Electronic Supplementary Material (ESI) for Dalton Transactions.

Electronic supplementary information

Postsynthetic Modifications of [2,2,2-(H)(PPh_3)$_2$-*closo*-2,1-$RhSB_8H_8$] (1) with Lewis Bases: Cluster Modular Tuning

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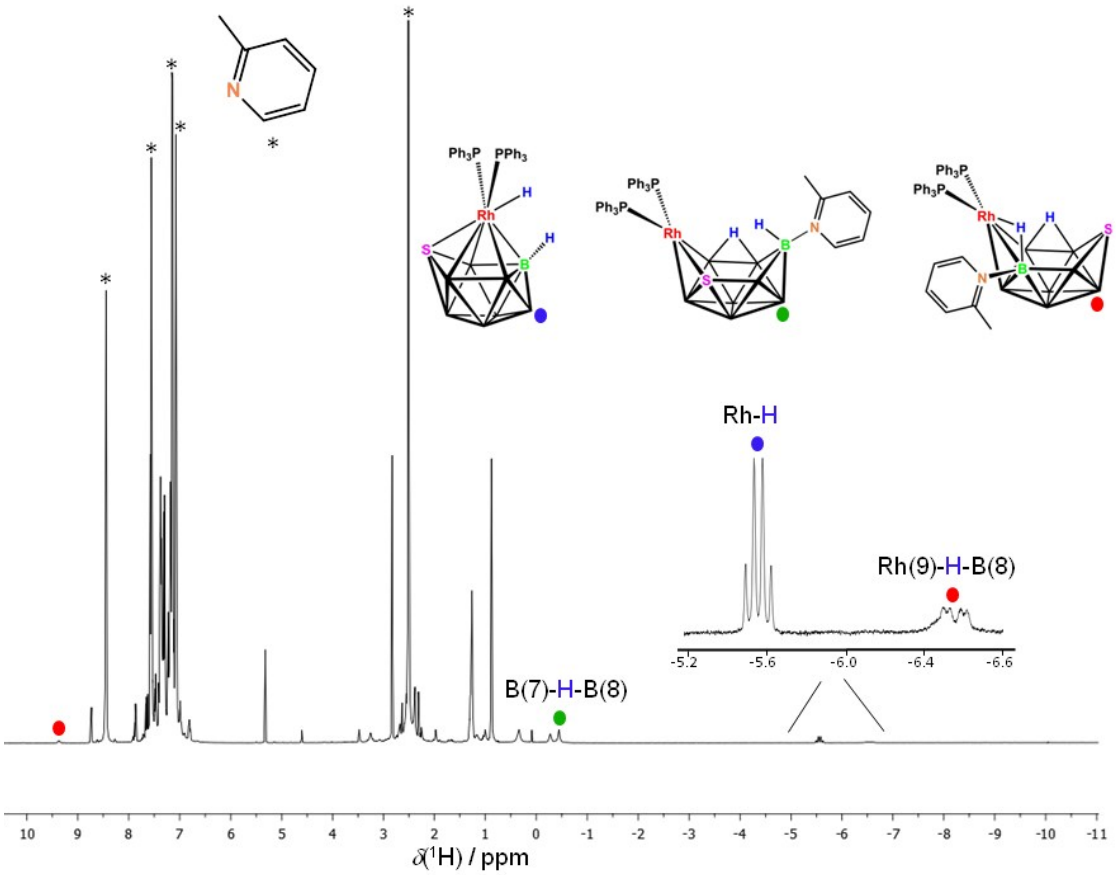

Figure S1. ^{1}H-{$^{11}B(BB)$} NMR data in CD_2Cl_2 at 283 K after the treatment of 10.4 mg of compound **1** (blue circles) with 10 equiv. of 2- Mepy (asterisk) to give the *arachno*-6,5-isomer (green circles) and the *arachno*-9,6-isomer (red circles) as major and minor products, respectively.

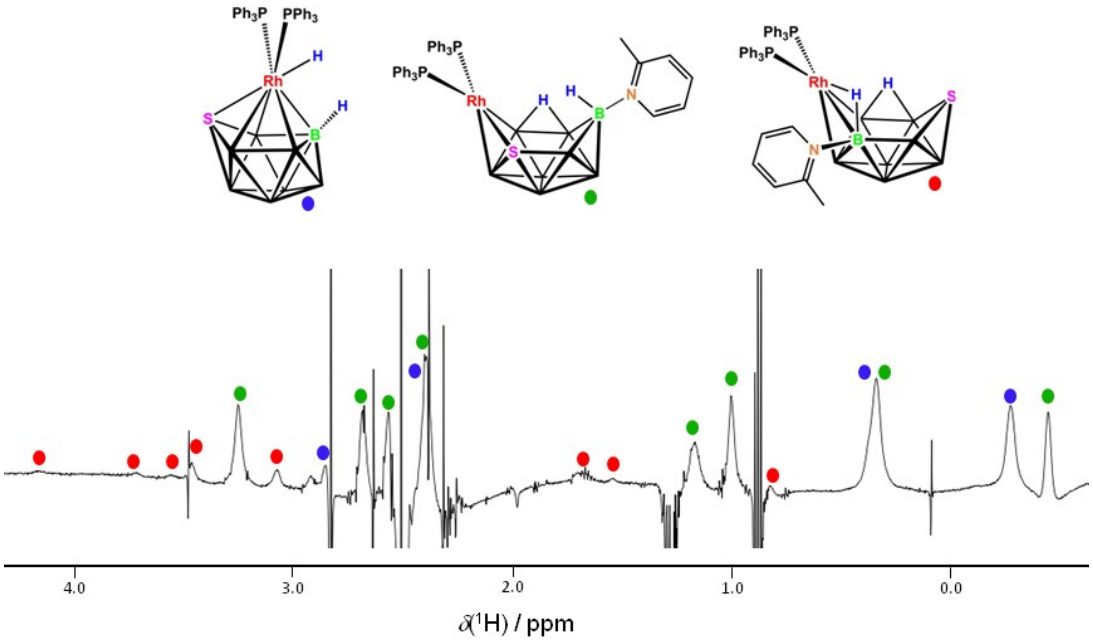

Figure S2. Spectrum that results when the ^{1}H-{^{11}B(off)} NMR spectrum is subtracted from the ^{1}H-{^{11}B(BB)} spectrum illustrated in Figure S1: only the resonances of the hydrogen atoms bound directly to boron atoms appear in the spectrum.

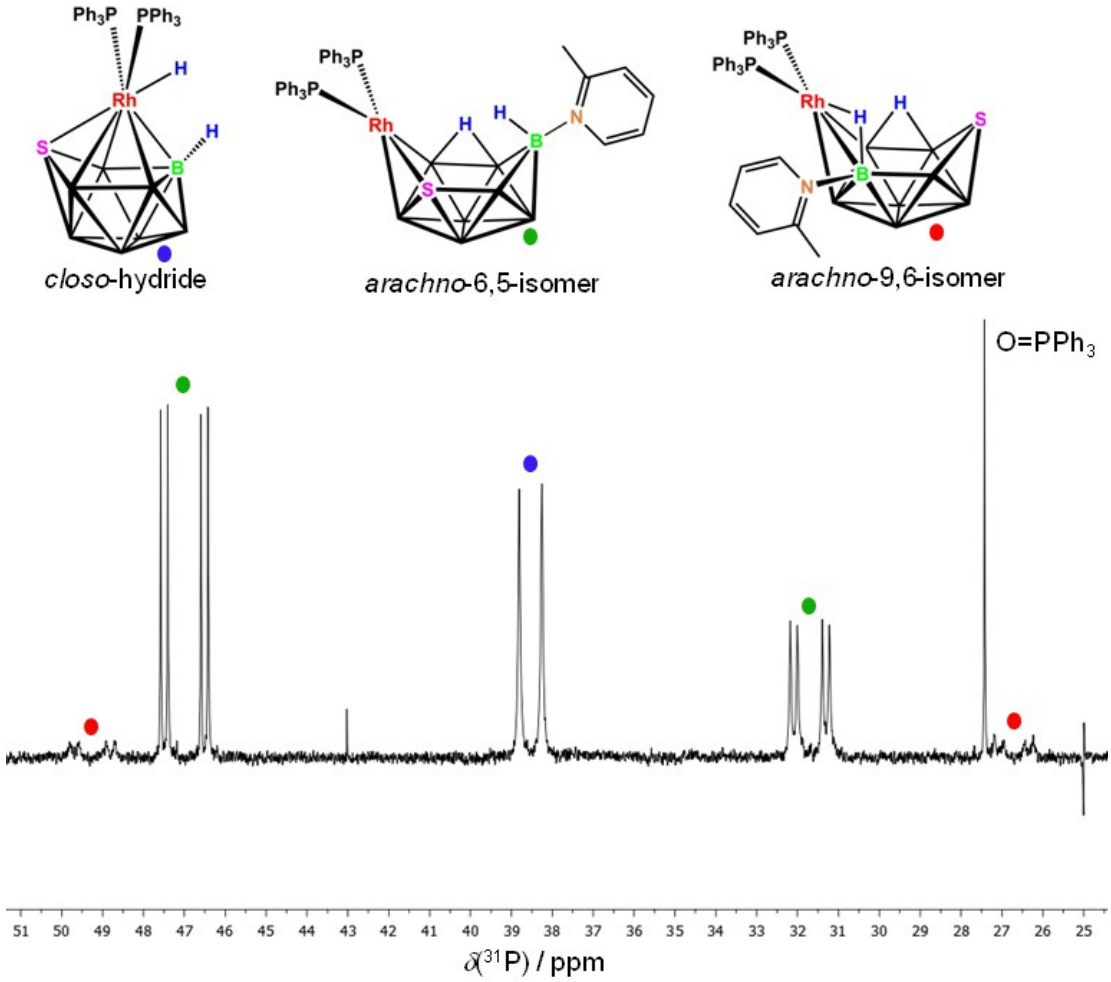

Figure S3. ^{31}P-{^{1}H} NMR spectrum in CD_2Cl_2 at 283 K after the treatment of 10.4 mg of compound **1** (blue circles) with 10 equiv. of 2- Mepy to give the *arachno*-6,5-isomer (green circles) and the *arachno*-9,6-isomer (red circles) as major and minor products, respectively.

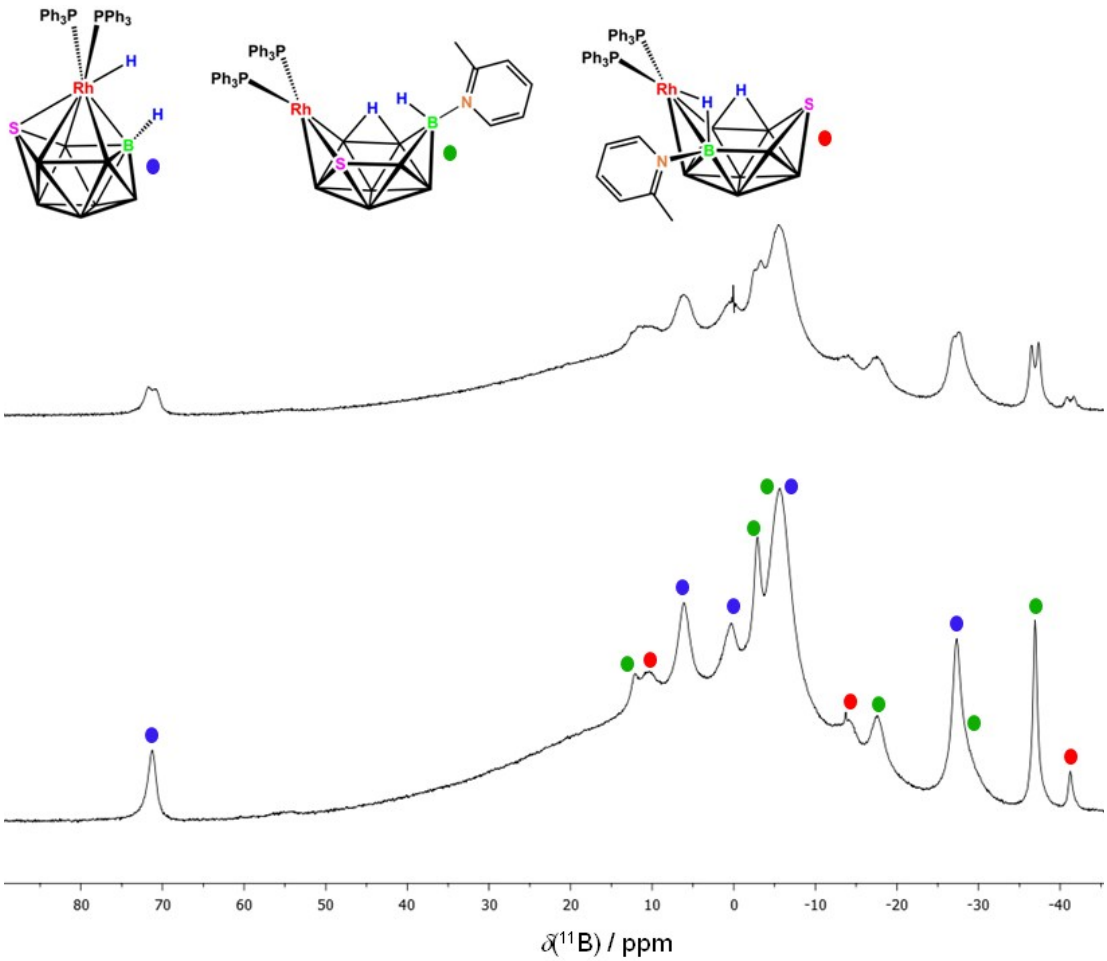

Figure S4. ^{11}B-{^{1}H} NMR data in CD_2Cl_2 at 283 K after the treatment of 10.4 mg of compound **1** (blue circles) with 10 equiv. of 2- Mepy to give the *arachno*-6,5-isomer (green circles) and the *arachno*-9,6-isomer (red circles) as major and minor products, respectively.

1. Tables of the optimized geometries (Cartesian coordinates, in Angstroms). Energies (in Hartrees) in parenthesis.

Table S1. [6,6-$(PPh_3)_2$-9-(PPh_3)-*arachno*-6,5-$RhSB_8H_9$] (**2**) (-3820.95865915)

	x	y	z
Rh	-1.08481200	-0.08041700	-1.04446500
S	0.41554300	1.21604000	-2.46181100
P	-1.94117400	1.87000800	0.04483400
P	-2.49095800	-1.70045400	-0.12845000
P	4.37067900	-0.23395900	-0.00688400
B	1.88589300	-1.96101400	-1.47556400

B	2.66114800	-0.80843600	-2.55059500
B	2.30263300	0.85222200	-2.20268600
B	2.62444400	-0.32747100	-0.87146100
B	-0.16902800	-0.66143100	-3.04426600
B	1.50578600	-0.02047000	-3.60514900
B	1.24188000	-1.70205400	-3.14400500
H	-0.46915400	-2.97615600	-1.80198300
H	2.36441700	-3.01940100	-1.20053000
H	1.34987800	-2.52381500	-4.00077800
H	-0.99299500	-0.64465200	-3.90641800
H	3.74868000	-1.08650700	-2.94837000
H	1.66606500	0.34755300	-4.72309200
H	2.99109500	1.79079500	-2.46432800
H	0.79434400	-1.74859900	-0.75244200
H	1.84263700	-0.02103500	-0.02185000
B	0.06458100	-1.91324400	-1.83721200
C	4.79219800	1.49524900	0.45373200
C	6.12685000	1.89769900	0.63053200
C	3.76413100	2.42947700	0.65034800
C	6.42428100	3.20786100	1.00722500
H	6.93532500	1.19294200	0.46154600
C	4.06691800	3.73946200	1.02430200
H	2.73036300	2.14326100	0.49034700
C	5.39454700	4.13035300	1.20475600
H	7.46052200	3.50828700	1.13685400
H	3.25904400	4.45300600	1.15510500
H	5.62808800	5.15288300	1.48946100
C	4.42392800	-1.18203600	1.56940500
C	5.13367800	-0.71930000	2.68903200
C	3.76080900	-2.41796900	1.64243800
C	5.18669500	-1.48283300	3.85573100
H	5.63998600	0.23950300	2.65580200
C	3.82557600	-3.18204900	2.80950200
H	3.19258800	-2.78057700	0.79268700
C	4.53706300	-2.71734200	3.91714000
H	5.73592400	-1.11077000	4.71641100
H	3.31203500	-4.13842500	2.84839800
H	4.58275400	-3.31217900	4.82557600
C	5.81405200	-0.80820400	-0.98362000
C	6.54723900	-1.94813200	-0.62944400
C	6.16691600	-0.09416100	-2.14195300
C	7.62160800	-2.36564800	-1.41898700
H	6.28400700	-2.51183900	0.25935600
C	7.24186200	-0.51259200	-2.92322200
H	5.59853500	0.78362400	-2.43485100
C	7.97107000	-1.64943400	-2.56345200
H	8.18284300	-3.25178300	-1.13559100
H	7.50483200	0.04506600	-3.81763700
H	8.80660400	-1.97614900	-3.17657300
C	-0.93786900	3.44393700	-0.07352400

C	-0.84200400	4.07546500	-1.32699500
C	-0.28545600	4.03389800	1.01870900
C	-0.11593100	5.25539400	-1.48217300
H	-1.34672700	3.64946700	-2.18825400
C	0.43626200	5.22198200	0.86309500
H	-0.35243700	3.58538400	2.00358000
C	0.52657100	5.83567900	-0.38620300
H	-0.05623500	5.72231400	-2.46154400
H	0.91303400	5.67364100	1.73010200
H	1.08556800	6.76008200	-0.50515900
C	-2.17814400	1.74003900	1.87807800
C	-3.33311100	2.12103900	2.57282600
C	-1.09496300	1.22142200	2.61072800
C	-3.39576600	2.00489300	3.96403700
H	-4.19709500	2.49238900	2.03398800
C	-1.15240500	1.11997000	4.00078700
H	-0.19983100	0.90047900	2.08272700
C	-2.30568100	1.51519200	4.68299900
H	-4.30426200	2.29761400	4.48373800
H	-0.29989100	0.72673800	4.54872600
H	-2.35620400	1.43223400	5.76549100
C	-3.53225300	2.51526500	-0.65647100
C	-4.12446400	3.71311700	-0.22011700
C	-4.11094300	1.83168100	-1.73562000
C	-5.29061200	4.18834700	-0.81981500
H	-3.66362300	4.28606600	0.57929100
C	-5.27339400	2.31381100	-2.34402200
H	-3.62997600	0.92771600	-2.10230700
C	-5.86991900	3.48699700	-1.88122900
H	-5.74013600	5.11320500	-0.46755700
H	-5.70569900	1.77418200	-3.18255900
H	-6.77368000	3.86333300	-2.35346900
C	-3.85747200	-1.27010900	1.07391400
C	-4.99327700	-0.60447300	0.58102100
C	-3.82597400	-1.60591200	2.43468500
C	-6.06261400	-0.28900300	1.41800200
H	-5.05466800	-0.34542800	-0.47024500
C	-4.89798100	-1.29032600	3.27436100
H	-2.97032600	-2.12681800	2.84848400
C	-6.02031000	-0.63397700	2.77108400
H	-6.93148300	0.22004000	1.00868900
H	-4.85168400	-1.56637600	4.32474400
H	-6.85609900	-0.39596600	3.42413100
C	-3.50876600	-2.68150000	-1.33848100
C	-4.52500100	-3.55028500	-0.89955200
C	-3.29548200	-2.54062300	-2.71584900
C	-5.29226800	-4.26945800	-1.81540800
H	-4.72398100	-3.65978500	0.16226000
C	-4.06968000	-3.25665300	-3.63320900
H	-2.52258300	-1.86918900	-3.06913100

C	-5.06631800	-4.12383500	-3.18686800
H	-6.07098600	-4.93822800	-1.45753900
H	-3.88762400	-3.13319100	-4.69751800
H	-5.66780300	-4.68086800	-3.90071500
C	-1.56114900	-2.98430700	0.84513300
C	-1.71565800	-4.36578300	0.66728200
C	-0.64658100	-2.53163700	1.81021600
C	-0.98903300	-5.26942200	1.44648700
H	-2.39514900	-4.74506700	-0.08742500
C	0.06507600	-3.43358500	2.60208500
H	-0.49474900	-1.46474900	1.94164800
C	-0.10449500	-4.80841000	2.42177400
H	-1.11710800	-6.33697400	1.28692600
H	0.76006200	-3.06026800	3.34934700
H	0.45179400	-5.51469200	3.03314800

Table S2. [9,9-$(PPh_3)_2$-8-(PPh_3)-*arachno*-9,6-$RhSB_8H_9$] (-3820.95000167)

	x	y	z
H	-3.84923300	0.22640000	-3.00585800
H	-3.24685200	-2.60192500	-2.15680100
H	-1.18669500	0.45824000	-1.19995500
H	-0.84216200	-2.94213900	-0.75719700
H	-2.74001200	-1.86629200	-5.01470700
H	-0.74712300	-3.51425900	-3.63266900
H	0.66204100	-0.46584200	-3.20680000
H	1.52900200	-2.18179800	-2.74219300
H	0.39870000	-1.10579800	-5.14650000
B	-1.97046100	-0.54724300	-1.27750000
B	-2.74707500	-0.20477900	-2.85318200
B	-2.35817800	-1.86286200	-2.44082400
B	-0.87507800	-1.99089000	-1.47771400
B	-2.13688500	-1.41413600	-4.09621400
B	-0.88635600	-2.39373200	-3.24681500
B	0.51639900	-1.58062800	-2.56328700
B	-0.21576700	-0.98632800	-4.13296100
P	1.09370100	1.96853500	0.02896100
P	2.26194400	-1.54765400	0.00292200
S	-1.54364200	0.43317400	-4.24831100
Rh	0.41709800	-0.30729700	-0.71342000
C	0.22572600	3.27993800	-0.97183100
C	-0.05941900	4.56332500	-0.47828900
C	-0.10949000	2.98555900	-2.30205700
C	-0.65781900	5.52317400	-1.29761600
H	0.18146400	4.82054800	0.54722300
C	-0.70362500	3.94646700	-3.12351300
H	0.08172800	1.99296700	-2.69663100
C	-0.97939100	5.21951000	-2.62292200
H	-0.86913200	6.51183400	-0.89745500

H	-0.95769900	3.68938600	-4.14783000
H	-1.44482300	5.96840200	-3.25832000
C	2.86705700	2.44412300	-0.28991300
C	3.86716600	2.16009500	0.65565200
C	3.25216700	3.02160600	-1.51136400
C	5.20638500	2.44795200	0.38820400
H	3.60462300	1.72446100	1.61243200
C	4.59347000	3.30309500	-1.77897500
H	2.50519300	3.26484200	-2.25931800
C	5.57670600	3.01761400	-0.83074300
H	5.95928100	2.22128000	1.13839700
H	4.86503700	3.75498500	-2.72957900
H	6.62007200	3.23973600	-1.03812800
C	0.81521300	2.58872500	1.75924600
C	1.56179600	3.62241100	2.34996600
C	-0.23467600	2.01929500	2.49431500
C	1.26642200	4.06761200	3.63991800
H	2.38139800	4.07952900	1.80500900
C	-0.53605200	2.46913200	3.78128800
H	-0.81178700	1.20736300	2.06251400
C	0.21625600	3.49298900	4.35918100
H	1.85805300	4.86562000	4.08126600
H	-1.35273700	2.00901200	4.32999000
H	-0.01194200	3.84037400	5.36353000
C	3.74317100	-1.68890900	-1.09960000
C	4.62093800	-2.78381600	-1.05227500
C	4.01361800	-0.64419300	-1.99396800
C	5.74591700	-2.82618200	-1.87840500
H	4.42308200	-3.60999200	-0.37665800
C	5.14074100	-0.68459000	-2.81509800
H	3.33161800	0.19722700	-2.05126800
C	6.00899900	-1.77642400	-2.76048500
H	6.41273600	-3.68351200	-1.83516800
H	5.33349000	0.13502500	-3.50181900
H	6.88242700	-1.81309300	-3.40639600
C	3.00219300	-0.99862600	1.61659200
C	2.13600500	-0.52569100	2.61471500
C	4.37529400	-1.06848300	1.89774100
C	2.62644000	-0.12593700	3.85963000
H	1.07108500	-0.46799800	2.41391200
C	4.86678100	-0.66654200	3.14163000
H	5.06697400	-1.42799000	1.14382500
C	3.99571300	-0.19223100	4.12513200
H	1.93781300	0.24948600	4.61144300
H	5.93410700	-0.72332600	3.34027000
H	4.38167300	0.12415100	5.09072100
C	1.89602800	-3.33511200	0.40404700
C	1.63503800	-4.24892600	-0.63221700
C	1.85849400	-3.80532800	1.72664300
C	1.34748700	-5.58436100	-0.35264300

H	1.65061300	-3.91880400	-1.66345200
C	1.56297900	-5.14323900	2.00507800
H	2.07468900	-3.13600600	2.55128600
C	1.30597000	-6.03810000	0.96726600
H	1.14867400	-6.26829100	-1.17324100
H	1.54830500	-5.48374700	3.03767300
H	1.07939100	-7.07898200	1.18290500
P	-3.28574600	-0.43249000	0.17868400
C	-2.69129700	-0.85537600	1.87434700
C	-3.23637900	-0.26099500	3.02425900
C	-1.72721300	-1.86675700	2.02026000
C	-2.82993300	-0.67528600	4.29401500
H	-3.97432300	0.52861000	2.93463800
C	-1.33121000	-2.28315900	3.29396700
H	-1.28796600	-2.32770600	1.14288100
C	-1.87920200	-1.68929500	4.43180400
H	-3.26237100	-0.20774000	5.17488600
H	-0.59119200	-3.07271400	3.38529000
H	-1.56894000	-2.01468500	5.42128400
C	-4.05034300	1.23350000	0.32448700
C	-5.30888000	1.40465000	0.92873700
C	-3.37171000	2.35851600	-0.16406800
C	-5.86578300	2.67740000	1.05291500
H	-5.86344900	0.54249700	1.28625100
C	-3.93219600	3.63131800	-0.03706700
H	-2.41566300	2.24781900	-0.66123400
C	-5.17648000	3.79336800	0.57249500
H	-6.84122900	2.79445000	1.51733600
H	-3.39112900	4.48912200	-0.42436000
H	-5.61357200	4.78403000	0.66545100
C	-4.72068200	-1.55834700	-0.07069300
C	-4.83849700	-2.75649500	0.64706900
C	-5.69356600	-1.23789100	-1.03229900
C	-5.90991500	-3.61899100	0.40736000
H	-4.09762000	-3.02443100	1.39227900
C	-6.76258100	-2.10114500	-1.26528200
H	-5.61250400	-0.32116700	-1.60579200
C	-6.87333500	-3.29414000	-0.54732900
H	-5.98724000	-4.54536600	0.96980600
H	-7.50558200	-1.84276100	-2.01458800
H	-7.70588200	-3.96715800	-0.73360100

Table S3. [6,6-$(PH_3)_2$-9-(PCy_3)-*arachno*-6,5-$RhSB_8H_9$]: PH_3 model of compound **3** (-2445.55557138)

	x	**y**	**z**
C	1.78728300	4.65099400	1.62718100
C	1.58336600	3.51408200	2.63695900
C	1.19852200	2.19714100	1.94083300

C	2.81697800	4.25726800	0.55914600
C	2.43435400	2.94411300	-0.14698600
C	2.24657500	1.79867000	0.87540400
C	3.16329000	-0.09627800	-1.22710600
C	1.98500200	-1.07709700	1.50826300
C	3.09766500	-1.45241500	-1.96544900
C	1.62648400	-2.53339400	1.13313500
C	4.03659000	-1.44557800	-3.18441500
C	1.51174900	-3.40676100	2.39484300
C	3.29769900	-1.04412300	2.32072500
C	4.61683300	0.18811900	-0.78399500
C	5.56099100	0.19731900	-2.00014800
C	3.18274600	-1.91956200	3.58218000
C	5.48351600	-1.11715600	-2.78993600
C	2.79389400	-3.36410300	3.23785700
H	-4.13672100	-0.08975300	-2.95150500
H	-3.28771200	2.55265400	-1.37826500
H	-1.84229700	1.69292900	-3.75692700
H	-1.84348000	1.48330500	-0.37139200
H	-1.60744500	-1.26012200	-4.01729100
H	-0.41242400	2.65025600	-1.27734300
H	0.82887400	4.87963700	1.13983400
H	0.22129900	2.31063000	1.45636600
H	0.71951000	0.42257700	-2.88345800
H	2.10470400	5.56585900	2.14318100
H	1.50479000	3.08843400	-0.70599000
H	0.80661300	3.78188100	3.36425100
H	2.91799100	5.05462200	-0.18761300
H	-0.66517300	-0.11370200	0.44076900
H	0.06263600	-2.32931700	-1.81210100
H	1.08770200	1.40894400	2.69506200
H	3.20866100	2.69141800	-0.87936100
H	2.51067000	3.36510600	3.21027600
H	3.80481600	4.14332800	1.03103500
H	2.87877700	0.67289000	-1.96045700
H	2.07599000	-1.67306600	-2.28084600
H	1.17910700	-0.71876100	2.16638500
H	3.20744400	1.65290300	1.38840900
H	0.69296600	-2.56406500	0.56559700
H	3.67477500	-0.70331300	-3.91018500
H	0.66428000	-3.05450400	3.00159600
H	3.98982700	-2.41979000	-3.68654700
H	3.40526600	-2.25663600	-1.28405200
H	3.56297300	-0.02183800	2.61186400
H	5.28949300	1.03577900	-2.65808900
H	4.69858200	1.14229500	-0.25337400
H	2.42466500	-1.48713700	4.25172000
H	2.40592600	-2.95036100	0.48256100
H	1.27925600	-4.43899300	2.10486800
H	4.12246400	-1.42084700	1.70243300

H	4.94644000	-0.59012400	-0.08437200
H	6.11989400	-1.06110700	-3.68194500
H	4.13258500	-1.89815600	4.13133700
H	2.66869900	-3.95253000	4.15542200
H	6.58932100	0.38350600	-1.66499000
H	5.88431200	-1.93362700	-2.17076600
H	3.61333600	-3.83398800	2.67398100
B	-2.74355600	1.48882700	-1.33898900
B	-3.16723500	0.05033300	-2.27560000
B	-1.80111300	1.03423300	-2.76481700
B	-1.59068400	-0.70550100	-2.96779400
B	-0.89471800	1.56102600	-1.29397400
B	-0.28259600	0.23231100	-2.26084500
B	-0.56478200	-1.34154600	-1.58769000
B	-0.01550900	0.04267100	-0.54903500
P	-5.02739500	1.51348700	0.58826300
P	-4.22886200	-1.66708700	1.59952800
P	1.83863800	0.14334600	0.08135600
S	-2.46213100	-1.72039200	-1.46439600
Rh	-3.65512700	-0.15065600	-0.07284700
H	-4.24358300	-3.06025900	1.33324300
H	-3.44599600	-1.75226600	2.78296000
H	-5.48404000	-1.62609200	2.26335700
H	-4.52222400	2.71444900	1.14952800
H	-5.84878900	2.11698700	-0.39316900
H	-6.04594800	1.30035400	1.55803400

Table S4. [6,6-$(PPh_3)_2$-9-(2-Mepy)-*arachno*-6,5-$RhSB_8H_9$] (**4**) (-3072.28412376)

	x	**y**	**z**
Rh	-0.07308700	-0.32345000	-0.75941400
P	1.76075900	-1.45754600	0.09582500
P	0.38825900	1.89694400	-0.00009600
S	-1.68020400	0.42810000	-2.42593900
B	-2.61024800	-1.16593800	-3.22700700
B	-0.88054400	-1.47002200	-2.55153800
B	-2.17521700	-2.64387100	-2.36114600
B	-3.68663100	-1.77688000	-1.99039300
B	-0.99729600	-2.39634800	-1.06318000
B	-2.80936400	-2.52912400	-0.67411400
B	-3.74594400	-0.87143900	-0.49859000
B	-3.51892000	-0.05578700	-2.09056700
C	2.44691500	-2.61912200	-1.18203200
C	2.61471600	-2.11754700	-2.48402000
H	2.30872800	-1.09921700	-2.70438900
C	3.14023500	-2.91933400	-3.49710800
H	3.26313100	-2.51092900	-4.49673100
C	3.48191700	-4.24726800	-3.23303800
H	3.87909900	-4.87766900	-4.02429000

C	3.29345800	-4.76372400	-1.95121500
H	3.53866500	-5.80139600	-1.73961800
C	2.78287500	-3.95648200	-0.93152100
H	2.63462800	-4.38327300	0.05374400
C	1.56447000	-2.51263600	1.61812300
C	0.29596900	-2.70153700	2.18230400
H	-0.56433300	-2.23827000	1.71250200
C	0.12917200	-3.47372700	3.33511900
H	-0.86497200	-3.60885600	3.75343300
C	1.23237000	-4.07211600	3.94295500
H	1.10473200	-4.67494600	4.83833200
C	2.50513700	-3.88815400	3.39636500
H	3.37224300	-4.34553400	3.86584400
C	2.66992200	-3.11175200	2.24941700
H	3.66750300	-2.96371000	1.84751200
C	3.30171400	-0.51863300	0.59576900
C	3.39852600	0.02147500	1.89015100
H	2.59195500	-0.11968900	2.60085400
C	4.53478000	0.72235800	2.29447100
H	4.58749500	1.11874000	3.30543100
C	5.59921500	0.90619000	1.41019100
H	6.48783800	1.44700000	1.72542000
C	5.51141100	0.38716900	0.11889500
H	6.33167500	0.52228700	-0.58126900
C	4.37571400	-0.31882500	-0.28421700
H	4.34228000	-0.73026700	-1.28646500
C	0.35802500	2.22745200	1.82704400
C	0.17937000	1.15181400	2.70746000
H	0.09838300	0.14772500	2.30271100
C	0.09224100	1.36115800	4.08664200
H	-0.04410500	0.51225100	4.75183400
C	0.17921400	2.65390700	4.60393600
H	0.11279600	2.81989600	5.67609000
C	0.33805300	3.73762400	3.73553000
H	0.39013600	4.74921200	4.12985000
C	0.41643300	3.52752100	2.35864000
H	0.50574400	4.38120500	1.69307900
C	1.97172200	2.61162600	-0.63778400
C	2.90343700	3.32032200	0.13102500
H	2.74216900	3.45744000	1.19446200
C	4.05722700	3.84417000	-0.45875400
H	4.77306400	4.38537400	0.15452800
C	4.29202100	3.67415100	-1.82278600
H	5.18744100	4.08789400	-2.27935700
C	3.37410600	2.96004000	-2.59749700
H	3.55113600	2.81433300	-3.66000700
C	2.22984400	2.42390100	-2.00816800
H	1.52756700	1.85381100	-2.61160200
C	-0.84824800	3.18430400	-0.53069600
C	-0.50756500	4.35563700	-1.22076200

H	0.52431300	4.54632900	-1.49533900
C	-1.49058200	5.28896100	-1.56399700
H	-1.20813200	6.19028300	-2.10213700
C	-2.82331600	5.06750900	-1.21966900
H	-3.58601000	5.79356100	-1.48871400
C	-3.17289000	3.90191000	-0.53280000
H	-4.21029600	3.71417600	-0.26867600
C	-2.19554300	2.96729500	-0.19593100
H	-2.48200600	2.05446200	0.31890100
C	-6.27658700	-0.66707500	-0.64865900
H	-6.05612000	-0.47563000	-1.68886400
C	-7.57274700	-0.65741500	-0.16446200
H	-8.39277600	-0.46358600	-0.84698000
C	-7.78396000	-0.89212300	1.19318000
H	-8.78579300	-0.89277200	1.61196900
C	-6.67838400	-1.12439500	2.00339900
H	-6.79997100	-1.31238100	3.06470200
C	-5.38570400	-1.12808700	1.47319900
C	-4.20147700	-1.38843100	2.35680300
H	-3.59624300	-2.20837000	1.95900400
H	-4.53938600	-1.64361400	3.36463300
H	-3.54960400	-0.51029200	2.41677400
N	-5.19708600	-0.90074000	0.13917000
H	-4.74337000	-2.26343000	-2.26567800
H	-2.78516600	-1.11181300	-4.40062500
H	-2.19368200	-3.66142200	-2.98158500
H	-0.05489500	-1.57824800	-3.40077700
H	-4.30503200	0.70314900	-2.57563000
H	-3.19391500	-3.50171500	-0.09519100
H	-0.35722700	-3.34880600	-0.74528000
H	-3.00877000	-0.29985900	0.23860200
H	-1.76280500	-2.01517800	-0.05282600

Table S5. [9,6-$(PPh_3)_2$-8-(2-Mepy)-*arachno*-9,6-$RhSB_8H_9$] (-3072.27589729)

	x	**y**	**z**
C	2.74500000	1.05612700	-1.12952200
C	2.04851300	1.38344300	-2.30378900
C	2.43727600	2.46922900	-3.08915700
C	3.53237600	3.25002900	-2.71013500
C	4.23498400	2.93147800	-1.54669300
C	3.84719600	1.84139200	-0.76338200
C	3.14506200	-0.45433200	1.35646900
C	3.01042100	0.66047900	2.20202700
C	3.61264800	0.67846300	3.46010700
C	4.34825000	-0.42263500	3.90388600
C	4.47903500	-1.53899400	3.07755500

C	3.88462200	-1.55646600	1.81385800
C	3.22348000	-1.66687700	-1.29714500
C	4.62325000	-1.54897900	-1.35282000
C	5.37276100	-2.36278800	-2.20082000
C	4.73481800	-3.29899100	-3.01905600
C	3.34614300	-3.41442400	-2.97961200
C	2.59470200	-2.60456900	-2.12337200
C	0.19869100	2.82311700	1.09908400
C	0.15392000	3.03117100	2.48857400
C	0.94225000	4.01143500	3.09308800
C	1.79123400	4.80736000	2.32181700
C	1.84659800	4.61000600	0.94176600
C	1.06328600	3.62544500	0.33568600
C	-1.39585100	2.26026100	-1.25598700
C	-1.65915000	3.63385400	-1.39300800
C	-2.12435200	4.15168700	-2.60323500
C	-2.33419900	3.30657700	-3.69568600
C	-2.07300300	1.94076300	-3.57324100
C	-1.60429400	1.42432500	-2.36336600
C	-2.30468300	1.51979400	1.41608800
C	-3.40089600	2.36724100	1.19483300
C	-4.48670100	2.37256000	2.07442700
C	-4.49272700	1.53639800	3.19292400
C	-3.40535100	0.69170400	3.42715800
C	-2.32394700	0.68036100	2.54329100
C	-4.22276200	-0.76798400	-0.30511600
C	-5.33874100	-0.21283700	-0.90094800
C	-5.57554500	-0.47424200	-2.24927000
C	-4.66015600	-1.26161400	-2.93355600
C	-3.52377400	-1.77982500	-2.30043500
N	-3.31706000	-1.53447100	-0.97158300
B	0.61630500	-2.92924100	0.72415900
B	-0.63385800	-2.96918600	-0.55120500
B	-2.13384300	-2.10559900	-0.05461900
B	-0.41850700	-4.35458900	0.58739000
B	-2.03820800	-3.87339900	0.07532100
B	-0.13727100	-3.66924400	2.22270100
B	-1.82808000	-4.49046400	1.69110000
B	-2.84342000	-3.00679500	1.35309200
P	2.22179200	-0.49795400	-0.24747500
P	-0.80356300	1.45921900	0.31074300
S	-1.81041200	-3.03584900	2.99364600
Rh	-0.06664100	-0.84590700	0.07498100
H	-2.69190200	3.71289400	-4.63818800
H	-2.22394200	1.27824500	-4.42166200
H	0.45209900	-2.45355100	1.90987400
H	1.76922800	-3.20196700	0.60814300
H	-0.31935500	-3.23485000	-1.67015300
H	1.19430200	0.78291100	-2.60167900
H	1.88280500	2.70573700	-3.99350900

H	-1.76645900	-1.17868100	0.70716100
H	3.83789700	4.09673400	-3.31934900
H	0.08372400	-5.38007500	0.24371900
H	-2.71524300	-4.48666900	-0.69637500
H	5.09077500	3.53044500	-1.24535300
H	0.55188700	-4.20685900	3.03073300
H	4.40496300	1.61008900	0.13815000
H	-2.20709300	-5.55026800	2.07136600
H	-4.02163200	-3.01183900	1.55261900
H	2.43572400	1.52215900	1.88110600
H	3.49951700	1.55483000	4.09293100
H	4.81230800	-0.41146300	4.88660300
H	5.04311400	-2.40483300	3.41404900
H	3.99364000	-2.43499100	1.18841600
H	5.13391300	-0.81969000	-0.73130500
H	6.45492900	-2.26289400	-2.22469200
H	5.31911000	-3.93281300	-3.68115900
H	2.83972200	-4.14279700	-3.60753600
H	1.51848300	-2.71446300	-2.08422600
H	-0.50469800	2.43361400	3.10899500
H	0.88383200	4.15584700	4.16881100
H	2.40177700	5.57381900	2.79174300
H	2.50507300	5.21718200	0.32679200
H	1.12870700	3.49088000	-0.73784300
H	-1.48771800	4.30574000	-0.55760500
H	-2.31901200	5.21727900	-2.69310700
H	-1.37322700	0.36602700	-2.26257600
H	-3.41965700	3.02051400	0.32930000
H	-5.32786100	3.03472900	1.88405000
H	-5.33856600	1.54055400	3.87520400
H	-3.39969400	0.02869100	4.28763500
H	-1.49899800	-0.00503300	2.71834500
H	-4.02075000	-0.62822200	0.74631500
H	-6.00687200	0.39563100	-0.30259500
H	-6.45093700	-0.07660500	-2.75401400
H	-4.80427000	-1.48715900	-3.98458100
C	-2.53956200	-2.57570400	-3.10229700
H	-1.54951800	-2.11332100	-3.07214500
H	-2.42146700	-3.58778200	-2.70824500
H	-2.87772100	-2.63404500	-4.14019400

Table S6. [6,6-$(PPh_3)_2$-9-(2-Etpy)-*arachno*-6,5-$RhSB_8H_9$] (**5**) (-3111.59429238)

	x	**y**	**z**
Rh	0.05182300	-0.07539100	-0.88077000
B	-1.07256600	-1.89415200	-1.71479700
B	-2.89343000	-1.95515000	-1.36531300
B	-3.32315600	0.86096000	-2.07260400
B	-3.66779100	-0.79859500	-2.43138200

B	-2.24098500	-1.68019400	-3.02698400
B	-2.51735000	0.00510700	-3.47583100
B	-0.84142500	-0.62498600	-2.90882600
P	1.54622300	-1.67805700	-0.08396300
P	0.81779700	1.96249300	0.17641700
S	-1.44271200	1.22924700	-2.30059000
B	-3.67804900	-0.32187000	-0.75376400
C	-6.15681000	0.20663600	-0.88346000
H	-5.86187500	0.64341100	-1.82621400
C	-7.47001000	0.24124400	-0.44916500
H	-8.22417100	0.70710900	-1.07365800
C	-7.77843500	-0.32288900	0.78579500
H	-8.79586000	-0.31807000	1.16549900
C	-6.75151000	-0.89363600	1.52985000
H	-6.96425900	-1.33973000	2.49273300
C	-5.43731500	-0.91057100	1.05524600
N	-5.15365200	-0.35596400	-0.16454900
H	-4.75839900	-1.08829500	-2.82531500
H	-2.66461000	0.38074400	-4.59302200
H	-2.33847100	-2.49531200	-3.89139500
H	-0.01873300	-0.58766300	-3.77053900
H	-4.01345700	1.80315300	-2.32572200
H	-3.37903800	-3.00710600	-1.07475300
H	-0.53491600	-2.95532700	-1.68471000
H	-2.90931400	-0.04212400	0.10853700
H	-1.81059800	-1.73346700	-0.63216200
C	-4.31271000	-1.52948200	1.84940800
H	-3.77441500	-2.22203400	1.19271300
H	-3.58447100	-0.74229100	2.08343600
C	-4.73009800	-2.24493300	3.13740600
H	-5.18691700	-1.56338900	3.86407500
H	-5.43332300	-3.06229100	2.94209300
H	-3.84549300	-2.68113400	3.61063300
C	0.70397900	-3.05144600	0.84887000
C	0.96540100	-4.41249300	0.64190000
C	-0.24171100	-2.69379900	1.82438900
C	0.30962100	-5.38823500	1.39737900
H	1.67470500	-4.71984400	-0.11844100
C	-0.87785100	-3.66685800	2.59589100
H	-0.48689800	-1.64517800	1.97064300
C	-0.60603700	-5.02035200	2.38284100
H	0.51858600	-6.43867100	1.21207600
H	-1.58817500	-3.36774600	3.36266400
H	-1.10883500	-5.78014100	2.97540800
C	0.97804300	2.19781600	2.01380900
C	1.05232600	3.47742100	2.59466500
C	0.98161300	1.08228500	2.85940500
C	1.15187500	3.62794700	3.97761900
H	1.01689500	4.36114600	1.96481100
C	1.07884100	1.23080700	4.24511000

H	0.91317200	0.09131400	2.42969000
C	1.16690400	2.50368400	4.80755600
H	1.20959300	4.62467100	4.40752900
H	1.08602800	0.34927300	4.88063900
H	1.24012800	2.62231000	5.88553600
C	2.91610900	-1.24015600	1.10912700
C	3.90267300	-0.33710800	0.67871300
C	3.03114600	-1.78798100	2.39596600
C	4.96337000	0.01583000	1.51243600
H	3.84948900	0.08892200	-0.31792800
C	4.09321700	-1.43151500	3.23229100
H	2.29576300	-2.50137400	2.75198100
C	5.06148900	-0.52820400	2.79516900
H	5.71078000	0.71936200	1.15617600
H	4.16315600	-1.86947500	4.22499600
H	5.88754000	-0.25274600	3.44563700
C	-0.28031200	3.42122300	-0.18704600
C	0.11961700	4.51785000	-0.96134900
C	-1.58417800	3.40659200	0.33784400
C	-0.76101000	5.57767000	-1.20085300
H	1.11908200	4.55240600	-1.38161700
C	-2.45800500	4.46628800	0.10401100
H	-1.91964200	2.55651900	0.92613900
C	-2.04874200	5.55740700	-0.66782400
H	-0.43371500	6.41880200	-1.80660600
H	-3.46256300	4.43690900	0.51791000
H	-2.73205500	6.38141500	-0.85547400
C	2.44352100	2.52322800	-0.51945700
C	2.69420700	2.21681500	-1.86872200
C	3.42048900	3.21954100	0.20599200
C	3.88564700	2.61130800	-2.47925900
H	1.95574100	1.64901900	-2.42946500
C	4.61736800	3.60450300	-0.40387300
C	4.85244700	3.30473700	-1.74679400
H	4.06116900	2.36704400	-3.52356900
H	5.36676600	4.13879800	0.17483300
H	5.78448200	3.60473100	-2.21862700
C	2.58403400	-2.55857900	-1.35448600
C	2.29404200	-2.42916000	-2.71876100
C	3.68685900	-3.34518000	-0.97309500
C	3.07567200	-3.07880100	-3.67803700
H	1.45895000	-1.81552400	-3.03026300
C	4.46271500	-3.99756900	-1.93100400
H	3.94807200	-3.44355600	0.07605300
C	4.15855600	-3.86612200	-3.28834300
H	2.83278100	-2.96436000	-4.73115300
H	5.30922200	-4.60258700	-1.61612000
H	4.76658100	-4.37033100	-4.03514600
H	3.25964500	3.45238800	1.25310800

Table S7. [6,6-$(PPh_3)_2$-9-(py)-*arachno*-6,5-$RhSB_8H_9$] (**6a**) (-3032.96576796)

	x	y	z
Rh	-0.16799100	-0.36872800	-0.69943300
B	-1.05207100	-2.46984800	-0.92379300
B	-2.84872800	-2.63539700	-0.49411300
B	-3.64908700	-0.21395900	-1.95822800
B	-3.76959100	-1.94054300	-1.80896200
B	-2.24899300	-2.78263600	-2.19041900
B	-2.73806400	-1.33822500	-3.08524200
B	-0.98793400	-1.58317700	-2.44047300
P	1.71467800	-1.43539700	0.13636700
P	0.26735100	1.88198000	-0.02041000
S	-1.82859300	0.29885600	-2.35146100
B	-3.81348600	-0.98482900	-0.34976600
C	-6.38793000	-0.94954900	-0.37369500
H	-6.27333900	-0.83747800	-1.44288200
C	-7.63186700	-0.98347200	0.24162400
H	-8.52439600	-0.90362000	-0.36937900
C	-7.70806100	-1.11184100	1.62770000
H	-8.66934600	-1.14067500	2.13135300
C	-6.51900900	-1.19912800	2.35393400
H	-6.52044800	-1.29932200	3.43388300
C	-5.30962600	-1.16268100	1.67831400
N	-5.23745400	-1.04247300	0.33169900
H	-4.82248700	-2.45596000	-2.04500000
H	-2.94156300	-1.32007500	-4.25532900
H	-2.25617600	-3.81559000	-2.78515500
H	-0.17784600	-1.69533600	-3.30381300
H	-4.46920000	0.50521000	-2.44785800
H	-3.20905800	-3.58306200	0.13804100
H	-0.38250300	-3.39565000	-0.58908100
H	-3.08485000	-0.40149700	0.39150800
H	-1.80498800	-2.07448800	0.08853500
H	-4.35639500	-1.23237500	2.18712100
C	0.29342400	2.27362100	1.79419600
C	0.15340800	1.22589300	2.71404500
C	0.35453600	3.59110700	2.28027300
C	0.10725300	1.47972000	4.08772100
H	0.06989100	0.20875100	2.34370600
C	0.31732300	3.84568000	3.65130000
H	0.41372700	4.42288700	1.58438500
C	0.19725200	2.78962000	4.55918700
H	-0.00012700	0.65209000	4.78426100
H	0.37095800	4.87012700	4.01070200
H	0.16273000	2.99038200	5.62689800
C	-1.01591900	3.12349700	-0.54860200
C	-0.72447900	4.28324500	-1.27942600
C	-2.34669200	2.88358400	-0.16672700
C	-1.73986100	5.18324600	-1.61730300

H	0.29394500	4.49029000	-1.59007100
C	-3.35613700	3.78545500	-0.49838600
H	-2.59516800	1.97868100	0.38098800
C	-3.05585400	4.93965500	-1.22656600
H	-1.49597900	6.07596900	-2.18769000
H	-4.38024600	3.58071000	-0.19756000
H	-3.84382000	5.63977900	-1.49151800
C	3.24782500	-0.45248900	0.57152200
C	3.36304900	0.12566000	1.84785700
C	4.29798900	-0.25780800	-0.33781100
C	4.49409600	0.85897400	2.20646900
H	2.57555800	-0.01069700	2.58057400
C	5.42876700	0.47989800	0.01971900
H	4.25020700	-0.69805300	-1.32704000
C	5.53516000	1.03704400	1.29361800
H	4.56146600	1.28478700	3.20449500
H	6.23067900	0.60998900	-0.70233300
H	6.42018700	1.60267200	1.57347800
C	2.39078300	-2.61761200	-1.12776500
C	2.74531100	-3.94531500	-0.85275800
C	2.52784400	-2.14542800	-2.44436700
C	3.24353900	-4.77159300	-1.86330600
H	2.62115900	-4.35002600	0.14508300
C	3.04110000	-2.96596600	-3.44864500
H	2.20840000	-1.13536300	-2.68317800
C	3.40108500	-4.28402700	-3.16046700
H	3.50333800	-5.80154300	-1.63230200
H	3.14030400	-2.58007000	-4.45978000
H	3.78865600	-4.92917000	-3.94457000
C	1.81262400	2.60498900	-0.73740900
C	2.76166600	3.34693700	-0.02297800
C	2.02392600	2.38250600	-2.11063200
C	3.88643800	3.86841800	-0.66835200
H	2.63751000	3.51167600	1.04147400
C	3.13909100	2.91594700	-2.75546900
H	1.30824400	1.78736400	-2.67244900
C	4.07466800	3.66293900	-2.03466000
H	4.61636200	4.43528200	-0.09627600
H	3.27971400	2.74265500	-3.81928000
H	4.94758600	4.07452300	-2.53467200
C	1.57667200	-2.45226200	1.69020300
C	2.70824400	-3.01536700	2.30816500
C	0.32593700	-2.64763100	2.29061000
C	2.58579900	-3.76398700	3.47858100
H	3.69254600	-2.86117100	1.87670600
C	0.20174500	-3.39191000	3.46688200
H	-0.55397800	-2.21275200	1.82999900
C	1.33033000	-3.95508500	4.06169600
H	3.47218200	-4.19425700	3.93759500
H	-0.77926300	-3.53334200	3.91308600

H	1.23572800	-4.53645600	4.97520100

Table S8. [9,9-$(PPh_3)_2$-8-(py)-*arachno*-9,6-$RhSB_8H_9$] (**6b**) (-3032.96436392)

	x	y	z
C	-4.72444500	-1.40884100	3.26286300
C	-4.89264000	-0.82715100	2.00434100
C	-3.63825900	-2.26018900	3.46267800
C	-3.99201100	-1.12325700	0.99418900
C	-2.75877300	-2.50189200	2.41556400
H	-5.42582600	-1.20493400	4.06612900
H	-5.72097500	-0.15964900	1.79408900
H	-3.46108500	-2.73769500	4.42039300
H	-1.88925500	-3.13832900	2.51421400
H	-3.97382800	-3.39088800	-1.32099000
H	-2.17449100	-4.73718000	0.63950200
H	-1.81179200	-1.25463500	-0.70824500
H	0.11717000	-3.21236200	1.38497900
H	-1.94392300	-5.63514700	-2.24116100
H	0.55195500	-5.25319500	-0.75348000
H	0.28663100	-2.22187000	-2.24868700
H	1.88037100	-2.82959100	-1.23473900
H	0.46312700	-3.88048500	-3.48615000
N	-2.93301900	-1.94395600	1.19536700
B	-1.97109000	-2.28674700	-0.00218700
B	-2.79125200	-3.22157400	-1.29353400
B	-1.69012100	-4.03279700	-0.19684700
B	-0.33968200	-2.99615500	0.29695500
B	-1.65082000	-4.55119200	-1.85304600
B	-0.11403000	-4.28378700	-0.94845500
B	0.70066000	-2.72798700	-1.13395000
B	-0.17032600	-3.48466700	-2.55882600
P	-0.97384700	1.44830900	-0.35439600
P	2.14569900	-0.39901700	0.28226000
S	-2.00480700	-3.05925400	-3.06193800
Rh	-0.09911100	-0.80518400	-0.20743200
H	-4.08835900	-0.72291500	-0.00714300
C	-2.53384700	1.45727200	-1.37702700
C	-3.62704800	2.29716500	-1.11079300
C	-2.61421500	0.58357300	-2.47464000
C	-4.76647300	2.26129800	-1.91829800
H	-3.59784900	2.98016600	-0.26863800
C	-3.74880000	0.55551800	-3.28802200
H	-1.79268900	-0.09628800	-2.68264100
C	-4.83056300	1.39325100	-3.01003000
H	-5.60438000	2.91606800	-1.69206100
H	-3.78774700	-0.13340600	-4.12701400
H	-5.71860500	1.36552900	-3.63580600
C	0.01963000	2.76343000	-1.21886600

C	0.97957600	3.51343600	-0.51819200
C	-0.10735900	2.96847700	-2.60254100
C	1.78046600	4.44377400	-1.18231000
H	1.10110800	3.38214700	0.55091400
C	0.69933500	3.89525700	-3.26501500
H	-0.84623800	2.41287300	-3.17030800
C	1.64606800	4.63743600	-2.55788100
H	2.51301200	5.01443000	-0.61774900
H	0.57918900	4.04032500	-4.33554200
H	2.27191700	5.36108200	-3.07328400
C	-1.53412700	2.30362300	1.19796900
C	-1.68894800	3.69471200	1.31473800
C	-1.85462600	1.50091900	2.30364000
C	-2.14702900	4.26385100	2.50503700
H	-1.44247300	4.33942800	0.47701000
C	-2.31940600	2.06769200	3.49191500
H	-1.71645200	0.42520300	2.23106400
C	-2.46447400	3.45256400	3.59657200
H	-2.25465900	5.34296200	2.57821800
H	-2.56028400	1.42729500	4.33663400
H	-2.81849200	3.89751600	4.52284700
C	3.27145800	-0.12955600	-1.15976000
C	4.67261700	-0.20455000	-1.06946200
C	2.69495100	0.19354800	-2.39646900
C	5.47140100	0.04273000	-2.18686900
H	5.14349300	-0.46966700	-0.12779600
C	3.49432500	0.44372900	-3.51342000
H	1.61319100	0.23797900	-2.47816100
C	4.88375100	0.36851500	-3.41141500
H	6.55281400	-0.02488400	-2.10085700
H	3.02841600	0.69032600	-4.46356500
H	5.50683300	0.55634800	-4.28193000
C	2.48912500	1.06450200	1.38276200
C	1.59362100	1.30995200	2.43588800
C	3.58967000	1.92202500	1.23337400
C	1.79476300	2.36808800	3.32382100
H	0.72037300	0.67587300	2.54720600
C	3.79020200	2.98458200	2.11766300
H	4.28774800	1.77697600	0.41698200
C	2.89669600	3.21072600	3.16663000
H	1.08091600	2.54013000	4.12481300
H	4.64783500	3.63875100	1.98187700
H	3.05489300	4.03972000	3.85147500
C	2.99533500	-1.73974700	1.26529000
C	3.75278900	-2.74728600	0.64633600
C	2.82882600	-1.79921000	2.65825300
C	4.32833500	-3.77395500	1.39714200
H	3.89790200	-2.73871100	-0.42688100
C	3.40227800	-2.82646000	3.40751400
H	2.25633400	-1.03639600	3.17405100

C	4.15549700	-3.81959500	2.78004400
H	4.90875400	-4.54162800	0.89237400
H	3.26049500	-2.84630600	4.48514300
H	4.60247800	-4.62050500	3.36299300

Table S9. [6,6-$(PPh_3)_2$-9-(3-Mepy)-*arachno*-6,5-$RhSB_8H_9$] (**7a**) (-3072.28449727)

	x	**y**	**z**
Rh	0.00169500	-0.30299300	-0.80991300
B	-0.95135200	-2.34925800	-1.20301800
B	-2.77957900	-2.44951100	-0.91084700
B	-3.36383000	0.07045500	-2.30678500
B	-3.57032700	-1.65334400	-2.25270100
B	-2.06318500	-2.54782600	-2.56587300
B	-2.42252200	-1.04283500	-3.42033700
B	-0.73605100	-1.39718600	-2.66479900
P	1.75281100	-1.49637000	0.13444800
P	0.47252100	1.88896500	0.01732500
S	-1.49743100	0.51415000	-2.54501500
B	-3.68115200	-0.76448700	-0.75505800
C	-6.24047100	-0.59850100	-0.95550400
H	-6.04816700	-0.42847600	-2.00561900
C	-7.52188500	-0.60935900	-0.42061800
H	-8.37019500	-0.44967200	-1.07741200
C	-7.69423300	-0.81698200	0.94443100
C	-6.57126700	-1.00994600	1.76204000
C	-5.32397500	-0.98717200	1.14891700
N	-5.15216100	-0.78997600	-0.17978800
H	-4.62419000	-2.10760800	-2.58870500
H	-2.53763900	-0.96129500	-4.59975700
H	-2.07054000	-3.55127400	-3.20912200
H	0.12962100	-1.50948100	-3.47264900
H	-4.11167900	0.84976100	-2.81957400
H	-3.22468100	-3.40744700	-0.35216500
H	-0.34895300	-3.31931000	-0.86582700
H	-2.98193700	-0.25219300	0.06314700
H	-1.75680500	-1.96597800	-0.22833600
H	-4.40934300	-1.13361900	1.71079000
C	0.38400200	2.19145600	1.84755900
C	0.12645700	1.11125900	2.70239000
C	0.47316800	3.48006900	2.40244700
C	-0.00623000	1.30365700	4.08039900
H	0.02033300	0.11694400	2.27974500
C	0.34984400	3.67276600	3.77851600
H	0.62206400	4.33931000	1.75497400
C	0.11347600	2.58363700	4.62215500
H	-0.20353100	0.45123600	4.72548100
H	0.42726500	4.67543300	4.19108900
H	0.01222400	2.73615500	5.69360900

C	-0.71279900	3.21504100	-0.53424300
C	-0.31492500	4.40550300	-1.15833900
C	-2.07957000	3.01192600	-0.27973900
C	-1.26125300	5.37091300	-1.51523900
H	0.73334200	4.58635400	-1.37101300
C	-3.02060500	3.97830700	-0.63069100
H	-2.41000200	2.08580700	0.18212000
C	-2.61431200	5.16266500	-1.25078300
H	-0.93444600	6.28663400	-2.00148900
H	-4.07389900	3.80057100	-0.43017000
H	-3.34856000	5.91352800	-1.53073100
C	3.29062400	-0.60330100	0.71902000
C	3.34104500	-0.07592500	2.02120100
C	4.40927000	-0.42383400	-0.10868600
C	4.47488900	0.59235400	2.48384300
H	2.49879000	-0.20103100	2.69214100
C	5.54251500	0.24947000	0.35271900
H	4.41218100	-0.82553700	-1.11548100
C	5.58351000	0.75572500	1.65146700
H	4.49048800	0.97937300	3.49968000
H	6.39742400	0.36916800	-0.30767600
H	6.46999100	1.27094100	2.01234300
C	2.47768900	-2.67410000	-1.10786000
C	2.78080000	-4.01533000	-0.83669800
C	2.71586100	-2.18078100	-2.40173200
C	3.32704100	-4.83478000	-1.82765700
H	2.57889900	-4.43567400	0.14179300
C	3.27700000	-2.99498000	-3.38554900
H	2.43600000	-1.15926400	-2.64022800
C	3.58499500	-4.32683600	-3.10073900
H	3.54566100	-5.87517800	-1.60073300
H	3.45393500	-2.59268300	-4.37952300
H	4.00989300	-4.96667700	-3.86972400
C	2.09387700	2.57560600	-0.55293000
C	3.02238400	3.23796000	0.25979900
C	2.38778300	2.41193400	-1.91929200
C	4.20784200	3.74140300	-0.28349100
H	2.83444900	3.35398900	1.32133400
C	3.56404600	2.92734900	-2.46184700
H	1.68828000	1.87614400	-2.55637400
C	4.47833600	3.59653800	-1.64377000
H	4.92039600	4.24665400	0.36337600
H	3.76860000	2.80068500	-3.52184400
H	5.39847200	3.99441000	-2.06388300
C	1.44095400	-2.55253300	1.63732900
C	2.49272800	-3.17192400	2.33715800
C	0.13467400	-2.72628800	2.11410900
C	2.24052500	-3.95210200	3.46561200
H	3.51709500	-3.03670200	2.00418800
C	-0.11974900	-3.50347800	3.24740900

H	-0.68667700	-2.24823300	1.59238200
C	0.93150700	-4.12129300	3.92404900
H	3.06782300	-4.42443100	3.98906000
H	-1.14178700	-3.62716100	3.59620000
H	0.73550200	-4.72775900	4.80452400
H	-8.69104200	-0.82778900	1.37748800
C	-6.69636100	-1.24142000	3.24746000
H	-7.26760200	-2.15353200	3.45660100
H	-5.71538600	-1.34445300	3.71999600
H	-7.21917400	-0.40952100	3.73357700

Table S10. [9,9-$(PPh_3)_2$-8-(3-Mepy)-*arachno*-9,6-$RhSB_8H_9$] (**7b**) (-3072.28309155)

	x	**y**	**z**
C	-5.09329900	-1.26343800	2.49147300
C	-5.04918400	-0.39766000	1.39925900
C	-4.17148200	-2.31399600	2.57904900
C	-4.10267800	-0.60007200	0.40826000
C	-3.23548700	-2.43746800	1.55435000
H	-5.74954000	0.42473800	1.30274700
H	-2.47636200	-3.20929400	1.55827100
H	-4.18389500	-2.32112500	-2.34350400
H	-2.77869500	-4.30869300	-0.61828300
H	-1.81939200	-0.71800500	-1.14309900
H	-0.38828600	-3.34914400	0.58701000
H	-2.40624900	-4.61646100	-3.60037200
H	-0.03109500	-4.93647800	-1.91371900
H	0.26464900	-1.65545700	-2.71964100
H	1.65781600	-2.70299500	-1.76762900
H	0.33130500	-3.02880700	-4.27983700
N	-3.20173100	-1.60619000	0.48747400
B	-2.18302600	-1.83850700	-0.68987800
B	-2.99735800	-2.34670600	-2.20492500
B	-2.12698900	-3.52764600	-1.24699500
B	-0.70072400	-2.83716800	-0.45187600
B	-2.00546500	-3.69332500	-2.96882200
B	-0.53613400	-3.85667100	-1.93486500
B	0.49908800	-2.44241700	-1.72147200
B	-0.32798900	-2.74255100	-3.33048900
P	-0.63111600	1.70152100	-0.20799600
P	2.09145100	-0.72315100	0.30265500
S	-2.03327200	-1.94916000	-3.84351900
Rh	-0.11278100	-0.65430600	-0.45264600
H	-4.03585300	0.02340900	-0.47431400
C	-2.02141900	2.15834000	-1.36324400
C	-3.01266400	3.10245000	-1.05034400
C	-2.06936800	1.53190600	-2.62015200
C	-4.01935400	3.40974300	-1.96887700
H	-3.00862600	3.60033000	-0.08671500

C	-3.06854500	1.84816700	-3.54266300
H	-1.33284900	0.77398800	-2.87162500
C	-4.04883600	2.78761300	-3.21833700
H	-4.78057300	4.13965400	-1.70479200
H	-3.08526800	1.34515300	-4.50530700
H	-4.83347700	3.02761000	-3.93087500
C	0.64405500	2.97512100	-0.67333800
C	1.58702200	3.42261700	0.26768300
C	0.74567300	3.44410700	-1.99340900
C	2.59418700	4.31582400	-0.10103200
H	1.53489200	3.08441000	1.29634300
C	1.75724400	4.33328100	-2.36047700
H	0.02733700	3.12619000	-2.74178900
C	2.68540000	4.77380600	-1.41613500
H	3.30949300	4.64861600	0.64634100
H	1.81228000	4.68640400	-3.38704900
H	3.47127800	5.46780400	-1.70206900
C	-1.26413900	2.33271900	1.42199000
C	-1.25979100	3.68771100	1.79306500
C	-1.80705200	1.39773500	2.31600000
C	-1.78372400	4.09187500	3.02282500
H	-0.83658100	4.43114600	1.12486100
C	-2.33765800	1.80075900	3.54306100
H	-1.79260300	0.34480300	2.04721000
C	-2.32533500	3.15033800	3.90081400
H	-1.76697700	5.14420500	3.29446300
H	-2.75304900	1.05912000	4.22061400
H	-2.73058700	3.46685400	4.85836800
C	3.41168500	-0.36385900	-0.94107800
C	4.76421100	-0.69516600	-0.74774800
C	3.04224300	0.29084900	-2.12441500
C	5.71957000	-0.37248900	-1.71257200
H	5.07203500	-1.21895700	0.15220100
C	3.99850300	0.61627400	-3.08804300
H	1.99638500	0.53324000	-2.28718000
C	5.33861200	0.28531600	-2.88451700
H	6.76032700	-0.64078300	-1.55043900
H	3.69265600	1.12143900	-4.00015500
H	6.08282800	0.53163200	-3.63738000
C	2.49833300	0.42167700	1.71360600
C	1.52415700	0.60200900	2.70821100
C	3.71996900	1.09798100	1.84890200
C	1.76275400	1.42261100	3.81216700
H	0.56435500	0.10699400	2.60308500
C	3.95941200	1.92294500	2.95015900
H	4.48588700	0.99806800	1.08853200
C	2.98430800	2.08740500	3.93603100
H	0.98777600	1.55248100	4.56277100
H	4.91178700	2.44047600	3.03405200
H	3.17297300	2.73203900	4.79053000

C	2.61976800	-2.35152600	1.04516500
C	3.26400100	-3.33760500	0.28033600
C	2.31515400	-2.64705400	2.38362200
C	3.59641600	-4.57309800	0.83873400
H	3.51001600	-3.14874600	-0.75733300
C	2.64578900	-3.88268600	2.94025700
H	1.82494800	-1.90907200	3.00890000
C	3.28854300	-4.85249900	2.16988300
H	4.09377500	-5.31856600	0.22399200
H	2.40210400	-4.08338200	3.98056700
H	3.54654900	-5.81550100	2.60253200
H	-5.83891000	-1.12610400	3.27036200
C	-4.18139400	-3.29353500	3.72652100
H	-5.04173200	-3.97019700	3.65415200
H	-3.27658200	-3.90784600	3.73492000
H	-4.25230500	-2.77630800	4.68981000

Table S11. [6,6-$(PPh_3)_2$-9-(4-Mepy)-*arachno*-6,5-$RhSB_8H_9$] (**8a**) (-3072.28585866)

	x	**y**	**z**
Rh	0.03506700	-0.32640200	-0.76675900
B	-0.92771300	-2.37978900	-1.09644600
B	-2.74959200	-2.47332300	-0.76305800
B	-3.36235900	0.01924400	-2.19448900
B	-3.56820900	-1.70293900	-2.10249000
B	-2.06873100	-2.60462500	-2.43068700
B	-2.44632600	-1.11632200	-3.30688300
B	-0.74403400	-1.45761000	-2.58228800
P	1.80345600	-1.50254000	0.16533100
P	0.52617100	1.88377200	-0.00159900
S	-1.50215800	0.45678200	-2.48296900
B	-3.64668900	-0.78574700	-0.62058900
C	-6.21325000	-0.61603800	-0.77137200
H	-6.04043100	-0.45756300	-1.82698700
C	-7.48634600	-0.61455400	-0.22266300
H	-8.33680300	-0.45574700	-0.87832100
C	-7.66858000	-0.80573600	1.15204300
C	-6.50873500	-0.98404000	1.91952100
H	-6.57010600	-1.13091800	2.99336600
C	-5.26415900	-0.97862700	1.31468500
N	-5.10651500	-0.80093100	-0.01746000
H	-4.62998700	-2.16213600	-2.40610100
H	-2.58766400	-1.05803500	-4.48487400
H	-2.09005300	-3.62037900	-3.05414500
H	0.10443300	-1.58612200	-3.40586800
H	-4.12092800	0.78858100	-2.70685700
H	-3.18275200	-3.42107600	-0.17801600
H	-0.31730700	-3.34314300	-0.75426000
H	-2.93258200	-0.25586500	0.17337100

H	-1.71220500	-1.97937200	-0.11084200
H	-4.34766300	-1.11817800	1.87436200
C	0.47432100	2.23261600	1.82166500
C	0.24540800	1.17274300	2.70933100
C	0.56483300	3.53576400	2.34112600
C	0.14131600	1.39944700	4.08459900
H	0.13867100	0.16732500	2.31413800
C	0.47016800	3.76284100	3.71420700
H	0.69208400	4.37897100	1.66844300
C	0.26179500	2.69393000	4.59047000
H	-0.03485800	0.56240800	4.75541100
H	0.54794100	4.77638600	4.09922800
H	0.18253200	2.87325200	5.65962400
C	-0.67130600	3.19499400	-0.56203000
C	-0.29026000	4.36110500	-1.23995200
C	-2.03039700	3.00432300	-0.26050200
C	-1.24533600	5.31551500	-1.60329700
H	0.75157800	4.53132100	-1.48963000
C	-2.97983300	3.96003600	-0.61763400
H	-2.34818300	2.09583700	0.24352800
C	-2.59020400	5.12042500	-1.29158600
H	-0.93167800	6.21233700	-2.13161800
H	-4.02697600	3.79252400	-0.37958100
H	-3.33126600	5.86275200	-1.57632900
C	3.35549600	-0.59855100	0.69377600
C	3.43834900	-0.04404800	1.98297900
C	4.45259500	-0.43566600	-0.16545400
C	4.58277800	0.63450400	2.40261300
H	2.61371400	-0.15558400	2.67782500
C	5.59637600	0.24789000	0.25273900
H	4.43016800	-0.85835700	-1.16332000
C	5.66972300	0.78125700	1.53915000
H	4.62365000	1.04274900	3.40940500
H	6.43403200	0.35441100	-0.43158400
H	6.56438400	1.30464400	1.86652200
C	2.49815900	-2.71099800	-1.06497900
C	2.80287400	-4.04664800	-0.76918900
C	2.70990000	-2.24920400	-2.37510600
C	3.32457200	-4.89128700	-1.75216600
H	2.62102300	-4.44347900	0.22294700
C	3.24669400	-3.08850000	-3.35137600
H	2.42850200	-1.23256000	-2.63214400
C	3.55632900	-4.41453700	-3.04219500
H	3.54461400	-5.92687700	-1.50545200
H	3.40338200	-2.71018900	-4.35809500
H	3.96222200	-5.07385500	-3.80496800
C	2.13636200	2.55592700	-0.61937200
C	3.07630400	3.24286400	0.15909500
C	2.40896900	2.35320300	-1.98484400
C	4.25228200	3.73177100	-0.41692400

H	2.90432200	3.38960400	1.21952800
C	3.57565800	2.85449900	-2.56051600
H	1.70055000	1.79794500	-2.59480300
C	4.50160400	3.54795700	-1.77654900
H	4.97401000	4.25647600	0.20377300
H	3.76380500	2.69758100	-3.61951400
H	5.41442300	3.93453700	-2.22239400
C	1.52330200	-2.52253600	1.69897100
C	2.58924100	-3.12863800	2.38896200
C	0.22782300	-2.68087400	2.20955300
C	2.36097500	-3.88105400	3.54105500
H	3.60598400	-3.00469200	2.02932600
C	-0.00250300	-3.43003000	3.36667500
H	-0.60440200	-2.21274200	1.69605800
C	1.06243500	-4.03490500	4.03348800
H	3.19880700	-4.34363900	4.05640700
H	-1.01654600	-3.54183200	3.74177300
H	0.88520600	-4.61957300	4.93249300
C	-9.03971900	-0.83984800	1.77340500
H	-9.41558200	-1.87061000	1.81646900
H	-9.02470500	-0.45451300	2.79776900
H	-9.75745900	-0.25314500	1.19210600

Table S12. [9,9-$(PPh_3)_2$-8-(4-Mepy)-*arachno*-9,6-$RhSB_8H_9$] (**8b**) (-3072.28428584)

	x	**y**	**z**
C	-5.11061900	-1.27029600	2.46259100
C	-5.05309200	-0.60326700	1.22877800
C	-4.09507500	-2.19691200	2.72269100
C	-4.04365200	-0.88660300	0.32792200
C	-3.09597900	-2.42844800	1.78785400
H	-5.80410200	0.13223300	0.95805700
H	-4.07159100	-2.74671000	3.65845200
H	-2.28759300	-3.12772900	1.95784800
H	-3.85855700	-3.00130800	-2.11818300
H	-2.40499900	-4.58441700	-0.04849900
H	-1.66587600	-1.05772400	-1.09446000
H	-0.14368700	-3.26308100	1.07925500
H	-1.86595300	-5.31631200	-2.93319500
H	0.43948800	-5.19546200	-1.12772900
H	0.55249500	-2.06916700	-2.43207200
H	1.96117500	-2.84527900	-1.27015800
H	0.78179400	-3.65715300	-3.74846300
N	-3.06746600	-1.78634200	0.59925800
B	-1.97892000	-2.11810500	-0.48741200
B	-2.68150700	-2.91178400	-1.93165700
B	-1.77829300	-3.86369700	-0.76842300
B	-0.44582700	-2.95122400	-0.03923200
B	-1.56120400	-4.27999900	-2.43818400

B	-0.13640800	-4.17257700	-1.33615000
B	0.78670200	-2.66838100	-1.31096400
B	0.06017900	-3.27573000	-2.88135800
P	-0.69425600	1.56019500	-0.44603100
P	2.17258700	-0.55858500	0.46269600
S	-1.66749700	-2.69727700	-3.57578900
Rh	-0.00567700	-0.76066500	-0.35507300
H	-3.98199100	-0.40900800	-0.64188100
C	-2.07475000	1.75989100	-1.68452500
C	-3.12805400	2.67472200	-1.52745500
C	-2.05029100	0.96085300	-2.84019000
C	-4.12731900	2.78413500	-2.49741800
H	-3.17807700	3.30315000	-0.64485900
C	-3.04344400	1.07802600	-3.81483800
H	-1.26073100	0.22590400	-2.96931800
C	-4.08729400	1.98914400	-3.64446500
H	-4.93769600	3.49465900	-2.35436800
H	-3.00431700	0.44420900	-4.69619400
H	-4.86658800	2.07479400	-4.39707600
C	0.49911900	2.85999600	-1.03612800
C	1.39704900	3.46391700	-0.13939300
C	0.58817700	3.19507100	-2.39707500
C	2.34885400	4.37877900	-0.59191500
H	1.35215000	3.23012700	0.91828500
C	1.54563700	4.10578900	-2.84766800
H	-0.09721700	2.75327800	-3.11279400
C	2.42946500	4.70187000	-1.94737200
H	3.02994900	4.83518800	0.12139000
H	1.59285000	4.35314000	-3.90509600
H	3.17303500	5.41252900	-2.29820100
C	-1.42780600	2.34037800	1.07356800
C	-1.51643300	3.72705400	1.27893500
C	-1.95224300	1.48447600	2.05395400
C	-2.11230500	4.23973100	2.43323900
H	-1.11054300	4.41097300	0.54012900
C	-2.55408400	1.99542500	3.20552800
H	-1.86455400	0.41042100	1.91299500
C	-2.63406300	3.37605900	3.39892900
H	-2.16688900	5.31565600	2.57764700
H	-2.95058100	1.31444100	3.95441300
H	-3.09456600	3.77730600	4.29800300
C	3.49182000	-0.22225000	-0.78879000
C	4.86423600	-0.39299400	-0.53526600
C	3.09452400	0.24833500	-2.04818100
C	5.81045600	-0.09299500	-1.51627800
H	5.19624300	-0.77536000	0.42517000
C	4.04134700	0.55172100	-3.02819700
H	2.03467900	0.36485300	-2.25397200
C	5.40086200	0.38132300	-2.76469200
H	6.86730400	-0.23583200	-1.30620700

H	3.71369000	0.91454200	-3.99857700
H	6.13876400	0.61023700	-3.52917200
C	2.43519800	0.76631800	1.74733500
C	1.40930300	0.98277100	2.68100100
C	3.59829700	1.54460100	1.84589500
C	1.54167200	1.93788400	3.69057500
H	0.49147500	0.40969600	2.60132100
C	3.73115500	2.50395700	2.85229000
H	4.40103800	1.41874000	1.12870100
C	2.70585100	2.70326600	3.77903800
H	0.72778000	2.09209600	4.39389000
H	4.63959400	3.09853100	2.90840700
H	2.81118500	3.45226600	4.55956500
C	2.81602000	-2.03622900	1.40321000
C	3.60774300	-3.02131100	0.79139700
C	2.45266400	-2.22024200	2.74696000
C	4.02806400	-4.14628800	1.50341700
H	3.90086100	-2.91853900	-0.24620800
C	2.87080600	-3.34545500	3.45712300
H	1.84531300	-1.47950400	3.25520500
C	3.66184000	-4.31439600	2.83834300
H	4.63928900	-4.89409000	1.00522900
H	2.57777900	-3.46123500	4.49756000
H	3.98804100	-5.19162500	3.39076500
C	-6.22408600	-1.01032400	3.44263200
H	-6.40392100	0.06371400	3.56337100
H	-7.16193000	-1.45737000	3.08869700
H	-6.00234300	-1.43656200	4.42521500

2. Kinetic studies of the reaction between 1 and 2-Mepy

Table S13. Reaction de **1** with 5 equivalents of 2-Mepy at 298 K in CD_2Cl_2. The change in the concentration of **1** with time was monitored by ^1H-{^{11}B} NMR spectroscopy, using the solvent residual signal as internal standard.

t (min)	[1]	ln(C/Co)
0.0	0.04000	0.00000
0.8	0.03893	-0.02714
1.6	0.03846	-0.03936
2.4	0.03749	-0.06470
3.1	0.03652	-0.09103
3.9	0.03601	-0.10518
4.7	0.03565	-0.11507
5.5	0.03477	-0.14013
6.3	0.03380	-0.16830
7.1	0.03342	-0.17968
7.8	0.03237	-0.21158
8.6	0.03179	-0.22978
9.4	0.03109	-0.25193
10.2	0.03097	-0.25592
11.0	0.02999	-0.28810
11.8	0.02921	-0.31420
12.5	0.02878	-0.32923
13.3	0.02812	-0.35246
14.1	0.02733	-0.38099
14.9	0.02737	-0.37926
15.7	0.02659	-0.40832
16.5	0.02602	-0.43008
17.2	0.02562	-0.44560
18.0	0.02493	-0.47292
18.8	0.02443	-0.49309
19.6	0.02395	-0.51271
20.4	0.02364	-0.52588
21.2	0.02337	-0.53764
21.9	0.02290	-0.55757
22.7	0.02220	-0.58867
23.5	0.02149	-0.62122
24.3	0.02152	-0.61984
25.1	0.02129	-0.63084
25.9	0.02069	-0.65945
26.6	0.01992	-0.69702
27.4	0.01963	-0.71202
28.2	0.01934	-0.72662
29.0	0.01881	-0.75452
29.8	0.01822	-0.78625
30.6	0.01813	-0.79150

31.3	0.01786	-0.80654
32.1	0.01767	-0.81673
32.9	0.01675	-0.87057
33.7	0.01654	-0.88303
34.5	0.01605	-0.91297
35.3	0.01568	-0.93657
36.0	0.01574	-0.93294
36.8	0.01518	-0.96897
37.6	0.01441	-1.02091
38.4	0.01453	-1.01257
39.2	0.01409	-1.04365
40.0	0.01369	-1.07220
40.7	0.01357	-1.08137
41.5	0.01351	-1.08510
42.3	0.01315	-1.11230
43.1	0.01277	-1.14179
43.9	0.01263	-1.15284
44.7	0.01251	-1.16208
45.4	0.01225	-1.18352
46.2	0.01184	-1.21778
47.0	0.01141	-1.25408
47.8	0.01148	-1.24790
48.6	0.01068	-1.32078
49.4	0.01048	-1.33987
50.1	0.01051	-1.33666
50.9	0.01056	-1.33197
51.7	0.01004	-1.38198
52.5	0.00998	-1.38833
53.3	0.00960	-1.42716
54.1	0.00968	-1.41844
54.8	0.00900	-1.49193

Table S14. Reaction of **1** with 7 equivalents of 2-Mepy at 298 K in CD_2Cl_2. The change in the concentration of 1 with time was monitored by 1H-{11B} NMR spectroscopy, using the solvent residual signal as internal standard.

t (min)	[1]	ln(C/Co)
0.0	0.040	0.000
0.9	0.036	0.126
1.8	0.033	0.048
2.7	0.029	-0.124
3.5	0.025	-0.262
4.4	0.024	-0.281
5.3	0.022	-0.410
6.2	0.019	-0.445
7.1	0.018	-0.551

8.0	0.016	-0.645
8.8	0.015	-0.713
9.7	0.011	-1.019
10.6	0.013	-0.915
11.5	0.011	-1.022
12.4	0.011	-1.088
13.3	0.009	-1.249
14.1	0.007	-1.460
15.0	0.009	-1.277
15.9	0.007	-1.458
16.8	0.006	-1.719
17.7	0.006	-1.743
18.6	0.005	-1.825
19.4	0.004	-2.140
20.3	0.006	-1.706
21.2	0.002	-2.803
22.1	0.004	-2.194
23.0	0.003	-2.515

Table S15. Reaction of **1** with 10 equivalents of 2-Mepy at 298 K in CD_2Cl_2. The change in the concentration of **1** with time was monitored by ^{1}H-{^{11}B} NMR spectroscopy, using the solvent residual signal as internal standard.

t (min)	[1]	ln(C/Co)
0.0	0.040	0.000
0.9	0.038	-0.043
1.7	0.038	-0.051
2.6	0.034	-0.157
3.5	0.034	-0.156
4.3	0.032	-0.225
5.2	0.029	-0.307
6.1	0.031	-0.258
6.9	0.029	-0.317
7.8	0.028	-0.372
8.7	0.029	-0.334
9.5	0.026	-0.447
10.4	0.023	-0.550
11.3	0.022	-0.599
12.1	0.020	-0.669
13.0	0.022	-0.604
13.9	0.023	-0.557
14.7	0.021	-0.621
15.6	0.018	-0.794
16.5	0.016	-0.911
17.3	0.016	-0.942

18.2	0.016	-0.934
19.1	0.014	-1.045
19.9	0.017	-0.872
20.8	0.013	-1.116
21.7	0.014	-1.068
22.5	0.011	-1.268
23.4	0.013	-1.163
24.3	0.010	-1.379
25.1	0.010	-1.399
26.0	0.007	-1.678

Tabe S16. Reaction of **1** with 15 equivalents of 2-Mepy at 298 K in CD_2Cl_2. The change in the concentration of **1** with time was monitored by 1H-{11B} NMR spectroscopy, using the solvent residual signal as internal standard.

t (min)	[1]	ln(C/Co)
0.0	0.04000	0.00000
0.8	0.03853	-0.03740
1.6	0.03666	-0.08710
2.4	0.03579	-0.11121
3.1	0.03625	-0.09833
3.9	0.03398	-0.16321
4.7	0.03330	-0.18343
5.5	0.03210	-0.22013
6.3	0.03050	-0.27128
7.1	0.02842	-0.34184
7.8	0.02878	-0.32926
8.6	0.02590	-0.43457
9.4	0.02466	-0.48355
10.2	0.02506	-0.46774
11.0	0.02207	-0.59478
11.8	0.02296	-0.55492
12.5	0.02012	-0.68721
13.3	0.01932	-0.72751
14.1	0.01916	-0.73617
14.9	0.01716	-0.84618
15.7	0.01594	-0.92020
16.5	0.01451	-1.01387
17.2	0.01318	-1.11005
18.0	0.01625	-0.90108
18.8	0.01311	-1.11514
19.6	0.01237	-1.17361
20.4	0.01225	-1.18304
21.2	0.01048	-1.33924
21.9	0.01042	-1.34520

22.7	0.01030	-1.35670
23.5	0.01157	-1.24007
24.3	0.00915	-1.47466
25.1	0.00866	-1.53039
25.85	0.00762	-1.65808
26.6	0.00722	-1.71185
27.4	0.00672	-1.78439
28.2	0.00940	-1.44832
29.0	0.00639	-1.83486
29.8	0.00645	-1.82488
30.6	0.00540	-2.00274
31.3	0.00446	-2.19340
32.1	0.00475	-2.13153
32.9	0.00403	-2.29558
33.7	0.00377	-2.36241

Table S17. Reaction of **1** with 15 equivalents of 2-Mepy at 298 K in CD_2Cl_2. The change in the concentration of **1** with time was monitored by ^{1}H-{^{11}B} NMR spectroscopy, using the solvent residual signal as internal standard.

t (min)	**[3]**	**ln(C/Co)**
0.0	0.0400	0.0000
0.7	0.0372	-0.0736
1.4	0.0350	-0.1322
2.1	0.0334	-0.1817
2.8	0.0313	-0.2461
3.5	0.0301	-0.2829
4.2	0.0289	-0.3265
4.9	0.0262	-0.4235
5.6	0.0252	-0.4628
6.3	0.0239	-0.5163
7.0	0.0223	-0.5839
7.7	0.0220	-0.5986
8.4	0.0210	-0.6434
9.1	0.0195	-0.7209
9.8	0.0188	-0.7553
10.5	0.0181	-0.7909
11.2	0.0166	-0.8772
11.9	0.0160	-0.9162
12.6	0.0151	-0.9739
13.3	0.0148	-0.9930
14	0.0136	-1.0813
14.7	0.0129	-1.1346
15.4	0.0125	-1.1647
16.1	0.0111	-1.2808
16.8	0.0110	-1.2895

17.5	0.0102	-1.3651
18.2	0.0098	-1.4087
18.9	0.0091	-1.4762
19.6	0.0085	-1.5452
20.3	0.0080	-1.6053
21	0.0082	-1.5789
21.7	0.0072	-1.7210
22.4	0.0067	-1.7886
23.1	0.0064	-1.8342
23.8	0.0059	-1.9165
24.5	0.0056	-1.9611
25.2	0.0058	-1.9240
25.9	0.0006	-2.0229