

Supporting Information

Theoretical study on homolytic B-B cleavages of diboron(4) compounds

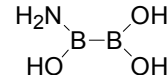
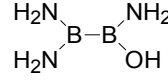
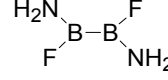
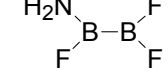
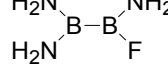
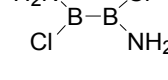
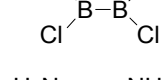
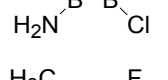
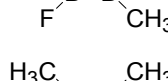
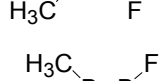
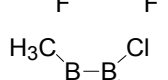
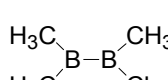
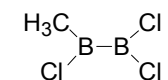

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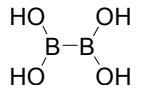
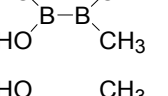
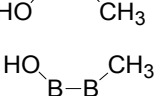
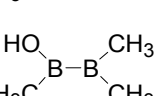
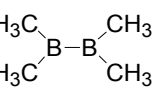
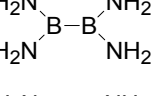
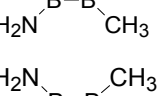
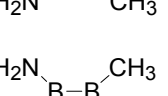
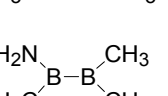
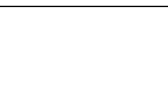

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Table S1 The 34 B-B BDEs calculated by using 28 kinds of DFT methods (kJ/mol)

Entry	Molecules	M06-HF	M05-2X	WB97	MN12-SX	BMK	SOGGA11-X	WB97XD	M06-2X	M06	KMLYP
1		429.0	447.2	444.1	423.5	425.6	434.8	423.1	414.6	425.3	445.1
2		409.9	425.0	423.2	402.6	404.1	413.1	403.8	396.2	404.4	422.7
3		402.9	416.7	415.4	391.7	396.5	406.6	398.2	388.7	393.7	413.5
4		388.3	399.8	399.0	378.3	379.2	387.7	382.6	374.7	381.1	396.1
5		390.1	401.8	400.9	377.9	382.1	391.5	386.9	377.4	380.5	397.9
6		404.2	413.2	411.6	388.0	393.9	402.1	399.3	390.4	390.7	408.5
7		408.3	435.3	437.0	400.9	410.2	423.9	415.0	400.5	409.8	427.2
8		402.6	425.1	426.6	393.9	401.8	413.8	406.9	393.5	401.3	418.5
9		400.3	418.0	418.8	389.7	395.5	405.6	400.6	389.7	395.3	411.5
10		397.4	415.7	417.0	386.9	394.6	405.2	399.8	387.2	392.4	410.8
11		396.8	410.8	410.9	383.9	390.7	400.2	396.0	385.1	387.8	406.2
12		423.1	457.0	451.0	429.5	432.9	445.4	428.5	414.8	427.2	450.1
13		424.9	430.5	430.1	410.5	416.6	423.6	411.2	407.2	414.6	433.0
14		420.3	420.9	419.2	396.0	409.2	408.9	401.7	400.4	403.3	422.2
15		418.5	420.9	419.8	395.7	407.3	409.9	404.3	399.9	402.0	421.2
16		413.6	417.9	416.8	392.1	403.0	406.9	402.3	396.5	397.2	416.8
17		416.7	420.4	419.0	395.0	404.6	409.2	404.4	398.4	400.5	418.8
18		410.2	416.9	415.5	391.5	399.3	405.7	402.1	394.6	395.7	413.9
19		415.2	438.0	437.6	408.8	414.7	426.4	415.9	404.2	414.4	432.6
20		402.8	426.3	426.4	397.8	403.2	415.7	406.2	392.5	402.3	420.5

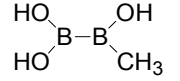
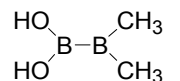
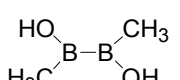
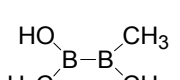
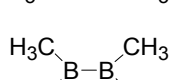
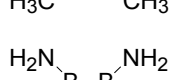
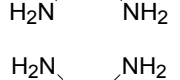
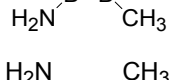
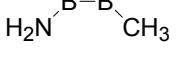
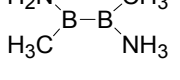
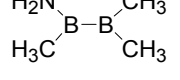
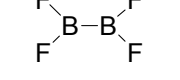
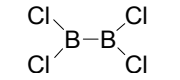
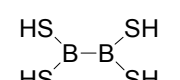
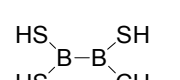
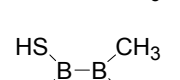
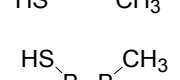
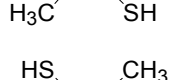
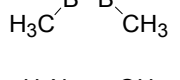
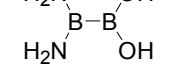
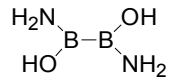
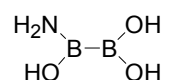
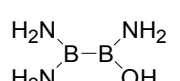
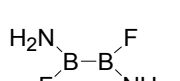
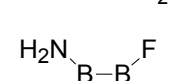
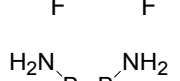
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E-mail address: wrzheng@sues.edu.cn (W.R. Zheng).

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22		403.1	428.6	429.1	397.9	404.3	417.3	407.2	394.7	404.9	421.6
23		431.0	458.5	455.8	428.9	433.8	446.9	433.7	419.6	431.0	451.4
24		431.2	462.0	457.4	433.5	438.0	450.5	435.3	421.4	433.8	455.1
25		419.1	446.5	446.3	414.6	421.8	434.9	423.8	409.7	420.4	439.1
26		436.6	455.0	455.3	429.8	436.6	444.5	433.7	425.4	434.5	453.0
27		428.2	440.5	441.0	419.6	424.3	431.0	419.1	414.4	423.3	440.4
28		421.5	444.5	445.5	414.6	422.7	433.2	423.8	412.2	421.6	439.4
29		398.3	412.6	410.4	390.6	393.3	403.6	393.1	383.2	388.9	409.8
30		401.1	413.5	411.9	389.4	394.0	403.6	396.8	387.1	390.5	410.0
31		413.2	437.6	434.1	412.6	416.4	428.2	414.1	401.4	411.0	433.1
32		416.8	424.0	422.5	401.9	407.4	414.7	406.3	401.4	406.5	423.5
33		412.7	421.8	420.1	397.6	403.6	411.3	405.8	399.0	401.7	419.2
34		422.5	429.4	428.4	408.2	414.3	421.3	410.9	406.4	412.3	430.6

Entry	Molecules	MN12-L	M11	N12-SX	MPW1B95	BP86-D3	MPW1P86	N12	B3P86	B3LYP-D3	M05
1		414.3	417.3	427.3	420.7	409.7	411.8	410.0	411.2	413.6	428.7
2		395.1	397.3	406.5	400.0	391.1	391.2	390.4	390.6	393.0	406.9
3		382.7	388.9	399.7	391.4	384.3	383.7	384.8	383.5	386.3	400.4
4		372.4	373.3	381.7	375.0	370.4	367.0	366.7	366.5	370.1	382.0
5		370.7	374.9	386.0	377.4	373.7	370.2	372.8	370.2	373.5	386.3
6		381.1	386.9	397.0	388.1	385.8	380.7	384.4	380.6	385.1	395.9
7		390.9	400.5	414.5	407.4	398.8	397.1	398.8	395.7	400.7	417.3
8		384.5	393.1	405.6	398.5	390.8	388.6	390.3	387.4	392.3	407.1
9		382.6	388.9	398.4	391.2	385.6	381.6	383.7	380.3	386.2	398.8
10		377.2	385.7	398.1	390.6	383.5	381.4	383.2	380.6	384.5	398.4
11		375.2	383.0	394.1	385.6	380.4	377.4	380.0	376.9	381.0	393.9

12		421.2	424.7	436.0	425.7	408.8	417.9	422.8	417.4	414.9	442.3
13		409.5	404.0	416.0	408.8	402.6	402.5	407.1	401.8	402.7	416.4
14		392.3	394.0	403.9	399.4	399.3	391.5	396.7	389.8	397.3	397.9
15		390.2	393.9	404.6	398.6	397.5	390.9	396.6	389.5	396.2	401.4
16		386.4	391.7	401.9	394.4	393.0	387.1	391.3	386.2	392.3	399.8
17		388.8	393.3	403.9	396.9	394.8	389.2	394.9	388.1	393.9	402.4
18		384.9	390.5	400.6	392.4	390.1	385.0	389.6	384.3	389.6	399.7
19		399.3	405.8	418.1	411.3	402.0	401.6	402.1	400.7	404.5	420.0
20		388.2	393.9	407.4	400.6	392.9	391.6	392.7	391.0	394.1	409.8
21		401.5	405.3	416.3	409.8	399.7	400.4	400.2	399.6	402.5	417.7
22		388.6	395.5	408.1	401.6	392.8	391.5	392.5	390.3	395.1	411.4
23		420.0	426.5	439.1	429.8	416.7	420.5	425.1	419.9	421.4	442.3
24		425.1	429.6	442.2	432.3	417.3	423.6	428.9	423.1	422.6	446.7
25		405.6	413.7	426.9	418.4	407.3	408.4	412.0	407.3	410.8	429.7
26		427.3	426.7	436.6	430.7	423.3	421.4	424.3	420.0	424.9	436.2
27		419.6	414.0	423.2	417.3	409.9	409.0	412.3	407.6	410.5	422.0
28		408.4	413.1	424.9	418.1	410.0	408.4	410.8	406.9	411.9	426.1
29		385.3	387.6	397.7	387.2	377.2	380.5	384.0	380.9	380.2	399.6
30		383.2	388.0	398.4	388.3	381.5	381.2	385.2	381.5	383.1	399.0
31		405.7	409.2	420.6	409.6	396.3	402.5	407.4	402.7	400.8	424.5
32		398.9	398.8	408.7	400.2	395.6	393.8	397.4	393.3	396.2	410.7
33		392.9	396.0	406.0	397.0	393.5	390.2	393.7	389.9	393.6	406.6
34		406.5	403.3	414.6	406.6	401.2	400.3	404.3	399.7	401.6	415.7

Entry	Molucules	M06-L	CAM-B3LYP	PBE1PBE	SOGGA11	MPW1K	B3LYP	M11-L	B97D
1		412.1	414.7	407.9	400.9	407.8	402.4	384.1	406.0

2		391.2	393.2	387.7	384.3	386.4	381.1	366.4	388.2
3		380.0	385.2	380.5	377.7	379.4	374.6	358.0	383.8
4		367.5	367.8	364.0	366.4	361.6	356.5	345.2	370.2
5		367.6	370.4	367.5	371.6	365.1	360.6	346.9	374.8
6		376.5	381.0	378.3	386.6	375.4	371.0	357.4	388.3
7		394.6	400.2	393.5	397.1	390.8	387.9	365.3	403.9
8		385.9	391.1	385.2	390.1	382.6	379.0	359.5	395.2
9		379.5	383.6	378.3	384.6	375.1	371.7	357.2	390.4
10		377.1	383.2	378.3	383.4	376.0	371.7	353.9	386.7
11		372.8	378.5	374.6	381.3	372.4	367.7	352.3	383.5
12		416.9	421.4	413.4	413.2	413.3	410.8	388.2	413.4
13		400.9	402.3	399.6	396.6	398.2	391.2	376.0	389.2
14		382.0	390.0	389.2	399.0	386.0	378.0	368.7	381.1
15		381.7	390.2	388.7	398.9	386.0	378.7	368.0	384.2
16		379.4	386.9	384.9	395.7	382.5	375.8	363.6	385.3
17		381.0	388.8	386.8	397.0	384.1	377.8	366.1	386.5
18		378.7	385.0	382.6	392.6	379.9	374.5	362.2	387.3
19		400.8	404.5	397.9	395.4	396.2	392.5	371.8	402.4
20		389.5	393.5	388.1	387.5	385.9	382.4	362.9	393.0
21		400.5	402.9	396.6	392.5	395.3	390.9	372.9	397.7
22		391.0	394.3	387.7	389.1	385.3	382.6	361.0	396.0
23		419.2	424.2	416.5	417.2	415.0	413.3	388.7	420.3
24		422.8	427.1	419.4	419.0	418.5	416.5	393.2	421.3
25		407.2	412.0	404.5	406.4	402.5	400.3	376.4	411.8
26		420.1	423.1	417.8	418.7	415.5	410.7	395.1	417.0
27		409.0	409.5	405.6	403.2	403.4	396.9	384.0	400.0

28	$\begin{array}{c} \text{H}_2\text{N} \\ \text{H}_2\text{N} \end{array} \text{B}-\text{B} \begin{array}{c} \text{NH}_2 \\ \text{Cl} \end{array}$	406.7	410.9	404.7	407.7	402.4	398.4	379.3	409.7
29	$\begin{array}{c} \text{H}_3\text{C} \\ \text{F} \end{array} \text{B}-\text{B} \begin{array}{c} \text{F} \\ \text{CH}_3 \end{array}$	377.9	382.2	377.1	375.4	376.2	372.7	351.3	378.9
30	$\begin{array}{c} \text{H}_3\text{C} \\ \text{H}_3\text{C} \end{array} \text{B}-\text{B} \begin{array}{c} \text{CH}_3 \\ \text{F} \end{array}$	377.9	382.4	378.3	379.6	376.6	372.7	354.9	383.8
31	$\begin{array}{c} \text{H}_3\text{C} \\ \text{F} \end{array} \text{B}-\text{B} \begin{array}{c} \text{F} \\ \text{F} \end{array}$	400.2	405.0	398.5	395.9	398.1	395.2	371.9	399.3
32	$\begin{array}{c} \text{H}_3\text{C} \\ \text{Cl} \end{array} \text{B}-\text{B} \begin{array}{c} \text{Cl} \\ \text{CH}_3 \end{array}$	391.5	393.9	390.9	392.5	389.2	383.5	369.4	389.2
33	$\begin{array}{c} \text{H}_3\text{C} \\ \text{H}_3\text{C} \end{array} \text{B}-\text{B} \begin{array}{c} \text{CH}_3 \\ \text{Cl} \end{array}$	387.0	390.5	387.5	392.3	385.4	380.3	366.2	391.4
34	$\begin{array}{c} \text{H}_3\text{C} \\ \text{Cl} \end{array} \text{B}-\text{B} \begin{array}{c} \text{Cl} \\ \text{Cl} \end{array}$	398.1	400.2	397.4	397.0	395.9	389.4	374.4	391.3

Table S2 The B-B BDE predictions of several diboron(4) compounds by using SOGGA11-X method

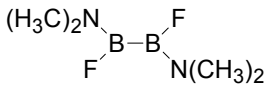
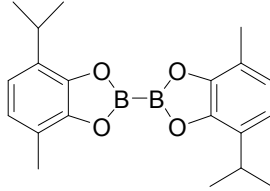
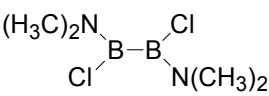
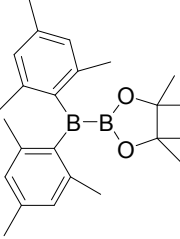
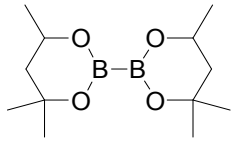
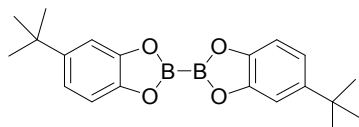
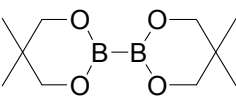
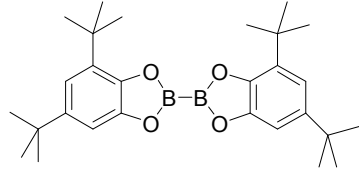
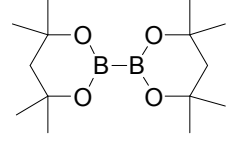
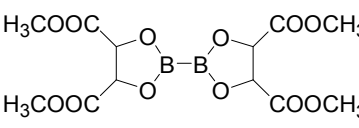
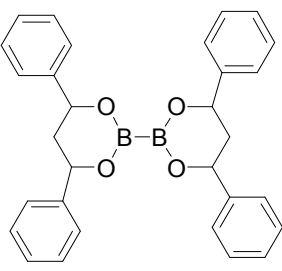
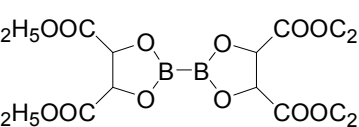
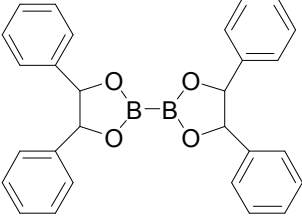
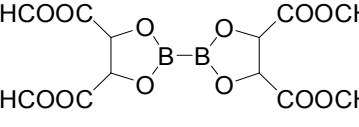
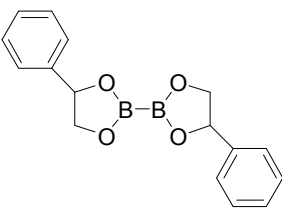
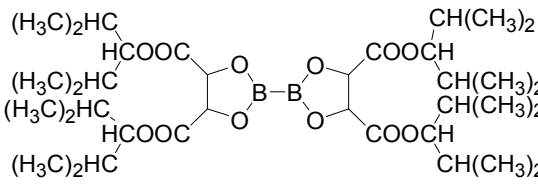
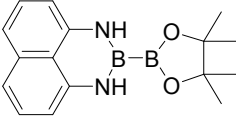
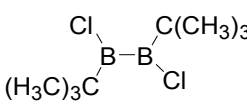
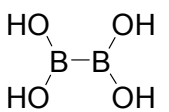
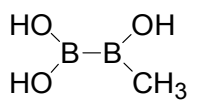
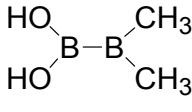
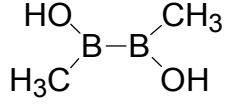
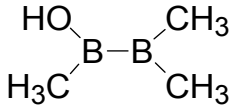
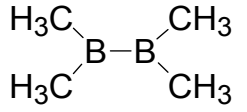
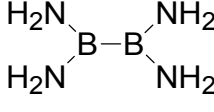
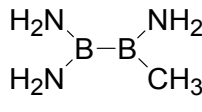
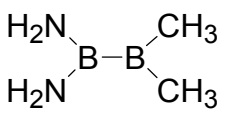
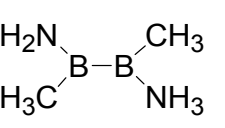
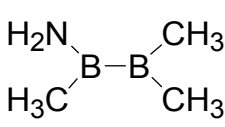
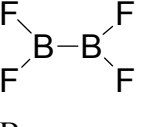
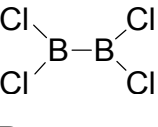
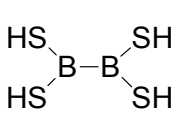
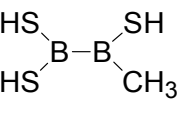
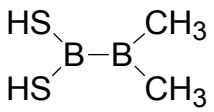
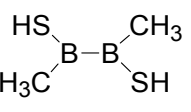
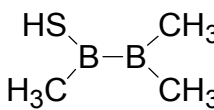
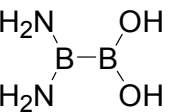
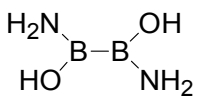
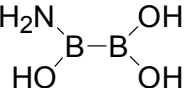
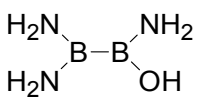
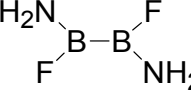
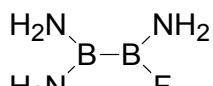
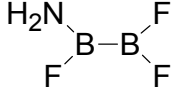
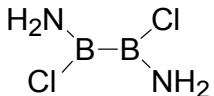
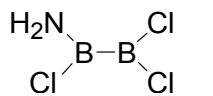
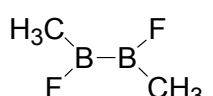
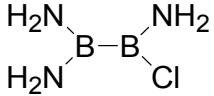
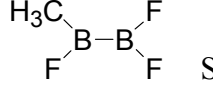
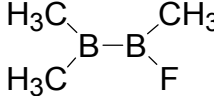
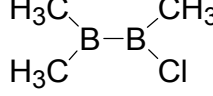
Entry	Compounds	B-B BDEs	Entry	Compounds	B-B BDEs
1		437.9	10		487.7
2		426.5	11		373.6
3		452.6	12		488.0
4		442.9	13		486.1
5		435.7	14		465.2
6		446.9	15		464.0
7		469.0	16		455.6
8		468.4	17		520.9
9		469.6	18		411.1

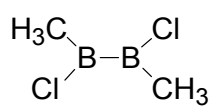
Table S3 The Cartesian coordinates and absolute energy values (hartrees) of selected molecules and radicals

Molecules:							
 SCF energy=-353.2265494				 SCF energy=-317.2640759			
B	0.21608500	-0.80020300	-0.22538200	B	-0.86790400	0.12276500	0.00000900
B	-0.21608500	0.80020300	0.22538200	B	0.84572800	-0.13045000	-0.00002600
O	1.52957800	-1.05408800	-0.53456200	O	-1.63719400	-1.01813800	0.00007700
H	1.68896400	-1.98179000	-0.77839800	H	-2.59327100	-0.84062800	0.00040100
O	0.67522100	1.84189000	0.29512900	O	1.27000200	-1.43083200	-0.00007300
H	1.57619400	1.57261600	0.06064900	H	0.52457000	-2.05481700	-0.00026900
O	-1.52957800	1.05408800	0.53456200	O	-1.54256600	1.32285000	-0.00010800
H	-1.68896400	1.98179000	0.77839800	H	-0.96099000	2.09576200	-0.00007900
O	-0.67522100	-1.84189000	-0.29512900	C	1.95553000	0.99321100	0.00007900
H	-1.57619400	-1.57261600	-0.06064900	H	1.85589100	1.65149900	-0.87733200
				H	1.85603900	1.65111100	0.87780400
				H	2.97352600	0.58518300	-0.00008600
 SCF energy =-281.3000649				 SCF energy =-281.300114			
B	0.89790100	0.00150000	-0.00403300	B	-0.84269300	-0.22431000	-0.00000300
B	-0.81633700	-0.00093800	0.00289400	B	0.84269300	0.22431000	0.00000200
O	1.54986800	0.06945800	-1.21058800	O	1.20459300	1.54842700	-0.00001400
H	2.51720900	0.05609500	-1.10469500	H	0.44710100	2.15373000	0.00011000
O	1.71650700	-0.06187900	1.11282900	O	-1.20459300	-1.54842700	0.00001400
H	1.25211800	-0.12115500	1.95835300	H	-0.44710100	-2.15373000	-0.00011100
C	-1.61723900	1.36057900	0.04065900	C	-2.03877900	0.81336700	-0.00001900
H	-1.66850300	1.66470700	1.10315700	H	-1.99454300	1.47635000	0.87870900
H	-1.12696100	2.19340600	-0.47902200	H	-1.99402100	1.47720600	-0.87806400
H	-2.65725400	1.28321700	-0.30430900	H	-3.02212800	0.32757300	-0.00052300
C	-1.61605200	-1.36175500	-0.04338200	C	2.03877900	-0.81336700	0.00002000
H	-1.68252600	-1.61725500	-1.11768900	H	1.99402200	-1.47720300	0.87806700
H	-1.12215400	-2.22024000	0.42935700	H	1.99454200	-1.47635300	-0.87870600
H	-2.65100300	-1.29516900	0.31895000	H	3.02212800	-0.32757300	0.00052000
 SCF energy =-245.3402161				 SCF energy =-209.3832803			
B	0.82233200	-0.00399700	-0.00217500	B	0.84098400	-0.00006500	-0.00000300
B	-0.88177900	0.04628500	0.09579200	B	-0.84098200	-0.00007300	0.00001500
O	-1.56135100	0.51368500	1.20382900	C	-1.66469100	1.01159000	0.90416000
H	-0.99395000	0.80607500	1.93178700	H	-1.15316600	1.37426500	1.80459200
C	-1.80796500	-0.45291200	-1.09024000	H	-1.84489400	1.90257700	0.27560200
H	-1.53380200	0.00891400	-2.04981600	H	-2.65918300	0.63904400	1.18844200
H	-1.69052700	-1.53757500	-1.23893600	C	1.66467700	1.01160600	-0.90415500
H	-2.87069100	-0.25298200	-0.90112700	H	1.15314100	1.37427400	-1.80458400
C	1.62699200	-1.30869500	0.39365400	H	1.84486900	1.90259600	-0.27559900
H	1.16266100	-1.94034100	1.16172900	H	2.65917300	0.63907300	-1.18844200
H	1.65776500	-1.92795900	-0.52220200	C	1.66501700	-1.01158300	0.90398200
H	2.67565900	-1.12489400	0.66653900	H	1.15354900	-1.37493300	1.80416600
C	1.64417000	1.24443800	-0.52613100	H	1.84591300	-1.90217400	0.27505900
H	1.10458900	1.91875000	-1.20272300	H	2.65923900	-0.63855200	1.18858500
H	1.88490600	1.84731400	0.36976300	C	-1.66500300	-1.01158400	-0.90399100
H	2.61224900	0.98479700	-0.97742700	H	-1.15352300	-1.37492600	-1.80417100
				H	-1.84590900	-1.90217900	-0.27507700
				H	-2.65922000	-0.63854900	-1.18860400
 SCF energy =-273.7172393				 SCF energy=-257.6401357			
B	0.85885300	0.00002700	0.00000200	B	0.83546700	-0.07526700	0.01992200
B	-0.85885700	-0.00002000	0.00001400	B	-0.88014300	0.04841400	-0.00697300
N	-1.58094400	-1.15005400	-0.44873700				
H	-2.59120000	-1.21522600	-0.49625700				

H	-1.11923400	-1.93841300	-0.87912400	N	-1.53614500	1.23652700	0.43924300
N	-1.58103000	1.14996900	0.44877100	H	-2.54061600	1.36676200	0.46901600
H	-2.59129800	1.21521400	0.49595500	H	-1.03044100	2.03995000	0.78278200
H	-1.11938900	1.93842200	0.87906000	N	-1.67338000	-1.05410600	-0.46194600
N	1.58094900	1.15006700	-0.44869400	H	-2.68394300	-1.04096000	-0.54097200
H	2.59120800	1.21524900	-0.49611800	H	-1.26412200	-1.87650600	-0.88140400
H	1.11928500	1.93828000	-0.87939400	N	1.41804600	-1.28005600	0.46997600
N	1.58101900	-1.14995600	0.44880400	H	2.41950500	-1.43425500	0.52292700
H	2.59129400	-1.21536500	0.49561800	H	0.88175400	-2.06319500	0.82301800
H	1.11939100	-1.93837600	0.87917000	C	1.80905900	1.09635600	-0.44373000
				H	1.62251500	1.36974000	-1.49284900
SCF energy=-241.5473718				H	1.62498000	2.01640800	0.13213100
B	0.81511500	-0.00002600	0.00001900	H	2.87974700	0.86162700	-0.34792300
B	-0.90952100	-0.00003600	0.00000400				
N	-1.62901100	-1.19070600	-0.32350700	SCF energy=-241.5637118			
H	-2.63776500	-1.26272000	-0.38686200	B	-0.85772400	-0.04631500	-0.03265800
H	-1.16324100	-2.06239800	-0.53007300	B	0.85786100	-0.04610500	0.03304900
N	-1.62888400	1.19071900	0.32352300	N	1.53268800	-1.08715300	0.70875900
H	-2.63762400	1.26285700	0.38697000	H	2.54248600	-1.13128500	0.80094100
H	-1.16299400	2.06235800	0.53004400	H	1.06451200	-1.85041800	1.18129800
C	1.64221500	-1.31413800	0.30805300	N	-1.53182100	-1.08747100	-0.70894700
H	1.80651100	-1.31393700	1.40189200	H	-1.06314000	-1.85046100	-1.18143700
H	1.13610400	-2.26332000	0.08795700	H	-2.54155400	-1.13194900	-0.80173000
H	2.64412100	-1.33472700	-0.14381300	C	-1.74124600	1.09910500	0.63508400
C	1.64209800	1.31414900	-0.30807500	H	-1.53734700	1.18317000	1.71300700
H	1.80636900	1.31386900	-1.40192100	H	-1.48705300	2.08272100	0.21258800
H	1.13592400	2.26331100	-0.08805300	H	-2.82621800	0.95975500	0.51530000
H	2.64401500	1.33485700	0.14376500	C	1.74034800	1.09995400	-0.63499200
				H	1.53654900	1.18308500	-1.71300700
SCF energy=-225.4720442				H	1.48493100	2.08354000	-0.21315700
B	-0.83454100	-0.00963400	-0.01905600	H	2.82547400	0.96195600	-0.51499400
B	0.86839100	-0.04580800	-0.06570200				
N	1.57452900	-0.75642800	-1.06089800	SCF energy=-449.3030824			
H	1.14101400	-1.28243700	-1.80898900	B	0.00000000	0.00000000	0.86367300
H	2.58778000	-0.79022600	-1.10200900	B	0.00000000	0.00000000	-0.86367300
C	-1.65230700	1.16971200	-0.69103800	F	0.00000000	-1.13309400	-1.55436200
H	-1.71595500	1.96478000	0.07520800	F	0.00000000	1.13309400	-1.55436200
H	-1.17864000	1.63524300	-1.56471400	F	0.00000000	1.13309400	1.55436200
H	-2.69143000	0.91212500	-0.94112800	F	0.00000000	-1.13309400	1.55436200
C	-1.65409600	-1.12944600	0.74657400				
H	-1.84307000	-1.92363100	-0.00005900	SCF energy=-1890.7313303			
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C	1.72221500	0.73465500	1.03483300	Cl	-1.07298700	-1.07431000	1.73444600
H	1.51111400	1.81399800	1.00697500	Cl	1.07298700	1.07431000	1.73444600
H	1.46170200	0.40846100	2.05238500	Cl	-1.07298700	1.07431000	-1.73444600
H	2.80960000	0.61111200	0.91909300	Cl	1.07298700	-1.07431000	-1.73444600
							
SCF energy=-1645.069131				SCF energy=-1286.1523706			
B	-0.84773700	-0.01667400	-0.01346000	B	-0.65344000	0.01155600	-0.07849800
B	0.84773800	0.01667300	-0.01346100	B	1.00625900	0.14382300	-0.37751800
H	-3.00271900	1.00400600	-0.56004000	H	-2.73184600	-1.28286800	0.02701400
H	0.77182200	2.13699500	1.14842000	H	1.39461600	-0.75295000	1.86948500
H	3.00272300	-1.00397900	-0.56007800	H	-0.69785100	2.38439800	0.45257900
H	-0.77182900	-2.13698100	1.14845200	C	1.58855900	0.68847800	-1.74104500
S	1.80037500	1.35880400	0.74726900	H	1.29077000	0.01512200	-2.55909400
S	1.71951800	-1.37564700	-0.77983200	H	1.14766300	1.66377100	-1.99308900
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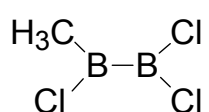
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B -0.36303900 -0.00239500 0.00008400 B 1.33199500 0.01966900 -0.00008600 H -2.53048200 -1.16133600 -0.00196400 H -0.32688100 2.43709600 0.00212700 C 2.11944300 -0.01209500 1.36986900 H 1.61087200 0.49563000 2.19933700 H 2.17361700 -1.07387600 1.67192200 H 3.15393900 0.34939000 1.30733900 C 2.11953200 -0.00556100 -1.37003200 H 2.19182800 -1.06861800 -1.66413900 H 1.60461300 0.48874300 -2.20347500 H 3.14845200 0.37173000 -1.30801000 S -1.33653100 1.53740800 0.00152500 S -1.24500600 -1.58860800 -0.00165900	 SCF energy=-927.2350775			
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B 0.85929200 -0.06277000 -0.00140200 B -0.85929400 0.06272100 -0.00139100 O -1.53770700 1.17768700 -0.48421700 H -0.94760300 1.84370800 -0.85985500 O 1.53781900 -1.17773600 -0.48405500 H 0.94788000 -1.84341300 -0.86055800 N 1.68602900 0.98553900 0.47316700 H 1.33639400 1.80810200 0.94336000 H 2.69747500 0.91086200 0.48484500 N -1.68615200 -0.98555100 0.47306900 H -1.33661200 -1.80800400 0.94352300 H -2.69756600 -0.91053900 0.48517200	 SCF energy=-333.3474872			
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H	-2.56097000	1.31705000	0.26411600	F	1.39593800	-1.34531900	-0.00002300
H	-1.04947800	2.06952300	0.35151700				
N	1.65483300	-1.12744200	0.23440800				
H	2.66888000	-1.14044000	0.25434200				
H	1.25375000	-2.01372300	0.50897900				
							
			SCF energy=-405.4147637				SCF energy=-317.6198949
B	-0.84598200	-0.07991600	-0.00004700	B	-0.86345500	-0.04538000	-0.00196800
B	0.86978200	0.01040000	-0.00002300	B	0.85103300	0.02987200	-0.01590400
N	-1.63028500	1.07795100	0.00004100	N	-1.56955600	-1.27778700	-0.15419400
H	-2.64425600	1.06046600	0.00001200	H	-2.57947500	-1.35684600	-0.16586400
H	-1.23367500	2.00856400	0.00006300	H	-1.11420700	-2.14970600	-0.38083400
F	1.49075500	1.19758000	-0.00002500	F	1.45124800	1.24621200	-0.22162800
F	-1.46994100	-1.28202500	-0.00001600	N	-1.57042000	1.17439600	0.18917200
F	1.66484400	-1.05634500	0.00004000	H	-2.57818900	1.27033600	0.21610000
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				N	1.73687800	-1.04560300	0.18568300
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				H	1.43544600	-1.98404200	0.40714600
							
			SCF energy=-1082.2486222				SCF energy=-1486.4888125
B	-0.71331700	-0.46629600	0.00021600	B	-0.91478300	0.59316900	-0.00001500
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N	-0.70853900	-1.85830700	-0.00010300	N	-1.09567800	1.97459600	-0.00005000
H	-1.54289900	-2.43301000	-0.00028700	H	-2.00454800	2.42338800	-0.00006400
H	0.15882000	-2.38252800	0.00095000	H	-0.31463900	2.62019800	-0.00006600
N	0.70852700	1.85834300	0.00015600	Cl	-2.36922600	-0.45149800	0.00002900
H	-0.15882500	2.38257600	-0.00032100	Cl	0.96168400	-1.80946100	-0.00002600
H	1.54288600	2.43304400	-0.00029900	Cl	2.07012100	1.00025000	0.00002900
Cl	-2.32341000	0.36090400	-0.00003800				
Cl	2.32341900	-0.36092100	-0.00005800				
							SCF energy=-329.3392881
				B	0.01487900	0.86201400	-0.03159500
			SCF energy=-677.9825222	B	-0.01487900	-0.86201400	-0.03159500
B	-1.18209500	-0.15837000	-0.00554400	F	-0.96505000	-1.45225100	-0.79669900
B	0.41357700	0.45793600	-0.06846000	F	0.96505000	1.45225100	-0.79669900
N	-2.26489100	0.69875100	0.36441300	C	-0.96505000	1.80593200	0.75349400
H	-3.22838500	0.39449600	0.43991900	H	-1.93797900	1.80449700	0.23462600
H	-2.12520100	1.62507900	0.74112900	H	-1.17549000	1.45067100	1.77123000
N	-1.42133100	-1.51272000	-0.36286800	H	-0.61609400	2.84467200	0.80144400
H	-2.32788000	-1.96349300	-0.36508000	C	0.96505000	-1.80593200	0.75349400
H	-0.66623300	-2.14065000	-0.60092600	H	1.93797900	-1.80449700	0.23462600
N	0.73146000	1.79331200	-0.34348800	H	1.17549000	-1.45067100	1.77123000
H	1.67934700	2.14892900	-0.39504700	H	0.61609400	-2.84467200	0.80144400
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							SCF energy=-389.322592
				B	-0.82665300	0.11243200	0.00328600
			SCF energy=-269.3615151	B	0.89037000	-0.03532500	-0.00076900
B	0.83535000	0.01337400	-0.03096300	C	-1.83393300	-1.08616800	-0.03258300
B	-0.86317000	-0.04602400	0.08619200	H	-1.66537900	-1.70604100	-0.92619800
C	1.65268000	-1.28036300	-0.42892500	H	-1.66547200	-1.75820100	0.82249100
H	1.83721700	-1.81344300	0.52221600	H	-2.88217800	-0.76607600	-0.02319400
H	1.12815400	-1.99721600	-1.07297900	F	1.59756200	-0.06552100	-1.13294400
H	2.64217500	-1.07087600	-0.85785200	F	-1.31580300	1.36776500	0.04035400
C	1.62212400	1.35705300	0.24584600	F	1.59580100	-0.15093500	1.12701300
H	1.63106900	1.90750400	-0.71318500				
H	1.15733100	2.03409500	0.97352100				
H	2.67538300	1.20682300	0.51935800				SCF energy=-629.725515
C	-1.91109900	0.33565300	-1.02846600	B	1.13176200	0.03812400	-0.01656500
H	-2.25560700	1.36571900	-0.83729300	B	-0.51289500	0.40577000	-0.09465000
H	-1.51212700	0.32109200	-2.04957900	C	1.89569200	-0.48801200	-1.29827600
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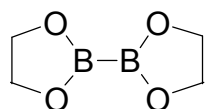
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C	1.09345300	-1.69826800	1.14567900
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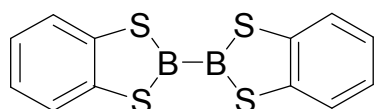
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C	-1.63242500	0.09885000	1.84333000
H	-1.06035900	-0.46647300	2.59041500
H	-1.57901000	1.15391900	2.16121300
H	-2.68468300	-0.20228500	1.88794800
Cl	-2.08076200	-0.06075400	-1.00921200
Cl	1.54271400	-1.51897600	-0.02903700
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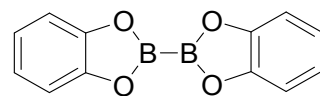
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C	0.07365900	0.77003800	3.00415500
H	1.03885500	1.10335600	3.40066300
C	-0.07365900	-0.77003800	3.00415500
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O	1.14211100	0.08935900	-1.61311100
C	-0.77318500	0.01915200	-3.00394300
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H	1.22405900	0.81236000	-3.55342100
H	-0.72753900	1.27843300	3.54852900
H	1.17343600	-0.96113400	-3.39450400
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H	-1.17343600	0.96113400	-3.39450400
H	0.72753900	-1.27843300	3.54852900
H	-1.03885500	-1.10335600	3.40066300



SCF energy=-2104.7940281

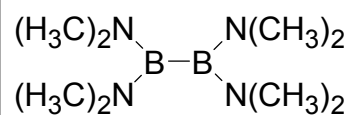
B	0.00001800	0.84014300	0.00003900
B	-0.00001800	-0.84014300	0.00003900
S	0.53843400	-1.84287000	1.40339400
S	-0.53850300	-1.84282300	-1.40334200
S	-0.53843400	1.84287000	1.40339400
S	0.53850300	1.84282300	-1.40334200
C	0.25243200	3.42563800	-0.65722300
C	0.50773600	4.63871600	-1.31185100
C	0.25341500	5.84031100	-0.65399500
C	-0.25350300	5.84033000	0.65390700
C	-0.50773600	4.63874400	1.31180600

H	1.77445100	-1.58620400	-1.28790300
H	1.49714900	-0.15162900	-2.26330600
H	2.97776000	-0.30062000	-1.27284000
C	1.93379800	0.20511600	1.33697700
H	2.29673100	1.24913300	1.35086200
H	1.34351100	0.07837700	2.25262300
H	2.82909300	-0.42831000	1.39916500
C	-1.17991400	1.80572500	-0.34542200
H	-1.45881000	2.22262300	0.63694900
H	-0.51271000	2.53500800	-0.82058300
H	-2.10957100	1.73906800	-0.92465000
Cl	-1.62525800	-0.98317000	0.19565200



SCF energy=-812.8733548

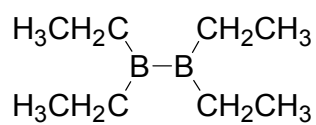
B	0.00000100	-0.84339600	0.00022100
B	-0.00000100	0.84339600	0.00022100
O	-1.14464600	1.63578100	0.00024900
O	1.14464200	1.63584100	0.00013200
O	1.14464600	-1.63578100	0.00024900
O	-1.14464200	-1.63584100	0.00013200
C	0.69758300	-2.94145400	0.00019800
C	1.43441600	-4.11513300	0.00025700
C	0.70154800	-5.31160000	-0.00019300
C	-0.70157800	-5.31156700	-0.00044800
C	-1.43441600	-4.11510100	-0.00025400
C	-0.69753400	-2.94146700	-0.00006200
H	2.51964700	-4.10293100	0.00037000
H	1.23430900	-6.25834400	-0.00033700
H	-2.51964900	-4.10278400	-0.00042500
C	0.70157800	5.31156700	-0.00044800
C	1.43441600	4.11510100	-0.00025400
C	0.69753400	2.94146700	-0.00006200
C	-0.69758300	2.94145400	0.00019800
C	-1.43441600	4.11513300	0.00025700
C	-0.70154800	5.31160000	-0.00019300
H	2.51964900	4.10278400	-0.00042500
H	-2.51964700	4.10293100	0.00037000
H	-1.23430900	6.25834400	-0.00033700
H	1.23434400	6.25830200	-0.00074300
H	-1.23434400	-6.25830200	-0.00074300



SCF energy=-588.1503337

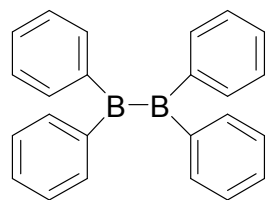
B	0.87006600	0.00021000	-0.00015700
B	-0.87009800	0.00021000	0.00014400
N	1.57547000	-1.02096500	-0.73529000
N	-1.57546900	-1.02106600	0.73516500
C	0.91814200	-1.82862800	-1.75242900
H	1.42253200	-1.72931700	-2.72766900
H	0.92921100	-2.89857500	-1.48527600
H	-0.12117400	-1.51797400	-1.87961500
C	2.94169000	-1.46945800	-0.50306500
H	2.95998200	-2.56662500	-0.40701200
H	3.62541000	-1.20701500	-1.32821000
H	3.33955300	-1.05276900	0.42337500
C	-0.91808600	-1.82866900	1.75231400
H	-1.42201500	-1.72884400	2.72774600
H	-0.92973000	-2.89868900	1.48549800
H	0.12142000	-1.51842000	1.87896600
C	-2.94175800	-1.46942200	0.50316500
H	-2.96019800	-2.56660500	0.40732200
H	-3.62538900	-1.20674900	1.32831700

C	-0.25235300	3.42566400	0.65721500
H	0.89919700	4.63691800	-2.32542600
H	0.44958700	6.78133000	-1.16055400
H	-0.44971000	6.78136500	1.16042200
H	-0.89920300	4.63694100	2.32537800
C	-0.25341500	-5.84031100	-0.65399500
C	-0.50773600	-4.63871600	-1.31185100
C	-0.25243200	-3.42563800	-0.65722300
C	0.25235300	-3.42566400	0.65721500
C	0.50773600	-4.63874400	1.31180600
C	0.25350300	-5.84033000	0.65390700
H	0.44958700	-6.78133000	-1.16055400
H	-0.89919700	-4.63691800	-2.32542600
H	0.89920300	-4.63694100	2.32537800
H	0.44971000	-6.78136500	1.16042200



SCF energy= -366.6410246

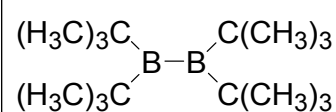
B	0.84625700	0.14245200	-0.05326500
B	-0.83803200	0.15920000	0.07871500
C	1.69354800	1.05439200	0.94455900
H	1.16979500	2.00463600	1.13650100
H	1.62981000	0.52702700	1.91595600
C	1.62265900	-0.75276900	-1.11172600
H	2.38371400	-1.33282200	-0.55986200
H	2.22798600	-0.06651400	-1.73076700
C	-1.64204800	-0.83146100	1.02489500
H	-2.32976000	-0.23282400	1.64684900
H	-2.32597100	-1.39674700	0.36504400
C	-1.64929500	1.21000400	-0.80766100
H	-1.15502700	2.19377000	-0.73886300
H	-1.47499300	0.91528900	-1.85910200
C	3.17319200	1.34141000	0.62841400
H	3.75425800	0.41743300	0.52324000
H	3.28037000	1.90078700	-0.30976100
H	3.64613200	1.93813300	1.41885500
C	-0.86001200	-1.81256200	1.91457200
H	-0.21348300	-2.46873200	1.31739400
H	-0.21557900	-1.28043200	2.62597900
H	-1.52671700	-2.45797400	2.50090000
C	0.81845500	-1.69543600	-2.02309100
H	0.23982900	-2.42182600	-1.43781700
H	0.10691300	-1.13973700	-2.64724600
H	1.46719000	-2.26597700	-2.70020900
C	-3.16173900	1.38212100	-0.57766600
H	-3.70301300	0.43803300	-0.71439300
H	-3.37570300	1.73397400	0.43945500
H	-3.59543800	2.11204800	-1.27318100



SCF energy= -976.3392887

B	-0.85019800	-0.00023600	-0.00022600
B	0.85018200	-0.00013100	0.00019100
C	1.63186600	0.95705800	0.96972700
C	1.09054500	2.20280800	1.36391700
C	2.87930100	0.59537100	1.52929700
C	1.76740400	3.05360300	2.23904500
H	0.12948700	2.51627500	0.96226900
C	3.54618800	1.42555200	2.43276600
H	3.32444000	-0.36002700	1.26278600
C	2.99592700	2.66270100	2.78190400
H	1.33353700	4.01386000	2.50793900

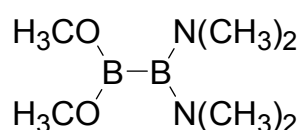
H	-3.33966300	-1.05286300	-0.42331600
N	1.57588800	1.02124500	0.73474700
N	-1.57585300	1.02140000	-0.73458700
C	0.91913100	1.82895800	1.75220800
H	1.42305000	1.72849500	2.72758300
H	0.93148400	2.89904700	1.48572400
H	-0.12058100	1.51937700	1.87879300
C	2.94240200	1.46883700	0.50255200
H	3.33973300	1.05240000	-0.42424300
H	2.96150700	2.56604300	0.40717700
H	3.62613100	1.20537500	1.32737300
C	-2.94247800	1.46879900	-0.50267400
H	-2.96176300	2.56601300	-0.40746600
H	-3.62604600	1.20511100	-1.32755600
H	-3.33987500	1.05243700	0.42412100
C	-0.91905000	1.82902900	-1.75208600
H	-1.42227900	1.72775500	-2.72774000
H	-0.93231000	2.89922700	-1.48612100
H	0.12095900	1.52009900	-1.87785300



SCF energy= -681.1507897

B	-0.86422700	-0.01554600	0.01443000
B	0.86416400	-0.01560900	-0.01442400
C	1.68223100	1.02953800	-0.97504500
C	1.62738300	-1.06995400	0.99020100
C	-1.62740300	-1.07004400	-0.99011300
C	-1.68224000	1.02970600	0.97491700
C	-2.53557200	-0.30624800	-1.99243000
H	-2.98374000	-1.02182500	-2.69747100
H	-1.97873800	0.42644900	-2.58820900
H	-3.35834500	0.21712400	-1.49579900
C	-0.62565300	-1.90432600	-1.82904100
H	-1.15960200	-2.54107100	-2.54982400
H	-0.03040700	-2.57167400	-1.19694600
H	0.06580500	-1.27902500	-2.40406600
C	-2.52387200	-2.10248500	-0.25123300
H	-2.90174300	-2.83386500	-0.98069800
H	-3.39102200	-1.64905700	0.23064900
H	-1.97549700	-2.66686200	0.51125200
C	-3.05581100	0.55368700	1.50756100
H	-3.48646100	1.32875500	2.15860800
H	-2.97220700	-0.36098000	2.10625600
H	-3.77943800	0.37056400	0.70755500
C	-1.94817500	2.32266000	0.14392200
H	-2.49559500	3.04097000	0.77140900
H	-2.55820200	2.13722800	-0.74513700
H	-1.02713800	2.81663300	-0.17837400
C	-0.86390400	1.46314600	2.21841300
H	-1.38954800	2.26327600	2.76009300
H	0.12707200	1.84693100	1.95661500
H	-0.72538800	0.63811400	2.92625500
C	0.86390400	1.46302900	-2.21853600
H	1.38957000	2.26315200	-2.76020700
H	-0.12706400	1.84684600	-1.95675900
H	0.72537600	0.63802500	-2.92640200
C	1.94845400	2.32249000	-0.14415100
H	2.49573000	3.04076300	-0.77180700
H	2.55872000	2.13706400	0.74474600
H	1.02754200	2.81653000	0.17840500
C	3.05568600	0.55330200	-1.50779600
H	3.48642600	1.32831300	-2.15885000
H	2.97186200	-0.36132300	-2.10653600
H	3.77935400	0.36999500	-0.70787300
C	0.62564100	-1.90409100	1.82928700

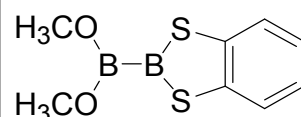
H	4.49734600	1.11319500	2.85778800
H	3.51896800	3.31668400	3.47578900
C	1.63261000	-0.95712200	-0.96894000
C	1.09189400	-2.20311200	-1.36321700
C	2.88015500	-0.59507700	-1.52802700
C	1.76944200	-3.05380600	-2.23791200
H	0.13075800	-2.51685900	-0.96197500
C	3.54774500	-1.42516100	-2.43106300
H	3.32483100	0.36052500	-1.26148100
C	2.99807600	-2.66255900	-2.78026300
H	1.33602400	-4.01424800	-2.50687400
H	4.49898000	-1.11252500	-2.85570600
H	3.52165000	-3.31646800	-3.47381600
C	-1.63186300	0.96926000	-0.95748100
C	-2.87928300	1.52886700	-0.59580800
C	-1.09053100	1.36340400	-2.20323900
C	-3.54614000	2.43233800	-1.42600900
H	-3.32444700	1.26237200	0.35958500
C	-1.76739100	2.23850100	-3.05407500
H	-0.12946000	0.96176100	-2.51667600
C	-2.99588800	2.78141400	-2.66318400
H	-4.49729000	2.85738200	-1.11365700
H	-1.33351600	2.50735900	-4.01434100
H	-3.51891000	3.47528900	-3.31719200
C	-1.63262300	-0.96952100	0.95659200
C	-2.88012600	-1.52860600	0.59438700
C	-1.09196100	-1.36395700	2.20255200
C	-3.54772500	-2.43179000	1.42430000
H	-3.32476700	-1.26192900	-0.36119200
C	-1.76950900	-2.23882700	3.05306600
H	-0.13085400	-0.96272200	2.51640200
C	-2.99810600	-2.78115900	2.66167300
H	-4.49892900	-2.85642100	1.11155000
H	-1.33613000	-2.50791800	4.01349100
H	-3.52168900	-3.47483000	3.31544700



SCF energy=-549.2836958

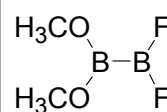
B	1.16517100	0.01928700	0.07551500
B	-0.56548000	0.04160700	0.10050200
N	-1.27042200	-1.19954600	0.28785600
N	-1.23924100	1.29974500	-0.06366000
O	1.95817000	-0.35873800	-0.98811400
O	1.83409300	0.40320600	1.21306100
C	-0.61335600	-2.38478700	0.82081700
H	-0.65023100	-3.22180500	0.10410600
H	-1.09900200	-2.72513500	1.74934100
H	0.43256000	-2.17593000	1.05796700
C	-2.65807400	-1.46870700	-0.06367800
H	-2.71948000	-2.40669600	-0.63724800
H	-3.06401800	-0.67270900	-0.68990900
H	-3.30745200	-1.58734800	0.81990000
C	-2.58687700	1.61993200	0.38942800
H	-3.28470800	1.80001300	-0.44520100
H	-2.56380700	2.53751400	0.99713800
H	-2.98918600	0.82330700	1.01618400
C	-0.55467500	2.48132300	-0.56976800
H	-1.07493700	2.89685500	-1.44761000
H	0.46689800	2.24015400	-0.87384500
H	-0.50654400	3.27488200	0.19326800
C	1.44205000	-0.77882100	-2.24327100
H	1.87624500	-1.75302800	-2.49391200
H	1.73593900	-0.05635400	-3.01365300
H	0.34930100	-0.86513700	-2.22703300
C	3.26072100	0.41075700	1.28358100

H	1.15958600	-2.54084100	2.55007200
H	0.03030000	-2.57141900	1.19726100
H	-0.06574700	-1.27871000	2.40431600
C	2.53543000	-0.30581900	1.99240400
H	2.98370700	-1.02121500	2.69756000
H	1.97849500	0.42688000	2.58807900
H	3.35811600	0.21758000	1.49566100
C	2.52392700	-2.10251700	0.25163600
H	2.90163600	-2.83381700	0.98125500
H	3.39116100	-1.64924700	-0.23023700
H	1.97558100	-2.66692900	-0.51084500



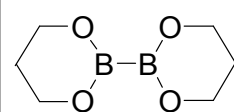
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B	0.75575400	-0.01101100	0.00006800
B	2.46599100	-0.09252100	0.00004300
S	-0.22927300	-1.52537200	0.00006700
S	-0.27875500	1.47349200	0.00007100
C	-1.85068300	0.65356100	0.00002300
C	-3.07426000	1.33756100	-0.00003100
C	-4.26418700	0.61287600	-0.00007700
C	-4.24024300	-0.78997700	-0.00008000
C	-3.02726200	-1.47516300	-0.00001100
C	-1.82416000	-0.75413900	0.00003600
H	-3.08970600	2.42407400	-0.00003000
H	-5.21430500	1.14013300	-0.00012900
H	-5.17228500	-1.34863300	-0.00013300
H	-3.00770800	-2.56157800	-0.00000700
O	3.35842900	0.94759300	0.00005400
O	2.98636100	-1.35787400	-0.00004400
C	3.00178800	2.32558600	-0.00008500
H	3.93093400	2.90146800	-0.00122200
H	2.42402200	2.58489100	0.89452400
H	2.42218800	2.58430500	-0.89367700
C	4.39587400	-1.59350500	-0.00011200
H	4.53975800	-2.67673700	-0.00613500
H	4.86262400	-1.16457600	0.89330700
H	4.86467900	-1.15416500	-0.88733100



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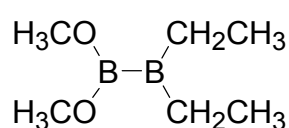
B	-0.34185400	-0.06485200	0.00173800
B	1.32764000	-0.50010200	-0.02197300
O	-0.84405600	1.19912600	0.11086600
O	-1.21165300	-1.10577600	-0.11903000
C	-0.07586900	2.39325500	0.24074200
H	-0.49889900	2.98066400	1.06085700
H	-0.15280600	2.96885500	-0.68734700
H	0.97901500	2.18653400	0.44759400
C	-2.62884900	-0.90644700	-0.15110900
H	-3.08765600	-1.89187200	-0.25815100
H	-2.91291400	-0.27197800	-0.99729400
H	-2.97384600	-0.43635700	0.77579000
F	2.27221500	0.26071300	-0.59379600
F	1.77135700	-1.63612600	0.51460100



SCF energy=-586.6535429

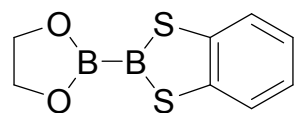
B	-0.85909800	-0.00000700	0.12199500
B	0.85909500	-0.00003200	0.12199100
O	1.52909200	1.20087800	0.12121300
O	1.52912300	-1.20092700	0.12092600
C	2.96052300	1.24664100	0.11087900

H	3.53177700	0.72081700	2.29654400
H	3.68633600	1.11548400	0.55993100
H	3.67265300	-0.58467600	1.08235600



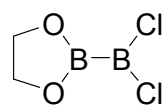
SCF energy=-438.5269983

B	-0.83988400	-0.08520700	-0.13190200
B	0.86990000	-0.23590000	-0.02072100
C	-1.71614200	-1.38532100	0.11784700
H	-1.36408800	-2.11869500	-0.63159100
H	-1.40205300	-1.84432600	1.07157600
C	-1.54352600	1.26664600	-0.56115900
H	-2.37575000	1.46958100	0.13528600
H	-2.06422300	1.04022300	-1.51057700
C	-3.25092700	-1.29388800	0.06816100
H	-3.64028500	-0.61872200	0.84095800
H	-3.60223800	-0.91423700	-0.89921300
H	-3.72061200	-2.27331800	0.22484000
C	-0.68121100	2.52745700	-0.73695500
H	-0.19627600	2.81549400	0.20492000
H	0.11408400	2.36419100	-1.47461300
H	-1.27293300	3.38819600	-1.07430600
O	1.65033000	0.01529700	1.08504300
O	1.51630800	-0.65970700	-1.15455100
C	1.11797100	0.44484100	2.32932900
H	1.70343100	1.29923600	2.68442600
H	0.06569200	0.74794700	2.24741200
C	2.93586700	-0.82734500	-1.19953400
H	3.18892700	-1.15967200	-2.20972400
H	3.26453200	-1.57896200	-0.47325300
H	3.44895200	0.11653600	-0.98462900
H	1.19745800	-0.36700400	3.06153700



SCF energy=-1306.4030762

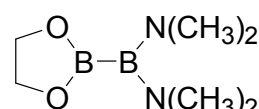
C	0.00000000	0.77398100	4.51707900
C	0.00000000	-0.77398100	4.51707900
H	-0.84259800	1.20418400	5.06614000
H	0.93126600	1.19766300	4.90853100
H	-0.93126600	-1.19766300	4.90853100
H	0.84259800	-1.20418400	5.06614000
B	0.00000000	0.00000000	2.36498500
B	0.00000000	0.00000000	0.67214100
O	0.11607100	-1.13976500	3.12678900
O	-0.11607100	1.13976500	3.12678900
S	0.08343400	-1.50025000	-0.32458800
S	-0.08343400	1.50025000	-0.32458800
C	-0.03881000	0.70326000	-1.90744700
C	0.03881000	-0.70326000	-1.90744700
C	0.07696200	-1.40447700	-3.12117600
C	0.03828300	-0.70048500	-4.32269500
C	-0.03828300	0.70048500	-4.32269500
C	-0.07696200	1.40447700	-3.12117600
H	0.13618200	-2.48946200	-3.11907400
H	0.06784600	-1.24274600	-5.26387700
H	-0.06784600	1.24274600	-5.26387700
H	-0.13618200	2.48946200	-3.11907400



SCF energy=-1199.3712593

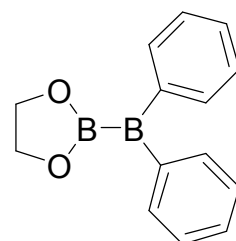
B	-0.64413400	-0.00023000	-0.00038200
B	1.05604900	-0.00010100	-0.00021400
C	-2.78840400	0.04489300	0.77233600

H	3.24708200	2.15705700	-0.42592500
C	2.96052800	-1.24666700	0.11059800
C	3.55145400	0.00006400	-0.54325000
O	-1.52911300	-1.20091600	0.12115200
O	-1.52909500	1.20090400	0.12099700
C	-2.96054900	-1.24660500	0.11093300
C	-2.96052600	1.24668700	0.11055700
H	-3.30988000	1.34383600	1.14807200
C	-3.55143800	-0.00005300	-0.54327300
H	3.30979400	1.34351800	1.14844800
H	-3.24702400	2.15696000	-0.42650600
H	-3.24718800	-2.15705500	-0.42575100
H	-3.30977900	-1.34333500	1.14853000
H	3.24712400	-2.15695600	-0.42639100
H	3.30984200	-1.34374500	1.14814100
H	-4.64486500	-0.00002000	-0.44518500
H	-3.31471600	-0.00022800	-1.61558900
H	4.64487700	0.00004900	-0.44514900
H	3.31473600	0.00019800	-1.61556900



SCF energy=-548.0829406

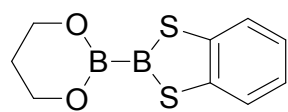
B	1.03582300	0.00003200	0.00004300
B	-0.68687200	-0.00002100	0.00000200
N	-1.39145400	-1.24651200	-0.14173700
N	-1.39148600	1.24639300	0.14209400
C	-0.78243500	-2.54761000	0.10653100
H	-0.71645300	-3.14105700	-0.82076100
H	-1.38679400	-3.12682400	0.82248400
H	0.21746300	-2.43708500	0.52614300
C	-2.73808700	-1.38405800	-0.68086700
H	-2.73619600	-2.12855400	-1.49209500
H	-3.09036600	-0.44042400	-1.09991900
H	-3.46483900	-1.72890200	0.07341600
C	-2.73831800	1.38385400	0.68078800
H	-3.46487400	1.72860300	-0.07374000
H	-2.73671400	2.12842400	1.49195900
H	-3.09063800	0.44024400	1.09983900
C	-0.78283500	2.54757300	-0.10668100
H	-1.38630000	3.12574100	-0.82427200
H	0.21783100	2.43719200	-0.52447300
H	-0.71882300	3.14202700	0.82010100
C	3.20810600	-0.46254700	0.61783100
C	3.20803500	0.46276800	-0.61786600
H	3.58499900	0.03516500	1.51878900
H	3.77319900	-1.38691400	0.46370800
H	3.77307800	1.38716900	-0.46378200
H	3.58491400	-0.03493400	-1.51883900
O	1.82064700	-0.79068100	0.82407400
O	1.82054600	0.79080900	-0.82403700



SCF energy=-742.1757615

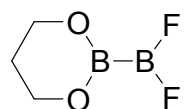
B	0.00018300	1.78208900	-0.00017200
B	-0.00002200	0.07158700	0.00003800
C	-0.29615500	3.94303500	0.71238400
C	0.29705200	3.94321700	-0.71193700
H	-1.21782800	4.52613800	0.79646900
H	0.41685500	4.29486700	1.46673500
H	-0.41584000	4.29556200	-1.46616300
H	1.21892300	4.52603600	-0.79581600

C	-2.78886400	-0.04503200	-0.77178300
H	-3.16780300	-0.86416900	1.25046400
H	-3.34205100	0.90682800	1.15428900
H	-3.34284900	-0.90687700	-1.15343500
H	-3.16835500	0.86409400	-1.24970500
O	-1.39515800	0.19535300	1.13003100
O	-1.39581800	-0.19573400	-1.13031200
Cl	1.96293700	1.51146500	-0.07559500
Cl	1.96370400	-1.51113200	0.07561200



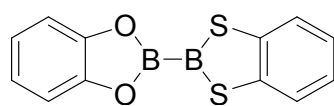
SCF energy=-1345.7256658

B	2.05807800	-0.00050400	-0.08954300
O	2.72145300	1.20181500	-0.10507600
O	2.72226300	-1.20236500	-0.10410700
S	-0.64289900	1.50189100	-0.02743200
S	-0.64358900	-1.50264100	-0.02761100
B	0.35778700	-0.00062600	-0.04886700
C	4.15551000	1.24863800	-0.12968400
H	4.47579700	1.34721200	-1.17576900
H	4.45248600	2.15808300	0.40180900
C	4.15634800	-1.24797500	-0.12944000
H	4.47624700	-1.34619900	-1.17568300
H	4.45434700	-2.15719000	0.40185900
C	4.75998900	0.00058900	0.50898200
H	5.85030400	0.00095300	0.38348000
H	4.55074100	0.00058500	1.58680000
C	-3.43966700	1.40637800	0.03114600
C	-4.64157300	0.70199300	0.05580400
C	-4.64188900	-0.70095300	0.05570000
C	-3.44029600	-1.40587300	0.03094700
C	-2.22638700	-0.70442800	0.00585700
C	-2.22606200	0.70440400	0.00595300
H	-3.43728400	2.49304100	0.03109200
H	-5.58239100	1.24549600	0.07522600
H	-5.58295000	-1.24403700	0.07505300
H	-3.43839400	-2.49253800	0.03074600



SCF energy=-517.9823974

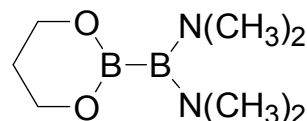
B	0.22423000	-0.00001000	0.07112100
O	-0.42664500	1.20212500	0.10549600
O	-0.42662900	-1.20217300	0.10498700
B	1.94035500	0.00001100	-0.02346800
C	-1.86189700	1.24992500	0.16820900
H	-2.15100100	1.35217700	1.22241300
H	-2.17052400	2.15817600	-0.35774200
C	-1.86186700	-1.25003300	0.16760000
H	-2.15102100	-1.35282600	1.22174000
H	-2.17047500	-2.15802300	-0.35881800
C	-2.48316700	0.00009200	-0.45132300
H	-3.56907000	0.00003400	-0.29348900
H	-2.30721900	0.00035900	-1.53503700
F	2.65362800	-1.12782000	-0.06213900
F	2.65350200	1.12788500	-0.06320700



SCF energy=-1458.8344917

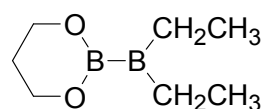
B	1.22217300	0.00058600	0.00001500
B	-0.45935600	0.00067100	0.00020400
O	2.01967000	-1.14429600	0.00006500
O	2.02022000	1.14502400	-0.00024600
S	-1.45420800	1.50392800	0.00046300

O	-0.59429200	2.55631500	0.97847500
O	0.59474100	2.55649900	-0.97856800
C	1.36288400	-0.69521000	0.06403600
C	2.54498900	-0.12337600	-0.46368900
C	1.48237400	-1.96385900	0.67851000
C	3.76706900	-0.79574700	-0.41595500
H	2.49575300	0.85684900	-0.93104700
C	2.70856100	-2.62557900	0.76162400
H	0.60188700	-2.42771100	1.11554600
C	3.85293400	-2.04705700	0.20323500
H	4.65525800	-0.34027100	-0.84777700
H	2.77243800	-3.59257500	1.25518200
H	4.80768200	-2.56521700	0.25670100
C	-1.36308500	-0.69495200	-0.06380500
C	-1.48251400	-1.96386900	-0.67776700
C	-2.54535100	-0.12272500	0.46312200
C	-2.70876300	-2.62545000	-0.76114500
H	-0.60194100	-2.42807400	-1.11424300
C	-3.76751200	-0.79491800	0.41510600
H	-2.49617600	0.85768500	0.93009900
C	-3.85330300	-2.04649700	-0.20355900
H	-2.77255800	-3.59265100	-1.25431100
H	-4.65582100	-0.33911200	0.84633300
H	-4.80811600	-2.56451200	-0.25725000



SCF energy=-587.4021763

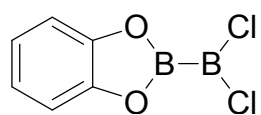
B	-0.74560600	0.08047000	0.04725300
O	-1.41504300	0.74299200	-0.96378800
O	-1.44326100	-0.51139700	1.08244000
B	0.97884100	-0.00692000	0.01055900
C	-2.84444300	0.83658900	-0.97935900
H	-3.13414900	1.78748900	-0.50969200
H	-3.15169200	0.87455000	-2.02981700
C	-2.87426000	-0.46604600	1.14341700
H	-3.16734400	0.38567300	1.77347400
H	-3.20240500	-1.38241600	1.64541900
C	-3.48652900	-0.33986900	-0.24901800
H	-4.57277500	-0.19777100	-0.17692400
H	-3.31124400	-1.26484300	-0.81446500
N	1.61066800	-1.29163600	-0.12193000
N	1.73434200	1.21284300	0.11076900
C	0.88960800	-2.46747600	-0.58435800
H	0.85980100	-3.25134600	0.18996500
H	1.36722600	-2.90131400	-1.47787900
H	-0.13828800	-2.21194600	-0.85111400
C	2.96912000	-1.62320300	0.28425900
H	2.95539000	-2.51945900	0.92398700
H	3.62891900	-1.84525200	-0.57142100
H	3.41175100	-0.81236500	0.86460200
C	3.09404600	1.41990800	-0.36670300
H	3.81463200	1.58214500	0.45266000
H	3.43054300	0.57171200	-0.96448700
H	3.12846000	2.31313900	-1.01002900
C	1.14987500	2.44820700	0.60990900
H	1.15034900	3.23476100	-0.16219200
H	1.71276500	2.83243800	1.47597200
H	0.11874100	2.28719400	0.93290800



SCF energy=-476.6471516

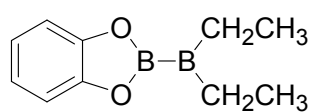
B	-0.40372800	-0.04201300	-0.00008600
O	-1.07788700	-0.04044900	-1.20338500
O	-1.07787500	-0.03917000	1.20320500

S	-1.45343700	-1.50315400	0.00016700
C	5.69584000	0.70094800	-0.00031200
C	4.49919700	1.43393500	-0.00024100
C	3.32517900	0.69776100	-0.00019000
C	3.32480000	-0.69768600	0.00007300
C	4.49851300	-1.43437300	0.00029100
C	5.69549300	-0.70194100	-0.00008600
H	6.64254200	1.23378000	-0.00051100
H	4.48748700	2.51918500	-0.00044600
H	4.48632600	-2.51962000	0.00043700
H	6.64194000	-1.23522800	-0.00010400
C	-3.03601000	0.70421700	0.00017100
C	-4.24961400	1.40660900	0.00001300
C	-5.45058800	0.70092000	-0.00030800
C	-5.45023000	-0.70219300	-0.00047900
C	-4.24890200	-1.40727500	-0.00025700
C	-3.03563300	-0.70428500	0.00005300
H	-4.24776300	2.49312600	0.00011700
H	-6.39190500	1.24359900	-0.00045900
H	-6.39126900	-1.24535300	-0.00075600
H	-4.24651700	-2.49379300	-0.00036700



SCF energy=-1351.8016363

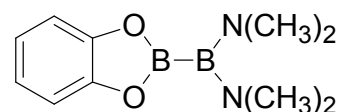
B	0.51252600	-0.00009700	0.00016500
B	2.20723700	0.00004600	0.00002800
O	-0.27778600	-1.14364200	0.00015800
O	-0.27771400	1.14353400	0.00010400
C	-3.95201600	0.70205500	-0.00011700
C	-2.75690300	1.43559300	0.00001900
C	-1.58330800	0.69776600	0.00009900
C	-1.58336000	-0.69777600	-0.00000800
C	-2.75698300	-1.43554700	-0.00006200
C	-3.95205700	-0.70194300	-0.00007400
H	-4.89902200	1.23416300	-0.00017800
H	-2.74477000	2.52071900	-0.00001400
H	-2.74489900	-2.52067300	-0.00006200
H	-4.89909500	-1.23399400	-0.00006300
Cl	3.10705000	-1.51335100	-0.00004700
Cl	3.10711000	1.51335300	-0.00006400



SCF energy=-589.7575639

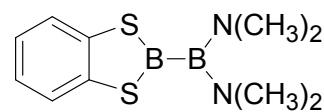
B	0.47425200	-0.08276500	0.00789500
B	2.18033200	-0.08398900	0.00976200
O	-0.32804700	-0.22934000	-1.12944500
O	-0.33055900	0.04358400	1.14602200
C	-4.00907100	-0.05550700	0.70567300
C	-2.81139500	0.04569100	1.43193100
C	-1.63684000	-0.02584600	0.70101000
C	-1.63533100	-0.19039000	-0.68365600
C	-2.80828400	-0.29158700	-1.41363900
C	-4.00756000	-0.22041500	-0.68645900
H	-4.95575600	-0.00445200	1.23628500
H	-2.80086700	0.17347400	2.50979700
H	-2.79537200	-0.41945200	-2.49146800
H	-4.95308500	-0.29529500	-1.21630600
C	2.90751600	-1.48844200	0.09153600
H	2.51858200	-2.09871800	-0.74393100
H	2.50643500	-2.01027800	0.97926300
C	4.44415300	-1.54679200	0.10590800
H	4.86097700	-0.99619700	0.95835300
H	4.87332500	-1.10967300	-0.80410000
H	4.80722200	-2.57978500	0.17457300

B	1.30948200	-0.07016800	-0.00004700
C	-2.51211800	-0.03921900	-1.24719300
H	-2.85311900	1.00109500	-1.34117500
H	-2.80419200	-0.57335600	-2.15714700
C	-2.51208600	-0.03863700	1.24730200
H	-2.85353800	1.00153800	1.34114000
H	-2.80372300	-0.57270600	2.15744300
C	-3.10375800	-0.69093800	0.00020800
H	-4.19689400	-0.59004400	0.00021600
H	-2.87029400	-1.76395700	0.00041400
C	2.02666200	-1.48605200	0.00006500
H	1.62614500	-2.04698300	0.86383700
H	1.62650900	-2.04674200	-0.86404300
C	2.17414700	1.25607700	-0.00011600
H	2.85933800	1.19899400	-0.86506000
H	2.85903200	1.19921000	0.86508400
C	1.44417500	2.60931600	-0.00039600
H	0.80208100	2.71309100	0.88347000
H	2.14298600	3.45603500	-0.00036700
H	0.80240700	2.71289500	-0.88452100
C	3.56298000	-1.56605600	0.00037200
H	3.99262500	-1.07627900	0.88330800
H	3.99298500	-1.07617000	-0.88232900
H	3.91496200	-2.60570400	0.00037900



SCF energy=-700.5151074

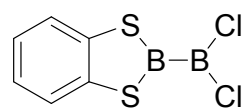
B	0.05603100	-0.00008500	0.00005800
B	1.77204300	-0.00002800	0.00006500
O	-0.75755100	0.86415400	0.74866500
O	-0.75755800	-0.86432300	-0.74855700
C	-4.43481400	-0.52826700	-0.46098800
C	-3.23635300	-1.07986800	-0.94158400
C	-2.06147400	-0.52626700	-0.45792800
C	-2.06147300	0.52613300	0.45800800
C	-3.23634300	1.07980000	0.94160600
C	-4.43481100	0.52825800	0.46095700
H	-5.38119100	-0.93057800	-0.81176600
H	-3.22469900	-1.89823600	-1.65472000
H	-3.22467700	1.89817200	1.65473800
H	-5.38118400	0.93062800	0.81167500
N	2.45553400	1.24296500	-0.21524100
N	2.45586500	-1.24285700	0.21540200
C	3.82026000	1.54346500	0.19764500
H	3.83619400	2.49756400	0.74589700
H	4.20403200	0.77233000	0.86689500
H	4.51024700	1.64688800	-0.65595800
C	1.81505500	2.39934000	-0.82763600
H	1.82520800	3.26637500	-0.14895700
H	0.77646200	2.18115000	-1.08484100
H	2.33401400	2.69375300	-1.75352000
C	1.81553200	-2.39952200	0.82739700
H	2.33441000	-2.69414600	1.75325900
H	1.82593500	-3.26637600	0.14847500
H	0.77685500	-2.18161600	1.08449700
C	3.82065200	-1.54300500	-0.19766600
H	4.51081200	-1.64628100	0.65580400
H	4.20414800	-0.77178900	-0.86698400
H	3.83674800	-2.49708100	-0.74596100



SCF energy=-1346.4746702

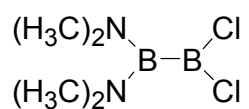
B	0.35522100	-0.00010400	0.00008500
B	2.07412700	0.00001600	0.00002400

C	3.01385100	1.25640300	-0.04518100
H	3.60496900	1.27929000	0.88979900
H	3.78774800	1.14839600	-0.82448100
C	2.26612600	2.58820700	-0.22124500
H	2.95065600	3.44578100	-0.22328900
H	1.54128900	2.74849700	0.58667100
H	1.71080700	2.61030100	-1.16733000



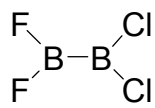
SCF energy=-1997.763129

B	-0.77761600	0.00006400	0.00012700
B	-2.46762800	-0.00000400	0.00001300
C	4.20915800	0.70187100	0.00002400
C	3.00930400	1.40786000	0.00021400
C	1.79534900	0.70482100	0.00016000
C	1.79531600	-0.70481100	-0.00010000
C	3.00922600	-1.40792100	-0.00031000
C	4.20912000	-0.70200000	-0.00023900
H	5.15065500	1.24406600	0.00006500
H	3.00754700	2.49427900	0.00041500
H	3.00740600	-2.49434000	-0.00051500
H	5.15058600	-1.24424800	-0.00040100
Cl	-3.38754600	-1.51020300	0.00036900
Cl	-3.38763100	1.51014900	-0.00051500
S	0.21629200	-1.50320500	-0.00015700
S	0.21640800	1.50332700	0.00039000



SCF energy=-1239.4459239

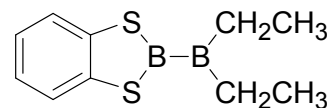
B	-1.16251400	-0.00008700	0.00002500
B	0.55584300	0.00000900	0.00007900
N	1.22361800	1.26022800	-0.12247700
N	1.22385800	-1.26011600	0.12249200
C	2.59504100	1.54404800	0.28246500
H	2.61355100	2.44894400	0.90792100
H	3.00422500	0.72585000	0.87635800
H	3.26051700	1.72581200	-0.57693500
C	0.54217800	2.45970900	-0.59227000
H	0.53117000	3.24235600	0.18200800
H	-0.49191700	2.24135400	-0.87277300
H	1.03974800	2.87509400	-1.48221400
C	0.54277800	-2.45956100	0.59276400
H	1.03959200	-2.87372500	1.48372000
H	0.53323100	-3.24302900	-0.18070600
H	-0.49181000	-2.24166600	0.87179500
C	2.59525800	-1.54368400	-0.28259300
H	3.26043300	-1.72667400	0.57677100
H	3.00467200	-0.72471600	-0.87524400
H	2.61367300	-2.44777600	-0.90921000
Cl	-2.10811500	0.44837700	1.43900800
Cl	-2.10762500	-0.44868900	-1.43926200



SCF energy=-1170.016851

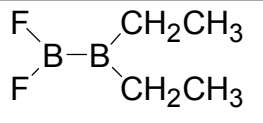
B	0.00000000	0.00000000	-0.34951200
B	0.00000000	0.00000000	1.35659600
F	-1.13304700	-0.00094100	2.05398800
F	1.13304700	0.00094100	2.05398800
Cl	0.00000000	-1.51743000	-1.23550600
Cl	0.00000000	1.51743000	-1.23550600

C	-4.66929400	-0.34640600	-0.60958300
C	-3.46635800	-0.69528000	-1.22182800
C	-2.25337000	-0.34952000	-0.61088600
C	-2.25337200	0.34928100	0.61099900
C	-3.46636300	0.69536800	1.22175100
C	-4.66929800	0.34663500	0.60942100
H	-5.61019400	-0.61523800	-1.08218400
H	-3.46448000	-1.23362500	-2.16579700
H	-3.46448800	1.23381800	2.16566100
H	-5.61020000	0.61571900	1.08187500
N	2.75880500	1.20966200	-0.35790900
N	2.75915200	-1.20940800	0.35796400
C	4.12350000	1.55660300	0.01785400
H	4.13860500	2.56609100	0.45582600
H	4.50949300	0.86647900	0.76924800
H	4.81255600	1.56464800	-0.84266100
C	2.10865200	2.29635100	-1.07903900
H	2.09933400	3.22218600	-0.48247800
H	1.07711200	2.03710200	-1.32722200
H	2.63438300	2.51286400	-2.02236600
C	2.10925900	-2.29635000	1.07889200
H	2.63534600	-2.51325400	2.02192700
H	2.09970600	-3.22200000	0.48200800
H	1.07781500	-2.03719800	1.32756400
C	4.12386100	-1.55606000	-0.01807900
H	4.81299000	-1.56430700	0.84236700
H	4.50968600	-0.86568800	-0.76930600
H	4.13903900	-2.56543300	-0.45635100
S	-0.66538100	-0.75017800	-1.29721800
S	-0.66539700	0.74972500	1.29746500



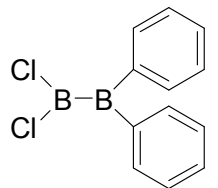
SCF energy=-1235.7183898

B	0.75458400	0.03946300	0.07102600
B	2.45385700	0.04137400	0.07580100
C	-4.26056900	0.66227600	-0.26724000
C	-3.05668100	1.27068500	-0.61997000
C	-1.84578600	0.65744900	-0.27264500
C	-1.84790500	-0.56255800	0.42680400
C	-3.06093800	-1.16887900	0.77877000
C	-4.26268700	-0.55405100	0.42989000
H	-5.20049400	1.13645300	-0.53635700
H	-3.05317900	2.21319900	-1.16065800
H	-3.06074700	-2.11146600	1.31934200
H	-5.20425900	-1.02345100	0.70161900
C	3.18709100	0.78449800	1.27001300
H	2.80315100	0.34263000	2.20713400
H	2.78862500	1.81398200	1.30848900
C	4.72432800	0.82051700	1.30541600
H	5.13696000	1.32469000	0.42275100
H	5.15234900	-0.18928100	1.33139000
H	5.09360700	1.35528600	2.18933100
C	3.29821200	-0.68109000	-1.04928900
H	4.04055500	0.04514600	-1.42466200
H	3.92620100	-1.42586800	-0.52564200
C	2.57257900	-1.34801900	-2.22860900
H	3.27678000	-1.82175500	-2.92418300
H	1.98607200	-0.61814900	-2.79995300
H	1.87707700	-2.12295900	-1.88422400
S	-0.25680900	1.34606400	-0.67159100
S	-0.26136400	-1.25903900	0.82175700



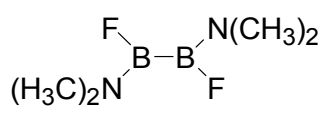
SCF energy=-407.9764397

B	0.0000000	0.0000000	-0.5774300
B	0.0000000	0.0000000	1.1305150
F	1.1251360	0.1038020	1.8521690
F	-1.1251360	-0.1038020	1.8521690
C	-0.2845800	1.3289930	-1.3792960
H	-1.3717510	1.2517600	-1.5869600
H	0.1799040	1.2890670	-2.3768840
C	0.0000000	2.6828960	-0.7049360
H	-0.3064750	3.5245420	-1.3378240
H	-0.5353340	2.7789900	0.2484520
H	1.0693950	2.8053380	-0.4936270
C	0.2845800	-1.3289930	-1.3792960
H	-0.1799040	-1.2890670	-2.3768840
H	1.3717510	-1.2517600	-1.5869600
C	0.0000000	-2.6828960	-0.7049360
H	0.5353340	-2.7789900	0.2484520
H	-1.0693950	-2.8053380	-0.4936270
H	0.3064750	-3.5245420	-1.3378240



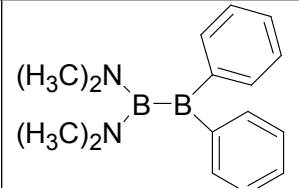
SCF energy=-1433.538708

B	0.0000170	0.1786240	-0.0001070
B	-0.0000200	1.8747980	-0.0001060
C	-1.3672980	-0.5797280	-0.0397550
C	-2.5471520	-0.0128430	0.4968640
C	-1.4885550	-1.8433770	-0.6639860
C	-3.7703200	-0.6812620	0.4452000
H	-2.5031960	0.9605420	0.9796990
C	-2.7154300	-2.5035480	-0.7472140
H	-0.6105390	-2.3034990	-1.1090620
C	-3.8579020	-1.9280860	-0.1826960
H	-4.6563460	-0.2273710	0.8821510
H	-2.7807820	-3.4669650	-1.2470240
H	-4.8130450	-2.4448650	-0.2375700
C	1.3673390	-0.5796880	0.0396270
C	2.5471900	-0.0127860	-0.4969880
C	1.4886220	-1.8433310	0.6638760
C	3.7703750	-0.6811650	-0.4452980
H	2.5032060	0.9605970	-0.9798280
C	2.7155110	-2.5034660	0.7471230
H	0.6106130	-2.3034630	1.1089580
C	3.8579790	-1.9279820	0.1826140
H	4.6563960	-0.2272470	-0.8822320
H	2.7808810	-3.4668830	1.2469320
H	4.8131330	-2.4447340	0.2375180
Cl	0.1453030	2.8019910	1.5059990
Cl	0.1451580	2.8027350	-1.5056860



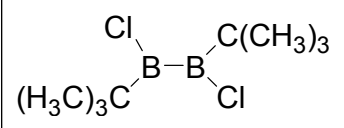
SCF energy=-518.7521252

B	0.7485010	-0.4264100	0.1825440
B	-0.7484920	0.4264670	0.1826400
N	2.0148130	0.1186940	-0.0882560
N	-2.0146890	-0.1188000	-0.0882730
C	2.2554670	1.5122890	-0.4474690
H	2.9404090	1.9812230	0.2734340
H	2.7193150	1.5772810	-1.4423620
H	1.3238010	2.0768330	-0.4529060
C	3.2405490	-0.6759590	-0.0475280



SCF energy=-782.2431752

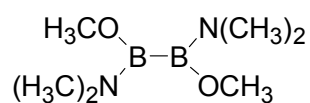
B	0.0000900	-0.1542550	0.0002470
B	-0.0001970	1.5791400	0.0000800
N	0.4119900	2.2690920	1.1938390
N	-0.4125890	2.2684150	-1.1941300
C	0.8867710	3.6433490	1.2876980
H	1.8354590	3.6684830	1.8457320
H	1.0782960	4.0606730	0.2983090
H	0.1810130	4.3044190	1.8181450
C	0.5176820	1.5801520	2.4725290
H	1.5504610	1.6001710	2.8560110
H	0.2114650	0.5347500	2.3795790
H	-0.1283570	2.0471760	3.2335300
C	-0.5183240	1.5788760	-2.4724900
H	0.1267390	2.0463450	-3.2340450
H	-1.5513570	1.5975940	-2.8553650
H	-0.2108460	0.5338600	-2.3793840
C	-0.8879090	3.6424640	-1.2885370
H	-0.1821190	4.3037670	-1.8186620
H	-1.0802650	4.0598280	-0.2993220
H	-1.8362580	3.6670410	-1.8471640
C	1.3634790	-0.9357380	-0.0761590
C	2.4932900	-0.3414040	-0.6843690
C	1.5494080	-2.2184720	0.4895930
C	3.7218370	-0.9984930	-0.7636920
H	2.4004020	0.6568410	-1.1073920
C	2.7839360	-2.8702110	0.4471900
H	0.7156880	-2.7043620	0.9900280
C	3.8713150	-2.2662780	-0.1917110
H	4.5658100	-0.5191890	-1.2545600
H	2.8977710	-3.8497230	0.9062180
H	4.8310470	-2.7760470	-0.2359510
C	-1.3631100	-0.9361090	0.0765200
C	-2.4930660	-0.3421670	0.6848430
C	-1.5487560	-2.2187660	-0.4895070
C	-3.7214680	-0.9995490	0.7640250
H	-2.4004240	0.6560150	1.1080660
C	-2.7831390	-2.8707870	-0.4472560
H	-0.7149340	-2.7043600	-0.9900600
C	-3.8706610	-2.2672410	0.1917670
H	-4.5655470	-0.5205350	1.2549930
H	-2.8967500	-3.8502240	-0.9065010
H	-4.8302760	-2.7772410	0.2358890



SCF energy=-1285.9622398

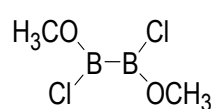
B	-0.2026760	0.8221240	-0.2645810
B	0.2026760	-0.8221240	-0.2645810
C	0.5106880	1.9940800	0.5354760
C	-0.5106880	-1.9940800	0.5354760
C	1.4889560	1.4331270	1.5932660
H	2.2573690	0.7940540	1.1406180
H	2.0080030	2.2515490	2.1108850
H	0.9664410	0.8443940	2.3581730
C	1.3209770	2.8228060	-0.5023050
H	1.8618980	3.6271400	0.0159710
H	2.0640140	2.2103440	-1.0276570
H	0.6679950	3.2835500	-1.2513590
C	-0.5106880	2.9238190	1.2329500
H	-1.2046840	3.3765820	0.5174280
H	-1.1041070	2.3854650	1.9830550

H	3.73959800	-0.66344500	-1.02698500
H	3.94070800	-0.26298700	0.69254400
H	3.01554700	-1.70897600	0.21970500
C	3.24038400	0.67600900	-0.04755700
H	-3.73918000	0.66393000	-1.02715000
H	-3.94077400	0.26280800	0.69217000
H	-3.01536300	1.70889500	0.22015100
C	-2.25560500	-1.51233200	-0.44743200
H	-2.94037900	-1.98117900	0.27368500
H	-2.71978900	-1.57724900	-1.44217600
H	-1.32402100	-2.07700400	-0.45321900
F	0.72826300	-1.76902600	0.49015500
F	-0.72836700	1.76905800	0.49015800



SCF energy=-549.2942233

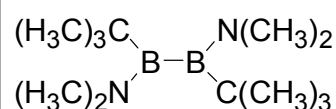
B	0.83398500	-0.15278800	-0.24907100
B	-0.82856900	-0.15575600	0.23995800
N	-1.78993900	0.72632100	-0.32566300
N	1.80849800	0.68527200	0.35689400
C	-3.19727800	0.72737900	0.05446900
H	-3.83924300	0.53729500	-0.81949500
H	-3.48935500	1.70210300	0.47519200
H	-3.38087900	-0.04653800	0.80067200
C	-1.47115600	1.72864300	-1.32869500
H	-2.05092700	1.56632700	-2.25102200
H	-0.40834100	1.69577300	-1.58236200
H	-1.70581100	2.74210200	-0.96644600
C	1.50777500	1.63340900	1.41666100
H	2.08799900	1.41016600	2.32574000
H	0.44529600	1.60113000	1.67156400
H	1.75622800	2.66205200	1.11116000
C	3.21336200	0.69004100	-0.03271800
H	3.85820500	0.44197200	0.82433700
H	3.51506600	1.68357100	-0.39887100
H	3.38166200	-0.04195700	-0.82351900
O	-1.31991700	-1.03460300	1.19867800
O	1.31027500	-0.98557300	-1.25836500
C	0.46963900	-1.90833900	-1.93247700
H	1.00350300	-2.25596100	-2.82251600
H	-0.47660200	-1.44745700	-2.24386200
H	0.24660900	-2.77627900	-1.29741900
C	-0.52852700	-2.00915500	1.85401900
H	-0.80938200	-3.01049400	1.50292100
H	-0.72164100	-1.95307400	2.93157500
H	0.54485800	-1.85962000	1.67922600



SCF energy=-1200.5823951

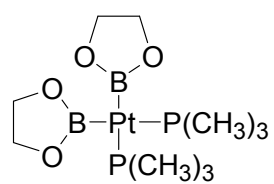
B	0.85165500	-0.02361200	0.11237600
B	-0.85164800	0.02355700	0.11236500
O	-1.55921500	-0.79761400	0.90440700
O	1.55915000	0.79786100	0.90418700
C	2.99064400	0.86264100	0.98121400
H	3.23043200	1.62779300	1.72159000
H	3.41182400	1.13799400	0.01002000
H	3.39988500	-0.10197400	1.29493400
C	-2.99071300	-0.86223800	0.98144400
H	-3.23066000	-1.62746000	1.72170000
H	-3.41188800	-1.13734800	0.01018300
H	-3.39974900	0.10241000	1.29531600
Cl	1.69648900	-1.18318300	-0.98281100
Cl	-1.69642700	1.18285700	-0.98319800

H	0.01707100	3.73594800	1.75199800
C	0.51068800	-2.92381900	1.23295000
H	1.20468400	-3.37658200	0.51742800
H	1.10410700	-2.38546500	1.98305500
H	-0.01707100	-3.73594800	1.75199800
C	-1.32097700	-2.82280600	-0.50230500
H	-1.86189800	-3.62714000	0.01597100
H	-2.06401400	-2.21034400	-1.02765700
H	-0.66799500	-3.28355000	-1.25135900
C	-1.48895600	-1.43312700	1.59326600
H	-2.25736900	-0.79405400	1.14061800
H	-2.00800300	-2.25154900	2.11088500
H	-0.96644100	-0.84439400	2.35817300
Cl	1.55353000	-1.23003500	-1.37838400
Cl	-1.55353000	1.23003500	-1.37838400



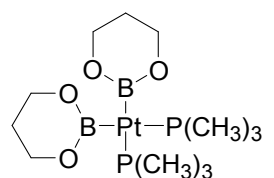
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B	0.85794700	-0.15207900	0.16072800
B	-0.85791400	0.15233800	0.16054400
C	1.84902600	0.71929300	-0.81796700
C	-1.84915100	-0.72029800	-0.81695000
C	1.03255500	1.78678000	-1.58962500
H	0.50550500	2.46953300	-0.91216300
H	1.69316700	2.39610900	-2.22432100
H	0.28289600	1.33069600	-2.24666000
C	2.92008200	1.50024300	-0.00974700
H	3.53846000	2.10581700	-0.68951000
H	2.45733500	2.19256900	0.70502300
H	3.59946700	0.85550400	0.55630700
C	2.55494900	-0.14820100	-1.89312700
H	3.22012700	-0.91054500	-1.47524500
H	1.82860300	-0.66828500	-2.52921300
H	3.16516500	0.48855600	-2.55181100
C	-2.55485900	0.14528700	-1.89377300
H	-3.22054700	0.90801100	-1.47740200
H	-1.82846400	0.66461800	-2.53041500
H	-3.16459900	-0.49276100	-2.55164700
C	-2.92050400	-1.49942000	-0.00737900
H	-3.53924500	-2.10583200	-0.68607700
H	-2.45802700	-2.19080100	0.70848200
H	-3.59949200	-0.85337300	0.55766400
C	-1.03289500	-1.78935700	-1.58667000
H	-0.50572800	-2.47083300	-0.90802400
H	-1.69367300	-2.39986400	-2.22006300
H	-0.28336000	-1.33457200	-2.24476100
N	-1.35207100	1.15732100	1.03655200
N	1.35228500	-1.15581200	1.03805600
C	-2.72335400	1.64548200	1.17781000
H	-2.76298900	2.72974400	0.99411700
H	-3.09467900	1.47026100	2.19894100
H	-3.39920200	1.16062000	0.48049600
C	-0.48486900	1.89081300	1.95872700
H	-0.46476800	2.96388000	1.71329900
H	0.53492800	1.50644600	1.92417700
H	-0.85116700	1.79591400	2.99233100
C	0.48519100	-1.88857100	1.96087600
H	0.46561100	-2.96195100	1.71675200
H	-0.53475100	-1.50466200	1.92558500
H	0.85118300	-1.79226000	2.99446000
C	2.72362700	-1.64365600	1.17971800
H	2.76386400	-2.72772500	0.99493000
H	3.09411200	-1.46933600	2.20130000
H	3.39981800	-1.15771100	0.48348000



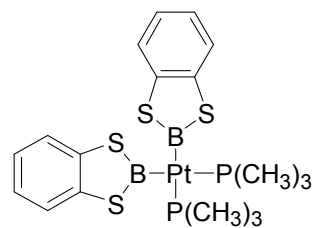
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Pt	-0.19831200	0.00180000	0.00011400
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C	-1.27287100	-3.18000900	-1.30699600
H	-1.96516600	-4.03002300	-1.26495700
H	-0.25487600	-3.53730700	-1.12766100
H	-1.30481100	-2.73775000	-2.30812700
C	-1.66132900	-2.86245500	1.52976100
H	-2.23808500	-3.79203100	1.44565500
H	-2.07523200	-2.25687900	2.34311000
H	-0.61835700	-3.08823000	1.76951400
C	-3.53386000	-1.75150800	-0.33524300
H	-4.01392700	-2.73813900	-0.32766200
H	-3.72191800	-1.27676600	-1.30428100
H	-3.98962900	-1.13375800	0.44440200
P	-1.65904000	1.93137700	0.04479300
C	-1.19612100	3.20954800	1.30346800
H	-1.86920300	4.07486300	1.26156100
H	-0.17090900	3.54378400	1.12089400
H	-1.23530600	2.77001500	2.30552400
C	-1.59662300	2.89702500	-1.53158000
H	-2.15167200	3.83976600	-1.44766700
H	-2.02555500	2.30056400	-2.34388000
H	-0.54909200	3.09867600	-1.77306800
C	-3.49243500	1.83529900	0.33850300
H	-3.94614300	2.83429100	0.33236200
H	-3.69052800	1.36558100	1.30796400
H	-3.96677600	1.23018300	-0.44004600
B	1.40475600	-1.31201100	-0.05472500
B	1.43347700	1.27953300	0.05484100
O	2.37993200	-1.37746000	-1.04934600
O	1.64430600	-2.29136100	0.91519400
O	2.40566100	1.32828300	1.05338600
O	1.69842900	2.24882600	-0.91858600
C	3.26209200	-2.47775900	-0.77885200
H	3.05879200	-3.28201600	-1.49889900
H	4.29881900	-2.14958400	-0.90682000
C	2.92926100	-2.88665000	0.66823900
H	2.86005400	-3.97063200	0.80881500
H	3.64865000	-2.48163700	1.39115600
C	3.31293700	2.40754800	0.78128000
H	4.34162000	2.05746400	0.91589600
H	3.12404400	3.21996000	1.49611300
C	2.99573700	2.81578800	-0.66942400
H	3.70862900	2.39009000	-1.38687000
H	2.95225500	3.90025400	-0.81639800



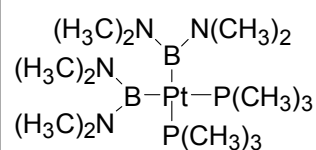
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Pt	-0.37306100	0.02195000	-0.00225400
P	-1.86565800	-1.88712100	-0.09439000
C	-1.36365800	-3.19642800	-1.30648000
H	-2.05062400	-4.05180700	-1.28411200
H	-0.35311000	-3.54107400	-1.07013500
H	-1.34769900	-2.77240700	-2.31593700
C	-1.90882800	-2.83313000	1.49563800
H	-2.45980600	-3.77659400	1.39349400
H	-2.38307000	-2.22330100	2.27205900
H	-0.87777900	-3.03050200	1.80260900



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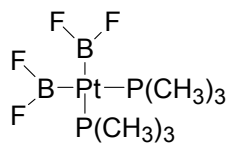
Pt	0.00932600	1.11818100	0.03334600
P	1.90282500	2.66801400	0.09420100
C	2.58119700	3.06077200	-1.58167800
H	3.47530600	3.69228600	-1.51428800
H	1.82353500	3.57559300	-2.18139800
H	2.83919300	2.12578500	-2.08883900
C	1.72745200	4.35667700	0.84702300
H	2.66928300	4.91534800	0.78548700
H	1.44816300	4.25898900	1.90157000
H	0.94813000	4.93175000	0.33750300
C	3.40475000	2.06674600	0.98714800
H	4.20129000	2.82010600	0.96369900
H	3.76641800	1.14501700	0.52355500
H	3.15038000	1.84005900	2.02723700
P	-1.77886400	2.77480400	-0.08755400
C	-3.48361500	2.14535500	-0.41964100
H	-4.19836300	2.97444900	-0.48568000
H	-3.78905600	1.46723600	0.38274100
H	-3.49482100	1.57988400	-1.35632000
C	-2.06842100	3.79694500	1.43087100
H	-2.90704900	4.48966000	1.29030500
H	-1.17149400	4.36967200	1.68385700
H	-2.29468800	3.13163800	2.27052700
C	-1.62400900	4.05724400	-1.41876400
H	-2.48441900	4.73744200	-1.42063500
H	-1.56669100	3.55777300	-2.39162500
H	-0.71106700	4.64548700	-1.28582100
B	-1.34611100	-0.42954400	-0.00613900
B	1.31138500	-0.47944300	0.04177000
C	4.65647000	-4.27214300	0.66895400
C	3.00999400	-2.49967600	0.69915700
C	3.18629500	-2.31646000	-0.68597100
C	4.09828000	-3.11529700	-1.38894600
C	4.83114100	-4.08964000	-0.71007200
H	5.22725000	-5.03382700	1.19378300
H	4.22899400	-2.97481600	-2.45880900
H	5.53758400	-4.70933000	-1.25627200
C	3.74812800	-3.48173900	1.37413700
H	3.60806900	-3.62509400	2.44237700
C	-3.26576400	-2.23533900	0.67303800
C	-4.18835100	-3.03825100	1.35738300
C	-4.97349400	-3.94851600	0.64857600
C	-4.84075600	-4.06351100	-0.74228500
C	-3.92240500	-3.26872300	-1.42947700
C	-3.13251300	-2.35052900	-0.72417100
H	-4.28677100	-2.95058900	2.43629700
H	-5.68813200	-4.57109700	1.18067800
H	-5.45207000	-4.77562300	-1.29055900
H	-3.81481000	-3.35950600	-2.50723200
S	2.20405500	-1.04910700	-1.45218800
S	1.82687700	-1.44567600	1.50332300
S	-2.21977200	-1.04605000	1.47936400
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SCF energy=-1629.6527587

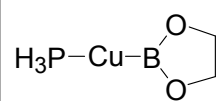
Pt	0.32755800	-0.00039400	-0.00004900
P	1.93335500	1.80778700	-0.37706300

H	4.55507100	1.10441100	-0.88662600
H	3.15806400	2.17147800	-1.17334100
H	3.32306400	0.67204000	-2.10086300
C	3.05286400	1.02362100	1.72763300
H	4.14684700	1.02211500	1.81160800
H	2.62953100	0.48555400	2.58193000
H	2.69705300	2.05745400	1.77132900
B	-1.98419500	-0.39873900	0.03270300
B	0.07298600	-2.04344500	-0.30104300
C	-0.00236600	-2.67624000	-1.77941300
H	-0.55148600	-2.02620100	-2.47141300
H	-0.55825700	-3.62989000	-1.74130700
C	1.38092200	-2.97128800	-2.40481700
H	1.28105700	-3.45744600	-3.38424200
H	1.98405400	-3.63740300	-1.77363900
H	1.95195100	-2.04671600	-2.55912300
C	0.17660800	-3.12827700	0.86623200
H	0.92710800	-3.88732900	0.57879500
H	-0.77767200	-3.68607200	0.80812200
C	0.40652200	-2.69575100	2.32272600
H	0.37474200	-3.54754800	3.01656700
H	-0.34865700	-1.96972100	2.64282800
H	1.38205400	-2.20985300	2.44980200
C	-2.86980500	-0.66794100	-1.27494400
H	-2.90533000	-1.77082200	-1.36001600
H	-2.34397100	-0.35110900	-2.18593900
C	-4.32014000	-0.13963200	-1.31311900
H	-4.83079300	-0.42943900	-2.24123000
H	-4.35561300	0.95730800	-1.25967300
H	-4.92052600	-0.51766400	-0.47811800
C	-2.74569200	-0.41797000	1.44534400
H	-3.53107400	0.35984900	1.41896100
H	-2.08235400	-0.14987400	2.27774700
C	-3.43348000	-1.76396800	1.78340200
H	-3.97808900	-1.70713500	2.73521300
H	-2.69890600	-2.57229100	1.87738000
H	-4.15122000	-2.06383900	1.01087700



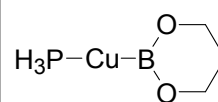
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Pt	-0.01110700	0.31247800	-0.01716500
P	-1.90085000	-1.20933600	-0.00403300
C	-3.56990600	-0.41473700	-0.04550900
H	-4.36837300	-1.16653900	-0.03545000
H	-3.66417100	0.19618600	-0.94899700
H	-3.68749400	0.24363600	0.82119600
C	-2.04205000	-2.40832000	-1.40859100
H	-2.95525700	-3.01011600	-1.32667200
H	-1.17671400	-3.07705000	-1.42500600
H	-2.06409000	-1.85573800	-2.35353800
C	-2.05540700	-2.30116400	1.48396100
H	-2.96425500	-2.91324800	1.43780300
H	-2.09019200	-1.67918800	2.38423800
H	-1.18655200	-2.96203400	1.56175800
P	1.85364700	-1.25073400	-0.01213900
C	3.14715400	-0.88565900	-1.28251300
H	3.98579100	-1.58852600	-1.21022900
H	3.52031900	0.13459200	-1.15304300
H	2.70573300	-0.95256500	-2.28220100
C	2.80444300	-1.19575600	1.57227800
H	3.70575700	-1.81799300	1.51901100
H	2.17131300	-1.55081500	2.39212300
H	3.08541000	-0.16135800	1.79082400
C	1.64112900	-3.07894600	-0.25328700



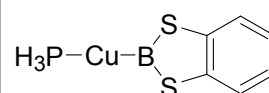
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Cu	-0.94065800	0.00139900	-0.00196900
P	-3.29964600	-0.00105100	0.00187800
H	-4.00234800	-0.37334300	1.17167500
H	-4.00504900	-0.82900400	-0.90247000
H	-4.00776300	1.19517800	-0.26011100
B	1.06577200	0.00072800	-0.00065700
O	1.85326200	-1.14249400	0.05076700
O	1.85538400	1.14247200	-0.05077000
C	3.24302000	-0.77065000	-0.05445700
H	3.80433300	-1.26152300	0.74722300
H	3.62745700	-1.12347400	-1.01924100
C	3.24425800	0.76821900	0.05716400
H	3.62752600	1.12065400	1.02254000
H	3.80791600	1.25783100	-0.74361400



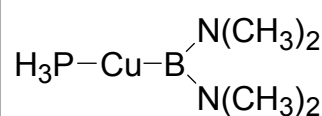
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P	3.62045200	-0.00074900	0.06126500
B	-0.76440300	0.00061400	-0.08598700
O	-1.45742700	-1.20013200	-0.10814500
O	-1.45873000	1.20059500	-0.10775900
C	-3.50413900	-0.00094200	0.48892300
H	-4.59501000	-0.00153200	0.35884300
H	-3.29764100	-0.00085300	1.56749800
C	-2.89089800	1.24319500	-0.14873000
H	-3.20759600	1.33283200	-1.19809700
H	-3.20009400	2.15575900	0.37311800
C	-2.88955600	-1.24437700	-0.14881800
H	-3.20634400	-1.33441600	-1.19812100
H	-3.19759900	-2.15728400	0.37311800
Cu	1.25058100	0.00092400	-0.01503900
H	4.35461000	-0.90677200	-0.74096100
H	4.34251600	1.16534500	-0.28853200
H	4.29235800	-0.26267400	1.27921100



SCF energy=-1591.6519952

P	4.76638000	0.00043800	-0.00142700
B	0.42522700	-0.00029300	0.00084300
C	-2.20092600	-0.70391200	-0.00032300
C	-3.41512300	-1.40522400	-0.00041900
C	-4.61891600	-0.70114200	-0.00060900
C	-4.61874100	0.70184900	-0.00061500
C	-3.41477200	1.40563000	-0.00042400
C	-2.20074900	0.70401600	-0.00032200
H	-3.41346300	-2.49211000	-0.00028900
H	-5.56020200	-1.24466700	-0.00066200
H	-5.55989100	1.24561000	-0.00066700
H	-3.41284000	2.49251600	-0.00030800
S	-0.60567300	-1.49156900	0.00044300
S	-0.60528700	1.49125500	0.00044800
H	5.46515000	1.06430300	0.61360400
H	5.46585300	0.00178100	-1.22977000
H	5.46706700	-1.06288800	0.61234600
Cu	2.41783500	-0.00041100	0.00086000



SCF energy=-833.3171975

P	-3.55273300	0.00036000	-0.00075700
B	0.89843600	0.00019400	0.00026500

H	2.60359400	-3.59958200	-0.17835600
H	1.21420700	-3.27756400	-1.24168900
H	0.96513600	-3.48714400	0.50488200
B	-1.28255500	1.92853800	0.02485300
B	1.35259800	1.85656200	-0.00234800
F	1.97966900	2.28716800	1.11789400
F	1.79596400	2.49098500	-1.10931600
F	-1.77060500	2.47158300	1.16327900
F	-1.79704900	2.50968800	-1.08138600



P	3.21503900	-0.26677200	0.00095900
B	-1.22730700	-0.06892500	-0.00018900
C	-2.00620300	1.31095200	-0.00980700
H	-2.71377700	1.29798600	0.84040300
H	-2.67013500	1.29655700	-0.89519700
C	-1.20333200	2.62108100	0.00852600
H	-1.85102000	3.50895600	-0.00809200
H	-0.53229500	2.68180700	-0.85806400
H	-0.57589500	2.68396400	0.90708400
C	-2.06468000	-1.42500900	0.00639400
H	-1.71737600	-2.01190200	0.87510100
H	-1.71154700	-2.02686700	-0.84940800
C	-3.60592600	-1.37809500	0.00082100
H	-4.04470100	-2.38516500	0.00496900
H	-3.99073700	-0.85828900	-0.88600600
H	-3.99699600	-0.84839600	0.87898600
H	3.96694900	0.89289600	-0.30806100
H	3.90478700	-1.15057300	-0.86462900
H	3.91250400	-0.60978900	1.18488300
Cu	0.80041500	-0.16891600	-0.00244900

Radicals:

$$\text{HO}-\text{B} \cdot$$

$$\text{HO}$$
 SCF energy=-176.5281004

B	0.00000000	0.00000000	0.47792100
O	0.00000000	-1.17583400	-0.19627200
H	0.00000000	-1.95475800	0.37537500
O	0.00000000	1.17583400	-0.19627200
H	0.00000000	1.95475800	0.37537500

$$\text{HO}-\text{B} \cdot$$

$$\text{H}_3\text{C}$$
 SCF energy=-140.573956

B	-0.13589600	-0.52995300	0.00005300
O	-1.26078800	0.21868500	0.00001300
H	-2.08412600	-0.29062700	-0.00015600
C	1.30442600	0.08566000	0.00000800
H	1.87071300	-0.25515100	0.87677000
H	1.86981100	-0.25369600	-0.87792000
H	1.28283300	1.18580100	0.00088700

$$\text{H}_3\text{C}-\text{B} \cdot$$

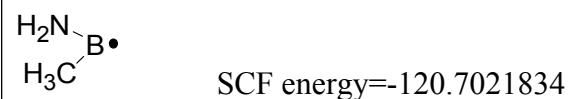
$$\text{H}_3\text{C}$$
 SCF energy=-104.612532

B	0.00000400	0.57026500	-0.00000200
C	-1.40572800	-0.09869000	0.01077800
H	-2.20050600	0.50259400	0.46633100

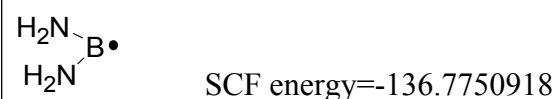
N	1.62059000	1.25031400	-0.01737800
N	1.61784900	-1.25156900	0.01742000
C	0.99944400	2.51572000	0.32988600
H	1.54178200	3.02182900	1.14564200
H	-0.02797600	2.34521700	0.66292700
H	0.97959600	3.20612300	-0.53196800
C	2.95571100	1.43990200	-0.56989900
H	3.69603600	1.73940600	0.19177300
H	3.30717100	0.52762200	-1.05510200
H	2.93740700	2.23638800	-1.33172800
C	0.99346600	-2.51564300	-0.32886900
H	1.53313800	-3.02280400	-1.14574100
H	-0.03424900	-2.34288500	-0.65990200
H	0.97375700	-3.20610100	0.53293900
C	2.95326700	-1.44405900	0.56824600
H	3.69192500	-1.74531000	-0.19434600
H	2.93414400	-2.24039300	1.33021200
H	3.30734200	-0.53248500	1.05286500
H	-4.26730200	-0.29979900	-1.18669400
H	-4.26919000	-0.87530800	0.85196800
H	-4.26892100	1.17696700	0.33099600
Cu	-1.14883600	0.00132500	0.00068000



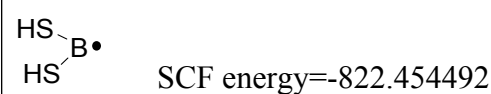
P	2.57453000	0.00061600	0.00068200
B	-1.78767700	0.00037100	0.00022100
H	3.27632800	-1.18400200	-0.31853600
H	3.27300800	0.87313900	-0.86448400
H	3.26940300	0.31741800	1.18999600
Cu	0.21439900	-0.00130400	-0.00110700
F	-2.54088800	-1.12086200	0.00077100
F	-2.53865500	1.12310500	0.00075900



B	0.08584200	0.55685600	0.00002600
N	1.30946500	-0.10347400	0.00004300
H	2.20377700	0.36926600	-0.00021200
H	1.39851100	-1.11941500	-0.00003600
C	-1.34117100	-0.09389800	-0.00001600
H	-1.91909900	0.22464800	0.87772100
H	-1.91955600	0.22618600	-0.87685400
H	-1.31206900	-1.19726300	-0.00095400

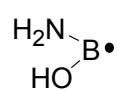


B	0.00001400	0.52944300	0.00003700
N	1.26270500	-0.09317900	-0.00003700
H	2.12622700	0.42879100	-0.00062100
H	1.40586100	-1.10018200	0.00102300
N	-1.26270700	-0.09317800	0.00004300
H	-2.12618600	0.42885900	0.00039800
H	-1.40595800	-1.10017600	-0.00102300



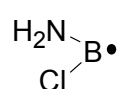
B	0.00000000	0.00000000	0.64399100
H	0.00000000	-2.36057100	0.95309000
H	0.00000000	2.36057100	0.95309000
S	0.00000000	-1.59358100	-0.16019200

H	-1.68977400	-0.23173400	-1.04859700
H	-1.41198800	-1.10435200	0.46375800
C	1.40574000	-0.09867200	-0.01077900
H	2.20070200	0.50282800	-0.46571400
H	1.68940700	-0.23243400	1.04861100
H	1.41206500	-1.10405900	-0.46437200



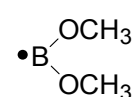
SCF energy=-156.6531282

B	-0.04962800	0.51767200	0.00011700
O	-1.20689700	-0.21044400	0.00034300
H	-2.01036000	0.32488200	-0.00204900
N	1.21396300	-0.08288900	-0.00027400
H	1.34083400	-1.09195600	-0.00032700
H	2.07510100	0.44248700	0.00095900



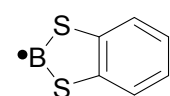
SCF energy=-541.0372644

B	-0.52464200	0.61357300	-0.00014300
N	-1.68636000	-0.14224700	0.00000200
H	-1.70057300	-1.15964900	-0.00028400
H	-2.60586800	0.27943700	0.00051600
Cl	1.10201000	-0.07011300	0.00002700



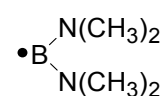
SCF energy= -255.1247803

B	0.02861200	0.79695800	0.00027300
O	-1.31165800	0.69455600	-0.00016400
O	0.86887200	-0.26527100	0.00016400
C	-1.97710100	-0.58382800	-0.00005500
H	-3.05026100	-0.38364000	-0.01531300
H	-1.69418900	-1.16264200	-0.88502300
H	-1.71749300	-1.14928200	0.90059800
C	2.29285300	-0.14182400	-0.00012000
H	2.68407700	-0.63950200	-0.89256100
H	2.59815200	0.90973000	-0.00000300
H	2.68443300	-0.63982300	0.89198400



SCF energy= -1052.307241

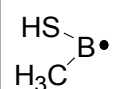
B	-0.00002000	2.39091100	0.00000000
S	0.00003200	1.45150800	1.51432500
S	0.00003200	1.45150800	-1.51432500
C	0.00002800	-2.55813800	-0.70084500
C	-0.00004100	-1.35562400	-1.40664400
C	-0.00009700	-0.14424300	-0.70408000
C	-0.00009700	-0.14424300	0.70408000
C	-0.00004100	-1.35562400	1.40664400
C	0.00002800	-2.55813800	0.70084500
H	0.00016600	-3.49892700	-1.24449200
H	0.00002600	-1.35445000	-2.49322700
H	0.00002600	-1.35445000	2.49322700
H	0.00016600	-3.49892700	1.24449200



SCF energy= -293.9997491

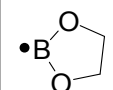
B	-0.00003100	-0.74564400	-0.00008300
N	1.28069200	-0.15425800	-0.02388900
C	2.47181800	-0.91698100	0.32742500
H	3.16551100	-0.98184800	-0.52595800
H	3.01047400	-0.44780900	1.16507800
H	2.18663300	-1.92979900	0.62200800
C	1.58091300	1.19270400	-0.50287200
H	1.95713700	1.84135400	0.30434800

S	0.00000000	1.59358100	-0.16019200
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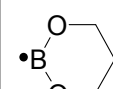
SCF energy=-463.5373344

B	0.46944500	-0.60173800	0.00002200
H	-1.91779600	-0.95152900	-0.00004700
C	1.85553300	0.11102100	-0.00000100
H	2.43944500	-0.20400900	0.87628200
H	2.43923500	-0.20377400	-0.87651000
H	1.80766200	1.21038700	0.00014700
S	-1.14056100	0.15571800	0.00000100



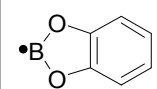
SCF energy=-253.9140393

B	0.00000000	0.00000000	1.28166300
O	0.00000000	1.15161000	0.56104700
O	0.00000000	-1.15161000	0.56104700
C	0.06147900	0.77191800	-0.84546000
C	-0.06147900	-0.77191800	-0.84546000
H	0.75742700	-1.26973600	-1.37081600
H	-1.01545500	-1.12395700	-1.24896200
H	-0.75742700	1.26973600	-1.37081600
H	1.01545500	1.12395700	-1.24896200



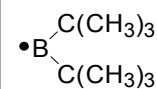
SCF energy= -293.2404155

B	0.11520700	-1.47193900	0.00000000
O	0.11355600	-0.85522100	1.20589800
O	0.11355600	-0.85522100	-1.20589800
C	0.11355600	0.59342600	1.25424400
C	0.11355600	0.59342600	-1.25424400
H	1.15421400	0.92429100	-1.36042600
C	-0.52954900	1.18165500	0.00000000
H	-0.43159200	0.87512300	-2.15915500
H	-0.43159200	0.87512300	2.15915500
H	1.15421400	0.92429100	1.36042600
H	-0.41917100	2.27409000	0.00000000
H	-1.60437600	0.95927700	0.00000000



SCF energy= -406.3415352

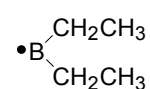
B	-0.00008600	-2.40492200	0.00000000
O	-0.00061200	-1.64463200	1.14918200
O	-0.00061200	-1.64463200	-1.14918200
C	0.00106700	2.04139600	-0.70099400
C	0.00011700	0.84413000	-1.43442100
C	-0.00061200	-0.32723000	-0.69706000
C	-0.00061200	-0.32723000	0.69706000
C	0.00011700	0.84413000	1.43442100
C	0.00106700	2.04139600	0.70099400
H	-0.00006200	0.83161400	-2.51957000
H	-0.00006200	0.83161400	2.51957000
H	0.00174300	2.98797400	1.23400400
H	0.00174300	2.98797400	-1.23400400



SCF energy= -340.4838129

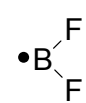
B	0.00000000	-0.00000100	-0.68470000
C	1.46566300	-0.00497600	-0.10902600
C	-1.46566300	0.00497700	-0.10902600
C	2.47816400	-0.52666600	-1.15773600
H	3.50686100	-0.45256000	-0.77421500
H	2.41786100	0.04690200	-2.08951600

H	2.35463500	1.15291300	-1.28416200
H	0.69102700	1.65385300	-0.93604900
N	-1.28078900	-0.15426800	0.02392500
C	-2.47195700	-0.91684300	-0.32740600
H	-3.16598400	-0.98097000	0.52575500
H	-3.01022800	-0.44813200	-1.16558600
H	-2.18692500	-1.92993500	-0.62122100
C	-1.58069900	1.19276900	0.50287000
H	-1.95688800	1.84149800	-0.30431300
H	-2.35434900	1.15314500	1.28424100
H	-0.69066100	1.65373900	0.93592200



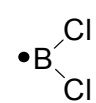
SCF energy= -183.2424985

B	0.05076500	0.77596700	0.00000000
C	1.10067700	-0.37382000	0.00000000
H	0.86974100	-1.01676900	0.87077100
H	0.86974100	-1.01677000	-0.87076900
C	-1.50964400	0.73318000	0.00000000
H	-1.85445600	1.32607100	0.86423500
H	-1.85445600	1.32607100	-0.86423500
C	2.59461600	-0.00329100	0.00000000
H	2.85031400	0.59454500	-0.88246500
H	2.85031400	0.59454600	0.88246400
H	3.23390300	-0.89515700	0.00000000
C	-2.19978100	-0.65040200	0.00000000
H	-1.92059100	-1.23641200	-0.88399100
H	-1.92059100	-1.23641200	0.88399100
H	-3.29295500	-0.55354900	0.00000000



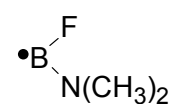
SCF energy=-224.5645921

B	0.00000000	0.00000000	0.50753500
F	0.00000000	-1.14830700	-0.14098200
F	0.00000000	1.14830700	-0.14098200



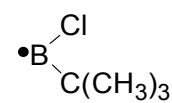
SCF energy=-945.283087

B	0.00000000	0.00000000	0.69219800
Cl	0.00000000	-1.54501300	-0.10179400
Cl	0.00000000	1.54501300	-0.10179400



SCF energy= -259.3007283

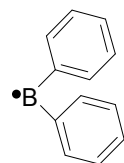
B	0.83448700	0.78827100	0.00001000
N	-0.36577600	0.08547500	0.00011300
C	-0.43443200	-1.37776200	-0.00001400
H	-0.96772700	-1.73766200	0.89047300
H	-0.96891500	-1.73741100	-0.88987500
H	0.57291300	-1.79872500	-0.00075400
C	-1.66160000	0.75391700	-0.00003000
H	-2.24226000	0.47595900	-0.89072400
H	-2.24309400	0.47473200	0.88974500
H	-1.51786100	1.83711300	0.00076800
F	2.03679300	0.18771000	-0.00002300



SCF energy= -642.872846

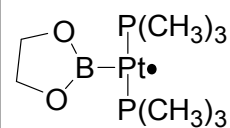
B	-0.57033000	0.18738000	-0.79704700
C	0.80271500	-0.00496500	-0.05317100
C	0.78541200	-1.24597500	0.87202100
H	-0.00363900	-1.17881200	1.62884400
H	0.63048800	-2.17141600	0.30374900
H	1.74849900	-1.33575500	1.39355200

H	2.28994800	-1.57871600	-1.40551200
C	1.78326400	1.49352500	0.17557400
H	2.82967000	1.58687400	0.49930200
H	1.15244800	1.90862100	0.96986700
H	1.66091800	2.11664200	-0.71950400
C	1.64433200	-0.81833300	1.19721400
H	2.68276700	-0.74161200	1.55177900
H	1.43338600	-1.88346600	1.04010300
H	0.99459200	-0.46147800	2.00328700
C	-2.47816500	0.52664800	-1.15774500
H	-3.50686300	0.45253900	-0.77422500
H	-2.41785600	-0.04693100	-2.08951800
H	-2.28995600	1.57869600	-1.40553300
C	-1.64433900	0.81834900	1.19720300
H	-2.68277500	0.74162500	1.55176800
H	-1.43340200	1.88348100	1.04007800
H	-0.99459800	0.46151000	2.00328200
C	-1.78325500	-1.49352200	0.17559300
H	-2.82966100	-1.58687300	0.49932400
H	-1.15243600	-1.90860500	0.96989000
H	-1.66090700	-2.11664900	-0.71947800



SCF energy= -488.107626

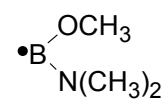
B	0.00001000	-1.10309800	0.00008700
C	-1.40655100	-0.50410000	0.01915600
C	-2.49962800	-1.15843000	-0.59861700
C	-1.67160100	0.71327600	0.69640400
C	-3.78186500	-0.61239400	-0.56997800
H	-2.32865700	-2.10578000	-1.10436600
C	-2.96157000	1.24055300	0.76029300
H	-0.85463400	1.24151700	1.18239400
C	-4.01729900	0.58403800	0.11817900
H	-4.60277600	-1.12484600	-1.06563200
H	-3.14375200	2.16861000	1.29705200
H	-5.02113500	1.00009000	0.15791800
C	1.40657000	-0.50409200	-0.01905400
C	1.67153200	0.71331100	-0.69628300
C	2.49970300	-1.15842800	0.59859900
C	2.96148700	1.24061600	-0.76027100
H	0.85450500	1.24154800	-1.18217400
C	3.78194100	-0.61239300	0.56983300
H	2.32877000	-2.10577900	1.10435900
C	4.01728200	0.58406800	-0.11830100
H	3.14360800	2.16870500	-1.29699200
H	4.60291100	-1.12485900	1.06537100
H	5.02111300	1.00012900	-0.15812800



SCF energy= -1295.4907836

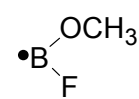
Pt	-0.00003800	-0.49233700	-0.00044700
P	2.30470100	-0.79415100	0.01901800
C	3.17291300	-0.09062800	-1.45393100
H	4.25921700	-0.22284000	-1.37595000
H	2.93477200	0.97459000	-1.52063500
H	2.81588000	-0.58571200	-2.36287800
C	3.18281500	0.02808500	1.42375900
H	4.26789600	-0.11884200	1.35509200
H	2.82487500	-0.38380900	2.37303800
H	2.95404800	1.09715700	1.39958400
C	3.01544000	-2.51135300	0.09164900
H	4.11430100	-2.49610100	0.09224300

C	1.00263700	1.27659000	0.80677300
H	1.97209000	1.21790500	1.32067300
H	1.00805300	2.18648700	0.19417000
H	0.22324100	1.38231300	1.57006800
C	1.96544500	-0.12367700	-1.06412700
H	2.01270800	0.74893300	-1.72568800
H	2.92554400	-0.20192000	-0.53494400
H	1.85871900	-1.01386200	-1.69566800
Cl	-2.16831200	0.00102300	-0.10814700



SCF energy= -274.5738129

B	0.34184100	-0.54982200	-0.00335100
N	-0.98047000	-0.09035200	0.00031400
C	-1.32679800	1.33004300	0.00220700
H	-1.91997300	1.58520800	0.89271300
H	-1.92149500	1.58729700	-0.88669200
H	-0.41624600	1.93254500	0.00204700
C	-2.12447500	-0.98942100	0.00082500
H	-2.75078500	-0.82957800	0.89139500
H	-1.77909600	-2.02645500	-0.00021700
H	-2.75269700	-0.82844300	-0.88820500
O	1.42799500	0.26793300	-0.00906500
C	2.76975000	-0.21013600	0.00518500
H	3.31003400	0.24397700	-0.83194400
H	2.80389800	-1.30157300	-0.08581000
H	3.24562700	0.09221100	0.94449300



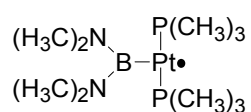
SCF energy= -239.8617844

B	-0.78707300	0.67370100	0.00001300
O	0.54422900	0.71155100	-0.00001000
C	1.39077200	-0.46003800	0.00000400
H	2.01951800	-0.41664100	-0.89235500
H	0.79783300	-1.37857400	-0.00102100
H	2.01813000	-0.41771200	0.89339200
F	-1.51095400	-0.45419500	-0.00000200



SCF energy= -584.9155109

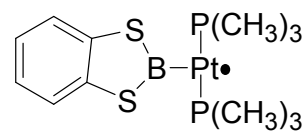
B	0.00000000	0.82262400	0.00000000
Cl	-0.68611200	-0.78948900	0.00000000
F	1.29598900	1.03424500	0.00000000



SCF energy= -1335.549395

Pt	0.01064700	-0.58825500	0.00305900
P	2.28804900	-0.96898300	0.14105800
C	3.33938000	0.03467600	-1.01041800
H	4.40786000	-0.14554800	-0.83770200
H	3.11883100	1.09674400	-0.86776700
H	3.09847300	-0.22521300	-2.04651500
C	3.07211600	-0.59730500	1.78038000
H	4.15175800	-0.79134700	1.75448600
H	2.61727900	-1.22272000	2.55530000
H	2.90321500	0.45118300	2.04437800
C	2.96479500	-2.67420500	-0.18666400
H	4.06107700	-2.70010200	-0.10963600
H	2.66684900	-2.99257600	-1.19088600
H	2.53485800	-3.37937100	0.53180500
P	-2.25557200	-1.03163200	-0.14585400
C	-3.14763800	-0.20899200	-1.54811500
H	-4.22502000	-0.41309100	-1.51218200
H	-2.75003600	-0.57231500	-2.50156700
H	-2.98128000	0.87144900	-1.49943000

H	2.66409600	-3.08747000	-0.77033800
H	2.66254000	-3.01186500	0.99910200
P	-2.30467100	-0.79411700	-0.01857800
C	-3.18382500	0.02725300	-1.42320800
H	-4.26879000	-0.12041900	-1.35424400
H	-2.82585600	-0.38440100	-2.37256800
H	-2.95584300	1.09649600	-1.39914500
C	-3.01530500	-2.51142700	-0.08972800
H	-4.11416800	-2.49640000	-0.08752200
H	-2.66161900	-3.08763700	0.77124300
H	-2.66466100	-3.01172200	-0.99817500
C	-3.17197800	-0.08965200	1.45442800
H	-4.25833800	-0.22162800	1.37690600
H	-2.93344900	0.97551800	1.52033600
H	-2.81475400	-0.58428200	2.36354500
B	-0.00002000	1.59300200	-0.00038400
O	1.13781500	2.40042000	-0.11385100
O	-1.13777700	2.40048800	0.11369500
C	0.74210300	3.78298600	-0.20490300
H	1.37387300	4.38243600	0.45841800
H	0.89047600	4.12461700	-1.23721800
C	-0.74189300	3.78297200	0.20534100
H	-0.89017700	4.12415300	1.23782600
H	-1.37361900	4.38280300	-0.45767800



SCF energy= -2093.8850835

Pt	-1.30877000	-0.00018200	-0.00001700
P	-1.69015000	-2.29945100	0.00021500
C	-0.96265600	-3.19375700	-1.44465000
H	-1.11404100	-4.27654400	-1.35796300
H	0.10834700	-2.97855900	-1.50535900
H	-1.43157900	-2.83938800	-2.36835800
C	-0.96084800	-3.19416600	1.44387300
H	-1.11184800	-4.27696600	1.35661500
H	-1.42899900	-2.84064000	2.36828800
H	0.11011200	-2.97853100	1.50369200
C	-3.43422700	-2.94178200	0.00119200
H	-3.46040900	-4.04000500	0.00186200
H	-3.95875000	-2.56991200	-0.88476800
H	-3.95828800	-2.56882000	0.88695500
P	-1.69158200	2.29885100	-0.00009900
C	-0.96334200	3.19399800	-1.44405700
H	-1.11534900	4.27667800	-1.35711200
H	-1.43132200	2.83974300	-2.36829000
H	0.10780700	2.97934100	-1.50402000
C	-3.43612200	2.93989400	-0.00074900
H	-3.46311000	4.03809900	-0.00036100
H	-3.96062900	2.56675300	0.88467700
H	-3.95966100	2.56742600	-0.88703800
C	-0.96438900	3.19384600	1.44444500
H	-1.11651300	4.27651400	1.35751900
H	0.10677700	2.97941400	1.50500100
H	-1.43284100	2.83941800	2.36836300
B	0.74797500	0.00041100	-0.00004000
C	3.39078600	0.00033700	-0.70398400
C	4.60473000	0.00008100	-1.40405100
C	5.81052100	0.00028800	-0.70081900
C	5.81049500	0.00071000	0.70090000
C	4.60467400	0.00094600	1.40408500
C	3.39076100	0.00077300	0.70396100
H	4.60290500	-0.00024700	-2.49106800
H	6.75111700	0.00009300	-1.24566400
H	6.75107000	0.00082300	1.24578100
H	4.60280400	0.00124000	2.49110100

H	-0.95060100	-3.02983900	1.48692800
H	0.11596700	-1.86327000	2.24475200
C	1.13337900	-3.61743900	1.47506600
H	1.09927300	-4.14721200	2.43635900
H	2.13495700	-3.17582900	1.38444700
H	1.03764300	-4.36782300	0.68102700