Supporting Information for

Theoretical Investigation on Borane Compounds Mimicking Transition Metals for N_2 Fixation and Activation

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1. Validations for Computational Methods

Table S1. Relative Gibbs free energies (ΔG) at 298.15 K, and relative potential energies (ΔE) of N_2 with simple silylborane compounds. (Unit: kcal/mol)

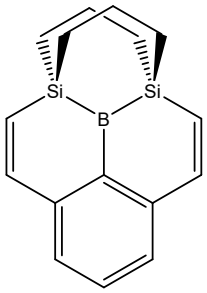
ΔG	H_2BSiH_3	$H_3C(H)BSiH_3$	$(H_3C)_2BSiH_3$	$HB(SiH_3)_2$	$H_3CB(SiH_3)_2$	$B(SiH_3)_3$
$N_2\cdots BR_3$	-	6.3	-	5.2	6.7	3.9
$[N_2\cdots BR_3]^{\neq}$	-	11.5	15.3	5.2	12.2	6.2
$N_2{:}BR_3$	2.1	10.5	15.6	-1.4	7.9	-4.8
$R_3B\cdots N_2{:}BR_3$	11.0	-	-	7.9	19.1	3.6
$[R_3B\cdots N_2{:}BR_3]^{\neq}$	10.9	24.2	33.6	8.5	22.2	6.2
$R_3B{:}N_2{:}BR_3$	5.9	22.9	33.4	-2.4	13.7	-10.8
ΔE	H_2BSiH_3	$H_3C(H)BSiH_3$	$(H_3C)_2BSiH_3$	$HB(SiH_3)_2$	$H_3CB(SiH_3)_2$	$B(SiH_3)_3$
$N_2\cdots BR_3$	-	-2.1	-	-3.3	-2.3	-3.2
$[N_2\cdots BR_3]^{\neq}$	-	-0.1	3.5	-3.3	-0.1	-3.0
$N_2{:}BR_3$	-10.9	-3.4	2.5	-14.4	-7.0	-18.1
$R_3B\cdots N_2{:}BR_3$	-13.8	-	-	-18.7	-11.4	-22.4
$[R_3B\cdots N_2{:}BR_3]^{\neq}$	-13.0	-2.0	7.4	-17.2	-7.3	-21.4
$R_3B{:}N_2{:}BR_3$	-20.6	-6.2	5.7	-29.8	-15.9	-38.4

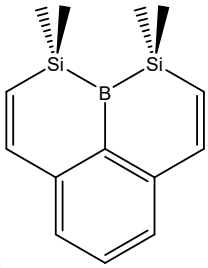
Table S2 Relative potential energies of G4 and 11 DFT methods for the reaction between N_2 and $H_3CB(SiH_3)_2$. (Unit: kcal/mol)[a]

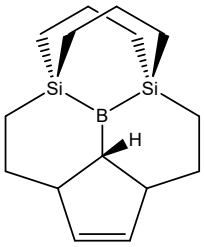
	$N_2\cdots BR_3$	$[N_2\cdots BR_3]^{\neq}$	$N_2{:}BR_3$	$R_3B\cdots N_2{:}BR_3$	$[R_3B\cdots N_2{:}BR_3]^{\neq}$	$R_3B{:}N_2{:}BR_3$
G4	-2.5	-1.4	-6.7	-10.6	-9.0	-16.8
BLYP	1.6	3.5	-5.6	0.7	-1.5	-14.0
PBE	-0.2	-0.9	-14.1	-12.5	-16.3	-32.1
B3LYP	0.8	3.1	-4.3	0.5	0.1	-10.6
ωB97XD	-1.5	0.5	-5.5	-8.7	-5.5	-13.5
M06-L	-2.6	-1.9	-11.9	-16.5	-15.5	-26.6
MN15-L	-3.2	-1.0	-9.6	-18.6	-14.1	-22.4
M06	-2.3	-0.6	-7.7	-12.4	-10.0	-18.7
M06-2X	-2.3	-0.1	-7.0	-11.4	-7.3	-15.9
MN15	-2.7	-2.2	-10.4	-17.4	-14.5	-24.4
PBE0DH	-0.9	-0.6	-9.2	-8.9	-9.4	-20.9
DSDPBEP86	-2.7	-2.3	-8.8	-13.2	-12.7	-22.0

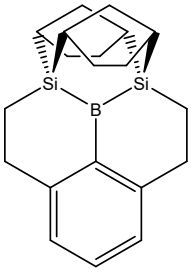
[a] Single-point energy calculations were performed on geometries optimized with the M06-2X/AVTZ method.

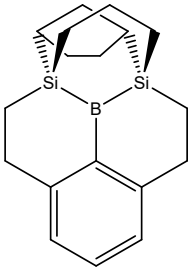
2. Structures of designed silylborane compounds

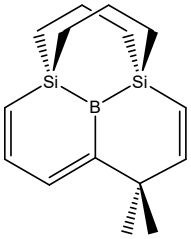
A-1: 

A-2: 

B-1: 

C-1: 

C-2: 

C-3: 

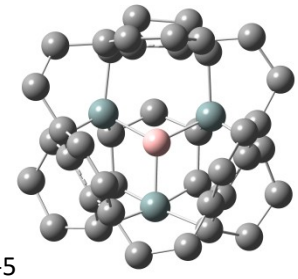
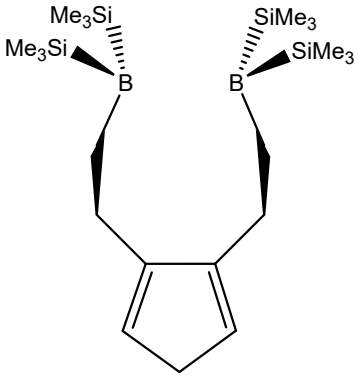
C-5 

Figure S1. Selected structures of designed silylborane compounds with single B center optimized by the M06-2X/SBS method in gas phase. H atoms were omitted for clarity.

Ring5-1:



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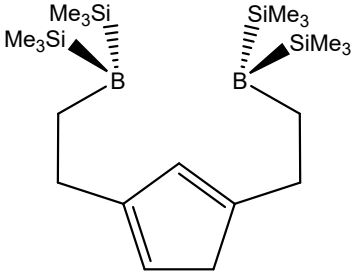

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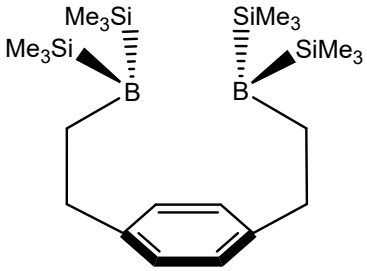

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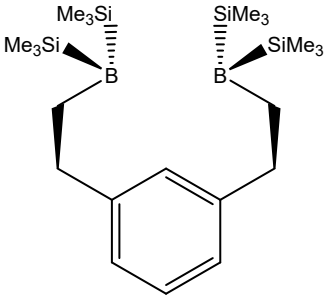
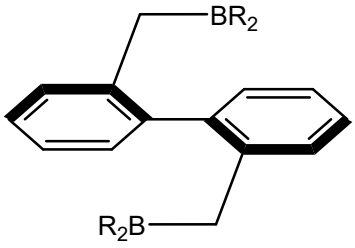


Biphenyl(R=SiH_3/$SiMe_3$):



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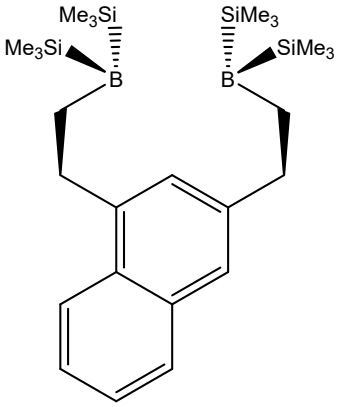

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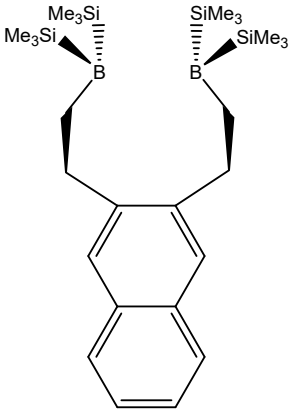

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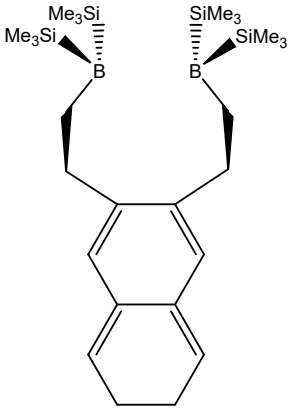

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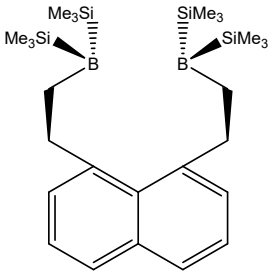
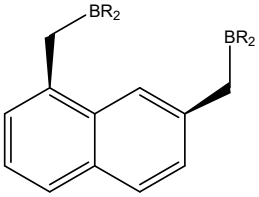


Naphthalene-5(R=SiH_3/$SiMe_3$):



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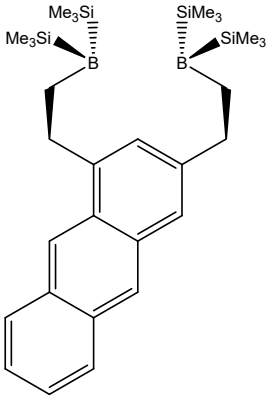

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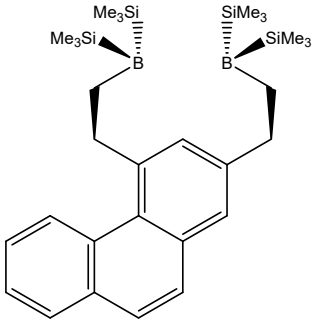

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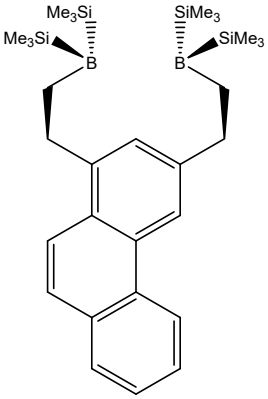

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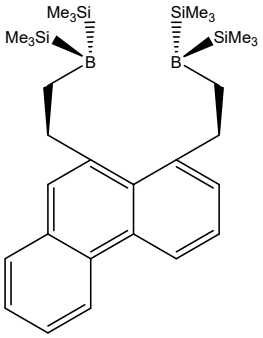

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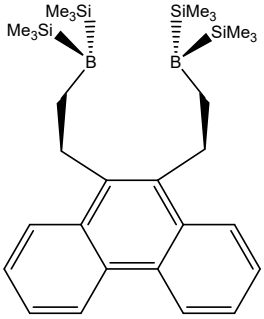
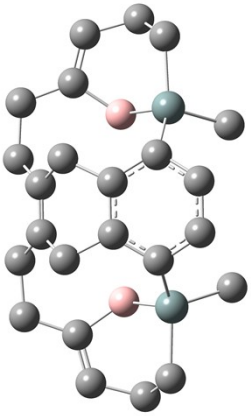
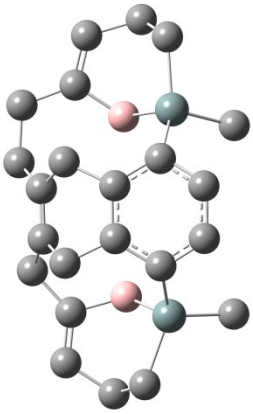
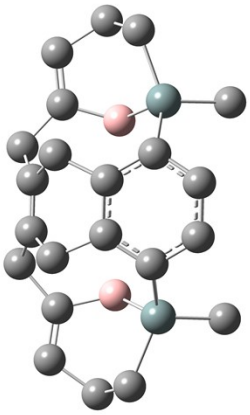


Cage-1:  Cage-2:  Cage-3: 

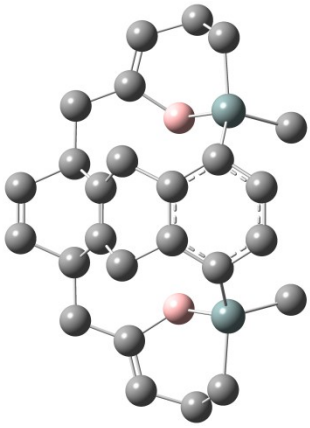
Cage-4: 

Figure S2. Selected structures of designed silylborane compounds with double B centers optimized by the M06-2X/SBS method in gas phase. H atoms were omitted for clarity.

Table S3. Relative Gibbs free energies (ΔG) at 298.15 K, and relative potential energies (ΔE) of N_2 with eight recommended silylborane compounds. (Unit: kcal/mol)

ΔG	$N_2\cdots BR_3$	$[N_2\cdots BR_3]^{\neq}$	$N_2{:}BR_3$	$R_3B\cdots N_2{:}BR_3$	$[R_3B\cdots N_2{:}BR_3]^{\neq}$	$R_3B{:}N_2{:}BR_3$
B-1	-	13.6	3.0	6.9	11.8	0.8
B-2	-	13.4	3.2	7.3	12.3	0.4
C-4	-	13.9	2.4	7.3	11.4	-6.7
C-5	-	22.8	-5.0	-	-	-
$B(SiPhMe_2)_3$	-	6.6	-6.3	1.3	7.7	-3.1
$B(SiPhMe_2)_2SiMe_3$	3.5	4.5	-8.4	-0.8	1.2	-13.3
Ring6-1	-	14.4	6.6	-	10.2	-0.1
Ring6-2	-	9.5	3.8	-	8.6	0.7
ΔE	$N_2\cdots BR_3$	$[N_2\cdots BR_3]^{\neq}$	$N_2{:}BR_3$	$R_3B\cdots N_2{:}BR_3$	$[R_3B\cdots N_2{:}BR_3]^{\neq}$	$R_3B{:}N_2{:}BR_3$
B-1	-	2.4	-11.6	-22.4	-19.1	-32.5
B-2	-	2.4	-10.8	-20.4	-17.3	-30.6
C-4	-	2.6	-11.6	-21.1	-19.3	-37.5
C-5	-	11.6	-20.3	-	-	-
$B(SiPhMe_2)_3$	-	0.2	-17.6	-23.0	-20.0	-35.2
$B(SiPhMe_2)_2SiMe_3$	-5.3	-5.4	-23.2	-34.4	-34.3	-50.8
Ring6-1	-	3.2	-5.1	-	-3.3	-16.5
Ring6-2	-	1.5	-7.4	-	-5.5	-14.8

Table S4. Binding Gibbs free energies (ΔG_{bin}) at 298.15 K and binding potential energies (ΔE_{bin}) of N_2 with single-boron-center silylborane compounds. (unit: kcal/mol)

	N_2:BR_3		R_3B:N_2:BR_3	
BR_3	ΔG_{bin}	ΔE_{bin}	ΔG_{bin}	ΔE_{bin}
$(SiMe_3)_2BMe$	4.5	-10.0	4.8	-27.4
$(SiEt_3)_2BMe$	4.7	-9.7	4.5	-27.7
$(Si(iPr)_3)_2BMe$	15.2	-0.3	-	-
$(SiPh_3)_2BMe$	8.9	-6.1	1.7	-37.6
$(SiPhMe_2)_2BMe$	3.7	-10.9	7.1	-27.3
$(SiPh_3)_2BCF_3$	-0.6	-15.0	-4.1	-42.6
$(SiPh_3)_2BCCl_3$	7.9	-6.1	33.1	-7.1
$(SiPh_3)_2BC(CN)_3$	3.9	-9.5	22.7	-16.3
$(SiPh_3)_2BC_6F_5$	4.9	-10.7	14.8	-27.0
$(SiMe_3)_3B$	-8.1	-23.4	-22.0	-55.4
$(SiEt_3)_3B$	-5.4	-20.1	-11.1	-48.9
$(SiPh_3)_3B$	7.3	-6.4	54.1	12.6
$(SiPhH_2)_3B$	-6.6	-20.3	-20.1	-56.8
$(SiPhMe_2)_3B$	-6.3	-17.6	-3.1	-35.2
$(SiPhMe_2)_2BSiMe_3$	-8.4	-23.2	-13.3	-50.8
A-1	1.9	-11.4	-7.5	-35.5
A-2	-	-	6.5	-23.5
B-3	4.5	-9.3	1.9	-28.5
C-1	7.0	-2.4	18.9	-12.9
C-2	1.4	-12.2	-4.1	-33.2
C-3	1.6	-12.1	-8.9	-39.3
C-5	-5.0	-20.3	-	-

Table S5. Binding Gibbs free energies (ΔG_{bin}) at 298.15 K and binding potential energies (ΔE_{bin}) of N_2 with double-boron-center silylborane compounds. (unit: kcal/mol)

	$R_3B:N_2:BR_3$	
$(R_3B)_2$	ΔG_{bin}	ΔE_{bin}
$(Me_3Si)_2B(CH_2)_3B(SiMe_3)_2$	15.6	-2.7
$(Me_3Si)_2B(CH_2)_4B(SiMe_3)_2$	10.0	-9.9
$(Me_3Si)_2B(CH_2)CH=CH(CH_2)B(SiMe_3)_2$	12.2	-3.6
$(Me_3Si)_2B(CH_2)_5B(SiMe_3)_2$	6.6	-14.9
$(H_3Si)_2B(CH_2)_6B(SiH_3)_2$	11.0	-7.2
$(Me_3Si)_2B(CH_2)_6B(SiMe_3)_2$	4.8	-18.4
$(Me_3Si)_2B(CH_2)_7B(SiMe_3)_2$	4.9	-20.1
Ring5-1	5.0	-11.7
Ring5-2	8.6	-9.1
Ring6-3	7.0	-11.0
Ring6-2-Ph	22.8	1.4
Biphenyl($R=SiH_3$)	10.5	-3.4
Biphenyl($R=SiMe_3$)	5.8	-12.9
Naphthalene-1	3.0	-14.5
Naphthalene-2	3.1	-14.9
Naphthalene-3	2.8	-14.2
Naphthalene-4	7.4	-8.1
Naphthalene-5($R=SiH_3$)	13.5	-8.1
Naphthalene-5($R=SiMe_3$)	8.9	-7.8
Anthracene-1	3.2	-13.0
Phenanthrene-1	3.2	-15.7
Phenanthrene-2	2.7	-13.6
Phenanthrene-3	6.9	-9.3
Phenanthrene-4	2.9	-12.7
Cage-1	-3.5	-21.1
Cage-2	-17.2	-34.4
Cage-3	-25.6	-43.1
Cage-4	1.7	-15.7

3. Cartesian coordinates of recommended silylborane compounds

B-1:

B	0.16383200	0.00000300	-0.37297900
C	1.61834300	-0.00002800	-0.87227800
Si	-0.92330500	1.57332200	-0.06005000
Si	-0.92336700	-1.57328200	-0.06009000
C	-2.26559900	1.34478100	-1.41074900
C	0.39722600	2.94707400	-0.16917000
C	-1.60980300	1.32762700	1.70877900
C	0.39712300	-2.94708000	-0.16914800
C	-2.26561100	-1.34468500	-1.41082600
C	-1.61002400	-1.32764300	1.70868400
C	-2.35542900	0.00004600	1.99369100
C	-3.04631700	0.00005000	-1.35870200
C	1.70892100	2.32087900	0.39474700
C	1.70882400	-2.32091300	0.39478500
C	2.43910200	1.27472900	-0.48862000
C	2.43905200	-1.27480900	-0.48859700
C	3.62695200	-0.66733800	0.22154300
C	3.62698000	0.66722500	0.22152900
H	1.44181100	-0.00003400	-1.96609400
H	-2.99946900	2.16007100	-1.40345300
H	-1.74776900	1.41962100	-2.37842700
H	0.16040700	3.86351400	0.38209900
H	0.54837800	3.23867200	-1.21734700
H	-2.26827400	2.16131000	1.98453700
H	-0.74432500	1.40105800	2.38385600
H	0.16025700	-3.86349400	0.38214300
H	0.54829300	-3.23871700	-1.21731200
H	-2.99949100	-2.15996800	-1.40355700
H	-1.74778700	-1.41948800	-2.37850900
H	-2.26870200	-2.16123200	1.98423600
H	-0.74465200	-1.40134800	2.38386600
H	-2.63560300	0.00002900	3.05473800
H	-3.30392200	0.00014800	1.44947800
H	-3.74110400	0.00007900	-2.20799400
H	-3.68368500	0.00002300	-0.47057200
H	2.42787500	3.12161200	0.61061200
H	1.49497000	1.84513700	1.36516500
H	2.42774800	-3.12166200	0.61068900
H	1.49486400	-1.84513600	1.36518500
H	2.78119800	1.80126800	-1.39291800
H	2.78113000	-1.80137800	-1.39288300
H	4.39680200	-1.28101200	0.68267400
H	4.39685400	1.28087700	0.68264800

B-2:

B	-0.44722900	0.36454000	0.00000000
C	-0.85153400	1.85064900	0.00000000
Si	-0.15563700	-0.71754000	1.58853900
Si	-0.15563700	-0.71754000	-1.58853900
C	-1.36987200	-2.16993000	1.32516200
C	-0.20654300	0.60450500	2.95907800
C	1.53773500	-1.54670800	1.30290400
C	-0.20654300	0.60450500	-2.95907800
C	-1.36987200	-2.16993000	-1.32516200
C	1.53773500	-1.54670800	-1.30290400
C	1.54465600	-2.39021000	0.00000000
C	-1.02959200	-2.92344200	0.00000000
C	0.43068600	1.87514200	2.31811500
C	0.43068600	1.87514200	-2.31811500
C	-0.41801800	2.64849300	1.27454300
C	-0.41801800	2.64849300	-1.27454300
C	0.35089400	3.79886000	-0.66713400
C	0.35089400	3.79886000	0.66713400
H	-1.95445200	1.74856100	0.00000000
H	-1.31156800	-2.89374800	2.14851000
H	-2.40937200	-1.82044300	1.29139400
H	0.33240200	0.34209700	3.87554000
H	-1.24408800	0.81708300	3.24880100
H	1.76916100	-2.20812200	2.14924000
H	2.34209000	-0.80109400	1.26479700
H	0.33240200	0.34209700	-3.87554000
H	-1.24408800	0.81708300	-3.24880100
H	-1.31156800	-2.89374800	-2.14851000
H	-2.40937200	-1.82044300	-1.29139400
H	1.76916100	-2.20812200	-2.14924000
H	2.34209000	-0.80109400	-1.26479700
H	2.48799000	-2.95420000	0.00000000
H	-1.66781200	-3.81790300	0.00000000
H	0.69505900	2.58522000	3.11197000
H	1.38306500	1.60027600	1.83693700
H	0.69505900	2.58522000	-3.11197000
H	1.38306500	1.60027600	-1.83693700
H	-1.30117000	3.03603200	1.80535900
H	-1.30117000	3.03603200	-1.80535900
H	0.85098300	4.54378800	-1.28103200
H	0.85098300	4.54378800	1.28103200
C	0.42128700	-3.44589300	0.00000000
H	0.55382300	-4.09060000	0.87944100
H	0.55382300	-4.09060000	-0.87944100

C-4:

B	0.08735600	-0.02130000	-0.17024700
C	-1.43257400	0.03504000	-0.42367400
Si	1.19921300	-1.58274900	0.09066600

Si	1.30172400	1.49475400	-0.20807700
C	2.50352900	-1.55128000	-1.30520300
C	-0.07456900	-2.94278400	-0.05386100
C	1.95402300	-1.19964300	1.81010700
C	0.11219600	2.88097800	-0.63098100
C	2.51462300	1.07463100	-1.62557900
C	2.16406200	1.44369700	1.50078800
C	2.81585600	0.08785400	1.88800900
C	3.31338400	-0.24239300	-1.47840200
C	-1.37306400	-2.61451100	-0.21157000
C	-1.21075200	2.62564500	-0.57665800
C	-2.20741400	-1.31188300	-0.15708700
C	-2.00742200	1.44012600	0.02316100
C	-2.84859500	-1.37283900	1.24465900
C	-3.31700200	-1.50992500	-1.21165300
H	3.20601700	-2.38800800	-1.20248300
H	1.94203300	-1.74766000	-2.22981800
H	0.14018500	-4.01133100	-0.08154800
H	2.55565400	-2.04024000	2.17745100
H	1.10786100	-1.11307500	2.50779300
H	0.39201400	3.85367100	-1.03589700
H	3.22245900	1.89830600	-1.78364900
H	1.90553100	1.02716900	-2.54002800
H	2.92762200	2.22752000	1.57987900
H	1.40028800	1.70010700	2.24774900
H	3.17252800	0.18336800	2.92123900
H	3.71796900	-0.05775100	1.28770600
H	3.93878600	-0.35613600	-2.37288400
H	4.01801700	-0.14054600	-0.64838600
H	-2.06286400	-3.45646600	-0.33292500
H	-1.87960700	3.42323300	-0.91277000
H	-3.65723200	-0.64640700	1.35590300
H	-2.10208000	-1.19779100	2.02546100
H	-3.27839000	-2.36598200	1.41197700
H	-4.03065600	-0.68575500	-1.21116500
H	-3.87554400	-2.43244900	-1.02052300
H	-2.88311800	-1.58279000	-2.21464100
C	-1.90488400	1.63473900	1.55510700
H	-2.62944400	1.03057800	2.10265100
H	-0.89958300	1.38052200	1.91044800
H	-2.08703000	2.68349200	1.81039600
C	-3.47158500	1.66434300	-0.38872800
H	-3.59582400	1.57803200	-1.47343500
H	-4.14680700	0.95468700	0.09319500
H	-3.79372800	2.66840900	-0.09203600
H	-1.35383200	0.10094700	-1.53527200

C-5:

B	-0.82993900	0.00188800	0.00027100

Si	-1.33761800	-1.66634100	-0.77410800
C	-3.25314100	1.27285100	-0.80583200
C	-3.73749300	-0.05586500	-1.43471200
C	-3.73401200	1.28458600	0.66345300
C	-3.25489100	0.07396200	1.50061600
C	-3.25888400	-1.32403400	-0.69088500
C	-3.73920400	-1.20269100	0.77546400
C	-0.74002100	-3.07685100	0.41022400
C	-0.73114000	1.18592400	-2.87046300
C	-0.53736700	-1.36969100	2.75128100
C	-0.72728400	1.89557500	2.46119500
C	-0.53986200	-1.69593300	-2.56239400
C	-0.52789800	3.06864400	-0.18841500
C	-1.54097800	-3.52001500	1.65863500
C	-1.53358000	0.32944900	-3.87992600
C	-1.52065200	-2.56343900	2.87690300
C	-1.52499000	3.20072600	2.22259300
C	-1.51924200	-1.20398100	-3.66081600
C	-1.50615200	3.77760500	0.78509000
H	-3.76624600	2.09347400	-1.32974500
H	-3.49639400	-0.10141400	-2.49370600
H	-4.83847400	-0.05209700	-1.38031900
H	-4.83509000	1.23882100	0.63755900
H	-3.49122400	2.22391700	1.15381000
H	-3.76931000	0.11915700	2.47248600
H	-3.77599600	-2.18640900	-1.13819900
H	-3.49964900	-2.09772800	1.34390600
H	-4.84011500	-1.15398000	0.74767500
H	-0.63562700	-3.98708900	-0.18428100
H	-0.62236900	2.15553800	-3.36123500
H	-0.27097500	-1.06542700	3.76921500
H	-0.62043500	1.83555500	3.54647200
H	-0.27701300	-2.73053600	-2.80766600
H	-0.26122800	3.79712500	-0.96163000
H	-1.07506600	-4.45930400	1.97679600
H	-2.56621300	-3.78245500	1.38130500
H	-2.55729100	0.70459700	-3.97028300
H	-1.06532700	0.52197400	-4.85163800
H	-1.21900200	-3.14989400	3.75095700
H	-2.52655400	-2.19460300	3.10252500
H	-1.05553300	3.94450700	2.87600900
H	-2.54971700	3.09475100	2.59079800
H	-2.52694700	-1.58015800	-3.45634700
H	-1.21731000	-1.66863600	-4.60518100
H	-2.51308100	3.79232700	0.35536800
H	-1.20044100	4.82663700	0.85539000
Si	-1.33230900	0.16691600	1.83343300
Si	-1.33046000	1.50835100	-1.05791000
C	0.74435000	2.64302700	0.54214300

C	0.64480500	2.03661600	1.82736100
C	1.79250200	1.56433500	2.48790900
C	3.03680400	1.73884600	1.88545800
C	3.14399800	2.37129700	0.65954400
C	2.01768900	2.83472400	-0.02599800
H	3.93044700	1.37862000	2.39029300
H	4.12513100	2.51618300	0.21528100
C	0.63943300	0.56217700	-2.67892000
C	0.73494600	-0.85434900	-2.56191500
C	2.00674800	-1.44607000	-2.44679600
C	3.13567500	-0.62410900	-2.39015700
C	3.03248100	0.75409200	-2.45471800
C	1.78974400	1.36683300	-2.60260500
H	4.11560500	-1.08427600	-2.29546300
H	3.92806800	1.36871600	-2.39666100
C	0.63324700	-2.60367000	0.85122000
C	0.73428600	-1.79425700	2.01910800
C	2.00853400	-1.40251200	2.47051700
C	3.13440900	-1.76816700	1.72751100
C	3.02585600	-2.51270400	0.56637100
C	1.78055500	-2.94316200	0.11294200
H	4.11621300	-1.45914200	2.07616000
H	3.91915000	-2.77242000	0.00265700
C	1.73861700	2.87921400	-2.62952800
C	2.26101700	3.55623200	-1.33586900
C	2.24560600	-2.94192700	-2.41752600
H	3.32710600	-3.09145500	-2.48973800
C	1.72336700	-3.72216900	-1.18338400
H	2.32901500	-4.63094800	-1.08604300
C	2.25320200	-0.62982800	3.75063700
C	1.73681900	0.83126500	3.81078900
H	2.34714500	1.36749200	4.54707400
H	3.33513600	-0.62174400	3.91364100
H	2.34752400	3.24658900	-3.46404900
H	3.34311600	3.68983400	-1.42754100
H	0.71141500	-4.06418800	-1.38964800
H	1.82138700	-3.40782400	-3.31598600
H	1.82894900	-1.17335400	4.60435200
H	0.72622600	0.82781300	4.21367400
H	1.84017900	4.56871400	-1.29090700
H	0.72854400	3.23302000	-2.82491800

$B(SiPhMe_2)_3$:

B	0.00323500	0.00009800	1.66960900
Si	-0.90409200	1.80670800	1.53504400
Si	2.02099500	-0.11710300	1.52946200
Si	-1.10760800	-1.68894800	1.53533500
C	-1.82219000	-1.59341100	-0.21506100
C	-0.98744800	-1.77207500	-1.33015500

C	-3.16498600	-1.25992700	-0.44877300
C	-1.46803800	-1.59705600	-2.62577900
H	0.05935900	-2.03538100	-1.19280000
C	-3.65260200	-1.08648000	-1.74337000
H	-3.84410300	-1.12962300	0.39113500
C	-2.80032900	-1.24556700	-2.83464600
H	-0.79437000	-1.72680500	-3.46780600
H	-4.69483100	-0.82571300	-1.89993500
H	-3.17613600	-1.10324400	-3.84329900
C	-0.46930300	2.37390500	-0.21805400
C	0.49101400	3.36866900	-0.45717900
C	-1.04607000	1.73876200	-1.32983500
C	0.88067300	3.70132700	-1.75388300
H	0.94721100	3.89281100	0.37998400
C	-0.65850800	2.06450800	-2.62756800
H	-1.79786800	0.96497900	-1.18828300
C	0.31228100	3.04116000	-2.84182600
H	1.62788100	4.47242000	-1.91464500
H	-1.11126700	1.54464500	-3.46688000
H	0.62016900	3.29314200	-3.85208600
C	2.28994700	-0.78069100	-0.22310600
C	2.67276700	-2.10968400	-0.46026900
C	2.02322200	0.03327500	-1.33596600
C	2.76305900	-2.61632300	-1.75606100
H	2.90273600	-2.76413700	0.37783400
C	2.10853500	-0.46812100	-2.63273700
H	1.72802600	1.07116700	-1.19580500
C	2.47079300	-1.79697000	-2.84501900
H	3.05893400	-3.64870300	-1.91542800
H	1.88121200	0.18139000	-3.47304900
H	2.53302200	-2.19166700	-3.85459000
C	-2.78521700	1.82215100	1.70658700
H	-3.25605800	1.13386900	0.99808100
H	-3.09686800	1.54295400	2.71819100
H	-3.16307900	2.82915700	1.50064300
C	-0.20943000	3.05460000	2.77407900
H	0.87520800	3.16072900	2.68900900
H	-0.66611000	4.03666400	2.60925300
H	-0.43777200	2.74855600	3.79990100
C	-2.53144400	-1.71435300	2.77939800
H	-3.15316900	-2.60141300	2.61583000
H	-2.14858600	-1.75974100	3.80385300
H	-3.16709300	-0.82883300	2.69753800
C	-0.17905500	-3.32555200	1.70137300
H	0.64974000	-3.38841100	0.98961800
H	0.22243900	-3.45671500	2.71132700
H	-0.86287000	-4.15621600	1.49728200
C	2.75884000	-1.33968700	2.76905300
H	2.30860800	-2.33253000	2.68795800

H	3.83717800	-1.43523200	2.60104800
H	2.61117200	-0.98645300	3.79450200
C	2.97421900	1.50534000	1.69500000
H	4.03480600	1.32943200	1.48649100
H	2.61103900	2.25563100	0.98606000
H	2.89075100	1.91679400	2.70602300

$B(SiPhMe_2)_2SiMe_3$:

B	0.16315600	1.05518100	0.42767000
Si	2.17629600	1.18512500	0.40647800
Si	-0.67242800	-0.39950200	1.55877600
Si	-0.99846300	2.18553000	-0.78418400
C	2.62358400	-0.49849700	-0.33128200
C	3.49174100	-1.39488300	0.30576200
C	1.98667100	-0.92888100	-1.50703900
C	3.71509900	-2.67138500	-0.20622600
H	3.99313000	-1.09970100	1.22498500
C	2.20013700	-2.20609100	-2.02217700
H	1.31050600	-0.25502800	-2.03345400
C	3.06431300	-3.08129700	-1.36771100
H	4.39191300	-3.34950300	0.30443200
H	1.69385500	-2.51734900	-2.93100300
H	3.23140800	-4.07833800	-1.76263200
C	-2.13923200	-1.09560900	0.59424500
C	-3.45460300	-1.05107300	1.07191900
C	-1.92923700	-1.59641000	-0.70073500
C	-4.52426100	-1.47519300	0.28444300
H	-3.65474000	-0.66299400	2.06834900
C	-2.99211100	-2.01814000	-1.49559900
H	-0.91505400	-1.65353300	-1.09858500
C	-4.29496900	-1.95202500	-1.00352400
H	-5.53689900	-1.42663300	0.67302400
H	-2.80720700	-2.39620400	-2.49660700
H	-5.12707500	-2.27478700	-1.62124700
C	2.93457100	2.55390600	-0.65216800
H	2.52901000	2.54433200	-1.66905900
H	2.73971400	3.54019700	-0.21885900
H	4.01910200	2.42043300	-0.72106200
C	2.91000500	1.31976300	2.14427800
H	2.56591600	0.51133500	2.79620600
H	4.00420400	1.28733900	2.10412400
H	2.62472800	2.26986000	2.60679300
C	-0.51050400	4.01103000	-0.63751100
H	-1.16102000	4.62191100	-1.27310600
H	-0.60899800	4.37918800	0.38880800
H	0.52319000	4.17037200	-0.95763600
C	-2.86151300	2.06109800	-0.49170400
H	-3.24848800	1.08948500	-0.81471000
H	-3.12444000	2.18860800	0.56378000

H	-3.37488400	2.84381300	-1.06186400
C	-1.30401600	0.40632900	3.15241800
H	-2.00275900	1.22305500	2.94633500
H	-1.81764900	-0.33501300	3.77400900
H	-0.47100900	0.81061000	3.73614000
C	0.45881300	-1.84552700	2.00040600
H	-0.08113500	-2.55417800	2.63738500
H	0.78612800	-2.37438400	1.09899600
H	1.35677500	-1.51599100	2.53265500
C	-0.68054100	1.64474400	-2.57547900
H	0.36492900	1.77849500	-2.87078600
H	-0.95891700	0.59688700	-2.72917600
H	-1.29935800	2.25451600	-3.24346000

Ring6-1:

C	3.10030100	3.77810300	-1.13889500
C	3.99010300	3.15776100	-0.26669700
C	3.50069200	2.32143600	0.73172500
C	2.13236300	2.07129900	0.87680800
C	1.23331600	2.71181400	0.00433900
C	1.73554500	3.55557500	-0.99119600
H	1.03433900	4.04409300	-1.66362400
C	-0.25434000	2.46445200	0.07857400
H	-0.77955900	3.28515300	-0.42411100
H	-0.59699700	2.47659600	1.11677600
C	1.66864800	1.16899100	2.00532200
H	1.85824400	1.68399800	2.95561500
H	0.58588300	1.01923400	1.95845000
C	2.36893400	-0.21677600	2.06514200
H	3.45488100	-0.05791800	2.08264100
H	2.10281400	-0.66043700	3.03431100
C	-0.65857000	1.13974300	-0.58757800
H	-0.04218700	0.31156200	-0.17384700
H	-0.34873400	1.15225700	-1.64372600
B	1.93663500	-1.15829100	0.85794600
B	-2.12592100	0.59242400	-0.42872600
H	3.46451800	4.43493400	-1.92201300
H	5.05815700	3.32853400	-0.35617200
Si	-3.51313400	1.35758400	0.84106500
Si	-2.66449500	-0.90768600	-1.68756100
Si	3.02766200	-1.21317100	-0.86140000
Si	0.46159800	-2.47063100	1.34962800
C	-4.86578800	0.08894000	1.21335600
H	-5.61140200	0.51824300	1.89136100
H	-5.38251100	-0.22148000	0.29917200
H	-4.45461900	-0.80850400	1.68835900
C	-3.34680600	-2.43918800	-0.80323100
H	-4.37881500	-2.26546700	-0.48509000
H	-3.34146100	-3.29528000	-1.48707500

H	-2.76414800	-2.71385200	0.08013400
C	-0.13250500	-3.69747500	0.04051600
H	0.69713900	-4.33853800	-0.27374100
H	-0.90942700	-4.34159200	0.46848500
H	-0.54797700	-3.22345100	-0.85235700
C	2.53632200	0.06448000	-2.16419200
H	1.50951000	-0.08065200	-2.51252800
H	2.63728800	1.08785000	-1.79276200
H	3.20186900	-0.05628600	-3.02709500
C	2.87807100	-2.91696200	-1.67789300
H	1.86373900	-3.08486700	-2.05501000
H	3.56800500	-2.98751700	-2.52614300
H	3.11754900	-3.72986300	-0.98364600
C	4.85626900	-0.94233300	-0.44443700
H	5.20956000	-1.64165800	0.32071500
H	5.47090400	-1.08604400	-1.33988100
H	5.02444600	0.07630600	-0.08180000
C	1.22238900	-3.53198500	2.73058800
H	1.49274100	-2.93413800	3.60604000
H	0.49969200	-4.29117600	3.04972300
H	2.12093900	-4.05446200	2.38569200
C	-1.03604000	-1.58364100	2.11264400
H	-1.59333100	-0.99240600	1.37583600
H	-1.73453000	-2.31410800	2.53714900
H	-0.72289500	-0.91007200	2.91818100
C	-2.86526000	1.98712000	2.50809700
H	-2.35211200	2.94800000	2.40811200
H	-3.70711000	2.12870200	3.19494200
H	-2.17392200	1.27649300	2.97317300
C	-4.31852900	2.81575000	-0.06804200
H	-4.75214900	2.50231100	-1.02310800
H	-5.12338300	3.23760500	0.54397200
H	-3.59489100	3.61227600	-0.26767800
C	-4.04193400	-0.25368100	-2.81609100
H	-4.32607700	-1.02052200	-3.54508300
H	-4.93430800	0.00784600	-2.23792800
H	-3.72522200	0.63516700	-3.37116700
C	-1.20288100	-1.39794100	-2.79349200
H	-1.40791900	-2.32441800	-3.34097000
H	-1.00222500	-0.61165100	-3.53013900
H	-0.28240300	-1.54606000	-2.21713800
H	4.19990300	1.85636700	1.42244400

Ring6-2:

C	-2.39935200	3.42361700	1.09070700
C	-2.85151300	2.77439900	-0.05215300
C	-1.94941600	2.14648700	-0.91875700
C	-0.58780800	2.20611400	-0.61582000
C	-0.11426300	2.85933500	0.52749800

C	-1.03702800	3.46214400	1.38236600
H	0.13101700	1.74351200	-1.28783400
H	-0.68572200	3.97286800	2.27507200
C	1.35864100	2.87216000	0.85856200
H	1.53951000	3.67239700	1.58472500
H	1.94114400	3.11911700	-0.03627000
C	-2.45422000	1.43729500	-2.15950500
H	-2.87084200	2.17577400	-2.85514400
H	-1.60592300	0.96927000	-2.67329700
C	-3.53843800	0.36752900	-1.85239300
H	-4.43653300	0.87187500	-1.47501700
H	-3.81021500	-0.10567900	-2.80672300
C	1.83526700	1.52639700	1.43505300
H	1.14718200	1.19078100	2.22306300
H	2.79154800	1.70225300	1.98170100
B	-2.93172700	-0.69387100	-0.84574600
B	2.39967800	0.36042300	0.54496100
H	-3.10939400	3.90708000	1.75508500
H	-3.91465100	2.75666800	-0.27836800
Si	3.36971000	0.68924300	-1.20843900
Si	2.82925500	-1.34641900	1.57101500
Si	-3.38023200	-0.78570500	1.12952000
Si	-1.47192800	-1.92260000	-1.55536100
C	3.94046000	-0.90822300	-2.04762800
H	4.61503400	-0.67105900	-2.87791000
H	4.47889400	-1.56330900	-1.35557200
H	3.09537700	-1.47157500	-2.45644200
C	2.35340900	-2.97469900	0.73407500
H	2.76667400	-3.05503800	-0.27625100
H	2.74304200	-3.80982900	1.32683100
H	1.26664300	-3.08853300	0.66806300
C	-1.40615500	-3.60537800	-0.69420800
H	-2.35057300	-4.15157200	-0.78228300
H	-0.61584600	-4.21891500	-1.14113200
H	-1.18073800	-3.49465400	0.37173600
C	-1.76483400	-0.39860400	2.04393200
H	-0.99463700	-1.13626800	1.78571100
H	-1.39074500	0.59550000	1.77014400
H	-1.90832900	-0.42459700	3.12985200
C	-3.95635400	-2.52469600	1.62222700
H	-3.19941300	-3.28832000	1.42916200
H	-4.18267700	-2.53639600	2.69426600
H	-4.86933300	-2.81045300	1.08950100
C	-4.74186700	0.38788200	1.72056200
H	-5.64908100	0.28260600	1.11584700
H	-5.00481300	0.15195500	2.75779300
H	-4.42306500	1.43165700	1.68269900
C	-1.63813000	-2.21884800	-3.41821500
H	-1.64423500	-1.27349900	-3.97160600

H	-0.80059900	-2.81945600	-3.78919700
H	-2.56392700	-2.75219800	-3.65744000
C	0.21302700	-1.09464400	-1.25572000
H	0.26074800	-0.66218700	-0.24664700
H	1.01301600	-1.83487100	-1.35623200
H	0.39389800	-0.29745500	-1.98189900
C	2.54843400	1.72790000	-2.56815600
H	2.21770800	2.71094700	-2.22142000
H	3.28723000	1.88704900	-3.36250100
H	1.69070600	1.22115200	-3.02194300
C	4.92371400	1.64130800	-0.66663800
H	5.49332700	1.08953900	0.08826600
H	5.58162100	1.81075200	-1.52619800
H	4.66148600	2.61774000	-0.24529500
C	4.71190800	-1.35614400	1.82603700
H	4.99999300	-2.21790700	2.43829400
H	5.25527100	-1.42003100	0.87805500
H	5.04781000	-0.45194500	2.34557900
C	2.04459400	-1.33846400	3.29403600
H	2.32042900	-2.24559300	3.84292100
H	2.38480700	-0.47769800	3.87986800
H	0.95171100	-1.29469200	3.24285400