

## Supporting Information

### Computational Study on C-B Homolytic Bond Dissociation Enthalpies of Organoboron Compounds

Jiaoyang Wang, Wenrui Zheng\*, Lanlan Ding, Yingxing Wang

College of Chemistry and Chemical Engineering, Shanghai University of Engineering Science, Shanghai 201620, China

**Table S1** The 64 C-B BDEs calculated by six composite high-level *ab initio* methods (kJ/mol)

Entry	Molecules	G3	G4	G3B3	series G		CBS-QB3	CBS-4M	CBS-Q	series CBS		Six methods Average
					Average	Max-Min				Average	Max-Min	
1	CH <sub>3</sub> CH=CH-B(OH) <sub>2</sub>	486.4	479.8	485.6	483.9	6.6	487.1	485.9	489.9	487.6	4.0	485.8
2	H <sub>2</sub> C=CH-B(OH) <sub>2</sub>	479.4	473.1	478.7	477.1	6.3	480.2	479.4	479.8	479.8	0.8	478.4
3	$\begin{array}{c} \text{H}_2\text{C}=\text{C}-\text{B}(\text{OH})_2 \\   \\ \text{CH}_3 \end{array}$	468.7	459.1	467.0	464.9	9.6	467.7	464.6	470.4	467.6	5.8	466.3
4	$\begin{array}{c} \text{H}_2\text{C}=\text{C}-\text{B}(\text{OH})_2 \\   \\ \text{CH}_2\text{CH}_3 \end{array}$	469.5	458.4	467.9	465.3	11.1	468.5	464.3	471.2	468.0	6.9	466.6
5	$\begin{array}{c} \text{H}_3\text{CHC}=\text{C}-\text{B}(\text{OH})_2 \\   \\ \text{CH}_3 \end{array}$	464.7	453.5	463.1	460.4	11.2	463.8	458.8	466.3	463.0	7.5	461.7
6	C <sub>2</sub> H <sub>5</sub> HC=CH-B(OH) <sub>2</sub>	488.2	478.1	486.6	484.3	10.1	488.1	487.1	494.5	489.9	7.4	487.1
7	$\begin{array}{c} \text{H}_2\text{C}=\text{CH}-\text{B}-\text{OH} \\   \\ \text{CH}_3 \end{array}$	479.2	472.4	477.2	476.3	6.8	479.8	480.1	480.5	480.1	0.7	478.2
8	$\begin{array}{c} \text{H}_3\text{CHC}=\text{CH}-\text{B}-\text{OH} \\   \\ \text{CH}_3 \end{array}$	488.8	479.8	486.3	485.0	9.0	488.9	491.7	494.9	491.8	6.0	488.4
9	$\begin{array}{c} (\text{H}_3\text{C})_2\text{C}=\text{CH}-\text{B}-\text{OH} \\   \\ \text{CH}_3 \end{array}$	486.6	476.3	484.4	482.4	10.3	486.5	482.4	495.6	488.2	13.2	485.3
10	$\begin{array}{c} \text{CH}_3 \\   \\ \text{H}_2\text{C}=\text{C}-\text{B}-\text{OH} \\   \\ \text{CH}_3 \end{array}$	472.3	458.6	465.3	465.4	13.7	471.6	469.9	473.9	471.8	4.0	468.6
11	$\begin{array}{c} \text{CH}_3 \\   \\ \text{H}_3\text{CHC}=\text{C}-\text{B}-\text{OH} \\   \\ \text{CH}_3 \end{array}$	473.0	457.6	466.3	465.6	15.4	468.1	465.2	477.2	470.2	12.0	467.9
12	$\begin{array}{c} \text{CH}_2\text{CH}_3 \\   \\ \text{H}_2\text{C}=\text{C}-\text{B}-\text{OH} \\   \\ \text{CH}_3 \end{array}$	473.7	462.7	470.8	469.1	11.0	472.7	470.7	476.7	473.4	6.0	471.2
13	H <sub>2</sub> C=CH-B(CH <sub>3</sub> ) <sub>2</sub>	477.3	471.9	475.6	474.9	5.4	478.5	480.4	478.6	479.2	1.9	477.1
14	H <sub>3</sub> CHC=CH-B(CH <sub>3</sub> ) <sub>2</sub>	486.2	479.0	484.4	483.2	7.2	487.1	488.5	490.4	488.7	3.3	485.9
15	(H <sub>3</sub> C) <sub>2</sub> C=CH-B(CH <sub>3</sub> ) <sub>2</sub>	478.4	470.0	476.5	475.0	8.4	479.0	478.3	485.6	481.0	7.3	478.0
16	$\begin{array}{c} \text{H}_2\text{C}=\text{C}-\text{B}(\text{CH}_3)_2 \\   \\ \text{CH}_3 \end{array}$	463.1	455.9	461.3	460.1	7.2	463.5	462.7	463.8	463.3	1.1	461.7
17	$\begin{array}{c} \text{H}_3\text{CHC}=\text{C}-\text{B}(\text{CH}_3)_2 \\   \\ \text{CH}_3 \end{array}$	464.4	455.4	462.5	460.8	9.0	464.6	462.9	466.2	464.6	3.3	462.7
18	$\begin{array}{c} \text{H}_2\text{C}=\text{C}-\text{B}(\text{CH}_3)_2 \\   \\ \text{C}_2\text{H}_5 \end{array}$	462.8	453.8	460.9	459.2	9.0	462.9	461.6	463.5	462.7	1.9	460.9
19	C <sub>2</sub> H <sub>5</sub> HC=CH-B(CH <sub>3</sub> ) <sub>2</sub>	473.0	464.1	470.5	469.2	8.9	473.1	472.8	481.8	475.9	9.0	472.6
20	$\begin{array}{c} \text{H}_2\text{C}=\text{CH}-\text{B}-\text{OH} \\   \\ \text{C}_2\text{H}_5 \end{array}$	475.1	474.6	473.6	474.4	1.5	475.6	476.1	476.9	476.2	1.3	475.3
21	$\begin{array}{c} \text{H}_2\text{C}=\text{CH}-\text{B}-\text{OH} \\   \\ \text{CH}(\text{CH}_3)_2 \end{array}$	482.9	473.1	480.6	478.9	9.8	482.9	482.9	487.5	484.4	4.6	481.7
22	$\begin{array}{c} \text{CH}_3 \\   \\ \text{H}_2\text{C}=\text{C}-\text{B}-\text{OH} \\   \\ \text{C}_2\text{H}_5 \end{array}$	465.9	462.8	463.9	464.2	3.1	465.2	461.1	468.4	464.9	7.3	464.6
23	$\begin{array}{c} \text{H}_3\text{CHC}=\text{CH}-\text{B}-\text{OH} \\   \\ \text{C}_2\text{H}_5 \end{array}$	482.8	480.2	481.0	481.3	2.6	482.9	482.8	489.2	485.0	6.4	483.2
24	H <sub>2</sub> C=CH-B(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub>	478.9	470.7	476.6	475.4	8.2	478.9	480.5	480.8	480.1	1.9	477.7
25	H <sub>3</sub> C-B(OH) <sub>2</sub>	438.5	435.4	438.5	437.5	3.1	442.3	441.3	440.8	441.5	1.5	439.5

\* Corresponding author. Tel.: +86 21 67791216; fax: +86 21 67791220.  
E-mail address: wrzheng@sues.edu.cn (W.R. Zheng).

26	$C_2H_5-B(OH)_2$	427.4	421.3	426.6	425.1	6.1	429.3	426.7	429.0	428.3	2.6	426.7
27	$(H_3C)_2HC-B(OH)_2$	416.1	406.4	414.8	412.4	9.7	415.1	412.2	417.0	414.8	4.8	413.6
28	$(H_3C)_3C-B(OH)_2$	412.1	399.7	411.0	407.6	12.4	409.9	406.1	413.8	409.9	7.7	408.8
29	$C_3H_7-B(OH)_2$	432.0	424.0	431.4	429.1	8.0	433.1	430.8	434.9	432.9	4.1	431.0
30	$C_4H_9-B(OH)_2$	431.8	422.5	431.2	428.5	9.3	432.7	430.1	435.8	432.9	5.7	430.7
31	$C_2H_5HC-B(OH)_2$ $CH_3$	417.5	406.9	416.6	413.7	10.6	416.5	412.9	419.3	416.2	6.4	415.0
32	$(H_3C)_2CHCH_2-B(OH)_2$	435.0	423.4	430.6	429.7	11.6	430.6	429.6	439.0	433.1	9.4	431.4
33	$H_3C-B(CH_3)_2$	430.0	427.9	429.7	429.2	2.1	434.8	436.1	433.9	434.9	2.2	432.1
34	$C_2H_5-B(C_2H_5)_2$	416.7	412.5	418.6	415.9	6.1	421.2	421.7	424.3	422.4	3.1	419.2
35	$HC\equiv C-BF_2$	612.4	601.6	605.8	606.6	10.8	608.8	598.3	615.7	607.6	17.4	607.1
36	$HC\equiv C-BCl_2$	599.7	589.6	592.8	594.0	10.1	595.3	591.9	600.7	596.0	8.8	595.0
37	$C_2H_5\overset{\text{CH}_3}{\underset{\text{CH}_3}{\text{B}}}-OH$	427.5	420.5	425.7	424.6	7.0	428.9	428.1	430.8	429.3	2.7	426.9
38	$(H_3C)_2HC\overset{\text{CH}_3}{\underset{\text{CH}_3}{\text{B}}}-OH$	415.8	406.2	413.5	411.8	9.6	415.0	414.2	418.4	415.9	4.2	413.9
39	$(H_3C)_3C\overset{\text{CH}_3}{\underset{\text{CH}_3}{\text{B}}}-OH$	410.2	398.5	408.1	405.6	11.7	408.2	406.1	413.1	409.1	7.0	407.4
40	$(H_3C)_2HC\overset{\text{C}_2H_5}{\underset{\text{C}_2H_5}{\text{B}}}-OH$	409.6	406.4	408.1	408.0	3.2	409.0	405.0	412.0	408.7	7.0	408.4
41	$C_3H_7\overset{\text{C}_2H_5}{\underset{\text{C}_2H_5}{\text{B}}}-OH$	425.2	423.2	424.2	424.2	2.0	426.5	423.4	430.0	426.6	6.6	425.4
42	$H_3C-BH_2$	434.5	436.6	434.7	435.3	2.1	441.2	440.9	440.0	440.7	1.2	438.0
43	$C_2H_5-BH_2$	423.1	422.2	422.6	422.6	0.9	427.4	427.0	427.4	427.3	0.4	425.0
44	$(H_3C)_2HC-BH_2$	411.6	408.3	410.7	410.2	3.3	413.8	412.2	414.7	413.6	2.5	411.9
45	$(H_3C)_3C-BH_2$	404.3	398.6	403.0	402.0	5.7	404.9	403.6	407.7	405.4	4.1	403.7
46	$H_3C-BH-OH$	440.8	439.7	440.2	440.2	1.1	445.7	445.8	445.1	445.5	0.7	442.9
47	$H_3CH_2C-BH-OH$	426.6	422.2	425.0	424.6	4.4	428.7	428.6	429.5	428.9	0.9	426.8
48	$(H_3C)_2HC-BH-OH$	416.7	409.6	414.6	413.6	7.1	416.5	415.7	418.3	416.8	2.6	415.2
49	$(H_3C)_3C-BH-OH$	412.2	402.7	410.2	408.4	9.5	411.1	409.3	414.9	411.8	5.6	410.1
50	$H_2C=CH-BH_2$	486.1	484.3	484.5	485.0	1.8	488.7	490.2	488.7	489.2	1.5	487.1
51	$H_2C=C-BH_2$ $CH_3$	472.6	468.8	470.7	470.7	3.8	474.2	473.3	475.3	474.3	2.0	472.5
52	$H_3CHC=CH-BH_2$	497.3	493.8	495.5	495.5	3.5	499.6	500.6	501.5	500.6	1.9	498.1
53	$(H_3C)_2C=CH-BH_2$	497.4	492.6	495.8	495.3	4.8	499.5	498.6	501.8	500.0	3.2	497.6
54	$H_3CHC=C-BH_2$ $CH_3$	472.9	467.3	470.9	470.4	5.6	474.1	472.4	476.9	474.5	4.5	472.4
55	$H_3CH_2CH_2C-BH_2$	427.4	425.2	427.1	426.6	2.2	431.5	431.1	432.1	431.6	1.0	429.1
56	$H_3C(H_2C)_2H_2C-BH_2$	426.9	423.7	426.8	425.8	3.2	431.1	430.2	431.8	431.0	1.6	428.4
57	$H_3C(H_2C)_3H_2C-BH_2$	425.8	420.9	425.2	424.0	4.9	429.8	429.6	431.2	430.2	1.6	427.1
58	$H_3C(H_2C)_4H_2C-BH_2$	425.9	419.5	425.3	423.6	6.4	429.8	429.7	430.5	430.0	0.8	426.8
59	$H_3CH_2CHC-BH_2$ $CH_3$	412.6	408.5	412.2	411.1	4.1	415.1	412.7	415.4	414.4	2.7	412.8
60	$H_3CHC-H_2C-BH_2$ $CH_3$	430.2	424.9	429.5	428.2	5.3	432.3	433.4	436.5	434.1	4.2	431.1
61	$(H_3C)_2HC-HC-BH_2$ $CH_3$	416.9	410.6	415.7	414.4	6.3	418.6	416.8	420.8	418.7	4.0	416.6
62	$C_2H_5-\overset{CH_3}{\underset{CH_3}{C}}-BH_2$	402.5	396.8	402.3	400.5	5.7	403.9	402.5	405.2	403.9	2.7	402.2
63	$(H_3C)_3C-H_2C-BH_2$	430.1	424.9	429.6	428.2	5.2	433.7	432.9	440.4	435.7	7.5	431.9
64	$(H_3C)_3C-HC-BH_2$ $CH_3$	411.4	403.3	410.0	408.2	8.1	412.7	410.7	416.9	413.4	6.2	410.8

**Table S2** The 64 C-B calculated BDEs using 34 kinds of DFTs (kJ/mol)

Entry	compounds	B3LYP	B3LYP-D3	CAM-B3LYP	B3P86	KMLYP	MPW1P86	B3PW91	B97D	B97D3
1	$\text{CH}_3\text{CH}=\text{CH}-\text{B}(\text{OH})_2$	456.0	466.9	467.6	469.2	504.1	469.3	456.6	455.7	458.1
2	$\text{H}_2\text{C}=\text{CH}-\text{B}(\text{OH})_2$	450.0	459.7	461.3	462.6	496.9	462.6	450.3	447.2	450.4
3	$\text{H}_2\text{C}=\overset{\text{CH}_3}{\underset{ }{\text{C}}}-\text{B}(\text{OH})_2$	427.6	441.9	441.8	441.3	479.6	442.6	428.1	430.0	431.3
4	$\text{H}_2\text{C}=\overset{\text{CH}_2\text{CH}_3}{\underset{ }{\text{C}}}-\text{B}(\text{OH})_2$	426.2	443.2	441.2	440.6	480.2	442.3	427.0	432.9	433.1
5	$\text{H}_3\text{CHC}=\overset{\text{CH}_3}{\underset{ }{\text{C}}}-\text{B}(\text{OH})_2$	420.2	437.7	435.3	435.3	474.2	437.0	421.6	428.6	428.2
6	$\text{C}_2\text{H}_5\text{HC}=\text{CH}-\text{B}(\text{OH})_2$	455.3	466.5	467.0	468.5	503.5	468.7	456.0	455.5	457.7
7	$\text{H}_2\text{C}=\overset{\text{CH}_3}{\underset{ }{\text{C}}}-\overset{\text{B}-\text{OH}}{\underset{ }{\text{B}}}$	439.5	449.6	450.3	452.6	484.4	452.3	440.3	440.4	442.5
8	$\text{H}_3\text{CHC}=\overset{\text{CH}_3}{\underset{ }{\text{C}}}-\overset{\text{B}-\text{OH}}{\underset{ }{\text{B}}}$	448.2	459.3	459.6	461.6	494.9	461.6	449.1	450.0	451.7
9	$(\text{H}_3\text{C})_2\text{C}=\overset{\text{CH}_3}{\underset{ }{\text{C}}}-\overset{\text{B}-\text{OH}}{\underset{ }{\text{B}}}$	444.0	457.4	456.1	458.6	493.3	459.1	444.9	449.0	449.1
10	$\text{H}_2\text{C}=\overset{\text{CH}_3}{\underset{ }{\text{C}}}-\overset{\text{B}-\text{OH}}{\underset{ }{\text{B}}}$	415.4	430.8	429.4	429.5	466.2	430.9	416.1	421.8	422.2
11	$\text{H}_3\text{CHC}=\overset{\text{CH}_3}{\underset{ }{\text{C}}}-\overset{\text{B}-\text{OH}}{\underset{ }{\text{B}}}$	414.6	432.2	429.2	430.4	468.3	431.9	416.2	425.4	424.3
12	$\text{H}_2\text{C}=\overset{\text{CH}_2\text{CH}_3}{\underset{ }{\text{C}}}-\overset{\text{B}-\text{OH}}{\underset{ }{\text{B}}}$	412.3	430.7	427.0	427.1	465.0	428.9	413.3	423.8	422.9
13	$\text{H}_2\text{C}=\text{CH}-\text{B}(\text{CH}_3)_2$	444.7	455.8	455.7	457.3	489.5	457.5	444.7	448.4	449.2
14	$\text{H}_3\text{CHC}=\text{CH}-\text{B}(\text{CH}_3)_2$	452.7	465.1	464.0	466.1	498.7	466.4	453.2	459.2	459.1
15	$(\text{H}_3\text{C})_2\text{C}=\text{CH}-\text{B}(\text{CH}_3)_2$	441.3	456.7	453.3	456.0	489.6	456.8	442.1	453.8	451.1
16	$\text{H}_2\text{C}=\overset{\text{CH}_3}{\underset{ }{\text{C}}}-\text{B}(\text{CH}_3)_2$	417.2	434.1	431.3	431.5	467.8	433.1	417.6	429.2	427.2
17	$\text{H}_3\text{CHC}=\overset{\text{CH}_3}{\underset{ }{\text{C}}}-\text{B}(\text{CH}_3)_2$	416.3	435.5	431.0	432.5	469.6	434.3	417.8	433.6	429.8
18	$\text{H}_2\text{C}=\overset{\text{C}_2\text{H}_5}{\underset{ }{\text{C}}}-\text{B}(\text{CH}_3)_2$	413.2	432.6	428.8	429.5	467.9	431.5	414.7	429.9	426.6
19	$\text{C}_2\text{H}_5\text{HC}=\text{CH}-\text{B}(\text{CH}_3)_2$	435.2	450.9	446.8	449.0	482.1	449.7	435.6	446.9	445.7
20	$\text{H}_2\text{C}=\overset{\text{C}_2\text{H}_5}{\underset{ }{\text{C}}}-\overset{\text{B}-\text{OH}}{\underset{ }{\text{B}}}$	441.5	453.5	453.4	455.3	489.2	455.5	442.6	444.8	445.5
21	$\text{H}_2\text{C}=\overset{\text{CH}(\text{CH}_3)_2}{\underset{ }{\text{C}}}-\overset{\text{B}-\text{OH}}{\underset{ }{\text{B}}}$	446.5	459.2	460.2	460.2	496.6	460.9	447.3	451.1	451.4
22	$\text{H}_2\text{C}=\overset{\text{CH}_3}{\underset{ }{\text{C}}}-\overset{\text{B}-\text{OH}}{\underset{ }{\text{B}}}$	418.8	436.2	433.7	434.1	472.0	435.7	420.2	429.7	427.9
23	$\text{H}_3\text{CHC}=\overset{\text{C}_2\text{H}_5}{\underset{ }{\text{C}}}-\overset{\text{B}-\text{OH}}{\underset{ }{\text{B}}}$	448.2	461.4	460.5	462.7	497.2	463.0	449.7	454.0	453.9
24	$\text{H}_2\text{C}=\text{CH}-\text{B}(\text{C}_2\text{H}_5)_2$	441.4	454.3	453.3	454.2	488.0	454.7	441.4	448.5	447.2
25	$\text{H}_3\text{C}-\text{B}(\text{OH})_2$	414.0	421.3	425.3	428.0	458.4	427.2	416.3	412.5	416.4
26	$\text{C}_2\text{H}_5-\text{B}(\text{OH})_2$	390.8	402.4	404.0	404.8	438.9	405.2	393.0	391.4	393.2
27	$(\text{H}_3\text{C})_2\text{HC}-\text{B}(\text{OH})_2$	368.7	385.6	383.9	383.6	420.8	385.1	371.0	375.8	374.0
28	$(\text{H}_3\text{C})_3\text{C}-\text{B}(\text{OH})_2$	350.7	372.7	368.4	366.7	407.7	369.5	353.0	364.0	359.1
29	$\text{C}_3\text{H}_7-\text{B}(\text{OH})_2$	394.2	406.8	408.2	408.8	444.2	409.4	396.7	396.4	397.2

30	$C_4H_9-B(OH)_2$	393.6	406.5	407.7	408.2	443.7	408.8	396.1	396.1	396.8
31	$C_2H_5HC(B(OH)_2)CH_3$	367.3	384.8	382.7	382.2	419.9	383.8	369.6	375.7	373.1
32	$(H_3C)_2CHCH_2-B(OH)_2$	391.6	406.6	405.8	406.5	442.1	407.3	394.1	398.8	397.9
33	$H_3C-B(CH_3)_2$	403.9	412.3	415.1	417.6	445.4	416.8	406.0	408.7	410.1
34	$C_2H_5-B(C_2H_5)_2$	375.9	391.6	389.5	389.8	422.7	390.6	377.8	389.0	385.4
35	$HC\equiv C-BF_2$	597.2	600.5	609.3	607.8	645.6	607.1	595.1	583.4	587.6
36	$HC\equiv C-BCl_2$	583.7	589.3	595.7	596.0	630.9	595.1	583.4	567.6	575.6
37	$C_2H_5\overset{\text{B-OH}}{\underset{CH_3}{\text{C}}}$	381.0	393.1	393.8	395.4	427.2	395.6	383.5	385.5	385.8
38	$(H_3C)_2HC\overset{\text{B-OH}}{\underset{CH_3}{\text{C}}}$	356.5	373.7	370.9	371.1	405.8	372.5	358.8	367.0	364.3
39	$(H_3C)_3C\overset{\text{B-OH}}{\underset{CH_3}{\text{C}}}$	337.3	360.8	354.9	353.6	392.9	356.5	339.7	355.9	349.7
40	$(H_3C)_2HC\overset{\text{B-OH}}{\underset{C_2H_5}{\text{C}}}$	355.4	375.3	371.3	371.6	408.2	373.4	358.4	371.0	365.9
41	$C_3H_7\overset{\text{B-OH}}{\underset{C_2H_5}{\text{C}}}$	383.0	398.3	397.5	398.9	433.2	399.6	386.4	393.5	390.7
42	$H_3C-BH_2$	422.3	425.2	430.3	435.8	457.7	433.6	424.5	424.6	428.8
43	$C_2H_5-BH_2$	401.4	407.4	410.8	415.0	439.2	413.7	403.8	404.8	407.2
44	$(H_3C)_2HC-BH_2$	379.9	389.3	390.9	393.9	420.6	393.5	382.3	386.3	386.5
45	$(H_3C)_3C-BH_2$	360.9	374.4	373.7	376.0	405.2	376.6	363.4	373.5	370.6
46	$H_3C-BH-OH$	419.8	424.2	429.7	433.2	459.7	431.9	421.8	418.7	423.1
47	$H_3CH_2C-BH-OH$	395.0	402.7	406.1	408.2	437.1	407.8	397.0	395.5	397.8
48	$(H_3C)_2HC-BH-OH$	373.8	385.4	386.3	387.3	418.4	387.8	375.6	378.5	378.3
49	$(H_3C)_3C-BH-OH$	357.4	373.8	372.7	372.1	407.6	374.0	359.2	367.1	364.3
50	$H_2C=CH-BH_2$	469.5	474.1	476.5	481.0	506.4	479.7	469.1	468.8	472.5
51	$H_2C=C(BH_2)CH_3$	446.6	454.4	455.6	459.0	486.5	458.5	446.5	450.0	452.3
52	$H_3CHC=CH-BH_2$	481.6	487.2	488.7	494.0	519.5	492.7	481.8	483.3	486.3
53	$(H_3C)_2C=CH-BH_2$	480.9	487.8	488.4	494.7	520.6	493.5	481.7	486.2	487.1
54	$H_3CHC=C(BH_2)CH_3$	446.1	455.7	455.2	459.9	487.5	459.5	446.7	454.7	455.0
55	$H_3CH_2CH_2C-BH_2$	404.9	411.7	415.1	419.0	444.6	417.9	407.5	409.5	411.1
56	$H_3C(H_2C)_2H_2C-BH_2$	404.4	411.4	414.7	418.5	444.2	417.4	407.1	409.2	410.6
57	$H_3C(H_2C)_3H_2C-BH_2$	402.8	409.7	412.5	416.5	441.3	415.3	405.2	408.0	409.5
58	$H_3C(H_2C)_4H_2C-BH_2$	402.7	409.7	412.4	416.5	441.3	415.3	405.1	408.0	409.5
59	$H_3CH_2CHC(BH_2)CH_3$	380.0	390.6	392.0	394.9	423.1	394.8	382.8	388.7	387.3
60	$H_3CHC(H_2C)C(BH_2)CH_3$	403.3	411.8	413.6	417.8	443.5	416.8	406.1	411.8	412.1
61	$(H_3C)_2HC-CH(BH_2)CH_3$	381.1	392.3	392.7	396.3	424.3	396.4	384.1	393.3	390.3

62	$\begin{array}{c} \text{CH}_3 \\   \\ \text{C}_2\text{H}_5-\text{C}-\text{BH}_2 \\   \\ \text{CH}_3 \end{array}$	357.3	372.6	370.6	373.2	403.0	374.0	360.3	373.4	369.3
63	$(\text{H}_3\text{C})_3\text{C}-\text{H}_2\text{C}-\text{BH}_2$	402.6	412.9	413.9	418.0	445.3	417.4	405.7	414.2	412.6
64	$\begin{array}{c} (\text{H}_3\text{C})_3\text{C}-\text{HC}-\text{BH}_2 \\   \\ \text{CH}_3 \end{array}$	372.5	386.2	384.7	388.8	417.6	389.0	375.9	389.9	384.6

Entry	compounds	BB1K	BMK	BP86	BP86-D3	M05	M05-2X	M06	M06-2X	M06-HF
1	$\text{CH}_3\text{CH}=\text{CH}-\text{B}(\text{OH})_2$	477.8	488.4	454.3	466.6	469.5	494.0	477.4	475.4	481.6
2	$\text{H}_2\text{C}=\text{CH}-\text{B}(\text{OH})_2$	471.0	481.9	447.8	458.8	463.2	486.9	470.0	468.7	476.3
3	$\begin{array}{c} \text{H}_2\text{C}=\text{C}-\text{B}(\text{OH})_2 \\   \\ \text{CH}_3 \end{array}$	451.5	463.7	424.5	440.7	440.3	473.0	453.5	455.2	470.5
4	$\begin{array}{c} \text{H}_2\text{C}=\text{C}-\text{B}(\text{OH})_2 \\   \\ \text{CH}_2\text{CH}_3 \end{array}$	451.6	464.0	423.3	442.5	440.4	474.6	455.5	456.7	472.5
5	$\begin{array}{c} \text{H}_3\text{CHC}=\text{C}-\text{B}(\text{OH})_2 \\   \\ \text{CH}_3 \end{array}$	446.0	457.9	418.5	438.4	434.4	468.8	448.6	451.0	465.6
6	$\text{C}_2\text{H}_5\text{HC}=\text{CH}-\text{B}(\text{OH})_2$	477.1	487.7	453.4	466.1	468.8	493.4	476.8	474.8	481.1
7	$\begin{array}{c} \text{H}_2\text{C}=\text{CH}-\text{B}-\text{OH} \\   \\ \text{CH}_3 \end{array}$	459.6	471.1	439.0	450.7	451.4	475.1	459.0	460.4	469.9
8	$\begin{array}{c} \text{H}_3\text{CHC}=\text{CH}-\text{B}-\text{OH} \\   \\ \text{CH}_3 \end{array}$	469.1	480.8	447.5	460.2	460.2	485.0	469.2	469.5	477.8
9	$\begin{array}{c} (\text{H}_3\text{C})_2\text{C}=\text{CH}-\text{B}-\text{OH} \\   \\ \text{CH}_3 \end{array}$	465.6	476.6	444.7	459.8	456.3	481.2	467.7	466.2	471.1
10	$\begin{array}{c} \text{CH}_3 \\   \\ \text{H}_2\text{C}=\text{C}-\text{B}-\text{OH} \\   \\ \text{CH}_3 \end{array}$	438.8	452.1	413.6	431.3	426.9	460.4	442.0	445.9	463.4
11	$\begin{array}{c} \text{CH}_3 \\   \\ \text{H}_3\text{CHC}=\text{C}-\text{B}-\text{OH} \\   \\ \text{CH}_3 \end{array}$	440.3	453.3	414.2	434.2	426.9	461.5	444.1	447.0	461.6
12	$\begin{array}{c} \text{CH}_2\text{CH}_3 \\   \\ \text{H}_2\text{C}=\text{C}-\text{B}-\text{OH} \\   \\ \text{CH}_3 \end{array}$	437.3	450.7	410.9	432.0	425.3	460.3	442.8	446.0	463.5
13	$\text{H}_2\text{C}=\text{CH}-\text{B}(\text{CH}_3)_2$	464.3	477.7	444.0	456.8	454.0	481.2	463.4	467.4	480.7
14	$\text{H}_3\text{CHC}=\text{CH}-\text{B}(\text{CH}_3)_2$	473.1	486.4	452.9	467.1	461.9	490.1	472.8	475.8	487.2
15	$(\text{H}_3\text{C})_2\text{C}=\text{CH}-\text{B}(\text{CH}_3)_2$	463.2	475.6	443.2	460.7	451.4	480.7	465.6	467.3	475.2
16	$\begin{array}{c} \text{H}_2\text{C}=\text{C}-\text{B}(\text{CH}_3)_2 \\   \\ \text{CH}_3 \end{array}$	440.5	455.7	416.3	435.7	426.0	463.5	443.5	450.3	470.8
17	$\begin{array}{c} \text{H}_3\text{CHC}=\text{C}-\text{B}(\text{CH}_3)_2 \\   \\ \text{CH}_3 \end{array}$	442.0	456.4	417.4	439.2	425.5	464.3	445.6	451.0	468.7
18	$\begin{array}{c} \text{H}_2\text{C}=\text{C}-\text{B}(\text{CH}_3)_2 \\   \\ \text{C}_2\text{H}_5 \end{array}$	440.1	454.0	413.5	435.7	423.1	463.5	444.6	450.8	469.2
19	$\text{C}_2\text{H}_5\text{HC}=\text{CH}-\text{B}(\text{CH}_3)_2$	456.1	469.7	435.8	453.9	446.5	474.6	458.8	461.7	473.0
20	$\begin{array}{c} \text{H}_2\text{C}=\text{CH}-\text{B}-\text{OH} \\   \\ \text{C}_2\text{H}_5 \end{array}$	463.5	475.3	440.9	454.6	453.7	479.9	464.6	464.8	474.0

21	$\text{H}_2\text{C}=\overset{\text{CH}_3}{\underset{\text{CH}(\text{CH}_3)_2}{\text{C}}}-\text{B}(\text{OH})_2$	470.2	482.0	444.3	459.0	461.5	488.4	471.5	469.8	477.0
22	$\text{H}_2\text{C}=\overset{\text{CH}_3}{\underset{\text{C}_2\text{H}_5}{\text{C}}}-\text{B}(\text{OH})_2$	444.4	457.9	417.9	437.8	429.9	466.8	448.9	452.2	468.9
23	$\text{H}_3\text{C}-\text{CH}=\overset{\text{CH}_3}{\underset{\text{C}_2\text{H}_5}{\text{C}}}-\text{B}(\text{OH})_2$	471.0	482.8	448.2	463.2	460.5	487.6	472.7	472.0	479.3
24	$\text{H}_2\text{C}=\text{CH}-\text{B}(\text{C}_2\text{H}_5)_2$	462.4	476.4	440.1	454.7	451.9	481.7	464.6	467.8	484.4
25	$\text{H}_3\text{C}-\text{B}(\text{OH})_2$	437.2	444.8	416.4	424.9	432.7	448.1	439.3	434.3	431.5
26	$\text{C}_2\text{H}_5-\text{B}(\text{OH})_2$	415.7	425.6	390.8	404.2	408.4	430.8	419.0	417.6	424.4
27	$(\text{H}_3\text{C})_2\text{HC}-\text{B}(\text{OH})_2$	396.2	408.5	368.0	387.0	385.0	416.9	399.8	403.1	420.1
28	$(\text{H}_3\text{C})_3\text{C}-\text{B}(\text{OH})_2$	381.1	396.4	349.4	374.3	366.5	409.0	387.8	393.8	420.4
29	$\text{C}_3\text{H}_7-\text{B}(\text{OH})_2$	420.0	429.4	394.3	408.8	412.5	435.0	424.9	421.4	425.6
30	$\text{C}_4\text{H}_9-\text{B}(\text{OH})_2$	419.5	428.5	393.6	408.3	411.9	434.3	424.2	420.8	424.9
31	$\text{C}_2\text{H}_5\text{HC}-\overset{\text{CH}_3}{\text{B}(\text{OH})_2}$	394.6	407.2	366.5	386.3	384.2	415.3	400.1	401.6	417.1
32	$(\text{H}_3\text{C})_2\text{CHCH}_2-\text{B}(\text{OH})_2$	418.3	427.8	392.0	409.1	410.7	434.8	424.3	421.1	426.8
33	$\text{H}_3\text{C}-\text{B}(\text{CH}_3)_2$	425.1	435.2	407.9	418.0	419.9	436.8	427.8	428.1	428.6
34	$\text{C}_2\text{H}_5-\text{B}(\text{C}_2\text{H}_5)_2$	400.1	414.5	377.0	395.3	392.3	419.8	408.0	411.3	427.5
35	$\text{HC}\equiv\text{C}-\text{BF}_2$	614.8	625.4	590.5	594.2	606.6	631.8	602.3	598.6	603.1
36	$\text{HC}\equiv\text{C}-\text{BCl}_2$	601.1	612.4	580.6	586.9	585.2	612.5	589.2	588.2	601.5
37	$\text{C}_2\text{H}_5-\overset{\text{CH}_3}{\text{B}(\text{OH})_2}$	404.9	415.6	382.7	396.8	397.1	419.2	408.9	409.8	417.2
38	$(\text{H}_3\text{C})_2\text{HC}-\overset{\text{CH}_3}{\text{B}(\text{OH})_2}$	382.0	396.1	356.9	376.6	371.9	402.9	387.9	392.8	411.8
39	$(\text{H}_3\text{C})_3\text{C}-\overset{\text{CH}_3}{\text{B}(\text{OH})_2}$	367.0	383.4	337.5	364.4	352.5	395.4	377.2	384.3	412.1
40	$(\text{H}_3\text{C})_2\text{HC}-\overset{\text{C}_2\text{H}_5}{\text{B}(\text{OH})_2}$	384.0	397.8	356.7	379.5	370.8	405.3	391.4	395.4	411.9
41	$\text{C}_3\text{H}_7-\overset{\text{C}_2\text{H}_5}{\text{B}(\text{OH})_2}$	409.8	420.1	385.4	402.9	399.8	424.7	416.8	414.8	418.6
42	$\text{H}_3\text{C}-\text{BH}_2$	440.3	449.3	429.9	433.4	440.9	448.3	443.8	438.8	431.0
43	$\text{C}_2\text{H}_5-\text{BH}_2$	420.4	431.3	407.4	414.3	418.4	431.4	423.7	422.3	422.7
44	$(\text{H}_3\text{C})_2\text{HC}-\text{BH}_2$	400.6	414.4	384.9	395.6	394.6	416.2	404.2	406.6	416.9
45	$(\text{H}_3\text{C})_3\text{C}-\text{BH}_2$	383.8	401.6	365.7	381.2	375.8	407.8	390.9	396.2	418.2
46	$\text{H}_3\text{C}-\text{BH}-\text{OH}$	440.3	448.2	423.9	429.0	438.9	449.1	441.6	436.4	432.0
47	$\text{H}_3\text{CH}_2\text{C}-\text{BH}-\text{OH}$	416.5	426.9	397.1	405.9	412.7	428.8	417.4	416.5	421.8
48	$(\text{H}_3\text{C})_2\text{HC}-\text{BH}-\text{OH}$	396.5	409.9	374.8	387.9	390.2	414.5	397.9	401.4	417.4
49	$(\text{H}_3\text{C})_3\text{C}-\text{BH}-\text{OH}$	383.3	399.5	357.6	376.4	373.4	408.5	388.7	394.2	419.4
50	$\text{H}_2\text{C}=\text{CH}-\text{BH}_2$	484.5	497.1	472.0	477.2	479.7	497.6	483.3	482.1	487.8
51	$\text{H}_2\text{C}=\overset{\text{CH}_3}{\text{C}}-\text{BH}_2$	463.2	477.6	448.8	457.6	455.6	480.8	464.0	465.7	478.6
52	$\text{H}_3\text{C}-\text{CH}=\text{CH}-\text{BH}_2$	497.2	509.6	485.4	491.7	491.5	509.7	496.5	493.9	496.1

53	$(\text{H}_3\text{C})_2\text{C}=\text{CH}-\text{BH}_2$	497.8	509.0	486.5	494.1	490.8	509.1	498.7	493.7	491.1
54	$\text{H}_3\text{CHC}=\underset{\text{CH}_3}{\text{C}}-\text{BH}_2$	463.9	478.3	450.4	461.2	455.3	481.0	466.7	466.2	474.0
55	$\text{H}_3\text{CH}_2\text{CH}_2\text{C}-\text{BH}_2$	424.6	435.3	410.9	418.8	422.5	435.6	429.7	426.2	423.9
56	$\text{H}_3\text{C}(\text{H}_2\text{C})_2\text{H}_2\text{C}-\text{BH}_2$	424.2	434.6	410.3	418.3	422.1	435.1	429.2	425.7	423.2
57	$\text{H}_3\text{C}(\text{H}_2\text{C})_3\text{H}_2\text{C}-\text{BH}_2$	422.0	433.4	408.7	416.7	420.2	433.5	426.5	424.2	423.8
58	$\text{H}_3\text{C}(\text{H}_2\text{C})_4\text{H}_2\text{C}-\text{BH}_2$	422.0	433.3	408.7	416.7	420.2	433.5	426.5	424.2	423.5
59	$\text{H}_3\text{CH}_2\text{CHC}-\underset{\text{CH}_3}{\text{BH}_2}$	402.2	415.4	385.4	397.4	395.2	417.7	407.0	408.0	415.3
60	$\text{H}_3\text{CHC}-\underset{\text{CH}_3}{\text{H}_2\text{C}}-\text{BH}_2$	423.7	435.1	409.7	419.5	421.5	436.3	430.5	426.7	425.6
61	$(\text{H}_3\text{C})_2\text{HC}-\underset{\text{CH}_3}{\text{HC}}-\text{BH}_2$	403.4	417.1	387.2	399.9	397.3	421.7	409.6	410.8	421.7
62	$\text{C}_2\text{H}_5-\underset{\text{CH}_3}{\overset{\text{CH}_3}{\text{C}}}-\text{BH}_2$	381.7	399.0	362.7	380.3	373.0	406.2	390.8	394.6	415.5
63	$(\text{H}_3\text{C})_3\text{C}-\text{H}_2\text{C}-\text{BH}_2$	425.1	435.7	409.4	421.2	421.2	437.6	433.3	427.7	423.7
64	$(\text{H}_3\text{C})_3\text{C}-\underset{\text{CH}_3}{\text{HC}}-\text{BH}_2$	397.3	411.0	379.3	394.9	389.1	415.4	404.8	404.8	413.3

Entry	compounds	M06-L	MPW1B95	MPW1K	MPW1KCIS	M11	M11-L	N12	N12-SX	MN12-L
1	$\text{CH}_3\text{CH}=\text{CH}-\text{B}(\text{OH})_2$	468.6	479.0	464.7	460.2	470.2	461.6	469.3	481.7	482.3
2	$\text{H}_2\text{C}=\text{CH}-\text{B}(\text{OH})_2$	460.9	472.1	458.1	453.6	463.5	453.2	462.7	474.6	474.2
3	$\text{H}_2\text{C}=\underset{\text{CH}_3}{\text{C}}-\text{B}(\text{OH})_2$	440.3	452.3	438.6	430.4	446.9	430.7	438.8	453.5	454.0
4	$\text{H}_2\text{C}=\underset{\text{CH}_2\text{CH}_3}{\text{C}}-\text{B}(\text{OH})_2$	441.5	452.5	438.2	429.4	448.8	431.2	437.2	453.4	455.7
5	$\text{H}_3\text{CHC}=\underset{\text{CH}_3}{\text{C}}-\text{B}(\text{OH})_2$	435.9	447.2	432.4	424.3	443.1	425.5	432.3	448.1	449.1
6	$\text{C}_2\text{H}_5\text{HC}=\text{CH}-\text{B}(\text{OH})_2$	467.8	478.3	464.1	459.5	469.6	460.5	468.6	481.1	481.4
7	$\text{H}_2\text{C}=\text{CH}-\underset{\text{CH}_3}{\overset{\text{B}-\text{OH}}{\text{C}}}$	449.8	461.4	446.8	444.4	453.4	441.9	453.5	463.6	464.3
8	$\text{H}_3\text{CHC}=\text{CH}-\underset{\text{CH}_3}{\overset{\text{B}-\text{OH}}{\text{C}}}$	459.6	470.9	456.3	453.3	462.9	451.9	462.4	473.7	474.9
9	$(\text{H}_3\text{C})_2\text{C}=\text{CH}-\underset{\text{CH}_3}{\overset{\text{B}-\text{OH}}{\text{C}}}$	458.5	468.1	452.3	449.8	460.6	451.1	459.7	470.6	473.9
10	$\text{H}_2\text{C}=\underset{\text{CH}_3}{\overset{\text{CH}_3}{\text{C}}}-\underset{\text{CH}_3}{\overset{\text{B}-\text{OH}}{\text{C}}}$	428.0	440.3	425.8	419.2	436.3	417.9	427.1	441.2	443.5
11	$\text{H}_3\text{CHC}=\underset{\text{CH}_3}{\overset{\text{CH}_3}{\text{C}}}-\underset{\text{CH}_3}{\overset{\text{B}-\text{OH}}{\text{C}}}$	432.3	442.1	426.2	419.3	438.7	419.4	427.8	443.0	447.4

12	$\begin{array}{c} \text{CH}_2\text{CH}_3 \\   \\ \text{H}_2\text{C}=\text{C}-\text{B}-\text{OH} \\   \\ \text{CH}_3 \end{array}$	427.8	439.0	423.5	416.4	436.6	417.3	424.2	439.4	444.1
13	$\text{H}_2\text{C}=\text{CH}-\text{B}(\text{CH}_3)_2$	451.5	466.6	451.2	448.9	460.1	444.8	458.9	468.6	468.7
14	$\text{H}_3\text{CCH}=\text{CH}-\text{B}(\text{CH}_3)_2$	461.3	475.7	459.7	457.7	468.4	455.2	467.7	477.7	479.2
15	$(\text{H}_3\text{C})_2\text{C}=\text{CH}-\text{B}(\text{CH}_3)_2$	454.5	466.5	448.7	447.4	461.0	449.2	457.7	467.5	473.0
16	$\begin{array}{c} \text{H}_2\text{C}=\text{C}-\text{B}(\text{CH}_3)_2 \\   \\ \text{CH}_3 \end{array}$	427.5	442.7	426.8	420.8	440.1	418.6	429.4	442.8	445.7
17	$\begin{array}{c} \text{H}_3\text{CCH}=\text{C}-\text{B}(\text{CH}_3)_2 \\   \\ \text{CH}_3 \end{array}$	432.0	444.6	427.1	421.1	442.0	420.1	430.4	444.3	449.6
18	$\begin{array}{c} \text{H}_2\text{C}=\text{C}-\text{B}(\text{CH}_3)_2 \\   \\ \text{C}_2\text{H}_5 \end{array}$	429.9	442.3	424.8	417.7	442.3	418.7	426.6	441.4	448.6
19	$\text{C}_2\text{H}_5\text{HC}=\text{CH}-\text{B}(\text{CH}_3)_2$	447.8	459.1	442.3	440.5	454.4	439.3	450.2	461.1	463.6
20	$\begin{array}{c} \text{H}_2\text{C}=\text{CH}-\text{B}-\text{OH} \\   \\ \text{C}_2\text{H}_5 \end{array}$	455.5	465.3	450.2	446.3	459.4	444.1	455.3	467.4	470.0
21	$\begin{array}{c} \text{H}_2\text{C}=\text{CH}-\text{B}-\text{OH} \\   \\ \text{CH}(\text{CH}_3)_2 \end{array}$	462.0	471.6	456.2	450.5	469.2	449.8	459.9	474.4	476.1
22	$\begin{array}{c} \text{CH}_3 \\   \\ \text{H}_2\text{C}=\text{C}-\text{B}-\text{OH} \\   \\ \text{C}_2\text{H}_5 \end{array}$	436.4	446.0	430.4	422.8	443.4	422.6	430.5	446.0	451.8
23	$\begin{array}{c} \text{H}_3\text{CCH}=\text{CH}-\text{B}-\text{OH} \\   \\ \text{C}_2\text{H}_5 \end{array}$	464.1	472.9	457.4	453.6	466.6	453.3	462.4	475.3	478.9
24	$\text{H}_2\text{C}=\text{CH}-\text{B}(\text{C}_2\text{H}_5)_2$	450.3	464.5	448.9	445.2	460.8	443.0	456.4	466.0	466.7
25	$\text{H}_3\text{C}-\text{B}(\text{OH})_2$	433.0	439.5	421.2	423.5	433.2	431.6	430.3	441.3	446.0
26	$\text{C}_2\text{H}_5-\text{B}(\text{OH})_2$	408.5	417.2	400.8	398.3	414.1	404.7	406.0	418.4	422.2
27	$(\text{H}_3\text{C})_2\text{HC}-\text{B}(\text{OH})_2$	385.2	397.3	381.2	374.8	397.1	379.8	382.8	396.9	400.7
28	$(\text{H}_3\text{C})_3\text{C}-\text{B}(\text{OH})_2$	367.8	382.0	365.6	355.4	386.1	361.1	362.6	379.8	385.9
29	$\text{C}_3\text{H}_7-\text{B}(\text{OH})_2$	413.7	421.4	405.0	402.2	418.7	410.8	409.5	422.6	427.5
30	$\text{C}_4\text{H}_9-\text{B}(\text{OH})_2$	412.9	420.9	404.6	401.7	418.2	410.5	409.2	422.1	427.0
31	$\begin{array}{c} \text{C}_2\text{H}_5\text{HC}-\text{B}(\text{OH})_2 \\   \\ \text{CH}_3 \end{array}$	384.9	395.8	379.8	373.5	395.9	379.0	381.5	395.6	399.5
32	$(\text{H}_3\text{C})_2\text{CHCH}_2-\text{B}(\text{OH})_2$	412.6	420.0	402.7	399.5	418.6	408.9	407.5	420.9	427.4
33	$\text{H}_3\text{C}-\text{B}(\text{CH}_3)_2$	420.0	428.7	409.2	414.4	425.2	419.6	422.2	430.8	435.4
34	$\text{C}_2\text{H}_5-\text{B}(\text{C}_2\text{H}_5)_2$	392.1	402.8	384.9	383.8	405.3	388.5	393.3	403.6	407.4
35	$\text{HC}\equiv\text{C}-\text{BF}_2$	642.4	615.3	602.6	597.6	603.1	585.2	610.5	621.1	613.9
36	$\text{HC}\equiv\text{C}-\text{BCl}_2$	628.2	602.6	589.4	586.4	587.8	567.0	599.0	605.9	604.9
37	$\begin{array}{c} \text{C}_2\text{H}_5-\text{B}-\text{OH} \\   \\ \text{CH}_3 \end{array}$	398.6	407.2	390.1	389.7	404.2	394.7	397.5	408.2	413.8
38	$\begin{array}{c} (\text{H}_3\text{C})_2\text{HC}-\text{B}-\text{OH} \\   \\ \text{CH}_3 \end{array}$	372.5	383.9	367.5	363.3	384.1	365.9	371.5	383.7	388.0
39	$\begin{array}{c} (\text{H}_3\text{C})_3\text{C}-\text{B}-\text{OH} \\   \\ \text{CH}_3 \end{array}$	356.5	368.8	351.3	343.0	374.8	348.7	350.4	365.9	376.1
40	$\begin{array}{c} (\text{H}_3\text{C})_2\text{HC}-\text{B}-\text{OH} \\   \\ \text{C}_2\text{H}_5 \end{array}$	378.0	386.1	368.1	362.5	388.7	368.3	370.1	384.7	394.2
41	$\begin{array}{c} \text{C}_3\text{H}_7-\text{B}-\text{OH} \\   \\ \text{C}_2\text{H}_5 \end{array}$	407.2	412.2	394.0	392.3	411.4	400.2	399.4	412.6	421.9
42	$\text{H}_3\text{C}-\text{BH}_2$	438.3	445.4	423.6	435.6	440.5	440.6	444.1	448.1	457.6
43	$\text{C}_2\text{H}_5-\text{BH}_2$	414.3	424.7	404.9	413.3	421.0	416.3	422.4	426.8	434.3



44	$(\text{H}_3\text{C})_2\text{HC}-\text{BH}_2$	390.7	404.4	385.4	390.2	402.6	391.2	399.1	404.9	412.1
45	$(\text{H}_3\text{C})_3\text{C}-\text{BH}_2$	370.8	387.4	368.4	369.8	389.8	369.0	378.6	386.7	393.6
46	$\text{H}_3\text{C}-\text{BH}-\text{OH}$	435.8	443.8	424.3	430.5	437.4	436.0	439.3	446.3	452.7
47	$\text{H}_3\text{CH}_2\text{C}-\text{BH}-\text{OH}$	407.8	419.1	401.8	403.8	414.4	406.5	413.3	421.2	424.9
48	$(\text{H}_3\text{C})_2\text{HC}-\text{BH}-\text{OH}$	383.7	398.7	382.3	380.9	396.1	380.9	390.9	399.7	401.5
49	$(\text{H}_3\text{C})_3\text{C}-\text{BH}-\text{OH}$	368.8	385.2	368.5	363.3	387.6	364.3	372.1	384.4	389.4
50	$\text{H}_2\text{C}=\text{CH}-\text{BH}_2$	472.9	488.3	470.9	476.0	478.2	469.7	486.7	490.7	494.4
51	$\begin{array}{c} \text{H}_2\text{C}=\text{C}-\text{BH}_2 \\   \\ \text{CH}_3 \end{array}$	450.2	466.7	450.0	452.7	457.8	445.4	462.1	468.2	470.6
52	$\text{H}_3\text{CHC}=\text{CH}-\text{BH}_2$	487.2	501.5	483.2	489.4	489.8	484.3	499.8	503.7	509.0
53	$(\text{H}_3\text{C})_2\text{C}=\text{CH}-\text{BH}_2$	490.9	502.6	482.9	489.9	491.1	487.7	500.7	504.0	512.6
54	$\begin{array}{c} \text{H}_3\text{CHC}=\text{C}-\text{BH}_2 \\   \\ \text{CH}_3 \end{array}$	455.1	468.1	449.7	453.4	459.0	448.6	462.7	469.4	475.0
55	$\text{H}_3\text{CH}_2\text{CH}_2\text{C}-\text{BH}_2$	419.8	428.9	409.2	417.3	425.8	422.3	426.0	431.1	439.5
56	$\text{H}_3\text{C}(\text{H}_2\text{C})_2\text{H}_2\text{C}-\text{BH}_2$	419.1	428.4	408.8	416.8	425.3	421.9	425.6	430.7	439.1
57	$\text{H}_3\text{C}(\text{H}_2\text{C})_3\text{H}_2\text{C}-\text{BH}_2$	416.7	426.3	406.6	414.7	423.1	418.7	423.7	428.7	436.4
58	$\text{H}_3\text{C}(\text{H}_2\text{C})_4\text{H}_2\text{C}-\text{BH}_2$	416.8	426.3	406.6	414.7	423.0	418.6	423.8	428.6	436.5
59	$\begin{array}{c} \text{H}_3\text{CH}_2\text{CHC}-\text{BH}_2 \\   \\ \text{CH}_3 \end{array}$	393.4	406.1	386.4	390.9	405.5	394.2	399.6	406.1	415.7
60	$\begin{array}{c} \text{H}_3\text{CHC}-\text{H}_2\text{C}-\text{BH}_2 \\   \\ \text{CH}_3 \end{array}$	419.9	428.2	407.9	415.6	426.4	421.3	424.6	430.2	440.1
61	$\begin{array}{c} (\text{H}_3\text{C})_2\text{HC}-\text{HC}-\text{BH}_2 \\   \\ \text{CH}_3 \end{array}$	394.2	407.5	387.7	392.0	407.8	394.6	402.2	407.7	416.4
62	$\begin{array}{c} \text{CH}_3 \\   \\ \text{C}_2\text{H}_5-\text{C}-\text{BH}_2 \\   \\ \text{CH}_3 \end{array}$	370.8	385.3	365.6	366.6	389.8	367.0	375.6	384.5	393.7
63	$(\text{H}_3\text{C})_3\text{C}-\text{H}_2\text{C}-\text{BH}_2$	422.9	429.6	408.1	415.3	430.1	423.9	424.7	430.6	444.6
64	$\begin{array}{c} (\text{H}_3\text{C})_3\text{C}-\text{HC}-\text{BH}_2 \\   \\ \text{CH}_3 \end{array}$	390.9	401.5	379.9	383.5	404.8	388.0	393.8	400.8	413.8

Entry	compounds	MN12-SX	PBE1PBE	SOGGA11	SOGGA11-X	TPSS	wB97	wB97XD
1	$\text{CH}_3\text{CH}=\text{CH}-\text{B}(\text{OH})_2$	485.2	466.1	460.2	489.4	446.1	490.6	479.1
2	$\text{H}_2\text{C}=\text{CH}-\text{B}(\text{OH})_2$	477.6	459.3	454.2	483.1	440.0	483.5	471.5
3	$\begin{array}{c} \text{H}_2\text{C}=\text{C}-\text{B}(\text{OH})_2 \\   \\ \text{CH}_3 \end{array}$	461.0	439.0	427.5	463.0	417.7	467.9	455.0

4	$\text{H}_2\text{C}=\underset{\text{CH}_2\text{CH}_3}{\text{C}}-\text{B}(\text{OH})_2$	461.8	438.7	427.0	462.5	416.6	469.2	456.8
5	$\text{H}_3\text{CHC}=\underset{\text{CH}_3}{\text{C}}-\text{B}(\text{OH})_2$	455.7	433.5	419.0	456.8	411.2	464.3	452.1
6	$\text{C}_2\text{H}_5\text{HC}=\text{CH}-\text{B}(\text{OH})_2$	484.3	465.5	459.4	488.7	445.4	490.1	479.0
7	$\text{H}_2\text{C}=\underset{\text{CH}_3}{\text{CH}}-\overset{\text{B}-\text{OH}}{\text{B}}$	466.6	449.4	447.6	471.5	430.2	472.7	462.7
8	$\text{H}_3\text{CHC}=\underset{\text{CH}_3}{\text{CH}}-\overset{\text{B}-\text{OH}}{\text{B}}$	476.8	458.7	456.3	480.6	438.4	482.2	472.4
9	$(\text{H}_3\text{C})_2\text{C}=\underset{\text{CH}_3}{\text{CH}}-\overset{\text{B}-\text{OH}}{\text{B}}$	474.0	455.8	448.2	477.8	434.7	480.2	470.6
10	$\text{H}_2\text{C}=\underset{\text{CH}_3}{\overset{\text{CH}_3}{\text{C}}}-\overset{\text{B}-\text{OH}}{\text{B}}$	449.2	427.5	420.1	450.2	406.0	456.2	445.5
11	$\text{H}_3\text{CHC}=\underset{\text{CH}_3}{\overset{\text{CH}_3}{\text{C}}}-\overset{\text{B}-\text{OH}}{\text{B}}$	450.8	428.5	416.1	450.9	406.2	458.1	447.8
12	$\text{H}_2\text{C}=\underset{\text{CH}_3}{\overset{\text{CH}_2\text{CH}_3}{\text{C}}}-\overset{\text{B}-\text{OH}}{\text{B}}$	448.7	425.5	417.3	448.2	403.4	456.3	446.7
13	$\text{H}_2\text{C}=\text{CH}-\text{B}(\text{CH}_3)_2$	470.8	454.4	452.6	477.4	435.3	478.7	469.5
14	$\text{H}_3\text{CHC}=\text{CH}-\text{B}(\text{CH}_3)_2$	480.4	463.3	461.9	485.5	443.6	487.3	479.2
15	$(\text{H}_3\text{C})_2\text{C}=\text{CH}-\text{B}(\text{CH}_3)_2$	472.4	453.5	449.0	475.4	433.0	479.1	471.9
16	$\text{H}_2\text{C}=\underset{\text{CH}_3}{\text{C}}-\text{B}(\text{CH}_3)_2$	450.5	429.5	421.5	452.9	408.6	459.5	449.9
17	$\text{H}_3\text{CHC}=\underset{\text{CH}_3}{\text{C}}-\text{B}(\text{CH}_3)_2$	451.9	430.6	418.2	453.3	409.2	461.1	452.4
18	$\text{H}_2\text{C}=\underset{\text{C}_2\text{H}_5}{\text{C}}-\text{B}(\text{CH}_3)_2$	450.7	427.8	414.9	450.9	405.4	460.0	450.4
19	$\text{C}_2\text{H}_5\text{HC}=\text{CH}-\text{B}(\text{CH}_3)_2$	465.1	446.5	445.1	469.0	426.8	472.8	465.9
20	$\text{H}_2\text{C}=\underset{\text{C}_2\text{H}_5}{\text{CH}}-\overset{\text{B}-\text{OH}}{\text{B}}$	470.5	452.6	447.3	474.5	432.6	476.9	467.0
21	$\text{H}_2\text{C}=\underset{\text{CH}(\text{CH}_3)_2}{\text{CH}}-\overset{\text{B}-\text{OH}}{\text{B}}$	476.1	458.0	451.9	482.0	437.3	487.6	475.5
22	$\text{H}_2\text{C}=\underset{\text{C}_2\text{H}_5}{\overset{\text{CH}_3}{\text{C}}}-\overset{\text{B}-\text{OH}}{\text{B}}$	454.8	432.4	419.4	454.6	410.7	461.9	451.6
23	$\text{H}_3\text{CHC}=\underset{\text{C}_2\text{H}_5}{\text{CH}}-\overset{\text{B}-\text{OH}}{\text{B}}$	478.8	460.2	454.5	481.4	439.4	484.4	475.1
24	$\text{H}_2\text{C}=\text{CH}-\text{B}(\text{C}_2\text{H}_5)_2$	469.4	451.6	451.7	474.5	432.2	477.1	469.4
25	$\text{H}_3\text{C}-\text{B}(\text{OH})_2$	445.9	425.0	427.3	447.5	403.6	449.8	436.9
26	$\text{C}_2\text{H}_5-\text{B}(\text{OH})_2$	424.9	403.0	400.2	426.0	380.9	430.6	418.0
27	$(\text{H}_3\text{C})_2\text{HC}-\text{B}(\text{OH})_2$	405.4	382.7	376.9	405.5	360.1	413.0	401.0
28	$(\text{H}_3\text{C})_3\text{C}-\text{B}(\text{OH})_2$	392.3	366.5	355.7	389.5	342.7	401.0	387.9
29	$\text{C}_3\text{H}_7-\text{B}(\text{OH})_2$	429.7	407.3	403.8	430.0	383.6	435.6	423.0
30	$\text{C}_4\text{H}_9-\text{B}(\text{OH})_2$	429.2	406.8	403.7	429.3	383.0	435.0	422.9
31	$\text{C}_2\text{H}_5\text{HC}-\underset{\text{CH}_3}{\text{B}(\text{OH})_2}$	404.4	381.4	374.2	404.4	358.2	412.5	400.8
32	$(\text{H}_3\text{C})_2\text{CHCH}_2-\text{B}(\text{OH})_2$	428.5	405.2	402.6	427.6	382.1	434.7	423.5
33	$\text{H}_3\text{C}-\text{B}(\text{CH}_3)_2$	434.3	415.0	424.5	435.8	394.0	440.0	429.8
34	$\text{C}_2\text{H}_5-\text{B}(\text{C}_2\text{H}_5)_2$	410.5	388.9	397.5	409.8	367.1	417.8	410.8

35	$\text{HC}\equiv\text{C}-\text{BF}_2$	618.7	602.8	604.6	629.3	583.1	625.1	611.5
36	$\text{HC}\equiv\text{C}-\text{BCl}_2$	604.8	591.5	591.1	613.5	571.5	610.1	597.1
37	$\text{C}_2\text{H}_5-\overset{\text{OH}}{\underset{\text{CH}_3}{\text{B}}}$	414.9	393.7	395.1	415.0	371.8	420.3	409.8
38	$(\text{H}_3\text{C})_2\text{HC}-\overset{\text{OH}}{\underset{\text{CH}_3}{\text{B}}}$	392.3	370.3	370.3	391.8	348.4	400.2	390.5
39	$(\text{H}_3\text{C})_3\text{C}-\overset{\text{OH}}{\underset{\text{CH}_3}{\text{B}}}$	380.5	353.7	347.4	375.6	330.0	389.3	378.8
40	$(\text{H}_3\text{C})_2\text{HC}-\overset{\text{OH}}{\underset{\text{C}_2\text{H}_5}{\text{B}}}$	395.0	371.2	366.2	392.3	348.6	402.7	393.3
41	$\text{C}_3\text{H}_7-\overset{\text{OH}}{\underset{\text{C}_2\text{H}_5}{\text{B}}}$	420.2	397.9	395.6	418.3	374.3	426.3	416.4
42	$\text{H}_3\text{C}-\text{BH}_2$	448.1	432.0	448.8	451.2	412.6	451.9	439.9
43	$\text{C}_2\text{H}_5-\text{BH}_2$	428.0	412.1	426.4	431.6	392.0	433.9	422.4
44	$(\text{H}_3\text{C})_2\text{HC}-\text{BH}_2$	408.2	391.8	403.4	411.4	371.4	415.9	404.2
45	$(\text{H}_3\text{C})_3\text{C}-\text{BH}_2$	392.4	374.4	384.9	393.9	353.6	402.1	389.6
46	$\text{H}_3\text{C}-\text{BH}-\text{OH}$	447.2	430.0	439.9	451.6	410.3	453.6	439.9
47	$\text{H}_3\text{CH}_2\text{C}-\text{BH}-\text{OH}$	423.0	406.0	412.8	428.1	386.1	431.5	418.4
48	$(\text{H}_3\text{C})_2\text{HC}-\text{BH}-\text{OH}$	402.7	385.8	391.9	408.0	365.8	413.8	401.1
49	$(\text{H}_3\text{C})_3\text{C}-\text{BH}-\text{OH}$	391.9	371.4	371.8	393.8	349.6	404.1	389.8
50	$\text{H}_2\text{C}=\text{CH}-\text{BH}_2$	488.7	476.7	485.8	497.9	460.0	493.8	483.8
51	$\text{H}_2\text{C}=\overset{\text{BH}_2}{\underset{\text{CH}_3}{\text{C}}}$	469.5	455.3	462.1	476.5	437.2	476.0	465.6
52	$\text{H}_3\text{CCH}=\text{CH}-\text{BH}_2$	501.7	489.8	500.3	509.7	472.2	505.9	497.0
53	$(\text{H}_3\text{C})_2\text{C}=\text{CH}-\text{BH}_2$	502.7	490.5	497.3	509.7	472.2	506.5	498.1
54	$\text{H}_3\text{CCH}=\overset{\text{BH}_2}{\underset{\text{CH}_3}{\text{C}}}$	471.1	456.3	460.1	476.4	437.9	477.0	467.2
55	$\text{H}_3\text{CH}_2\text{CH}_2\text{C}-\text{BH}_2$	432.8	416.4	431.2	435.7	394.7	439.0	427.5
56	$\text{H}_3\text{C}(\text{H}_2\text{C})_2\text{H}_2\text{C}-\text{BH}_2$	432.4	416.0	431.1	435.2	394.1	438.7	427.3
57	$\text{H}_3\text{C}(\text{H}_2\text{C})_3\text{H}_2\text{C}-\text{BH}_2$	429.9	413.8	429.4	433.1	393.2	436.1	425.1
58	$\text{H}_3\text{C}(\text{H}_2\text{C})_4\text{H}_2\text{C}-\text{BH}_2$	429.9	413.8	429.5	433.1	393.1	436.2	425.3
59	$\text{H}_3\text{CH}_2\text{CHC}-\overset{\text{BH}_2}{\underset{\text{CH}_3}{\text{C}}}$	410.3	393.0	402.7	412.5	371.2	418.2	406.4
60	$\text{H}_3\text{CHC}-\overset{\text{H}_2\text{C}-\text{BH}_2}{\underset{\text{CH}_3}{\text{C}}}$	432.4	415.3	431.4	434.3	393.9	439.0	428.2
61	$(\text{H}_3\text{C})_2\text{HC}-\overset{\text{HC}-\text{BH}_2}{\underset{\text{CH}_3}{\text{C}}}$	411.3	394.5	408.3	413.2	373.3	419.5	408.5
62	$\text{C}_2\text{H}_5-\overset{\text{CH}_3}{\underset{\text{CH}_3}{\text{C}}}-\text{BH}_2$	390.9	371.7	380.3	391.1	350.4	401.1	389.4
63	$(\text{H}_3\text{C})_3\text{C}-\text{H}_2\text{C}-\text{BH}_2$	434.1	415.8	428.0	434.8	393.1	441.0	430.6
64	$(\text{H}_3\text{C})_3\text{C}-\overset{\text{HC}-\text{BH}_2}{\underset{\text{CH}_3}{\text{C}}}$	405.5	387.0	395.3	406.0	365.9	413.8	403.4

**Table S3** The Cartesian coordinates and absolute energy values (hartrees) of selected molecules and radicals

<b>Molecules:</b>							
$\begin{array}{c} \text{H}_2\text{C}=\text{C}-\text{B}(\text{OH})_2 \\   \\ \text{CH}_3 \end{array}$				$\begin{array}{c} \text{H}_2\text{C}=\text{C}-\text{B}(\text{OH})_2 \\   \\ \text{C}_2\text{H}_5 \end{array}$			
SCF energy=-293.9569145				SCF energy=-333.2715555			
C	0.78031200	0.15783800	0.00105200	C	-0.22711600	0.65296300	-0.22328800
C	1.33128500	1.38290600	0.05708100	C	-0.11905600	1.99213300	-0.15768600
H	2.41007800	1.53646200	0.06364700	H	0.82805100	2.50141300	0.02263000
H	0.73943100	2.29731500	0.10795700	H	-0.97393800	2.65202000	-0.30580400
C	1.64905200	-1.08028000	-0.05213700	C	-1.56734200	-0.00273300	-0.49982300
H	2.71628700	-0.83006500	-0.04115900	H	-2.29349800	0.75836700	-0.81572100
H	1.43855000	-1.74215800	0.79712100	H	-1.45621000	-0.70717500	-1.33461700
H	1.44083300	-1.66865500	-0.95479800	C	-2.12668700	-0.76688000	0.71445200
B	-0.78284400	-0.03840600	0.00146500	H	-2.28093600	-0.09317300	1.56612500
O	-1.27082100	-1.31729500	0.06216500	H	-3.09049000	-1.22927800	0.46909800
H	-2.24088900	-1.33624500	0.05653300	H	-1.44473400	-1.56480600	1.02977200
O	-1.70776400	0.98059700	-0.05610600	B	1.04376700	-0.26295500	-0.05146800
H	-1.32528400	1.86618000	-0.12108000	O	0.99008400	-1.54960400	-0.52003500
C <sub>2</sub> H <sub>5</sub> HC=CH-B(OH) <sub>2</sub> SCF energy=-333.2710475				$\begin{array}{c} \text{CH}_3 \\   \\ \text{H}_3\text{C}-\text{C}=\text{C}-\text{B}-\text{OH} \\   \\ \text{CH}_3 \end{array}$			
C	0.26840200	-0.58669600	-0.11574800	SCF energy=-297.2945035			
H	0.14416400	-1.66912000	-0.03544600	C	-0.29677900	0.26104300	0.00003600
C	-0.83632500	0.14781700	-0.33551000	C	-1.31847800	-0.62583500	0.00008200
H	-0.75304700	1.23807400	-0.41875500	H	-1.04919000	-1.68261800	0.00018800
C	-2.24090600	-0.37167600	-0.47508800	C	-2.79936800	-0.37233300	0.00003200
H	-2.61552600	-0.12227400	-1.47985800	H	-3.06692300	0.68764600	0.00012600
H	-2.23587600	-1.46639700	-0.40204800	H	-3.26608600	-0.83938600	-0.87907500
C	-3.20227800	0.22306100	0.57037100	H	-3.26622900	-0.83961500	0.87893800
H	-3.23330400	1.31801600	0.50482700	C	-0.49707200	1.76497000	-0.00009700
H	-4.22196900	-0.14924000	0.41759700	H	-1.54897000	2.06570600	0.00052700
H	-2.89075500	-0.04318400	1.58695200	H	-0.02557300	2.22757600	0.87793500
B	1.71774300	-0.02556600	0.03150700	H	-0.02670700	2.22728600	-0.87890300
O	2.06204100	1.30921100	-0.04014600	B	1.17246300	-0.29448900	0.00000700
H	1.31550400	1.90464200	-0.19255300	C	2.44523000	0.65612700	0.00010500
O	2.73468500	-0.91926300	0.24902500	H	2.44235200	1.32176100	0.87546300
H	3.59492100	-0.47730400	0.32656300	H	3.40500400	0.12085200	0.00000000
(H <sub>3</sub> C) <sub>2</sub> C=CH-B(OH) <sub>2</sub> SCF energy=-297.2964235				H	2.44224600	1.32193700	-0.87512200
C	-0.04443200	-0.68636600	0.00012800	O	1.32988400	-1.66310900	-0.00012200
H	-0.03174700	-1.78085200	0.00018400	H	2.25749100	-1.93765900	-0.00008300
C	-1.28333800	-0.13571700	0.00003200	(H <sub>3</sub> C) <sub>2</sub> C=CH-B(CH <sub>3</sub> ) <sub>2</sub> SCF energy=-261.3157029			
C	-1.56510600	1.34663500	-0.00005800	C	-0.07591400	0.69816300	-0.08294500
H	-0.65578200	1.94625300	0.00039500	H	-0.10983800	1.78858500	-0.18608800
H	-2.16765400	1.61651600	-0.87971900	C	-1.30415800	0.12280600	-0.00425200
H	-2.16873500	1.61645800	0.87884600	C	-1.57123400	-1.34773200	0.20292400
C	-2.52461600	-0.99795900	-0.00002300	H	-2.25417900	-1.49191300	1.05194200
H	-3.14798900	-0.78232600	-0.87967100	H	-2.08110000	-1.76987900	-0.67554300
H	-2.28593500	-2.06613400	-0.00029800	H	-0.67010900	-1.92994400	0.38851300
H	-3.14777500	-0.78274400	0.87987900	C	-2.56348500	0.95393800	-0.09378700
B	1.36551700	-0.02342200	0.00007500				

C	2.66348300	-0.94146000	-0.00010100	H	-2.34741400	2.00925500	-0.28564200
H	2.67025800	-1.60591900	-0.87655900	H	-3.21746700	0.58200700	-0.89567400
H	3.61372300	-0.38902500	0.00033900	H	-3.14570200	0.88363700	0.83628200
H	2.66981500	-1.60668900	0.87576900	B	1.36429400	0.10579200	-0.02639700
O	1.49150600	1.35042100	0.00007600	C	2.56263800	1.12809500	0.16010000
H	2.41625200	1.63740000	-0.00001500	H	3.34206600	0.73815200	0.83053800
H <sub>3</sub> CHC=CH-B(CH <sub>3</sub> ) <sub>2</sub> SCF energy=-222.0019484							
C	0.38978300	0.52420400	-0.02371900	H	3.06174700	1.25505200	-0.81673200
H	0.58899000	1.60100300	-0.06497000	H	2.27317500	2.12877300	0.50448100
C	1.47425700	-0.27931700	0.01414500	C	1.74701500	-1.42845400	-0.18697700
H	1.32653100	-1.36026700	0.05611600	H	2.79916200	-1.56205100	-0.47184900
C	2.90659600	0.16601500	0.00360000	H	1.63082300	-1.93873500	0.78428300
H	3.43298200	-0.19124800	0.90006000	H	1.12819400	-1.98279500	-0.90290700
H	3.44085500	-0.25930200	-0.85785200	H <sub>3</sub> CHC=C-B(CH <sub>3</sub> ) <sub>2</sub> CH <sub>3</sub> SCF energy=-261.3151649			
H	2.99411900	1.25693700	-0.03835300	C	-0.32094500	0.26682800	-0.01148800
B	-1.08961000	0.03548100	-0.01396300	C	-1.31250800	-0.65876800	0.00253400
C	-1.49353400	-1.49580400	-0.00271300	H	-1.01783700	-1.70750200	0.01023200
H	-2.28010400	-1.68868100	0.74183600	C	-2.80224200	-0.46535700	0.01683800
H	-1.95273700	-1.74399300	-0.97384200	H	-3.11462300	0.58156500	0.00914000
H	-0.68393100	-2.21529500	0.16570100	H	-3.25870500	-0.96402300	-0.85019800
C	-2.24459000	1.11983900	0.00485100	H	-3.23682600	-0.94196400	0.90722800
H	-3.20771500	0.75867800	-0.37834900	C	-0.61200900	1.75816600	-0.02427300
H	-2.42063900	1.40323900	1.05780600	H	-0.07387600	2.25557200	-0.84134600
H	-1.98536400	2.05189800	-0.51531600	H	-1.67283100	1.99981800	-0.13815100
C <sub>2</sub> H <sub>5</sub> HC=CH-B(CH <sub>3</sub> ) <sub>2</sub> SCF energy=-261.3106173							
C	-0.39593200	-1.07202100	0.19387200	H	-0.26662200	2.23459500	0.90353000
H	-0.78996700	-2.04334000	0.51266200	B	1.17722500	-0.20624600	0.00609600
C	0.93130500	-1.07811600	-0.06943700	C	2.33374500	0.88182000	0.03253700
H	1.47847700	-2.01370700	0.08596500	H	3.32988800	0.46519900	0.22593500
C	1.79811400	0.03347500	-0.59308800	H	2.38253900	1.38139200	-0.95021300
H	1.20681600	0.92412000	-0.81869600	H	2.15321900	1.68934700	0.75592500
H	2.24204100	-0.29896900	-1.54447000	C	1.62949300	-1.72460000	-0.01908300
C	2.94044300	0.38818000	0.37843400	H	0.85180700	-2.48672700	-0.13599900
H	3.55755700	-0.49047000	0.60457600	H	2.36908400	-1.87571000	-0.82060400
H	3.59439700	1.15508700	-0.05306200	H	2.17545300	-1.94886500	0.91165100
H	2.54518300	0.77107100	1.32647100	H <sub>2</sub> C=C-B-OH CH <sub>3</sub> C <sub>2</sub> H <sub>5</sub> SCF energy=-297.2924721			
B	-1.46291000	0.06131100	0.05554600	C	-1.30277600	-0.26451100	-0.00003700
C	-1.14647500	1.61548300	0.05696300	C	-1.60225600	-1.57712700	-0.00010900
H	-1.01859700	1.95181800	-0.98644600	H	-0.83327000	-2.34685600	-0.00016400
H	-1.98797500	2.20107000	0.45211700	H	-2.63138200	-1.93830500	-0.00019300
H	-0.23916300	1.90953300	0.59667000	C	-2.40206800	0.77750700	0.00009300
C	-2.98264400	-0.37788300	-0.03549200	H	-2.32388400	1.43312500	0.87679300
H	-3.40072500	-0.33536200	0.98647100	H	-2.32357800	1.43385500	-0.87597300
H	-3.59705700	0.30965900	-0.63235700	H	-3.39874500	0.31978600	-0.00019200
H	-3.14530600	-1.40177800	-0.39514600	B	0.19695400	0.21283600	-0.00000100
H <sub>2</sub> C=CH-B-OH CH(CH <sub>3</sub> ) <sub>2</sub> SCF energy=-297.2879671							
C	1.64091300	-0.61899800	0.31776900	O	0.37155000	1.57504200	-0.00012000
H	1.52132600	-1.61772300	0.74529700	H	1.30223100	1.84552000	-0.00008700
C	2.89290100	-0.20704400	0.05370600	C	1.44880800	-0.77274800	0.00014200
H	3.76818000	-0.82595400	0.24843300	H	1.36644200	-1.44279800	-0.86951300
H	3.08281000	0.77708500	-0.37099100	H	1.36651500	-1.44250800	0.87003600
B	0.36605700	0.25532700	0.05971600	C	2.83958500	-0.11283400	-0.00001900
O	0.57686200	1.50614100	-0.46540200	H	3.64273100	-0.85932900	0.00012200
H	-0.23968200	2.01070000	-0.59515800	H	2.99397200	0.51545800	-0.88832400
C	-1.09751300	-0.29030800	0.38454400	H	2.99404500	0.51580700	0.88803900
H	-1.05412700	-0.70976500	1.40420100	(H <sub>3</sub> C) <sub>2</sub> HCH <sub>2</sub> C-B(OH) <sub>2</sub> SCF energy=-334.4949524			
C	-2.20765900	0.77604800	0.36442800	C	-0.01960000	-0.81039300	-0.02362800
H	-2.34097400	1.20629100	-0.63999800	H	-0.03556300	-1.59303300	-0.80201100
H	-3.17864100	0.34854000	0.64689000	H	-0.14536700	-1.35389000	0.92791600
				C	-1.23264700	0.12333900	-0.23688300

H	-2.00309900	1.60010400	1.06107400	H	-1.06247700	0.68069700	-1.16848500
C	-1.45362000	-1.46355900	-0.56212900	C	-2.53307600	-0.68022200	-0.39294600
H	-0.70448100	-2.26297400	-0.52476300	H	-3.39161900	-0.01909700	-0.56729800
H	-2.42407300	-1.90316800	-0.29529400	H	-2.47277300	-1.38006000	-1.23615700
H	-1.52255100	-1.12573300	-1.60495800	H	-2.74400900	-1.26684900	0.51227600
H <sub>2</sub> C=CH-B(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> SCF energy=-261.3042316				C	-1.35949600	1.14543700	0.90394000
C	1.67001100	-0.70714000	-0.09233600	H	-0.45910200	1.76482900	0.99187200
H	1.79626700	-1.78506600	-0.23772700	H	-2.21009200	1.81852900	0.73864200
C	2.80114500	0.00651500	0.06499900	H	-1.52004500	0.63950900	1.86664600
H	2.78755100	1.08772700	0.19261300	B	1.41034200	-0.13184700	-0.09548400
H	3.78946500	-0.45253000	0.05695400	O	1.60759700	0.96216900	-0.89634700
B	0.21999900	-0.11426500	-0.16199200	H	2.53165800	1.25862800	-0.88269400
C	-0.08837300	1.34339100	0.38356300	O	2.51673800	-0.61016700	0.57804200
H	0.79690200	1.99223900	0.31539600	H	2.33192000	-1.37500100	1.14025900
H	-0.23254900	1.20932700	1.47284200	C <sub>2</sub> H <sub>5</sub> -B(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> SCF energy=-262.5269456			
C	-1.31269200	2.08203000	-0.18781000	B	0.16254900	-0.04339200	0.12131300
H	-1.44819700	3.06373700	0.28339400	C	1.65592400	0.03310400	0.65177500
H	-1.21060800	2.24970500	-1.26766500	H	1.82288300	-0.61776500	1.52265500
H	-2.23810100	1.51460100	-0.03367500	H	1.91820900	1.05691100	0.95928200
C	-0.94435400	-1.06060300	-0.67781100	C	2.63321600	-0.39577800	-0.47523200
H	-1.68585500	-0.50894200	-1.27188500	H	2.53833200	0.24764100	-1.35891800
H	-0.55554700	-1.86352100	-1.32065500	H	3.67561300	-0.33964100	-0.13848800
C	-1.67606400	-1.71250400	0.52757200	H	2.44941400	-1.42877800	-0.79740300
H	-2.13763400	-0.95665600	1.17474700	C	-0.69057400	-1.33437200	0.45864200
H	-2.47125700	-2.38793500	0.18861900	H	-0.03627500	-2.22042700	0.40292000
H	-0.98847500	-2.30149100	1.14793500	H	-0.90643900	-1.25062000	1.54158600
C <sub>2</sub> H <sub>5</sub> -B(OH) <sub>2</sub> SCF energy=-255.8636894				C	-1.99937400	-1.59760500	-0.30354600
C	-0.79205000	0.77190200	-0.00015300	H	-1.81617400	-1.73220900	-1.37721300
H	-0.81760400	1.44660100	0.87167900	H	-2.50599800	-2.50209900	0.05625100
H	-0.81752100	1.44583700	-0.87259900	H	-2.70453300	-0.76393900	-0.19820000
C	-2.04688100	-0.11747300	0.00013500	C	-0.43974700	1.18540100	-0.67809400
H	-2.07026000	-0.76890200	-0.88059500	H	-1.13825200	0.87027400	-1.46583000
H	-2.07012800	-0.76832900	0.88128400	H	0.34932200	1.77593100	-1.16612600
H	-2.96512900	0.48259900	0.00000200	C	-1.20269300	2.11656400	0.30407500
B	0.59316400	0.00368400	-0.00003600	H	-1.61747200	2.98689100	-0.21892100
O	0.62706600	-1.36446800	-0.00008500	H	-2.03773100	1.59646400	0.78961800
H	1.53646100	-1.70375700	0.00022600	H	-0.54415100	2.49444800	1.09649700
O	1.81360600	0.65242800	0.00008200	HC≡C-BF <sub>2</sub> SCF energy=-301.4515863			
H	1.74656800	1.61728100	0.00032200	B	-0.00002900	-0.47023800	0.00000000
(H <sub>3</sub> C) <sub>3</sub> C-B(OH) <sub>2</sub> SCF energy=-334.4954048				F	-0.00002900	-1.15888700	-1.13624300
C	0.61906300	0.00265400	0.00002600	F	-0.00002900	-1.15888700	1.13624300
C	1.10455700	0.76161800	-1.25951100	C	0.00009800	1.04981900	0.00000000
H	0.80290200	0.25112300	-2.18392900	C	0.00001700	2.26330700	0.00000000
H	0.69853000	1.77840300	-1.29254100	H	-0.00001500	3.33239200	0.00000000
H	2.20179500	0.83337600	-1.26560900	HC≡C-BCl <sub>2</sub> SCF energy=-1022.1357			
C	1.22994000	-1.41450000	0.00017000	B	-0.02110500	0.00043000	-0.00019900
H	2.32735800	-1.36396200	0.00010300	C	-1.52873300	0.00276000	-0.00016400
H	0.94066200	-1.99001100	0.89125500	C	-2.74457200	0.00441000	0.00010300
H	0.94050300	-1.99020900	-0.89071600	H	-3.81358200	0.00581100	0.00021400
C	1.10460000	0.76196900	1.25931100	Cl	0.86619600	-1.52049700	0.00003400
H	0.69837800	1.77867900	1.29207500	Cl	0.87256500	1.51749800	0.00003400
H	0.80316300	0.25165700	2.18390000	(H <sub>3</sub> C) <sub>3</sub> C-B(OH) <sub>2</sub> CH <sub>3</sub> SCF energy=-298.51686			
H	2.20182400	0.83392800	1.26522900	B	0.93785900	-0.16663600	-0.04077700
B	-0.97818200	-0.02389700	-0.00000100	C	-0.64513400	0.04721800	-0.01515400
O	-1.65503000	1.16861800	-0.00000300	C	-1.40579900	-1.18495800	-0.54799400
H	-2.61694600	1.04095000	0.00002000	H	-1.15061700	-2.09055800	0.01261200
O	-1.74789400	-1.16724300	0.00003100	H	-2.49215700	-1.03178700	-0.47185200
H	-1.23283300	-1.98589700	0.00001600	C <sub>4</sub> H <sub>9</sub> -B(OH) <sub>2</sub> SCF energy=-334.491898			

C	-0.37652600	0.71065500	-0.00016800
H	-0.33307100	1.38482800	-0.87304700
H	-0.33298800	1.38518500	0.87242400
C	0.86209800	-0.20213300	-0.00001300
H	0.82537200	-0.86513100	0.87551200
H	0.82532600	-0.86548100	-0.87527100
C	2.19060600	0.56637000	-0.00024100
H	2.22715400	1.22707100	-0.87953400
H	2.22700600	1.22783400	0.87848500
C	3.41985500	-0.35033100	0.00026900
H	4.35223800	0.22746100	-0.00027300
H	3.42976700	-0.99877900	0.88590000
H	3.42954900	-1.00007200	-0.88441900
B	-1.78008600	-0.02309100	-0.00002400
O	-2.98355400	0.65641200	0.00022700
H	-2.89182800	1.61930200	0.00053500
O	-1.84974900	-1.39006800	-0.00014700
H	-2.76785600	-1.70488500	0.00008500
C <sub>3</sub> H <sub>7</sub> -B-OH C <sub>2</sub> H <sub>5</sub> SCF energy=-298.5110754			
B	0.61106100	0.06229500	0.00014900
C	1.91067300	-0.84356100	0.00044900
H	1.85185500	-1.52323400	-0.86652300
H	1.85227700	-1.52174000	0.86863300
C	3.26365300	-0.11319700	-0.00046400
H	4.10424900	-0.81864200	-0.00004200
H	3.36722800	0.53051500	-0.88163600
H	3.36759400	0.53203800	0.87954500
O	0.79415200	1.42138000	0.00014500
H	-0.03567900	1.92291700	0.00003800
C	-0.84848500	-0.57631600	-0.00008700
H	-0.92419300	-1.25195600	-0.86893500
H	-0.92429700	-1.25251800	0.86831200
C	-2.04977300	0.38559100	0.00013200
H	-1.99952200	1.04352600	0.88187800
H	-1.99939400	1.04408000	-0.88119500
C	-3.40866600	-0.32661500	-0.00021000
H	-4.23985000	0.38931100	-0.00003100
H	-3.51653700	-0.96581300	-0.88573000
H	-3.51666500	-0.96640500	0.88486500
(H <sub>3</sub> C) <sub>2</sub> HC-BH <sub>2</sub> SCF energy=-144.556945			
B	0.76119900	1.43461100	0.00000000
H	1.10134700	1.94696900	1.02995700
H	1.10134700	1.94696900	-1.02995700
C	-0.20362700	0.20873900	0.00000000
H	-1.15810800	0.79158600	0.00000000
C	-0.20362700	-0.65275400	1.27776300
H	-0.27032400	-0.03547200	2.18102600
H	-1.04232600	-1.36136000	1.28708200
H	0.71999900	-1.24214800	1.34834600
C	-0.20362700	-0.65275400	-1.27776300
H	-1.04232600	-1.36136000	-1.28708200
H	-0.27032400	-0.03547200	-2.18102600
H	0.71999900	-1.24214800	-1.34834600
H <sub>3</sub> C-BH-OH SCF energy=-141.245016			
B	-0.13109300	0.49241800	-0.00009800
H	-0.30219300	1.68600700	0.00010200
C	1.30092800	-0.14596900	-0.00000500
H	1.87308100	0.19553300	0.87547700
H	-1.17151800	-1.37698600	-1.60293400
C	1.98176900	1.02997800	-0.02988000
H	1.69633000	1.82974500	0.66586200
H	3.00751600	0.72363400	0.21976700
H	2.02074700	1.50113200	-1.02386500
O	1.38078300	-1.46586100	-0.04502900
H	2.34608800	-1.54383600	-0.01198300
C	-1.03359000	0.26838900	1.47265200
H	-0.53588900	1.14722200	1.90314400
H	-2.11784100	0.42988800	1.56151700
H	-0.77819700	-0.60138400	2.09123600
C	-1.06566300	1.29390400	-0.82507200
H	-0.58255100	2.20745500	-0.45701800
H	-0.81456700	1.19038500	-1.88927500
H	-2.15240400	1.44797400	-0.76040900
(H <sub>3</sub> C) <sub>2</sub> C=CH-BH <sub>2</sub> SCF energy=-182.6603762			
B	2.24738400	-0.09727500	0.00014700
H	2.43525300	1.08573200	0.00056700
C	0.84433000	-0.71095300	-0.00022300
C	-0.34856500	-0.04746900	-0.00002000
H	3.20837200	-0.81347200	0.00007600
C	-1.65986500	-0.79248700	0.00011200
H	-1.51800800	-1.87716300	-0.00068000
H	-2.25990500	-0.51985200	0.88000300
H	-2.26096400	-0.51860300	-0.87864600
H	0.76110600	-1.80113200	-0.00043400
C	-0.49225000	1.45207400	-0.00004600
H	-1.06687700	1.77723700	0.87862900
H	0.46751600	1.96950500	0.00066200
H	-1.06531300	1.77713900	-0.87983900
H <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> C-BH <sub>2</sub> SCF energy=-144.557365			
B	2.14283700	0.12802600	0.00859100
H	3.08158000	-0.61329200	-0.07830000
H	2.35888900	1.30191400	0.13407200
C	0.69303000	-0.45212500	-0.00588300
H	0.60721200	-1.19171000	-0.82174900
H	0.63241000	-1.08600500	0.90288900
C	-0.48841700	0.53161100	-0.03765800
H	-0.39394100	1.23617900	0.80046400
H	-0.42496400	1.14181300	-0.94975700
C	-1.85981700	-0.15159700	0.02050900
H	-1.97054500	-0.73924100	0.94151200
H	-2.67640700	0.58038600	-0.00808600
H	-1.99719300	-0.83750700	-0.82581000
H <sub>3</sub> C(H <sub>2</sub> C) <sub>4</sub> H <sub>2</sub> C-BH <sub>2</sub> SCF energy=-262.499149			
B	-4.06238600	-0.34913400	0.01639900
H	-5.09288000	0.25775800	-0.07225300
H	-4.11779600	-1.54046100	0.15019800
C	-2.70492300	0.42203800	-0.01037400
H	-2.72195800	1.14826800	-0.84248900
H	-2.72976800	1.07812000	0.88375200
C	-1.40144300	-0.39362200	-0.02717200
H	-1.39673700	-1.08556700	0.82771600
H	-1.38360900	-1.02858500	-0.92534000
C	-0.12971500	0.46513800	0.00730400
H	-0.14588100	1.09824600	0.90825400
H	-0.13765900	1.15731600	-0.84903700
C	1.16861600	-0.35278700	-0.01439200
H	1.18458100	-0.98497300	-0.91560000
H	1.17648000	-1.04450100	0.84204400
C	2.43998500	0.50673000	0.02071100

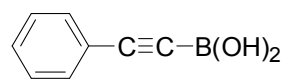
H	1.28664600	-1.24191300	-0.00024900	H	2.43341100	1.19749500	0.83518500
H	1.87377400	0.19581200	-0.87494800	H	2.42531700	1.13755800	0.92164500
O	-1.22696200	-0.32282900	0.00003200	C	3.73128700	-0.32007900	-0.00162000
H	-2.06571400	0.16091900	-0.00012500	H	3.79280900	-0.93468900	-0.90908300
(H <sub>3</sub> C) <sub>2</sub> HC-BH-OH SCF energy=-219.8694666				H	4.61962000	0.32262400	0.02599600
B	0.97040700	-0.00055600	0.44686400	H	3.78315500	-0.99743900	0.86064700
H	1.02715800	-0.00139300	1.65236600	$\begin{array}{c} \text{CH}_3 \\   \\ \text{C}_2\text{H}_5-\text{C}-\text{BH}_2 \\   \\ \text{CH}_3 \end{array}$			
C	-0.40911400	-0.00000100	-0.31334600	SCF energy=-223.1868666			
H	-0.21905500	0.00010600	-1.39708800	B	-1.68380800	-0.64268400	-0.88561500
O	2.13535600	-0.00001500	-0.26470500	H	-2.75420800	-0.10219600	-0.90911400
H	2.92848300	-0.00030900	0.29108400	H	-1.58295200	-1.73141200	-1.37873900
C	-1.21882700	-1.26884800	0.03738700	C	-0.47837500	0.00519700	-0.11992200
H	-1.41930100	-1.32891800	1.11553000	C	0.89352300	-0.46557700	-0.67707700
H	-2.18898400	-1.26842800	-0.47814600	H	0.98395600	-0.11130400	-1.71490000
H	-0.69129200	-2.18587100	-0.25450900	C	2.14688200	-0.02135200	0.09363100
C	-1.21797200	1.26931300	0.03766400	H	3.04740000	-0.42078400	-0.38869200
H	-2.18820700	1.26948900	-0.47772400	H	2.24917200	1.06965600	0.12128400
H	-1.41831200	1.32944500	1.11583800	H	2.14552400	-0.38340000	1.12869100
H	-0.68989300	2.18600100	-0.25426300	C	-0.57078200	1.54356700	-0.04317900
H <sub>2</sub> C=CH-BH <sub>2</sub> SCF energy=-104.0243734				H	-1.56343500	1.86163200	0.29726000
B	-1.35553400	0.20777900	-0.00008900	H	0.16724900	1.96564400	0.65163700
H	-1.40432500	1.40548700	0.00012400	H	-0.39717600	2.00193400	-1.02584700
C	0.02223100	-0.48586300	-0.00000500	C	-0.72725600	-0.59123500	1.30556500
C	1.16796800	0.22952500	0.00001900	H	-1.72740500	-0.34567700	1.68645900
H	1.14867800	1.31851200	-0.00000300	H	-0.61219800	-1.68233500	1.32508500
H	2.15605000	-0.23091800	0.00007900	H	-0.00587400	-0.16905300	2.01724400
H	-2.37492700	-0.41956500	0.00012800	H	0.88503600	-1.56288100	-0.73640000
H	0.11100000	-1.57438100	0.00003400	(H <sub>3</sub> C) <sub>3</sub> C-CH-BH <sub>2</sub>			
(H <sub>3</sub> C) <sub>2</sub> HC-CH-BH <sub>2</sub> SCF energy=-223.1882981				$\begin{array}{c} \text{CH}_3 \\   \\ \text{CH}_3 \\   \\ \text{CH}_3 \end{array}$			
B	1.56073500	1.36165900	-0.06983400	SCF energy=-262.5040402			
H	2.37472900	1.83458600	0.67245400	B	1.68504800	1.36812000	-0.03669900
H	1.47845200	1.80895100	-1.18089800	H	2.62524200	1.72326800	-0.69088500
C	0.72246800	0.10589100	0.34257000	H	1.46842700	1.95390500	0.98597600
H	0.60417200	0.04763800	1.43640600	C	0.87372500	0.10024000	-0.47269400
C	-0.67618800	0.00173800	-0.31273400	C	-0.61541900	-0.00213700	-0.00638800
H	-0.53163500	0.02232300	-1.40471400	C	-1.30003500	-1.22267100	-0.65833700
C	-1.41879000	-1.29636600	0.04461100	H	-2.36493800	-1.25684700	-0.39441700
H	-2.41753300	-1.31168500	-0.40979800	H	-1.23051800	-1.17740100	-1.75329800
H	-0.88804900	-2.18943700	-0.30398200	H	-0.85415100	-2.16978300	-0.33226500
H	-1.54906000	-1.38589900	1.13220500	H	0.87146800	0.03321300	-1.57261500
C	-1.53215900	1.22166400	0.06912000	C	-1.34935800	1.27118100	-0.47908600
H	-1.69507400	1.26065000	1.15504500	H	-0.93097200	2.17112400	-0.00893400
H	-1.05023500	2.16199400	-0.23070800	H	-1.27280900	1.39159800	-1.56801100
H	-2.51695800	1.18758700	-0.41334600	H	-2.41612000	1.23183200	-0.22296600
C	1.67698300	-1.05909000	-0.07280200	C	-0.74448800	-0.11620700	1.52572300
H	2.68727700	-0.93335600	0.33789700	H	-1.80242100	-0.12058600	1.81809800
H	1.30158600	-2.01961500	0.29812800	H	-0.29820000	-1.04394900	1.90310600
H	1.76476700	-1.13505100	-1.16410900	H	-0.26311900	0.72417000	2.03860900
H <sub>3</sub> C-C≡C-B(OH) <sub>2</sub> SCF energy=-292.7252471				C	1.79430200	-1.06372100	0.01905500
C	1.57505200	-0.01778600	-0.00179400	H	1.35810200	-2.03796900	-0.23038000
C	0.35775000	-0.03600600	-0.00124400	H	2.77846300	-1.01813800	-0.46203300
B	-1.17302000	-0.01950000	-0.00009100	H	1.95394700	-1.04514600	1.10387500
O	-1.86942100	-1.19434700	0.00032400	C	3.26983300	0.21253800	-0.00178100
H	-2.82768100	-1.04015700	0.00090400	H	3.36116800	1.19074300	0.46384700
C	3.03491900	-0.02044600	0.00005600	H	4.18012200	-0.26285800	-0.35549100
H	3.43607000	0.83839800	-0.55150000	C	1.97034400	-0.52186800	0.01866100
H	3.42209000	0.02936300	1.02523200	H	1.93663700	-1.24388400	-0.81112700
				H	1.89995500	-1.13797300	0.93688500
				C	0.73549400	0.39553600	-0.04152700
				H	0.77619700	0.99049200	-0.96515100
				H	0.78354400	1.11472800	0.78994300
				C	-0.59475500	-0.36637100	0.02047800



H	3.42710400	-0.93443000	-0.46187300
O	-1.88921300	1.15725200	0.00025000
H	-1.32973000	1.94651200	0.00099800

(H<sub>3</sub>C)<sub>2</sub>N-C≡C-B(OH)<sub>2</sub> SCF energy=-387.3864165

C	-0.60632600	0.00586000	-0.11371800
C	0.61831900	-0.01436600	-0.05896500
B	2.13205200	-0.01817100	0.00342400
O	2.82057900	-1.20386800	0.04134900
H	3.77767400	-1.05016600	0.07727300
O	2.87709600	1.14757900	0.02626000
H	2.33534700	1.94792700	-0.00698600
N	-1.93623600	-0.00315300	-0.21112400
C	-2.63878600	-1.25757800	0.07147700
H	-3.60984200	-1.24555400	-0.43492200
H	-2.04888300	-2.09310000	-0.31021900
H	-2.80171900	-1.39859400	1.15133400
C	-2.66762400	1.22758900	0.09362700
H	-2.10508000	2.08461000	-0.28279100
H	-3.64235500	1.19777600	-0.40485800
H	-2.82664700	1.35130900	1.17651500



SCF energy=-484.4909988

C	0.46252200	0.00283500	0.00030200
C	1.68272800	-0.02512800	0.00045100
B	3.21317200	-0.02104200	0.00004400
O	3.89557000	-1.20391600	-0.00055200
H	4.85569300	-1.06272100	-0.00078000
O	3.93891200	1.14914800	0.00014600
H	3.38945100	1.94543100	0.00055100
C	-0.96560600	0.00227400	0.00013000
C	-1.67437000	-1.21670800	0.00024600
C	-1.68653400	1.21365600	-0.00013600
C	-3.06825000	-1.21878700	0.00009100
H	-1.12035600	-2.15063700	0.00045500
C	-3.08049200	1.20263600	-0.00029400
H	-1.14383300	2.15446600	-0.00022200
C	-3.77499200	-0.01156400	-0.00018100
H	-3.60460400	-2.16406800	0.00018300
H	-3.62625000	2.14254800	-0.00050600
H	-4.86185500	-0.01695100	-0.00030300

Cl-C≡C-B(OH)<sub>2</sub> SCF energy=-713.0142443

C	-1.06736500	-0.01597900	-0.00000100
C	0.14826600	-0.03873900	-0.00000200
B	1.68273600	-0.01835900	-0.00000100
O	2.39151600	1.15889900	-0.00000200
H	1.83711700	1.95186800	0.00001500
O	2.36914900	-1.19568900	0.00000000
H	3.32932800	-1.05370200	0.00000900
Cl	-2.71475600	-0.01080900	0.00000100

NC-C≡C-B(OH)<sub>2</sub> SCF energy=-345.6516774

C	-1.19871400	-0.03091600	0.00004400
C	0.02008300	-0.04771400	0.00009600
B	1.56529200	-0.01495500	0.00008800
O	2.23669200	-1.19443600	-0.00004000
H	3.20019300	-1.07408200	-0.00010900
O	2.25447900	1.16649000	-0.00005200
H	1.70612900	1.96400600	0.00001200
C	-2.57063700	-0.01811900	-0.00001100

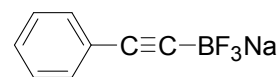
H	-0.63085400	-0.96196200	0.94576400
H	-0.63915600	-1.08908800	-0.80880900
C	-1.82770700	0.54597800	-0.04040400
H	-1.79270400	1.14000500	-0.96532800
H	-1.78438900	1.26821900	0.78790900
C	-3.15338700	-0.22224900	0.02221800
H	-3.23496100	-0.79752800	0.95355900
H	-4.01282800	0.45743400	-0.02540400
H	-3.24166300	-0.92971700	-0.81246700

H<sub>3</sub>C-C≡C-BF<sub>3</sub>Na SCF energy=-603.025059

C	2.42719100	0.00065600	-0.00073000
C	1.21139600	-0.00017400	-0.00151100
B	-0.33923100	-0.00076500	-0.00017300
F	-0.95329800	-0.61841000	1.16012700
F	-0.95567000	1.31287200	-0.04492400
F	-0.95606900	-0.69649300	-1.11468600
Na	-2.77637600	0.00125400	0.00054500
C	3.88879600	0.00055200	0.00025600
H	4.28620900	0.93057700	-0.42556400
H	4.28481900	-0.09487900	1.01923000
H	4.28629600	-0.83359100	-0.59153300

(H<sub>3</sub>C)<sub>2</sub>N-C≡C-BF<sub>3</sub>Na SCF energy=-697.6821603

C	1.53381000	-0.00617500	-0.17347800
C	0.31519400	-0.00999300	-0.10662600
B	-1.22675900	-0.00768500	-0.03301400
F	-1.82394400	1.30475300	0.14750800
F	-1.92120800	-0.52828000	-1.20259100
F	-1.80597700	-0.78874100	1.05157300
Na	-3.65988900	0.01549700	0.09518400
N	2.88006900	0.00009200	-0.28010700
C	3.56360400	-1.22979200	0.12459800
H	3.04675400	-2.08816200	-0.31076200
H	4.59203200	-1.20670100	-0.25239100
H	3.58922700	-1.34987600	1.22105400
C	3.55124000	1.23745800	0.12252100
H	4.57967900	1.22439400	-0.25492000
H	3.02531300	2.08992900	-0.31353000
H	3.57615800	1.35914600	1.21884300



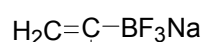
SCF energy=-794.7918993

C	-0.52871900	-0.00066000	-0.00118000
C	0.68972800	-0.00108000	-0.00297000
B	2.24340700	-0.00064400	-0.00155100
F	2.85390500	1.03101500	-0.81447100
F	2.85254400	0.18935000	1.29943600
F	2.85356800	-1.22146200	-0.48614700
Na	4.68146600	0.00129500	0.00276900
C	-1.95864200	-0.00031200	-0.00044100
C	-2.67728200	-1.21320600	-0.00014900
C	-2.67643200	1.21310300	-0.00016200
C	-4.07183200	-1.20873700	0.00071500
H	-2.12949200	-2.15106600	-0.00058000
C	-4.07097600	1.20966400	0.00063300
H	-2.12795600	2.15055900	-0.00064000
C	-4.77447400	0.00071500	0.00112400
H	-4.61204500	-2.15230600	0.00104200
H	-4.61049700	2.15363100	0.00085900
H	-5.86155300	0.00110500	0.00182600

NC-C≡C-BF<sub>3</sub>Na SCF energy=-655.9597341

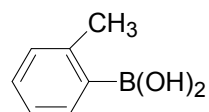


O	1.09345300	-1.52436300	-0.00049000
O	2.82237400	-0.11823200	0.00047900
H	3.26366100	-0.98789300	0.00032500



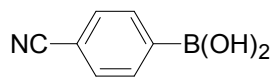
SCF energy=-796.026522

C	-0.87494500	1.39623600	1.42305600
H	-1.90972900	1.49741900	1.74884600
C	-0.48099500	0.34052900	0.67189200
B	-1.58171800	-0.72642000	0.10030800
F	-1.43382300	-2.03980600	0.48053400
F	-2.91925200	-0.24283600	0.42738900
F	-1.55376200	-0.60571600	-1.36673700
Na	-2.41969900	1.37828900	-0.99862200
H	-0.17472000	2.12477400	1.83077000
C	0.95531000	0.18298100	0.30363800
C	1.52579500	-1.09989900	0.19909000
C	1.78622200	1.29413000	0.05920800
C	2.87881700	-1.26038800	-0.10697700
H	0.90424400	-1.97206100	0.37198700
C	3.13632800	1.13418000	-0.25487500
H	1.36742900	2.29696700	0.10364700
C	3.69116400	-0.14677400	-0.33592800
H	3.29744400	-2.26188200	-0.17073000
H	3.75357000	2.00939300	-0.44455000
H	4.74239600	-0.27443700	-0.58197600



SCF energy=-447.6341618

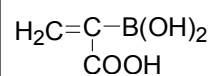
C	1.96235700	-1.49267200	-0.14295200
C	0.56760200	-1.45225400	-0.13265900
C	-0.15338400	-0.24586000	-0.02550000
C	0.58124400	0.96497800	0.07732400
C	1.98275300	0.91096100	0.07922300
C	2.67356600	-0.29786200	-0.03159200
H	2.48390900	-2.44162300	-0.23816300
H	0.02798300	-2.39299500	-0.23967300
H	2.54487900	1.83826800	0.16839100
H	3.76098900	-0.30289900	-0.03169400
B	-1.72427700	-0.32252700	-0.02696500
O	-2.48575200	0.72648100	-0.47082000
H	-3.43305800	0.52324300	-0.41252700
O	-2.41575500	-1.43995200	0.39586200
H	-1.85760700	-2.13280100	0.77485000
C	-0.09330400	2.31602100	0.18770500
H	-0.63891000	2.56554700	-0.72859700
H	-0.82686700	2.34211700	1.00085300
H	0.64711400	3.10167800	0.37175000



SCF energy=-500.5763613

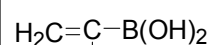
C	1.19859300	1.22028900	-0.00091100
C	-0.19419600	1.21813000	-0.00094400
C	-0.93344400	0.02124200	-0.00009900
C	-0.21581700	-1.19072000	0.00070800
C	1.17633100	-1.21252100	0.00080200
C	1.89178800	-0.00212900	0.00000100
H	1.75260700	2.15397100	-0.00161500
H	-0.70116700	2.18192100	-0.00184100
B	-2.50721500	-0.00686500	-0.00000900

H	1.10173600	2.54687100	0.17208600
H	-0.75368600	2.57473300	0.17805100
C	-1.12349900	-0.08688900	-0.02513500
F	-1.17227100	-1.08867800	0.91379600
F	-2.22324800	0.67141600	0.16455100
F	-1.27511300	-0.71091200	-1.22757200



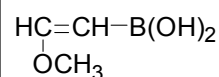
SCF energy=-443.2454103

C	-0.05579000	0.57596900	-0.00016400
B	1.35075800	-0.15104900	-0.00002400
O	2.46839700	0.64195000	0.00000700
H	3.28197200	0.11394400	-0.00017300
O	1.48106000	-1.50630000	0.00021600
H	0.60198500	-1.93662900	-0.00002000
C	-0.15636100	1.91889700	-0.00004200
H	0.74028300	2.53267600	0.00005100
H	-1.11417100	2.43232800	0.00017100
C	-1.27998500	-0.26383100	-0.00008300
O	-1.26811800	-1.49103000	-0.00021400
O	-2.44974600	0.41494400	0.00014700
H	-3.16377600	-0.24979500	0.00058100



SCF energy=-485.7238447

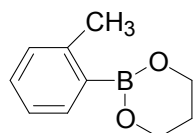
C	0.99072000	0.62268300	-0.27721400
B	2.16106100	-0.35894300	0.12968500
O	2.04980500	-1.70924500	-0.06388900
H	2.84310300	-2.18032900	0.23800300
O	3.34232200	0.09501300	0.67346500
H	3.34411500	1.04384700	0.86229100
C	1.32755800	1.82246600	-0.79744600
H	2.36515600	2.12289600	-0.93561400
H	0.58405600	2.53402200	-1.15231400
C	-0.44529100	0.25652600	-0.10674000
C	-0.90862300	-1.04708900	-0.36577400
C	-1.38094100	1.21979700	0.31746400
C	-2.26300400	-1.36230900	-0.23627800
H	-0.20492500	-1.81073600	-0.67754000
C	-2.73293200	0.90165400	0.45369600
H	-1.03960400	2.22183200	0.56446100
C	-3.18189100	-0.39194400	0.17228200
H	-2.59975400	-2.37319000	-0.45341500
H	-3.43377800	1.66216300	0.78972600
H	-4.23427000	-0.64263800	0.27943500



SCF energy=-369.1833673

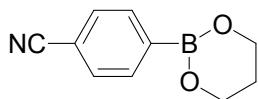
C	0.86529500	0.68557100	0.00014500
H	0.57640600	1.73587700	0.00035600
C	-0.03189500	-0.31987600	-0.00019800
H	0.32389900	-1.34801400	-0.00046600
B	-1.56848700	-0.10689400	-0.00003900
O	-2.36667700	-1.22453500	0.00016100
H	-3.30868000	-0.99308300	0.00013900
O	-2.22019200	1.11370200	-0.00010400
H	-1.64313500	1.88859200	-0.00019100
O	2.21561700	0.61995700	0.00010100
C	2.81813300	-0.67388500	-0.00004800
H	3.89498600	-0.49985700	-0.00061200
H	2.53034400	-1.23636000	0.89638600

O	-3.30825300	1.10990500	0.00152200
H	-2.84493600	1.95838100	0.00372400
O	-3.12558700	-1.22661200	-0.00160300
H	-4.09253200	-1.15067200	-0.00114300
H	-0.76451600	-2.12772500	0.00127100
H	1.71558100	-2.15497200	0.00146800
C	3.32731300	-0.01289700	0.00007900
N	4.49119300	-0.02018600	0.00014500



SCF energy=-564.3594424

C	0.81079800	-0.18854600	0.02784800
C	1.67261200	0.94053500	-0.00975400
C	3.05997600	0.73415900	-0.05368200
C	3.61469000	-0.54726600	-0.06107500
C	2.77639000	-1.66227400	-0.02444800
C	1.39537700	-1.47214000	0.01918900
H	3.71964500	1.59924600	-0.08276700
H	4.69499200	-0.66984800	-0.09505500
H	3.19200000	-2.66706700	-0.02940300
H	0.73982900	-2.33792800	0.04780000
B	-0.75815700	-0.12559200	0.08202500
O	-1.41994900	1.07875900	0.11351900
O	-1.44164200	-1.32169500	0.09385700
C	-2.85071300	1.13210200	0.16456700
H	-3.15240700	2.05105600	-0.34837400
H	-3.15413000	1.21754200	1.21725300
C	-2.87050400	-1.35747100	0.14252300
H	-3.17848600	-1.45831600	1.19279700
H	-3.18578400	-2.26156000	-0.38852200
C	-3.47598500	-0.10199600	-0.47861900
H	-3.28241000	-0.09394500	-1.55937000
H	-4.56415700	-0.09404400	-0.33575300
C	1.16294500	2.36687700	-0.00553400
H	0.50780400	2.56613100	-0.86052800
H	0.57270900	2.58429700	0.89103900
H	2.00039700	3.07200200	-0.04433900



SCF energy=-617.30447

C	0.18428700	-0.00001700	0.04652700
C	0.90802600	-1.20692900	0.03003600
C	2.30037800	-1.21736900	-0.00283800
C	3.00421500	0.00000400	-0.01940000
C	2.30036000	1.21736900	-0.00283500
C	0.90800800	1.20691300	0.03007000
B	-1.38519000	0.00000400	0.08590300
O	-2.04042300	1.20384700	0.10057900
O	-2.04048500	-1.20375000	0.10091000
C	-3.47400500	1.24900700	0.13636800
H	-3.77614900	2.15756500	-0.39333900
H	-3.78634900	1.34724400	1.18477300
C	-3.47404800	-1.24909000	0.13613600
H	-3.78678500	-1.34780300	1.18437900
H	-3.77587800	-2.15747400	-0.39405100
C	-4.08093500	0.00003800	-0.49804500
H	-3.88061500	0.00016500	-1.57750700
H	-5.16997300	0.00003900	-0.36356800
H	0.36768800	-2.14932600	0.04334100
H	2.84865700	-2.15468000	-0.01549000
H	0.36765400	2.14929800	0.04331500

H	2.52943000	-1.23652600	-0.89607500
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H<sub>2</sub>N-CH=CH-B(OH)<sub>2</sub> SCF energy=-310.0118784

C	1.44221100	-0.26898400	-0.02104500
H	1.33717200	-1.35379000	-0.07965400
C	0.35548200	0.53561700	0.02422800
H	0.52783700	1.61303900	0.07315700
B	-1.10986600	0.05059500	0.00488600
O	-2.10910100	0.99608300	-0.02599000
H	-2.98734700	0.58478400	-0.03055000
O	-1.52735500	-1.27313100	0.01089800
H	-0.81368200	-1.92159200	0.06966700
N	2.76490400	0.11980300	0.06206500
H	3.46734600	-0.50009100	-0.31743700
H	2.96917100	1.10265200	-0.07242500

HC=CH-B(OH)<sub>2</sub>  
COOCH<sub>3</sub> SCF energy=-482.5364827

C	-0.04061500	0.65846400	-0.00007300
H	0.25832200	1.70621700	-0.00035800
C	0.85170200	-0.34672300	0.00021500
H	0.46409200	-1.36472900	0.00043000
B	2.41156700	-0.15968100	0.00009700
O	3.17560000	-1.29280000	-0.00034500
H	4.12634100	-1.09756300	-0.00051400
O	3.05848800	1.05302800	0.00028200
H	2.47972900	1.82807900	0.00053400
C	-1.51980700	0.51373600	-0.00012900
O	-2.27864700	1.46746800	-0.00027400
O	-1.93608200	-0.76975000	0.00010000
C	-3.36193000	-0.96738900	0.00013400
H	-3.50210500	-2.04856000	-0.00027000
H	-3.80751800	-0.51892700	0.89210600
H	-3.80767400	-0.51820600	-0.89138900

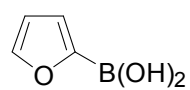
F<sub>3</sub>C-CH=CH-B(OH)<sub>2</sub> SCF energy=-591.7296029

C	-0.24985800	0.41709100	-0.00017600
H	-0.13088000	1.50023400	-0.00065200
C	0.78069300	-0.43611400	0.00023900
H	0.55573100	-1.50208800	0.00059300
B	2.29774100	-0.02081400	0.00004200
O	3.21137800	-1.03471100	-0.00014800
H	4.12663100	-0.71172700	-0.00032700
O	2.76437200	1.27099100	0.00003100
H	2.08829300	1.96213400	0.00032000
C	-1.69254900	0.00598500	-0.00003800
F	-2.33968300	0.50205600	1.08930500
F	-1.87216100	-1.33173900	0.00050500
F	-2.33973400	0.50118400	-1.08974000

H<sub>2</sub>N-CH=CH-BF<sub>3</sub>Na SCF energy=-620.3082647

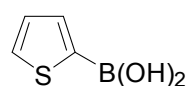
C	1.73520200	-0.20061100	0.26400900
H	1.58102700	0.01399600	1.32275900
C	0.67845600	-0.48673400	-0.52729700
H	0.89031600	-0.74596100	-1.57070600
B	-0.85042400	-0.54685300	-0.01986800
F	-1.43031700	-1.78880200	0.08586400
F	-0.94750200	0.18216000	1.25569500
F	-1.65577800	0.30107800	-0.92776600
Na	-0.45567300	1.89811100	-0.05056200
N	3.07922100	-0.09438000	-0.12010900
H	3.75206500	-0.33182500	0.59997700

H	2.84863200	2.15468600	-0.01537800
C	4.43932700	0.00003500	-0.05270800
N	5.60323600	-0.00004000	-0.07968100



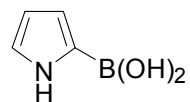
SCF energy=-406.1056026

C	2.13062000	-0.71812600	-0.00035300
C	2.29734100	0.63720800	-0.00004800
C	0.98038900	1.19429200	0.00042700
C	0.08971100	0.15110600	0.00034400
H	2.81828600	-1.55122500	-0.00065100
H	3.23942100	1.16869800	-0.00007100
B	-1.45526400	0.02337800	0.00012600
O	-2.21255000	1.16245400	-0.00049700
H	-3.16252900	0.96768300	-0.00059500
O	-2.08114900	-1.19949600	0.00026100
H	-1.46019400	-1.94366100	0.00048100
O	0.81115700	-1.03644900	-0.00012400
H	0.71329700	2.24266900	0.00087000



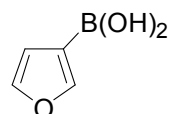
SCF energy=-729.0963492

C	2.36438100	-0.20278700	-0.00006300
C	2.05903000	1.13683800	0.00016500
C	0.65395200	1.36348200	0.00025500
C	-0.10912600	0.20984900	0.00009300
H	3.34642100	-0.65913400	-0.00016200
H	2.80455800	1.92509700	0.00025300
B	-1.65567000	0.05023000	0.00002900
O	-2.18990900	-1.21016700	0.00039800
H	-3.15958000	-1.19797800	0.00022000
O	-2.52966600	1.11541100	-0.00033300
H	-2.10911300	1.98595100	-0.00088500
H	0.22353600	2.36228400	0.00042900
S	0.94498100	-1.18460100	-0.00020200



SCF energy=-386.258404

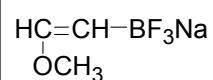
C	-2.19157200	-0.72002700	-0.00001100
C	-2.30025700	0.66288800	0.00001500
C	-0.98038400	1.17975800	-0.00015900
C	-0.08325100	0.11021900	-0.00000600
N	-0.86431000	-1.03501700	0.00010700
H	-0.47733000	-1.96873400	0.00026300
H	-2.95323500	-1.48773200	0.00001700
H	-3.22358100	1.22696400	0.00007300
B	1.45615200	0.02100800	0.00001500
O	2.30447800	1.10591700	-0.00002000
H	1.85462800	1.96200000	0.00105200
O	2.02334500	-1.23350700	-0.00009200
H	2.99223300	-1.19902600	-0.00007400
H	-0.71311300	2.23029500	-0.00028800



SCF energy=-406.1036528

C	-2.22602700	0.67181800	-0.00025500
C	-0.95185800	1.14187600	-0.00039500
C	-0.07296800	-0.00860700	0.00002400
C	-0.92144000	-1.08572500	0.00034600
H	-3.20130300	1.13445500	-0.00051100

H	3.30698900	-0.54636000	-1.00016000
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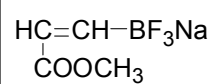


SCF energy=-679.4805313

C	1.27417600	0.08509200	0.64520200
H	0.93715100	0.43584600	1.61908200
C	0.42581000	-0.44026500	-0.25973200
H	0.82939900	-0.82274700	-1.19809700
B	-1.15863000	-0.60541600	-0.00371200
F	-1.63283400	-1.88544400	0.14250500
F	-1.54401400	0.22909800	1.14419500
F	-1.85770800	0.06040100	-1.12524900
Na	-1.08673600	1.88182600	-0.22522500
O	2.62952500	0.24052100	0.56707300
C	3.27940900	-0.26076700	-0.59510600
H	2.93225800	0.25969800	-1.49825600
H	4.34473400	-0.07338100	-0.44927500
H	3.10214300	-1.33745600	-0.70924100

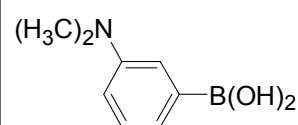
F<sub>3</sub>C-CH=CH-BF<sub>3</sub>Na SCF energy=-902.0365143

C	-1.05783000	0.37507400	-0.00085700
H	-0.84670800	1.44227000	-0.00287100
C	-0.08481100	-0.54085800	0.00071200
H	-0.37161200	-1.59326000	0.00259800
B	1.45767500	-0.17949600	-0.00059000
F	2.19511100	-0.69510100	-1.13706600
F	1.76161300	1.23396100	-0.00184300
F	2.19620300	-0.69289800	1.13650700
Na	3.84496500	0.34414900	0.00120900
C	-2.51912800	0.05971500	0.00012200
F	-3.14591400	0.59273300	-1.08872900
F	-3.14478200	0.59395600	1.08900400
F	-2.79490500	-1.26606700	0.00102300



SCF energy=-792.837831

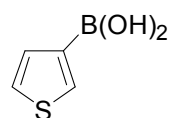
C	-0.56128100	0.24685700	-0.54001600
H	-0.19043600	1.02102800	-1.21298300
C	0.26783900	-0.67258300	-0.00694100
H	-0.18393300	-1.44279800	0.62079900
B	1.87710400	-0.63924400	-0.14063500
F	2.48044900	-1.79500500	-0.55795900
F	2.27127200	0.49708300	-0.97467000
F	2.38214600	-0.23992200	1.19082800
Na	1.77329200	1.78836500	0.70632200
C	-2.02806400	0.33415600	-0.34020500
O	-2.55080800	-0.71782500	0.32875200
O	-2.70112700	1.27590200	-0.72979100
C	-3.97116900	-0.67994400	0.55034400
H	-4.24264400	0.19524500	1.14737700
H	-4.50454000	-0.64399900	-0.40338200
H	-4.20344800	-1.60020300	1.08724600



SCF energy=-542.2993941

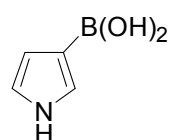
C	-0.02911800	2.31872800	0.01793600
C	1.20286100	1.66518400	0.02336300
C	1.25212200	0.25987000	-0.00706500
C	0.04607300	-0.45669400	-0.04876600
C	-1.21364400	0.18461800	-0.07418700
C	-1.22246100	1.59900600	-0.02453600

H	-0.64326900	2.17823300	-0.00075700
O	-2.22368100	-0.69974400	0.00026000
B	1.48123100	0.01012600	0.00007500
O	2.11193900	1.22572500	0.00051900
H	3.07761300	1.13429700	0.00018700
O	2.28120800	-1.11369600	-0.00044000
H	1.80703800	-1.95579900	-0.00130700
H	-0.76820700	-2.15626800	0.00097700



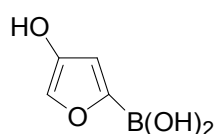
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C	-1.82179000	1.13919100	-0.00001600
C	-0.46339300	1.29118000	0.00000400
C	0.26000800	0.04546400	0.00002100
C	-0.61257300	-1.02322600	0.00000700
H	-2.58554700	1.90631300	-0.00003000
H	0.03028300	2.25685200	0.00002700
B	1.81824300	-0.04850400	0.00000600
O	2.53561700	1.11864000	0.00000200
H	3.49220100	0.95805800	-0.00001700
O	2.53385400	-1.22644500	-0.00001700
H	1.99702700	-2.03017100	0.00000700
H	-0.38260100	-2.08273400	0.00002800
S	-2.27324100	-0.53868900	-0.00000100



SCF energy=-386.2556559

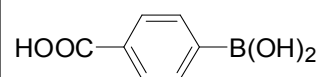
C	-2.24662700	0.69326400	-0.00008500
C	-0.95140500	1.15860800	-0.00023300
C	-0.06129600	0.02761000	-0.00014600
C	-0.88164400	-1.09406100	0.00061500
N	-2.18734200	-0.68602100	-0.00008900
H	-2.98833900	-1.30082900	-0.00009200
H	-3.19431800	1.21296300	-0.00020700
H	-0.67522900	2.20674900	-0.00035900
B	1.48526100	-0.00408500	-0.00006500
O	2.13473100	-1.21578600	-0.00039400
H	3.09800800	-1.10448800	-0.00049400
O	2.28095900	1.12607900	0.00036900
H	1.78543300	1.95625200	0.00044300
H	-0.62015000	-2.14295100	0.00095300



SCF energy=-481.3286515

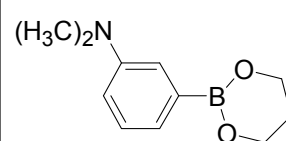
C	-1.53775600	1.16789400	0.00058100
C	-1.91482100	-0.14746900	-0.00018500
C	-0.71410000	-0.91965800	0.00010700
C	0.33366000	-0.03157800	0.00010100
H	-2.08930300	2.09477000	0.00113400
H	-0.62394000	-1.99884000	-0.00027100
B	1.87789000	-0.16701700	-0.00001500
O	2.43065400	-1.41847600	0.00014300
H	3.39993100	-1.38847200	0.00010700
O	2.69920500	0.93300400	-0.00049300
H	2.21226800	1.77127900	0.00046400
O	-3.21132200	-0.57997800	-0.00133000
H	-3.23047100	-1.54844900	0.00666900

H	-0.07065800	3.40504800	0.05243600
H	2.11299600	2.26233300	0.06087900
B	2.60728800	-0.52919300	0.00715900
O	2.58116700	-1.90109300	0.00597700
H	3.47502300	-2.27685300	0.01217100
O	3.85107000	0.06541400	0.01901200
H	3.83081300	1.03217600	0.01356700
H	-2.15854800	2.14525400	-0.02016200
H	0.10629600	-1.53786400	-0.06380900
N	-2.39736700	-0.54521100	-0.15702000
C	-2.35744500	-1.98435800	0.05748900
H	-1.99135800	-2.25612000	1.06172800
H	-3.36463500	-2.38893700	-0.06387600
H	-1.71467300	-2.47313100	-0.68301900
C	-3.66279900	0.13268400	0.07472600
H	-3.81656900	0.93605800	-0.65520000
H	-4.47821100	-0.58283600	-0.05096500
H	-3.73676700	0.56851100	1.08591900



SCF energy=-596.

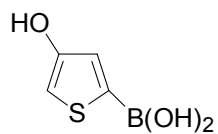
C	-0.75450100	-1.18073500	-0.00001600
C	0.63938500	-1.18039000	-0.00001000
C	1.37364600	0.02111400	0.00003200
C	0.64954100	1.22841300	0.00003700
C	-0.74276300	1.24460300	0.00004600
C	-1.45341000	0.03595600	0.00001300
H	1.16962200	2.18560900	0.00008300
H	-1.29412900	2.17958200	0.00004600
B	2.94621500	-0.02470500	0.00000600
O	3.75793000	1.08556200	-0.00006800
H	3.29711800	1.93552500	-0.00011300
O	3.55781000	-1.24881400	0.00004200
H	4.52491500	-1.17539200	-0.00003300
H	1.17551400	-2.12489000	-0.00003800
H	-1.30291100	-2.11663800	-0.00005700
C	-2.93979900	0.09679900	-0.00000200
O	-3.59624200	1.12125500	-0.00002600
O	-3.52515400	-1.12993300	-0.00002300
H	-4.48855900	-0.97940100	0.00007700



SCF energy=-659.0241595

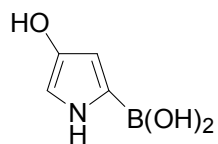
C	-2.49995300	1.49590200	-0.00743500
C	-2.23115300	0.10972800	0.07384800
C	-0.87511700	-0.28706000	0.08716000
C	0.17619800	0.64266100	0.05324700
C	-0.12653500	2.01459600	-0.00863100
C	-1.45883800	2.42469200	-0.04236600
H	0.67631100	2.74545200	-0.03689600
H	-1.70247300	3.48345800	-0.10119400
B	1.66069400	0.14844100	0.08647200
O	1.91463300	-1.20340700	0.13673200
O	2.67157400	1.08024800	0.06226900
C	3.25896400	-1.69277800	0.17488600
H	3.25825200	-2.66845600	-0.32201100
H	3.54015400	-1.84924900	1.22590300
C	4.04288200	0.67354700	0.09484200
H	4.38512400	0.69572300	1.13910800
H	4.61249300	1.42483400	-0.46182200
C	4.22181700	-0.72032000	-0.50166000
H	4.01710500	-0.68908000	-1.57996000

O -0.17601800 1.25165800 0.00022300



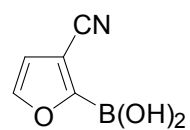
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C -1.87719400 0.94797900 -0.00010800  
C -1.89188800 -0.42584300 0.00005400  
C -0.58534900 -0.99654700 0.00011100  
C 0.42836300 -0.06088100 0.00001600  
S -0.25577900 1.54735500 -0.00016500  
H -2.72754200 1.61570500 -0.00006200  
H -0.38862600 -2.06509600 0.00021000  
B 1.95898100 -0.33847500 0.00002600  
O 2.36869000 -1.64578500 -0.00034900  
H 3.33552900 -1.72244600 -0.00028200  
O 2.93379500 0.63413700 0.00035900  
H 2.61748900 1.54826400 0.00074900  
O -3.06587200 -1.13181800 0.00011500  
H -2.87578500 -2.08224500 0.00045300



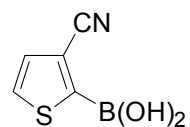
SCF energy=-461.4815069

C 1.58879300 1.19305900 0.00010200  
C 1.92270100 -0.15286800 0.00006300  
C 0.72058800 -0.89815100 -0.00006800  
C -0.34715600 0.00858800 -0.00011500  
N 0.22111600 1.26498800 -0.00008200  
H -0.32158100 2.11712200 0.00063200  
H 2.21977200 2.06946100 0.00016000  
H 0.64116400 -1.97992500 -0.00021600  
O 3.21875400 -0.60711000 0.00007300  
H 3.21822400 -1.57555100 -0.00086100  
B -1.87842800 -0.16916300 0.00000200  
O -2.52834900 -1.38373900 0.00016100  
H -1.93915400 -2.15044800 0.00024000  
O -2.65086700 0.97008000 -0.00013700  
H -3.59994800 0.77263000 -0.00005600



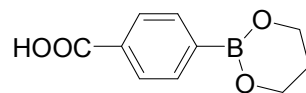
SCF energy=-498.3615079

C -1.57370800 -1.87576000 0.00014900  
C -2.15677900 -0.64493700 -0.00007100  
C -1.06374400 0.28507900 -0.00005500  
C 0.11399700 -0.44523100 0.00003600  
O -0.21967100 -1.76935100 0.00024300  
B 1.62330300 -0.02864800 0.00017500  
O 2.55751000 -1.01982700 -0.00050300  
H 3.46139800 -0.66677800 -0.00096500  
O 2.02745800 1.27784400 0.00051000  
H 1.33492000 1.95696800 0.00052600  
H -3.21240900 -0.41439000 -0.00033200  
H -1.96761600 -2.88105000 0.00004800  
C -1.12396600 1.70511500 -0.00018100  
N -1.11857000 2.87051100 -0.00020300



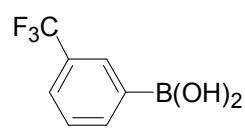
SCF energy=-821.358191

H 5.25748900 -1.05901400 -0.36962500  
H -3.52080300 1.85892600 -0.04068400  
N -3.26601300 -0.82759300 0.15597800  
C -4.62147800 -0.40109500 -0.15244400  
H -4.73029200 -0.02273800 -1.18408600  
H -5.29871000 -1.24866800 -0.02398300  
H -4.95004300 0.38630200 0.53532200  
C -2.95574800 -2.23284000 -0.05711500  
H -3.86867100 -2.82035900 0.06618300  
H -2.54425500 -2.43487200 -1.06129800  
H -2.23314300 -2.59016000 0.68442700  
H -0.61580400 -1.33808000 0.12839800



SCF energy=-713.6414182

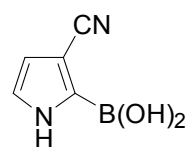
C -0.26928700 0.01368400 -0.05150700  
C 0.46468700 -1.18706800 -0.03707300  
C 1.85843100 -1.18400800 -0.00753700  
C 2.55317100 0.03561100 0.00743700  
C 1.83822400 1.24300400 -0.00711100  
C 0.44600900 1.22659700 -0.03647800  
H 2.38842600 2.17881500 0.00445400  
H -0.10147500 2.16508000 -0.04810800  
B -1.83817500 0.00068000 -0.08693100  
O -2.48607100 -1.20844600 -0.10204100  
O -2.50591500 1.19874000 -0.09880600  
C -3.91837800 -1.26489000 -0.13435200  
H -4.21248400 -2.17691800 0.39427800  
H -4.23354400 -1.36356400 -1.18207100  
C -3.93891400 1.23213400 -0.13085700  
H -4.25575600 1.32871100 -1.17826200  
H -4.24765000 2.13774900 0.40040300  
C -4.53445100 -0.02223500 0.50366100  
H -4.33067500 -0.02205600 1.58250500  
H -5.62393100 -0.03103200 0.37232100  
H -0.06825700 -2.13390800 -0.04923000  
C 4.03740400 0.09797000 0.03789600  
O 4.69690500 1.12109900 0.05219400  
O 4.62703900 -1.12901500 0.04890300  
H 5.58904000 -0.97206400 0.06838200  
H 2.41013100 -2.11803900 0.00350700



SCF energy=-745.4108457

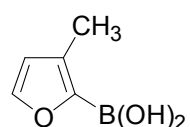
C 0.28134500 2.37386900 0.00071100  
C 1.47679900 1.65229800 0.00786300  
C 1.48910700 0.24675500 -0.00361600  
C 0.24943400 -0.41773100 -0.02246400  
C -0.94963000 0.29826600 -0.03204500  
C -0.93846900 1.69791800 -0.01837000  
H 0.29760300 3.46023100 0.00720600  
H 2.41156200 2.21176400 0.02137100  
B 2.81779200 -0.59434200 0.00061200  
O 2.71567200 -1.95804900 -0.00417400  
H 3.58189100 -2.39409000 -0.00206400  
O 4.08252300 -0.05391300 0.00867000  
H 4.12243200 0.91191400 0.01029200  
H -1.87242700 2.25101800 -0.02917300  
H 0.23210200 -1.50268100 -0.03539400  
C -2.26572700 -0.43458300 -0.00323300  
F -2.69791300 -0.64802800 1.27115600  
F -2.19540100 -1.65085000 -0.59483100  
F -3.25166500 0.25759900 -0.63014000

C	-2.50249200	0.07992300	0.00002400
C	-1.81116800	1.26173800	-0.00066900
C	-0.39751900	1.04230000	0.00001700
C	-0.02166100	-0.29958600	-0.00002500
S	-1.44659800	-1.28785700	0.00031600
B	1.40761500	-0.94608300	-0.00008300
O	2.57724900	-0.24112100	-0.00006200
H	2.51075200	0.72716400	-0.00014900
O	1.46199000	-2.31280000	-0.00029200
H	2.37351600	-2.64473200	0.00006700
H	-2.26919300	2.24404900	-0.00123400
C	0.56702900	2.09476600	0.00023500
N	1.39282400	2.91753500	0.00027400
H	-3.57640100	-0.05656500	0.00009700



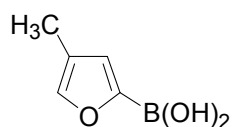
SCF energy=-478.5236267

C	-1.65965400	-1.85152600	0.00004100
C	-2.18266500	-0.57402700	-0.00031400
C	-1.06924400	0.31684000	-0.00003600
C	0.11299600	-0.43977800	-0.00035900
N	-0.29355500	-1.75104900	0.00037200
H	0.35589100	-2.52681800	0.00055400
B	1.61415200	-0.03588400	-0.00012600
O	2.07397700	1.24979600	-0.00009900
H	1.39818600	1.94685900	0.00023100
O	2.51844300	-1.06969300	-0.00002200
H	3.43701200	-0.75798400	0.00027800
H	-3.22861100	-0.30187000	-0.00047700
H	-2.15399700	-2.81259100	0.00025200
C	-1.08768100	1.73707700	0.00010800
N	-1.03517600	2.90240300	0.00021800



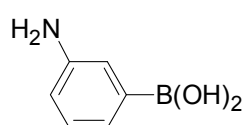
SCF energy=-445.4237039

C	-1.82084200	-1.41695000	0.00004500
C	-2.23719500	-0.11885000	-0.00012000
C	-1.05189900	0.69204900	0.00003900
C	0.01746300	-0.17513100	0.00000900
O	-0.46765100	-1.48306700	-0.00000700
H	-2.34231700	-2.36334600	0.00011100
H	-3.26306700	0.22688500	-0.00024400
C	-1.00389700	2.19234200	0.00007700
H	-1.51186000	2.60041500	-0.88321100
H	-1.51278600	2.60038300	0.88281900
H	0.02698200	2.55354900	0.00056800
B	1.56071000	-0.04679800	0.00001500
O	2.14475000	1.19357600	-0.00006000
H	3.11272200	1.13256300	-0.00013500
O	2.37198700	-1.15673200	0.00002700
H	1.87231500	-1.98743300	0.00002900



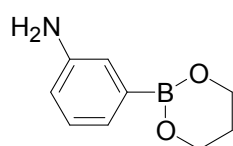
SCF energy=-445.4222621

C	1.48521000	1.17629400	-0.00002500
C	1.90091700	-0.12652200	-0.00000100
C	0.69290500	-0.90079300	-0.00016000
C	-0.36917600	-0.03431600	0.00000200
O	0.12802400	1.26132100	-0.00009700



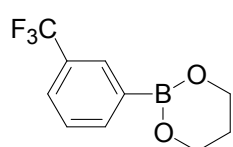
SCF energy=-463.6851068

C	1.21597700	1.86320000	0.01865600
C	-0.13864900	1.52467600	0.01865500
C	-0.53592100	0.17441300	0.00264200
C	0.46109200	-0.81362900	-0.01169100
C	1.82678700	-0.48701700	-0.01318200
C	2.19457300	0.86994600	0.00168900
H	1.51710100	2.90800800	0.03281000
H	-0.87551600	2.32648000	0.03614100
B	-2.04415900	-0.25662900	0.00172400
O	-3.10408500	0.62322300	-0.03213000
H	-2.85020500	1.55560000	-0.06752500
O	-2.35094800	-1.59295500	0.03543400
H	-3.30889200	-1.74324500	0.02490200
H	3.24814300	1.14304200	-0.00622400
H	0.16390400	-1.85992100	-0.02701100
N	2.80087400	-1.48983200	-0.09018100
H	3.71235500	-1.24393100	0.27700600
H	2.50490100	-2.40575100	0.22550100



SCF energy=-580.410381

C	-3.33078300	0.69646900	0.05262800
C	-2.81706500	-0.61081400	0.01310300
C	-1.42509800	-0.78593900	-0.03182700
C	-0.54495200	0.30786500	-0.03690900
C	-1.08313700	1.60792900	0.00351600
C	-2.46626800	1.79233200	0.04857300
H	-4.40819200	0.85087100	0.07956800
H	-0.41644400	2.46526900	0.00081100
H	-2.88159900	2.79718600	0.08081500
B	1.00291900	0.08052700	-0.08589700
O	1.83397300	1.17532500	-0.09848600
O	1.48781700	-1.20653100	-0.10897500
C	3.25514000	1.01311500	-0.14448800
H	3.69135500	1.86711300	0.38370900
H	3.57502800	1.06617000	-1.19462700
C	2.89676500	-1.45557700	-0.15339100
H	3.19055600	-1.59098500	-1.20374200
H	3.07059200	-2.40179100	0.36930000
C	3.68136800	-0.31141900	0.48365900
H	4.75887900	-0.46760600	0.34486500
H	3.48548600	-0.28678800	1.56378000
H	-1.01727300	-1.79438900	-0.06813300
N	-3.68065200	-1.71739300	-0.04486900
H	-3.27371700	-2.59017000	0.27088200
H	-4.59484500	-1.56987700	0.36684500

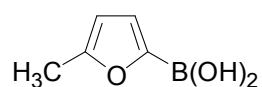


SCF energy=-862.1387866

C	2.21106400	1.65064400	-0.06980400
C	1.96140600	0.27352100	-0.04393100
C	0.64903300	-0.20451600	0.00627300
C	-0.44061900	0.68197800	0.02755800
C	-0.17208600	2.06229900	-0.00054100
C	1.13805400	2.54316700	-0.04954800

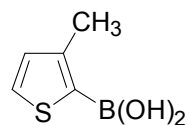


H	2.01836700	2.11656600	0.00006400
B	-1.91180600	-0.18339400	-0.00000700
O	-2.45825900	-1.43785400	0.00003500
H	-3.42755600	-1.41075200	-0.00017400
O	-2.74378500	0.91027300	0.00013100
H	-2.26166800	1.75126200	-0.00017000
C	3.31378800	-0.63410000	0.00010900
H	3.51587500	-1.25234000	0.88364400
H	3.51596300	-1.25225200	-0.88346000
H	4.03297700	0.19205400	0.00019000
H	0.61537400	-1.98086100	-0.00016400



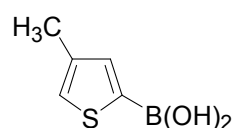
SCF energy=-445.426003

C	-1.81309700	-0.04793100	0.00003100
C	-1.63623200	1.31013500	0.00010800
C	-0.22574200	1.53835500	0.00001500
C	0.39048200	0.31393000	-0.00013800
O	-0.59860900	-0.66633000	-0.00011100
B	1.85699100	-0.18025100	-0.00002000
O	2.86974300	0.74079100	-0.00004000
H	3.74285300	0.31908500	0.00008700
O	2.17137600	-1.51905300	0.00011500
H	1.38785900	-2.08958400	0.00012100
H	0.28356500	2.49301700	-0.00001800
H	-2.42306000	2.05289600	0.00023000
C	-3.01732200	-0.92440100	-0.00000900
H	-3.92424000	-0.31292700	0.00044100
H	-3.04049300	-1.57217100	-0.88559300
H	-3.04005900	-1.57285500	0.88507900



SCF energy=-768.4127401

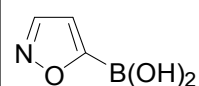
C	2.33167600	-0.63942700	-0.00002500
C	2.10047800	0.70973500	0.00005000
C	0.70981800	1.05473100	0.00005200
C	-0.11912600	-0.05861900	-0.00003500
S	0.85210000	-1.52618800	-0.00011000
H	3.28254300	-1.15688300	-0.00004700
H	2.89615100	1.44905800	0.00011100
B	-1.67157300	-0.17978200	-0.00002300
O	-2.34579700	-1.38414700	0.00028100
H	-1.79626700	-2.18006500	0.00063900
O	-2.45210100	0.94907700	-0.00030500
H	-3.39564600	0.72222600	-0.00021700
C	0.25503200	2.49244500	0.00014100
H	-0.83187700	2.57441900	0.00015700
H	0.64264500	3.01821800	0.88273900
H	0.64261700	3.01830800	-0.88241500



SCF energy=-768.4128054

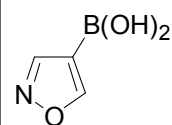
C	1.79601800	1.01300100	-0.00000300
C	1.90069500	-0.35882700	0.00008800
C	0.60605500	-0.96421400	0.00016600
C	-0.45444500	-0.07894000	0.00006800
S	0.15687600	1.55808100	-0.00006400
H	2.60793700	1.73051900	0.00001800
B	-1.98104800	-0.37153000	0.00000100
O	-2.51113800	-1.64396200	-0.00011500
H	-1.85661900	-2.35560600	-0.00028900

H	-1.00312100	2.76248400	0.01452600
H	1.32727800	3.61313600	-0.07395800
B	-1.91119500	0.13936800	0.08206100
O	-2.94494500	1.04069900	0.10690700
O	-2.10931400	-1.21726800	0.09985900
C	-4.30322300	0.58312800	0.15903600
H	-4.91024500	1.33077500	-0.36070500
H	-4.61729700	0.56251300	1.21146700
C	-3.43627300	-1.75896900	0.14517500
H	-3.68655200	-1.96346300	1.19500500
H	-3.40771600	-2.71413700	-0.38800500
C	-4.44545300	-0.79728000	-0.47735400
H	-4.26798000	-0.72495600	-1.55840000
H	-5.46551800	-1.17551600	-0.33375800
H	3.23141100	2.01928100	-0.11081500
C	3.11177200	-0.69607900	-0.01225000
H	0.46430800	-1.27402100	0.02390000
F	3.49040100	-0.99633200	1.26322200
F	4.21806100	-0.20924300	-0.63193000
F	2.81191900	-1.87750800	-0.60811100



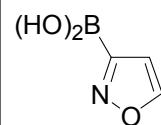
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C	-2.27467800	0.54303300	0.00028000
C	-1.00369900	1.18164700	-0.00011000
C	-0.10664500	0.14877000	0.00000500
O	-0.80341400	-1.02502200	-0.00005000
H	-3.26164300	0.98890800	0.00040800
H	-0.78470300	2.23941100	-0.00018800
N	-2.17225900	-0.76709800	-0.00019900
B	1.45311900	0.02796100	-0.00001900
O	2.07646500	-1.18902300	0.00010700
H	1.46576000	-1.94236100	0.00009800
O	2.18794300	1.17632900	-0.00003900
H	3.14297600	1.00496500	-0.00002800



SCF energy=-422.1108391

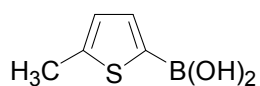
C	-0.97294500	-1.09260200	0.00095000
C	-0.07926400	0.03258600	-0.00009900
C	-0.96304300	1.07858100	-0.00054800
O	-2.23410300	0.65386500	-0.00045200
H	-0.71009000	-2.14330200	0.00164300
N	-2.23678500	-0.75468500	0.00032900
H	-0.84540100	2.15488500	-0.00130200
B	1.47528700	0.00100500	-0.00033000
O	2.08127000	-1.22501200	-0.00087900
H	3.04912900	-1.15809700	-0.00049200
O	2.28421400	1.11447300	0.00077900
H	1.82789300	1.96627800	0.00208400



SCF energy=-422.1120029

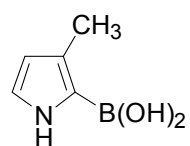
C	-0.10249100	0.07249200	-0.00007700
C	-1.01787900	1.17267000	0.00014500
C	-2.24127200	0.57948100	-0.00002000
O	-2.11102100	-0.76391500	-0.00013900
N	-0.75402200	-1.07667900	0.00017100
H	-3.25673200	0.94977000	-0.00006900
H	-0.78264000	2.22661100	0.00025900
B	1.46837900	0.02264800	-0.00009400

O	-2.85745900	0.68033900	0.00008400
H	-3.78180800	0.38721200	0.00000800
C	3.19785600	-1.12571000	-0.00006300
H	4.05868500	-0.44934100	0.00154300
H	3.28057600	-1.77237500	0.88288800
H	3.28188500	-1.76979500	-0.88479000
H	0.47627400	-2.04512600	0.00035100



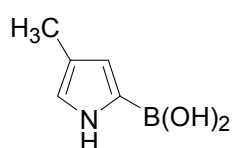
SCF energy=-768.4135705

C	-1.95899300	0.09364800	-0.00011300
C	-1.49507600	1.38944000	-0.00012400
C	-0.07464500	1.47311200	-0.00002900
C	0.56808900	0.25058300	0.00000700
S	-0.62890900	-1.02770600	-0.00001300
B	2.08791200	-0.06612300	0.00001700
O	3.06748100	0.90444300	0.00012700
H	2.73731200	1.81315000	0.00025100
O	2.49373400	-1.37447800	-0.00007600
H	3.45985000	-1.45745600	-0.00014900
H	0.45306100	2.42424400	-0.00008300
H	-2.15407100	2.25257200	-0.00022600
C	-3.38510600	-0.37603300	0.00013800
H	-3.61318400	-0.98539900	-0.88315200
H	-3.61378400	-0.98244100	0.88532700
H	-4.06153100	0.48501800	-0.00151900



SCF energy=-425.574224

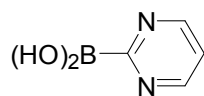
C	-1.90933500	-1.40305000	0.00011100
C	-2.24643900	-0.05742200	0.00029000
C	-1.03854000	0.68878700	-0.00008300
C	0.02482000	-0.22460500	-0.00010700
N	-0.55101000	-1.48801100	-0.00024600
H	-0.00937600	-2.34125000	0.00087700
H	-2.53209100	-2.28721300	-0.00004500
H	-3.25173700	0.34526100	0.00019200
C	-0.93987400	2.19204400	-0.00018200
H	-1.93726600	2.64444300	-0.00055100
H	-0.42073100	2.57667800	0.88929600
H	-0.42014500	2.57636700	-0.88943200
B	1.55763300	-0.07238300	-0.00005200
O	2.23402900	1.12868500	0.00026800
H	1.65979100	1.90652700	0.00038100
O	2.31254100	-1.22580600	-0.00013700
H	3.26411400	-1.04038000	0.00003900



SCF energy=-425.5736636

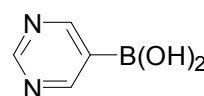
C	1.53784000	1.21032800	-0.00000700
C	1.90876300	-0.12803100	-0.00016700
C	0.69594500	-0.86963300	-0.00019300
C	-0.38284000	0.01571500	0.00004400
N	0.17371800	1.28310600	0.00010400
H	-0.37491000	2.13156900	-0.00054000
H	2.15037100	2.10247400	-0.00019300
B	-1.91135800	-0.18570600	0.00003900
O	-2.53815700	-1.41251600	0.00001200
H	-1.93139900	-2.16565800	-0.00000100

O	2.15608900	1.20111000	-0.00005300
H	3.11725900	1.06753400	-0.00002300
O	2.14055400	-1.16667400	0.00004300
H	1.54324500	-1.93242700	0.00002400



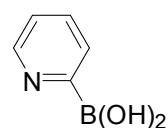
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C	-0.11405900	0.00000000	0.00000700
N	0.51224800	1.19569200	0.00000400
C	1.84858300	1.18402200	0.00000100
C	2.58550200	0.00000000	-0.00000300
C	1.84858300	-1.18402200	-0.00000400
N	0.51224800	-1.19569200	0.00000100
H	2.34119200	2.15560800	0.00000000
H	3.67159100	0.00000000	-0.00000600
H	2.34119200	-2.15560800	-0.00000500
B	-1.70389200	0.00000000	0.00000100
O	-2.33793200	-1.21330600	0.00000200
H	-3.30536800	-1.18578600	-0.00000100
O	-2.33793200	1.21330600	-0.00000300
H	-3.30536800	1.18578500	-0.00002600



SCF energy=-440.4067698

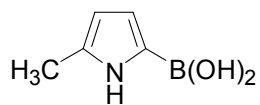
C	2.54518400	-0.01792100	0.00003600
N	1.93143300	-1.20736300	0.00068400
C	0.59362700	-1.17430500	0.00067200
C	-0.15226600	0.01777100	0.00005600
C	0.62549800	1.18370400	-0.00073200
N	1.96343700	1.18736900	-0.00072600
H	0.08773600	-2.13720000	0.00123900
H	3.63286300	-0.03151700	-0.00002000
H	0.16542600	2.17363600	-0.00137500
B	-1.72217900	0.00008400	0.00029400
O	-2.34351700	-1.21708600	-0.00128900
H	-3.31063300	-1.14096000	-0.00115100
O	-2.51327700	1.12335100	0.00098500
H	-2.04649000	1.96996700	0.00236800



SCF energy=-424.3645256

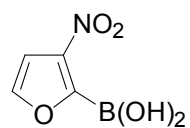
C	-0.15829500	0.06597100	-0.00012500
C	0.59133900	1.25040000	-0.00024500
C	1.98553000	1.17877700	-0.00012300
C	2.59106100	-0.07806300	0.00010700
C	1.77262800	-1.21273400	0.00020900
N	0.43754500	-1.15270200	0.00011800
H	2.58791900	2.08391400	-0.00021800
H	0.07776400	2.20748600	-0.00045700
H	3.67233300	-0.18480200	0.00020900
H	2.20950100	-2.20991500	0.00039600
B	-1.73557200	0.01212400	-0.00032500
O	-2.45832900	1.17357200	0.00043600
H	-3.41453000	1.01132900	0.00062600
O	-2.35842500	-1.20162900	-0.00021500
H	-1.67747700	-1.90136100	-0.00046200

O	-2.70703500	0.93798600	0.00002600
H	-3.65150900	0.71908500	0.00017400
C	3.31108500	-0.66994900	0.00013900
H	3.50517300	-1.29416700	-0.88178900
H	4.04861700	0.14058900	-0.00286800
H	3.50687900	-1.28909600	0.88528800
H	0.62432700	-1.95234900	-0.00019900



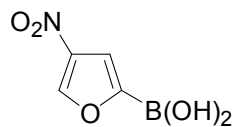
SCF energy=-425.5761166

C	-1.85233800	-0.07472900	-0.00011600
C	-1.63040900	1.29781700	-0.00026400
C	-0.22814000	1.50411700	0.00016700
C	0.40168600	0.26011000	0.00054700
N	-0.62430200	-0.67636600	0.00044100
H	-0.45911500	-1.67405900	0.00050800
B	1.87804200	-0.17711800	0.00013600
O	2.95232100	0.68642900	-0.00031900
H	2.70738400	1.62202100	0.00027100
O	2.14799500	-1.52823000	-0.00024900
H	3.10014100	-1.71077100	0.00000100
H	0.27016400	2.46687300	0.00029300
H	-2.40235000	2.05693900	-0.00062500
C	-3.12806300	-0.85818500	-0.00018300
H	-3.21484100	-1.50205400	-0.88590900
H	-3.21545300	-1.50108800	0.88618400
H	-3.98496600	-0.17807500	-0.00085700



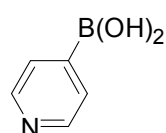
SCF energy=-610.6064583

C	0.39492600	2.45481600	-0.00001900
C	1.44552600	1.59389800	-0.00010100
C	0.84538000	0.29807100	0.00005600
C	-0.53615800	0.43349800	0.00009300
O	-0.78494200	1.77362300	0.00010600
B	-1.80516700	-0.50879200	-0.00009900
O	-3.01353600	0.12323900	-0.00005800
H	-3.74792600	-0.51088100	0.00043600
O	-1.72394300	-1.86110100	-0.00018900
H	-0.79866800	-2.17839300	-0.00008800
H	2.50062000	1.82075200	-0.00013900
N	1.60835400	-0.91947300	0.00005500
O	1.01430800	-2.01327200	0.00028600
O	2.83315500	-0.81802100	-0.00019200
H	0.31494200	3.53134400	0.00010600



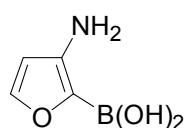
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C	-0.74153000	1.38157500	0.00015700
C	-1.21291600	0.09534500	0.00014400
C	-0.08931100	-0.78227500	0.00021300
C	1.01800600	0.01912000	0.00019900
O	0.60047600	1.35414200	0.00022800
B	2.55468700	-0.23487600	-0.00002400
O	2.98405600	-1.52844500	0.00028300
H	3.95119900	-1.60184300	0.00012100
O	3.46170100	0.79084800	-0.00053200
H	3.06522100	1.67492200	-0.00090500
H	-1.22989300	2.34362200	0.00024800
H	-0.10875700	-1.86219200	0.00029600



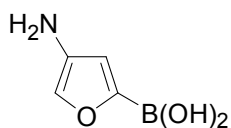
SCF energy=-424.3583455

C	-1.95114800	-1.15424300	0.00079000
C	-0.55533500	-1.18740300	0.00068200
C	0.17042400	0.01550900	-0.00011000
C	-0.58831500	1.19684300	-0.00084300
C	-1.98344100	1.13038100	-0.00073700
N	-2.66771600	-0.02091400	0.00010900
H	-2.52493300	-2.07936400	0.00143100
H	-0.03343100	-2.13980600	0.00121000
H	-0.11787600	2.17944800	-0.00168200
H	-2.57982100	2.04121000	-0.00132000
B	1.74526200	-0.00068400	-0.00007100
O	2.53135900	1.12646100	0.00132900
H	2.05029800	1.96533100	0.00316700
O	2.37592900	-1.21350000	-0.00143900
H	3.34205300	-1.12722000	-0.00103000



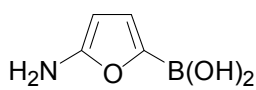
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C	-1.98103200	-1.26373600	0.00009200
C	-2.23611900	0.07791900	0.00016300
C	-0.94720000	0.70556500	-0.00008700
C	0.00157400	-0.29099700	-0.00025100
O	-0.64650100	-1.50417900	-0.00012500
H	-2.61680100	-2.13725400	0.00014500
H	-3.20809800	0.55394000	0.00022500
B	1.55334800	-0.16261700	-0.00002400
O	2.34413400	-1.27799800	0.00010200
H	3.28547800	-1.04365200	0.00004800
O	2.10931500	1.08820100	0.00005200
H	1.40282300	1.77198000	0.00003300
N	-0.59631300	2.09882900	-0.00005700
H	-0.96774200	2.57793100	-0.81947600
H	-0.96713600	2.57765000	0.81981100



SCF energy=-461.4628897

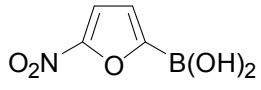
C	1.51798200	1.17012700	-0.00883200
C	1.91291000	-0.14342700	0.00450900
C	0.70331600	-0.91052100	0.01201700
C	-0.34824900	-0.02988100	0.00105900
O	0.15316200	1.25640000	-0.00547500
H	2.05658400	2.10604100	-0.00708800
B	-1.89144300	-0.17287100	-0.00108800
O	-2.44359200	-1.42513700	-0.00360900
H	-3.41276100	-1.39371100	-0.00236900
O	-2.71762800	0.92497500	-0.00168400
H	-2.22965900	1.76267100	0.00261800
N	3.21453100	-0.66297000	0.08769600
H	3.33199200	-1.53884600	-0.41031100
H	3.93888300	-0.00902900	-0.18880600
H	0.61917100	-1.98967500	0.03115800



SCF energy=-461.4718521

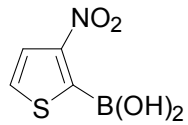
C	-1.82004800	-0.09026500	0.00199100
C	-1.68155700	1.27759000	0.00385400

N	-2.60341500	-0.27276300	-0.00008400
O	-3.43544800	0.64024700	0.00004500
O	-2.86988500	-1.47596300	-0.00044100



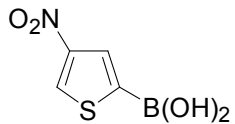
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C	-1.16264400	0.28839600	-0.00014800
C	-0.86290300	1.62498900	0.00029200
C	0.55735600	1.68055600	0.00040100
C	1.02432700	0.38436400	-0.00003800
O	-0.05344600	-0.47630700	-0.00041800
B	2.43844300	-0.27898800	-0.00006600
O	3.52183600	0.54788000	0.00000400
H	4.36247400	0.06360500	0.00004800
O	2.60112100	-1.63530900	-0.00017300
H	1.77380700	-2.14130400	-0.00023900
H	1.17664800	2.56717100	0.00068400
H	-1.57468500	2.43710500	0.00041000
N	-2.42576600	-0.38395200	0.00001200
O	-3.42744100	0.34053400	-0.00077400
O	-2.42793400	-1.61602300	0.00090000



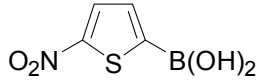
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C	0.25705700	2.51319300	-0.00024500
C	1.31200400	1.64662800	-0.00016300
C	0.86426900	0.29207800	-0.00001600
C	-0.51683200	0.10977900	0.00030200
S	-1.25701800	1.68016000	0.00013600
B	-1.51795100	-1.11815600	0.00005400
O	-1.16601700	-2.42409500	-0.00002500
H	-0.19394300	-2.53254400	-0.00010100
O	-2.84299900	-0.76608300	-0.00011400
H	-3.42531700	-1.54167200	-0.00012100
H	2.35565800	1.93051800	-0.00034300
N	1.85626800	-0.77066400	0.00003200
O	1.49157000	-1.95928000	-0.00020800
O	3.04033800	-0.44037700	0.00022800
H	0.28965100	3.59517700	-0.00040600



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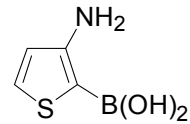
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C	1.30445000	0.05138300	0.00000400
C	0.14481600	-0.77104900	-0.00007100
C	-1.02162500	-0.04061200	-0.00014200
S	-0.65154200	1.67639000	0.00016200
B	-2.50372500	-0.53229700	-0.00005500
O	-2.86821200	-1.85469200	0.00047400
H	-2.14174600	-2.49301500	0.00057900
O	-3.48606000	0.41698000	-0.00052200
H	-4.37795200	0.03564100	-0.00020300
H	1.75746200	2.20692200	0.00030300
N	2.65441900	-0.47828100	-0.00005500
O	2.78037700	-1.70636300	-0.00021700
O	3.58998800	0.32535000	0.00005400
H	0.20474800	-1.85327300	-0.00028400



SCF energy=-933.5908182

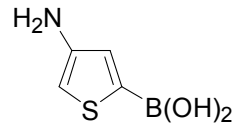
C	-1.30659200	0.23825600	-0.00001600
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C	-0.27454400	1.51738600	0.00498300
C	0.37381700	0.31031900	0.00097800
O	-0.61447800	-0.69650600	0.00101300
B	1.84097100	-0.15613400	-0.00178900
O	2.84046800	0.78273300	-0.02007800
H	3.71873100	0.37233100	-0.01265900
O	2.18825800	-1.48999100	0.01361000
H	1.41996800	-2.07943300	0.03878400
H	0.21686100	2.48168500	0.00530300
H	-2.47981400	2.00699800	0.00791100
N	-2.91728100	-0.93035600	0.07390600
H	-3.78589300	-0.50630700	-0.22827100
H	-2.77373000	-1.84217800	-0.34666200



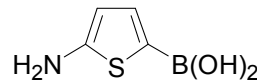
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C	-2.05163700	0.83328700	0.01313800
C	-0.63564900	1.07247700	-0.01488000
C	0.12033000	-0.10008100	-0.01873800
S	-0.95538200	-1.49497100	-0.00392100
B	1.65182800	-0.23289800	-0.00042900
O	2.35855800	-1.41832000	-0.00578500
H	1.82103700	-2.22180000	-0.03571700
O	2.40523900	0.92629700	0.03604500
H	3.35632700	0.73593700	0.05034400
H	-2.79359500	1.62605900	0.00941400
N	-0.10912200	2.35128100	-0.09726000
H	-0.65516900	3.09063100	0.32547000
H	0.88806200	2.42388700	0.07243900
H	-3.34991900	-0.94430500	0.04235100



SCF energy=-784.4561087

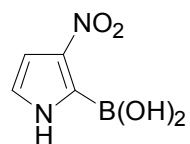
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C	1.90580900	-0.39402500	0.00111300
C	0.60454200	-0.98502300	-0.00025500
C	-0.43747600	-0.07844300	-0.00208000
S	0.19527100	1.54621100	0.01067600
B	-1.96855900	-0.34698300	-0.00404700
O	-2.51906600	-1.61060900	0.02597300
H	-1.87665300	-2.33193900	0.06608900
O	-2.82805100	0.71805800	-0.03854300
H	-3.75690200	0.43985100	-0.02947400
H	2.65456100	1.68655700	0.01002700
N	3.08736400	-1.15430600	0.07220100
H	3.04874500	-2.02521300	-0.44673400
H	3.92494700	-0.63943500	-0.17582700
H	0.46213100	-2.06391500	0.00848600



SCF energy=-784.4569426

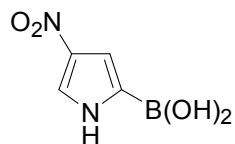
C	-1.97116700	0.07481900	-0.00298100
C	-1.52809900	1.38294100	-0.00908200
C	-0.11039200	1.46671100	-0.00437400
C	0.55324500	0.25648800	0.00399800
S	-0.63620900	-1.04659800	0.01981200
B	2.06685300	-0.05136500	-0.00419300
O	3.04683700	0.92224000	0.00375000
H	2.71348200	1.82943000	0.02457100
O	2.48156700	-1.35965000	-0.02063200

C	-0.83445700	1.53106100	-0.00006500
C	0.57999100	1.54615200	0.00002300
C	1.16175600	0.28619200	-0.00003800
S	-0.05541700	-0.95735400	-0.00006500
B	2.67842700	-0.10076600	0.00003700
O	3.69625600	0.81905100	0.00004300
H	3.42637100	1.74748000	0.00008300
O	2.99434100	-1.42801500	-0.00000300
H	3.95050100	-1.59104600	0.00005600
H	1.15313900	2.46922900	0.00008000
N	-2.69257900	-0.15014500	0.00002200
O	-3.53775000	0.74885800	0.00000300
O	-2.94178800	-1.36033000	0.00009200
H	-1.48006400	2.40035000	-0.00002600



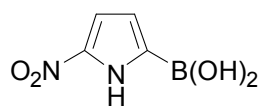
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C	0.39844500	2.48941000	-0.00010200
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C	0.85745900	0.30602500	-0.00008100
C	-0.54337500	0.41659600	0.00019800
N	-0.76989500	1.76677100	0.00023000
H	-1.70682600	2.15130000	0.00012600
B	-1.77812700	-0.55061400	-0.00001300
O	-1.71108600	-1.90063000	-0.00045800
H	-0.77873200	-2.20424200	-0.00028600
O	-2.99423200	0.09476600	0.00017400
H	-3.73940000	-0.52582000	-0.00019200
H	2.50331200	1.82188900	-0.00044900
N	1.61841700	-0.90393900	0.00007000
O	1.02451500	-2.00282400	0.00036400
O	2.84603400	-0.81193500	-0.00002900
H	0.39169000	3.56996700	-0.00008800



SCF energy=-590.7635787

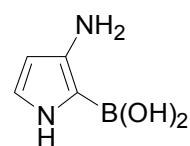
C	-0.77903200	-1.42700700	-0.00017600
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C	-0.10153500	0.75239400	0.00023800
C	1.02886600	-0.05121400	-0.00008000
N	0.57129300	-1.36886600	-0.00059400
H	1.19390500	-2.16693600	0.00050400
B	2.54923400	0.25040500	0.00001300
O	3.10099900	1.50485500	-0.00021400
H	2.46846500	2.23664800	-0.00083600
O	3.38687700	-0.83700400	0.00047300
H	4.32502500	-0.59117200	0.00023400
H	-1.33639700	-2.35132900	-0.00070700
N	-2.60186500	0.28287900	0.00008400
O	-2.85157000	1.49329000	-0.00009200
O	-3.45838600	-0.61032700	0.00018200
H	-0.14454100	1.83253600	0.00044100



SCF energy=-590.758702

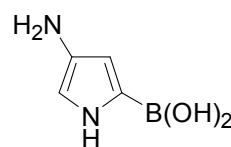
C	-1.19813700	0.26653900	0.00002800
C	-0.85870600	1.61424500	-0.00000500
C	0.54833900	1.65109100	-0.00001900

H	3.44819500	-1.43431700	-0.02028500
H	0.40893200	2.42261900	-0.01550700
N	-3.28297200	-0.37959800	0.07096800
H	-3.97774100	0.30178700	-0.21296500
H	-3.46259300	-1.28730100	-0.34246800
H	-2.19313600	2.24088500	-0.01644700



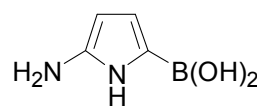
SCF energy=-441.6255869

C	-2.04468300	-1.24045600	-0.00011600
C	-2.23599900	0.13256000	-0.00023400
C	-0.94147500	0.72120900	0.00006600
C	0.01079800	-0.29576400	0.00039000
N	-0.69852300	-1.48090600	0.00018100
H	-0.26414000	-2.39306400	0.00024000
B	1.55183100	-0.15334500	0.00010400
O	2.13126200	1.08478700	-0.00000300
H	1.42318300	1.77001500	-0.00012900
O	2.32970000	-1.28990700	-0.00018900
H	3.27587300	-1.07702600	-0.00066700
H	-3.19087500	0.64318300	-0.00044300
H	-2.76146900	-2.05017700	0.00004300
N	-0.56069400	2.11138700	-0.00004300
H	-0.92381500	2.59809000	-0.81859300
H	-0.92293500	2.59800000	0.81895000



SCF energy=-441.6141907

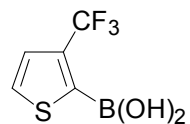
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C	0.70623800	-0.88589200	0.00646100
C	-0.36310000	0.01574800	0.00218800
N	0.20095900	1.27342200	0.00511400
H	-0.34051200	2.12590300	-0.00010600
B	-1.89253100	-0.17282700	-0.00273100
O	-2.53022800	-1.39445400	0.00726300
H	-1.92981800	-2.15234300	0.02693500
O	-2.67914100	0.95744600	-0.01853200
H	-3.62520100	0.74598600	-0.01583100
H	2.19049400	2.08237600	0.01048000
N	3.22130000	-0.69121200	0.08299400
H	3.31827400	-1.56036100	-0.43222500
H	3.94211500	-0.04415000	-0.21978900
H	0.62825500	-1.96751500	0.01991000



SCF energy=-441.6196457

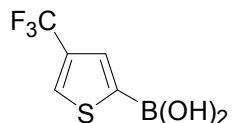
C	-1.85940800	-0.11350900	0.00664900
C	-1.66925000	1.26451900	-0.01400800
C	-0.26782600	1.48427000	-0.01342400
C	0.38380200	0.25317700	-0.00304700
N	-0.63154300	-0.70434400	0.01661200
H	-0.46506400	-1.69719400	0.10999900
B	1.86405800	-0.15797300	-0.00284900
O	2.92525200	0.72403000	0.00550500
H	2.66383000	1.65502200	0.01575200
O	2.15958200	-1.50483900	-0.00695000
H	3.11508700	-1.66810400	0.00100600

C	1.03603100	0.33402600	0.00001900
N	-0.06271300	-0.48736100	0.00003600
H	-0.04844900	-1.50051500	0.00012700
B	2.47293100	-0.26349200	0.00001200
O	3.62214900	0.48298300	-0.00002300
H	3.49586800	1.44182800	0.00010000
O	2.56923000	-1.62865700	-0.00001400
H	3.48524300	-1.94712700	-0.00003700
H	1.15396600	2.54910100	-0.00003800
N	-2.47747700	-0.35588800	0.00001600
O	-2.50248400	-1.59736800	-0.00003800
O	-3.47376700	0.37337300	-0.00000600
H	-1.55614500	2.43884700	-0.00006100



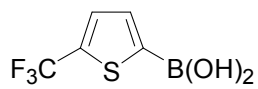
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C	-0.43997000	-0.64330900	0.02193200
C	0.78900600	0.00492500	0.02636200
S	2.05550900	-1.18912400	0.04246100
B	1.21512100	1.51755200	0.01353800
O	0.39551800	2.58094000	0.26250300
H	-0.51422500	2.36255700	0.51303700
O	2.53460700	1.76590100	-0.25693600
H	2.74256600	2.71253200	-0.21739400
H	-1.22015900	-2.72225000	0.03009100
C	-1.75894700	0.06349100	-0.04831600
F	-2.80337200	-0.77838700	0.09698900
F	-1.93971800	0.72603100	-1.22021500
F	-1.89570900	1.01893400	0.93442000
H	1.29469500	-3.52562700	0.07022000



SCF energy=-1066.1869872

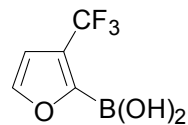
C	0.62936500	1.51152300	0.00660500
C	0.98324500	0.18381200	0.00602000
C	-0.14804300	-0.68383100	0.00221800
C	-1.35591200	-0.01943900	0.00065700
S	-1.07830700	1.70807800	0.00295400
B	-2.80487600	-0.59665800	-0.00133000
O	-3.09065100	-1.94049600	0.00737200
H	-2.32509300	-2.53107100	0.01778500
O	-3.84844100	0.28605700	-0.01226800
H	-4.71147400	-0.15650400	-0.01194400
H	1.29054400	2.36778900	0.00979500
H	-0.05228600	-1.76590400	0.00205400
C	2.39426400	-0.30836000	-0.00061100
F	2.64450400	-1.14703600	1.04128100
F	3.29194400	0.70230900	0.07519000
F	2.68253400	-1.01382700	-1.12852200



SCF energy=-1066.1822182

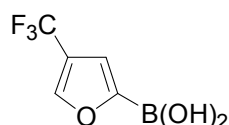
C	-0.97707000	0.28288100	-0.01470300
C	-0.46228900	1.55755300	-0.01427800
C	0.95784300	1.55380000	-0.00727000
C	1.52013500	0.29100800	-0.00116000
S	0.26872000	-0.92247700	-0.00560400
B	3.02466500	-0.12542000	0.00279200

H	0.21508500	2.45460100	-0.03679100
H	-2.45235800	2.01114500	-0.04536400
N	-3.02504800	-0.89617500	0.07781300
H	-3.85738300	-0.32524200	0.17947500
H	-3.14593500	-1.52099800	-0.71626000



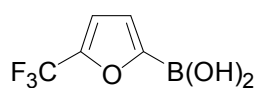
SCF energy=-743.191903

C	-0.47859400	2.59686600	0.03617400
C	0.75358000	2.01494500	0.03095300
C	0.50429800	0.60700900	0.03469700
C	-0.86436800	0.41360800	0.03555500
O	-1.45048100	1.65482100	0.03763800
B	-1.84397000	-0.81256800	0.01387100
O	-3.16940300	-0.53825800	-0.15467300
H	-3.70563000	-1.34682900	-0.14814000
O	-1.44909200	-2.11432400	0.14484900
H	-0.50757900	-2.25468900	0.32353400
H	1.71462300	2.50864600	0.03108100
H	-0.81346600	3.62342100	0.04498900
C	1.56809500	-0.43323200	-0.02789500
F	2.76027800	0.03713700	0.39744800
F	1.75890600	-0.91878400	-1.28232500
F	1.27922000	-1.52733100	0.75151800



SCF energy=-743.1949147

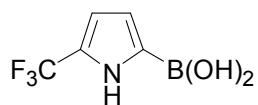
C	0.33940700	1.43851400	0.00000600
C	0.86432000	0.17688000	0.00019500
C	-0.24692600	-0.72528200	0.00054000
C	-1.38188300	0.03865700	0.00024500
O	-1.00856100	1.37904200	0.00045400
B	-2.90694000	-0.26637800	-0.00012900
O	-3.30223900	-1.57256300	-0.00000900
H	-4.26738100	-1.66760700	-0.00025200
O	-3.84711000	0.73102400	-0.00044900
H	-3.47115500	1.62418900	-0.00007400
H	0.78597900	2.42133700	-0.00016000
C	2.30912100	-0.17542300	-0.00007700
F	3.09508300	0.93080300	0.00025300
F	2.65575000	-0.91359400	1.08658500
F	2.65554900	-0.91277000	-1.08739800
H	-0.21114500	-1.80608100	0.00076100



SCF energy=-743.1902735

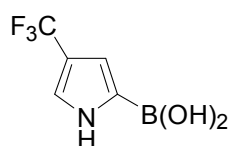
C	-0.82635400	0.41924800	0.00011400
C	-0.44784000	1.73127100	0.00027500
C	0.98002100	1.71693700	0.00012800
C	1.38145700	0.40487800	-0.00016400
O	0.25408600	-0.39938600	-0.00014400
B	2.75677000	-0.32519000	-0.00006900
O	3.88804000	0.43833500	-0.00029700
H	4.69647300	-0.09756800	-0.00004700
O	2.85451300	-1.69102900	0.00034800
H	1.99969800	-2.14809600	0.00043800
H	1.64089200	2.57302400	0.00012100
H	-1.10606300	2.58846100	0.00051600
C	-2.16333900	-0.23802800	-0.00002600
F	-3.14190200	0.69429400	0.00108500
F	-2.34783900	-1.02837600	-1.08721200

O	4.06126400	0.77624500	0.01560700
H	3.80257500	1.70780000	0.02566600
O	3.32455700	-1.45806900	-0.00678600
H	4.27943500	-1.62772900	-0.00249800
H	1.54282800	2.46968800	-0.00932700
C	-2.42432600	-0.08694800	0.00136700
F	-2.79076800	-0.69172000	1.16261200
F	-3.21196200	1.00509200	-0.14247700
F	-2.74648300	-0.95205600	-0.99479400
H	-1.07708800	2.44995200	-0.02051900



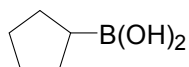
SCF energy=-723.3462432

C	-0.84915500	0.36746500	-0.02165100
C	-0.44292500	1.69334100	-0.01122100
C	0.97144800	1.68077700	0.00161900
C	1.40578800	0.35374100	-0.00017200
N	0.26566600	-0.42328400	-0.01168500
H	0.27678700	-1.43518100	-0.03095300
B	2.80888600	-0.30459600	0.00276300
O	3.99467200	0.38714200	0.01291500
H	3.90522700	1.35009900	0.01804000
O	2.85287200	-1.67618300	-0.00534900
H	3.75810500	-2.02380500	-0.00357000
H	1.60841900	2.55703400	0.00774700
H	-1.09692400	2.55404400	-0.01475600
C	-2.21491900	-0.21597600	-0.00039000
F	-3.15561400	0.71650600	-0.26011700
F	-2.35472200	-1.21477300	-0.91799500
F	-2.52938500	-0.77728800	1.20275900



SCF energy=-723.351531

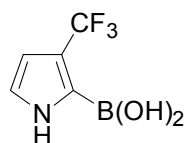
C	0.37286600	1.49073900	-0.00138600
C	0.87344800	0.19698200	-0.00163100
C	-0.23636000	-0.68901900	-0.00091300
C	-1.39719000	0.07558400	-0.00029700
N	-0.98215000	1.40030000	-0.00062100
H	-1.62435200	2.18160600	-0.00086900
B	-2.90320900	-0.28103400	0.00036600
O	-3.40735300	-1.55804200	-0.00062500
H	-2.74291900	-2.26083400	-0.00269000
O	-3.78985500	0.76832600	0.00188300
H	-4.71449200	0.47594700	0.00180400
H	0.88908100	2.43967900	-0.00230200
C	2.30826600	-0.17978900	0.00004000
F	3.11941700	0.91000200	-0.01936500
F	2.65585200	-0.91059900	1.09694200
F	2.64850000	-0.94520400	-1.07507900
H	-0.17866200	-1.77037200	-0.00083700



SCF energy=-372.6048645

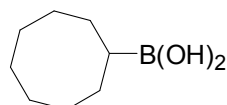
C	-2.22032400	0.78302100	0.32636300
C	-0.71315100	1.08526200	0.54671000
C	0.03924500	0.11565600	-0.40905100
C	-0.83244200	-1.15500500	-0.32408800
C	-2.28529000	-0.62804400	-0.33057000
H	-2.77490400	0.81953100	1.27110900
H	-2.67194500	1.53463700	-0.33156500

F	-2.34710800	-1.03025800	1.08591700
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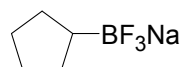
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C	-0.49249200	2.62751300	0.02564800
C	0.74741300	2.01679100	0.03843200
C	0.51054700	0.61683200	0.04153300
C	-0.87148300	0.38918500	0.02552400
N	-1.44008700	1.64499600	0.01651500
H	-2.44215600	1.78480500	0.00785900
B	-1.81211900	-0.85244600	0.00978300
O	-1.43435100	-2.15973000	0.10842200
H	-0.48645100	-2.29797000	0.25687700
O	-3.15285300	-0.56346200	-0.11238700
H	-3.70289000	-1.36198000	-0.09989800
H	1.70931400	2.50937600	0.04875500
H	-0.76206700	3.67417500	0.02832400
C	1.57980500	-0.41063700	-0.02026500
F	2.76437100	0.04981900	0.43986900
F	1.28183400	-1.53085700	0.72573300
F	1.80716700	-0.87604100	-1.28115200



SCF energy=-490.5390877

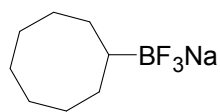
C	-2.80958500	-0.39658200	-0.23261500
C	-2.46800100	1.00817200	0.31012300
C	0.14446700	-0.97376200	-0.82125400
C	-1.30015800	1.77907200	-0.35681700
C	0.92539100	0.36378100	-0.63391800
C	0.13938400	1.46879400	0.11461500
H	-2.67699000	-0.38886600	-1.32395400
H	-2.29699300	0.96131700	1.39655900
H	-1.37408200	1.67239400	-1.45036500
H	-0.61407900	-0.82762100	-1.59931000
H	1.12535300	0.74139500	-1.65270400
H	-3.88267000	-0.57563600	-0.07714700
H	-3.36542700	1.62848400	0.18011100
H	0.82475000	-1.73539500	-1.22801200
H	-1.47743500	2.84432800	-0.15464800
H	0.73100900	2.39051400	0.02566900
H	0.12163900	1.25272700	1.18991100
C	-2.06692000	-1.60191700	0.38033800
H	-2.33868500	-2.49143300	-0.20744800
H	-2.45689500	-1.78076100	1.39291500
C	-0.53161800	-1.50120300	0.46775400
H	-0.26383000	-0.85790100	1.31306200
H	-0.13746900	-2.49296100	0.72479900
B	2.33575900	0.07628000	0.04243000
O	2.52741300	0.30003800	1.38048500
H	3.42364600	0.05674400	1.66319500
O	3.41458000	-0.43598900	-0.65276000
H	3.24565600	-0.56926400	-1.59593400



SCF energy=-682.9085354

B	0.81543900	-0.02302900	-0.19381900
F	1.57530300	-1.21324800	-0.56040600
F	1.58589700	1.05365500	-0.80772200
F	1.12526500	0.13117200	1.22629000
Na	3.18646500	0.02802100	0.36923800
C	-0.72704500	-0.05626700	-0.56023700

H	-0.43752100	0.87066100	1.58934600
H	-0.45700900	2.13352200	0.36012700
H	-0.05207100	0.52467100	-1.42763100
H	-0.63747900	-1.86883000	-1.13374400
H	-0.64549500	-1.68600600	0.62456600
H	-2.64259800	-0.54912400	-1.36468500
H	-2.97363200	-1.30335700	0.19045700
B	1.58166100	-0.01815100	-0.08056600
O	2.13091500	-1.01353900	0.70123200
H	1.48602700	-1.66752100	1.00545700
O	2.44546600	0.92727200	-0.57033600
H	3.35904900	0.76736700	-0.28396000



SCF energy=-800.8428766

B	1.64299100	0.12262600	0.20704900
F	2.48837100	1.31045400	0.12629300
F	2.43666300	-0.77654900	1.04001900
F	1.78939700	-0.46351800	-1.12266200
Na	3.93671000	-0.26321500	-0.53179100
C	0.15236300	0.37923800	0.71366800
C	-0.63038100	-0.94616700	0.92454800
H	0.26169100	0.83814600	1.71149500
C	-0.55307600	1.42761000	-0.18313000
C	-1.26725000	-1.54308700	-0.35521300
H	-1.41607500	-0.78132600	1.67311200
H	0.04752100	-1.67786300	1.38145300
H	-0.51471500	1.11345900	-1.23614400
H	0.05698400	2.33937900	-0.13623300
C	-2.01068000	1.81864000	0.15549800
C	-2.80656900	-1.60361900	-0.32909800
H	-0.94581400	-0.96978400	-1.23094300
H	-0.89051300	-2.56023900	-0.52683900
C	-3.15872500	1.00638300	-0.49407400
H	-2.15138200	1.83022600	1.24773000
H	-2.14737100	2.85996300	-0.16978100
C	-3.54482200	-0.33968400	0.15614700
H	-3.16180500	-1.85359000	-1.34025700
H	-3.12405900	-2.43761900	0.31531500
H	-2.93860100	0.85896200	-1.56301700
H	-4.05124900	1.64736500	-0.46386100
H	-4.61674100	-0.51328100	-0.01633100
H	-3.44167200	-0.24093200	1.24582700

### Radicals:

H<sub>2</sub>C=CH• SCF energy=-77.8995094

C	0.04894900	0.72398000	0.00000000
H	-0.67678200	1.52819600	0.00000000
C	0.04894900	-0.58885300	0.00000000
H	-0.88172100	-1.16842200	0.00000000
H	0.97111000	-1.17053400	0.00000000

H<sub>3</sub>CHC=CH• SCF energy=-117.2164276

C	1.31908300	-0.31973400	-0.00006700
H	2.38621600	-0.13534500	0.00025100
C	0.21178700	0.39071800	-0.00003800
H	0.29800800	1.48718400	0.00003500
C	-1.19627700	-0.15370300	-0.00002500
H	-1.74635500	0.19626500	0.88331300
H	-1.74683700	0.19578100	-0.88323600
H	-1.19859100	-1.24757400	0.00041900

C	1.52932800	-1.20924800	0.09212300
C	-1.51821400	1.23516400	-0.16778300
H	-0.80447600	-0.18282100	-1.65182700
C	-2.98985900	-0.73561700	0.00782300
H	-1.24117400	-1.32735200	1.14710500
H	-1.35676000	-2.17277000	-0.40229800
C	-2.90027500	0.76049200	0.37124100
H	-1.63091600	1.89599500	-1.03524500
H	-0.98792800	1.81502200	0.59691200
H	-3.35538400	-0.85483400	-1.02264200
H	-3.67042000	-1.29375700	0.66346800
H	-3.73571000	1.34457000	-0.03374100
H	-2.93540100	0.87150300	1.46329400

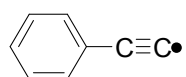
H<sub>3</sub>CHC=C•  
CH<sub>3</sub> SCF energy=-156.5369412

C	0.55977500	-0.27426700	0.00007900
C	-0.56945200	0.40402600	0.00001300
H	-0.51211500	1.50406800	0.00008600
C	-1.96243100	-0.17843900	-0.00002600
H	-2.52552700	0.15198300	-0.88321000
H	-1.93327900	-1.27241000	0.00007800
H	-2.52566900	0.15213800	0.88301900
C	2.01602500	-0.04904200	-0.00002300
H	2.49307000	-0.49075200	-0.88426300
H	2.24692900	1.03126400	-0.00058900
H	2.49309200	-0.48995200	0.88461900



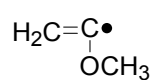
$(\text{H}_3\text{C})_2\text{C}=\text{CH}\bullet$ SCF energy=-156.5351293				$\text{H}_3\text{CCH}_2\text{CHC}=\text{CH}\bullet$ SCF energy=-156.5303901			
C	-0.33057300	1.47090000	-0.00001800	C	1.90945800	-0.05483300	-0.34164300
H	-1.23595700	2.06657400	0.00022100	H	2.90521400	-0.47922000	-0.30870900
C	-0.01695100	0.18930200	-0.00010300	C	0.80166500	-0.11555400	0.36484500
C	1.41782400	-0.29641100	0.00000200	H	0.78448100	-0.75844400	1.25827200
H	1.61442400	-0.91942400	0.88353900	C	-0.49171500	0.61031100	0.06466800
H	1.61435100	-0.92013700	-0.88299300	H	-0.72552400	1.27690300	0.90775300
H	2.12534200	0.53720600	-0.00025600	H	-0.35426400	1.24662200	-0.81683800
C	-1.08286300	-0.89746700	0.00003000	C	-1.66915400	-0.35421600	-0.15560000
H	-0.97405500	-1.53990400	-0.88463600	H	-2.59796400	0.20036400	-0.33494900
H	-0.97363000	-1.54023200	0.88435400	H	-1.48708200	-1.00398200	-1.01932500
H	-2.09509400	-0.48202700	0.00030700	H	-1.82637900	-0.99649500	0.72017800
$\text{H}_2\text{C}=\text{C}\bullet$   $\text{CH}_3$ SCF energy=-117.2203814				$\text{CH}_3\bullet$ SCF energy=-39.8299442			
C	-0.12423100	-0.38187500	0.00016900	C	0.00000000	0.00000000	0.00000000
C	-1.34907400	0.09821700	-0.00002200	H	0.00000000	1.08405000	0.00000000
C	1.27541100	0.07659300	-0.00003300	H	-0.93881500	-0.54202500	0.00000000
H	1.81506200	-0.28679200	0.88352400	H	0.93881500	-0.54202500	0.00000000
H	1.81404700	-0.28533600	-0.88486200	$\text{C}_2\text{H}_5\bullet$ SCF energy=-79.144171			
H	1.33135700	1.17947400	0.00087600	C	0.00965000	0.79584000	0.00000000
H	-2.22918300	-0.54365900	-0.00031900	H	-0.05850700	1.35504200	0.92844000
H	-1.54391700	1.17870300	0.00009700	H	-0.05850700	1.35504200	-0.92844000
$\text{H}_2\text{C}=\text{C}\bullet$   $\text{CH}_2\text{CH}_3$ SCF energy=-156.5342737				$\text{C}_2\text{H}_5\bullet$ SCF energy=-79.144171			
C	0.73114500	-0.03987200	-0.36400300	C	0.00965000	-0.69521000	0.00000000
C	1.94593100	-0.17812200	0.12289700	H	-1.01555300	-1.10853800	0.00000000
C	-0.55929000	0.59954200	-0.04021200	H	0.50838100	-1.10266500	-0.88850300
H	-0.80134600	1.34208300	-0.81391600	H	0.50838100	-1.10266500	0.88850300
H	-0.44744200	1.16504800	0.90400600	$\text{B}(\text{OH})_2\bullet$ SCF energy=-176.5509514			
H	2.71973900	-0.75124000	-0.38633800	B	0.00001400	0.47804400	-0.00001800
H	2.23958900	0.28369700	1.07474000	O	1.17573200	-0.19626300	0.00001800
C	-1.72587000	-0.39753000	0.09022700	H	1.95494100	0.37502200	-0.00003800
H	-2.65602400	0.13123200	0.32816400	O	-1.17576700	-0.19630600	-0.00002000
H	-1.87465300	-0.94867200	-0.84483900	H	-1.95473300	0.37531300	0.00014500
H	-1.53135300	-1.12625300	0.88472100	$\text{B}(\text{OH})_2\bullet$   $\text{CH}(\text{CH}_3)_2$ SCF energy=-219.1991128			
$(\text{CH}_3)_3\text{C}-\text{CH}\bullet$   $\text{CH}_3$ SCF energy=-236.4087037				$\text{B}(\text{OH})_2\bullet$   $\text{CH}(\text{CH}_3)_2$ SCF energy=-219.1991128			
C	0.89204000	-0.69949100	-0.32789000	B	0.99692500	0.00006700	-0.51573700
H	0.84714600	-1.76870300	-0.53316100	C	-0.37604000	0.00003900	0.26747300
C	-0.41784800	-0.01165200	-0.01753300	H	-0.14957700	0.00015200	1.35286200
C	2.23336700	-0.09147900	-0.06604000	O	2.24012500	0.00013400	-0.00976300
H	2.37552900	0.17393000	0.99730800	H	2.30470700	0.00039000	0.96741200
H	3.04031500	-0.78107300	-0.33609800	C	-1.19550800	1.27126700	-0.04377100
H	2.38974100	0.83895900	-0.63211400	H	-1.45061300	1.32122200	-1.10919600
C	-1.54619300	-0.67649100	-0.83471000	H	-2.13313800	1.27468300	0.52774200
H	-2.51931100	-0.22631400	-0.60017700	H	-0.64778400	2.18731800	0.20970100
H	-1.37015400	-0.56490600	-1.91155200	C	-1.19502200	-1.27148400	-0.04371900
H	-1.61186600	-1.74982700	-0.61456200	H	-0.64669800	-2.18744000	0.20885500
C	-0.73728900	-0.16992200	1.49551400	H	-2.13221400	-1.27562800	0.52849000
H	-0.81499000	-1.22824300	1.77260900	H	-1.45088500	-1.32102900	-1.10898300
H	0.04353800	0.28587100	2.11625000	$\text{B}(\text{F})_2\bullet$ SCF energy=-224.6008483			
H	-1.69071000	0.31662800	1.74326600	B	0.00000000	0.00000000	0.50759900
C	-0.36205300	1.49357900	-0.35968600	F	0.00000000	1.14812900	-0.14100000
H	-0.12763400	1.64967100	-1.42003800	F	0.00000000	-1.14812900	-0.14100000
H	-1.32934800	1.96932800	-0.15460500	$(\text{CH}_3)_2\text{CH}\bullet$ SCF energy=-118.4604299			
H	0.39559700	2.01740800	0.23495000	C	0.01018200	0.53712000	0.00000000
$\text{H}_3\text{C}-\text{CH}(\text{CH}_3)-\text{CH}\bullet$   $\text{CH}_3$ SCF energy=-197.0899191				$(\text{CH}_3)_2\text{CH}\bullet$ SCF energy=-118.4604299			
C	0.87210800	-0.38960400	0.62296600	H	-0.21267400	1.60190200	0.00000000
H	1.11473800	-1.16192000	1.35157100	C	0.01018200	-0.19814800	1.30019700
C	-0.58018100	-0.01837900	0.47904000	H	0.20076500	0.46849100	2.14901200
H	-1.03094200	-0.05848100	1.48276500	H	-0.95721600	-0.69893000	1.49410700





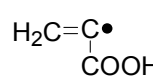
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C	2.07770800	0.00002300	-0.01678700
C	-3.36043600	-0.00001700	0.01946600
C	-0.67983000	0.00001500	-0.00677200
C	0.04684000	-1.22708300	-0.00340600
C	0.04686800	1.22710400	-0.00339900
C	1.43386300	-1.21988800	0.00223000
H	-0.51012700	-2.15872800	-0.00524300
C	1.43389000	1.21986900	0.00222500
H	-0.51008500	2.15875900	-0.00523400
C	2.12943100	-0.00001900	0.00501300
H	1.98318500	-2.15712000	0.00468300
H	1.98323500	2.15708800	0.00467000
H	3.21628900	-0.00003400	0.00971100



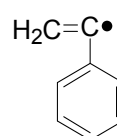
SCF energy=-192.440436

C	-0.63137800	-0.25746600	-0.29394300
C	-1.85688900	-0.03857200	0.16190900
H	-2.67304300	-0.70004300	-0.10744100
H	-2.07234500	0.80144200	0.82617400
O	0.46558500	0.48688000	-0.22010800
C	1.67218300	-0.19560500	0.17249000
H	2.45704700	0.56172700	0.17303600
H	1.55333000	-0.62275600	1.17401800
H	1.90683700	-0.98554200	-0.54766100



SCF energy=-266.4877224

C	0.87687800	-0.03529600	-0.16668500
C	2.15750200	-0.05211100	0.06179600
H	2.88691700	-0.15897000	-0.74309500
H	2.56502800	0.03561000	1.07377800
C	-0.52931800	0.11088300	-0.02436200
O	-1.18478500	-1.08319000	0.02663700
H	-2.13583000	-0.87589000	0.09736000
O	-1.10852500	1.19049000	0.01679600



SCF energy=-308.9936799

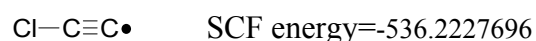
C	-3.22908700	-0.00010400	-0.00034200
H	-3.81242700	0.00030400	-0.92610000
C	-1.92507300	0.00031900	0.00042300
H	-3.81342500	-0.00061100	0.92477300
C	-0.55116900	0.00025500	0.00024300
C	0.19169000	-1.22857500	0.00011600
C	0.19213600	1.22879000	0.00015400
C	1.57740300	-1.21411800	-0.00012200
H	-0.35268200	-2.16826800	0.00018400
C	1.57786500	1.21382400	-0.00004900
H	-0.35174700	2.16876900	0.00010900
C	2.28570300	-0.00026400	-0.00014900
H	2.12035100	-2.15620600	-0.00022200
H	2.12111400	2.15573900	-0.00013300
H	3.37200700	-0.00049200	-0.00025900



SCF energy=-133.2613215

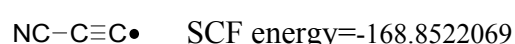
C	-0.13885100	0.44054500	-0.00827600
H	-0.05239000	1.52820100	-0.03230000
C	-1.33863300	-0.11486400	0.02821900
H	-1.80801900	-1.08801200	-0.00180700
N	1.11183200	-0.20773400	-0.09057500

C	-1.08367000	0.00012800	-0.00000500
C	-2.36768400	0.00005700	0.00005600
N	0.22478000	0.00001500	-0.00022800
C	0.99811100	-1.24826800	0.00004500
H	0.30783200	-2.09123200	-0.00093200
H	1.63571700	-1.28911100	-0.89140500
H	1.63399800	-1.28977400	0.89269200
C	0.99833900	1.24814400	0.00005100
H	1.63517200	1.28937200	-0.89193900
H	0.30822500	2.09124600	0.00013600
H	1.63501700	1.28902800	0.89215900



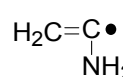
SCF energy=-536.2227696

C	0.00000000	0.70895300	0.00000000
C	0.48471700	1.89681500	0.00000000
Cl	-0.17107700	-0.91968300	0.00000000



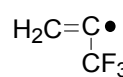
SCF energy=-168.8522069

C	0.16989300	-0.72425400	0.00000000
C	-0.03398700	-1.98613500	0.00000000
C	0.00000000	0.62006100	0.00000000
N	-0.11649100	1.79171000	0.00000000



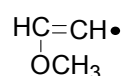
SCF energy=-133.2724356

C	-0.06513200	-0.41948000	-0.04153500
C	-1.28146000	0.10878700	0.01601200
H	-2.16052100	-0.47191100	-0.24797500
H	-1.44867600	1.13078100	0.37127900
N	1.18326200	0.13040800	0.05077100
H	1.47146900	0.76628200	-0.68739700
H	1.93445200	-0.47384800	0.36183000



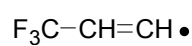
SCF energy=-414.9868411

C	-1.01075400	-0.56199900	-0.00112200
C	-2.22365800	-0.06477300	-0.00016000
H	-2.39530200	1.01601800	0.00196100
H	-3.10667200	-0.70137700	-0.00079600
C	0.37136400	-0.04224500	0.00016500
F	1.05959700	-0.45549700	1.09035900
F	1.06049600	-0.45397300	-1.09044000
F	0.39993600	1.32052200	0.00069600



SCF energy=-192.43425

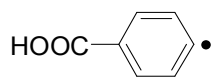
C	-0.83646300	-0.52244400	0.00003400
H	-1.34726600	-1.48313700	0.00012500
C	-1.49751500	0.62049700	-0.00001000
H	-1.37731500	1.69149800	-0.00008500
O	0.52060200	-0.72074100	-0.00006500
C	1.32406100	0.45582300	0.00002900
H	2.36078400	0.11546000	0.00038300
H	1.12951000	1.05931200	-0.89646000
H	1.12897000	1.05953900	0.89624500



SCF energy=-414.989447

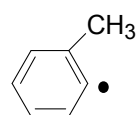
C	-1.02836300	-0.69692700	0.00001000
H	-0.96834600	-1.78525300	-0.00004800
C	-2.17148900	-0.05372200	0.00004100
H	-2.53243400	0.96583500	0.00010300
C	0.31622900	-0.01212100	0.00003800
F	1.04468300	-0.36781700	-1.08887700
F	1.04511500	-0.36846100	1.08842200
F	0.22159200	1.33583800	0.00038900

H	1.85372300	0.25847300	0.42167700
H	1.08876800	-1.19860800	0.12679900



SCF energy=-420.1717637

C	-0.50443700	-1.21088300	0.00013000
C	-1.90609600	-1.26067000	0.00009200
C	-2.56820800	-0.05081300	-0.00001900
C	-1.97902500	1.19703000	-0.00010900
C	-0.57843900	1.22794500	-0.00009800
C	0.15516900	0.02986800	0.00002800
H	-2.55814800	2.11632600	-0.00020000
H	-0.04320500	2.17298800	-0.00018300
H	-2.42999300	-2.21256200	0.00015800
H	0.07287600	-2.12982000	0.00022100
C	1.63831600	0.12587800	0.00002800
O	2.27210800	1.16448500	0.00024800
O	2.25317900	-1.08749100	-0.00025100
H	3.21249700	-0.91302100	-0.00028900



SCF energy=-270.8930393

C	1.89846300	0.00081700	-0.00001500
C	1.22770900	-1.23627700	-0.00000300
C	-0.14802200	-1.19431500	0.00002300
C	-0.94826100	-0.06441300	0.00003300
C	-0.24174800	1.15509000	0.00002300
C	1.15788700	1.18580300	0.00000200
H	2.98577200	0.02865000	-0.00004500
H	1.77913500	-2.17333000	-0.00001500
H	-0.80262900	2.08869500	0.00000600
H	1.67131400	2.14391800	-0.00004300
C	-2.45861000	-0.12343000	-0.00002400
H	-2.83359100	-0.65512600	-0.88274500
H	-2.83367600	-0.65502500	0.88271800
H	-2.89083600	0.88257300	-0.00010500



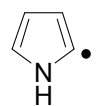
SCF energy=-229.3460489

C	0.82823400	0.73902700	-0.00025600
C	-0.50380300	1.02265200	0.00010200
C	-1.21079400	-0.23974800	0.00006300
C	-0.21321200	-1.16255600	0.00013300
H	1.73240000	1.32739400	0.00111500
H	-0.94903700	2.00920500	-0.00028400
O	1.01131100	-0.63520100	-0.00009400
H	-2.27639400	-0.41124000	-0.00033400



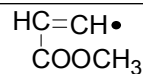
SCF energy=-552.3393404

C	0.04350000	1.18857400	-0.00017100
C	-1.24052400	0.71175500	-0.00006200
C	-1.31996600	-0.72857200	-0.00001700
C	-0.06823200	-1.25242600	-0.00008200
H	0.38052700	2.21747100	0.00026100
H	-2.11515500	1.35505600	0.00052500
H	-2.24271400	-1.29708300	0.00030100
S	1.21804200	-0.11196400	0.00005700



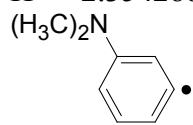
SCF energy=-209.4955011

C	-0.69108000	0.88891400	0.00004900
C	0.68801800	0.92918500	-0.00004100
C	1.18362000	-0.42100200	0.00003300



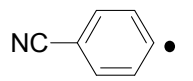
SCF energy=-305.7971308

C	-1.58035600	0.29991900	0.00007000
H	-2.12443700	1.24321800	0.00017600
C	-2.19798700	-0.86365600	-0.00002600
H	-1.92883300	-1.91204200	-0.00015300
C	-0.09338100	0.47004200	-0.00000300
O	0.45467400	1.55454200	-0.00005500
O	0.56818000	-0.70734700	-0.00002400
C	2.00593000	-0.61872500	0.00003700
H	2.35656900	-1.65103900	0.00012700
H	2.35434500	-0.09166000	-0.89206000
H	2.35428800	-0.09151500	0.89206800



SCF energy=-365.5563974

C	2.03710400	1.07859000	0.01141000
C	2.71944200	-0.15031600	0.03877000
C	1.90326500	-1.26011500	0.02271900
C	0.53012200	-1.28248200	-0.01943700
C	-0.15099500	-0.03263100	-0.06694300
C	0.64417200	1.14118400	-0.03564900
H	2.60451800	2.00741300	0.03000800
H	3.80326200	-0.20340000	0.07442100
H	0.17488500	2.11753300	-0.05071000
H	-0.01112300	-2.22194100	-0.01534800
N	-1.53770600	0.02935500	-0.15130200
C	-2.31459600	-1.18364400	0.04994100
H	-2.18204600	-1.61382300	1.05704700
H	-3.37341200	-0.95580000	-0.09011200
H	-2.04271900	-1.94772800	-0.68734400
C	-2.20574600	1.30360400	0.06573500
H	-1.88601900	2.04486100	-0.67569500
H	-3.28244400	1.16489400	-0.05298400
H	-2.01756900	1.71736100	1.07055400



SCF energy=-323.8330989

C	0.15562200	-1.22424100	0.00000000
C	1.55691000	-1.22954900	0.00000000
C	2.18181300	0.00000000	0.00000000
C	1.55690900	1.22955000	0.00000000
C	0.15562200	1.22424100	0.00000000
C	-0.53963500	0.00000000	0.00000000
H	-0.39823700	-2.15885800	0.00000000
H	2.10876700	-2.16553200	0.00000000
H	2.10876700	2.16553200	0.00000000
H	-0.39823800	2.15885800	0.00000000
C	-1.97514900	0.00000000	0.00000000
N	-3.13908800	0.00000000	0.00000000



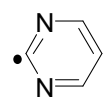
SCF energy=-229.3450925

C	-0.74737300	0.79593800	-0.00000200
C	-1.12401600	-0.51815100	0.00000100
C	0.11242800	-1.22509900	0.00002700
C	1.14319700	-0.34918400	-0.00004100
H	-1.30068700	1.72352900	-0.00000300
H	-2.13063200	-0.91088100	-0.00005000
O	0.61343700	0.92345100	0.00001400
H	2.21840900	-0.42127900	0.00003600



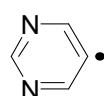
SCF energy=-552.3424759

C	0.05904100	-1.20368700	0.00001800
N	-1.07127300	-0.44630400	-0.00006000
H	-2.01789500	-0.79543100	0.00003700
H	-1.42942100	1.67845200	0.00010500
H	1.29465400	1.82619100	-0.00008300
H	2.21397400	-0.74554900	0.00000700



SCF energy=-263.6644967

C	-0.00000700	1.32778400	-0.00000700
N	1.19225800	0.78564400	-0.00000300
C	1.19230800	-0.56256400	0.00000500
C	0.00000800	-1.28928500	0.00000700
C	-1.19230100	-0.56257500	0.00000200
N	-1.19227000	0.78563100	-0.00000600
H	2.16379700	-1.05225200	0.00000900
H	0.00001300	-2.37455900	0.00001300
H	-2.16378300	-1.05227700	0.00000400



SCF energy=-263.6544223

C	0.00012000	1.24311800	-0.00000100
N	1.20019500	0.65294200	-0.00000100
C	1.20386800	-0.69544100	0.00002500
C	-0.00020800	-1.36803500	0.00000600
C	-1.20400600	-0.69519700	-0.00003600
N	-1.19997600	0.65320700	0.00000000
H	2.17149700	-1.19056200	0.00000300
H	0.00026400	2.33079700	0.00000600
H	-2.17193200	-1.18995600	0.00002800



SCF energy=-247.6236929

C	-0.24015300	-1.35757700	-0.00026700
C	-1.33649800	-0.49542400	-0.00011200
C	-1.02422300	0.86749900	0.00007300
C	0.31943000	1.27056200	0.00023100
C	1.31576000	0.29697200	0.00017600
N	1.00210900	-1.01783800	-0.00015700
H	-1.81939700	1.61018100	0.00014500
H	-2.36045000	-0.85391600	-0.00021600
H	0.58720400	2.32322400	0.00038900
H	2.37198900	0.55317900	0.00018300



SCF energy=-247.6165635

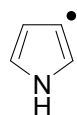
C	1.14641300	-0.65981500	0.00009900
C	1.21462200	0.74714500	0.00022300
C	0.00000100	1.39350100	0.00007500
C	-1.21462000	0.74714700	-0.00013300
C	-1.14641400	-0.65981400	-0.00016500
N	-0.00000100	-1.34753200	-0.00008000
H	2.06393800	-1.24687800	0.00019300
H	2.17294000	1.25874500	0.00038100
H	-2.17293900	1.25874600	-0.00025500
H	-2.06394100	-1.24687300	-0.00035700



SCF energy=-245.3548079

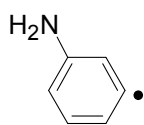
C	-0.21640200	-1.15260900	0.00010400
C	1.07902200	-0.56600900	0.00002900

C	0.43727100	-1.13168100	0.00003100
C	1.49112500	-0.25028300	0.00022500
C	1.00179900	1.08039700	-0.00013500
C	-0.33632700	1.26050300	0.00000500
H	0.47382900	-2.21410700	-0.00023500
H	2.53523500	-0.53944300	-0.00049100
H	-0.93266000	2.16203900	0.00023600
S	-1.10247600	-0.32263200	-0.00001700



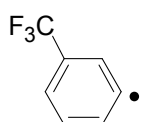
SCF energy=-209.4962866

C	0.67481100	0.88822300	-0.00000200
C	1.19067600	-0.40013500	0.00000600
C	0.05942600	-1.24607800	0.00000600
C	-1.10088400	-0.51625700	-0.00000600
N	-0.69911100	0.80969000	-0.00001100
H	-1.32249500	1.60465000	0.00009300
H	1.17827600	1.84559100	-0.00002600
H	2.23645100	-0.67336100	-0.00000100
H	-2.14263600	-0.79922800	-0.00000900



SCF energy=-286.9416104

C	0.09668900	-1.16552200	-0.00459400
C	0.90925400	-0.01516400	-0.00750300
C	0.28560600	1.25428900	-0.00294700
C	-1.08911700	1.27781700	0.00367500
C	-1.93442800	0.18860300	0.00766600
C	-1.29511600	-1.06482600	0.00352200
H	0.56539100	-2.14726900	-0.01566000
H	-3.01671800	0.27558300	0.01285300
H	-1.89466300	-1.97302400	0.00676100
H	0.88252200	2.16432600	-0.01061600
N	2.30218800	-0.12263500	-0.07501700
H	2.82021500	0.67966700	0.26224500
H	2.69060100	-0.99202400	0.27062900



SCF energy=-568.6664025

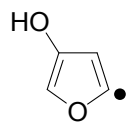
C	-0.82618600	1.13747300	-0.01619900
C	-0.08648500	-0.05243200	-0.02546700
C	-0.73913200	-1.29777900	-0.01527900
C	-2.11585000	-1.26396500	0.00221100
C	-2.89964800	-0.13134500	0.01062500
C	-2.22188200	1.10090800	0.00112800
H	-3.98543300	-0.17348600	0.02233400
H	-2.78805100	2.02899800	0.00488200
H	-0.30969600	2.09234300	-0.02698700
C	1.41932900	0.01559400	-0.00306400
H	-0.17648400	-2.22587200	-0.02526100
F	1.89175400	0.32540800	1.23527800
F	1.89834600	0.96797900	-0.84374100
F	1.99643200	-1.15702100	-0.35805900



SCF energy=-245.3513867

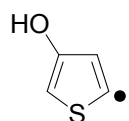
C	-0.66839700	0.85695900	0.00010000
C	-1.11129500	-0.49878300	0.00004200
C	0.08377800	-1.15343100	-0.00008000
O	1.13342300	-0.37738500	-0.00006000
H	-1.26823000	1.75986200	0.00017100
H	-2.11185100	-0.90004200	0.00007000
N	0.64116900	0.99011400	-0.00001900

C	0.75773600	0.75943500	0.00005400
O	-0.57892000	0.94905800	-0.00030200
N	-1.21340400	-0.35159500	0.00017600
H	1.35442900	1.66195800	0.00001800
H	2.04863000	-1.03816200	0.00004800



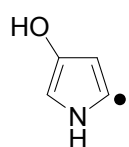
SCF energy=-304.5694113

C	0.24514400	-1.07135500	0.01324900
C	-0.65321500	-0.04479300	0.00620400
C	0.08768400	1.19935400	-0.00114900
C	1.38271500	0.78439100	-0.01124100
H	0.17211500	-2.14600900	0.00082800
H	-0.29315800	2.21015400	-0.01651300
O	-2.00813200	-0.20474400	-0.03803200
H	-2.44670100	0.61447700	0.23689300
O	1.53235400	-0.53078100	0.00508400



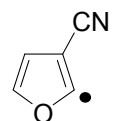
SCF energy=-627.517477

C	-0.01042400	-1.04911600	0.00006700
C	0.97143300	-0.09415600	0.00005500
C	0.47021800	1.26199100	0.00002900
C	-0.88550600	1.23450400	-0.00012400
S	-1.60705000	-0.31832300	0.00002400
H	0.10680600	-2.12427300	-0.00017000
H	1.08949100	2.15299600	0.00002400
O	2.29965300	-0.42843100	-0.00015800
H	2.84494600	0.37254700	0.00086400



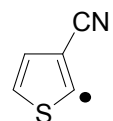
SCF energy=-284.7159724

C	0.25876400	-1.07244800	-0.03392600
C	-0.66792400	-0.03914700	-0.02826700
C	0.02801200	1.20432900	-0.03145700
C	1.36711800	0.86871300	0.08419000
N	1.51513100	-0.48018800	-0.03855900
H	2.38863500	-0.98059200	0.03018300
H	0.11943600	-2.13604900	0.09582700
H	-0.39620600	2.19898700	-0.05840700
O	-2.01794000	-0.25629400	0.05333700
H	-2.49008400	0.56063700	-0.16762900



SCF energy=-321.5994532

C	-0.47552100	-1.11714600	-0.00009800
C	0.37476700	-0.04350800	-0.00021200
C	-0.52099700	1.10219700	-0.00012700
C	-1.78665600	0.61297400	0.00013300
O	-1.75141300	-0.77798200	0.00010200
H	-0.22002500	2.14080800	0.00010100
H	-2.77252900	1.04997800	0.00005000
C	1.79314100	-0.03981000	-0.00004100
N	2.95649300	-0.00788300	0.00015700



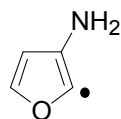
SCF energy=-644.5932019

C	-0.18355000	-1.04308000	-0.00029000
C	0.71322600	-0.01050100	-0.00058700
C	-0.00124000	1.25104500	0.00013700



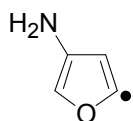
SCF energy=-245.3478016

C	1.11615600	0.38897000	-0.00016700
C	-0.02742500	1.22086100	0.00018900
C	-1.10023500	0.39437200	0.00004700
O	-0.65221700	-0.88202900	-0.00049200
H	2.16717100	0.64399400	0.00010700
N	0.75579900	-0.87781100	0.00049200
H	-2.17099900	0.53169500	-0.00003700



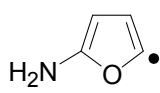
SCF energy=-284.7047019

C	0.07844800	-1.22917600	0.00008900
C	-0.69001400	0.01247200	0.00000800
C	0.17793200	1.14272700	0.00008200
C	1.43036200	0.60064800	-0.00001300
O	1.38215200	-0.77245100	-0.00001400
H	-0.06921600	2.19643100	0.00009800
H	2.41584200	1.04787800	-0.00025000
N	-2.03930800	-0.01735900	-0.00029400
H	-2.50010000	-0.91904600	0.00058900
H	-2.60896100	0.81583200	0.00074500



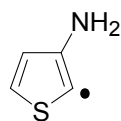
SCF energy=-284.7040514

C	-1.42480000	0.75524500	-0.01519200
C	-0.14149500	1.20007500	-0.00153000
C	0.64523500	-0.01967100	0.00542700
C	-0.23858000	-1.06419300	0.02133300
O	-1.54537100	-0.56382500	0.01124400
H	-0.14799600	-2.13849300	-0.00637000
H	0.21548100	2.21884500	-0.03061300
N	2.04316800	-0.05906300	-0.09400100
H	2.51390100	0.60099300	0.51673200
H	2.43724900	-0.98603500	0.02807300



SCF energy=-284.7016582

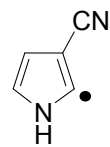
C	1.39610500	0.90327400	-0.09794200
C	1.56956600	-0.49789800	0.02675200
C	0.31803700	-1.13312200	0.01375200
C	-0.61469600	-0.09280400	0.04057100
O	0.00594500	1.10610000	0.05362600
H	2.53657400	-0.98432700	0.04580700
H	0.08964100	-2.19012900	-0.03839100
N	-1.96440400	-0.08024600	-0.07155500
H	-2.47565800	-0.94964400	-0.02757300
H	-2.46136500	0.76031700	0.19323800



SCF energy=-607.6979249

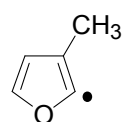
C	-0.08522900	-1.20009900	-0.00012400
C	-0.97324500	-0.06046500	-0.00007600
C	-0.38100200	1.25569300	-0.00009200
C	0.97809300	1.17586800	0.00022100
S	1.48883700	-0.53125400	-0.00000300
H	-0.94065600	2.18676300	-0.00035100
H	1.68531400	1.99818200	-0.00018200
N	-2.31000500	-0.27788500	0.00022900
H	-2.63789500	-1.23580200	-0.00002400
H	-2.98983000	0.47012500	-0.00056300

C	-1.35715200	1.09579000	0.00037300
S	-1.82915000	-0.59400100	0.00010500
H	0.50372500	2.21074400	-0.00140500
H	-2.12056000	1.86336400	-0.00036800
C	2.13288000	-0.13717900	-0.00009800
N	3.29403700	-0.21521900	0.00041200



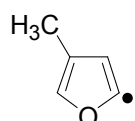
SCF energy=-301.7536573

C	-1.77704400	0.66916200	0.00003500
C	-0.47729500	1.11158000	-0.00014800
C	0.39070700	-0.04475600	0.00004500
C	-0.46615700	-1.12708900	0.00004800
N	-1.75377400	-0.72311500	-0.00003500
H	-2.56084200	-1.33010800	0.00000900
H	-0.14309000	2.14019300	-0.00027200
C	1.80927800	-0.05522400	0.00004900
N	2.97382100	-0.03980400	0.00003800
H	-2.71332400	1.20830800	0.00007000



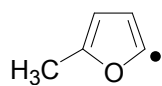
SCF energy=-268.662901

C	-0.15978500	-1.10494200	0.00003100
C	0.69639300	-0.04689200	-0.00011100
C	-0.20779900	1.08968100	-0.00002900
C	-1.48139700	0.60937700	-0.00001700
O	-1.45554200	-0.77351400	0.00000800
H	0.08240300	2.13345200	0.00015200
H	-2.46305300	1.05738800	0.00015600
C	2.19480600	-0.03318500	0.00003300
H	2.58898000	0.48343600	0.88403500
H	2.59353600	-1.05209400	0.00106300
H	2.58915700	0.48169700	-0.88490800



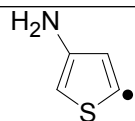
SCF energy=-268.6633416

C	1.46501700	0.74542800	-0.00026300
C	0.18631100	1.20158800	0.00020800
C	-0.61960800	-0.00793500	0.00024500
C	0.25748900	-1.05207400	0.00007900
O	1.56539400	-0.58221000	-0.00001600
H	0.15032500	-2.12616800	0.00001100
H	-0.15421000	2.22664800	0.00000600
C	-2.11836600	-0.07884700	-0.00013100
H	-2.46160900	-1.11920800	-0.00128900
H	-2.54154100	0.41281100	0.88457900
H	-2.54116800	0.41463800	-0.88400600



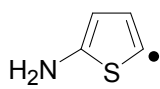
SCF energy=-268.666376

C	-1.36086000	0.85796300	-0.00022700
C	-1.65690200	-0.46601000	0.00001900
C	-0.35529100	-1.10169600	0.00011900
C	0.59207000	-0.11981300	0.00016800
O	-0.05063000	1.11816900	0.00016500
H	-2.63073200	-0.93168600	-0.00030200
H	-0.16394800	-2.16744600	-0.00010300
C	2.07914400	-0.09617000	-0.00012600
H	2.47595200	0.41453500	0.88633800
H	2.45925800	-1.12258000	-0.00117000
H	2.47554000	0.41618700	-0.88580100



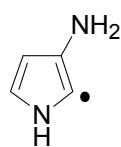
SCF energy=-607.6513752

C	-0.93034600	1.22141800	-0.00896200
C	0.42227300	1.27799800	-0.00133900
C	0.97122800	-0.06413500	0.00299300
C	-0.00131700	-1.03567000	0.01393800
S	-1.62156700	-0.34685900	0.00481600
H	0.12350500	-2.11116600	-0.00619800
H	1.02148500	2.18159200	-0.02744900
N	2.35470400	-0.28829500	-0.09098300
H	2.91540900	0.34765700	0.46665900
H	2.63071900	-1.24794800	0.08703400



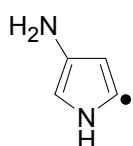
SCF energy=-607.6936163

C	-1.67926900	-0.30257400	-0.11494100
C	-1.44575700	1.04151100	0.02769800
C	-0.05156700	1.35791900	0.02983100
C	0.75713200	0.23655300	0.06930200
S	-0.23229600	-1.24135000	0.01669300
H	-2.22914700	1.78546000	0.13332200
H	0.34306400	2.37021000	-0.00176600
N	2.12540600	0.16126400	-0.10232200
H	2.60366900	1.03953900	-0.26354300
H	2.63808300	-0.46291000	0.50981000



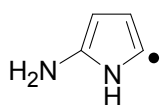
SCF energy=-264.8614106

C	1.41785400	0.67631700	-0.00009700
C	0.12860100	1.15857400	0.00010800
C	-0.69986400	-0.00204900	0.00013700
C	0.09299000	-1.23762100	0.00002500
N	1.35560100	-0.72189000	-0.00004700
H	2.17856700	-1.30859000	-0.00031900
H	-0.16633200	2.20048800	-0.00009300
H	2.36227900	1.20741200	-0.00001800
N	-2.05282300	-0.05891500	0.00047300
H	-2.49456200	-0.96919200	-0.00134500
H	-2.63688700	0.76418900	-0.00224200



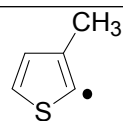
SCF energy=-264.8481215

C	-0.24807400	-1.06667700	0.04046200
C	0.66159400	-0.00788900	0.02965000
C	-0.08757300	1.20762000	0.03310900
C	-1.41694100	0.83822900	-0.08771200
N	-1.52296600	-0.51674600	0.04178700
H	-2.38133600	-1.04413100	-0.00750500
H	-0.08769400	-2.12635700	-0.11022400
H	0.30951800	2.21347200	0.03441700
N	2.05324600	-0.11054800	-0.11121400
H	2.57379100	0.56469600	0.43856700
H	2.41972900	-1.04431900	0.03768300



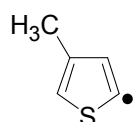
SCF energy=-264.8483926

C	0.62834300	-0.08117700	0.05281700
C	-0.29208300	-1.13931100	0.01506600
C	-1.56816100	-0.55055800	0.01806800
C	-1.44669600	0.86376100	-0.10413500



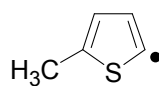
SCF energy=-591.6564999

C	-0.06289400	-1.05652600	-0.00001800
C	-1.01196000	-0.08439500	-0.00007100
C	-0.34357900	1.20076500	0.00005800
C	1.02241100	1.12539500	-0.00003300
S	1.57766700	-0.53608800	0.00001800
H	-0.88582000	2.14279900	0.00000500
H	1.74129500	1.93523600	-0.00008400
C	-2.50530200	-0.27458900	0.00002000
H	-2.76516100	-1.33701100	0.00110400
H	-2.96259700	0.18718000	0.88410600
H	-2.96244000	0.18530500	-0.88514600



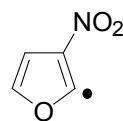
SCF energy=-591.656623

C	0.97802200	1.21579900	0.00000500
C	-0.37451800	1.29006100	0.00000400
C	-0.95071000	-0.04063900	0.00000500
C	0.00831000	-1.02067500	0.00002600
S	1.63857100	-0.37022900	-0.00001000
H	-0.13742200	-2.09426400	0.00001100
H	-0.95541500	2.20611200	0.00001000
C	-2.43517500	-0.29546000	-0.00000700
H	-2.91509500	0.14341800	0.88398900
H	-2.91502800	0.14322600	-0.88414700
H	-2.64974700	-1.36934200	0.00008900



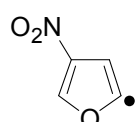
SCF energy=-591.6567476

C	-1.67726600	-0.33267200	-0.00004900
C	-1.52591400	1.01288000	0.00001000
C	-0.11937200	1.34178500	0.00001300
C	0.71975400	0.25799300	0.00001800
S	-0.21673800	-1.24323400	0.00001400
H	-2.32902600	1.74095300	0.00000500
H	0.24688400	2.36508600	0.00000500
C	2.21988800	0.23229100	-0.00001800
H	2.62384400	-0.27421400	0.88547600
H	2.62381700	-0.27382200	-0.88575200
H	2.59976200	1.26008400	0.00020400



SCF energy=-433.8400976

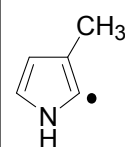
C	0.78203000	-1.11959300	-0.00035200
C	-0.02575900	-0.01841600	0.00008500
C	0.86315500	1.11495200	0.00063900
C	2.11820500	0.59909700	0.00030200
O	2.05838100	-0.79834200	-0.00039300
H	0.57160800	2.15534000	0.00004200
N	-1.45815000	-0.01509600	0.00010900
O	-2.03475600	-1.10474300	0.00048300
O	-2.01167700	1.08827100	-0.00066500
H	3.11406600	1.01261000	-0.00024700



SCF energy=-433.8425076

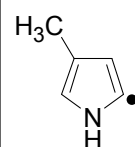
C	-2.09660400	0.72934900	0.00032700
C	-0.83870000	1.23219000	-0.00028100
C	-0.03413900	0.03647600	-0.00095000
C	-0.85650100	-1.05540600	-0.00021900
O	-2.14984800	-0.61231600	0.00027800

N	-0.09297200	1.10171600	0.07909700
H	0.33128900	1.99571900	-0.12979300
H	-2.51063400	-1.07989300	0.08460600
H	-0.03528900	-2.19201200	-0.00922200
N	1.99683900	-0.08357900	-0.10105500
H	2.52480900	0.58881200	0.44492300
H	2.43433900	-0.99587300	-0.12770700



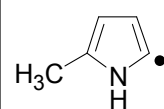
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C	-1.46705700	0.67614900	0.00261900
C	-0.15372400	1.09635400	-0.00259800
C	0.71197900	-0.05771300	-0.00220600
C	-0.15898400	-1.11759200	-0.00666800
N	-1.46013700	-0.71002100	0.00620300
H	-2.26983900	-1.31086900	-0.00840900
H	-2.39547400	1.23012800	-0.00345300
H	0.17949300	2.12777600	-0.00619900
C	2.21313200	-0.07196500	0.00265400
H	2.61744900	0.43073500	0.89063800
H	2.59369700	-1.09838800	-0.00121800
H	2.62355900	0.43936800	-0.87759000



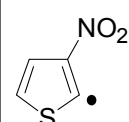
SCF energy=-248.811542

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C	-0.63170200	-0.01353100	-0.00038400
C	0.12598700	1.21570400	-0.00038400
C	1.43947700	0.82958200	0.00060000
N	1.55530100	-0.52404300	0.00011000
H	2.41698100	-1.04771600	0.00050500
H	0.11271000	-2.12869000	0.00003100
H	-0.26651500	2.22280700	-0.00095300
C	-2.13064200	-0.12470800	0.00035800
H	-2.57232300	0.34966400	0.88621800
H	-2.57363200	0.35608100	-0.88133900
H	-2.44395300	-1.17516800	-0.00319800



SCF energy=-248.8126106

C	-0.60245300	0.09331000	-0.02796600
C	0.33923000	1.10473300	-0.00590100
C	1.65372300	0.52106300	0.00172900
C	1.43518500	-0.83066000	0.04012800
N	0.10125800	-1.10863000	-0.03652400
H	-0.31081100	-2.02757900	0.03296200
H	2.60283800	1.03685000	-0.01689000
H	0.11743800	2.16525100	0.01123600
C	-2.09724300	0.13198400	0.01652300
H	-2.55083800	-0.43068800	-0.81082100
H	-2.49920600	-0.27485200	0.95524800
H	-2.43888000	1.16883900	-0.06314200

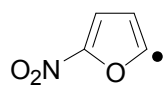


SCF energy=-756.8361033

C	0.50815600	-1.02133200	0.00030300
C	-0.34782400	0.03809800	-0.00009000
C	0.35302500	1.29108000	-0.00048300
C	1.70619900	1.11041100	-0.00036000
S	2.15488600	-0.59181900	0.00023100

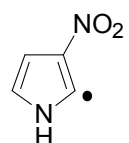


H	-0.69364000	-2.12098900	0.00109600
H	-0.50452500	2.25706600	0.00004800
N	1.40484100	-0.02215400	-0.00004900
O	2.01375000	1.04854800	0.00041500
O	1.92609100	-1.14081400	0.00004900



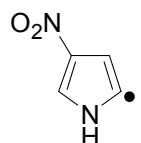
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C	-1.99199200	-0.82649200	0.00007700
C	-2.23770300	0.51787500	-0.00002000
C	-0.92963000	1.10223900	-0.00013000
C	-0.04408000	0.05815100	0.00001700
O	-0.70427200	-1.14704700	0.00007000
H	-3.19414700	1.01791600	-0.00002300
H	-0.67246500	2.15207200	-0.00016700
N	1.38075800	0.03356600	-0.00005800
O	1.94854400	-1.05803400	-0.00010900
O	1.93344500	1.14063300	0.00015500



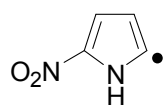
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C	2.11242400	0.65712300	-0.00027500
C	0.82365700	1.13073800	0.00028900
C	-0.03902800	-0.01246500	0.00037300
C	0.77399500	-1.12380900	0.00032800
N	2.06410100	-0.73964200	-0.00037400
H	2.86279300	-1.35871500	0.00026600
H	0.50151700	2.16208900	0.00030700
N	-1.46733400	-0.02777700	-0.00003700
O	-2.04734700	1.06346700	-0.00019500
O	-2.03125900	-1.12792600	-0.00007000
H	3.06088500	1.17470100	0.00013000



SCF energy=-413.9994541

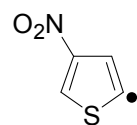
C	0.86078200	-1.05667300	0.00043900
C	0.02262700	0.04438700	0.00030000
C	0.79359000	1.25443200	-0.00001300
C	2.08148000	0.80653500	-0.00060400
N	2.14043900	-0.56085000	0.00006700
H	2.98474100	-1.11576600	0.00036700
H	0.63767600	-2.11267000	-0.00008300
N	-1.40964300	-0.03705500	-0.00002500
O	-2.04409900	1.02145800	0.00021000
O	-1.91923300	-1.16439900	-0.00041100
H	0.41779000	2.26521500	0.00029500



SCF energy=-413.9977575

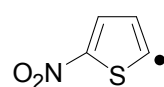
C	-0.03624900	0.06435200	0.00000600
C	-0.93837300	1.11752700	0.00009200
C	-2.24300500	0.55342700	0.00016500
C	-2.04316600	-0.81398900	-0.00037600
N	-0.73453200	-1.13089700	0.00019700
H	-0.29905300	-2.04437700	-0.00163600
H	-3.18579700	1.07997200	0.00036300
N	1.37935400	0.05866100	0.00007900
O	1.94065100	-1.05115600	0.00031800
O	1.96105600	1.14806900	-0.00036000
H	-0.67779700	2.16685700	0.00035300

H	-0.14935000	2.25078700	-0.00055500
H	2.48546800	1.86208100	-0.00042000
N	-1.78700300	-0.09987400	0.00006400
O	-2.45553800	0.93662900	0.00074800
O	-2.24728700	-1.24340200	-0.00067200



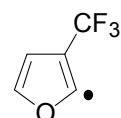
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C	-1.66204700	1.20361000	0.00001100
C	-0.32110300	1.38030400	-0.00002700
C	0.29613900	0.08081300	0.00000100
C	-0.56810500	-0.98466700	-0.00001500
S	-2.21139600	-0.43079000	0.00001100
H	-0.31957800	-2.03720000	-0.00009200
H	0.22120800	2.31621900	-0.00006600
N	1.73837000	-0.10174300	0.00000600
O	2.16809400	-1.25756000	0.00000100
O	2.43725700	0.91324300	0.00001400



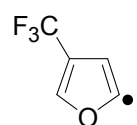
SCF energy=-756.8346301

C	-2.23314100	-0.22017100	0.00029400
C	-2.00178600	1.12306000	-0.00018600
C	-0.59188200	1.36259000	-0.00000800
C	0.13106300	0.19305000	-0.00010600
S	-0.86673800	-1.25009200	-0.00008300
H	-2.75996800	1.89706200	0.00030200
H	-0.12805500	2.34240700	0.00027300
N	1.55976200	0.07767400	0.00002700
O	2.21635300	1.12224800	-0.00002400
O	2.03514400	-1.06385900	0.00009900



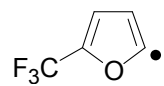
SCF energy=-566.4335807

C	-2.43927900	0.60008100	-0.00001400
C	-1.17765500	1.10365300	-0.00004900
C	-0.27849400	-0.03041300	0.00006100
C	-1.10586400	-1.11027200	-0.00001600
O	-2.39051000	-0.78913300	0.00002400
H	-3.42934600	1.02783100	-0.00002400
H	-0.89517200	2.14791300	-0.00003600
C	1.20668600	-0.01847800	-0.00001200
F	1.70805600	0.62862800	1.08587300
F	1.71898800	-1.26879900	0.00164100
F	1.70809300	0.62571400	-1.08750800



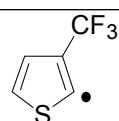
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C	1.16457100	-1.04660600	0.00017800
C	0.32885500	0.03055700	0.00015900
C	1.14865900	1.22341200	0.00010700
C	2.40998900	0.72691900	-0.00018900
O	2.46802600	-0.60866500	-0.00003900
H	1.01639300	-2.11477400	0.00010100
H	0.82932800	2.25416400	0.00008000
C	-1.15942800	-0.01612200	-0.00007600
F	-1.68808600	0.60191700	-1.08735900
F	-1.68824200	0.60326900	1.08656800
F	-1.61764900	-1.29174600	0.00068600



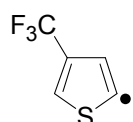
SCF energy=-566.4301594

C	-0.34239300	0.07796800	0.00048400
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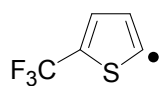
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C	-2.04648400	1.10011000	-0.00005400
C	-0.69192200	1.27871900	-0.00000700
C	0.03694000	0.03357700	0.00011100
C	-0.82906100	-1.01320600	0.00007300
S	-2.48784300	-0.59768600	-0.00000300
H	-2.82297900	1.85460800	0.00007400
H	-0.20956700	2.25062300	0.00020400
C	1.52714100	-0.07006400	-0.00002200
F	2.07406900	0.53683500	-1.08708800
F	1.94706200	-1.35336700	-0.00002500
F	2.07424200	0.53685800	1.08702000



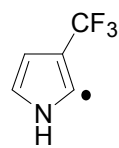
SCF energy=-889.429343

C	0.87604700	-0.97520400	0.00028000
C	0.00733600	0.08455000	0.00035300
C	0.65595200	1.37454000	0.00022900
C	1.99730800	1.19265900	-0.00022400
S	2.53513500	-0.44075600	-0.00004500
H	0.63900700	-2.03079000	0.00003700
H	0.13833800	2.32626900	0.00005500
C	-1.48169000	-0.06554400	-0.00006100
F	-1.86441900	-1.36434100	0.00128700
F	-2.04974000	0.52176800	1.08627500
F	-2.04908900	0.51930800	-1.08787500



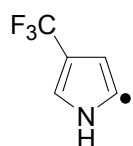
SCF energy=-889.42572

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C	0.88523900	1.34590900	0.00063700
C	2.30506100	1.12223200	-0.00003500
C	2.54974800	-0.21257600	-0.00103100
S	1.17900700	-1.24147400	0.00032600
H	0.43325600	2.33190900	0.00033200
H	3.05402100	1.90507300	-0.00027400
C	-1.33431700	0.06441600	-0.00004900
F	-1.92294200	1.28266600	0.00550500
F	-1.79935000	-0.60359300	-1.08921100
F	-1.79970800	-0.61384100	1.08273800



SCF energy=-546.5867249

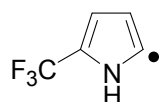
C	-2.43814000	0.65889200	-0.00003800
C	-1.14180200	1.11702200	-0.00006100
C	-0.26929900	-0.02657200	-0.00009200
C	-1.10207700	-1.11652000	0.00000200
N	-2.39909800	-0.73165800	0.00008800
H	-3.19804300	-1.34881500	-0.00044200
H	-0.82698000	2.15228200	0.00001800
H	-3.38052200	1.18774400	0.00036300
C	1.21335600	-0.02649500	-0.00000400
F	1.73075500	0.61380600	-1.08577000
F	1.73066500	0.61289200	1.08633600
F	1.71935900	-1.28309400	-0.00049800



SCF energy=-546.5883699

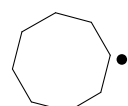
C	1.17065000	1.04802300	-0.00009100
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C	-1.24347300	1.10148700	0.00041600
C	-2.55523800	0.50420200	-0.00019400
C	-2.29849300	-0.83182900	-0.00030500
O	-1.00301700	-1.13628500	0.00008000
H	-1.01110800	2.15783000	0.00058300
H	-3.51471500	0.99809300	-0.00014600
C	1.14355600	0.03049300	-0.00028100
F	1.63867300	1.28980300	0.00031300
F	1.64336100	-0.60986900	1.08550300
F	1.64310000	-0.60877500	-1.08601600



SCF energy=-546.5843536

C	-0.33645900	-0.05556400	-0.02940200
C	-1.23354000	-1.10577200	-0.01349800
C	-2.55683100	-0.56102800	0.01123100
C	-2.37542200	0.79940300	0.01847100
N	-1.06181700	1.12914100	-0.00682000
H	-0.67634600	2.06236300	-0.04100700
H	-3.48987200	-1.10441700	0.02158300
C	1.14460400	-0.04702100	-0.00285000
F	1.65007300	-1.26057300	-0.30667800
F	1.65685200	0.30533900	1.21329900
F	1.66179900	0.85679900	-0.88665500
H	-0.97369400	-2.15613000	-0.01623600



SCF energy=-313.8277421

C	1.42200900	1.29929600	-0.19131200
C	1.75086400	-0.05435100	0.47300900
C	-2.01504900	0.06747800	0.14504400
C	1.26124500	-1.34612200	-0.21452300
C	-1.31682300	-1.11121300	-0.46334600
C	-0.17106100	-1.82782300	0.17765300
H	2.01958200	1.39475800	-1.10980300
H	1.38929000	-0.05676800	1.51160100
H	1.32925600	-1.25031900	-1.30776700
H	-2.76095200	0.44364600	-0.56784900
H	-1.60463900	-1.42532700	-1.46545600
H	1.78777400	2.08571000	0.48571100
H	2.84605800	-0.10219100	0.55212200
H	-2.58180100	-0.24218900	1.04190600
H	1.95110600	-2.15520000	0.06352000
H	-0.23395400	-2.89358700	-0.08807900
H	-0.25360700	-1.77797100	1.27490100
C	-0.05001200	1.59687300	-0.54646100
H	-0.31170100	1.05694200	-1.46596200
H	-0.12130400	2.66309200	-0.79912500
C	-1.07927800	1.23831700	0.55241200
H	-0.56021600	0.97885800	1.48316500
H	-1.70626500	2.10581800	0.79626400



SCF energy=-195.8896683

C	-0.73809000	0.99023700	0.22249700
C	-1.23678500	-0.43538300	-0.12061700
C	-0.00038200	-1.27861600	-0.00021600
C	1.23646600	-0.43613600	0.12074400
C	0.73875000	0.98981100	-0.22256800
H	-1.32884300	1.77911900	-0.25691200
H	-0.79779000	1.14798900	1.30793300
H	-1.64373100	-0.46364500	-1.14869600
H	-2.05637100	-0.76912400	0.53273600
H	-0.00074100	-2.36468500	0.00020800

C	0.32193300	-0.04053700	-0.00002300	H	1.64296300	-0.46452500	1.14901500
C	1.10850400	-1.24567600	-0.00010900	H	2.05612600	-0.77035900	-0.53224300
C	2.40040500	-0.80284700	-0.00008900	H	1.32995300	1.77830900	0.25691900
N	2.46078400	0.55872800	-0.00002100	H	0.79867700	1.14744300	-1.30800100
H	3.30276000	1.11546000	-0.00005000				
H	0.96236200	2.10767700	-0.00010200				
C	-1.16204500	0.02496700	0.00005100				
F	-1.60913600	1.30797000	0.00008300				
F	-1.71085800	-0.58585400	-1.08595300				
F	-1.71076200	-0.58587900	1.08609000				
H	0.74952200	-2.26394400	-0.00011700				