	2.637137
129	1	0	-2.851461	6.894037	0.308205
130	1	0	-5.079287	3.230551	4.303027
131	1	0	-2.135004	6.988367	-2.018679
132	6	0	-2.138404	5.324538	-3.314730
133	1	0	-2.205139	3.446879	-4.386499
134	1	0	0.791450	-6.350425	-3.738662
135	1	0	4.430831	-2.122469	3.472008
136	1	0	-4.500761	5.623459	4.533066
137	1	0	-1.754588	5.867733	-4.155685

TSr4a ONIOM: extrapolated energy = -6284.061097495909 A.U.
SCF Done: E(RM052X+HF-M052X) = -6307.31388026 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.418659	-0.017395	4.457806
2	6	0	1.859963	0.439306	5.834801
3	6	0	3.384455	0.428338	5.732810
4	6	0	3.651055	0.000410	4.287062
5	7	0	2.437706	-0.282312	3.661473
6	1	0	1.434388	1.424273	6.027342
7	1	0	3.862190	-0.288893	6.400084
8	8	0	4.733113	-0.070881	3.756478
9	8	0	0.189852	-0.092283	4.189273
10	1	0	3.845012	1.400264	5.904623
11	1	0	1.455652	-0.246638	6.579368
12	35	0	2.367371	-1.124039	1.582404
13	6	0	2.724014	-3.116486	-0.398285
14	6	0	2.119926	-1.807378	-0.454291
15	6	0	2.837747	-0.775107	-1.186148
16	6	0	4.121065	-0.993060	-1.701386
17	6	0	4.616453	-2.308664	-1.654858
18	6	0	3.941418	-3.342064	-0.944730
19	1	0	2.170447	-3.899372	0.100962
20	1	0	1.038136	-1.766678	-0.527846
21	1	0	4.426355	-4.305087	-0.916754
22	8	0	2.280978	0.395621	-1.342407
23	1	0	-0.227421	-0.276072	3.113308
24	8	0	5.736511	-2.690410	-2.282692
25	1	0	5.867707	-2.200319	-3.128424
26	6	0	4.914595	0.145820	-2.285979
27	6	0	5.423062	0.052124	-3.572695
28	6	0	5.226011	1.294076	-1.546564
29	6	0	6.164103	1.056161	-4.154394
30	6	0	5.967571	2.307801	-2.130832
31	6	0	6.425798	2.199094	-3.429574
32	1	0	6.542174	0.918849	-5.146362
33	1	0	6.199603	3.160955	-1.533931
34	1	0	7.005179	2.990074	-3.862024
35	6	0	4.790370	1.460335	-0.104024
36	1	0	3.722738	1.608266	-0.063761
37	1	0	5.040493	0.571757	0.464417
38	8	0	5.462502	2.604107	0.446568
39	8	0	5.250724	-1.147925	-4.277375
40	6	0	5.162005	2.834938	1.836258
41	1	0	5.338851	1.945450	2.426841
42	1	0	5.815516	3.630314	2.163069
43	1	0	4.128786	3.141199	1.958366
44	6	0	4.110459	-1.234924	-5.182283
45	1	0	4.208507	-0.494195	-5.962425
46	1	0	4.137886	-2.226860	-5.602666
47	1	0	3.191118	-1.078689	-4.637584
48	1	0	1.433324	0.514524	-0.772728
49	8	0	-0.932225	-0.430898	2.111246
50	15	0	-0.921340	0.200125	0.735673
51	8	0	-2.163817	1.252718	0.761611
52	8	0	-1.415454	-0.921986	-0.355249
53	8	0	0.306187	0.810092	0.149060
54	6	0	-2.590421	1.706138	-0.474381
55	6	0	-2.723316	-1.361838	-0.262488
56	6	0	-3.358404	0.833132	-1.246028
57	6	0	-2.270710	2.993887	-0.895479
58	6	0	-2.983913	-2.654513	0.179198
59	6	0	-3.740009	-0.486400	-0.651281
60	6	0	-3.713898	1.202966	-2.556711
61	6	0	-2.707786	3.363744	-2.162167
62	6	0	-1.533858	3.972729	-0.017249
63	6	0	-4.318970	-3.024628	0.295432
64	6	0	-1.898017	-3.664456	0.449657
65	6	0	-5.081598	-0.855089	-0.439461
66	6	0	-3.390305	2.487138	-3.007764
67	6	0	-4.337171	0.173347	-3.513494
68	1	0	-2.480418	4.365207	-2.508622
69	6	0	-2.248883	4.684695	0.950817
70	6	0	-0.168439	4.201958	-0.202479
71	6	0	-5.366467	-2.141399	0.032112
72	1	0	-4.544006	-4.030742	0.629546
73	6	0	-1.359031	-4.378041	-0.626719
74	6	0	-1.510666	-3.958720	1.758949
75	6	0	-6.205415	0.181189	-0.604432
76	6	0	-3.803526	2.987657	-4.399363
77	1	0	-5.018084	-0.471919	-2.981122
78	1	0	-3.527214	-0.452892	-3.879183
79	6	0	-5.039575	0.828364	-4.712173
80	6	0	-1.574492	5.648296	1.753916
81	6	0	-3.654394	4.490613	1.172595
82	6	0	0.500709	5.157023	0.619125
83	6	0	0.611202	3.494638	-1.178952
84	6	0	-6.807054	-2.635870	0.226860
85	6	0	-0.421155	-5.422182	-0.380075
86	6	0	-1.722713	-4.109862	-1.990421
87	6	0	-0.582785	-5.016136	1.996457
88	6	0	-2.009196	-3.230251	2.892616
89	1	0	-6.197058	0.800522	0.288746
90	1	0	-5.999075	0.831378	-1.439827
91	6	0	-7.591260	-0.464541	-0.750876
92	1	0	-4.698322	3.594615	-4.290698
93	1	0	-3.021283	3.627217	-4.791371
94	6	0	-4.095975	1.840751	-5.377860
95	1	0	-5.334896	0.060182	-5.418514
96	1	0	-5.940121	1.336586	-4.380661
97	6	0	-2.319626	6.378519	2.737613
98	6	0	-0.217481	5.859694	1.570984
99	6	0	-4.316710	5.198398	2.107822
100	1	0	-4.167226	3.765807	0.577178
101	6	0	1.913614	5.349486	0.454133
102	6	0	1.934670	3.705370	-1.301365
103	1	0	0.123807	2.760015	-1.780349
104	1	0	-6.843588	-3.282718	1.095688
105	1	0	-7.082192	-3.233455	-0.638119
106	6	0	-7.811632	-1.484046	0.376228
107	6	0	0.116730	-6.151849	-1.491884
108	6	0	-0.061414	-5.722296	0.925046
109	6	0	-1.190875	-4.817625	-3.005670
110	1	0	-2.427988	-3.330035	-2.183009
111	6	0	-0.219327	-5.332282	3.347750
112	6	0	-1.635864	-3.557173	4.144020
113	1	0	-2.647019	-2.392948	2.717528
114	1	0	-7.667496	-0.964802	-1.711782
115	1	0	-8.351258	0.308416	-0.719761
116	1	0	-3.170111	1.344366	-5.650390
117	1	0	-4.538542	2.239521	-6.283928
118	6	0	-3.637168	6.164940	2.909506
119	1	0	-1.796620	7.101320	3.333651
120	1	0	0.288478	6.581957	2.183553
121	1	0	-5.365711	5.039670	2.261255
122	1	0	2.404565	6.058669	1.092528
123	6	0	2.606147	4.645976	-0.460878
124	1	0	2.505502	3.133667	-2.003962
125	1	0	-7.672007	-0.996041	1.335334
126	1	0	-8.821972	-1.876636	0.346598
127	6	0	-0.250466	-5.862288	-2.753819
128	1	0	0.817788	-6.938485	-1.289243
129	1	0	0.625985	-6.526610	1.109521
130	1	0	-1.472412	-4.603314	-4.017487
131	1	0	0.469887	-6.137949	3.511577
132	6	0	-0.730778	-4.637001	4.379624

133	1	0	-2.002186	-2.992049	4.977163
134	1	0	-4.187686	6.714561	3.646957
135	1	0	3.668643	4.753456	-0.550445
136	1	0	0.154685	-6.413031	-3.579291
137	1	0	-0.456637	-4.879140	5.387331

TSs1a ONIOM: extrapolated energy = -6284.065162627510 A.U.
SCF Done: E(RM052X+HF-M052X) = -6307.31803822 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.848569	-2.653806	-3.753370
2	6	0	0.808521	-3.491114	-4.503975
3	6	0	-0.481954	-2.686872	-4.357924
4	6	0	-0.045432	-1.483381	-3.544219
5	7	0	1.248507	-1.504030	-3.262281
6	1	0	1.138849	-3.620822	-5.534344
7	1	0	-1.260747	-3.210124	-3.803213
8	8	0	-0.882176	-0.603544	-3.211502
9	8	0	3.012937	-2.952642	-3.612115
10	1	0	-0.908913	-2.344583	-5.301067
11	1	0	0.751790	-4.473156	-4.036962
12	35	0	2.200067	0.159394	-2.011272
13	6	0	3.310606	2.743372	-1.575384
14	6	0	2.669693	1.773775	-0.708809
15	6	0	3.511750	1.121930	0.284223
16	6	0	4.888383	1.358665	0.342641
17	6	0	5.439652	2.295710	-0.532012
18	6	0	4.638173	2.973618	-1.505647
19	1	0	2.682570	3.258409	-2.290485
20	1	0	1.661846	2.002873	-0.378358
21	1	0	5.149450	3.666010	-2.156284
22	8	0	2.977853	0.294680	1.136548
23	1	0	-0.694340	0.191922	-2.289038
24	8	0	6.728154	2.642485	-0.519408
25	1	0	7.161379	2.561908	0.371785
26	6	0	5.740674	0.412556	1.133621
27	6	0	5.836532	-0.889796	0.627314
28	6	0	6.425329	0.742074	2.289320
29	6	0	6.602629	-1.830958	1.288780
30	6	0	7.199454	-0.207756	2.945232
31	6	0	7.279838	-1.487833	2.445467
32	1	0	6.679538	-2.826313	0.907289
33	1	0	7.734265	0.062513	3.833717
34	1	0	7.875844	-2.224124	2.947310
35	6	0	6.397503	2.154989	2.806341
36	1	0	5.405304	2.580222	2.744113
37	1	0	6.743907	2.199260	3.829961
38	8	0	7.304395	2.921598	1.964643
39	8	0	5.150554	-1.138365	-0.514662
40	6	0	7.417852	4.322313	2.293510
41	1	0	7.823198	4.441869	3.290364
42	1	0	8.091663	4.756365	1.572120
43	1	0	6.453441	4.812702	2.234847
44	6	0	5.084687	-2.462088	-1.094011
45	1	0	4.672117	-3.162773	-0.380985
46	1	0	4.433102	-2.383511	-1.945490
47	1	0	6.069448	-2.789232	-1.405090
48	1	0	1.991776	0.178668	0.985726
49	8	0	-0.739259	0.931399	-1.368801
50	15	0	-0.833674	0.355126	0.044087
51	8	0	-1.615542	-1.062557	-0.193901
52	8	0	-1.912032	1.242734	0.880993
53	8	0	0.371571	0.238394	0.909597
54	6	0	-2.334257	-1.601697	0.855635
55	6	0	-3.179160	1.317777	0.331861
56	6	0	-3.511154	-0.962811	1.253980
57	6	0	-1.898158	-2.783039	1.446322
58	6	0	-3.592690	2.490226	-0.291746
59	6	0	-4.004451	0.201197	0.454296
60	6	0	-4.184304	-1.416249	2.404588
61	6	0	-2.632193	-3.259213	2.526161
62	6	0	-0.740039	-3.587679	0.915721
63	6	0	-4.864480	2.486535	-0.852064
64	6	0	-2.746541	3.736123	-0.326141
65	6	0	-5.250279	0.192554	-0.201324
66	6	0	-3.736528	-2.579030	3.040257
67	6	0	-5.318510	-0.579161	3.019360
68	1	0	-2.310652	-4.181804	2.995303
69	6	0	-0.969384	-4.492090	-0.126401
70	6	0	0.515970	-3.506610	1.518474
71	6	0	-5.681897	1.354650	-0.849269
72	1	0	-5.213904	3.391757	-1.334782
73	6	0	-2.675055	4.541452	0.815393
74	6	0	-2.114995	4.127228	-1.509494
75	6	0	-6.063663	-1.107950	-0.307285
76	6	0	-4.455010	-3.167557	4.262963
77	1	0	-5.917404	-0.128651	2.243907
78	1	0	-4.849967	0.232504	3.570067
79	6	0	-6.200100	-1.389963	3.980859
80	6	0	0.081818	-5.352628	-0.554130
81	6	0	-2.237016	-4.596294	-0.794046
82	6	0	1.555550	-4.386723	1.095941
83	6	0	0.817643	-2.550101	2.547295
84	6	0	-7.056027	1.443917	-1.528394
85	6	0	-1.957052	5.770393	0.764809
86	6	0	-3.308952	4.184873	2.053670
87	6	0	-1.411694	5.367238	-1.552704
88	6	0	-2.135880	3.323097	-2.700770
89	1	0	-5.607756	-1.702971	-1.094572
90	1	0	-5.983909	-1.677828	0.604955
91	6	0	-7.537372	-0.858678	-0.661151
92	1	0	-5.092086	-3.980731	3.925525
93	1	0	-3.717574	-3.588416	4.936550
94	6	0	-5.317849	-2.130477	4.996496
95	1	0	-6.886131	-0.720483	4.488091
96	1	0	-6.792051	-2.109510	3.422984
97	6	0	-0.166223	-6.278392	-1.621512
98	6	0	1.314433	-5.289134	0.075028
99	6	0	-2.427003	-5.476177	-1.797613
100	1	0	-3.031157	-3.954008	-0.478221
101	6	0	2.834879	-4.310769	1.740682
102	6	0	2.040940	-2.496932	3.106496
103	1	0	0.063383	-1.847513	2.826810
104	1	0	-6.971034	2.057580	-2.417661
105	1	0	-7.740201	1.945190	-0.848961
106	6	0	-7.629451	0.064659	-1.884778
107	6	0	-1.894062	6.589430	1.940271
108	6	0	-1.348075	6.156862	-0.417869
109	6	0	-3.225265	4.983573	3.134862
110	1	0	-3.848761	3.263744	2.101004
111	6	0	-0.788538	5.772283	-2.780414
112	6	0	-1.537559	3.742006	-3.831502
113	1	0	-2.604280	2.365401	-2.657579
114	1	0	-8.047004	-0.397446	0.179606
115	1	0	-8.023134	-1.807404	-0.861651
116	1	0	-4.680147	-1.416327	5.507351
117	1	0	-5.926693	-2.626986	5.743925
118	6	0	-1.370209	-6.338701	-2.222310
119	1	0	0.633924	-6.925725	-1.925158
120	1	0	2.100201	-5.948881	-0.240707
121	1	0	-3.379914	-5.540904	-2.284577
122	1	0	3.600294	-4.994014	1.426224
123	6	0	3.070428	-3.401824	2.704305
124	1	0	2.261428	-1.756083	3.847779
125	1	0	-7.065309	-0.367338	-2.705001
126	1	0	-8.658892	0.171172	-2.208538
127	6	0	-2.502108	6.213542	3.080290
128	1	0	-1.348957	7.511907	1.884756
129	1	0	-0.819332	7.090574	-0.455812
130	1	0	-3.701754	4.700081	4.052223
131	1	0	-0.272450	6.712875	-2.799019
132	6	0	-0.854799	4.996363	-3.877466
133	1	0	-1.552725	3.124043	-4.706805
134	1	0	-1.549669	-7.036137	-3.016406
135	1	0	4.034805	-3.332612	3.165931
136	1	0	-2.451032	6.830644	3.955267
137	1	0	-0.390927	5.306317	-4.793081

TSs2a ONIOM: extrapolated energy = -6284.062617098327 A.U.
SCF Done: E(RM052X+HF-M052X) = -6307.31376027 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.454236	-0.678649	-4.269996
2	6	0	1.817681	-1.754486	-5.154241
3	6	0	0.320720	-1.604806	-4.885863
4	6	0	0.276261	-0.478820	-3.876558
5	7	0	1.454781	0.035097	-3.609618
6	1	0	2.105395	-1.579903	-6.190611
7	1	0	-0.130663	-2.486863	-4.432652
8	8	0	-0.841166	-0.127523	-3.378958
9	8	0	3.639977	-0.477447	-4.147328
10	1	0	-0.269632	-1.330032	-5.760511
11	1	0	2.207572	-2.724541	-4.848700
12	35	0	1.976925	1.499641	-1.863820
13	6	0	2.786594	3.882709	-0.523552
14	6	0	2.282566	2.591316	-0.093028
15	6	0	3.244056	1.672362	0.518692
16	6	0	4.625171	1.908756	0.451142
17	6	0	5.035784	3.084477	-0.196834
18	6	0	4.112930	4.114468	-0.570804
19	1	0	2.067698	4.611800	-0.872942
20	1	0	1.292446	2.559179	0.350065
21	1	0	4.540935	5.021082	-0.969013
22	8	0	2.793391	0.583219	1.063479
23	1	0	-0.843521	0.483076	-2.451574
24	8	0	6.305675	3.323464	-0.534462
25	1	0	6.759208	2.493296	-0.838558
26	6	0	5.622205	0.898857	0.957436
27	6	0	6.579164	0.390310	0.088527
28	6	0	5.671188	0.488873	2.293604
29	6	0	7.524394	-0.527495	0.490152
30	6	0	6.626755	-0.427228	2.700911
31	6	0	7.540696	-0.945629	1.803587
32	1	0	8.244818	-0.874561	-0.221090
33	1	0	6.647806	-0.706574	3.730279
34	1	0	8.277084	-1.650119	2.135390

35	6	0	4.712514	1.048951	3.323827
36	1	0	4.809138	2.130448	3.359868
37	1	0	3.703209	0.787949	3.053442
38	8	0	5.029860	0.484358	4.609299
39	8	0	6.658203	0.903331	-1.207607
40	6	0	4.267486	1.031205	5.696047
41	1	0	3.204800	0.867670	5.553064
42	1	0	4.593027	0.522990	6.590533
43	1	0	4.446002	2.096169	5.801569
44	6	0	5.912457	0.222890	-2.279422
45	1	0	6.247022	-0.800738	-2.351083
46	1	0	4.856593	0.260657	-2.088977
47	1	0	6.141402	0.757573	-3.184363
48	1	0	1.773113	0.481617	0.971113
49	8	0	-1.042510	1.093017	-1.287027
50	15	0	-0.927891	0.328504	0.014810
51	8	0	-1.157669	-1.231601	-0.433997
52	8	0	-2.238201	0.628026	0.942343
53	8	0	0.255847	0.510218	0.915004
54	6	0	-1.808263	-2.128858	0.385657
55	6	0	-3.438624	0.485801	0.268094
56	6	0	-3.168921	-1.950708	0.649439
57	6	0	-1.099152	-3.219085	0.880102
58	6	0	-4.144758	1.618067	-0.126683
59	6	0	-3.895212	-0.807285	0.015639
60	6	0	-3.812481	-2.818596	1.554858
61	6	0	-1.783003	-4.116110	1.690456
62	6	0	0.361965	-3.406877	0.579367
63	6	0	-5.303925	1.408672	-0.863341
64	6	0	-3.731699	3.013027	0.265279
65	6	0	-5.016366	-0.988657	-0.817057
66	6	0	-3.114529	-3.921707	2.058203
67	6	0	-5.219493	-2.487535	2.082910
68	1	0	-1.243172	-4.972639	2.077437
69	6	0	0.757914	-4.017510	-0.611933
70	6	0	1.311603	-2.995968	1.516744
71	6	0	-5.726235	0.135055	-1.250716
72	1	0	-5.877110	2.274493	-1.173983
73	6	0	-3.990114	3.457382	1.566762
74	6	0	-3.189214	3.882831	-0.684335
75	6	0	-5.379092	-2.389482	-1.336677
76	6	0	-3.775604	-4.952480	2.984503
77	1	0	-5.822900	-2.050186	1.304500
78	1	0	-5.096646	-1.728953	2.851961
79	6	0	-5.928754	-3.705197	2.693734
80	6	0	2.144354	-4.218247	-0.870516
81	6	0	-0.185169	-4.466122	-1.597939
82	6	0	2.697049	-3.194763	1.247408
83	6	0	0.948654	-2.360419	2.752827
84	6	0	-6.997144	0.014862	-2.104004
85	6	0	-3.701741	4.806912	1.919205
86	6	0	-4.550447	2.605418	2.578009
87	6	0	-2.925096	5.237865	-0.325914
88	6	0	-2.876412	3.466679	-2.024326
89	1	0	-4.698848	-2.608015	-2.155791
90	1	0	-5.203015	-3.131776	-0.574146
91	6	0	-6.823268	-2.474330	-1.852551
92	1	0	-4.081193	-5.804319	2.382796
93	1	0	-3.042710	-5.305464	3.700742
94	6	0	-5.005746	-4.390599	3.711329
95	1	0	-6.847983	-3.381644	3.169717
96	1	0	-6.192312	-4.410785	1.911386
97	6	0	2.536495	-4.857263	-2.093755
98	6	0	3.080130	-3.800684	0.062128
99	6	0	0.225428	-5.069009	-2.731613
100	1	0	-1.226848	-4.316269	-1.406967
101	6	0	3.663035	-2.741735	2.205123
102	6	0	1.890441	-1.962837	3.628310
103	1	0	-0.087380	-2.195874	2.956831
104	1	0	-7.025679	0.834832	-2.812189
105	1	0	-7.858437	0.117866	-1.449320
106	6	0	-7.089447	-1.329330	-2.840889
107	6	0	-3.972252	5.251586	3.255471
108	6	0	-3.183941	5.666444	0.964198
109	6	0	-4.789983	3.063584	3.821653
110	1	0	-4.771421	1.591602	2.322660
111	6	0	-2.402654	6.131893	-1.319493
112	6	0	-2.386887	4.339964	-2.924519
113	1	0	-2.999154	2.437143	-2.274261
114	1	0	-7.518579	-2.404249	-1.021245
115	1	0	-6.977174	-3.435120	-2.331621
116	1	0	-4.693848	-3.668052	4.458566
117	1	0	-5.525818	-5.193687	4.221730
118	6	0	1.617500	-5.270496	-2.987579
119	1	0	3.583841	-5.006116	-2.272968
120	1	0	4.124506	-3.947654	-0.137802
121	1	0	-0.492071	-5.412864	-3.450644
122	1	0	4.702633	-2.859377	1.972049
123	6	0	3.279089	-2.147086	3.349587
124	1	0	1.602806	-1.482737	4.542742
125	1	0	-6.352851	-1.363213	-3.637079
126	1	0	-8.070906	-1.430922	-3.290791
127	6	0	-4.494324	4.415813	4.171701
128	1	0	-3.747504	6.270824	3.504031
129	1	0	-2.984461	6.687560	1.229429
130	1	0	-5.205513	2.412405	4.564823
131	1	0	-2.222009	7.151303	-1.037354
132	6	0	-2.152921	5.704235	-2.570345
133	1	0	-2.149187	4.011399	-3.916506
134	1	0	1.918448	-5.761753	-3.891969
135	1	0	4.004223	-1.755336	4.033197
136	1	0	-4.693959	4.754835	5.168800
137	1	0	-1.767838	6.378330	-3.309933

TSs3a ONIOM: extrapolated energy = -6284.062556781846 A.U.
SCF Done: E(RM052X+HF-M052X) = -6307.32176842 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.063855	-1.260116	3.327998
2	6	0	0.542235	-1.905380	4.563782
3	6	0	-0.247970	-3.202981	4.714304
4	6	0	-1.211408	-3.189919	3.524792
5	7	0	-1.032905	-2.007870	2.807481
6	1	0	0.451649	-1.220027	5.406413
7	1	0	0.366248	-4.098607	4.639695
8	8	0	-2.007622	-4.054109	3.255844
9	8	0	0.345601	-0.152469	2.918142
10	1	0	-0.826723	-3.262896	5.635778
11	1	0	1.603627	-2.062123	4.370614
12	35	0	-1.998824	-1.847730	0.822010
13	6	0	-3.760273	-2.872904	-1.153454
14	6	0	-2.855217	-1.749283	-1.197405
15	6	0	-3.456033	-0.432380	-1.175997
16	6	0	-4.805613	-0.261716	-0.846073
17	6	0	-5.598893	-1.394001	-0.670108
18	6	0	-5.073377	-2.704246	-0.873222
19	1	0	-3.331444	-3.856891	-1.274999
20	1	0	-1.946059	-1.848708	-1.778121
21	1	0	-5.759116	-3.529045	-0.758174
22	8	0	-2.733341	0.625988	-1.419809
23	1	0	-0.006408	0.353001	1.746551
24	8	0	-6.887534	-1.333118	-0.299958
25	1	0	-7.071989	-0.584292	0.324064
26	6	0	-5.389035	1.116662	-0.905274
27	6	0	-5.535337	1.695520	-2.168130
28	6	0	-5.773543	1.835103	0.213645
29	6	0	-6.058295	2.967170	-2.292322
30	6	0	-6.308410	3.110649	0.083001
31	6	0	-6.444949	3.671641	-1.165923
32	1	0	-6.168855	3.416142	-3.256236
33	1	0	-6.609771	3.652685	0.956857
34	1	0	-6.852482	4.657177	-1.272434
35	6	0	-5.656181	1.213350	1.579889
36	1	0	-5.742884	1.962898	2.354626
37	1	0	-4.716869	0.689759	1.690767
38	8	0	-6.754482	0.267301	1.706446
39	8	0	-5.138272	0.938543	-3.232118
40	6	0	-6.739050	-0.530963	2.910043
41	1	0	-5.817915	-1.095963	2.984924
42	1	0	-7.576703	-1.206937	2.843661
43	1	0	-6.847916	0.101825	3.782069
44	6	0	-5.015975	1.508609	-4.545411
45	1	0	-5.982299	1.792140	-4.943333
46	1	0	-4.589252	0.730291	-5.156022
47	1	0	-4.359188	2.369025	-4.537754
48	1	0	-1.766446	0.391202	-1.571946
49	8	0	-0.220685	-0.030288	-1.648292
50	15	0	0.585039	0.390657	-0.465987
51	8	0	1.597931	1.559858	-0.964413
52	8	0	1.594317	-0.758356	0.099806
53	8	0	-0.143964	0.885667	0.789386
54	6	0	2.626901	1.896332	-0.099649
55	6	0	2.655542	-1.112049	-0.718601
56	6	0	3.708418	1.019300	-0.012065
57	6	0	2.570868	3.083170	0.622355
58	6	0	2.667647	-2.365033	-1.320589
59	6	0	3.704919	-0.203958	-0.869599
60	6	0	4.729295	1.269229	0.923867
61	6	0	3.637471	3.349454	1.474483
62	6	0	1.448676	4.079296	0.501262
63	6	0	3.727341	-2.642451	-2.176831
64	6	0	1.654664	-3.432675	-1.005174
65	6	0	4.715398	-0.471806	-1.811842
66	6	0	4.695062	2.459322	1.658433
67	6	0	5.789872	0.197798	1.228010
68	1	0	3.619368	4.274697	2.038119
69	6	0	1.416022	4.945865	-0.595058
70	6	0	0.515026	4.202732	1.533279
71	6	0	4.720746	-1.706762	-2.468256
72	1	0	3.760132	-3.616796	-2.650284
73	6	0	1.794776	-4.166667	0.177228
74	6	0	0.659542	-3.759880	-1.927219
75	6	0	5.727242	0.620918	-2.193511
76	6	0	5.808185	2.838941	2.645244
77	1	0	6.071172	-0.322930	0.326794
78	1	0	5.323150	-0.532790	1.884127
79	6	0	7.031223	0.772649	1.926678
80	6	0	0.426657	5.968591	-0.651486
81	6	0	2.353630	4.857205	-1.679042

82	6	0	-0.457708	5.243330	1.475566
83	6	0	0.480453	3.310724	2.660075
84	6	0	5.825288	-2.095433	-3.461542
85	6	0	0.913602	-5.254687	0.436892
86	6	0	2.810690	-3.877478	1.150877
87	6	0	-0.189453	-4.878034	-1.677126
88	6	0	0.444931	-3.003786	-3.131134
89	1	0	5.222221	1.293165	-2.882272
90	1	0	5.997268	1.203255	-1.326550
91	6	0	6.979495	0.054003	-2.878637
92	1	0	6.486140	3.525712	2.145643
93	1	0	5.370683	3.365419	3.485386
94	6	0	6.604597	1.620433	3.133795
95	1	0	7.674620	-0.042066	2.240589
96	1	0	7.593811	1.389328	1.232146
97	6	0	0.404370	6.854217	-1.779072
98	6	0	-0.480046	6.098423	0.387498
99	6	0	2.297781	5.710282	-2.719687
100	1	0	3.097941	4.090834	-1.645723
101	6	0	-1.391719	5.384801	2.555445
102	6	0	-0.418603	3.476626	3.647907
103	1	0	1.153989	2.482788	2.684469
104	1	0	5.388803	-2.678250	-4.264321
105	1	0	6.538562	-2.732117	-2.945058
106	6	0	6.565748	-0.875477	-4.029185
107	6	0	1.061306	-5.996647	1.655151
108	6	0	-0.049337	-5.592543	-0.500008
109	6	0	2.923724	-4.608300	2.277285
110	1	0	3.481998	-3.067986	0.960125
111	6	0	-1.169315	-5.240114	-2.661781
112	6	0	-0.499282	-3.369526	-4.020037
113	1	0	1.025270	-2.120205	-3.286789
114	1	0	7.575864	-0.501245	-2.160695
115	1	0	7.586492	0.872527	-3.249441
116	1	0	5.989186	1.020259	3.796259
117	1	0	7.471126	1.952662	3.694687
118	6	0	1.301905	6.732265	-2.774167
119	1	0	-0.349120	7.617472	-1.807135
120	1	0	-1.215498	6.879515	0.348089
121	1	0	3.002665	5.627037	-3.522983
122	1	0	-2.109511	6.180399	2.501294
123	6	0	-1.368487	4.542633	3.603968
124	1	0	-0.440975	2.787775	4.468398
125	1	0	5.917110	-0.335959	-4.711649
126	1	0	7.434737	-1.205523	-4.587428
127	6	0	2.029627	-5.691264	2.539380
128	1	0	0.379246	-6.802778	1.841499
129	1	0	-0.697815	-6.426030	-0.308629
130	1	0	3.694274	-4.385100	2.988836
131	1	0	-1.779805	-6.102769	-2.474625
132	6	0	-1.314216	-4.521129	-3.790748
133	1	0	-0.656007	-2.788824	-4.906871
134	1	0	1.278981	7.397248	-3.614560
135	1	0	-2.068421	4.654397	4.408465
136	1	0	2.142302	-6.258802	3.441941
137	1	0	-2.046965	-4.797253	-4.522648

TSs4a ONIOM: extrapolated energy = -6284.063581804901 A.U.
SCF Done: E(RM052X+HF-M052X) = -6307.32272418 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.196573	-1.307871	3.435044
2	6	0	0.365933	-1.867003	4.725603
3	6	0	-0.403640	-3.172865	4.908441
4	6	0	-1.259731	-3.276162	3.645760
5	7	0	-1.086977	-2.109695	2.883674
6	1	0	0.226435	-1.139001	5.524245
7	1	0	0.232972	-4.053020	4.963440
8	8	0	-1.977585	-4.192837	3.346136
9	8	0	0.201711	-0.186147	3.015562
10	1	0	-1.063670	-3.171217	5.775846
11	1	0	1.437069	-2.013641	4.583704
12	35	0	-2.110787	-1.998274	0.938689
13	6	0	-3.960175	-3.035151	-0.924757
14	6	0	-3.030160	-1.946134	-1.064395
15	6	0	-3.583373	-0.610270	-1.114585
16	6	0	-4.941907	-0.362899	-0.862019
17	6	0	-5.791510	-1.476195	-0.770578
18	6	0	-5.284375	-2.804661	-0.753864
19	1	0	-3.558063	-4.037600	-0.937487
20	1	0	-2.123931	-2.113613	-1.633784
21	1	0	-6.004958	-3.597857	-0.630158
22	8	0	-2.802217	0.402249	-1.388452
23	1	0	-0.079983	0.214919	1.949847
24	8	0	-7.130527	-1.374858	-0.716539
25	1	0	-7.459597	-0.618158	-1.255155
26	6	0	-5.444194	1.047586	-0.708189
27	6	0	-6.502796	1.505050	-1.478580
28	6	0	-4.917682	1.916828	0.253455
29	6	0	-7.010131	2.779036	-1.360274
30	6	0	-5.421718	3.201172	0.371833
31	6	0	-6.454702	3.637051	-0.434174
32	1	0	-7.838841	3.069816	-1.972335
33	1	0	-5.002239	3.830493	1.124266
34	1	0	-6.838687	4.631588	-0.324433
35	6	0	-3.806987	1.490884	1.190060
36	1	0	-2.869113	1.460595	0.657202
37	1	0	-4.013374	0.500144	1.578772
38	8	0	-3.724678	2.437401	2.264735
39	8	0	-7.135731	0.610057	-2.354127
40	6	0	-2.543639	2.288516	3.073308
41	1	0	-2.576245	1.363117	3.640783
42	1	0	-2.525896	3.127108	3.750804
43	1	0	-1.650813	2.290315	2.463858
44	6	0	-6.666530	0.589616	-3.734403
45	1	0	-6.843076	1.551970	-4.192369
46	1	0	-7.240519	-0.173537	-4.234279
47	1	0	-5.612914	0.354633	-3.765388
48	1	0	-1.825371	0.123702	-1.487171
49	8	0	-0.341996	-0.284567	-1.500775
50	15	0	0.467040	0.278658	-0.372330
51	8	0	1.384650	1.457040	-1.020800
52	8	0	1.579390	-0.773364	0.200766
53	8	0	-0.244030	0.789207	0.874213
54	6	0	2.530717	1.869198	-0.368197
55	6	0	2.533719	-1.195232	-0.712176
56	6	0	3.629988	1.008562	-0.363544
57	6	0	2.584485	3.144102	0.187138
58	6	0	2.493642	-2.498912	-1.194773
59	6	0	3.530748	-0.294155	-1.088394
60	6	0	4.788405	1.368411	0.352059
61	6	0	3.782212	3.515396	0.790467
62	6	0	1.438290	4.118085	0.150836
63	6	0	3.440199	-2.846121	-2.152078
64	6	0	1.541605	-3.543234	-0.678309
65	6	0	4.410940	-0.638477	-2.132647
66	6	0	4.865399	2.646674	0.914113
67	6	0	5.901534	0.339020	0.610904
68	1	0	3.851817	4.510844	1.212568
69	6	0	1.061697	4.713596	-1.057005
70	6	0	0.828097	4.501575	1.350144
71	6	0	4.362680	-1.931826	-2.661606
72	1	0	3.432018	-3.860296	-2.533738
73	6	0	1.785093	-4.135130	0.565533
74	6	0	0.505025	-4.007816	-1.490230
75	6	0	5.328931	0.425160	-2.757789
76	6	0	6.127379	3.147766	1.630995
77	1	0	6.027139	-0.305909	-0.243582
78	1	0	5.568067	-0.287303	1.434811
79	6	0	7.237690	0.992896	0.993708
80	6	0	0.051953	5.718562	-1.059223
81	6	0	1.663429	4.365130	-2.313576
82	6	0	-0.160584	5.527907	1.338143
83	6	0	1.155213	3.902340	2.615921
84	6	0	5.334293	-2.403053	-3.753077
85	6	0	0.968911	-5.218535	0.999436
86	6	0	2.847538	-3.705526	1.431849
87	6	0	-0.277624	-5.120563	-1.064475
88	6	0	0.185015	-3.399536	-2.753484
89	1	0	4.714106	1.015622	-3.432218
90	1	0	5.698420	1.097002	-1.999760
91	6	0	6.491686	-0.187968	-3.552178
92	1	0	6.695620	3.756160	0.932590
93	1	0	5.835417	3.786122	2.456727
94	6	0	7.017802	2.001021	2.130827
95	1	0	7.939067	0.223080	1.296462
96	1	0	7.659047	1.504000	0.133218
97	6	0	-0.325659	6.325567	-2.302608
98	6	0	-0.529229	6.106539	0.136113
99	6	0	1.282047	4.963249	-3.457960
100	1	0	2.419018	3.610533	-2.324143
101	6	0	-0.742160	5.951714	2.579017
102	6	0	0.586150	4.332951	3.758302
103	1	0	1.852830	3.093103	2.631632
104	1	0	4.811645	-3.073482	-4.425397
105	1	0	6.130076	-2.970574	-3.278153
106	6	0	5.953326	-1.236436	-4.536625
107	6	0	1.227777	-5.820215	2.275524
108	6	0	-0.036066	-5.692596	0.172269
109	6	0	3.064524	-4.305613	2.618765
110	1	0	3.469641	-2.897915	1.111314
111	6	0	-1.294660	-5.630501	-1.939854
112	6	0	-0.787536	-3.903746	-3.538473
113	1	0	0.709728	-2.512696	-3.036215
114	1	0	7.197799	-0.657145	-2.873432
115	1	0	7.016570	0.598854	-4.082578
116	1	0	6.539993	1.501458	2.967505
117	1	0	7.964306	2.399924	2.478389
118	6	0	0.263833	5.964511	-3.456536
119	1	0	-1.092237	7.075820	-2.285915
120	1	0	-1.277827	6.875796	0.130975
121	1	0	1.738892	4.687045	-4.387422
122	1	0	-1.477166	6.732515	2.551140
123	6	0	-0.374676	5.389897	3.745009
124	1	0	0.841417	3.872345	4.692015
125	1	0	5.201767	-0.780204	-5.172700
126	1	0	6.747682	-1.607900	-5.174367
127	6	0	2.237999	-5.386985	3.053549
128	1	0	0.595817	-6.627465	2.589958

129	1	0	-0.636692	-6.520068	0.497575
130	1	0	3.869264	-3.979248	3.247766
131	1	0	-1.853669	-6.488731	-1.619415
132	6	0	-1.532648	-5.054725	-3.133655
133	1	0	-1.019633	-3.435654	-4.474279
134	1	0	-0.023444	6.421195	-4.382686
135	1	0	-0.807315	5.717733	4.669380
136	1	0	2.436908	-5.852594	3.998711
137	1	0	-2.287805	-5.445312	-3.786578

TSr1k ONIOM: extrapolated energy = -6322.890433255106 A.U.
SCF Done: E(RM052X+HF-M052X) = -6346.64216763 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.681388	-3.488095	3.390359
2	6	0	0.300230	-3.486851	4.563770
3	6	0	0.885353	-2.074254	4.557965
4	6	0	0.171112	-1.395075	3.400973
5	7	0	-0.687955	-2.220050	2.813110
6	1	0	1.041100	-4.263524	4.384181
7	1	0	0.702617	-1.507919	5.471292
8	8	0	0.403005	-0.206293	3.090678
9	8	0	-1.348912	-4.423072	3.021522
10	1	0	1.955883	-2.048887	4.353775
11	1	0	-0.242845	-3.734928	5.475368
12	35	0	-1.938860	-1.976003	1.058289
13	6	0	-4.088052	-3.066543	-0.401086
14	6	0	-3.127999	-2.052812	-0.792174
15	6	0	-3.600173	-0.694880	-0.925003
16	6	0	-4.907496	-0.332780	-0.582110
17	6	0	-5.777623	-1.339213	-0.162596
18	6	0	-5.354339	-2.694061	-0.078250
19	1	0	-2.324677	-2.343387	-1.460736
20	1	0	-6.091238	-3.406514	0.261050
21	8	0	-2.808117	0.240948	-1.386131
22	1	0	0.092069	0.278196	1.876082
23	8	0	-7.058650	-1.120614	0.173674
24	1	0	-7.481580	-0.361018	-0.299829
25	6	0	-5.226434	1.126848	-0.465411
26	6	0	-4.551903	1.832444	0.538970
27	6	0	-6.114288	1.804483	-1.282759
28	6	0	-4.762162	3.188659	0.693369
29	6	0	-6.338154	3.165370	-1.107170
30	6	0	-5.657106	3.850708	-0.128144
31	1	0	-4.228301	3.733478	1.442145
32	1	0	-7.037066	3.674653	-1.740369
33	1	0	-5.817223	4.902543	0.002768
34	6	0	-6.891934	1.067666	-2.339317
35	1	0	-6.283286	0.318391	-2.826435
36	1	0	-7.279219	1.752995	-3.081319
37	8	0	-8.007632	0.420320	-1.664477
38	8	0	-3.707081	1.109788	1.319206
39	6	0	-8.867011	-0.367068	-2.514091
40	1	0	-9.337269	0.261756	-3.260105
41	1	0	-9.620859	-0.800347	-1.876252
42	1	0	-8.309271	-1.154738	-3.006890
43	6	0	-2.776756	1.756418	2.215766
44	1	0	-2.128090	2.427210	1.677254
45	1	0	-2.187383	0.964774	2.639255
46	1	0	-3.304201	2.287743	2.996912
47	1	0	-1.848164	-0.038671	-1.447225
48	8	0	-0.243567	-0.284754	-1.449727
49	15	0	0.592267	0.305025	-0.369569
50	8	0	1.405365	1.559676	-1.010261
51	8	0	1.780177	-0.684111	0.155223
52	8	0	-0.050947	0.812224	0.932894
53	6	0	2.461000	2.063178	-0.269208
54	6	0	2.789621	-0.953225	-0.758624
55	6	0	3.641214	1.319652	-0.235607
56	6	0	2.336874	3.290072	0.372870
57	6	0	2.878825	-2.212643	-1.339169
58	6	0	3.708564	0.060595	-1.036695
59	6	0	4.705299	1.744661	0.580923
60	6	0	3.439811	3.732836	1.096461
61	6	0	1.109774	4.158139	0.292275
62	6	0	3.878180	-2.397965	-2.288710
63	6	0	2.024709	-3.383453	-0.932288
64	6	0	4.650930	-0.124474	-2.065478
65	6	0	4.601597	2.975144	1.238387
66	6	0	5.906745	0.820937	0.841467
67	1	0	3.370066	4.693196	1.593413
68	6	0	0.844705	4.873413	-0.879094
69	6	0	0.316169	4.340079	1.428938
70	6	0	4.733239	-1.372392	-2.691443
71	1	0	3.969446	-3.375606	-2.747176
72	6	0	2.359168	-4.094542	0.224717
73	6	0	1.006339	-3.837216	-1.772061
74	6	0	5.490775	1.059627	-2.571992
75	6	0	5.749031	3.544755	2.084637
76	1	0	6.159311	0.269073	-0.049870
77	1	0	5.592530	0.094138	1.586480
78	6	0	7.132727	1.579027	1.372305
79	6	0	-0.235203	5.802261	-0.905408
80	6	0	1.628776	4.721228	-2.072641
81	6	0	-0.742186	5.294654	1.400029
82	6	0	0.515183	3.592938	2.641194
83	6	0	5.776486	-1.671712	-3.777168
84	6	0	1.658831	-5.294219	0.538038
85	6	0	3.402997	-3.672809	1.117146
86	6	0	0.347902	-5.066278	-1.475951
87	6	0	0.584841	-3.107417	-2.937003
88	1	0	4.848768	1.647487	-3.222929
89	1	0	5.775895	1.698321	-1.751039
90	6	0	6.727759	0.611618	-3.364705
91	1	0	6.292050	4.265799	1.479613
92	1	0	5.332793	4.077179	2.931863
93	6	0	6.725323	2.459952	2.562384
94	1	0	7.894150	0.865828	1.668515
95	1	0	7.550748	2.201936	0.587172
96	6	0	-0.497383	6.532156	-2.111840
97	6	0	-0.994676	5.999369	0.235413
98	6	0	1.348937	5.427830	-3.184060
99	1	0	2.438886	4.024774	-2.063445
100	6	0	-1.516232	5.512904	2.588803
101	6	0	-0.238796	3.826026	3.732995
102	1	0	1.252772	2.820313	2.650006
103	1	0	5.336191	-2.329044	-4.517842
104	1	0	6.603585	-2.204978	-3.316280
105	6	0	6.315016	-0.398285	-4.445609
106	6	0	2.008304	-6.015252	1.727414
107	6	0	0.680674	-5.759842	-0.325589
108	6	0	3.706511	-4.384928	2.220121
109	1	0	3.939138	-2.777659	0.885163
110	6	0	-0.638924	-5.563572	-2.391877
111	6	0	-0.362205	-3.601368	-3.758144
112	1	0	1.007482	-2.142534	-3.112975
113	1	0	7.449872	0.152078	-2.696310
114	1	0	7.198644	1.479243	-3.813526
115	1	0	6.250121	1.844832	3.319747
116	1	0	7.595931	2.925777	3.010526
117	6	0	0.261841	6.353694	-3.207884
118	1	0	-1.317394	7.223792	-2.115787
119	1	0	-1.793776	6.715953	0.216971
120	1	0	1.940521	5.297217	-4.068257
121	1	0	-2.293482	6.252133	2.557107
122	6	0	-1.267769	4.817476	3.714291
123	1	0	-0.082805	3.251527	4.624097
124	1	0	5.546735	0.040814	-5.073704
125	1	0	7.158814	-0.649183	-5.078663
126	6	0	2.995074	-5.583163	2.535731
127	1	0	1.463309	-6.910839	1.953119
128	1	0	0.173072	-6.677438	-0.097725
129	1	0	4.493594	-4.059629	2.871606
130	1	0	-1.099603	-6.508038	-2.174905
131	6	0	-0.973803	-4.866187	-3.493738
132	1	0	-0.674170	-3.040845	-4.616600
133	1	0	0.059382	6.900779	-4.107049
134	1	0	-1.844476	4.990986	4.601257
135	1	0	3.260178	-6.134877	3.416006
136	1	0	-1.707861	-5.245541	-4.176743
137	6	0	-3.621194	-4.506944	-0.279644
138	1	0	-3.014102	-4.780015	-1.132152
139	1	0	-3.016955	-4.615041	0.615846
140	1	0	-4.469267	-5.175315	-0.213376

TSr3k ONIOM: extrapolated energy = -6322.892373109131 A.U.
SCF Done: E(RM052X+HF-M052X) = -6346.63661406 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.433604	-0.791612	-3.627130
2	6	0	0.420935	-1.964991	-4.587733
3	6	0	1.905697	-2.291858	-4.744958
4	6	0	2.603693	-1.242704	-3.872915
5	7	0	1.656930	-0.404496	-3.308972
6	1	0	-0.159432	-2.770940	-4.139423
7	1	0	2.276422	-2.207524	-5.766212
8	8	0	3.801146	-1.160953	-3.700500
9	8	0	-0.648945	-0.288587	-3.218826
10	1	0	2.161002	-3.282060	-4.370062
11	1	0	-0.072535	-1.665068	-5.512923
12	35	0	2.146107	1.095771	-1.607577
13	6	0	2.980852	3.564875	-0.513986
14	6	0	2.387569	2.353480	0.049065
15	6	0	3.262365	1.477148	0.826506
16	6	0	4.645196	1.580706	0.714250
17	6	0	5.164964	2.636723	-0.035419
18	6	0	4.328165	3.669862	-0.562823
19	1	0	1.378796	2.438990	0.439668
20	1	0	4.827992	4.494341	-1.048800
21	8	0	2.740826	0.520848	1.537729
22	1	0	-0.694797	0.408352	-2.235064
23	8	0	6.465872	2.734703	-0.322406
24	1	0	6.858384	1.834873	-0.515044
25	6	0	5.520574	0.663549	1.508728
26	6	0	5.633388	0.919049	2.876605
27	6	0	6.203303	-0.409221	0.960905

28	6	0	6.425307	0.112338	3.671373
29	6	0	7.005812	-1.211984	1.762486
30	6	0	7.111985	-0.950321	3.110468
31	1	0	6.519252	0.304729	4.718856
32	1	0	7.544275	-2.029430	1.326157
33	1	0	7.732616	-1.565640	3.731269
34	6	0	6.097192	-0.693534	-0.516865
35	1	0	6.576274	-1.633179	-0.757451
36	1	0	5.065809	-0.731603	-0.838268
37	8	0	6.772147	0.381762	-1.218082
38	8	0	4.925910	1.984321	3.353147
39	6	0	6.660299	0.321064	-2.666754
40	1	0	5.648790	0.081132	-2.961794
41	1	0	6.945451	1.294625	-3.034839
42	1	0	7.337460	-0.430303	-3.052428
43	6	0	4.888285	2.288763	4.756582
44	1	0	5.871197	2.548009	5.129626
45	1	0	4.231398	3.137781	4.846804
46	1	0	4.491587	1.458758	5.327554
47	1	0	1.748567	0.442318	1.399490
48	8	0	-0.941972	1.027336	-1.226489
49	15	0	-0.972707	0.304712	0.116349
50	8	0	-1.361967	-1.226069	-0.316511
51	8	0	-2.287592	0.799384	0.942435
52	8	0	0.165352	0.391838	1.073376
53	6	0	-2.044814	-2.037391	0.564694
54	6	0	-3.487999	0.675600	0.268637
55	6	0	-3.373212	-1.731630	0.870483
56	6	0	-1.410765	-3.167078	1.073111
57	6	0	-4.107425	1.809305	-0.247970
58	6	0	-4.040528	-0.599420	0.155261
59	6	0	-4.038377	-2.480395	1.861410
60	6	0	-2.122264	-3.943157	1.979207
61	6	0	-0.029886	-3.572040	0.630976
62	6	0	-5.288062	1.611905	-0.953365
63	6	0	-3.575677	3.199986	-0.015585
64	6	0	-5.185377	-0.781894	-0.644215
65	6	0	-3.404108	-3.599471	2.411252
66	6	0	-5.391335	-2.003079	2.415699
67	1	0	-1.645091	-4.829137	2.381708
68	6	0	0.119912	-4.310088	-0.547229
69	6	0	1.079211	-3.263174	1.418995
70	6	0	-5.814477	0.340818	-1.192085
71	1	0	-5.795621	2.480367	-1.356754
72	6	0	-3.800442	3.814282	1.221118
73	6	0	-2.943683	3.897889	-1.047988
74	6	0	-5.662006	-2.197897	-1.007801
75	6	0	-4.092664	-4.499925	3.447155
76	1	0	-5.994303	-1.581480	1.627521
77	1	0	-5.179710	-1.199778	3.116885
78	6	0	-6.159150	-3.113668	3.147734
79	6	0	1.414861	-4.757843	-0.935643
80	6	0	-0.990249	-4.645407	-1.394365
81	6	0	2.372200	-3.714249	1.020348
82	6	0	0.976787	-2.486904	2.623769
83	6	0	-7.104391	0.228251	-2.017516
84	6	0	-3.384426	5.161312	1.423263
85	6	0	-4.448702	3.141466	2.311733
86	6	0	-2.545682	5.251662	-0.839155
87	6	0	-2.666502	3.304215	-2.327355
88	1	0	-5.011658	-2.555959	-1.801829
89	1	0	-5.534004	-2.865381	-0.170391
90	6	0	-7.115426	-2.225597	-1.503607
91	1	0	-4.488185	-5.371406	2.932270
92	1	0	-3.353096	-4.848971	4.158463
93	6	0	-5.241589	-3.789276	4.177046
94	1	0	-7.028969	-2.686261	3.634456
95	1	0	-6.509722	-3.853670	2.434374
96	6	0	1.554139	-5.523736	-2.140478
97	6	0	2.508959	-4.452393	-0.142259
98	6	0	-0.816100	-5.365317	-2.520898
99	1	0	-1.964563	-4.309025	-1.110271
100	6	0	3.505405	-3.380565	1.833593
101	6	0	2.068602	-2.196448	3.354733
102	1	0	0.015939	-2.118944	2.912250
103	1	0	-7.083093	0.969138	-2.808259
104	1	0	-7.944975	0.464324	-1.370428
105	6	0	-7.308334	-1.174987	-2.606898
106	6	0	-3.622845	5.781179	2.694253
107	6	0	-2.772883	5.849478	0.388213
108	6	0	-4.653869	3.760932	3.489898
109	1	0	-4.763535	2.130208	2.169323
110	6	0	-1.921974	5.968430	-1.914782
111	6	0	-2.079088	4.013944	-3.309096
112	1	0	-2.900627	2.273019	-2.468007
113	1	0	-7.791610	-2.014574	-0.680423
114	1	0	-7.348129	-3.217227	-1.876186
115	1	0	-4.841306	-3.038036	4.850169
116	1	0	-5.794819	-4.507838	4.771612
117	6	0	0.484030	-5.817454	-2.904092
118	1	0	2.534949	-5.863211	-2.413173
119	1	0	3.483408	-4.792988	-0.437233
120	1	0	-1.656746	-5.611144	-3.139206
121	1	0	4.473975	-3.714415	1.516093
122	6	0	3.362079	-2.649827	2.953066
123	1	0	1.979301	-1.597656	4.238633
124	1	0	-6.587848	-1.349102	-3.399495
125	1	0	-8.300988	-1.248162	-3.037308
126	6	0	-4.232109	5.110423	3.688973
127	1	0	-3.302228	6.796080	2.829611
128	1	0	-2.473669	6.869426	0.540084
129	1	0	-5.136439	3.242321	4.294351
130	1	0	-1.639609	6.989682	-1.745146
131	6	0	-1.704548	5.377590	-3.103967
132	1	0	-1.870194	3.552304	-4.253333
133	1	0	0.594784	-6.397037	-3.799194
134	1	0	4.217285	-2.379228	3.537942
135	1	0	-4.406950	5.579802	4.636651
136	1	0	-1.243242	5.919932	-3.905666
137	6	0	2.033547	4.589200	-1.102977
138	1	0	1.384474	4.121514	-1.834460
139	1	0	1.404347	4.997413	-0.319285
140	1	0	2.578408	5.395768	-1.573729

TSs1k ONIOM: extrapolated energy = -6322.892728507000 A.U.
SCF Done: E(RM052X+HF-M052X) = -6346.63754008 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.856199	-2.539080	3.801777
2	6	0	-0.819146	-3.316696	4.618531
3	6	0	0.466815	-2.513187	4.436898
4	6	0	0.032308	-1.359042	3.550217
5	7	0	-1.262034	-1.417686	3.251119
6	1	0	-1.162599	-3.379852	5.650952
7	1	0	1.253110	-3.062455	3.919081
8	8	0	0.854631	-0.488578	3.181630
9	8	0	-3.015497	-2.863438	3.666270
10	1	0	0.884327	-2.114941	5.361973
11	1	0	-0.751338	-4.327162	4.218705
12	35	0	-2.181945	0.161467	1.890821
13	6	0	-3.204656	2.776253	1.327441
14	6	0	-2.620043	1.724207	0.510556
15	6	0	-3.491629	1.025050	-0.421309
16	6	0	-4.864356	1.261917	-0.457454
17	6	0	-5.377834	2.250490	0.387337
18	6	0	-4.542518	2.986954	1.279190
19	1	0	-1.615687	1.904458	0.141162
20	1	0	-5.030402	3.735867	1.884873
21	8	0	-2.975568	0.146047	-1.239168
22	1	0	0.689566	0.303804	2.158990
23	8	0	-6.667447	2.599991	0.399499
24	1	0	-7.125604	2.478420	-0.472708
25	6	0	-5.746312	0.290015	-1.181024
26	6	0	-5.848853	-0.987046	-0.615331
27	6	0	-6.451283	0.576753	-2.336305
28	6	0	-6.640242	-1.946241	-1.219235
29	6	0	-7.250423	-0.390461	-2.934107
30	6	0	-7.336215	-1.646092	-2.376602
31	1	0	-6.722560	-2.922398	-0.792014
32	1	0	-7.800361	-0.152244	-3.822565
33	1	0	-7.951294	-2.396030	-2.833252
34	6	0	-6.419176	1.965908	-2.913775
35	1	0	-5.421358	2.381680	-2.889487
36	1	0	-6.786156	1.970921	-3.931253
37	8	0	-7.300120	2.776977	-2.086712
38	8	0	-5.144417	-1.194948	0.522936
39	6	0	-7.396387	4.166132	-2.464818
40	1	0	-7.816883	4.256839	-3.458556
41	1	0	-8.050307	4.637583	-1.748587
42	1	0	-6.423312	4.642208	-2.440179
43	6	0	-5.104870	-2.486439	1.172049
44	1	0	-4.724114	-3.236625	0.492178
45	1	0	-4.436844	-2.380587	2.007610
46	1	0	-6.092993	-2.768892	1.514973
47	1	0	-1.994423	0.042376	-1.095787
48	8	0	0.759504	0.973394	1.256940
49	15	0	0.872077	0.323451	-0.131469
50	8	0	1.641421	-1.080861	0.189348
51	8	0	1.971034	1.178218	-0.971532
52	8	0	-0.321957	0.181082	-1.004556
53	6	0	2.356702	-1.674216	-0.836062
54	6	0	3.234260	1.250560	-0.409898
55	6	0	3.540268	-1.063491	-1.257135
56	6	0	1.907717	-2.872708	-1.380230
57	6	0	3.656150	2.431950	0.189843
58	6	0	4.046129	0.120495	-0.495956
59	6	0	4.209358	-1.567197	-2.388668
60	6	0	2.637385	-3.396632	-2.440964
61	6	0	0.740963	-3.643900	-0.820226
62	6	0	4.925076	2.426924	0.757721
63	6	0	2.826956	3.689446	0.203620
64	6	0	5.287535	0.113464	0.167522
65	6	0	3.748736	-2.747992	-2.980297
66	6	0	5.354216	-0.767011	-3.031723
67	1	0	2.306063	-4.332928	-2.874781
68	6	0	0.957806	-4.500406	0.264205
69	6	0	-0.510682	-3.581449	-1.434056
70	6	0	5.729737	1.286956	0.787405
71	1	0	5.280967	3.339146	1.222026

72	6	0	2.748252	4.469252	-0.954875
73	6	0	2.229439	4.122077	1.390542
74	6	0	6.083549	-1.193927	0.314445
75	6	0	4.460783	-3.389471	-4.179740
76	1	0	5.957026	-0.294933	-2.272154
77	1	0	4.896580	0.028956	-3.613598
78	6	0	6.227496	-1.623940	-3.960237
79	6	0	-0.103366	-5.329914	0.726885
80	6	0	2.221853	-4.586239	0.941127
81	6	0	-1.560824	-4.429638	-0.974175
82	6	0	-0.797845	-2.675473	-2.511719
83	6	0	7.101033	1.377599	1.471907
84	6	0	2.061622	5.716659	-0.917205
85	6	0	3.344724	4.068523	-2.198207
86	6	0	1.563991	5.383126	1.422168
87	6	0	2.249430	3.341051	2.597186
88	1	0	5.614654	-1.761388	1.114354
89	1	0	6.002817	-1.787487	-0.582380
90	6	0	7.557967	-0.953854	0.671779
91	1	0	5.086923	-4.197892	-3.811858
92	1	0	3.718681	-3.825124	-4.838605
93	6	0	5.337635	-2.390900	-4.949321
94	1	0	6.922551	-0.982416	-4.490717
95	1	0	6.809551	-2.329331	-3.374586
96	6	0	0.131229	-6.207506	1.836982
97	6	0	-1.332928	-5.283767	0.090263
98	6	0	2.399384	-5.421149	1.984528
99	1	0	3.023834	-3.967285	0.599586
100	6	0	-2.836968	-4.371808	-1.626883
101	6	0	-2.018351	-2.637781	-3.078275
102	1	0	-0.034648	-1.996619	-2.823935
103	1	0	7.019111	2.017204	2.342969
104	1	0	7.795331	1.850563	0.782558
105	6	0	7.654182	0.001551	1.870165
106	6	0	1.990470	6.509125	-2.110347
107	6	0	1.493856	6.147924	0.270468
108	6	0	3.254333	4.843263	-3.296082
109	1	0	3.860982	3.133634	-2.235863
110	6	0	0.987789	5.836155	2.656459
111	6	0	1.691614	3.802481	3.732497
112	1	0	2.684847	2.367297	2.564006
113	1	0	8.079220	-0.522689	-0.177745
114	1	0	8.029752	-1.902935	0.901657
115	1	0	4.709714	-1.688448	-5.487759
116	1	0	5.941417	-2.922352	-5.676503
117	6	0	1.332483	-6.252468	2.444498
118	1	0	-0.676921	-6.831237	2.167495
119	1	0	-2.126875	-5.918911	0.434532
120	1	0	3.349900	-5.472925	2.477691
121	1	0	-3.611231	-5.029291	-1.281057
122	6	0	-3.059638	-3.509438	-2.635036
123	1	0	-2.227752	-1.933553	-3.857537
124	1	0	7.079346	-0.400321	2.698226
125	1	0	8.682827	0.103831	2.197696
126	6	0	2.562060	6.091444	-3.254610
127	1	0	1.469374	7.445871	-2.064540
128	1	0	0.994133	7.097821	0.299420
129	1	0	3.701964	4.526652	-4.217093
130	1	0	0.506064	6.794931	2.667739
131	6	0	1.055859	5.081824	3.768697
132	1	0	1.706097	3.201644	4.619670
133	1	0	1.501998	-6.914123	3.270720
134	1	0	-4.022225	-3.451702	-3.101825
135	1	0	2.505026	6.688690	-4.142859
136	1	0	0.627859	5.427673	4.688831
137	6	0	-2.262019	3.613878	2.168719
138	1	0	-1.566347	2.982178	2.705060
139	1	0	-1.679617	4.259835	1.520228
140	1	0	-2.809614	4.225553	2.872593

TSs3k ONIOM: extrapolated energy = -6322.887462905739 A.U.
SCF Done: E(RM052X+HF-M052X) = -6346.64047779 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.336435	-1.268861	3.127453
2	6	0	1.200113	-1.718877	4.294290
3	6	0	0.913835	-3.216305	4.401339
4	6	0	-0.037536	-3.498431	3.237854
5	7	0	-0.317829	-2.296479	2.588411
6	1	0	0.937851	-1.141763	5.180661
7	1	0	1.795952	-3.840024	4.273566
8	8	0	-0.490377	-4.572920	2.933275
9	8	0	0.282605	-0.073889	2.771585
10	1	0	0.422966	-3.503069	5.331332
11	1	0	2.237488	-1.497279	4.042064
12	35	0	-1.516680	-2.386183	0.787796
13	6	0	-3.594679	-3.670813	-0.575085
14	6	0	-2.730043	-2.612063	-1.056715
15	6	0	-3.308645	-1.293368	-1.191047
16	6	0	-4.520777	-0.984672	-0.585173
17	6	0	-5.201229	-1.995223	0.092220
18	6	0	-4.779400	-3.346553	0.013824
19	1	0	-1.959673	-2.868523	-1.775233
20	1	0	-5.403460	-4.086409	0.492284
21	8	0	-2.693280	-0.339310	-1.848746
22	1	0	-0.234556	0.259634	1.550012
23	8	0	-6.275052	-1.731548	0.860399
24	1	0	-6.153148	-0.867616	1.327648
25	6	0	-5.112379	0.376676	-0.775320
26	6	0	-5.799541	0.623464	-1.963232
27	6	0	-4.983675	1.390543	0.156852
28	6	0	-6.350520	1.868839	-2.198117
29	6	0	-5.539407	2.639957	-0.081010
30	6	0	-6.217415	2.873562	-1.256581
31	1	0	-6.878255	2.067477	-3.106419
32	1	0	-5.430780	3.416264	0.649055
33	1	0	-6.646935	3.836799	-1.448549
34	6	0	-4.259506	1.109989	1.446137
35	1	0	-4.138629	2.009900	2.030005
36	1	0	-3.285053	0.681323	1.254805
37	8	0	-5.083951	0.162432	2.184747
38	8	0	-5.883918	-0.416147	-2.846180
39	6	0	-4.456303	-0.400751	3.354579
40	1	0	-3.534542	-0.903031	3.089498
41	1	0	-5.153119	-1.113419	3.768290
42	1	0	-4.248814	0.373233	4.083736
43	6	0	-6.479581	-0.243627	-4.140487
44	1	0	-7.530591	0.005953	-4.061867
45	1	0	-6.371210	-1.195302	-4.634140
46	1	0	-5.968512	0.522773	-4.709708
47	1	0	-1.713804	-0.495514	-1.976167
48	8	0	-0.110790	-0.317980	-1.826813
49	15	0	0.408805	0.359344	-0.609607
50	8	0	1.047086	1.783744	-1.064259
51	8	0	1.671066	-0.417325	0.073830
52	8	0	-0.539584	0.627656	0.578831
53	6	0	1.924456	2.394061	-0.182501
54	6	0	2.801058	-0.494530	-0.732898
55	6	0	3.207778	1.856555	-0.072661
56	6	0	1.529501	3.522090	0.526694
57	6	0	3.157874	-1.703716	-1.318772
58	6	0	3.553701	0.667686	-0.907913
59	6	0	4.107391	2.390802	0.867472
60	6	0	2.469910	4.083840	1.385349
61	6	0	0.181274	4.177679	0.390155
62	6	0	4.248895	-1.684275	-2.180923
63	6	0	2.505694	-3.016668	-0.974213
64	6	0	4.597445	0.679711	-1.850548
65	6	0	3.732723	3.530225	1.588124
66	6	0	5.424662	1.665164	1.188702
67	1	0	2.186347	4.971889	1.937531
68	6	0	-0.084802	4.980439	-0.722489
69	6	0	-0.739906	4.087751	1.437413
70	6	0	4.942267	-0.513999	-2.492256
71	1	0	4.549437	-2.617658	-2.642387
72	6	0	2.925560	-3.683885	0.181744
73	6	0	1.599918	-3.617773	-1.849290
74	6	0	5.265288	2.005254	-2.250234
75	6	0	4.684841	4.217661	2.576672
76	1	0	5.848680	1.237540	0.294297
77	1	0	5.178433	0.838026	1.850042
78	6	0	6.447223	2.573890	1.887504
79	6	0	-1.297425	5.725874	-0.776199
80	6	0	0.826444	5.098457	-1.826017
81	6	0	-1.934443	4.863888	1.387472
82	6	0	-0.540494	3.230647	2.574411
83	6	0	6.105626	-0.593953	-3.490827
84	6	0	2.416971	-4.982818	0.466489
85	6	0	3.876585	-3.119006	1.099085
86	6	0	1.129857	-4.935932	-1.575173
87	6	0	1.112757	-2.957667	-3.030086
88	1	0	4.590797	2.504360	-2.941031
89	1	0	5.368691	2.648938	-1.390546
90	6	0	6.621980	1.798427	-2.940064
91	1	0	5.145586	5.063107	2.072958
92	1	0	4.109670	4.607061	3.408531
93	6	0	5.788760	3.277916	3.082840
94	1	0	7.292043	1.977255	2.213841
95	1	0	6.818249	3.317850	1.188977
96	6	0	-1.558956	6.548575	-1.921345
97	6	0	-2.185860	5.661112	0.284016
98	6	0	0.541569	5.883036	-2.882614
99	1	0	1.736657	4.539468	-1.795650
100	6	0	-2.845655	4.811797	2.494851
101	6	0	-1.429797	3.201857	3.585602
102	1	0	0.308222	2.582338	2.592366
103	1	0	5.842838	-1.284565	-4.283620
104	1	0	6.970215	-1.001878	-2.974126
105	6	0	6.475594	0.776472	-4.077301
106	6	0	2.853588	-5.658455	1.653558
107	6	0	1.537986	-5.581549	-0.421264
108	6	0	4.272838	-3.794614	2.195882
109	1	0	4.272590	-2.148842	0.887792
110	6	0	0.250517	-5.570014	-2.515510
111	6	0	0.277068	-3.586884	-3.879310
112	1	0	1.387569	-1.939457	-3.194346
113	1	0	7.352501	1.438795	-2.221443
114	1	0	6.976754	2.748240	-3.324594
115	1	0	5.362533	2.534620	3.748952

116	1	0	6.521730	3.846417	3.644374
117	6	0	-0.677402	6.625289	-2.934722
118	1	0	-2.478609	7.100278	-1.947875
119	1	0	-3.087158	6.243343	0.249957
120	1	0	1.229413	5.954165	-3.701550
121	1	0	-3.724770	5.426182	2.455816
122	6	0	-2.599140	4.022668	3.557791
123	1	0	-1.270085	2.544752	4.416963
124	1	0	5.698984	1.106465	-4.759554
125	1	0	7.398890	0.693408	-4.639681
126	6	0	3.750665	-5.093091	2.483630
127	1	0	2.447480	-6.629119	1.859846
128	1	0	1.171290	-6.567955	-0.211284
129	1	0	4.993205	-3.363381	2.863062
130	1	0	-0.072245	-6.572176	-2.309155
131	6	0	-0.151405	-4.927597	-3.628268
132	1	0	-0.084984	-3.078595	-4.750546
133	1	0	-0.879948	7.240263	-3.788871
134	1	0	-3.279323	3.996382	4.386449
135	1	0	4.084174	-5.610952	3.361158
136	1	0	-0.801584	-5.409452	-4.331457
137	6	0	-3.068430	-5.094577	-0.584303
138	1	0	-3.865357	-5.795091	-0.374610
139	1	0	-2.629117	-5.328047	-1.545251
140	1	0	-2.300660	-5.199316	0.175594

TSs4k ONIOM: extrapolated energy = -6322.886998279779 A.U.
SCF Done: E(RM052X+HF-M052X) = -6346.63331728 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.009801	-1.457033	3.477811
2	6	0	0.667986	-2.147031	4.657759
3	6	0	-0.069562	-3.482758	4.747166
4	6	0	-1.046406	-3.445086	3.571327
5	7	0	-0.946666	-2.201557	2.942076
6	1	0	0.571600	-1.515734	5.541006
7	1	0	0.581988	-4.345321	4.621792
8	8	0	-1.788997	-4.332158	3.231660
9	8	0	0.379583	-0.315394	3.111774
10	1	0	-0.636073	-3.611221	5.669333
11	1	0	1.728690	-2.254569	4.431245
12	35	0	-2.096923	-2.008592	1.095788
13	6	0	-4.122108	-3.143624	-0.527972
14	6	0	-3.145703	-2.113461	-0.823185
15	6	0	-3.623672	-0.758455	-1.005249
16	6	0	-4.961882	-0.409956	-0.790433
17	6	0	-5.868366	-1.462864	-0.587140
18	6	0	-5.431572	-2.798424	-0.400914
19	1	0	-2.285272	-2.392253	-1.422663
20	1	0	-6.197404	-3.528017	-0.184983
21	8	0	-2.789596	0.184663	-1.371377
22	1	0	0.026311	0.162598	2.013662
23	8	0	-7.199629	-1.284582	-0.565851
24	1	0	-7.480526	-0.564908	-1.177201
25	6	0	-5.389060	1.031359	-0.762058
26	6	0	-6.416512	1.479803	-1.577746
27	6	0	-4.827965	1.942278	0.137687
28	6	0	-6.855453	2.784172	-1.565829
29	6	0	-5.262686	3.256963	0.150312
30	6	0	-6.262339	3.682116	-0.702205
31	1	0	-7.662874	3.069479	-2.208203
32	1	0	-4.819183	3.919499	0.859576
33	1	0	-6.593947	4.700925	-0.675602
34	6	0	-3.757094	1.527072	1.122270
35	1	0	-2.804475	1.447238	0.620612
36	1	0	-4.002490	0.559486	1.544747
37	8	0	-3.680769	2.514704	2.158563
38	8	0	-7.091559	0.549237	-2.382168
39	6	0	-2.589271	2.299310	3.071749
40	1	0	-2.748837	1.398887	3.657910
41	1	0	-2.559302	3.156269	3.724485
42	1	0	-1.651277	2.209781	2.541604
43	6	0	-6.606941	0.379207	-3.746690
44	1	0	-6.722489	1.305146	-4.291153
45	1	0	-7.217313	-0.392347	-4.187084
46	1	0	-5.568202	0.083978	-3.738266
47	1	0	-1.820459	-0.111409	-1.404993
48	8	0	-0.283021	-0.395165	-1.354494
49	15	0	0.517279	0.248736	-0.269166
50	8	0	1.285876	1.513346	-0.942325
51	8	0	1.740606	-0.693864	0.260222
52	8	0	-0.178767	0.713118	1.013474
53	6	0	2.407834	2.039633	-0.326028
54	6	0	2.693692	-1.011162	-0.698354
55	6	0	3.583087	1.286197	-0.352096
56	6	0	2.360255	3.320149	0.217270
57	6	0	2.747394	-2.298746	-1.218313
58	6	0	3.589167	-0.013804	-1.087846
59	6	0	4.722791	1.754679	0.328329
60	6	0	3.537947	3.804284	0.780133
61	6	0	1.134717	4.192863	0.210569
62	6	0	3.687297	-2.534426	-2.216497
63	6	0	1.913515	-3.451110	-0.725946
64	6	0	4.461295	-0.251834	-2.167509
65	6	0	4.698243	3.038995	0.880805
66	6	0	5.933493	0.833756	0.555662
67	1	0	3.528993	4.806699	1.190915
68	6	0	0.652428	4.719006	-0.992252
69	6	0	0.557008	4.567328	1.429474
70	6	0	4.509841	-1.531771	-2.728407
71	1	0	3.751362	-3.534320	-2.628852
72	6	0	2.252230	-4.081213	0.475919
73	6	0	0.923279	-3.989501	-1.550673
74	6	0	5.259070	0.903707	-2.794771
75	6	0	5.928582	3.658575	1.558775
76	1	0	6.092016	0.198631	-0.300927
77	1	0	5.684381	0.183951	1.391043
78	6	0	7.214044	1.610880	0.895970
79	6	0	-0.433614	5.640944	-0.969400
80	6	0	1.218631	4.383074	-2.268758
81	6	0	-0.507273	5.514903	1.440403
82	6	0	0.992853	4.037510	2.693673
83	6	0	5.481887	-1.889562	-3.861730
84	6	0	1.595124	-5.290692	0.843502
85	6	0	3.260800	-3.568259	1.360874
86	6	0	0.316127	-5.230645	-1.202684
87	6	0	0.484633	-3.334425	-2.753511
88	1	0	4.571335	1.452489	-3.433065
89	1	0	5.594464	1.588160	-2.032486
90	6	0	6.443175	0.415243	-3.642379
91	1	0	6.417693	4.312882	0.842223
92	1	0	5.602863	4.271788	2.390899
93	6	0	6.935048	2.601438	2.035697
94	1	0	7.992340	0.911260	1.180472
95	1	0	7.560843	2.153433	0.021549
96	6	0	-0.920680	6.177091	-2.207299
97	6	0	-0.981843	6.022157	0.243344
98	6	0	0.734231	4.914133	-3.407176
99	1	0	2.031804	3.691895	-2.299344
100	6	0	-1.052957	5.938396	2.697551
101	6	0	0.453263	4.464285	3.851759
102	1	0	1.749645	3.283209	2.696585
103	1	0	4.998662	-2.589795	-4.533090
104	1	0	6.340967	-2.392846	-3.426370
105	6	0	5.966737	-0.654876	-4.635303
106	6	0	1.952832	-5.931508	2.076014
107	6	0	0.657747	-5.847366	-0.011596
108	6	0	3.571259	-4.204966	2.507395
109	1	0	3.763885	-2.665427	1.089062
110	6	0	-0.623366	-5.822464	-2.112341
111	6	0	-0.419964	-3.914904	-3.566465
112	1	0	0.857810	-2.355395	-2.961724
113	1	0	7.211425	-0.003706	-2.999215
114	1	0	6.877067	1.257951	-4.169142
115	1	0	6.529851	2.065061	2.887728
116	1	0	7.850404	3.087886	2.353897
117	6	0	-0.361413	5.829515	-3.380103
118	1	0	-1.744340	6.863366	-2.170726
119	1	0	-1.787647	6.731131	0.255848
120	1	0	1.166586	4.647894	-4.351147
121	1	0	-1.845529	6.661095	2.685617
122	6	0	-0.582945	5.447334	3.858777
123	1	0	0.790372	4.055663	4.783711
124	1	0	5.155905	-0.254089	-5.234885
125	1	0	6.768561	-0.938920	-5.307665
126	6	0	2.903949	-5.413413	2.876491
127	1	0	1.446043	-6.839669	2.338535
128	1	0	0.191493	-6.776873	0.253659
129	1	0	4.332109	-3.811935	3.152584
130	1	0	-1.040993	-6.777577	-1.857872
131	6	0	-0.967650	-5.198143	-3.254550
132	1	0	-0.744928	-3.411687	-4.455189
133	1	0	-0.730485	6.232854	-4.302003
134	1	0	-0.989359	5.775303	4.794921
135	1	0	3.176164	-5.905377	3.789382
136	1	0	-1.664634	-5.648853	-3.933022
137	6	0	-3.647694	-4.569447	-0.311922
138	1	0	-3.188971	-4.649469	0.668923
139	1	0	-4.481275	-5.256693	-0.365923
140	1	0	-2.909182	-4.840694	-1.052986

TSr11 ONIOM: extrapolated energy = -6208.445681445866 A.U.
SCF Done: E(RM052X+HF-M052X) = -6230.90318364 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.083987	-3.084138	3.720147
2	6	0	-0.097097	-3.058354	4.887688
3	6	0	0.697060	-1.772243	4.672811
4	6	0	0.060512	-1.167484	3.437355
5	7	0	-0.917756	-1.916351	2.959797
6	1	0	0.510149	-3.959878	4.835992
7	1	0	0.632483	-1.058206	5.493678
8	8	0	0.479158	-0.067764	2.988175
9	8	0	-1.881080	-3.952668	3.484411
10	1	0	1.751797	-1.942617	4.456011
11	1	0	-0.658936	-3.076810	5.821122

12	35	0	-2.068857	-1.773417	1.102751
13	6	0	-3.997919	-2.877196	-0.599048
14	6	0	-3.108297	-1.774869	-0.857216
15	6	0	-3.694772	-0.457117	-0.945752
16	6	0	-5.047989	-0.253168	-0.643533
17	6	0	-5.811632	-1.350890	-0.262244
18	6	0	-5.297868	-2.673451	-0.270332
19	1	0	-3.570749	-3.869117	-0.608211
20	1	0	-2.231973	-1.949503	-1.469848
21	1	0	-5.967993	-3.470950	0.008796
22	8	0	-2.976894	0.561704	-1.335816
23	1	0	0.094587	0.348927	1.927809
24	8	0	-7.103352	-1.240478	0.118509
25	1	0	-7.428336	-0.329017	0.113396
26	6	0	-5.640103	1.118505	-0.670946
27	6	0	-5.138968	2.068821	0.218801
28	6	0	-6.678730	1.462330	-1.538297
29	6	0	-5.676283	3.341467	0.247574
30	6	0	-7.206165	2.751589	-1.499156
31	6	0	-6.708937	3.676959	-0.608057
32	1	0	-5.289675	4.064383	0.935161
33	1	0	-7.975262	3.027386	-2.190634
34	1	0	-7.115101	4.668824	-0.586001
35	8	0	-4.123379	1.681337	1.036802
36	6	0	-3.001590	2.581919	1.274713
37	1	0	-2.873169	3.253322	0.436947
38	1	0	-2.128346	1.963621	1.368862
39	1	0	-3.170604	3.148632	2.177929
40	1	0	-2.004774	0.313978	-1.448802
41	8	0	-0.474901	-0.109288	-1.504226
42	15	0	0.433488	0.349596	-0.411432
43	8	0	1.413422	1.478862	-1.058861
44	8	0	1.482904	-0.798875	0.092497
45	8	0	-0.147321	0.894111	0.891720
46	6	0	2.534558	1.823597	-0.325433
47	6	0	2.444384	-1.207337	-0.817092
48	6	0	3.604101	0.927528	-0.316791
49	6	0	2.581126	3.041637	0.343499
50	6	0	2.371881	-2.483336	-1.364496
51	6	0	3.487443	-0.329234	-1.116509
52	6	0	4.725426	1.193541	0.491079
53	6	0	3.739769	3.320471	1.061025
54	6	0	1.473968	4.060925	0.301073
55	6	0	3.331411	-2.818639	-2.313088
56	6	0	1.374766	-3.512953	-0.905779
57	6	0	4.388193	-0.656354	-2.147084
58	6	0	4.794363	2.414797	1.170077
59	6	0	5.794272	0.112993	0.725403
60	1	0	3.801399	4.270116	1.579198
61	6	0	1.316639	4.861093	-0.834377
62	6	0	0.690857	4.279870	1.437672
63	6	0	4.304967	-1.917430	-2.745975
64	1	0	3.296993	-3.811770	-2.745596
65	6	0	1.606209	-4.191298	0.295393
66	6	0	0.297555	-3.865173	-1.720295
67	6	0	5.370933	0.398696	-2.680325
68	6	0	6.016539	2.812133	2.009537
69	1	0	5.963071	-0.454069	-0.175831
70	1	0	5.391632	-0.576606	1.463316
71	6	0	7.116102	0.690375	1.253505
72	6	0	0.360379	5.916765	-0.822288
73	6	0	2.092213	4.670269	-2.027678
74	6	0	-0.242274	5.357863	1.448659
75	6	0	0.774510	3.449888	2.608903
76	6	0	5.292733	-2.369936	-3.830853
77	6	0	0.734323	-5.247722	0.684702
78	6	0	2.708162	-3.875673	1.161395
79	6	0	-0.542708	-4.953690	-1.342611
80	6	0	-0.010518	-3.163308	-2.936814
81	1	0	4.806247	1.051420	-3.340985
82	1	0	5.740420	1.011418	-1.873088
83	6	0	6.534678	-0.221175	-3.468062
84	1	0	6.645576	3.462446	1.407660
85	1	0	5.684577	3.383214	2.868709
86	6	0	6.842807	1.599070	2.460753
87	1	0	7.777058	-0.123713	1.530305
88	1	0	7.606912	1.263705	0.472775
89	6	0	0.208393	6.732222	-1.992127
90	6	0	-0.386897	6.147835	0.320893
91	6	0	1.917543	5.459376	-3.104784
92	1	0	2.809474	3.878369	-2.046320
93	6	0	-1.007177	5.604986	2.637792
94	6	0	0.029117	3.711534	3.699256
95	1	0	1.410844	2.592699	2.586919
96	1	0	4.765534	-2.977948	-4.556815
97	1	0	6.046944	-2.997714	-3.363978
98	6	0	5.987314	-1.190035	-4.526617
99	6	0	0.977042	-5.932902	1.921026
100	6	0	-0.311695	-5.612358	-0.147269
101	6	0	2.908715	-4.553494	2.308616
102	1	0	3.373006	-3.090418	0.872186
103	6	0	-1.608903	-5.345036	-2.220694
104	6	0	-1.032706	-3.554679	-3.722691
105	1	0	0.566175	-2.298422	-3.184208
106	1	0	7.195463	-0.757288	-2.793251
107	1	0	7.111168	0.568917	-3.936386
108	1	0	6.296583	1.041661	3.214939
109	1	0	7.772543	1.936679	2.905064
110	6	0	0.954771	6.513957	-3.090077
111	1	0	-0.518446	7.520902	-1.967682
112	1	0	-1.090508	6.958668	0.333333
113	1	0	2.500167	5.299099	-3.990049
114	1	0	-1.688773	6.433726	2.637165
115	6	0	-0.870565	4.821440	3.723485
116	1	0	0.091820	3.070641	4.555650
117	1	0	5.278267	-0.667206	-5.160215
118	1	0	6.787181	-1.560470	-5.158028
119	6	0	2.024526	-5.604923	2.700999
120	1	0	0.301716	-6.715654	2.205561
121	1	0	-0.953231	-6.422974	0.141063
122	1	0	3.743128	-4.312471	2.937582
123	1	0	-2.213195	-6.186126	-1.939179
124	6	0	-1.840194	-4.679395	-3.367743
125	1	0	-1.257475	-3.014634	-4.620560
126	1	0	0.834566	7.125615	-3.961975
127	1	0	-1.442163	5.013436	4.609942
128	1	0	2.208770	-6.132122	3.616262
129	1	0	-2.636629	-4.977808	-4.020024
130	6	0	-7.186820	0.474767	-2.523617
131	1	0	-6.456299	-0.213479	-2.903339
132	6	0	-8.438131	0.394961	-2.934838
133	1	0	-9.210978	1.037708	-2.557664
134	1	0	-8.738131	-0.333099	-3.663162

TSr21 ONIOM: extrapolated energy = -6208.445912801961 A.U.
SCF Done: E(RM052X+HF-M052X) = -6230.89348950 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.726118	0.533570	4.419784
2	6	0	-2.027023	0.944427	5.720087
3	6	0	-0.558252	1.078280	5.319848
4	6	0	-0.567339	0.735525	3.838395
5	7	0	-1.784534	0.411581	3.410502
6	1	0	-2.210260	0.175174	6.469976
7	1	0	-0.151793	2.081319	5.447886
8	8	0	0.474348	0.786746	3.147241
9	8	0	-3.917368	0.358405	4.292270
10	1	0	0.107860	0.384937	5.834282
11	1	0	-2.470678	1.871712	6.081109
12	35	0	-2.337692	-0.693279	1.514609
13	6	0	-3.734472	-2.747447	0.176244
14	6	0	-2.894020	-1.681859	-0.323313
15	6	0	-3.563983	-0.550290	-0.946297
16	6	0	-4.948048	-0.375406	-0.817048
17	6	0	-5.658010	-1.330924	-0.077590
18	6	0	-5.067300	-2.567934	0.313966
19	1	0	-3.241625	-3.644264	0.521989
20	1	0	-1.934206	-1.950873	-0.747468
21	1	0	-5.714489	-3.288426	0.788978
22	8	0	-2.862454	0.360668	-1.556099
23	1	0	0.302205	0.848661	1.834535
24	8	0	-6.926994	-1.144601	0.313316
25	1	0	-7.082001	-0.201662	0.571621
26	6	0	-5.617942	0.834626	-1.397320
27	6	0	-6.328144	1.687952	-0.566745
28	6	0	-5.581396	1.114177	-2.768979
29	6	0	-6.955875	2.818101	-1.040621
30	6	0	-6.221846	2.253552	-3.243004
31	6	0	-6.891057	3.106902	-2.388483
32	1	0	-7.500091	3.438196	-0.359163
33	1	0	-6.221421	2.450096	-4.295254
34	1	0	-7.382746	3.976423	-2.776139
35	8	0	-6.465037	1.337118	0.776696
36	6	0	-5.462921	1.856654	1.722589
37	1	0	-4.505222	1.928674	1.229902
38	1	0	-5.394759	1.162279	2.541626
39	1	0	-5.783590	2.829605	2.063508
40	1	0	-1.870424	0.167828	-1.530867
41	8	0	-0.335534	-0.209086	-1.423840
42	15	0	0.645434	0.212610	-0.383446
43	8	0	1.872370	0.963194	-1.138702
44	8	0	1.371494	-1.047457	0.356134
45	8	0	0.187188	1.113338	0.767883
46	6	0	2.938426	1.293365	-0.313224
47	6	0	2.361634	-1.726482	-0.337834
48	6	0	3.800041	0.264421	0.063058
49	6	0	3.123729	2.610200	0.093479
50	6	0	2.131049	-3.025318	-0.777265
51	6	0	3.586481	-1.084614	-0.541347
52	6	0	4.816382	0.521159	1.001527
53	6	0	4.194845	2.853024	0.946967
54	6	0	2.265596	3.752266	-0.381150
55	6	0	3.150840	-3.641153	-1.495961
56	6	0	0.885583	-3.818383	-0.477442
57	6	0	4.564906	-1.695815	-1.347040
58	6	0	5.016678	1.835813	1.433915
59	6	0	5.610053	-0.637416	1.626715
60	1	0	4.368825	3.873287	1.267895
61	6	0	2.424367	4.230935	-1.686133

62	6	0	1.400708	4.393677	0.510017
63	6	0	4.342274	-2.994027	-1.817928
64	1	0	2.989183	-4.656328	-1.838667
65	6	0	0.784599	-4.490735	0.743739
66	6	0	-0.083377	-3.998307	-1.468299
67	6	0	5.800826	-0.903855	-1.805739
68	6	0	6.148904	2.209180	2.401294
69	1	0	5.799072	-1.404863	0.892504
70	1	0	4.976777	-1.078475	2.392219
71	6	0	6.923454	-0.172868	2.273745
72	6	0	1.699953	5.383685	-2.103680
73	6	0	3.305151	3.612337	-2.636885
74	6	0	0.701369	5.562288	0.087467
75	6	0	1.173899	3.922473	1.849760
76	6	0	5.388833	-3.752219	-2.646431
77	6	0	-0.299097	-5.389584	0.964164
78	6	0	1.746308	-4.323667	1.797223
79	6	0	-1.151369	-4.917524	-1.247429
80	6	0	-0.053887	-3.283358	-2.714901
81	1	0	5.479468	-0.262090	-2.622136
82	1	0	6.149650	-0.257558	-1.016506
83	6	0	6.936531	-1.811087	-2.302124
84	1	0	6.975084	2.609279	1.819719
85	1	0	5.803571	2.995710	3.062044
86	6	0	6.648890	1.007772	3.216874
87	1	0	7.367362	-0.999794	2.817129
88	1	0	7.626889	0.133463	1.505208
89	6	0	1.869233	5.867011	-3.443065
90	6	0	0.863429	6.026014	-1.206123
91	6	0	3.436625	4.100050	-3.885289
92	1	0	3.854852	2.747708	-2.333866
93	6	0	-0.152247	6.241065	1.019732
94	6	0	0.365189	4.594020	2.690894
95	1	0	1.625345	3.005886	2.158699
96	1	0	4.880628	-4.363451	-3.383079
97	1	0	5.928951	-4.421198	-1.981921
98	6	0	6.392219	-2.812746	-3.330907
99	6	0	-0.385259	-6.081064	2.217876
100	6	0	-1.230533	-5.595515	-0.041119
101	6	0	1.625164	-4.989981	2.961092
102	1	0	2.559930	-3.648775	1.639110
103	6	0	-2.119466	-5.120422	-2.286529
104	6	0	-0.992083	-3.495663	-3.657659
105	1	0	0.708534	-2.550267	-2.863891
106	1	0	7.371531	-2.350809	-1.466203
107	1	0	7.716326	-1.198935	-2.741557
108	1	0	5.897585	0.719433	3.944887
109	1	0	7.547520	1.283855	3.757304
110	6	0	2.702521	5.251660	-4.301642
111	1	0	1.311925	6.733819	-3.741398
112	1	0	0.331949	6.904394	-1.519847
113	1	0	4.095591	3.622695	-4.583075
114	1	0	-0.662936	7.123783	0.686662
115	6	0	-0.306007	5.784203	2.275086
116	1	0	0.203504	4.226695	3.684846
117	1	0	5.902258	-2.273152	-4.134870
118	1	0	7.198274	-3.394623	-3.763741
119	6	0	0.537114	-5.889405	3.178500
120	1	0	-1.205342	-6.756149	2.368404
121	1	0	-2.026036	-6.300154	0.114920
122	1	0	2.347697	-4.849492	3.740109
123	1	0	-2.909069	-5.825606	-2.112788
124	6	0	-2.041067	-4.441748	-3.446036
125	1	0	-0.966033	-2.942056	-4.574577
126	1	0	2.823692	5.617284	-5.301883
127	1	0	-0.941938	6.297901	2.968626
128	1	0	0.465975	-6.408596	4.113422
129	1	0	-2.769240	-4.596595	-4.217119
130	6	0	-4.921050	0.185004	-3.714736
131	1	0	-4.942776	-0.849702	-3.430144
132	6	0	-4.333479	0.538439	-4.840656
133	1	0	-4.240304	1.562700	-5.146151
134	1	0	-3.892467	-0.193026	-5.489549

TSr31 ONIOM: extrapolated energy = -6208.442581994810 A.U.
SCF Done: E(RM052X+HF-M052X) = -6230.90109529 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.134346	-1.588483	3.773006
2	6	0	2.871287	-1.887891	5.062983
3	6	0	4.323390	-2.027557	4.607652
4	6	0	4.257916	-1.773624	3.099418
5	7	0	2.927348	-1.598703	2.720389
6	1	0	2.699780	-1.072602	5.765649
7	1	0	4.741673	-3.019456	4.777068
8	8	0	5.201734	-1.713883	2.348443
9	8	0	0.895613	-1.351618	3.808144
10	1	0	4.997101	-1.299279	5.057371
11	1	0	2.450867	-2.795565	5.496196
12	35	0	2.496614	-1.078123	0.574711
13	6	0	2.688299	-1.371705	-2.255776
14	6	0	2.091895	-0.354883	-1.418564
15	6	0	2.810834	0.900984	-1.275355
16	6	0	4.120787	1.018651	-1.743088
17	6	0	4.660690	-0.027724	-2.478280
18	6	0	3.937010	-1.221095	-2.756021
19	1	0	2.123600	-2.275286	-2.427687
20	1	0	1.010706	-0.295947	-1.394589
21	1	0	4.429464	-1.980056	-3.342928
22	8	0	2.278076	1.890478	-0.616333
23	1	0	0.283044	-1.100897	2.877688
24	8	0	5.915309	0.014040	-2.967583
25	1	0	6.391436	0.821254	-2.721863
26	6	0	4.946751	2.221854	-1.425105
27	6	0	4.753901	3.384929	-2.170974
28	6	0	5.904044	2.190767	-0.412408
29	6	0	5.519704	4.505498	-1.917581
30	6	0	6.667457	3.332301	-0.164678
31	6	0	6.474375	4.469559	-0.914365
32	1	0	5.380296	5.403134	-2.481119
33	1	0	7.379767	3.325573	0.633897
34	1	0	7.058749	5.345924	-0.714579
35	8	0	3.795926	3.324360	-3.142294
36	6	0	3.425802	4.490809	-3.896679
37	1	0	4.253092	4.852402	-4.494483
38	1	0	2.625151	4.170766	-4.542453
39	1	0	3.076188	5.282830	-3.246734
40	1	0	1.407834	1.616238	-0.180444
41	8	0	-0.653708	-0.866064	2.059266
42	15	0	-0.876399	0.012896	0.851944
43	8	0	-2.384373	0.601211	1.081256
44	8	0	-1.071643	-0.938360	-0.480523
45	8	0	0.066119	1.088640	0.431647
46	6	0	-2.990494	1.165087	-0.024803
47	6	0	-2.179760	-1.762314	-0.517207
48	6	0	-3.477357	0.299293	-1.006107
49	6	0	-3.131704	2.546916	-0.122762
50	6	0	-2.031984	-3.138318	-0.373471
51	6	0	-3.425336	-1.170358	-0.736384
52	6	0	-3.978840	0.826077	-2.210786
53	6	0	-3.708106	3.038730	-1.288509
54	6	0	-2.777720	3.497774	0.992383
55	6	0	-3.193218	-3.903325	-0.381852
56	6	0	-0.693515	-3.823613	-0.282912
57	6	0	-4.590079	-1.955658	-0.652105
58	6	0	-4.095563	2.213022	-2.344766
59	6	0	-4.282347	-0.102172	-3.398328
60	1	0	-3.835608	4.111243	-1.380051
61	6	0	-3.707466	3.706424	2.016290
62	6	0	-1.589479	4.230150	0.954736
63	6	0	-4.464528	-3.338200	-0.479705
64	1	0	-3.096940	-4.978015	-0.278768
65	6	0	0.007066	-4.099813	-1.461643
66	6	0	-0.214798	-4.281020	0.946424
67	6	0	-5.975478	-1.289002	-0.624964
68	6	0	-4.690674	2.862211	-3.602361
69	1	0	-4.709130	-1.030158	-3.051315
70	1	0	-3.330923	-0.345197	-3.864851
71	6	0	-5.195583	0.554689	-4.444303
72	6	0	-3.439564	4.680005	3.020695
73	6	0	-4.942458	2.977984	2.099777
74	6	0	-1.334748	5.207531	1.961419
75	6	0	-0.585952	4.023907	-0.051648
76	6	0	-5.685423	-4.267996	-0.439406
77	6	0	1.215196	-4.852667	-1.402982
78	6	0	-0.448031	-3.658512	-2.751036
79	6	0	0.985369	-5.050425	0.991610
80	6	0	-0.885777	-4.002214	2.186027
81	1	0	-6.118025	-0.897769	0.379091
82	1	0	-6.001486	-0.446420	-1.297576
83	6	0	-7.112931	-2.270461	-0.944750
84	1	0	-5.726590	3.118019	-3.396534
85	1	0	-4.161368	3.785553	-3.807459
86	6	0	-4.640592	1.935025	-4.825651
87	1	0	-5.259540	-0.085453	-5.317464
88	1	0	-6.198034	0.666375	-4.041976
89	6	0	-4.401825	4.887920	4.063288
90	6	0	-2.264178	5.411112	2.966305
91	6	0	-5.819314	3.204614	3.096728
92	1	0	-5.149892	2.242761	1.352144
93	6	0	-0.111186	5.955198	1.910914
94	6	0	0.559355	4.731291	-0.049189
95	1	0	-0.743603	3.251515	-0.770111
96	1	0	-5.496127	-5.068689	0.266081
97	1	0	-5.804696	-4.718038	-1.421394
98	6	0	-6.978728	-3.526367	-0.071249
99	6	0	1.923335	-5.128842	-2.619520
100	6	0	1.673422	-5.314204	-0.179705
101	6	0	0.247495	-3.940826	-3.870600
102	1	0	-1.356371	-3.097112	-2.803105
103	6	0	1.447112	-5.545349	2.256557
104	6	0	-0.414914	-4.484000	3.351701
105	1	0	-1.742006	-3.365120	2.168293
106	1	0	-7.074804	-2.552860	-1.992724
107	1	0	-8.065744	-1.783407	-0.768545
108	1	0	-3.615299	1.828942	-5.165417
109	1	0	-5.216017	2.369508	-5.635638
110	6	0	-5.545927	4.180594	4.102393
111	1	0	-4.183178	5.623573	4.813061

112	1	0	-2.069099	6.148949	3.721455
113	1	0	-6.734336	2.648346	3.146338
114	1	0	0.062307	6.692086	2.671262
115	6	0	0.798619	5.727457	0.946478
116	1	0	1.321922	4.514297	-0.769339
117	1	0	-6.951851	-3.236692	0.974173
118	1	0	-7.828662	-4.184809	-0.212532
119	6	0	1.460939	-4.691980	-3.806689
120	1	0	2.831556	-5.696574	-2.557636
121	1	0	2.577794	-5.891036	-0.140694
122	1	0	-0.105998	-3.602847	-4.824401
123	1	0	2.344066	-6.133784	2.272143
124	6	0	0.769190	-5.283113	3.389062
125	1	0	-0.916987	-4.251443	4.268947
126	1	0	-6.260013	4.340366	4.885690
127	1	0	1.718276	6.277866	0.924208
128	1	0	1.993762	-4.905169	-4.711999
129	1	0	1.112824	-5.665593	4.330214
130	6	0	6.078980	0.965035	0.406697
131	1	0	5.201218	0.376733	0.579731
132	6	0	7.220813	0.552686	0.924020
133	1	0	7.237935	-0.337533	1.520886
134	1	0	8.151700	1.065694	0.768104

TSr41 ONIOM: extrapolated energy = -6208.443125063459 A.U.
SCF Done: E(RM052X+HF-M052X) = -6230.89269492 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.731076	-1.385577	4.225055
2	6	0	2.289735	-1.511052	5.630303
3	6	0	3.801229	-1.481749	5.409319
4	6	0	3.943716	-1.297565	3.896175
5	7	0	2.681822	-1.347911	3.307694
6	1	0	1.912115	-0.684155	6.231680
7	1	0	4.302463	-2.406816	5.694155
8	8	0	4.976763	-1.114518	3.298382
9	8	0	0.488042	-1.312197	4.053459
10	1	0	4.305793	-0.659947	5.915208
11	1	0	1.919472	-2.437366	6.069967
12	35	0	2.515406	-1.185035	1.083482
13	6	0	2.796969	-1.956183	-1.691052
14	6	0	2.238799	-0.803254	-1.029230
15	6	0	2.955422	0.453773	-1.159959
16	6	0	4.178512	0.526478	-1.835761
17	6	0	4.597798	-0.608118	-2.547188
18	6	0	3.944569	-1.863864	-2.405160
19	1	0	2.260111	-2.889064	-1.610729
20	1	0	1.157428	-0.727943	-1.016069
21	1	0	4.373470	-2.703595	-2.929026
22	8	0	2.456663	1.536708	-0.625560
23	1	0	-0.028436	-1.071847	3.016421
24	8	0	5.624419	-0.579588	-3.410449
25	1	0	5.704331	0.294925	-3.854544
26	6	0	5.003436	1.779047	-1.775873
27	6	0	5.362017	2.441264	-2.937216
28	6	0	5.476353	2.275593	-0.552808
29	6	0	6.095957	3.606401	-2.927172
30	6	0	6.216448	3.452915	-0.546368
31	6	0	6.508408	4.125115	-1.716813
32	1	0	6.357966	4.070448	-3.855373
33	1	0	6.601501	3.816187	0.383904
34	1	0	7.089099	5.025167	-1.687818
35	8	0	5.041049	1.849842	-4.165571
36	6	0	3.809479	2.283585	-4.816370
37	1	0	3.874361	3.335333	-5.054539
38	1	0	3.728111	1.700316	-5.718804
39	1	0	2.963773	2.102710	-4.169620
40	1	0	1.624199	1.338370	-0.094254
41	8	0	-0.834719	-0.842530	2.137223
42	15	0	-0.873827	0.032770	0.901981
43	8	0	-2.331660	0.758936	1.006005
44	8	0	-1.052275	-0.934414	-0.419812
45	8	0	0.201186	0.998317	0.546552
46	6	0	-2.788603	1.352360	-0.156518
47	6	0	-2.227713	-1.652726	-0.535884
48	6	0	-3.279715	0.511541	-1.156731
49	6	0	-2.777512	2.737865	-0.291484
50	6	0	-2.222185	-3.033989	-0.368095
51	6	0	-3.390638	-0.949508	-0.857796
52	6	0	-3.629189	1.052134	-2.407677
53	6	0	-3.205371	3.251975	-1.510496
54	6	0	-2.413757	3.678837	0.828876
55	6	0	-3.447977	-3.685124	-0.454157
56	6	0	-0.964908	-3.843958	-0.181713
57	6	0	-4.627975	-1.619071	-0.853097
58	6	0	-3.592343	2.439908	-2.577475
59	6	0	-3.933118	0.126864	-3.597452
60	1	0	-3.213142	4.328656	-1.634146
61	6	0	-3.389765	4.001518	1.777427
62	6	0	-1.161038	4.295033	0.863002
63	6	0	-4.648590	-3.003759	-0.653714
64	1	0	-3.462901	-4.762041	-0.333297
65	6	0	-0.235260	-4.226213	-1.312584
66	6	0	-0.597829	-4.303723	1.084770
67	6	0	-5.940935	-0.823819	-0.942227
68	6	0	-4.018232	3.110629	-3.891276
69	1	0	-4.478981	-0.743158	-3.267667
70	1	0	-2.978504	-0.224260	-3.981390
71	6	0	-4.690097	0.843390	-4.725771
72	6	0	-3.102178	4.973364	2.778060
73	6	0	-4.691399	3.394497	1.785730
74	6	0	-0.887665	5.274175	1.863179
75	6	0	-0.111473	3.966450	-0.060591
76	6	0	-5.952875	-3.812509	-0.694159
77	6	0	0.884049	-5.096466	-1.167343
78	6	0	-0.570893	-3.778973	-2.636141
79	6	0	0.516759	-5.184141	1.217283
80	6	0	-1.299232	-3.917600	2.277511
81	1	0	-6.120805	-0.399883	0.042351
82	1	0	-5.834830	0.003195	-1.626346
83	6	0	-7.139888	-1.699740	-1.335384
84	1	0	-5.035353	3.474660	-3.773924
85	1	0	-3.383127	3.970321	-4.071127
86	6	0	-3.968700	2.149833	-5.088328
87	1	0	-4.751602	0.189118	-5.588554
88	1	0	-5.703909	1.066533	-4.407122
89	6	0	-4.111235	5.298640	3.743517
90	6	0	-1.862360	5.591183	2.792987
91	6	0	-5.610625	3.729089	2.711607
92	1	0	-4.915176	2.662014	1.040122
93	6	0	0.400008	5.906857	1.883447
94	6	0	1.091326	4.566963	0.008057
95	1	0	-0.287264	3.188686	-0.768821
96	1	0	-5.894857	-4.612186	0.035057
97	1	0	-6.040616	-4.270160	-1.675937
98	6	0	-7.192925	-2.944024	-0.436905
99	6	0	1.623099	-5.481851	-2.335485
100	6	0	1.230839	-5.557980	0.092248
101	6	0	0.152474	-4.162224	-3.706456
102	1	0	-1.411395	-3.128767	-2.753270
103	6	0	0.867457	-5.671597	2.519982
104	6	0	-0.930891	-4.393930	3.481579
105	1	0	-2.089229	-3.204855	2.194918
106	1	0	-7.050154	-2.006427	-2.373332
107	1	0	-8.052111	-1.121154	-1.239778
108	1	0	-2.936408	1.931729	-5.343025
109	1	0	-4.431976	2.617585	-5.950003
110	6	0	-5.317197	4.702302	3.714271
111	1	0	-3.877097	6.031282	4.491555
112	1	0	-1.652768	6.329937	3.543353
113	1	0	-6.575664	3.262381	2.705903
114	1	0	0.586103	6.649425	2.635280
115	6	0	1.349945	5.569283	0.992676
116	1	0	1.878886	4.260567	-0.649917
117	1	0	-7.217198	-2.636286	0.603392
118	1	0	-8.089031	-3.521885	-0.634084
119	6	0	1.274459	-5.033086	-3.556273
120	1	0	2.460160	-6.141161	-2.209093
121	1	0	2.067828	-6.222001	0.196829
122	1	0	-0.110089	-3.816221	-4.686312
123	1	0	1.701531	-6.341280	2.601874
124	6	0	0.167446	-5.298852	3.606793
125	1	0	-1.449197	-4.076917	4.363623
126	1	0	-6.066204	4.949367	4.440151
127	1	0	2.314189	6.036914	1.020454
128	1	0	1.830328	-5.326244	-4.424543
129	1	0	0.431213	-5.670099	4.577465
130	6	0	5.271063	1.519939	0.703895
131	1	0	5.239378	0.452370	0.609298
132	6	0	5.153791	2.049298	1.905610
133	1	0	5.058465	1.408957	2.758532
134	1	0	5.133343	3.108930	2.076652

TSs11 ONIOM: extrapolated energy = -6208.442786435227 A.U.
SCF Done: E(RM052X+HF-M052X) = -6230.89442747 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.258502	-2.540952	-3.596125
2	6	0	1.295838	-3.452716	-4.362030
3	6	0	-0.042177	-2.719037	-4.285808
4	6	0	0.297759	-1.477022	-3.489622
5	7	0	1.575095	-1.407489	-3.166086
6	1	0	1.672024	-3.588991	-5.375627
7	1	0	-0.812144	-3.271630	-3.747451
8	8	0	-0.609265	-0.641541	-3.205371
9	8	0	3.428162	-2.769116	-3.393549
10	1	0	-0.450021	-2.423546	-5.253052
11	1	0	1.273082	-4.424574	-3.871733
12	35	0	2.349232	0.345359	-1.928835
13	6	0	3.183328	3.043860	-1.448844
14	6	0	2.614451	2.005415	-0.613358
15	6	0	3.485853	1.392606	0.376402
16	6	0	4.852630	1.693754	0.405104
17	6	0	5.341210	2.636918	-0.484187
18	6	0	4.500650	3.340664	-1.398275
19	1	0	2.513745	3.548789	-2.133114

20	1	0	1.580146	2.130616	-0.312206
21	1	0	4.967005	4.073927	-2.037432
22	8	0	3.008641	0.537213	1.228159
23	1	0	-0.490943	0.127049	-2.337846
24	8	0	6.647296	2.960054	-0.546993
25	1	0	7.194780	2.462463	0.078664
26	6	0	5.782636	0.884837	1.248309
27	6	0	6.026772	-0.426356	0.826274
28	6	0	6.413345	1.383987	2.381581
29	6	0	6.890419	-1.229310	1.545336
30	6	0	7.283021	0.561422	3.098757
31	6	0	7.512119	-0.728860	2.677569
32	1	0	7.080886	-2.234418	1.235479
33	1	0	7.742951	0.929929	3.992163
34	1	0	8.174523	-1.361025	3.235417
35	8	0	5.386081	-0.808681	-0.304748
36	6	0	5.412467	-2.174225	-0.780903
37	1	0	6.420486	-2.464064	-1.051866
38	1	0	5.027988	-2.842391	-0.022254
39	1	0	4.775499	-2.193958	-1.647394
40	1	0	2.024450	0.357357	1.080640
41	8	0	-0.611129	0.908612	-1.363427
42	15	0	-0.729258	0.329860	0.039087
43	8	0	-1.454786	-1.115700	-0.223595
44	8	0	-1.859938	1.166677	0.862492
45	8	0	0.452088	0.243104	0.944225
46	6	0	-2.212949	-1.676723	0.783381
47	6	0	-3.101052	1.229134	0.258432
48	6	0	-3.427276	-1.073619	1.121872
49	6	0	-1.773667	-2.848144	1.391572
50	6	0	-3.508380	2.408490	-0.357027
51	6	0	-3.905520	0.092440	0.314670
52	6	0	-4.147906	-1.556927	2.231067
53	6	0	-2.550406	-3.355217	2.426388
54	6	0	-0.560477	-3.607179	0.919134
55	6	0	-4.749425	2.392718	-0.981270
56	6	0	-2.682167	3.667635	-0.302607
57	6	0	-5.116443	0.074546	-0.403602
58	6	0	-3.701975	-2.712399	2.881800
59	6	0	-5.335100	-0.756467	2.792590
60	1	0	-2.227136	-4.270853	2.907857
61	6	0	-0.704199	-4.519991	-0.131099
62	6	0	0.663548	-3.472756	1.576221
63	6	0	-5.539452	1.242635	-1.046695
64	1	0	-5.096071	3.302146	-1.458259
65	6	0	-2.703105	4.440365	0.863507
66	6	0	-1.961002	4.093526	-1.420966
67	6	0	-5.896553	-1.238892	-0.577589
68	6	0	-4.468962	-3.332212	4.058764
69	1	0	-5.904486	-0.313819	1.990947
70	1	0	-4.917594	0.061512	3.374164
71	6	0	-6.244117	-1.599410	3.699279
72	6	0	0.400337	-5.335219	-0.510690
73	6	0	-1.935015	-4.676177	-0.855227
74	6	0	1.758025	-4.306265	1.199589
75	6	0	0.878243	-2.506589	2.617827
76	6	0	-6.880055	1.319735	-1.791611
77	6	0	-1.982900	5.668203	0.906861
78	6	0	-3.434103	4.049473	2.036222
79	6	0	-1.250321	5.329266	-1.368680
80	6	0	-1.895174	3.330258	-2.637228
81	1	0	-5.391316	-1.806636	-1.354829
82	1	0	-5.848405	-1.827790	0.324869
83	6	0	-7.356339	-1.010308	-0.996877
84	1	0	-5.065200	-4.158271	3.680383
85	1	0	-3.757695	-3.740583	4.767268
86	6	0	-5.397252	-2.325984	4.754229
87	1	0	-6.973693	-0.953075	4.174791
88	1	0	-6.786269	-2.328951	3.104937
89	6	0	0.238544	-6.271200	-1.585872
90	6	0	1.600749	-5.218346	0.170926
91	6	0	-2.043152	-5.562549	-1.865400
92	1	0	-2.768412	-4.067596	-0.575851
93	6	0	3.003847	-4.175905	1.899088
94	6	0	2.071771	-2.402808	3.231639
95	1	0	0.082344	-1.838977	2.865457
96	1	0	-6.763734	1.953459	-2.663123
97	1	0	-7.606866	1.793550	-1.137212
98	6	0	-7.407737	-0.062235	-2.203921
99	6	0	-2.014160	6.452767	2.106795
100	6	0	-1.276550	6.084818	-0.209531
101	6	0	-3.437725	4.816664	3.143148
102	1	0	-3.976248	3.128781	2.013318
103	6	0	-0.523739	5.765143	-2.527270
104	6	0	-1.205125	3.779018	-3.702406
105	1	0	-2.374922	2.377903	-2.663156
106	1	0	-7.914914	-0.577390	-0.172323
107	1	0	-7.812875	-1.963407	-1.240663
108	1	0	-4.807147	-1.600200	5.304333
109	1	0	-6.031145	-2.845982	5.463913
110	6	0	-0.933698	-6.381035	-2.240208
111	1	0	1.076910	-6.886527	-1.850769
112	1	0	2.427129	-5.843991	-0.108592
113	1	0	-2.969768	-5.666593	-2.394465
114	1	0	3.810915	-4.825266	1.618784
115	6	0	3.156295	-3.261032	2.873918
116	1	0	2.226155	-1.657026	3.984665
117	1	0	-6.796087	-0.465513	-3.004502
118	1	0	-8.422254	0.031687	-2.575216
119	6	0	-2.712194	6.045742	3.182730
120	1	0	-1.465107	7.374375	2.122509
121	1	0	-0.741494	7.015044	-0.175636
122	1	0	-3.986509	4.508077	4.010643
123	1	0	-0.001543	6.701047	-2.473841
124	6	0	-0.506720	5.024748	-3.650996
125	1	0	-1.159071	3.192146	-4.597829
126	1	0	-1.048689	-7.086128	-3.039511
127	1	0	4.094029	-3.154928	3.381696
128	1	0	-2.730830	6.636720	4.076763
129	1	0	0.031154	5.359478	-4.516154
130	6	0	6.145047	2.775204	2.823668
131	1	0	5.145526	3.128160	2.656719
132	6	0	7.040990	3.572035	3.374557
133	1	0	8.059975	3.271482	3.529807
134	1	0	6.784981	4.566636	3.684011

TSs21 ONIOM: extrapolated energy = -6208.444617035833 A.U.
SCF Done: E(RM052X+HF-M052X) = -6230.89378444 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.842425	-1.460587	-3.576501
2	6	0	2.223047	-2.593037	-4.400873
3	6	0	0.725071	-2.286775	-4.373542
4	6	0	0.665785	-1.016358	-3.557312
5	7	0	1.839009	-0.573952	-3.180496
6	1	0	2.659069	-2.581972	-5.399697
7	1	0	0.132464	-3.051939	-3.871821
8	8	0	-0.468555	-0.485646	-3.302899
9	8	0	4.012666	-1.337456	-3.302760
10	1	0	0.284048	-2.106560	-5.354507
11	1	0	2.467155	-3.543878	-3.931428
12	35	0	2.265368	1.224083	-1.754759
13	6	0	3.008769	3.841042	-0.967730
14	6	0	2.417525	2.703480	-0.280542
15	6	0	3.280148	1.971913	0.650878
16	6	0	4.668036	2.188697	0.667996
17	6	0	5.186546	3.130603	-0.225735
18	6	0	4.341825	4.035784	-0.947913
19	1	0	2.352990	4.463434	-1.561763
20	1	0	1.386261	2.797626	0.043313
21	1	0	4.835653	4.801857	-1.525112
22	8	0	2.764096	1.056668	1.398876
23	1	0	-0.515191	0.239773	-2.504797
24	8	0	6.493313	3.243866	-0.485965
25	1	0	6.939348	2.358525	-0.479865
26	6	0	5.547092	1.356632	1.554328
27	6	0	6.562831	0.594557	0.997261
28	6	0	5.397750	1.354770	2.947887
29	6	0	7.392906	-0.192892	1.764923
30	6	0	6.242600	0.562456	3.717560
31	6	0	7.222757	-0.216604	3.134269
32	1	0	8.172810	-0.747915	1.286490
33	1	0	6.153855	0.590144	4.783926
34	1	0	7.871529	-0.809876	3.747055
35	8	0	6.813912	0.703937	-0.370193
36	6	0	6.162338	-0.253908	-1.282613
37	1	0	6.416754	-1.258851	-0.982156
38	1	0	5.096032	-0.121281	-1.277192
39	1	0	6.555796	-0.040479	-2.260879
40	1	0	1.770180	0.849917	1.180327
41	8	0	-0.800017	1.040976	-1.394242
42	15	0	-0.797204	0.406778	-0.024912
43	8	0	-1.157749	-1.166192	-0.343312
44	8	0	-2.082704	0.909432	0.847202
45	8	0	0.357800	0.549017	0.919389
46	6	0	-1.707387	-1.953706	0.643943
47	6	0	-3.322784	0.661080	0.296669
48	6	0	-3.003849	-1.674600	1.084406
49	6	0	-0.987169	-3.043146	1.126425
50	6	0	-4.054540	1.705865	-0.258479
51	6	0	-3.807590	-0.644470	0.355106
52	6	0	-3.517162	-2.370962	2.195908
53	6	0	-1.554676	-3.772432	2.163758
54	6	0	0.301976	-3.508025	0.499176
55	6	0	-5.282835	1.382359	-0.822058
56	6	0	-3.593711	3.139587	-0.213250
57	6	0	-5.012846	-0.960681	-0.301659
58	6	0	-2.778450	-3.426905	2.738843
59	6	0	-4.817342	-1.901152	2.869409
60	1	0	-1.008493	-4.626061	2.548358
61	6	0	0.239054	-4.386389	-0.588337
62	6	0	1.533919	-3.144976	1.043135
63	6	0	-5.756417	0.070608	-0.884834
64	1	0	-5.875316	2.181168	-1.252716
65	6	0	-3.754978	3.868833	0.969462
66	6	0	-3.103996	3.759334	-1.365428
67	6	0	-5.440795	-2.427073	-0.479163
68	6	0	-3.298459	-4.266408	3.914687
69	1	0	-5.524869	-1.564819	2.128117

70	1	0	-4.563460	-1.038397	3.479965
71	6	0	-5.444458	-2.978950	3.766098
72	6	0	1.441597	-4.933860	-1.121233
73	6	0	-1.002397	-4.767846	-1.202479
74	6	0	2.732367	-3.700388	0.503951
75	6	0	1.649998	-2.205144	2.122624
76	6	0	-7.110588	-0.184960	-1.561828
77	6	0	-3.426636	5.254604	0.991294
78	6	0	-4.251139	3.277026	2.180150
79	6	0	-2.799355	5.152296	-1.338217
80	6	0	-2.885046	3.045248	-2.593371
81	1	0	-4.847605	-2.833518	-1.294555
82	1	0	-5.199031	-2.999262	0.402335
83	6	0	-6.930138	-2.573670	-0.825052
84	1	0	-3.712694	-5.189935	3.518956
85	1	0	-2.464877	-4.530537	4.555136
86	6	0	-4.383376	-3.540652	4.723650
87	1	0	-6.269501	-2.546884	4.321807
88	1	0	-5.842810	-3.783560	3.155036
89	6	0	1.362165	-5.843714	-2.227886
90	6	0	2.658672	-4.584794	-0.557794
91	6	0	-1.032011	-5.615896	-2.250079
92	1	0	-1.908532	-4.357202	-0.811193
93	6	0	3.991595	-3.322002	1.076790
94	6	0	2.854634	-1.864052	2.616021
95	1	0	0.761754	-1.739193	2.489944
96	1	0	-7.208884	0.476061	-2.415101
97	1	0	-7.898051	0.070371	-0.857741
98	6	0	-7.286541	-1.647100	-1.996545
99	6	0	-3.598805	5.992069	2.209119
100	6	0	-2.965493	5.865186	-0.163600
101	6	0	-4.397536	4.006084	3.303094
102	1	0	-4.497816	2.237211	2.172731
103	6	0	-2.333896	5.786494	-2.538440
104	6	0	-2.445651	3.680323	-3.695929
105	1	0	-3.040198	1.989564	-2.598967
106	1	0	-7.537251	-2.315854	0.037657
107	1	0	-7.138953	-3.607335	-1.078620
108	1	0	-3.939429	-2.725854	5.286381
109	1	0	-4.831029	-4.229079	5.431910
110	6	0	0.175472	-6.170774	-2.774275
111	1	0	2.275898	-6.261924	-2.605094
112	1	0	3.562896	-5.006440	-0.954623
113	1	0	-1.967492	-5.887273	-2.697654
114	1	0	4.883770	-3.753974	0.665849
115	6	0	4.051748	-2.440178	2.090766
116	1	0	2.930577	-1.122981	3.384156
117	1	0	-6.634405	-1.861955	-2.836956
118	1	0	-8.309137	-1.810928	-2.318211
119	6	0	-4.064481	5.394460	3.321214
120	1	0	-3.346380	7.034888	2.208499
121	1	0	-2.736676	6.914129	-0.147875
122	1	0	-4.765003	3.547128	4.199357
123	1	0	-2.122328	6.837966	-2.505342
124	6	0	-2.172860	5.082661	-3.673553
125	1	0	-2.277178	3.131059	-4.600546
126	1	0	0.123936	-6.853110	-3.599495
127	1	0	4.994463	-2.141655	2.501380
128	1	0	-4.190222	5.951706	4.228241
129	1	0	-1.829087	5.563111	-4.568322
130	6	0	4.394526	2.225308	3.603773
131	1	0	4.160147	3.130192	3.077031
132	6	0	3.798586	1.971391	4.752392
133	1	0	3.964184	1.065395	5.303307
134	1	0	3.095180	2.661407	5.175608

TSs31 ONIOM: extrapolated energy = -6208.439641720448 A.U.
SCF Done: E(RM052X+HF-M052X) = -6230.89871273 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.102054	-1.255800	3.409484
2	6	0	0.510291	-1.873021	4.653037
3	6	0	-0.251075	-3.187491	4.803812
4	6	0	-1.204591	-3.199875	3.606342
5	7	0	-1.046719	-2.014324	2.881210
6	1	0	0.393509	-1.183883	5.489423
7	1	0	0.383977	-4.069170	4.738748
8	8	0	-1.977009	-4.081711	3.330901
9	8	0	0.302224	-0.135148	3.000657
10	1	0	-0.836166	-3.255482	5.720590
11	1	0	1.577342	-2.004094	4.472078
12	35	0	-2.080328	-1.892069	0.890358
13	6	0	-3.836168	-2.978155	-1.034444
14	6	0	-2.951664	-1.835560	-1.098632
15	6	0	-3.571935	-0.522267	-1.097578
16	6	0	-4.937938	-0.383189	-0.816030
17	6	0	-5.711313	-1.526477	-0.691169
18	6	0	-5.162493	-2.834780	-0.808341
19	1	0	-3.382336	-3.954560	-1.117929
20	1	0	-2.046422	-1.930191	-1.686907
21	1	0	-5.837263	-3.669463	-0.702366
22	8	0	-2.864965	0.544052	-1.312957
23	1	0	-0.051170	0.303706	1.921916
24	8	0	-7.038888	-1.479895	-0.454952
25	1	0	-7.378102	-0.577951	-0.360256
26	6	0	-5.558848	0.972424	-0.731544
27	6	0	-5.705653	1.708000	-1.908013
28	6	0	-5.998311	1.503586	0.477839
29	6	0	-6.283124	2.961265	-1.873331
30	6	0	-6.581206	2.770243	0.499753
31	6	0	-6.718973	3.485025	-0.667913
32	1	0	-6.393629	3.534288	-2.769153
33	1	0	-6.884756	3.194136	1.434375
34	1	0	-7.156843	4.463265	-0.646948
35	8	0	-5.269277	1.108569	-3.053167
36	6	0	-5.016647	1.879234	-4.242385
37	1	0	-5.939023	2.237885	-4.681265
38	1	0	-4.532174	1.201169	-4.925010
39	1	0	-4.363308	2.715244	-4.030276
40	1	0	-1.875727	0.328637	-1.441748
41	8	0	-0.388406	-0.064082	-1.544875
42	15	0	0.448437	0.377746	-0.384937
43	8	0	1.431269	1.548714	-0.945065
44	8	0	1.499910	-0.763749	0.128638
45	8	0	-0.232733	0.853012	0.890367
46	6	0	2.486776	1.911907	-0.126930
47	6	0	2.534760	-1.100906	-0.725540
48	6	0	3.581868	1.049437	-0.064870
49	6	0	2.445070	3.111587	0.575150
50	6	0	2.544912	-2.355505	-1.324788
51	6	0	3.567545	-0.180410	-0.912969
52	6	0	4.630745	1.324338	0.832401
53	6	0	3.536201	3.402073	1.386927
54	6	0	1.312579	4.097642	0.466884
55	6	0	3.580807	-2.623570	-2.212482
56	6	0	1.554146	-3.433726	-0.976856
57	6	0	4.551200	-0.439109	-1.886092
58	6	0	4.607688	2.524351	1.550814
59	6	0	5.714231	0.269889	1.114012
60	1	0	3.528366	4.336979	1.934694
61	6	0	1.248301	4.946974	-0.641694
62	6	0	0.401105	4.229550	1.517213
63	6	0	4.552785	-1.676737	-2.537549
64	1	0	3.611359	-3.599232	-2.683438
65	6	0	1.726259	-4.152873	0.210466
66	6	0	0.547015	-3.785984	-1.876485
67	6	0	5.535541	0.665291	-2.304626
68	6	0	5.748068	2.929987	2.495286
69	1	0	5.970345	-0.260102	0.210631
70	1	0	5.279818	-0.456986	1.795950
71	6	0	6.971742	0.869299	1.761209
72	6	0	0.249501	5.960767	-0.691628
73	6	0	2.162100	4.848972	-1.745033
74	6	0	-0.582454	5.260413	1.464797
75	6	0	0.400412	3.355728	2.658512
76	6	0	5.631445	-2.055563	-3.562608
77	6	0	0.867232	-5.251806	0.497187
78	6	0	2.753783	-3.836459	1.163141
79	6	0	-0.278146	-4.915954	-1.600947
80	6	0	0.296584	-3.043569	-3.082102
81	1	0	4.999475	1.327488	-2.979570
82	1	0	5.825250	1.255267	-1.449382
83	6	0	6.773006	0.112538	-3.027179
84	1	0	6.400072	3.619256	1.965453
85	1	0	5.331943	3.460988	3.343433
86	6	0	6.576275	1.727822	2.971380
87	1	0	7.636234	0.067005	2.063021
88	1	0	7.501751	1.483640	1.039482
89	6	0	0.195340	6.828984	-1.831599
90	6	0	-0.635717	6.098642	0.364837
91	6	0	2.076401	5.685484	-2.797140
92	1	0	2.913248	4.089067	-1.716530
93	6	0	-1.495555	5.408560	2.561449
94	6	0	-0.479270	3.527946	3.662372
95	1	0	1.083592	2.535838	2.680102
96	1	0	5.178850	-2.649342	-4.348295
97	1	0	6.369814	-2.678820	-3.065331
98	6	0	6.336043	-0.828445	-4.159614
99	6	0	1.047362	-5.977265	1.721063
100	6	0	-0.105600	-5.616090	-0.419426
101	6	0	2.897504	-4.552250	2.295605
102	1	0	3.408174	-3.018372	0.951808
103	6	0	-1.268059	-5.304482	-2.565502
104	6	0	-0.657031	-3.433241	-3.950760
105	1	0	0.859324	-2.151742	-3.255122
106	1	0	7.399867	-0.430739	-2.326246
107	1	0	7.356222	0.937654	-3.420920
108	1	0	5.991689	1.128909	3.662309
109	1	0	7.457318	2.077954	3.497760
110	6	0	1.071529	6.698908	-2.844644
111	1	0	-0.564217	7.586479	-1.853949
112	1	0	-1.378755	6.872783	0.329857
113	1	0	2.764107	5.595469	-3.614513
114	1	0	-2.224242	6.194266	2.509560
115	6	0	-1.442058	4.582378	3.621352
116	1	0	-0.478068	2.851916	4.493684
117	1	0	5.658259	-0.301580	-4.823414
118	1	0	7.191390	-1.149084	-4.743872
119	6	0	2.025407	-5.646144	2.585047

120	1	0	0.381412	-6.791680	1.928341
121	1	0	-0.735853	-6.458829	-0.208521
122	1	0	3.676127	-4.308490	2.991431
123	1	0	-1.858321	-6.177336	-2.361094
124	6	0	-1.446063	-4.597921	-3.697671
125	1	0	-0.839977	-2.863167	-4.839508
126	1	0	1.025002	7.351349	-3.693917
127	1	0	-2.129106	4.696276	4.436367
128	1	0	2.162340	-6.201354	3.491938
129	1	0	-2.185493	-4.894489	-4.414779
130	6	0	-5.820797	0.731180	1.733701
131	1	0	-4.916370	0.157815	1.802141
132	6	0	-6.693605	0.708688	2.722887
133	1	0	-7.624784	1.242079	2.681070
134	1	0	-6.508387	0.140800	3.613690

TSs41 ONIOM: extrapolated energy = -6208.445584960980 A.U.
SCF Done: E(RM052X+HF-M052X) = -6230.90087131 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.015995	-1.065221	3.546822
2	6	0	0.607014	-1.701371	4.791224
3	6	0	-0.316566	-2.888074	5.054302
4	6	0	-1.321702	-2.835981	3.902180
5	7	0	-1.049904	-1.715623	3.108543
6	1	0	0.633858	-0.962492	5.592053
7	1	0	0.188915	-3.851374	5.019319
8	8	0	-2.211247	-3.622782	3.705898
9	8	0	0.539222	-0.031910	3.057229
10	1	0	-0.859707	-2.822415	5.996675
11	1	0	1.633838	-1.989133	4.564638
12	35	0	-2.180417	-1.573982	1.201867
13	6	0	-4.126313	-2.662369	-0.474612
14	6	0	-3.188128	-1.601519	-0.745030
15	6	0	-3.732921	-0.268161	-0.906287
16	6	0	-5.081469	0.014767	-0.620064
17	6	0	-5.933286	-1.072540	-0.382125
18	6	0	-5.438634	-2.401804	-0.269425
19	1	0	-3.731916	-3.665195	-0.404815
20	1	0	-2.320248	-1.828762	-1.352779
21	1	0	-6.159419	-3.170720	-0.039749
22	8	0	-2.974152	0.693649	-1.348735
23	1	0	0.168525	0.411161	1.967233
24	8	0	-7.267670	-0.950222	-0.267152
25	1	0	-7.621158	-0.244913	-0.856586
26	6	0	-5.563453	1.438804	-0.586803
27	6	0	-6.657393	1.835642	-1.339024
28	6	0	-4.954311	2.395423	0.240121
29	6	0	-7.134827	3.127667	-1.333940
30	6	0	-5.438472	3.698070	0.242998
31	6	0	-6.510819	4.069401	-0.543634
32	1	0	-7.994299	3.368655	-1.924487
33	1	0	-4.982392	4.412852	0.896444
34	1	0	-6.873233	5.077479	-0.518423
35	8	0	-7.352501	0.871792	-2.082139
36	6	0	-6.951588	0.692317	-3.473597
37	1	0	-7.132965	1.604194	-4.023609
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39	1	0	-5.905447	0.430334	-3.527404
40	1	0	-1.997682	0.422950	-1.400551
41	8	0	-0.513283	-0.055720	-1.422378
42	15	0	0.458198	0.345108	-0.360928
43	8	0	1.505632	1.383228	-1.051369
44	8	0	1.426299	-0.881575	0.119792
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47	6	0	2.331826	-1.366265	-0.808038
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51	6	0	3.436036	-0.575316	-1.131427
52	6	0	4.816911	0.861219	0.438349
53	6	0	4.008694	3.062960	1.002789
54	6	0	1.796606	3.972731	0.270391
55	6	0	3.060451	-3.049775	-2.310378
56	6	0	1.071536	-3.576057	-0.878480
57	6	0	4.289583	-0.978381	-2.175092
58	6	0	4.991862	2.079406	1.103545
59	6	0	5.803065	-0.297014	0.665661
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61	6	0	1.692220	4.773965	-0.870427
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63	6	0	4.095864	-2.232116	-2.764128
64	1	0	2.938512	-4.038216	-2.737710
65	6	0	1.237114	-4.247286	0.337534
66	6	0	-0.018608	-3.863863	-1.701674
67	6	0	5.343403	-0.008063	-2.732962
68	6	0	6.256013	2.388364	1.917793
69	1	0	5.911509	-0.883779	-0.232247
70	1	0	5.361381	-0.946393	1.417539
71	6	0	7.174698	0.180998	1.165278
72	6	0	0.823590	5.902668	-0.858137
73	6	0	2.438335	4.513071	-2.069242
74	6	0	0.200483	5.410507	1.422796
75	6	0	1.079101	3.440253	2.591749
76	6	0	5.026625	-2.768531	-3.861148
77	6	0	0.286794	-5.232096	0.731476
78	6	0	2.346292	-3.994762	1.214572
79	6	0	-0.938034	-4.884957	-1.319920
80	6	0	-0.262313	-3.160317	-2.931912
81	1	0	4.820902	0.682567	-3.389826
82	1	0	5.773477	0.579326	-1.937073
83	6	0	6.441256	-0.723362	-3.534228
84	1	0	6.922659	2.982464	1.298513
85	1	0	5.984516	2.991202	2.776486
86	6	0	6.993721	1.118987	2.367501
87	1	0	7.775502	-0.679319	1.439380
88	1	0	7.694564	0.707528	0.370486
89	6	0	0.726098	6.719118	-2.033038
90	6	0	0.107743	6.200550	0.289693
91	6	0	2.317197	5.305860	-3.151071
92	1	0	3.090221	3.666458	-2.087903
93	6	0	-0.534475	5.724157	2.614980
94	6	0	0.364803	3.767387	3.685558
95	1	0	1.648914	2.537510	2.573614
96	1	0	4.441101	-3.337370	-4.574085
97	1	0	5.736078	-3.451332	-3.401415
98	6	0	5.801523	-1.652203	-4.576711
99	6	0	0.462091	-5.909276	1.983427
100	6	0	-0.769800	-5.538215	-0.110886
101	6	0	2.481122	-4.663230	2.376656
102	1	0	3.068898	-3.263638	0.922551
103	6	0	-2.016581	-5.215407	-2.208105
104	6	0	-1.299286	-3.491158	-3.726083
105	1	0	0.378557	-2.343300	-3.184460
106	1	0	7.068290	-1.306064	-2.865885
107	1	0	7.070943	0.015472	-4.017491
108	1	0	6.419253	0.612438	3.136403
109	1	0	7.954445	1.387451	2.792667
110	6	0	1.442100	6.434196	-3.136013
111	1	0	0.065091	7.563771	-2.008099
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113	1	0	2.877116	5.093351	-4.040046
114	1	0	-1.154189	6.600018	2.611039
115	6	0	-0.449996	4.940996	3.705575
116	1	0	0.387876	3.131623	4.547851
117	1	0	5.126209	-1.078487	-5.203120
118	1	0	6.559058	-2.089220	-5.217706
119	6	0	1.518334	-5.640982	2.773952
120	1	0	-0.271279	-6.636452	2.271701
121	1	0	-1.468442	-6.299658	0.179325
122	1	0	3.320965	-4.469674	3.014666
123	1	0	-2.681323	-6.008496	-1.923543
124	6	0	-2.186742	-4.552420	-3.367095
125	1	0	-1.474153	-2.950371	-4.634596
126	1	0	1.363209	7.047695	-4.011392
127	1	0	-1.002749	5.179884	4.592386
128	1	0	1.650046	-6.160958	3.702241
129	1	0	-2.993258	-4.805497	-4.026125
130	6	0	-3.824581	2.033235	1.125152
131	1	0	-3.886332	1.068847	1.591238
132	6	0	-2.767611	2.794850	1.323778
133	1	0	-2.643745	3.738742	0.828245
134	1	0	-1.952321	2.475470	1.938008

References

1) N. P. H. Tan, C. D. Donner, *Tetrahedron. Lett.* **2008**, *49*, 4160.

2) S. B. Jones, L. He, S. L. Castle, *Org. Lett.* **2006**, *8*, 3757.

3) K. Fuji, T. Morimoto, K. Tsutsumi, K. Kakiuchi, *Angew. Chem. Int. Ed.* **2003**, *42*, 2409.

4) A. Bengston, A. Hallberg, M. Larhed, *Org. Lett.* **2002**, *4*, 1231.

5) N. U. Hoflokken, L. Skattebol, *Acta Chemica Scandinavica* **1993**, *53*, 258.

6) N. Bajwa, M. P. Jennings, *J. Org. Chem.* **2006**, *71*, 3646.

7) (a) Matsumoto, T.; Konegawa, T.; Nakamura, T.; Suzuki, K. *Synlett* **2002**, 122. (b) Okuyama, K.; Shingubara, K.; Tsujiyama, S.; Suzuki, K.; Matsumoto, T. *Synlett* **2009**, 941.

8) Gaussian 03 (Revision E.01) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, M.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. Gaussian 03, Revision E.01.; Gaussian, Inc.: Wallingford, CT, 2004.

9) Zhao, Y.; Schultz, N. E.; Truhlar, D. G. *J. Chem. Theory Comp.* **2006**, *2*, 364.

10) M05-2X is a good level of theory for studying organocatalysis, see: Simòn, L.; Goodman, J. M. *Org. Biomol. Chem.* **2011**, *9*, 689.

11) Reed, A. E.; Weinstock, R. B.; Weinhold, F. *J. Chem. Phys.* **1985**, *83,* 735