Utilisation of a Lithium Boryl as a Reducing Agent in Low Oxidation State Group 15 Chemistry: Synthesis and Characterisation of an Amido-Distibene and a Boryl-Dibismuthene

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SUPPLEMENTARY INFORMATION

(31 pages)

Contents

1. Syntheses

General considerations. All manipulations were carried out using standard Schlenk and glove box techniques under an atmosphere of high purity dinitrogen. Diethyl ether and pentane were distilled over Na/K alloy (25:75), while THF, hexane and toluene were distilled over molten potassium. ^{1}H, ^{13}C{^{1}H}, ^{29}Si{^{1}H} and ^{11}B{^{1}H} NMR spectra were recorded on either Bruker AvanceIII 400 or Bruker DPX300 spectrometers and were referenced to the resonances of the solvent used, external $SiMe_4$ or $[BF_3(OEt_2)]$. IR spectra were recorded for solid samples using an Agilent Cary 630 attenuated total reflectance (ATR) spectrometer. UV/visible spectra were recorded on a Cary 1E spectrometer. Mass spectra were recorded on an Agilent Techonlogies 5975D inert MSD with a solid state probe. Melting points were determined in sealed glass capillaries under dinitrogen, and are uncorrected. Microanalyses were carried out at the Science Centre, London Metropolitan University. LK(THF) (L = L*, L', L† or L^{Ph}) were prepared by deprotonation of LH with KH in THF at ambient temperature,[1] while $(THF)_2$LiB(DAB) was prepared by a literature procedure.[2] All other reagents were used as received.

Synthesis of L*AsCl$_2$, 1a. A solution of L*K(THF) (0.50 g, 0.80 mmol) in THF (20 cm^3) was added to a solution of $AsCl_3$ (0.16 g, 74 μL, 0.88 mmol) in THF (10 cm^3) at -78 °C. The reaction mixture was warmed to room temperature over a period of 12 hrs whereupon volatiles were removed *in vacuo*, and the residue extracted with toluene (40 cm^3). The extract was concentrated to *ca.* 20 cm^3 and stored at -30°C overnight to give colourless crystals of **1a** (0.30 g, 69%). Mp: 98-100 °C; ^{1}H NMR (400 MHz, C_6D_6, 298 K): δ = 0.37 (s, 9H, Si(CH_3)$_3$), 1.73 (s, 3H, ArCH_3), 6.47 (s,

2H, C*H*Ph_2), 6.71-7.43 (m, 22H, Ar-*H*); $^{13}C\{^1H\}$ NMR (100 MHz, C_6D_6, 298 K): δ = 4.1 (Si(*C*H_3)$_3$), 21.0 (Ar*C*H_3), 51.9 (*C*HPh_2), 126.8, 126.9, 127.2, 128.8, 130.0, 130.4, 130.6, 131.9, 137.0, 143.7, 144.2, 145.1 (Ar-*C*); $^{29}Si\{^1H\}$ NMR (80 MHz, C_6D_6, 298 K): δ = 17.5; IR *ν*/cm^{-1} (ATR): 1598(w), 1493(m), 1447(m), 1376(w), 1253(m), 1196(w), 1120(w), 1077(w), 1031(w), 892(m), 863(m), 837(s), 746(m); MS (EI) *m/z* (%): 656.1 (M^+, 1), 510.4 (L^{*+}, 100), 439.3 (Ar*NH_2^+, 45), 167.1 ($CHPh_2^+$, 50), 73.1 ($SiMe_3^+$, 48); anal. calc. for $C_{36}H_{36}Cl_2NAsSi$: C 65.85%, H 5.53%, N 2.13%, found: C 65.69%, H 5.42%, N 2.21%.

Synthesis of L'AsCl$_2$, 1b. This compound was prepared by a similar procedure to that employed for the synthesis of **1a**, except using L'K(THF) (1.0 g, 1.53 mmol) and $AsCl_3$ (0.14 mL, 1.69 mmol). The compound was obtained as a colourless microcrystalline solid (0.80 g, 76%). Mp: 110-113 °C; ^1H NMR (300 MHz, C_6D_6, 298 K): δ = 0.37 (s, 9H, Si(CH_3)$_3$), 0.85 (d, $^3J_{HH}$ = 6.9 Hz, 6H, CH(CH_3)$_2$), 2.37 (sept., $^3J_{HH}$ = 6.9 Hz, 1H, C*H*(CH$_3$)$_2$), 6.49 (s, 2H, C*H*Ph_2), 6.99-7.28 (m, 22H, Ar-*H*); $^{13}C\{^1H\}$ NMR (75 MHz, C_6D_6, 298 K): δ = 4.0 (Si(*C*H_3)$_3$), 23.5 (CH(*C*H_3)$_2$), 33.6 (*C*H(CH$_3$)$_2$), 52.0 (*C*HPh_2), 126.9, 127.1, 128.6, 128.7, 128.8, 129.2, 130.3, 130.5, 143.8, 144.3, 144.9, 147.4 (Ar-*C*); $^{29}Si\{^1H\}$ NMR (C_6D_6, 80 MHz, 296 K): no signal observed, even for concentrated samples and long spectral acquisition times; IR *ν*/cm^{-1} (ATR): 1598(m), 1492(s), 1453(s), 1377(m), 1254(s), 1197(w), 1117(m), 1077(w), 1031(m), 894(s), 841(s), 817(s), 744(s); MS (EI) *m/z* (%): 538.5 ($L^{\dagger+}$, 100), 167.2 ($CHPh_2^+$, 50), 73.2 $(SiMe_3)^+$, 28). N.B. A reproducible microanalysis could not be obtained for this compound, though it was shown to have a purity of > 95% by ^1H NMR spectroscopy.

Synthesis of L'SbBr$_2$, 1c. This compound was prepared by a similar procedure to that employed for the synthesis of **1a**, except using L'K(THF) (1.0 g, 1.53 mmol) and $SbBr_3$ (0.58 g, 1.61 mmol). The compound was obtained as a colourless crystalline solid (0.90 g, 71%). Mp: 140-143 °C dec. ^1H NMR (300 MHz, C_6D_6): δ = 0.64 (s, 9H, Si(CH_3)$_3$), 1.03 (d, $^3J_{HH}$ = 6.9 Hz, 6H, CH(CH_3)$_2$), 2.56 (sept., $^3J_{HH}$ = 6.9 Hz, 1H, C*H*(CH$_3$)$_2$), 6.67 (s, 2H, C*H*Ph_2), 7.22-7.47 (m, 22H, Ar-*H*); $^{13}C\{^1H\}$ NMR (75 MHz, C_6D_6): δ = 4.7 (Si(*C*H_3)$_3$), 23.6 (CH(*C*H_3)$_2$), 33.5 (*C*H(CH$_3$)$_2$), 52.0 (*C*HPh_2), 126.9, 127.5, 128.5, 128.6, 128.7, 129.1, 130.3, 131.0, 144.1, 144.3, 144.5, 146.3 (Ar-*C*); $^{29}Si\{^1H\}$ NMR (C_6D_6, 80 MHz, 296 K): no signal observed, even for concentrated samples and long spectral acquisition times; IR *ν*/cm^{-1} (ATR): 1598(m), 1492(s), 1432(s), 1248(s), 1196(m), 1115(m), 1075(m), 1031(s), 881(s), 842(s), 743(s); MS (EI) *m/z* (%): 740 (L'SbBrH$^+$, 2), 538.5 (L'^+, 100), 467.4 (Ar†NH_2^+, 23), 167.2 ($CHPh_2^+$, 29), 73.2 ($SiMe_3^+$, 28); anal. calc. for $C_{38}H_{40}Br_2NSbSi$: C 55.63%, H 4.91%, N 1.71%, found: C 55.69%, H 5.01%, N 1.80%.

Synthesis of L†SbBr$_2$, 1d. This compound was prepared by a similar procedure to that employed for the synthesis of **1a**, except using L†K(THF) (1.0 g, 1.36 mmol) and $SbBr_3$ (0.52 g, 1.43 mmol). The compound was obtained as a colourless crystalline solid (0.86 g, 70%). Mp: 206-210 °C; ^{1}H NMR (C_6D_6, 300 MHz, 298 K): δ = 0.88 (d, 6H, $^3J_{HH}$ = 6.9 Hz, Ar-CH(CH_3)$_2$), 1.27 (d, 18H, $^3J_{HH}$= 7.5 Hz, SiCH(CH_3)$_2$), 1.91 (sept., 3H, $^3J_{HH}$ = 7.5 Hz , SiC*H*(CH$_3$)$_2$), 2.43 (sept., 1H, $^3J_{HH}$ = 6.9 Hz Ar-C*H*(CH$_3$)$_2$), 6.52 (s, 2H, C*H*Ph$_2$) 7.38-6.93 (m, 22H, Ar-*H*); ^{13}C{^{1}H} NMR (100 MHz, C_6D_6, 298 K): δ = 15.0 (Si*C*H(CH$_3$)$_2$), 19.9 (SiCH(*C*H$_3$)$_2$), 23.6 (Ar-CH(*C*H$_3$)$_2$), 33.6 (Ar-*C*H(CH$_3$)$_2$), 51.3 (*C*HPh$_2$), 126.6, 127.9, 128.5, 128.6, 128.9, 130.2, 131.5, 141.7, 144.6, 145.0, 145.2, 146.9 (Ar-*C*); ^{29}Si{^{1}H} NMR (80 MHz, C_6D_6, 298 K): δ = 16.6; IR *v*/cm^{-1} (Nujol): 1599(w), 1492(m), 1450(m), 1381(w), 1258(m), 1183(w), 1108(w), 1078(w), 865(m), 816(s), 863(m), 727(s); MS (EI) *m/z* (%): 467.4 (Ar†NH$_2^+$, 28), 167.2 (CHPh$_2^+$, 39); anal. calc. for $C_{44}H_{52}Br_2NSbSi$: C 58.42%, H 5.79%, N 1.55%, found: C 58.47%, H 5.71%, N 1.57%.

Synthesis of L'BiBr$_2$, 1e. This compound was prepared by a similar procedure to that employed for the synthesis of **1a**, except using L'K(THF) (1.0 g, 1.53 mmol) and $BiBr_3$ (0.72 g, 1.61 mmol). The compound was obtained as a yellow crystalline solid (0.68 g, 49%). Mp: 166-171 °C; ^{1}H NMR (400 MHz, C_6D_6, 298 K): δ = 0.51 (s, 9H, Si(CH_3)$_3$), 0.88 (d, $^3J_{HH}$ = 6.8 Hz, 6H, CH(CH_3)$_2$), 2.53 (sept., $^3J_{HH}$ = 6.8 Hz, 1H, C*H*(CH$_3$)$_2$), 6.69 (s, 2H, C*H*Ph$_2$), 7.25-6.91 (m, 22H, Ar-*H*); ^{13}C{^{1}H} NMR (100 MHz, C_6D_6, 298 K): δ = 5.6 (Si(*C*H$_3$)$_3$), 24.1 (CH(*C*H$_3$)$_2$), 33.5 (*C*H(CH$_3$)$_2$), 51.8 (*C*HPh$_2$), 126.8, 127.1, 128.5, 128.6, 129.4, 129.9, 130.2, 131.1, 144.1, 144.4, 145.6, 145.9 (Ar-*C*); ^{29}Si{^{1}H} NMR (80 MHz, C_6D_6, 298 K): δ = 0.1; IR *v*/cm^{-1} (ATR): 1596(w), 1491(m), 1449(s), 1377(m), 1242(s), 1198(m), 1118(m), 1074(m), 1031(m), 887(s), 843(s), 817(s), 744(s); MS(EI) *m/z* (%): 539.5 (L'H$^+$, 100), 467.4 (Ar†NH$_2^+$, 58), 167.2 (CHPh$_2^+$, 50), 73.1 (SiMe$_3^+$, 80); anal. calc. for $C_{38}H_{40}Br_2NBiSi$: C 50.29%, H 4.44%, N 1.54%, found: C 50.13%, H 4.48%, N 1.62%.

Synthesis of L†BiBr$_2$, 1f. This compound was prepared by a similar procedure to that employed for the synthesis of **1a**, except using L†K(THF) (1.0 g, 1.36 mmol) and $BiBr_3$ (0.64 g, 1.43 mmol). The compound was obtained as a yellow crystalline solid (0.76 g, 56%). Mp: 237-242 °C (decomp.); ^{1}H NMR (300 MHz, C_6D_6, 298 K): δ = 0.88 (d, 6H, $^3J_{HH}$ = 6.9 Hz, Ar-CH(CH_3)$_2$), 1.37 (d, 18H, $^3J_{HH}$= 7.5 Hz, SiCH(CH_3)$_2$), 1.91 (sept., 3H, $^3J_{HH}$ = 7.5 Hz , SiC*H*(CH$_3$)$_2$), 2.52 (sept., 1H, $^3J_{HH}$ = 6.9 Hz Ar-C*H*(CH$_3$)$_2$), 7.34-6.84 (m, 24H, C*H*Ph$_2$ and Ar-*H*); ^{13}C{^{1}H} NMR (100 MHz, C_6D_6, 298 K): δ = 16.4 (Si*C*H(CH$_3$)$_2$), 20.0 (SiCH(*C*H$_3$)$_2$), 24.1 (Ar-*C*H(CH$_3$)$_2$), 33.4 (Ar-CH(*C*H$_3$)$_2$), 51.0 (*C*HPh$_2$), 126.9, 127.4, 128.4, 128.7, 129.3, 130.1, 131.4, 141.9, 144.5, 146.6, 146.9, 147.8 (Ar-*C*); ^{29}Si{^{1}H} NMR (80 MHz, C_6D_6, 298 K): δ = 17.2; IR *v*/cm^{-1} (ATR): 1598(w), 1492(m), 1449(m), 1380(w),

1259(m), 1193(w), 1113(w), 1077(w), 875(m), 826(s), 863(m), 809(m); MS (EI) *m/z* (%): 623.5 ($L^{\dagger}H^{+}$, 35), 580.5 ($L^{\dagger}$-Pr^{i+}, 100), 167.0 ($CHPh_2^{+}$, 100); anal. calc. for $C_{44}H_{52}Br_2NBiSi$: C 53.29%, H 5.28%, N 1.41%, found: C 53.12%, H 5.24%, N 1.48%.

Synthesis of $L^{Ph}BiBr_2$, 1g. This compound was prepared by a similar procedure to that employed for the synthesis of **1a**, except using $L^{Ph}K(THF)$ (0.5 g, 0.61 mmol) and $BiBr_3$ (0.29 g, 0.64 mmol). The compound was obtained as a yellow crystalline solid (0.35 g, 54%). Mp: 157-162 °C (decomp.); ^{1}H NMR (400 MHz, C_6D_6, 298 K): δ = 2.17 (s, 3H, ArC*H*$_3$), 6.42 (m, 2H, C*H*Ph$_2$), 6.41-7.57 (m, 37H, Ar-*H*); ^{13}C{^{1}H} NMR (100 MHz, C_6D_6, 298 K): δ = 20.6 (Ar*C*H$_3$), 51.1 (*C*HPh$_2$), 125.9, 126.4, 128.4, 128.7, 129.3, 130.0, 130.1, 130.5, 130.9, 132.0, 136.4, 137.8, 144.4, 144.7, 145.5, 145.8 (Ar-*C*), ^{29}Si{^{1}H} NMR (800 MHz, C_6D_6, 298 K): δ = -12.7; IR ν/cm-1 (ATR): 1812(w), 1596(w), 1491(m), 1428(s), 1376(w), 1260(w), 1231(w), 1203(m), 1106(s), 1029(m), 898(s), 850.(m), 790(m), 763(w), 738(m), 703(s); MS (EI) *m/z* (%): 907.4 ($L^{Ph}Bi^{+}$, 4), 259.1 ($SiPh_3H^{+}$, 19), 167.0 ($CHPh_2^{+}$, 100); N.B. A reproducible microanalysis could not be obtained for this compound, though it was shown to have a purity of > 95% by ^{1}H NMR spectroscopy.

Synthesis of L*As(H){B(DAB)} 3a. The reaction of **1a** with two equivalents of **2** in toluene afforded a complex mixture of products, from which a few dark orange crystals of **3a** were isolated. The yield of the compound was too low for the acquisition of any characterising data. Details of the crystal structure of the compound can be found below.

Synthesis of L'As(H){B(DAB)} 3b. The reaction of **1b** with two equivalents of **2** in toluene afforded a complex mixture of products, from which a few dark orange crystals of **3b** were isolated. The yield of the compound was too low for the acquisition of any characterising data. Details of the crystal structure of the compound can be found below.

Synthesis of $L^{\dagger}Sb=SbL^{\dagger}$, 4, and {(DAB)B}Bi=Bi{B(DAB)}, 5. See main text for details.

Synthesis of $L^{Ph}Bi=Bi\{B(DAB)\}$. The reaction of **1g** with two equivalents of **2** in toluene resulted in deposition of bismuth metal, and a complex mixture of products, from which a few dark blue crystals of the title compound were isolated. The yield of the compound was too low for the acquisition of any characterising data. Details of the crystal structure of the compound can be found below.

2. X-Ray Crystallography

Crystals of **1a**, **1c-1g**, **3a**·(hexane)$_{0.25}$, **3b**·(pentane)$_{0.25}$, **4**·(pentane)$_2$, **5**, and L^{Ph}Bi=Bi{B(DAB)}·(pentane) (**1S**·(pentane)) suitable for X-ray structural determination were mounted in silicone oil. Crystallographic measurements were carried out with either a Bruker Apex X8 diffractometer using a graphite monochromator with Mo Kα radiation (λ = 0.71073 Å), or the MX1 beamline of the Australian Synchrotron (λ = 0.7108 Å). The software package Blu-Ice[3] was used for synchrotron data acquisition, while the program XDS[4] was employed for synchrotron data reduction. All structures were solved by direct methods and refined on F^2 by full matrix least squares (SHELX97)[5] using all unique data. Hydrogen atoms are included in calculated positions (riding model), except for the hydride ligands of **3a** and **3b**, the positional parameters of which were freely refined. Crystal data, details of data collections and refinements for all structures can be found in their CIF files and are summarized in Table S1.

Table S1. 1a, **1c-1g**, **3a**·(hexane)$_{0.25}$, **3b**·(pentane)$_{0.25}$, **4**·(pentane)$_2$, **5**, and L^{Ph}Bi=Bi{B(DAB)}·(pentane) (**1S**·(pentane))

	1a	**1c**	**1d**	**1e**	**1f**	**1g**	**3a**
empirical formula	$C_{36}H_{36}AsCl_2NSi$	$C_{38}H_{40}Br_2NSbSi$	$C_{44}H_{52}Br_2NSbSi$	$C_{38}H_{40}BiBr_2NSi$	$C_{44}H_{52}BiBr_2NSi$	$C_{51}H_{42}BiBr_2NSi$	$C_{63.50}H_{73.50}AsBN_3Si$
formula weight	656.57	820.37	904.53	907.60	991.76	1065.75	992.57
crystal system	triclinic	triclinic	monoclinic	triclinic	monoclinic	triclinic	triclinic
space group	*P*-1	*P*-1	$P2_1/c$	*P-1*	$P2_1/c$	*P-1*	*P-1*
a (Å)	8.8947(5)	10.1762(6)	10.104(2)	10.1646(5)	10.130(2)	10.3779(4)	12.3574(10)
b (Å)	12.7255(8)	11.2391(8)	17.041(3)	11.2590(6)	17.182(3)	12.1720(4)	12.6670(10)
c (Å)	15.2825(9)	15.5145(8)	23.615(5)	15.5011(7)	23.696(5)	18.3157(7)	19.7946(18)
α (deg.)	78.686(3)	95.865(5)	90	95.931(4)	90	82.925(2)	99.963(7)
β (deg)	73.993(3)	95.903(5)	101.92(3)	96.150(4)	102.26(3)	88.322(2)	104.228(7)
γ (deg.)	70.480(3)	100.813(5)	90	100.498(4)	90	66.682(2)	100.574(7)
vol (Å^3)	1556.81(16)	1720.21(18)	3978.4(14)	1720.51(15)	4030.3(14)	2108.00(13)	2874.0(4)
Z	2	2	4	2	4	2	2
ρ (calcd) (g.cm^{-3})	1.401	1.584	1.510	1.752	1.634	1.679	1.147
μ (mm^{-1})	1.329	3.187	2.764	7.508	6.418	6.143	0.652
F(000)	680	820	1832	884	1960	1044	1055
T (K)	123(2)	123(2)	123(2)	123(2)	100(2)	123(2)	123(2)
reflections collected	19087	13213	27969	15473	27660	20733	22745
unique reflections	5772	6406	7298	6404	6842	8685	10322
R_{int}	0.0237	0.0338	0.0921	0.0419	0.0796	0.0321	0.1102

R1 indices [$I>2\sigma(I)$]	0.0379	0.0274	0.0414	0.0307	0.0480	0.0289	0.1023
*w*R2 indices (all data)	0.0863	0.0619	0.1091	0.0661	0.1277	0.0655	0.3149
CCDC No.	1051441	1051442	1051443	1051444	1051445	1051446	1051448

Table S1 (contd.). 1a, **1c-1g**, **3a**·(hexane)$_{0.25}$, **3b**·(pentane)$_{0.25}$, **4**·(pentane)$_2$, **5**, and L^{Ph}Bi=Bi{B(DAB)}·(pentane) (**1S**·(pentane))

	3b	**4**	**5**	**1S**
empirical formula	$C_{65.25}H_{80}AsBN_3Si$	$C_{98}H_{128}N_2Sb_2Si_2$	$C_{52}H_{72}B_2Bi_2N_4$	$C_{82}H_{90}BBi_2N_3Si$
formula weight	1020.14	1633.70	1192.72	1574.43
crystal system	triclinic	triclinic	triclinic	triclinic
space group	*P*-1	*P*-1	*P-1*	*P-1*
a (Å)	12.4034(7)	12.6918(10)	10.5010(7)	13.6508(5)
b (Å)	13.3700(8)	13.6933(10)	12.7973(14)	14.2481(6)
c (Å)	20.1020(12)	14.0983(11)	21.8679(9)	20.2258(7)
α (deg.)	77.434(5)	72.740(7)	88.502(5)	97.059(3)
β (deg)	77.587(5)	77.066(7)	76.645 (4)	95.917(3)
γ (deg.)	65.731(6)	67.955(7)	67.584(8)	112.943(4)
vol (Å^3)	2936.5(3)	2151.2(3)	2636.9(4)	3545.8(2)
Z	2	1	2	2
ρ (calcd) (g.cm^{-3})	1.154	1.261	1.502	1.475
μ (mm^{-1})	0.640	0.702	6.700	5.019
F(000)	1089	860	1176	1576

T (K)	123(2)	123(2)	123(2)	123(2)
reflections collected	26319	16202	19674	27961
unique reflections	10880	7999	9810	13193
R_{int}	0.0357	0.0390	0.0418	0.0410
R1 indices [$I>2\sigma(I)$]	0.0492	0.0473	0.0406	0.0396
*w*R2 indices (all data)	0.1362	0.1285	0.0902	0.0924
CCDC No.	1051449	1051450	1051451	1051447

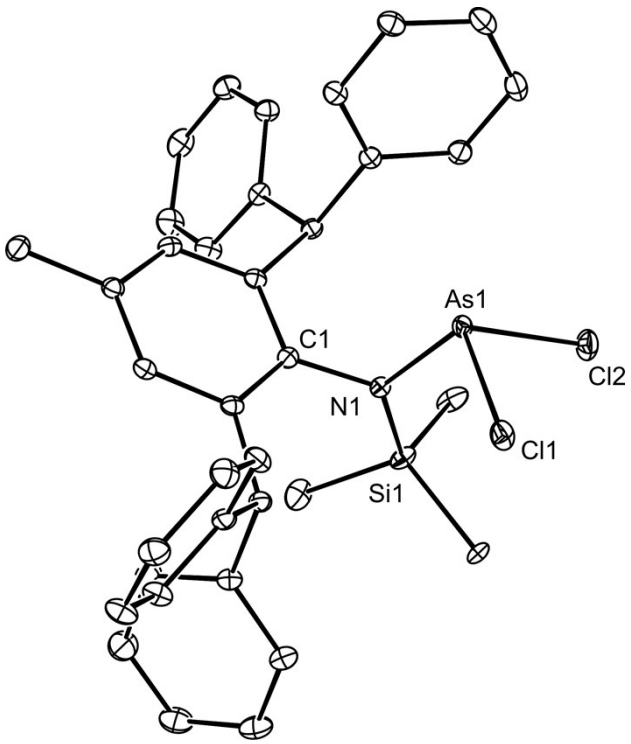

Fig. S1 Molecular structure of **1a** (25% thermal ellipsoids; hydrogen atoms omitted). Selected bond lengths (Å) and angles (º): As(1)-N(1) 1.818(4), As(1)-Cl(2) 2.1823(8), As(1)-Cl(1) 2.2300(8), N(1)-As(1)-Cl(2) 101.66(10), N(1)-As(1)-Cl(1) 102.86(10), Cl(2)-As(1)-Cl(1) 93.99(3).

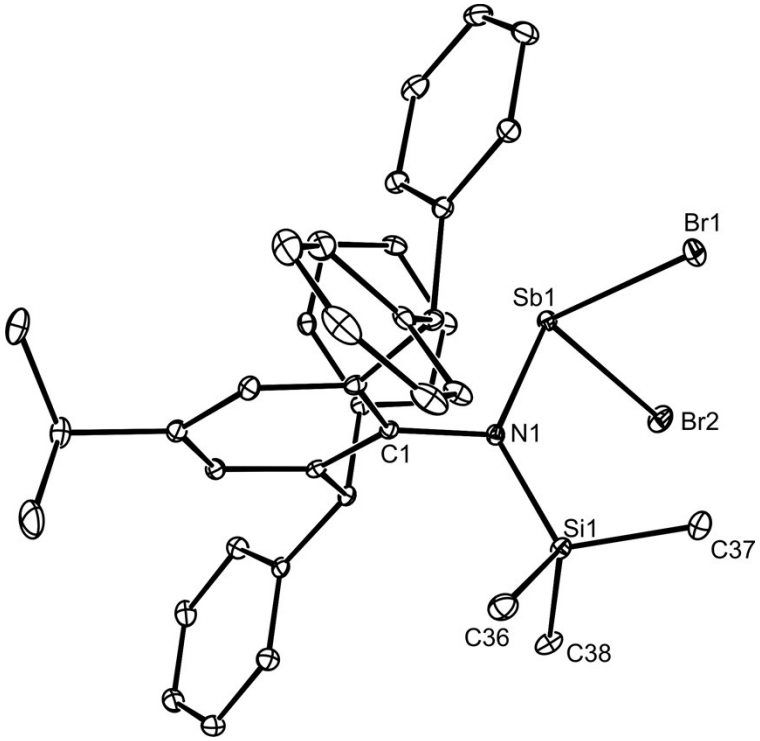

Fig. S2 Molecular structure of **1c** (25% thermal ellipsoids; hydrogen atoms omitted). Selected bond lengths (Å) and angles (º): Sb(1)-N(1) 2.0379(19), Sb(1)-Br(2) 2.5428(4), Sb(1)-Br(1) 2.5460(4), N(1)-Sb(1)-Br(2) 97.81(6), N(1)-Sb(1)-Br(1) 101.09(6), Br(2)-Sb(1)-Br(1) 91.420(13).

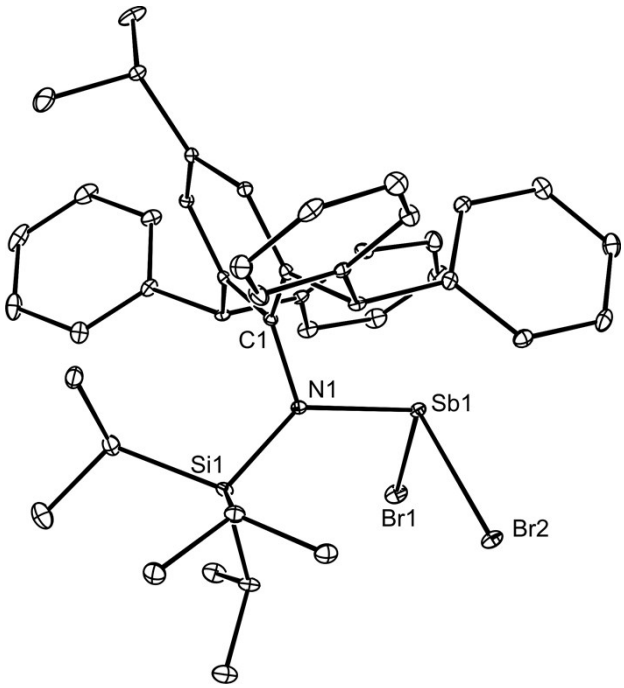

Fig. S3 Molecular structure of **1d** (25% thermal ellipsoids; hydrogen atoms omitted). Selected bond lengths (Å) and angles (º): Sb(1)-N(1) 2.055(3), Sb(1)-Br(1) 2.5381(5), Sb(1)-Br(2) 2.5487(6), N(1)-Sb(1)-Br(1) 103.83(8), N(1)-Sb(1)-Br(2) 103.43(8), Br(1)-Sb(1)-Br(2) 89.49(2).

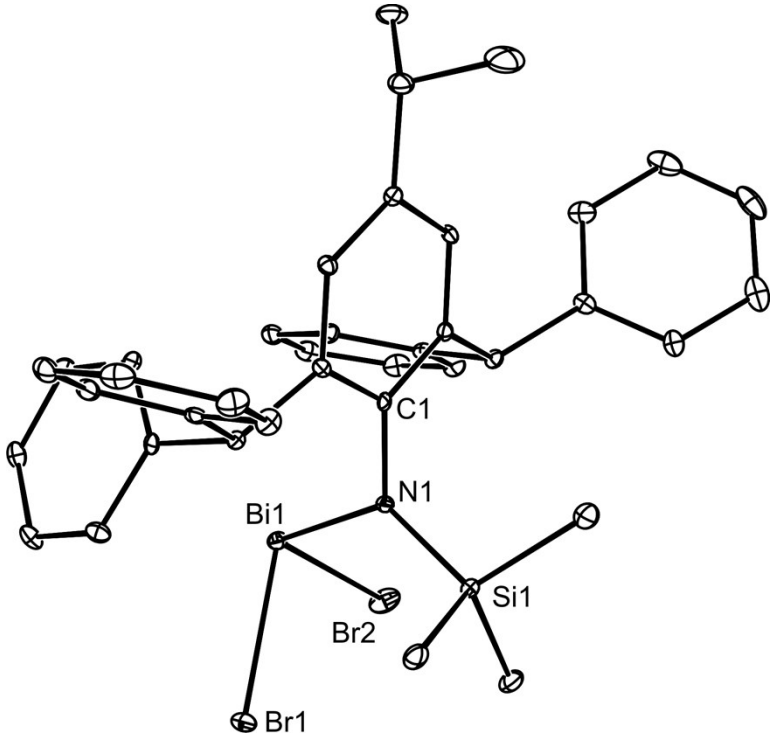

Fig. S4 Molecular structure of **1e** (25% thermal ellipsoids; hydrogen atoms omitted). Selected bond lengths (Å) and angles (º): Bi(1)-N(1) 2.155(3), Bi(1)-Br(2) 2.6380(5), Bi(1)-Br(1) 2.6425(5), N(1)-Bi(1)-Br(2) 101.14(8), N(1)-Bi(1)-Br(1) 96.85(8), Br(2)-Bi(1)-Br(1) 90.666(16).

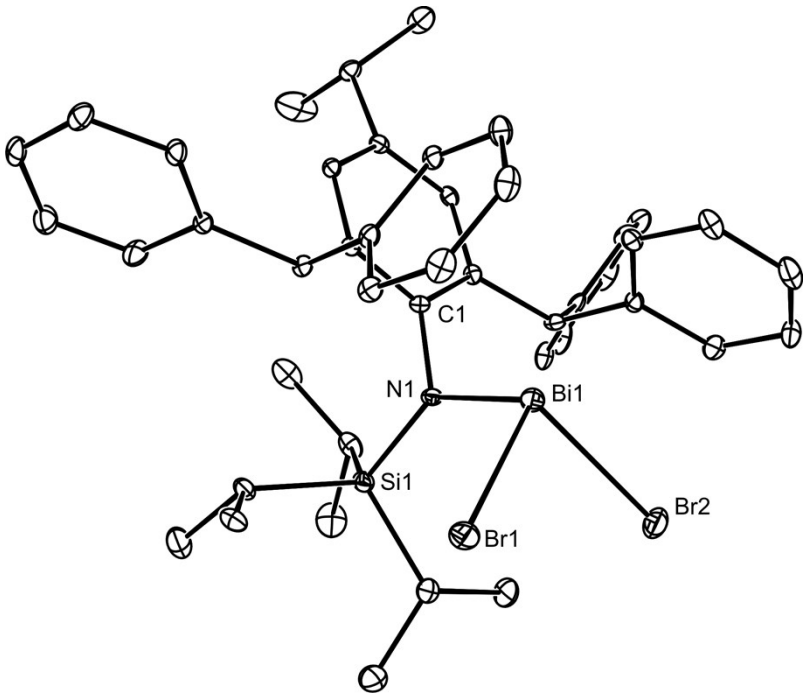

Fig. S5 Molecular structure of **1f** (25% thermal ellipsoids; hydrogen atoms omitted). Selected bond lengths (Å) and angles (º): Bi(1)-N(1) 2.164(5), Bi(1)-Br(2) 2.6277(9), Bi(1)-Br(1) 2.6449(9), N(1)-Bi(1)-Br(2) 103.53(15), N(1)-Bi(1)-Br(1) 104.04(14), Br(2)-Bi(1)-Br(1) 88.69(3).

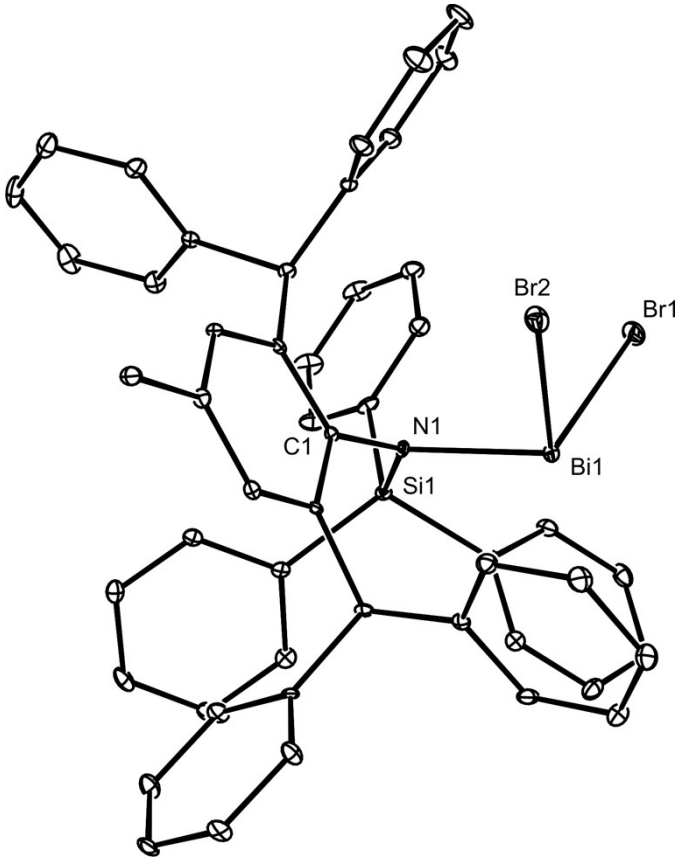

Fig. S6 Molecular structure of **1g** (25% thermal ellipsoids; hydrogen atoms omitted). Selected bond lengths (Å) and angles (º): Bi(1)-N(1) 2.183(3), Bi(1)-Br(2) 2.5895(4), Bi(1)-Br(1) 2.6392(4), N(1)-Bi(1)-Br(2) 96.93(7), N(1)-Bi(1)-Br(1) 103.26(7), Br(2)-Bi(1)-Br(1) 91.995(14).

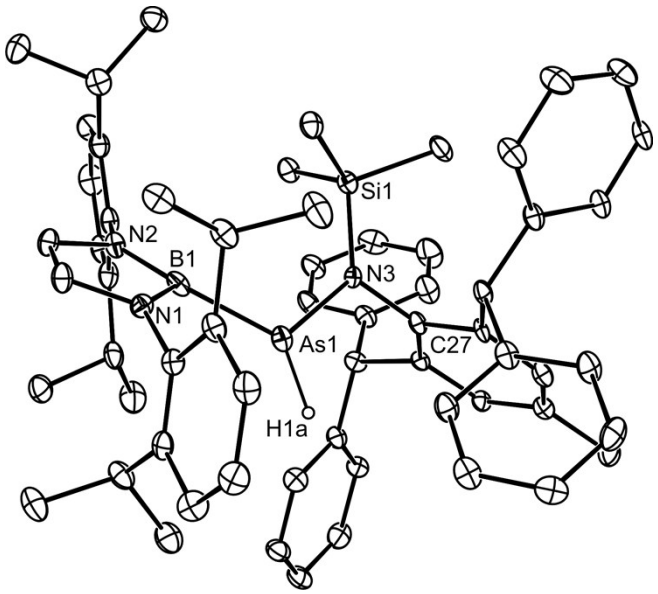

Fig. S7 Molecular structure of **3a** (25% thermal ellipsoids; hydrogen atoms, except H1a, omitted). Selected bond lengths (Å) and angles (º): As(1)-N(3) 1.877(6), As(1)-B(1) 2.042(9), As(1)-H(1a) 1.37(4), N(3)-As(1)-B(1) 113.6(3), N(3)-As(1)-H(1a) 105(1), B(1)-As(1)-H(1a) 137(1).

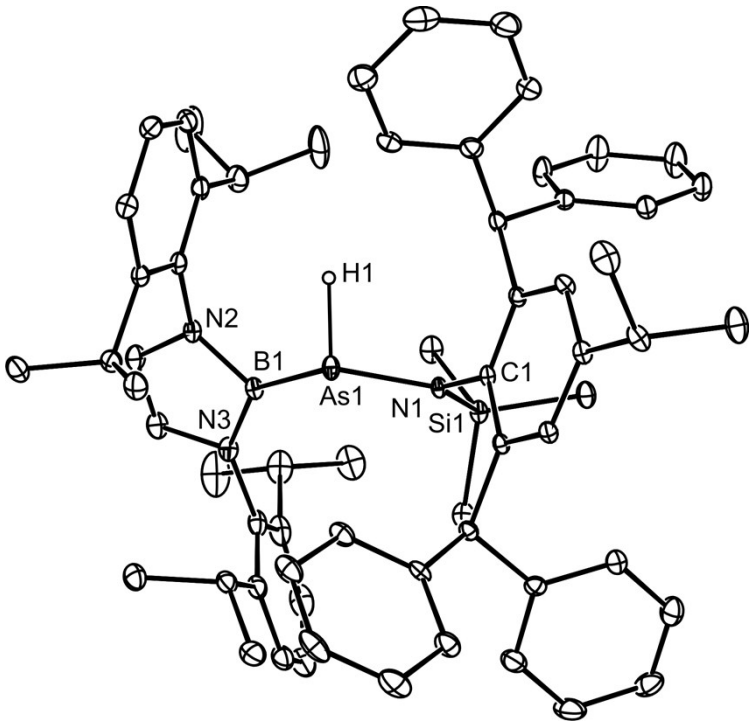

Fig. S8 Molecular structure of **3b** (25% thermal ellipsoids; hydrogen atoms, except H1, omitted). Selected bond lengths (Å) and angles (º): As(1)-N(1) 1.866(2), As(1)-B(1) 2.048(3), As(1)-H(1) 1.49(5), N(1)-As(1)-B(1) 115.48(11), N(3)-As(1)-H(1) 101 (1), B(1)-As(1)-H(1) 99(1).

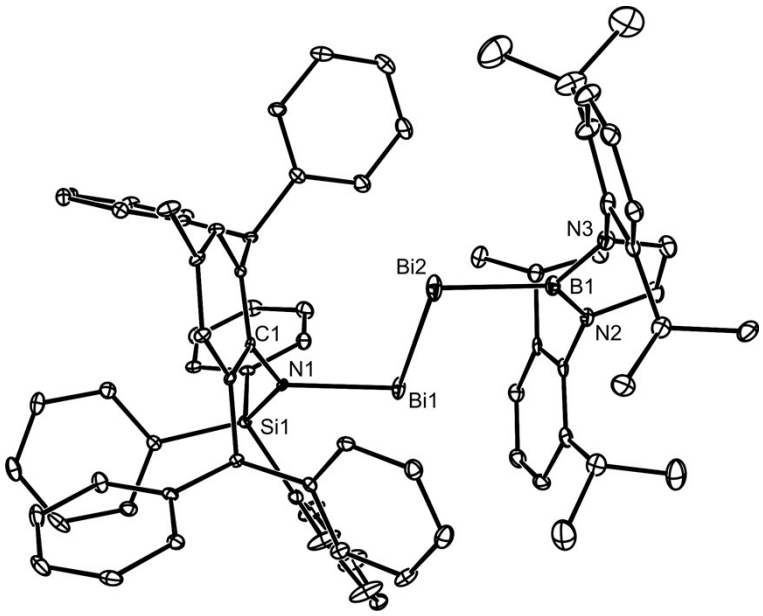

Fig. S9 Molecular structure of **1S** (25% thermal ellipsoids; hydrogen atoms omitted). Selected bond lengths (Å) and angles (º): Bi(1)-N(1) 2.259(4), Bi(1)-Bi(2) 2.8183(3), B(1)-Bi(2) 2.348(6), N(1)-Bi(1)-Bi(2) 99.82(10), B(1)-Bi(2)-Bi(1) 92.24(15).

3. Computational Studies

The DFT calculations were performed using the Amsterdam Density Functional (ADF) Package Software 2013.[6] Calculations were performed using the Vosko-Wilk-Nusair local density approximation with exchange from Becke,[7] and correlation corrections from Perdew (BP).[8] Slater-type orbitals (STOs)[9] were used for the triple zeta basis set with an additional set of polarization functions (TZP). Relativistic effects were handled using the Zeroth Order Regular Approximation approach (two component spin-orbit ZORA).[10] The large frozen core basis set approximation was applied with no molecular symmetry. General numerical integration was 6.

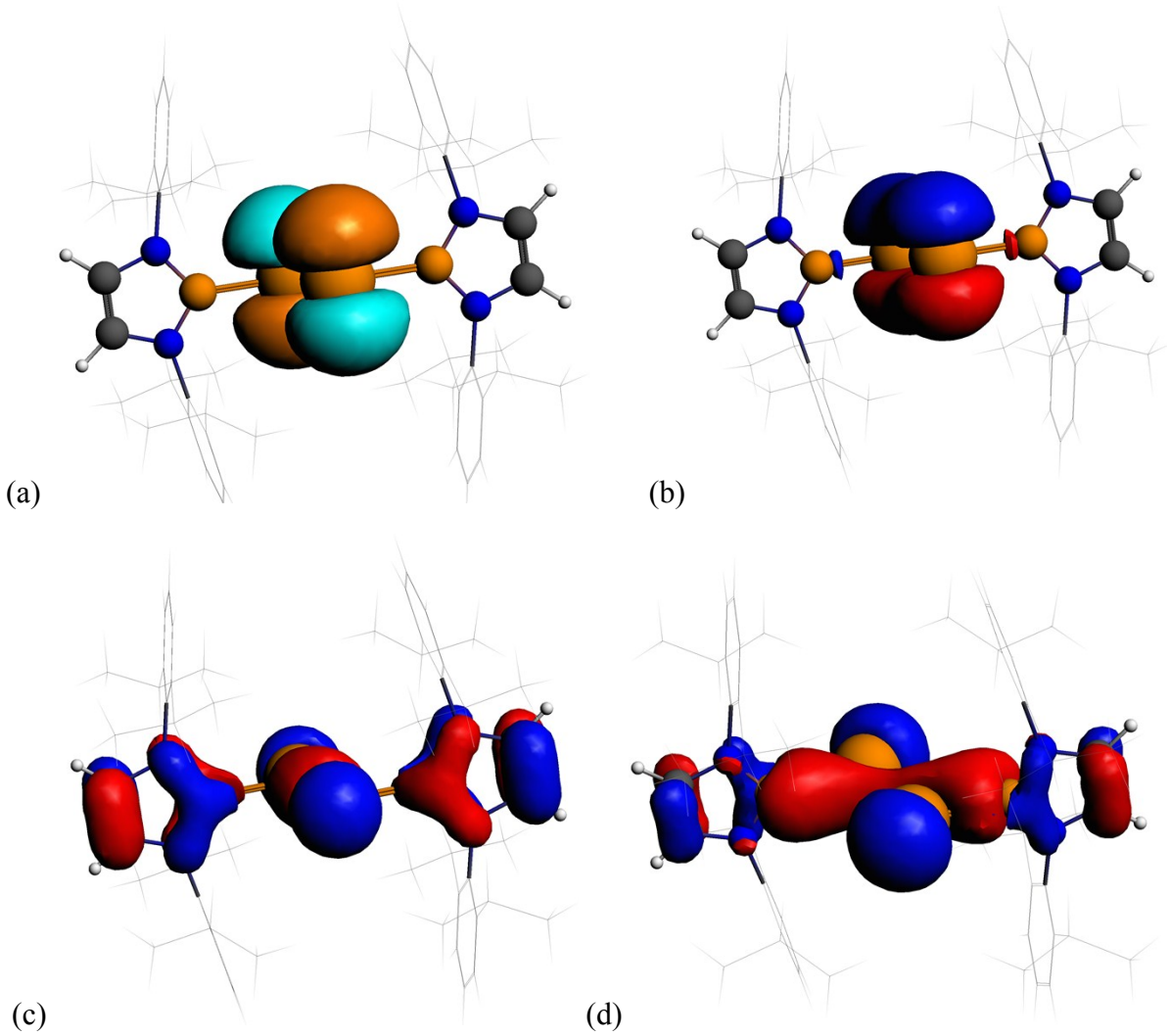

Fig. S10 (a) LUMO, (b) HOMO, (c) HOMO-1, and (d) HOMO-3 of $\mathbf{5}_{\mathbf{orth}}$.

Table S2. Absolute energies (kcal/mol) of the geometry optimised structures of **5** with variable tilt angles (°) between the boryl ligands and the Bi_2B_2 fragment.

Tilt angle	**Energy**
0 degrees (planar)	-17886.86
15 degrees	-17886.62
30 degrees	-17885.98
45 degrees	-17885.21
60 degrees	-17884.51
75 degrees	-17884.07
90 degrees (orthogonal)	-17884.07

Table S3. Cartesian coordinates of geometry optimized molecules

{(DAB)B}Bi=Bi{B(DAB)} planar

1 H	-4.083748687000	0.149003040100	-5.131746995000
2 H	-4.972625156000	1.120287948000	-3.931428361000
3 H	-2.930803719000	2.505423445000	-3.329147237000
4 C	-4.340348452000	0.228778347000	-4.063676638000
5 H	-2.007705642000	1.671141732000	-4.591665563000
6 H	1.549795588000	4.090887724000	-3.649590018000
7 H	-4.934789620000	-0.654722385500	-3.791416392000
8 H	2.220304692000	3.042872292000	-4.919153250000
9 H	3.797608073000	5.228396000000	-3.316057588000
10 C	-2.298630709000	1.627806960000	-3.531350643000
11 H	-7.145478211000	2.032265649000	0.087976610300
12 H	4.563907301000	4.213613689000	-4.559150931000
13 H	-1.390302205000	-0.332788782900	-5.248505439000
14 C	2.066145307000	3.136513773000	-3.833187666000
15 C	4.308425584000	4.269014779000	-3.489704619000
16 H	-4.911842947000	3.209243285000	0.361531207700
17 C	-3.066854061000	0.337555700400	-3.200945904000
18 H	-1.387073394000	1.713574453000	-2.923420374000
19 H	1.402580679000	2.319586299000	-3.515306627000
20 C	-6.926043560000	1.413180233000	0.971115297600
21 H	4.257303368000	1.948252793000	-5.384256815000
22 H	-7.362550507000	1.914505134000	1.848632147000
23 C	-1.406879014000	-1.101279411000	-4.473860263000
24 H	-3.380481903000	0.400703701500	-2.149784586000
25 H	-7.436869971000	0.447537505400	0.847832179200
26 H	5.248506924000	4.273531103000	-2.919787381000
27 C	3.402575035000	3.095476752000	-3.070565446000
28 H	0.039435112420	5.241274863000	0.105850630900
29 H	-0.016890321720	-2.373526477000	-5.525345026000
30 C	-4.697614403000	2.590869619000	1.246481820000
31 H	-5.038972180000	3.145947323000	2.133757677000
32 C	-2.204894280000	-0.914119020600	-3.335904771000
33 C	-0.632764548900	-2.249537018000	-4.633581293000
34 H	-5.031877857000	0.736865296700	0.223254786100
35 H	3.177156888000	3.212835657000	-2.002247368000
36 C	-5.405182810000	1.228249625000	1.131599577000
37 C	4.481756181000	1.319598997000	-4.520124806000
38 H	-3.607918009000	2.467527311000	1.324698069000

39 H	2.088424221000	6.264424797000	1.189530713000
40 C	0.001174535293	4.482896175000	0.902686122400
41 H	-0.660442260700	4.865313221000	1.694764503000
42 C	4.108334153000	1.753868171000	-3.239417944000
43 H	5.415894701000	-0.217245985500	-5.712945509000
44 H	-0.455491775600	3.571848351000	0.490865713100
45 H	-4.725939764000	-2.891273940000	-2.030485055000
46 C	5.133023874000	0.102029627700	-4.708822585000
47 C	-2.205115832000	-1.928636583000	-2.350594326000
48 H	-5.931147605000	1.660192615000	3.765545932000
49 C	-4.333988121000	-2.344169910000	-1.180224535000
50 H	1.494193328000	5.896175786000	2.825624281000
51 C	-0.641285466200	-3.233866842000	-3.647986422000
52 C	2.063215121000	5.492553068000	1.973847582000
53 H	2.024831724000	3.849153658000	0.592824403100
54 N	-3.049926395000	-1.785093996000	-1.193442552000
55 H	-5.915787329000	-2.365334765000	0.365011286600
56 C	1.416843352000	4.200754019000	1.437148933000
57 C	-5.070294763000	0.318741332000	2.309560173000
58 C	-4.928479098000	-2.082467941000	0.016868948820
59 H	-0.027968251670	-4.127954817000	-3.776533775000
60 C	-1.422310187000	-3.096749655000	-2.490402737000
61 C	-5.421931285000	0.706710129800	3.611069042000
62 H	3.093935737000	5.315477468000	2.312715885000
63 C	4.409345427000	0.919115483100	-2.139075519000
64 B	-2.811913618000	-1.124530562000	0.076246481620
65 Bi	1.002037785000	-0.136101740500	-1.071094448000
66 N	-4.044747353000	-1.344541889000	0.812177779100
67 H	-3.093946723000	-5.315467209000	-2.312726387000
68 C	5.421920299000	-0.706699870900	-3.611079544000
69 N	4.044736367000	1.344552148000	-0.812188281000
70 C	-4.409356413000	-0.919105224300	2.139065017000
71 B	2.811902631000	1.124540821000	-0.076256983550
72 H	5.915776342000	2.365345024000	-0.365021788500
73 H	0.027957265400	4.127965076000	3.776523273000
74 Bi	-1.002048771000	0.136111999300	1.071083946000
75 C	4.928468111000	2.082478200000	-0.016879450750
76 C	5.070283777000	-0.318731073200	-2.309570675000
77 H	5.931136618000	-1.660182356000	-3.765556434000
78 C	1.422299201000	3.096759913000	2.490392235000
79 H	-1.494204315000	-5.896165528000	-2.825634783000
80 C	-2.063226107000	-5.492542809000	-1.973858084000
81 C	-1.416854338000	-4.200743761000	-1.437159435000
82 C	-5.133034860000	-0.102019368800	4.708812083000
83 H	-2.024842710000	-3.849143399000	-0.592834905100
84 N	3.049915409000	1.785104255000	1.193432050000
85 H	-5.415905688000	0.217256244400	5.712935007000
86 C	4.333977135000	2.344180169000	1.180214033000
87 C	0.641274479900	3.233877101000	3.647975920000
88 H	4.725928778000	2.891284199000	2.030474553000
89 C	2.205104846000	1.928646842000	2.350583824000
90 H	-2.088435208000	-6.264414539000	-1.189541215000
91 C	-4.108345139000	-1.753857912000	3.239407442000
92 C	-4.481767167000	-1.319588738000	4.520114304000
93 H	0.660431274400	-4.865302963000	-1.694775005000
94 H	0.455480789300	-3.571838093000	-0.490876215000
95 C	-0.001185521563	-4.482885916000	-0.902696624400
96 C	5.405171824000	-1.228239366000	-1.131610079000
97 H	3.607907023000	-2.467517052000	-1.324708571000
98 H	5.031866871000	-0.736855037900	-0.223265288000
99 H	-3.177167874000	-3.212825399000	2.002236866000
100 C	0.632753562600	2.249547277000	4.633570791000
101 H	5.038961193000	-3.145937064000	-2.133768179000
102 H	7.436858985000	-0.447527246600	-0.847842681100

103 H	-5.248517911000	-4.273520845000	2.919776879000
104 H	7.362539520000	-1.914494876000	-1.848642649000
105 H	0.016879335450	2.373536736000	5.525334524000
106 C	4.697603416000	-2.590859360000	-1.246492322000
107 C	-3.402586022000	-3.095466493000	3.070554945000
108 H	-4.257314354000	-1.948242534000	5.384246313000
109 H	-0.039446098690	-5.241264604000	-0.105861132900
110 C	6.926032574000	-1.413169974000	-0.971125799500
111 C	2.204883294000	0.914129279400	3.335894269000
112 H	3.380470917000	-0.400693442600	2.149774084000
113 C	1.406868028000	1.101289669000	4.473849761000
114 C	-4.308436571000	-4.269004520000	3.489694117000
115 H	-1.402591665000	-2.319576040000	3.515296125000
116 H	4.911831961000	-3.209233026000	-0.361541709600
117 H	-4.563918288000	-4.213603430000	4.559140429000
118 H	1.387062408000	-1.713564194000	2.923409872000
119 C	3.066843075000	-0.337545441500	3.200935402000
120 H	7.145467224000	-2.032255390000	-0.087987112230
121 C	-2.066156293000	-3.136503515000	3.833177164000
122 H	-3.797619060000	-5.228385741000	3.316047086000
123 H	1.390291219000	0.332799041800	5.248494937000
124 H	-2.220315678000	-3.042862033000	4.919142748000
125 H	4.934778634000	0.654732644400	3.791405890000
126 C	2.298619723000	-1.627796701000	3.531340142000
127 H	-1.549806575000	-4.090877465000	3.649579516000
128 C	4.340337466000	-0.228768088100	4.063666136000
129 H	2.007694656000	-1.671131474000	4.591655061000
130 H	2.930792733000	-2.505413186000	3.329136735000
131 H	4.972614169000	-1.120277689000	3.931417859000
132 H	4.083737701000	-0.148992781200	5.131736493000

{(DAB)B}Bi=Bi{B(DAB)} othogonal

1 H	-2.726047263000	-2.081141994000	-6.155805120000
2 H	3.250276680000	-1.918668941000	-5.907276270000
3 H	-4.126625156000	-0.156693824200	-5.466303947000
4 H	2.214048541000	0.295288438700	-5.524950651000
5 C	-2.910502822000	-1.892747575000	-5.097117764000
6 H	1.043350676000	2.046200807000	-5.089284593000
7 C	3.348144112000	-1.433358685000	-4.935033222000
8 H	-4.192995229000	1.995036112000	-4.580244165000
9 C	-3.697153498000	-0.812630419500	-4.706285210000
10 H	3.478810876000	2.890616988000	-4.750376746000
11 C	2.768300284000	-0.183988418100	-4.717345549000
12 H	-1.724459287000	-3.564066256000	-4.447343892000
13 C	-2.351131763000	-2.729296462000	-4.131699654000
14 H	4.490054811000	-3.044488182000	-4.080787486000
15 C	0.915691779100	2.017848818000	-3.996636248000
16 C	4.043723883000	-2.063241252000	-3.906520977000
17 C	-4.222686943000	1.969549841000	-3.480296434000
18 H	-6.314842186000	0.418322726100	-4.547450797000
19 H	-3.197233839000	2.118415346000	-3.112691976000
20 H	0.452871969500	2.970310491000	-3.700002816000
21 H	0.214681948200	1.207556123000	-3.754171201000
22 C	3.235655504000	2.961799440000	-3.678478619000
23 H	2.785180701000	3.949406755000	-3.495508509000
24 H	-4.836024300000	2.819029068000	-3.143636722000
25 C	2.876825267000	0.463548722300	-3.478488072000
26 C	-3.947547607000	-0.549959790100	-3.350415307000
27 C	2.257051601000	1.841668289000	-3.268680100000
28 H	6.568998234000	-2.960246878000	-2.811726973000
29 H	4.173998234000	2.906371444000	-3.110413549000
30 C	-4.813967833000	0.644902986600	-2.964150964000

31	H	-3.081483979000	-5.241107444000	-2.345869407000
32	H	-0.623069234600	-4.662937519000	-2.969104923000
33	C	-6.266028320000	0.470806888500	-3.448861174000
34	H	0.101522741900	-3.153995794000	-2.359809123000
35	C	-2.572619554000	-2.513820397000	-2.763992285000
36	H	6.912055748000	-1.363511155000	-2.110197808000
37	C	4.181319661000	-1.459284743000	-2.646989467000
38	H	-6.884018605000	1.322139085000	-3.125183235000
39	C	3.595605880000	-0.188694125100	-2.449073612000
40	C	-3.382824588000	-1.416477474000	-2.387473563000
41	C	6.443123194000	-2.337846466000	-1.912383496000
42	C	-0.581872161100	-3.976875991000	-2.109623097000
43	H	-6.714576096000	-0.449543159300	-3.048725221000
44	H	2.067698129000	1.944901123000	-2.190154181000
45	H	-4.833341122000	0.695540880700	-1.867155123000
46	C	-2.923486491000	-4.640436997000	-1.436242592000
47	H	4.369665807000	-4.230472177000	-2.074170143000
48	C	-1.975559665000	-3.457878246000	-1.724901271000
49	H	5.647217769000	1.437183619000	-1.645181014000
50	H	6.991390389000	-2.821477983000	-1.089615618000
51	H	-2.492613784000	-5.296595395000	-0.664465294900
52	C	4.954484872000	-2.181033761000	-1.547611465000
53	H	-0.148131664900	-4.537393598000	-1.268809640000
54	H	-3.903242620000	-4.294920756000	-1.079742484000
55	N	3.754818963000	0.464378436600	-1.174183856000
56	C	4.328638518000	-3.547169557000	-1.212271223000
57	C	4.885229314000	1.248635528000	-0.897283387000
58	N	-3.658769934000	-1.185564063000	-0.991756951200
59	H	-5.531361893000	-2.298960152000	-0.935423027900
60	H	-1.871203760000	-2.881846816000	-0.793730762700
61	H	4.897116810000	-1.559316082000	-0.644005054500
62	H	3.274699675000	-3.440756198000	-0.917301281700
63	H	4.872073557000	-4.023835625000	-0.382423786300
64	C	-4.827507200000	-1.678847671000	-0.391765710300
65	Bi	-1.005775984000	0.987009396400	-0.406752775500
66	H	-4.872081189000	4.023836767000	0.382437512000
67	B	-2.940011246000	-0.392233213700	-0.019047749940
68	B	2.940003613000	0.392234355600	0.019061475620
69	C	4.827499567000	1.678848813000	0.391779436000
70	Bi	1.005768352000	-0.987008254500	0.406766501200
71	H	-3.274707307000	3.440757340000	0.917315007400
72	H	5.531354261000	2.298961294000	0.935436753600
73	H	-4.897124442000	1.559317223000	0.644018780100
74	C	-4.328646150000	3.547170699000	1.212284948000
75	H	-6.991398021000	2.821479125000	1.089629344000
76	C	-4.885236946000	-1.248634386000	0.897297112600
77	H	1.871196128000	2.881847958000	0.793744488400
78	H	3.903234988000	4.294921898000	1.079756209000
79	N	3.658762302000	1.185565205000	0.991770676800
80	N	-3.754826595000	-0.464377294700	1.174197582000
81	H	2.492606152000	5.296596537000	0.664479020500
82	C	-4.954492504000	2.181034903000	1.547625191000
83	H	-5.647225401000	-1.437182478000	1.645194740000
84	H	-4.369673439000	4.230473319000	2.074183869000
85	H	0.148124032900	4.537394740000	1.268823366000
86	C	2.923478859000	4.640438138000	1.436256317000
87	C	-6.443130826000	2.337847608000	1.912397221000
88	C	1.975552033000	3.457879388000	1.724914996000
89	H	6.714568464000	0.449544301200	3.048738947000
90	H	-6.912063380000	1.363512297000	2.110211533000
91	H	4.833333490000	-0.695539738800	1.867168848000
92	H	6.884010973000	-1.322137943000	3.125196961000
93	C	0.581864529100	3.976877132000	2.109636823000
94	H	-6.569005866000	2.960248020000	2.811740698000

95 H	-2.067705762000	-1.944899982000	2.190167907000
96 C	3.382816956000	1.416478616000	2.387487289000
97 C	-3.595613512000	0.188695267000	2.449087337000
98 C	6.266020688000	-0.470805746600	3.448874899000
99 H	3.081476347000	5.241108586000	2.345883132000
100 C	-4.181327293000	1.459285885000	2.647003192000
101 H	0.623061602500	4.662938661000	2.969118648000
102 C	2.572611922000	2.513821539000	2.764006010000
103 C	4.813960201000	-0.644901844700	2.964164690000
104 H	-0.101530374000	3.153996936000	2.359822849000
105 H	-4.174005866000	-2.906370302000	3.110427274000
106 H	4.836016668000	-2.819027926000	3.143650447000
107 H	6.314834554000	-0.418321584200	4.547464522000
108 C	3.947539975000	0.549960931900	3.350429033000
109 C	-2.257059233000	-1.841667148000	3.268693825000
110 C	-2.876832899000	-0.463547580400	3.478501798000
111 H	-2.785188333000	-3.949405613000	3.495522235000
112 C	-3.235663136000	-2.961798299000	3.678492345000
113 C	4.222679311000	-1.969548699000	3.480310160000
114 C	-4.043731515000	2.063242393000	3.906534703000
115 H	-4.490062443000	3.044489323000	4.080801212000
116 H	3.197226207000	-2.118414204000	3.112705702000
117 H	-0.452879601500	-2.970309349000	3.700016542000
118 H	-0.214689580300	-1.207554981000	3.754184927000
119 C	2.351124131000	2.729297604000	4.131713380000
120 C	-0.915699411100	-2.017847676000	3.996649974000
121 H	1.724451655000	3.564067398000	4.447357618000
122 H	-3.478818508000	-2.890615846000	4.750390471000
123 H	4.192987597000	-1.995034970000	4.580257891000
124 C	-2.768307916000	0.183989560000	4.717359275000
125 C	3.697145866000	0.812631561400	4.706298935000
126 C	-3.348151744000	1.433359827000	4.935046948000
127 C	2.910495190000	1.892748717000	5.097131489000
128 H	-1.043358308000	-2.046199665000	5.089298319000
129 H	4.126617524000	0.156694966100	5.466317672000
130 H	-2.214056173000	-0.295287296800	5.524964377000
131 H	-3.250284312000	1.918670083000	5.907289996000
132 H	2.726039631000	2.081143136000	6.155818846000

{(DAB)B}Bi=Bi{B(DAB)} 15° boryl tilt

1 H	-4.488696254000	0.921608455200	-4.690174727000
2 H	-5.290712823000	1.623367147000	-3.262438397000
3 H	-3.226851699000	2.936436617000	-2.577970977000
4 C	-4.657059067000	0.792616880200	-3.609436534000
5 H	-2.390713843000	2.375356570000	-4.036835591000
6 H	0.976018943500	4.574476745000	-2.972294516000
7 H	-5.212061518000	-0.144768981300	-3.462924141000
8 H	1.584931714000	3.798695107000	-4.451258489000
9 H	3.165672401000	5.827888497000	-2.659909240000
10 C	-2.598629743000	2.129689995000	-2.984661324000
11 H	-7.301230534000	1.521457982000	0.944843074900
12 H	3.869695445000	5.085625895000	-4.114349094000
13 H	-1.814105199000	0.548646779800	-5.108853603000
14 C	1.534811768000	3.707254344000	-3.355366049000
15 C	3.719570695000	4.952501011000	-3.031870487000
16 H	-5.162645942000	2.854212229000	1.249919498000
17 C	-3.318615483000	0.778695590600	-2.843792254000
18 H	-1.644820327000	2.128963918000	-2.438859442000
19 H	0.963687072500	2.798154434000	-3.118836083000
20 C	-6.952107264000	0.789882893700	1.689339470000
21 H	3.634769006000	2.960703969000	-5.267138637000
22 H	-7.352426135000	1.091147160000	2.669641010000

23	C	-1.753756777000	-0.350268301300	-4.493001912000
24	H	-3.545848156000	0.636557928200	-1.778286660000
25	H	-7.384669892000	-0.188693011800	1.436670287000
26	H	4.709614356000	4.945201587000	-2.554037027000
27	C	2.940718837000	3.657805718000	-2.731191616000
28	H	-0.038028008590	5.195586166000	1.117024191000
29	H	-0.447516413000	-1.367145450000	-5.877483992000
30	C	-4.821307858000	2.127120623000	2.002380341000
31	H	-5.135807114000	2.496318555000	2.990563215000
32	C	-2.452450184000	-0.399804930900	-3.278094690000
33	C	-0.984439399900	-1.427679817000	-4.929852802000
34	H	-5.077369459000	0.439267814200	0.705456392400
35	H	2.816445253000	3.588077862000	-1.642399144000
36	C	-5.412525532000	0.736281555300	1.708194254000
37	C	3.986037503000	2.225219300000	-4.540574298000
38	H	-3.722210219000	2.104158167000	1.985271175000
39	H	2.095859243000	6.048039621000	2.182173399000
40	C	0.002352748599	4.302250901000	1.758792826000
41	H	-0.584754533300	4.516446701000	2.664707152000
42	C	3.713636780000	2.421376792000	-3.178382456000
43	H	4.898849652000	0.976698668700	-6.045698839000
44	H	-0.486436021100	3.473139953000	1.227934773000
45	H	-4.781549334000	-2.744596372000	-2.137953892000
46	C	4.696422136000	1.110524218000	-4.982008768000
47	C	-2.354685075000	-1.578890443000	-2.503503103000
48	H	-5.701808628000	0.705379712000	4.413138498000
49	C	-4.340635341000	-2.317260921000	-1.244265848000
50	H	1.658053750000	5.369571840000	3.767784477000
51	C	-0.897432003900	-2.578423583000	-4.149937385000
52	C	2.148315112000	5.144129062000	2.808082968000
53	H	1.991959902000	3.784428082000	1.154103103000
54	N	-3.095341884000	-1.676437252000	-1.272593974000
55	H	-5.764985551000	-2.697769203000	0.403657210100
56	C	1.463278402000	3.958668332000	2.100787696000
57	C	-4.900680558000	-0.315223358800	2.687765417000
58	C	-4.832589606000	-2.293545614000	0.025276411020
59	H	-0.288574487600	-3.416393446000	-4.495234518000
60	C	-1.574698059000	-2.679333077000	-2.925269221000
61	C	-5.147125033000	-0.166731047000	4.060798554000
62	H	3.207111832000	4.932174211000	3.014365726000
63	C	4.178063238000	1.452498133000	-2.259997107000
64	B	-2.775322688000	-1.213920261000	0.064834306330
65	Bi	0.993866234400	-0.065574083620	-1.085472993000
66	N	-3.918816603000	-1.633941155000	0.854933699200
67	H	-3.207122607000	-4.932164365000	-3.014376081000
68	C	5.147114258000	0.166740892500	-4.060808909000
69	N	3.918805828000	1.633951000000	-0.854944054100
70	C	-4.178074013000	-1.452488287000	2.259986752000
71	B	2.775311913000	1.213930107000	-0.064844661310
72	H	5.764974777000	2.697779048000	-0.403667565100
73	H	0.288563712800	3.416403291000	4.495224163000
74	Bi	-0.993877009200	0.065583929110	1.085462638000
75	C	4.832578831000	2.293555459000	-0.025286765990
76	C	4.900669783000	0.315233204300	-2.687775772000
77	H	5.701797853000	-0.705369866500	-4.413148853000
78	C	1.574687284000	2.679342923000	2.925258866000
79	H	-1.658064525000	-5.369561994000	-3.767794832000
80	C	-2.148325887000	-5.144119216000	-2.808093323000
81	C	-1.463289177000	-3.958658487000	-2.100798051000
82	C	-4.696432911000	-1.110514372000	4.981998413000
83	H	-1.991970677000	-3.784418237000	-1.154113458000
84	N	3.095331109000	1.676447097000	1.272583619000
85	H	-4.898860427000	-0.976688823200	6.045688484000
86	C	4.340624567000	2.317270766000	1.244255493000

87 C	0.897421229000	2.578433429000	4.149927030000
88 H	4.781538559000	2.744606217000	2.137943537000
89 C	2.354674300000	1.578900288000	2.503492748000
90 H	-2.095870018000	-6.048029776000	-2.182183754000
91 C	-3.713647555000	-2.421366946000	3.178372101000
92 C	-3.986048278000	-2.225209455000	4.540563943000
93 H	0.584743758400	-4.516436855000	-2.664717507000
94 H	0.486425246200	-3.473130107000	-1.227945128000
95 C	-0.002363523473	-4.302241056000	-1.758803181000
96 C	5.412514757000	-0.736271709800	-1.708204609000
97 H	3.722199444000	-2.104148322000	-1.985281530000
98 H	5.077358684000	-0.439257968700	-0.705466747400
99 H	-2.816456028000	-3.588068016000	1.642388789000
100 C	0.984428625000	1.427689662000	4.929842447000
101 H	5.135796339000	-2.496308709000	-2.990573570000
102 H	7.384659117000	0.188702857300	-1.436680642000
103 H	-4.709625131000	-4.945191741000	2.554026672000
104 H	7.352415360000	-1.091137314000	-2.669651365000
105 H	0.447505638200	1.367155296000	5.877473637000
106 C	4.821297083000	-2.127110777000	-2.002390696000
107 C	-2.940729612000	-3.657795872000	2.731181261000
108 H	-3.634779781000	-2.960694123000	5.267128282000
109 H	0.038017233710	-5.195576321000	-1.117034546000
110 C	6.952096489000	-0.789873048200	-1.689349825000
111 C	2.452439410000	0.399814776400	3.278084335000
112 H	3.545837381000	-0.636548082700	1.778276305000
113 C	1.753746002000	0.350278146800	4.492991557000
114 C	-3.719581470000	-4.952491166000	3.031860132000
115 H	-0.963697847300	-2.798144588000	3.118825728000
116 H	5.162635167000	-2.854202384000	-1.249929853000
117 H	-3.869706220000	-5.085616049000	4.114338739000
118 H	1.644809552000	-2.128954072000	2.438849087000
119 C	3.318604708000	-0.778685745100	2.843781899000
120 H	7.301219759000	-1.521448137000	-0.944853429900
121 C	-1.534822543000	-3.707244498000	3.355355694000
122 H	-3.165683176000	-5.827878651000	2.659898885000
123 H	1.814094424000	-0.548636934300	5.108843248000
124 H	-1.584942489000	-3.798685261000	4.451248134000
125 H	5.212050743000	0.144778826800	3.462913786000
126 C	2.598618968000	-2.129680149000	2.984650969000
127 H	-0.976029718400	-4.574466899000	2.972284161000
128 C	4.657048292000	-0.792607034700	3.609426179000
129 H	2.390703068000	-2.375346724000	4.036825236000
130 H	3.226840924000	-2.936426772000	2.577960622000
131 H	5.290702048000	-1.623357302000	3.262428042000
132 H	4.488685479000	-0.921598609700	4.690164372000

{(DAB)B}Bi=Bi{B(DAB)} 30° boryl tilt

1 H	-5.116312089000	1.659316474000	-3.828803501000
2 H	-5.742759416000	2.002986088000	-2.196761610000
3 H	-3.641610968000	3.255611091000	-1.509732885000
4 C	-5.137832779000	1.298624586000	-2.788422165000
5 H	-2.987387039000	3.053054460000	-3.144644615000
6 H	0.330291103100	4.961887945000	-2.060065285000
7 H	-5.643115323000	0.322507489000	-2.779338446000
8 H	0.780816737300	4.537845714000	-3.726479857000
9 H	2.456717148000	6.326160158000	-1.770645121000
10 C	-3.050561779000	2.584642012000	-2.151067435000
11 H	-7.269267292000	0.770137445400	2.034103353000
12 H	3.000405705000	5.940164575000	-3.419024551000
13 H	-2.517105073000	1.522562506000	-4.644328535000
14 C	0.886843634200	4.236812362000	-2.672926139000

15	C	3.009694437000	5.591037542000	-2.374982889000
16	H	-5.237248697000	2.244065274000	2.399103737000
17	C	-3.710645235000	1.197746413000	-2.213316571000
18	H	-2.034322318000	2.521929685000	-1.738052604000
19	H	0.414173663000	3.251512232000	-2.554588755000
20	C	-6.770500601000	-0.052619422600	2.568652814000
21	H	2.750301208000	4.059535828000	-4.935427068000
22	H	-7.076437579000	-0.002164296963	3.625074608000
23	C	-2.353237691000	0.519375831000	-4.247178388000
24	H	-3.792901695000	0.825956175000	-1.182803712000
25	H	-7.140774642000	-1.002313771000	2.156987552000
26	H	4.054473296000	5.582827224000	-2.033015440000
27	C	2.364847576000	4.197873722000	-2.246372162000
28	H	0.038029370590	4.869135822000	2.305195061000
29	H	-1.225151781000	-0.119488479000	-5.972266908000
30	C	-4.747285749000	1.425606629000	2.948086273000
31	H	-4.978732897000	1.555607674000	4.016294170000
32	C	-2.879697881000	0.182322206000	-2.991756563000
33	C	-1.627269778000	-0.403166028000	-4.998738029000
34	H	-5.000832299000	0.011896213020	1.356122706000
35	H	2.395358296000	3.912221535000	-1.186574607000
36	C	-5.240573464000	0.063664207040	2.426635008000
37	C	3.245254304000	3.235123681000	-4.418133002000
38	H	-3.659901646000	1.530266179000	2.823677072000
39	H	2.328727322000	5.535641298000	3.146676960000
40	C	0.176499231000	3.868070416000	2.741088101000
41	H	-0.235281340300	3.891479922000	3.761336963000
42	C	3.147938079000	3.143668634000	-3.021600623000
43	H	4.027720611000	2.384748468000	-6.240700658000
44	H	-0.415663542800	3.151486358000	2.154756394000
45	H	-4.939287000000	-2.529115629000	-2.076915300000
46	C	3.962134616000	2.294680948000	-5.155407687000
47	C	-2.650002667000	-1.124957028000	-2.504564414000
48	H	-5.155326948000	-0.504910985000	5.085782907000
49	C	-4.399859929000	-2.249246045000	-1.178991282000
50	H	2.175543085000	4.526236099000	4.605007770000
51	C	-1.411567057000	-1.686179414000	-4.500931289000
52	C	2.483466741000	4.522337512000	3.547875602000
53	H	2.019189497000	3.530867324000	1.700257011000
54	N	-3.209260708000	-1.512743269000	-1.235376246000
55	H	-5.549463744000	-3.063595490000	0.524862408100
56	C	1.668873162000	3.492268994000	2.740569628000
57	C	-4.527149844000	-1.100074481000	3.108081936000
58	C	-4.705783780000	-2.515322147000	0.120537842200
59	H	-0.837863319400	-2.401909160000	-5.092834992000
60	C	-1.912329138000	-2.073789274000	-3.249125566000
61	C	-4.595447560000	-1.238696053000	4.502360827000
62	H	3.559829010000	4.302139910000	3.513053918000
63	C	3.795425611000	2.064889485000	-2.377998571000
64	B	-2.727252503000	-1.298132012000	0.116022495100
65	Bi	0.956995997500	-0.013693923830	-1.116169274000
66	N	-3.721687400000	-1.955170281000	0.943888033200
67	H	-3.559839847000	-4.302129872000	-3.513064415000
68	C	4.595436723000	1.238706091000	-4.502371325000
69	N	3.721676563000	1.955180319000	-0.943898530700
70	C	-3.795436448000	-2.064879447000	2.377988073000
71	B	2.727241666000	1.298142050000	-0.116032992600
72	H	5.549452907000	3.063605528000	-0.524872905600
73	H	0.837852482500	2.401919198000	5.092824494000
74	Bi	-0.957006834500	0.013703961600	1.116158776000
75	C	4.705772943000	2.515332185000	-0.120548339700
76	C	4.527139007000	1.100084518000	-3.108092434000
77	H	5.155316111000	0.504921022700	-5.085793405000
78	C	1.912318301000	2.073799311000	3.249115068000

79 H	-2.175553922000	-4.526226061000	-4.605018268000
80 C	-2.483477578000	-4.522327474000	-3.547886100000
81 C	-1.668883999000	-3.492258956000	-2.740580126000
82 C	-3.962145453000	-2.294670910000	5.155397189000
83 H	-2.019200334000	-3.530857286000	-1.700267508000
84 N	3.209249871000	1.512753306000	1.235365748000
85 H	-4.027731448000	-2.384738430000	6.240690160000
86 C	4.399849092000	2.249256083000	1.178980785000
87 C	1.411556220000	1.686189452000	4.500920791000
88 H	4.939276163000	2.529125667000	2.076904802000
89 C	2.649991830000	1.124967065000	2.504553916000
90 H	-2.328738159000	-5.535631260000	-3.146687457000
91 C	-3.147948916000	-3.143658596000	3.021590125000
92 C	-3.245265141000	-3.235113643000	4.418122505000
93 H	0.235270503300	-3.891469885000	-3.761347461000
94 H	0.415652705800	-3.151476320000	-2.154766892000
95 C	-0.176510068000	-3.868060378000	-2.741098598000
96 C	5.240562627000	-0.063654169270	-2.426645505000
97 H	3.659890809000	-1.530256142000	-2.823687569000
98 H	5.000821462000	-0.011886175250	-1.356133203000
99 H	-2.395369133000	-3.912211498000	1.186564110000
100 C	1.627258941000	0.403176065800	4.998727531000
101 H	4.978722060000	-1.555597636000	-4.016304668000
102 H	7.140763805000	1.002323808000	-2.156998049000
103 H	-4.054484133000	-5.582817186000	2.033004943000
104 H	7.076426742000	0.002174334737	-3.625085105000
105 H	1.225140944000	0.119498516700	5.972256410000
106 C	4.747274912000	-1.425596591000	-2.948096770000
107 C	-2.364858413000	-4.197863684000	2.246361664000
108 H	-2.750312045000	-4.059525790000	4.935416570000
109 H	-0.038040207560	-4.869125785000	-2.305205559000
110 C	6.770489764000	0.052629460380	-2.568663312000
111 C	2.879687044000	-0.182312168200	2.991746065000
112 H	3.792890858000	-0.825946137200	1.182793214000
113 C	2.353226854000	-0.519365793200	4.247167891000
114 C	-3.009705274000	-5.591027504000	2.374972391000
115 H	-0.414184499900	-3.251502194000	2.554578258000
116 H	5.237237860000	-2.244055236000	-2.399114234000
117 H	-3.000416542000	-5.940154537000	3.419014053000
118 H	2.034311481000	-2.521919647000	1.738042107000
119 C	3.710634398000	-1.197736376000	2.213306073000
120 H	7.269256455000	-0.770127407700	-2.034113851000
121 C	-0.886854471200	-4.236802324000	2.672915641000
122 H	-2.456727985000	-6.326150120000	1.770634624000
123 H	2.517094236000	-1.522552468000	4.644318038000
124 H	-0.780827574200	-4.537835676000	3.726469360000
125 H	5.643104486000	-0.322497451200	2.779327948000
126 C	3.050550942000	-2.584631974000	2.151056938000
127 H	-0.330301940100	-4.961877907000	2.060054788000
128 C	5.137821942000	-1.298614548000	2.788411667000
129 H	2.987376202000	-3.053044422000	3.144634117000
130 H	3.641600131000	-3.255601053000	1.509722387000
131 H	5.742748579000	-2.002976050000	2.196751112000
132 H	5.116301252000	-1.659306436000	3.828793004000

{(DAB)B}Bi=Bi{B(DAB)} 45° boryl tilt

1 H	-5.729240815000	2.249654296000	-2.790194558000
2 H	-6.216271577000	2.115079815000	-1.082421940000
3 H	-4.104601854000	3.266014140000	-0.265608875600
4 C	-5.644751261000	1.626200734000	-1.886376206000
5 H	-3.577851703000	3.518088896000	-1.940552728000
6 H	-0.252544343500	5.071797927000	-1.053622326000

7 H	-6.115855783000	0.656375214300	-2.100523895000
8 H	0.054080311210	5.062550418000	-2.802932078000
9 H	1.809145089000	6.505262029000	-0.661434934900
10 C	-3.547990324000	2.810491967000	-1.098453845000
11 H	-7.093724803000	-0.263258173500	2.907309968000
12 H	2.224044078000	6.509778477000	-2.391581917000
13 H	-3.340646051000	2.435781445000	-3.871550599000
14 C	0.279181067000	4.543098136000	-1.858952455000
15 C	2.345264364000	5.953895786000	-1.448917260000
16 H	-5.178150714000	1.319948811000	3.418070678000
17 C	-4.169676906000	1.454549109000	-1.471991553000
18 H	-2.499778651000	2.695279577000	-0.789011309200
19 H	-0.127069658100	3.524375092000	-1.928574333000
20 C	-6.459849051000	-1.121453070000	3.177709277000
21 H	1.828063396000	4.908193688000	-4.266313807000
22 H	-6.640395686000	-1.353273270000	4.238808436000
23 C	-3.054718017000	1.389692743000	-3.747065209000
24 H	-4.148190087000	0.823293093300	-0.573396004900
25 H	-6.785718616000	-1.987743616000	2.584608065000
26 H	3.415160989000	5.949676952000	-1.196273170000
27 C	1.790799981000	4.521571495000	-1.573827088000
28 H	0.220090832100	4.239442106000	3.376338765000
29 H	-2.132447375000	1.273513271000	-5.694405663000
30 C	-4.554607863000	0.461715189500	3.710979819000
31 H	-4.674895079000	0.318707136700	4.795626890000
32 C	-3.380437927000	0.725495502200	-2.555190616000
33 C	-2.378146397000	0.738233547100	-4.776197906000
34 H	-4.859842078000	-0.572011288600	1.856982737000
35 H	1.937575213000	4.021077541000	-0.607521695000
36 C	-4.975060538000	-0.794188352400	2.926434988000
37 C	2.462279175000	4.068726158000	-3.974562740000
38 H	-3.502995434000	0.719019796100	3.519518009000
39 H	2.593333657000	4.878283404000	3.961960827000
40 C	0.459943685100	3.186152907000	3.586614084000
41 H	0.227919740800	3.000619409000	4.646194794000
42 C	2.556981525000	3.718419227000	-2.619436931000
43 H	3.077388078000	3.656345954000	-6.001498904000
44 H	-0.203366968100	2.553930603000	2.980147205000
45 H	-5.089507228000	-2.331662380000	-2.052325508000
46 C	3.163257793000	3.366709317000	-4.953152021000
47 C	-2.995786860000	-0.628108544900	-2.421959650000
48 H	-4.476938939000	-1.905535633000	5.359873572000
49 C	-4.453036611000	-2.192508485000	-1.185899205000
50 H	2.717667472000	3.604044379000	5.199534012000
51 C	-2.013905669000	-0.598679733600	-4.628695263000
52 C	2.845766842000	3.819694777000	4.127344900000
53 H	2.109325597000	3.165980189000	2.218035364000
54 N	-3.338481778000	-1.342779425000	-1.219337062000
55 H	-5.296053072000	-3.454580538000	0.421096867600
56 C	1.940606520000	2.909600211000	3.272835362000
57 C	-4.082152070000	-1.990961287000	3.239167960000
58 C	-4.560068157000	-2.749427151000	0.051062197160
59 H	-1.482236721000	-1.101373130000	-5.438505553000
60 C	-2.310692480000	-1.308291855000	-3.455844190000
61 C	-3.946972088000	-2.432458459000	4.563855677000
62 H	3.907845781000	3.679992972000	3.881868840000
63 C	3.385126106000	2.627691218000	-2.270159852000
64 B	-2.701971765000	-1.359357379000	0.083404331450
65 Bi	0.967108552200	0.019266894760	-1.099616565000
66 N	-3.519926386000	-2.271193802000	0.858090655100
67 H	-3.913328636000	-3.546881153000	-3.869746410000
68 C	3.973086336000	2.292350757000	-4.589204299000
69 N	3.515922190000	2.258913554000	-0.884134251600
70 C	-3.384221258000	-2.691942404000	2.228821410000

71 B	2.700295405000	1.366524203000	-0.084042126670
72 H	5.293843607000	3.452441305000	-0.482714820500
73 H	1.483700042000	1.321345403000	5.436893260000
74 Bi	-0.959312690100	-0.040408659650	1.119835149000
75 C	4.558956466000	2.756853760000	-0.092956176530
76 C	4.101650984000	1.900310481000	-3.248477359000
77 H	4.517509205000	1.744702927000	-5.361110593000
78 C	2.315041369000	1.439924713000	3.448151600000
79 H	-2.788093406000	-3.426996393000	-5.240605750000
80 C	-2.863862636000	-3.672707585000	-4.169836341000
81 C	-1.921738751000	-2.779804204000	-3.336611226000
82 C	-3.149111084000	-3.530150018000	4.881708510000
83 H	-2.039016727000	-3.062330054000	-2.281227579000
84 N	3.345631566000	1.377141091000	1.214368471000
85 H	-3.057168331000	-3.857685072000	5.918340127000
86 C	4.457126564000	2.229449976000	1.157508657000
87 C	2.008308626000	0.780081998600	4.647316327000
88 H	5.093479853000	2.393835135000	2.019701988000
89 C	2.991741388000	0.711905403700	2.442048530000
90 H	-2.598398256000	-4.733751590000	-4.045285690000
91 C	-2.571535765000	-3.808349126000	2.530875180000
92 C	-2.468864056000	-4.207729784000	3.871769376000
93 H	-0.281885139900	-2.847133639000	-4.797794868000
94 H	0.233530947800	-2.417758156000	-3.151068885000
95 C	-0.458391451200	-3.044905810000	-3.729822861000
96 C	5.004408117000	0.725044868800	-2.885693453000
97 H	3.547133006000	-0.823326302900	-3.422086130000
98 H	4.887657482000	0.543835388100	-1.808709545000
99 H	-2.004573432000	-4.070898041000	0.497337228200
100 C	2.354459046000	-0.554795202000	4.846241293000
101 H	4.718304457000	-0.462663605100	-4.710538111000
102 H	6.804014186000	1.946182398000	-2.586070560000
103 H	-3.443481798000	-6.027557226000	1.096034889000
104 H	6.669757104000	1.245194136000	-4.214105696000
105 H	2.101942056000	-1.051318542000	5.784232906000
106 C	4.596903410000	-0.564378875100	-3.621384355000
107 C	-1.826455194000	-4.585523429000	1.450824807000
108 H	-1.845101862000	-5.066756279000	4.127053459000
109 H	-0.204556392300	-4.099659584000	-3.545441732000
110 C	6.487245064000	1.054342517000	-3.145239960000
111 C	3.355792985000	-0.641597438700	2.626210235000
112 H	4.080184548000	-0.842958146200	0.636563389000
113 C	3.021019074000	-1.254868106000	3.842424812000
114 C	-2.366341837000	-6.022291601000	1.315847739000
115 H	0.087503128390	-3.569220203000	1.764808188000
116 H	5.227175853000	-1.404977248000	-3.293789009000
117 H	-2.209330439000	-6.595302877000	2.242730811000
118 H	2.472741320000	-2.730271756000	1.006790425000
119 C	4.133793597000	-1.420050655000	1.569671761000
120 H	7.127089233000	0.212843801100	-2.838889438000
121 C	-0.307606100700	-4.592420418000	1.696540220000
122 H	-1.847636039000	-6.551419261000	0.501947905900
123 H	3.290762828000	-2.299562700000	4.006800648000
124 H	-0.053465204820	-5.116401772000	2.630639724000
125 H	6.077961090000	-0.550236251500	2.102287775000
126 C	3.531756263000	-2.806517127000	1.289550609000
127 H	0.210065504100	-5.107585935000	0.873377435900
128 C	5.620969688000	-1.539618472000	1.958930482000
129 H	3.603218726000	-3.467944926000	2.165984944000
130 H	4.073479147000	-3.294521748000	0.465411637500
131 H	6.183844195000	-2.066661338000	1.173135138000
132 H	5.736427810000	-2.104779493000	2.897067714000

{(DAB)B}Bi=Bi{B(DAB)} 60° boryl tilt

1 H	-6.382728786000	2.273745234000	-1.665883953000
2 H	-6.575424224000	1.799291081000	0.040364077270
3 H	-4.493001768000	3.066544949000	0.759596157700
4 C	-6.089595672000	1.528655822000	-0.909750532600
5 H	-4.283672267000	3.666406943000	-0.895598959300
6 H	-0.672904110100	4.961117170000	0.108522322200
7 H	-6.480756888000	0.552143044900	-1.228498559000
8 H	-0.546099999100	5.400361979000	-1.605945698000
9 H	1.374773055000	6.366764971000	0.641996094600
10 C	-4.035742627000	2.838258006000	-0.214810087800
11 H	-6.774226481000	-1.281263503000	3.451314135000
12 H	1.623287154000	6.798650631000	-1.067037711000
13 H	-4.170108406000	2.979035765000	-2.985032310000
14 C	-0.212885186200	4.674301718000	-0.848962032700
15 C	1.847409468000	6.043089333000	-0.297947157900
16 H	-4.967859570000	0.402240557600	4.031716583000
17 C	-4.557379050000	1.491217049000	-0.741042720400
18 H	-2.944494797000	2.820774168000	-0.086195558920
19 H	-0.599029614100	3.686085179000	-1.134257589000
20 C	-6.034214804000	-2.094570319000	3.499662548000
21 H	0.980062604200	5.585523816000	-3.251771707000
22 H	-6.060526420000	-2.514346213000	4.517158899000
23 C	-3.789493221000	1.963606971000	-3.108700759000
24 H	-4.325940022000	0.729603682800	0.015841921460
25 H	-6.347810852000	-2.884412730000	2.802394546000
26 H	2.936128287000	6.029446234000	-0.146428322300
27 C	1.319336349000	4.656552225000	-0.715793193900
28 H	0.522446330700	3.129356570000	4.384364512000
29 H	-3.168795576000	2.304783666000	-5.147073599000
30 C	-4.234140192000	-0.415279167800	4.098834441000
31 H	-4.202494973000	-0.748313374600	5.147348675000
32 C	-3.879192428000	1.061208246000	-2.038375302000
33 C	-3.230014666000	1.587013834000	-4.327844327000
34 H	-4.668624719000	-1.158655508000	2.134404336000
35 H	1.573574045000	3.947446402000	0.083431335140
36 C	-4.629003202000	-1.564893963000	3.154116422000
37 C	1.711144736000	4.775598783000	-3.217118709000
38 H	-3.243916746000	-0.010723521160	3.844433120000
39 H	2.908390726000	3.918813880000	4.668139239000
40 C	0.889718198300	2.093724204000	4.325972754000
41 H	0.903187268700	1.692785838000	5.350604056000
42 C	2.003350716000	4.166645204000	-1.987661348000
43 H	2.093578085000	4.851957824000	-5.339649673000
44 H	0.169029134700	1.505222815000	3.742041316000
45 H	-5.216604517000	-2.238687284000	-1.960591599000
46 C	2.335151997000	4.365057742000	-4.393695704000
47 C	-3.376267173000	-0.246935034400	-2.226586470000
48 H	-3.749945851000	-3.010125332000	5.284634954000
49 C	-4.489886226000	-2.176822722000	-1.158804446000
50 H	3.385555558000	2.443282232000	5.543934951000
51 C	-2.746852872000	0.291212932100	-4.496684713000
52 C	3.274560574000	2.888314734000	4.542812811000
53 H	2.215572493000	2.549993661000	2.702692791000
54 N	-3.479521294000	-1.203426848000	-1.153785499000
55 H	-4.989343097000	-3.790292361000	0.266266773600
56 C	2.288754748000	2.066803930000	3.686917134000
57 C	-3.595269201000	-2.687003783000	3.155612118000
58 C	-4.380054328000	-2.948879221000	-0.044349699600
59 H	-2.307637707000	0.003776525878	-5.453571287000
60 C	-2.806482385000	-0.649061226000	-3.457501575000
61 C	-3.266410838000	-3.328883640000	4.358999338000
62 H	4.271630689000	2.935081405000	4.083888242000

63 C	2.954227794000	3.120667861000	-1.972426882000
64 B	-2.682853744000	-1.371316063000	0.045946449530
65 Bi	0.970166248300	0.020968739610	-1.095089203000
66 N	-3.295477700000	-2.497172926000	0.719533706200
67 H	-4.271641499000	-2.935071308000	-4.083898862000
68 C	3.266400028000	3.328893736000	-4.359009957000
69 N	3.295466890000	2.497183023000	-0.719544325900
70 C	-2.954238603000	-3.120657764000	1.972416263000
71 B	2.682842934000	1.371326159000	-0.045957069160
72 H	4.989332287000	3.790302457000	-0.266277393200
73 H	2.307626897000	-0.003766429273	5.453560668000
74 Bi	-0.970177058300	-0.020958643000	1.095078583000
75 C	4.380043518000	2.948889318000	0.044339079980
76 C	3.595258391000	2.687013880000	-3.155622738000
77 H	3.749935041000	3.010135428000	-5.284645573000
78 C	2.806471575000	0.649071322700	3.457490955000
79 H	-3.385566368000	-2.443272136000	-5.543945570000
80 C	-3.274571384000	-2.888304637000	-4.542823430000
81 C	-2.288765558000	-2.066793833000	-3.686927754000
82 C	-2.335162807000	-4.365047646000	4.393685084000
83 H	-2.215583303000	-2.549983564000	-2.702703411000
84 N	3.479510484000	1.203436945000	1.153774880000
85 H	-2.093588895000	-4.851947728000	5.339639054000
86 C	4.489875416000	2.176832819000	1.158793827000
87 C	2.746842062000	-0.291202835500	4.496674094000
88 H	5.216593707000	2.238697381000	1.960580980000
89 C	3.376256363000	0.246945131000	2.226575851000
90 H	-2.908401535000	-3.918803784000	-4.668149858000
91 C	-2.003361526000	-4.166635107000	1.987650728000
92 C	-1.711155546000	-4.775588686000	3.217108089000
93 H	-0.903198078700	-1.692775741000	-5.350614675000
94 H	-0.169039944600	-1.505212718000	-3.742051935000
95 C	-0.889729008200	-2.093714107000	-4.325983374000
96 C	4.628992392000	1.564904059000	-3.154127042000
97 H	3.243905936000	0.010733617770	-3.844443740000
98 H	4.668613909000	1.158665605000	-2.134414956000
99 H	-1.573584855000	-3.947436305000	-0.083441954770
100 C	3.230003856000	-1.587003737000	4.327833707000
101 H	4.202484163000	0.748323471200	-5.147359294000
102 H	6.347800042000	2.884422826000	-2.802405165000
103 H	-2.936139097000	-6.029436137000	0.146417702600
104 H	6.060515610000	2.514356309000	-4.517169518000
105 H	3.168784766000	-2.304773570000	5.147062979000
106 C	4.234129382000	0.415289264400	-4.098845060000
107 C	-1.319347159000	-4.656542129000	0.715782574300
108 H	-0.980073414100	-5.585513720000	3.251761088000
109 H	-0.522457140600	-3.129346473000	-4.384375131000
110 C	6.034203994000	2.094580415000	-3.499673168000
111 C	3.879181618000	-1.061198150000	2.038364683000
112 H	4.325929212000	-0.729593586200	-0.015852541090
113 C	3.789482411000	-1.963596875000	3.108690140000
114 C	-1.847420278000	-6.043079237000	0.297936538200
115 H	0.599018804100	-3.686075083000	1.134246969000
116 H	4.967848760000	-0.402230461000	-4.031727203000
117 H	-1.623297964000	-6.798640534000	1.067027092000
118 H	2.944483988000	-2.820764071000	0.086184939300
119 C	4.557368240000	-1.491206952000	0.741032100800
120 H	6.774215671000	1.281273600000	-3.451324754000
121 C	0.212874376200	-4.674291621000	0.848951413100
122 H	-1.374783865000	-6.366754874000	-0.642006714300
123 H	4.170097597000	-2.979025668000	2.985021690000
124 H	0.546089189200	-5.400351882000	1.605935078000
125 H	6.480746078000	-0.552132948300	1.228487939000
126 C	4.035731817000	-2.838247909000	0.214799468200

127 H	0.672893300100	-4.961107073000	-0.108532941800
128 C	6.089584862000	-1.528645726000	0.909739913000
129 H	4.283661457000	-3.666396846000	0.895588339700
130 H	4.492990958000	-3.066534852000	-0.759606777300
131 H	6.575413414000	-1.799280985000	-0.040374696900
132 H	6.382717976000	-2.273735137000	1.665873334000

{(DAB)B}Bi=Bi{B(DAB)} 75° boryl tilt

1 H	-6.977317118000	2.056591988000	-0.387412429900
2 H	-6.938331179000	1.149917836000	1.144391540000
3 H	-4.899409202000	2.417214790000	1.970239414000
4 C	-6.544514521000	1.178566452000	0.116832266700
5 H	-4.896846931000	3.416175946000	0.503600337400
6 H	-1.180834669000	4.472454858000	0.986156376200
7 H	-6.895886329000	0.280165943900	-0.410117485000
8 H	-1.080495709000	5.493563569000	-0.455790582700
9 H	0.938798760100	5.581046006000	1.838357782000
10 C	-4.527240769000	2.474303837000	0.936351465900
11 H	-6.411327368000	-2.580033228000	3.690454940000
12 H	1.192965945000	6.509210482000	0.338061989600
13 H	-5.130710278000	3.234381720000	-1.721967284000
14 C	-0.769402835400	4.526566091000	-0.032348485310
15 C	1.380117472000	5.541903623000	0.830545103300
16 H	-4.819576640000	-0.750977939700	4.436154539000
17 C	-5.004848021000	1.253708590000	0.131307870000
18 H	-3.429552134000	2.525965220000	0.968716815100
19 H	-1.227872677000	3.726993339000	-0.630071989200
20 C	-5.558432267000	-3.256727912000	3.529274843000
21 H	0.058211870470	5.724674544000	-2.263890186000
22 H	-5.414124240000	-3.841267494000	4.450951104000
23 C	-4.620821916000	2.353094641000	-2.115863369000
24 H	-4.633418988000	0.355133040400	0.642147246900
25 H	-5.825017253000	-3.958060904000	2.725881590000
26 H	2.466553315000	5.419084327000	0.939134423000
27 C	0.759777960400	4.387656473000	0.016487519090
28 H	0.818957158700	1.673885840000	4.857396927000
29 H	-4.317679561000	3.234355008000	-4.062041910000
30 C	-3.969450717000	-1.433397593000	4.284999111000
31 H	-3.768619438000	-1.933578861000	5.244611806000
32 C	-4.443072637000	1.234922353000	-1.287057105000
33 C	-4.167659758000	2.355771601000	-3.432931208000
34 H	-4.502313741000	-1.888432797000	2.257970601000
35 H	0.989439833800	3.449782988000	0.542150035700
36 C	-4.292556967000	-2.452495049000	3.176702543000
37 C	0.913568102200	5.068130789000	-2.427762683000
38 H	-3.085914985000	-0.831346763100	4.028691676000
39 H	3.064759864000	2.835687265000	5.038834517000
40 C	1.345901649000	0.759990394000	4.545100865000
41 H	1.586586044000	0.193860177600	5.457388004000
42 C	1.396656673000	4.289809467000	-1.366181174000
43 H	1.112793149000	5.634458801000	-4.500601055000
44 H	0.655355105400	0.154423591900	3.942253157000
45 H	-5.309266451000	-2.152138644000	-1.827989626000
46 C	1.503838332000	5.017757176000	-3.690035609000
47 C	-3.779843076000	0.107017562500	-1.822798206000
48 H	-3.040147833000	-4.131293337000	4.908255782000
49 C	-4.498016692000	-2.148324723000	-1.109175015000
50 H	3.915182342000	1.339549445000	5.498777292000
51 C	-3.519536434000	1.233015466000	-3.944245986000
52 C	3.572527273000	1.942667440000	4.643421516000
53 H	2.307729861000	1.768804893000	2.913433815000
54 N	-3.611293909000	-1.065290768000	-1.002515055000

55 H	-4.627975013000	-4.058938917000	-0.007758229706
56 C	2.611851204000	1.127822809000	3.753013207000
57 C	-3.107577081000	-3.369502241000	2.888837054000
58 C	-4.160503453000	-3.099187723000	-0.197445560800
59 H	-3.162991578000	1.244331218000	-4.975428818000
60 C	-3.309421093000	0.091697145100	-3.156714415000
61 C	-2.587528217000	-4.172726518000	3.915409074000
62 H	4.460011615000	2.274794723000	4.087931708000
63 C	2.504851799000	3.445319006000	-1.612900600000
64 B	-2.661911330000	-1.350868928000	0.053693093750
65 Bi	0.970082958700	-0.029733610060	-1.096056093000
66 N	-3.047859249000	-2.659564501000	0.534223936200
67 H	-4.460022428000	-2.274784579000	-4.087942379000
68 C	2.587517403000	4.172736662000	-3.915419745000
69 N	3.047848435000	2.659574645000	-0.534234607200
70 C	-2.504862613000	-3.445308862000	1.612889929000
71 B	2.661900516000	1.350879072000	-0.053703764750
72 H	4.627964200000	4.058949061000	0.007747558704
73 H	3.162980764000	-1.244321074000	4.975418147000
74 Bi	-0.970093772400	0.029743753590	1.096045422000
75 C	4.160492639000	3.099197867000	0.197434889800
76 C	3.107566267000	3.369512385000	-2.888847725000
77 H	3.040137019000	4.131303480000	-4.908266453000
78 C	3.309410280000	-0.091687001570	3.156703744000
79 H	-3.915193156000	-1.339539302000	-5.498787963000
80 C	-3.572538087000	-1.942657296000	-4.643432187000
81 C	-2.611862017000	-1.127812665000	-3.753023878000
82 C	-1.503849145000	-5.017747032000	3.690024938000
83 H	-2.307740674000	-1.768794750000	-2.913444486000
84 N	3.611283095000	1.065300911000	1.002504384000
85 H	-1.112803963000	-5.634448658000	4.500590384000
86 C	4.498005878000	2.148334867000	1.109164344000
87 C	3.519525620000	-1.233005323000	3.944235315000
88 H	5.309255637000	2.152148787000	1.827978955000
89 C	3.779832263000	-0.107007419000	1.822787535000
90 H	-3.064770677000	-2.835677121000	-5.038845188000
91 C	-1.396667487000	-4.289799323000	1.366170503000
92 C	-0.913578915900	-5.068120645000	2.427752012000
93 H	-1.586596858000	-0.193850034100	-5.457398675000
94 H	-0.655365919100	-0.154413448300	-3.942263828000
95 C	-1.345912463000	-0.759980250500	-4.545111536000
96 C	4.292546153000	2.452505192000	-3.176713214000
97 H	3.085904171000	0.831356906700	-4.028702347000
98 H	4.502302928000	1.888442940000	-2.257981272000
99 H	-0.989450647500	-3.449772844000	-0.542160706700
100 C	4.167648944000	-2.355761457000	3.432920537000
101 H	3.768608624000	1.933589005000	-5.244622477000
102 H	5.825006439000	3.958071048000	-2.725892261000
103 H	-2.466564129000	-5.419074183000	-0.939145094000
104 H	5.414113426000	3.841277637000	-4.450961775000
105 H	4.317668748000	-3.234344865000	4.062031239000
106 C	3.969439904000	1.433407736000	-4.285009782000
107 C	-0.759788774100	-4.387646329000	-0.016498190090
108 H	-0.058222684170	-5.724664400000	2.263879515000
109 H	-0.818967972400	-1.673875697000	-4.857407598000
110 C	5.558421453000	3.256738055000	-3.529285514000
111 C	4.443061824000	-1.234912209000	1.287046434000
112 H	4.633408174000	-0.355122896800	-0.642157917900
113 C	4.620811102000	-2.353084498000	2.115852698000
114 C	-1.380128286000	-5.541893479000	-0.830555774300
115 H	1.227861864000	-3.726983195000	0.630061318200
116 H	4.819565826000	0.750988083300	-4.436165210000
117 H	-1.192976758000	-6.509200338000	-0.338072660600
118 H	3.429541320000	-2.525955077000	-0.968727486100

119	C	5.004837207000	-1.253698446000	-0.131318541000
120	H	6.411316555000	2.580043372000	-3.690465611000
121	C	0.769392021700	-4.526555948000	0.032337814310
122	H	-0.938809573800	-5.581035863000	-1.838368453000
123	H	5.130699464000	-3.234371577000	1.721956613000
124	H	1.080484895000	-5.493553425000	0.455779911700
125	H	6.895875515000	-0.280155800400	0.410106814000
126	C	4.527229955000	-2.474293694000	-0.936362136900
127	H	1.180823855000	-4.472444715000	-0.986167047200
128	C	6.544503707000	-1.178556308000	-0.116842937700
129	H	4.896836117000	-3.416165803000	-0.503611008400
130	H	4.899398388000	-2.417204647000	-1.970250085000
131	H	6.938320365000	-1.149907693000	-1.144402211000
132	H	6.977306305000	-2.056581844000	0.387401758900

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