Electronic Supplementary Information

Neutral cyclic sp^2-sp^3 and sp^3-sp^3 diboranes from N,N'-dicyclohexylcarbodiimide insertion into 1,2-dichlorodiboranes(4)

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General Methods:

All reactions were performed under dry argon atmosphere using standard Schlenk techniques. All solvents were dried by applying suitable procedures. $B_2(NMe_2)_4$,[1] $B_2Cl_2(NMe_2)_2$,[2] $B_2Cl_2Dur_2$ (Dur: 2,3,5,6-tetramethylphenyl[3] were prepared according to literature procedures. N,N'-Dicyclohexylcarbodiimide was purchased from Sigma-Aldrich and used directly. Infrared spectra were recorded on an ATR Spectrum-II, PerkinElmer spectrometer. Elemental analyses were done on a LECO CHNS-932 by METU Central Laboratory (Ankara, Turkey). ^{1}H, ^{11}B and ^{13}C NMR spectra were recorded with a Varian 400 spectrometer in $CDCl_3$. Residual signal of the solvent was used as reference for ^{1}H and ^{13}C NMR spectra. ^{11}B NMR spectra were referenced to external $BF_3.Et_2O$.

Preparation and characterization:

Synthesis of 1: A solution of CyN=C=NCy (1.03 g, 5.0 mmol) in 10 mL toluene was slowly added to a solution of $B_2Cl_2(NMe_2)_2$ (0.9 g, 5 mmol) in 5 mL toluene at room temperature. The mixture was stirred for 12 h. The resulting white precipitate was separated by filtration and washed with pentane. Compound **1** was obtained in 78% yield as a white powder. X-ray quality crystals were obtained from a saturated solution in CH_2Cl_2 at -30 °C.^{1}H NMR (400 MHz, $CDCl_3$, ppm): 0.83-3.08 (m, 20H, Cy-CH_2), 2.81 (s, 3H, B-NCH_3), 2.85 (s, 3H, C-NCH_3), 2.85 (s, 3H, C-NCH_3), 3.03 (s, 3H, B-NCH_3), 3.51 (m, 2H, Cy-CH); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): 25.3 (Cy-CH_2), 25.4 (Cy-CH_2), 26.7 (Cy-CH_2), 27.1 (Cy-CH_2), 31.6 (Cy-CH_2), 33.2 (Cy-CH_2), 41.1 (B-NCH_3), 41.6 (C-NCH_3), 42.4 (B-NCH_3), 59.5 (Cy-CH), 59.9 (Cy-CH), 173.5 (N-C(NMe_2)-N); ^{11}B NMR (128 MHz, $CDCl_3$, ppm): 2.8 (Cl_2-B-NCy), 41.6 (Me_2N-B-NCy); Elem. Anal. Calcd. (%) for $C_{17}H_{34}B_2Cl_2N_4$: C, 52.76; H, 8.86; N, 14.48; Found: C, 52.61; H, 8.53; N, 14.61; crystal data: M_r = 387.00; 0.517 × 0.365 × 0.307 mm; orthorhombic; space group $P2_12_12_1$; a= 9.1674(7), b= 10.6202(9), c= 22.2091(16) Å, V= 2162.3(3) Å^3, Z= 4, ρ_{calc}= 1.189 g/cm^3, MoK_α radiation (λ = 0.71073 Å), T = 294 K, 2Θ range for data collection= 6.71-51.358°, reflections collected 4857, independent reflections3563, R_{int}= 0.0271, final R indexes [$I>=2\sigma(I)$]: R_1= 0.0431, wR_2= 0.0806.

Synthesis of 2: A solution of CyN=C=NCy (0.41 g, 5.0 mmol) in 10 mL toluene was slowly added to a solution of $B_2Cl_2Dur_2$ (0.71 g, 2 mmol) in 5 mL toluene at room temperature. The mixture was stirred for 12 h. The resulting yellow precipitate was separated by filtration and washed with pentane. Compound **2** was obtained in 71% yield as a yellow solid. X-ray quality crystals were obtained from a saturated solution in CH_2Cl_2 at -30 °C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): 0.65-2.81 (m, 20H, Cy-CH_2), 2.16 (s, 12H, Dur-CH_3), 2.20 (s, 6H, Dur-CH_3), 2.29 (s, 6H, Dur-CH_3), 3.46 (m, 2H, Cy-CH), 6.84 (s, 1H, Dur-p-H), 7.15 (s, 1H, Dur-p-H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): 18.8 (Dur-CH_3), 19.1 (Dur-CH_3), 19.6 (Dur-CH_3), 20.0 (Dur-CH_3), 21.4 (Dur-CH_3), 23.0 (Dur-CH_3), 24.1 (Dur-CH_3), 25.1 (Cy-CH_2), 26.2 (Cy-CH_2), 27.8 (Cy-CH_2), 30.4 (Cy-CH_2), 32.2 (Cy-CH_2), 32.8 (Cy-CH_2), 63.0 (Cy-CH), 122.9 (Dur), 124.8 (Dur), 129.5 (Dur), 130.3 (Dur), 131.0 (Dur), 133.0 (Dur), 134.0 (Dur), 138.9 (Dur), 142.1 (Dur), 159.1 (N-C(Dur)-N); ^{11}B NMR (128 MHz, $CDCl_3$, ppm): 3.1 (Cl_2-B-NCy), 67.0 (Dur-B-NCy); Elem. Anal. Calcd. (%) for $C_{33}H_{48}B_2Cl_2N_2$: C, 70.12; H, 8.56; N, 4.96; Found: C, 70.38; H, 8.58; N, 4.81; crystal data: M_r = 565.25; 0.225 × 0.095 × 0.087 mm; monoclinic; space group $P2_1/n$; a= 10.335(3), b= 22.822(7), c= 13.912(4) Å, β= 102.12(3), V= 3208.0(17) Å^3, Z= 4, ρ_{calc}= 1.17 g/cm^3, MoK_α radiation (λ = 0.71073 Å), T = 293(2) K, 2Θ range for data collection= 5.736-49.426°, reflections collected 10635, independent reflections 5424, R_{int}= 0.1917, final R indexes [$I>=2\sigma(I)$]: R_1= 0.0956, wR_2= 0.1098.

Synthesis of 3: A solution of CyN=C=NCy (1.03 g, 5.0 mmol) in 10 mL toluene was slowly added to a solution of $B_2Cl_2(NMe_2)_2$ (0.45 g, 2.5 mmol) in 5 mL toluene at room temperature. The mixture was stirred for 12 h. The resulting white precipitate was separated by filtration and washed with pentane. Compound **3** was obtained in 74% yield as a white powder. X-ray quality crystals were obtained from a saturated solution in CH_2Cl_2 at -30 °C. ^{1}H NMR (400 MHz, C_6D_6, ppm): 0.87-1.95 (m, 40H, Cy-CH_2), 2.33 (s, 12 H, C-NCH_3), 3.29 (m, 4H, Cy-CH); ^{13}C NMR (100 MHz, C_6D_6, ppm): 26.2 (Cy-CH_2), 27.4 (Cy-CH_2), 33.7 (Cy-CH_2), 40.0 (C-NCH_3), 40.9 (C-NCH_3), 58.5 (Cy-CH), 170.5 (N-C(NMe_2)-N); ^{11}B NMR (128 MHz, C_6D_6, ppm): 6.1 (Cl-B-($NCy)_2$). Elem. Anal. Calcd. (%) for $C_{30}H_{56}B_2Cl_2N_6$: C, 60.73; H, 9.51; N, 14.16; Found: C, 60.77; H, 9.38; N, 14.01; crystal data: M_r = 593.32; 0.393 × 0.319 × 0.283 mm; tetragonal; space group $I4_1cd$; a= 17.6380(16), b= 17.6380(16), c= 24.541(3) Å, V= 7634.6(16) Å^3, Z= 4, ρ_{calc}= 1.189 g/cm^3, MoK_α radiation (λ = 0.71073 Å), T = 295 K, 2Θ range for data collection= 6.534-50.038°, reflections collected 5667, independent reflections 2016, R_{int}= 0.1050, final R indexes [$I>=2\sigma(I)$]: R_1= 0.0476, wR_2= 0.0887.

NMR Spectra:

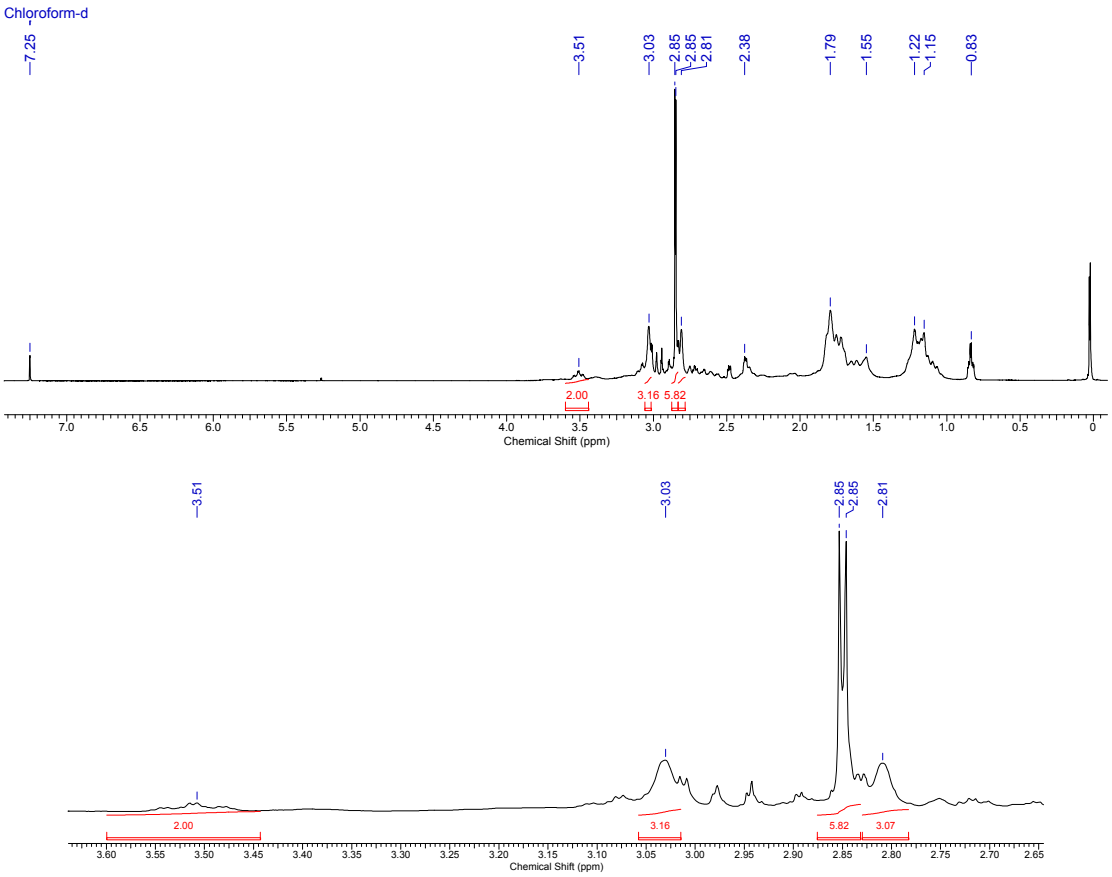


Fig. S1. ^{1}H NMR spectrum of **1**.

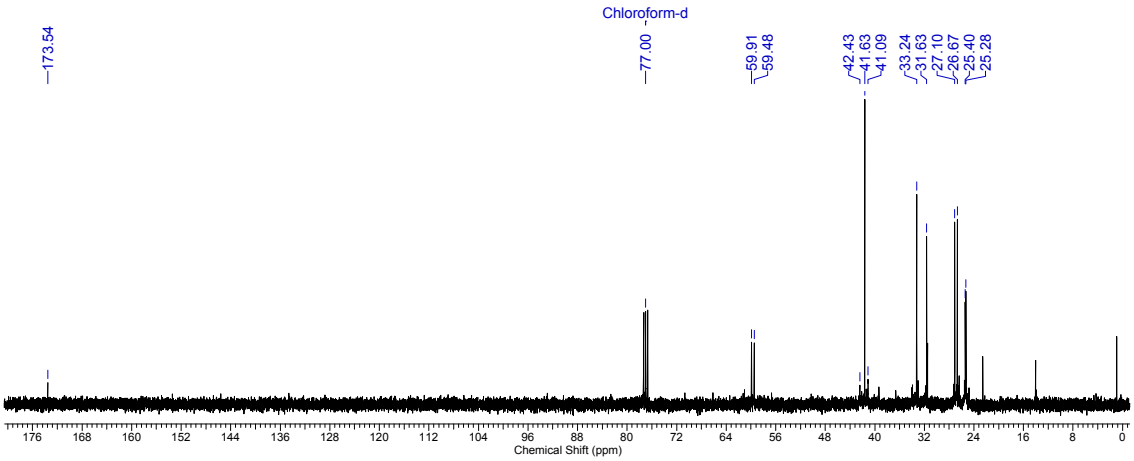


Fig. S2. ^{13}C NMR spectrum of **1**.

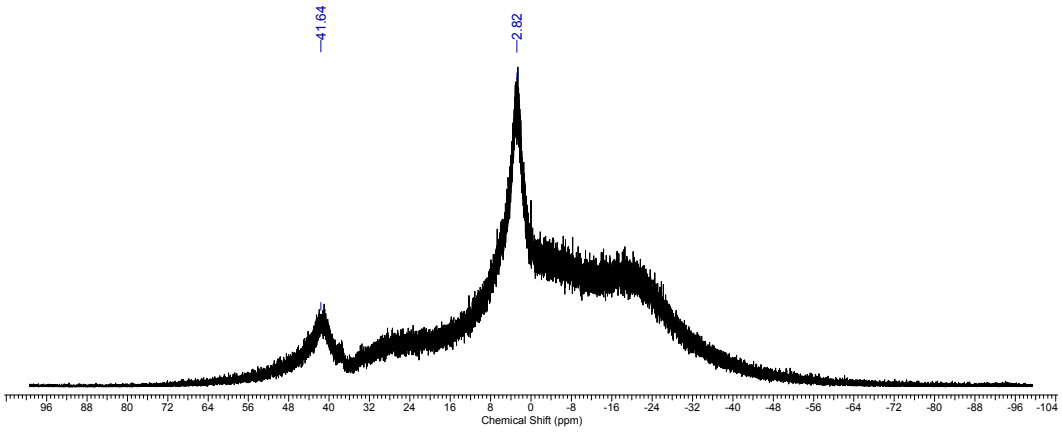


Fig. S3. ^{11}B NMR spectrum of **1**.

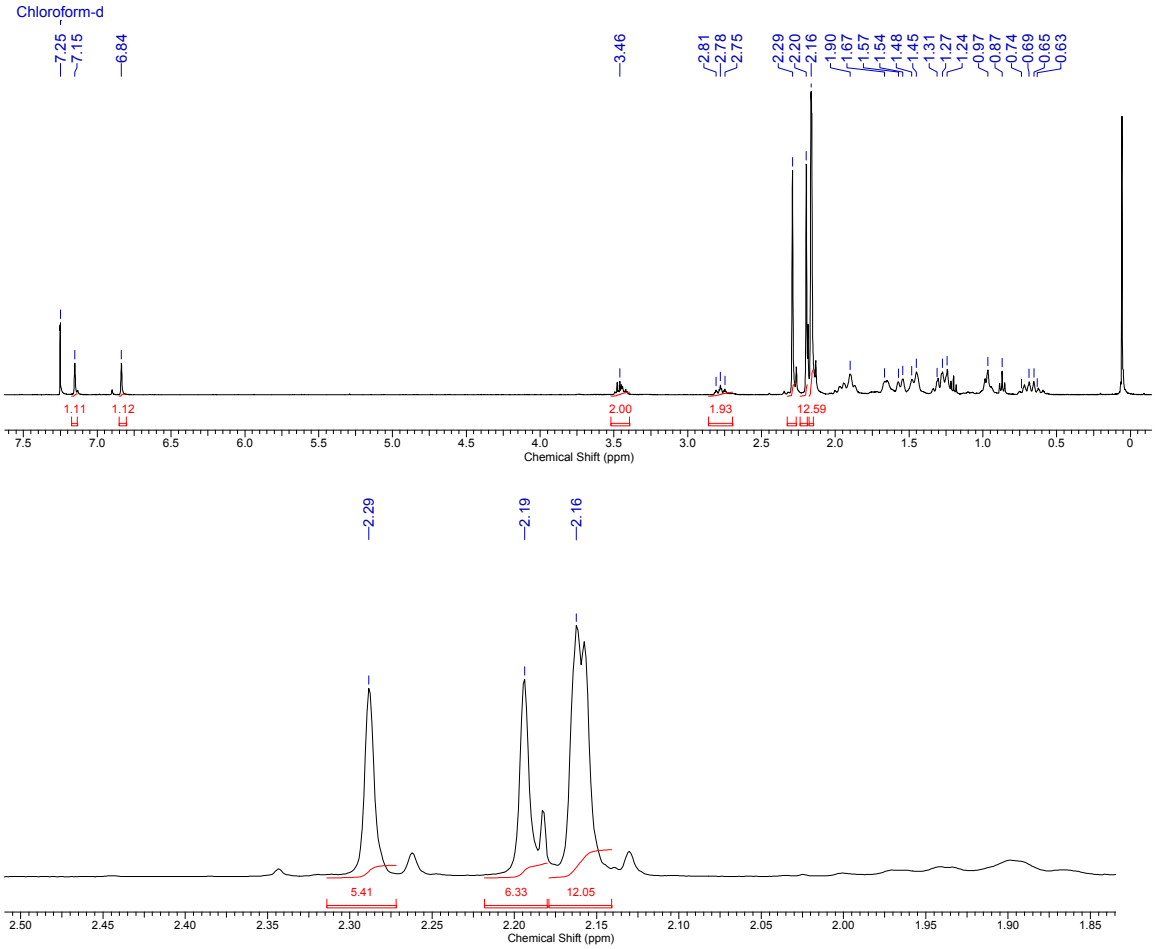


Fig. S4. ^{1}H NMR spectrum of **2**

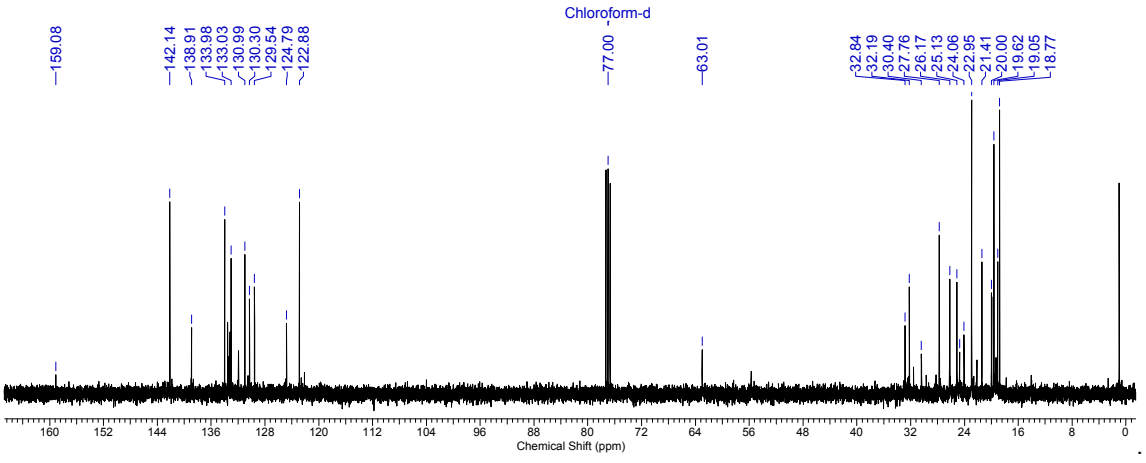


Fig. S5. ^{13}C NMR spectrum of **2**

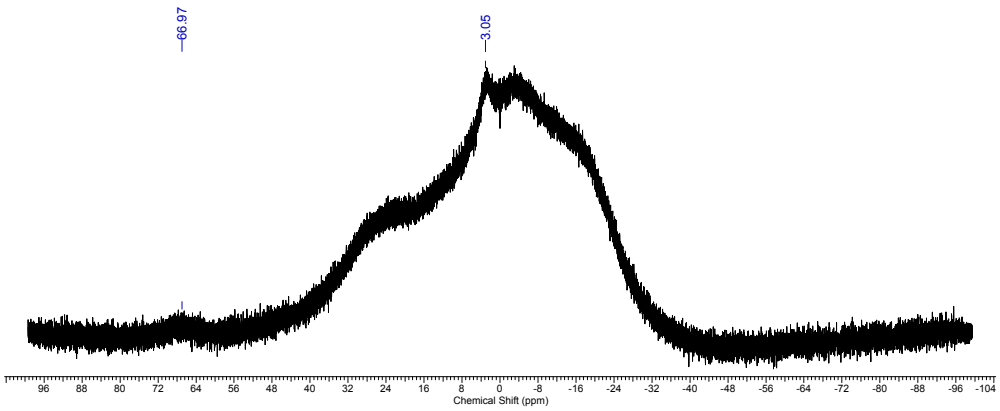


Fig. S6. ^{11}B NMR spectrum of **2**

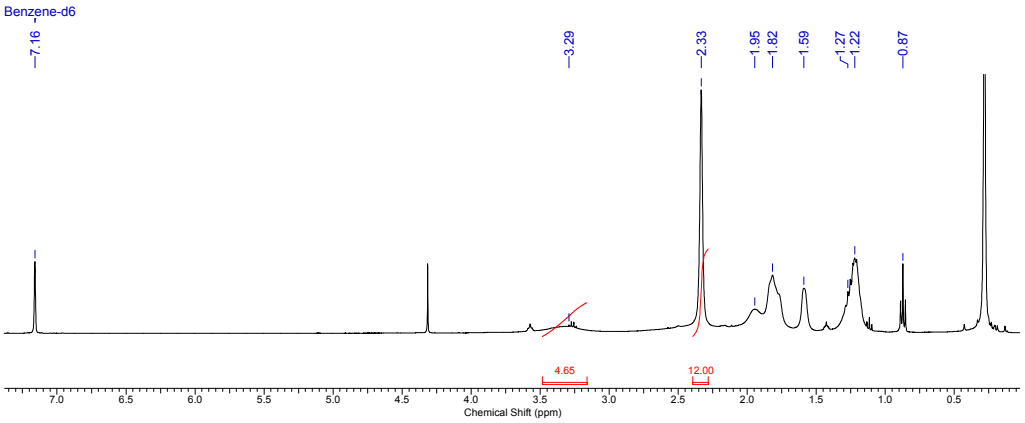


Fig. S7. ^{1}H NMR spectrum of **3**

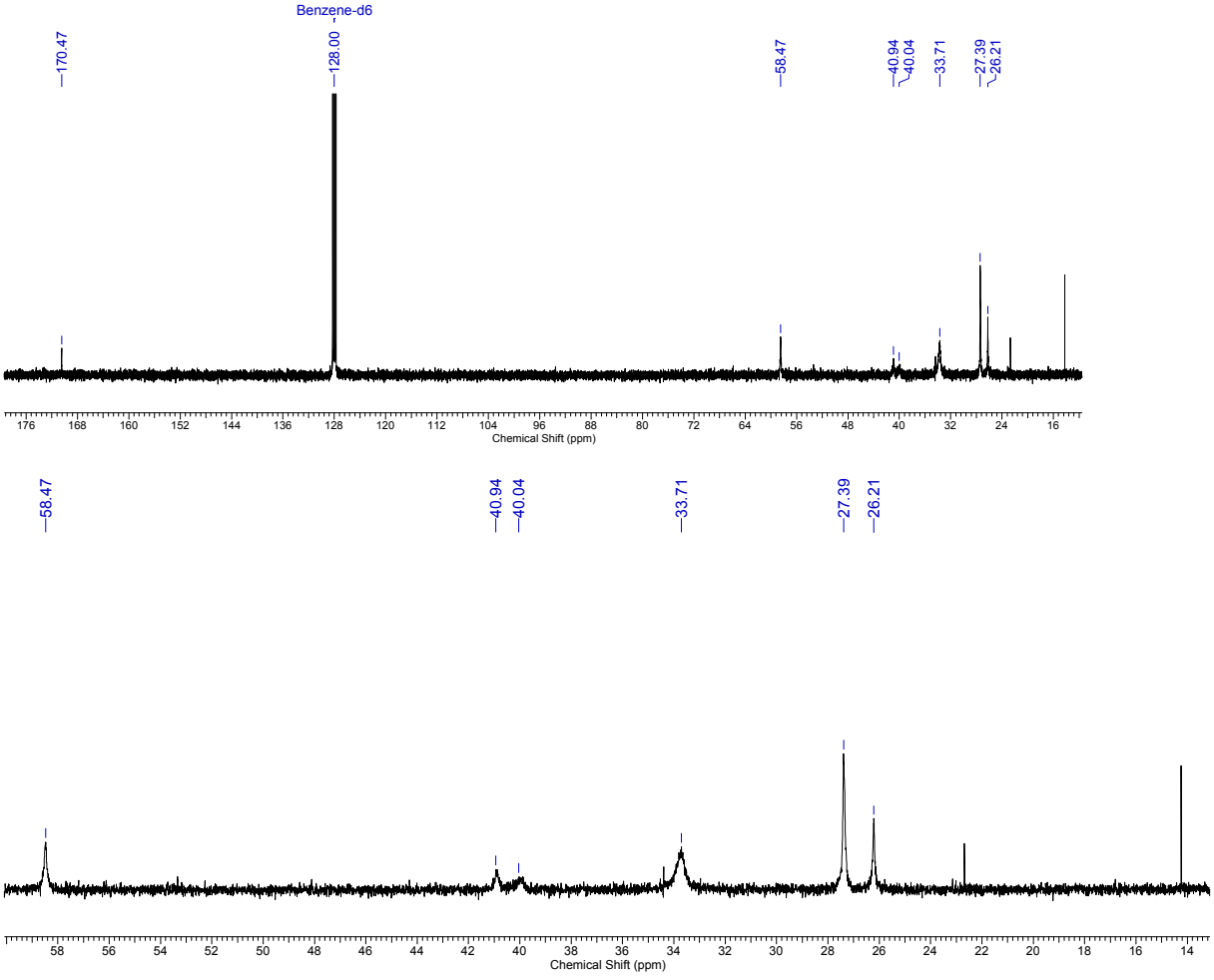


Fig. S8. ^{13}C NMR spectrum of **3**

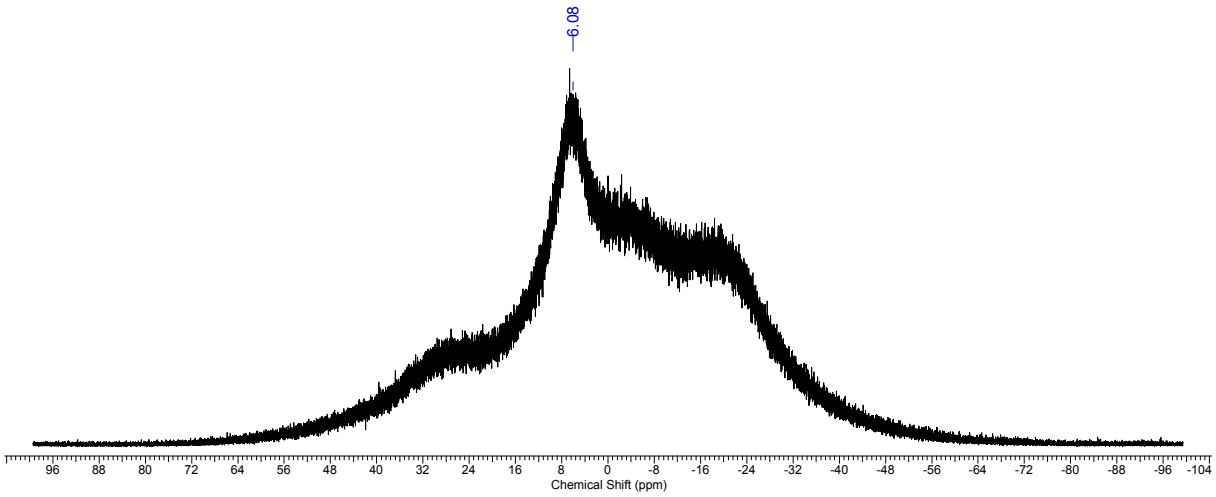


Fig. S9. ^{13}B NMR spectrum of **3**

X-Ray Crystallography:

The molecular structures of compounds were determined by single-crystal X-ray diffraction. Single-crystal data were collected at 293 (2) K by w-scan technique, on a Rigaku-Oxford Xcalibur diffractometer with an Eos CCD area detector using graphite monochromated radiation MoKα (λ=0.71073 Å) from an enhance X-ray source. The data collection, cell refinement and data reduction were performed using the CrysAlisPro program.[4] Solution, refinement and analysis of the structures were done using the OLEX2 system.[5] The crystal structures were solved with the ShelXT structure solution program using Direct Methods and refined by full-matrix least-squares method based on F^2 against all reflections using the SHELXL2016.[6] All non-H atoms were refined anisotropically while the H atoms were placed in calculated positions and refined using a riding model. CCDC 1995325 (**1**), 1995326 (**3**) and 1995327 (**2**) contain the supplementary crystallographic data for this paper. These data are provided free of charge by The Cambridge Crystallographic Data Centre.

Computational Details:

Quantum mechanical calculations were performed on Orca4[7] package program using DFT with the M06-2X[8] hybrid functional with the basis sets of 6-311G(d,p) for geometry optimizations, 6-311++G(2d,p)[9,10] for ^{1}H, ^{11}B and ^{13}C NMR calculations with the GIAO method[11,12]. To enlighten the reaction mechanism, transition states (*TS*) of the studied molecules were calculated with PM7 semiempirical methods on MOPAC2016 (Stewart, 2020) package program.[13] Natural Bond Orbital (NBO) analysis were performed using NBO6 program [14].

Table S1. Selected geometric parameters of the crystal structures and optimized geometries.

	1		**2**		**3**	
	X-ray	**Opt**	**X-ray**	**Opt**	**X-ray**	**Opt**
B1–B2	1.659(6)	1.689	1.663(1)	1.696	1.652(1)	1.699
B1–N1	1.560(5)	1.573	1.585(1)	1.574	1.578(7)	1.579
B2–N2	1.509(5)	1.514	1.469(1)	1.468	1.563(8)	1.573
N1–C1	1.330(4)	1.320	1.315(1)	1.316	1.309(7)	1.331
N2–C1	1.382(4)	1.374	1.399(1)	1.386	1.343(6)	1.333
N1–B1–B2	98.3(3)	97.5	98.5(7)	99.5	97.1(5)	97.6
B1–B2–N2	105.1(3)	104.5	105.4(9)	103.0	103.3(6)	101.8
N1–B1–B2–N2	13.9(4)	14.1	-4.5(9)	-3.3	16.5(5)	16.7

Comparison of Experimental and Theoretically Calculated Results

Table S2. Experimentally found and calculated chemical shift values for boron and carbon atoms.

	Exp δ_{13C} (ppm)	**Calc δ_{13C} (ppm)**	**Exp δ_{11B} (ppm)**	**Calc δ_{11B} (ppm)**
1	173.5	171.2	2.8, 41.6	3.0, 39.8
2	159.1	175.7	3.1, 67.0	4.0, 66.6
3	170.5	170.0	6.1	8.6

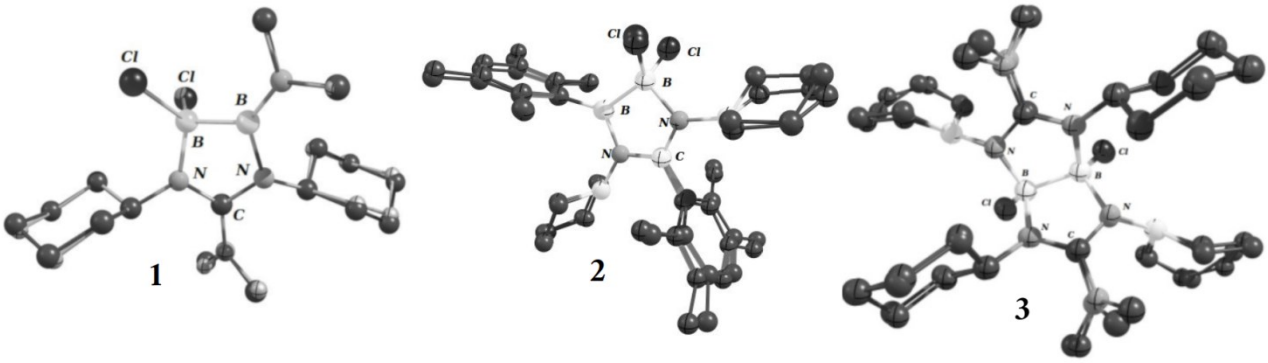


Fig. S10. Overlay of crystal structure and optimized geometries of the studied molecules. For clarity, H-atoms were omitted. RMSD values are 0.170Å, 0.377Å and 0.475 Å for **1**, **2** and **3**, respectively. Due to crystal structures of **2** and **3** have disordered 2 carbon atoms at one of cyclohexane groups, RMSD values are a little larger. Given RMSD values above are between optimized and main parts of the crystal structures. RMSD values between optimized and 2nd parts for **2** and **3** are 0.544 Å and 0.889 Å, respectively.

Reaction paths and transition geometries of the studied molecules 2 and 3.

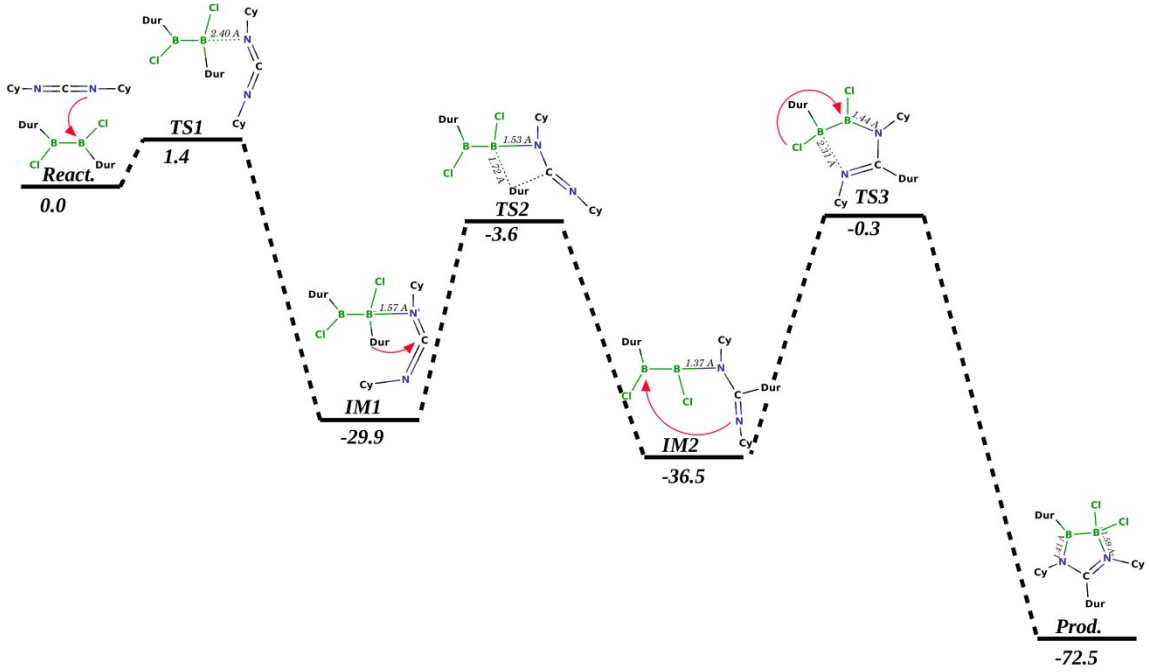


Fig. S11. Energy diagram of the reaction path of **2**. The calculated relative free energies are given in kcal/mol.

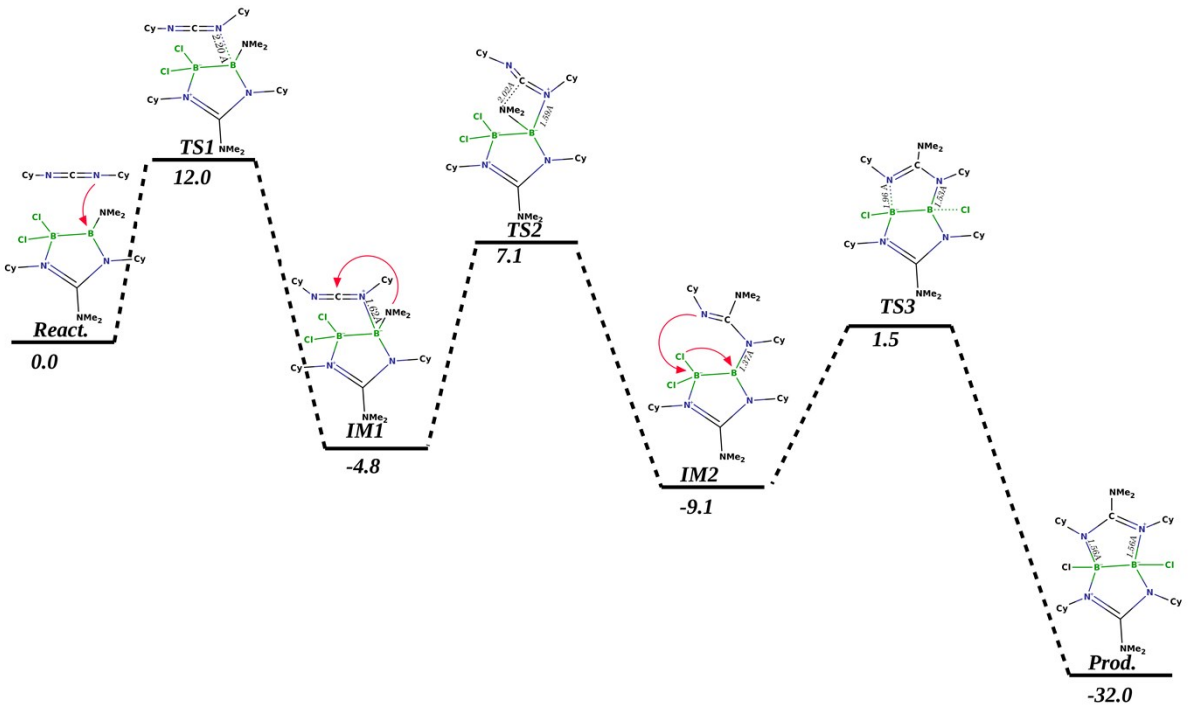
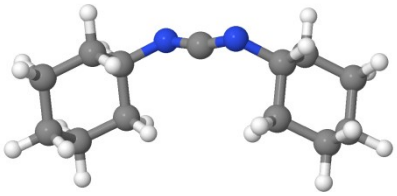


Fig. S12. Energy diagram of the reaction path of **3**. The calculated relative free energies are given in kcal/mol.

The computed geometries are given as follows.

Reactant 1:



Energy: -6.2542190 kcal/mol

C	-0.00006000	-1.22201100	-0.00027300
N	-0.97679400	-1.37985100	0.74444000
N	0.97665400	-1.37928900	-0.74513300
C	2.26430100	-0.70442500	-0.67618600
C	2.97296200	-0.98552500	0.66742800
C	2.10707200	0.81812000	-0.89441600
C	3.48457600	1.48748500	-0.87203700
C	4.20125500	1.20577000	0.45507700
C	4.34449500	-0.30495900	0.68209100
C	-2.26432800	-0.70469200	0.67591500
C	-2.97327100	-0.98535700	-0.66763900
C	-2.10681700	0.81777600	0.89447300
C	-4.34469400	-0.30456600	-0.68191100
C	-4.20117800	1.20608900	-0.45455500
C	-3.48421900	1.48736800	0.87250400
H	2.86840500	-1.14346200	-1.51856900
H	3.07845300	-2.07687700	0.81464000
H	2.35504400	-0.62485000	1.51022100
H	1.45886300	1.25221400	-0.11228300
H	1.59980800	1.00850900	-1.85819500
H	3.37703100	2.57771700	-1.02190300
H	4.09792800	1.12490800	-1.71844200
H	3.63963200	1.66161900	1.29192100
H	5.19617800	1.68653300	0.45897600
H	4.85082300	-0.49779200	1.64620200
H	4.99685200	-0.74514700	-0.09551700
H	-2.86837700	-1.14381100	1.51828900
H	-3.07896200	-2.07666000	-0.81508300
H	-2.35542800	-0.62458100	-1.51045800
H	-1.45868000	1.25195500	0.11231700
H	-1.59935300	1.00787500	1.85820700
H	-4.99698100	-0.74482800	0.09569900
H	-4.85122000	-0.49708600	-1.64597200
H	-5.19602900	1.68700700	-0.45816800
H	-3.63962500	1.66205900	-1.29139400
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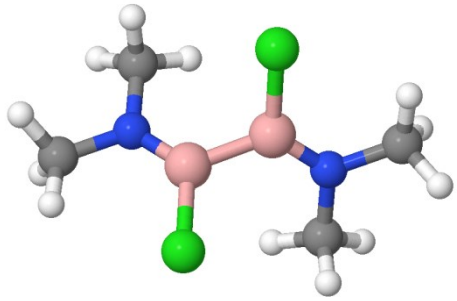
Reactant 2a:



Energy: -135.4762406 kcal/mol

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C	3.22182000	-0.12253700	0.31359100
N	-1.84502000	-0.35837100	0.42788100
C	-1.75838200	-1.64373100	1.12044100
C	-3.22189000	0.12247000	0.31363100
H	0.79643200	1.76543600	1.65260100
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H	2.55521200	1.76309400	1.87493100
H	3.30740900	-1.00028700	-0.35551900
H	3.61764000	-0.42732700	1.29937100
H	3.88423100	0.65808200	-0.10351900
H	-0.79614200	-1.76561300	1.65208100
H	-1.83979300	-2.48213100	0.39862100
H	-2.55482200	-1.76326100	1.87510100
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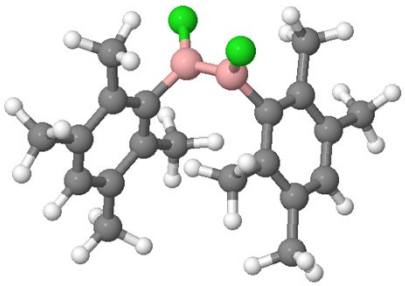
Reactant 2b:



Energy: -103.9738481 kcal/mol

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Cl	0.03495800	-2.34314600	-2.08618900
C	1.51361700	-0.36489900	-0.62674300
C	2.69505500	-0.65584500	0.05237200
C	1.28986300	0.87931800	-1.22538400
C	2.24456500	1.89012500	-1.05088000
C	3.40359300	1.62420000	-0.31978200
C	3.64566700	0.36242700	0.21933300
C	0.06194300	1.10930000	-2.04252400
C	2.97144200	-2.01940000	0.59387300
C	4.91075800	0.11717700	0.97150400
C	2.05267900	3.25614800	-1.62180900
C	-1.28991300	0.87915300	1.22571800
C	-2.69512900	-0.65582500	-0.05223600
C	-3.64568000	0.36249900	-0.21917400
C	-3.40354300	1.62422300	0.32003400
C	-2.24450700	1.89004600	1.05115400
C	-2.97154100	-2.01934100	-0.59383900
C	-0.06190700	1.10901700	2.04275800
C	-2.05255500	3.25604500	1.62212200
C	-4.91077900	0.11735500	-0.97136600
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H	-0.86427700	0.90687800	-1.48027600
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H	2.32853200	-2.80831000	0.18376500
H	2.86381900	-2.04071200	1.68960400
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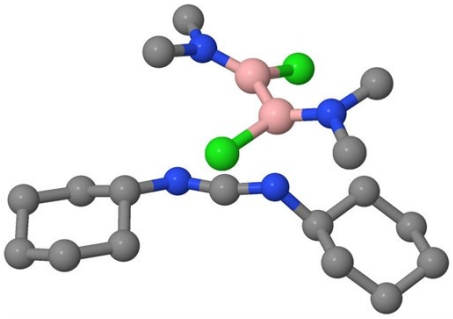
H	4.71183900	-0.31064500	1.96499500
H	1.12567500	3.71726100	-1.24934400
H	1.99332300	3.22437200	-2.71990000
H	2.87325700	3.93937600	-1.36742600
H	-4.13713200	2.41546800	0.17694300
H	-2.86410800	-2.04056100	-1.68958900
H	-4.00165900	-2.33555000	-0.36707600
H	-2.32854000	-2.80829000	-0.18395300
H	0.03418700	2.14245600	2.39960800
H	0.86416000	0.91082000	1.47868800
H	-0.05510800	0.47188000	2.94032600
H	-2.87233300	3.93975100	1.36645300
H	-1.12475000	3.71657700	1.25095600
H	-1.99481500	3.22432600	2.72031000
H	-5.56222000	-0.58682300	-0.43250000
H	-4.71193800	-0.31122400	-1.96455400
H	-5.49288500	1.03454000	-1.12922100

Molecule 1 – TS1

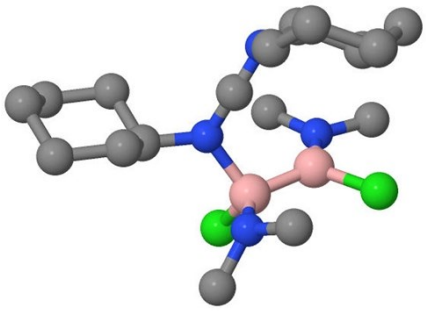


Energy: -140.26 kcal/mol

C	-0.42741500	-0.60354600	-0.72968700
N	-1.58851300	-0.39398400	-1.11209700
N	0.78655000	-0.53556800	-0.43203400
C	1.84475700	-1.48590100	-0.86066100
H	1.47024600	-2.16623400	-1.67081200
C	2.26631700	-2.34177700	0.35208300
H	1.41745900	-2.96033400	0.69509300
H	2.51806900	-1.67623900	1.21208300
C	3.01630900	-0.65204000	-1.41752300
H	3.31060800	0.13177200	-0.67952100
H	2.68412000	-0.08638900	-2.30992300
C	4.20897000	-1.55160700	-1.75364100
H	5.05647700	-0.93117300	-2.10131800
H	3.95358900	-2.21718100	-2.60072800
C	4.63716900	-2.39164200	-0.54208800
H	5.02056000	-1.72670300	0.25544100
H	5.47675700	-3.05507800	-0.82003900
C	3.46656400	-3.22578400	-0.00268700
H	3.78818500	-3.79432500	0.89005600
H	3.16872300	-3.98247200	-0.75415900
C	-2.85641500	-0.62990400	-0.39001500
H	-2.99408500	0.25448500	0.30754000
C	-2.85212100	-1.93316700	0.43604300
H	-2.05549000	-1.89417100	1.20473300
H	-2.61279000	-2.79450400	-0.21537900
C	-3.98314400	-0.64175400	-1.44326800
H	-3.79480200	-1.43902200	-2.18816700
H	-3.97595100	0.30605200	-2.01423100
C	-4.21600200	-2.14336900	1.10456700
H	-4.38964900	-1.35197300	1.85948400
H	-4.21425700	-3.09908200	1.66191300
C	-5.35301600	-2.14050700	0.07315400
H	-6.32699300	-2.24888300	0.58512500
H	-5.25599400	-3.02039900	-0.59173700
C	-5.34192600	-0.85496700	-0.76611600
H	-5.58576900	0.01400000	-0.12534500
H	-6.13720400	-0.89957700	-1.53393400
B	0.24634600	2.18016000	-0.09626300
B	0.79822900	1.17885300	1.10114100
Cl	1.38647700	2.40168200	-1.47898700
Cl	-0.49358800	0.28280700	2.03860300
N	2.06316200	1.22769700	1.70126700
C	3.16642900	1.95713300	1.05834700
H	2.84393800	2.96997200	0.75603300
H	3.51831900	1.42599000	0.14279300
H	4.02503600	2.07934200	1.73677900
C	2.43149100	0.30560500	2.78744600
H	2.46034300	-0.74777200	2.42523400
H	1.69818800	0.35891000	3.61274700
H	3.41804900	0.54526700	3.21309100

N	-0.96558300	2.85070600	-0.17652700
C	-1.99462000	2.72042100	0.86474700
H	-1.54720500	2.76420800	1.87507300
H	-2.53145300	1.74757200	0.77400800
H	-2.74096300	3.52865000	0.80712100
C	-1.32742900	3.61693600	-1.38204800
H	-2.32320300	4.07797000	-1.29933300
H	-1.33365700	2.96397600	-2.27652900
H	-0.59603000	4.42522900	-1.56722200

Molecule 1 – IM1

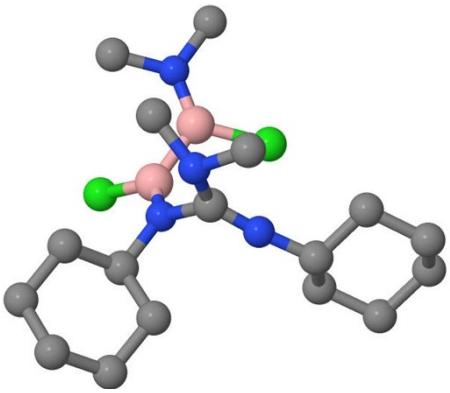


Energy: -147.96 kcal/mol

C	-0.09061100	0.53450300	-0.82387800
N	-1.03565600	-0.11696600	-0.29180700
N	0.79633000	0.98571800	-1.53767900
C	1.91417500	1.85097500	-1.17767300
H	2.17586800	2.40848900	-2.11903400
C	3.10441000	0.97044900	-0.74288500
H	3.35126400	0.23902400	-1.53448600
H	2.83501500	0.36758900	0.14742800
C	1.54424900	2.84988800	-0.06042900
H	1.21914500	2.30587900	0.84897800
H	0.68829900	3.47508100	-0.37066000
C	2.75716400	3.72785000	0.26373800
H	2.50260100	4.43860900	1.07206800
H	3.02441100	4.35023100	-0.61039700
C	3.95427000	2.86345400	0.68063000
H	3.72255800	2.32309100	1.61907200
H	4.82522800	3.50416100	0.90692900
C	4.30892100	1.85954300	-0.42410700
H	5.16229400	1.23066600	-0.10535900
H	4.64807600	2.39197500	-1.33123100
C	-2.40374800	0.42628500	-0.18626300
H	-3.03605300	-0.37451000	0.29256300
C	-2.96173900	0.74191100	-1.58875400
H	-2.94822200	-0.16963600	-2.21600700
H	-2.32732800	1.48380700	-2.10658900
C	-2.41566900	1.68141700	0.71007100
H	-1.75292400	2.46303600	0.30092100
H	-2.00896400	1.42356800	1.71086000
C	-4.39319900	1.27108200	-1.45154500
H	-5.05027000	0.48483200	-1.03211200
H	-4.80579900	1.50828800	-2.44924100
C	-4.42772100	2.51696900	-0.55656900
H	-5.46482000	2.88613100	-0.46069100
H	-3.85707600	3.33798300	-1.02857800
C	-3.84908300	2.20486700	0.82994100
H	-4.48391700	1.46022900	1.34755400
H	-3.86929700	3.11032400	1.46390900
B	-0.50768900	-1.37116000	0.69197800
B	0.85835600	-2.10162800	-0.08768200
Cl	-1.74304700	-2.70331700	0.50282000
Cl	2.30854000	-2.21423300	0.90829300
N	0.84851600	-2.63539700	-1.33632600
C	2.01665400	-3.36409200	-1.84691800
H	2.87412600	-2.68044200	-1.99217100
H	1.81948800	-3.86047000	-2.81019300
H	2.33553000	-4.15483500	-1.13880700
C	-0.25797800	-2.62670000	-2.28738100
H	-1.02452300	-1.86949500	-2.04448500
H	-0.77513200	-3.60718700	-2.28986600
H	0.08981800	-2.40502100	-3.31188800

N	-0.44172900	-0.74494200	2.02568700
C	0.79599000	-0.23539800	2.60518500
H	1.45626000	0.18840500	1.83173400
H	1.36475200	-1.00373000	3.16023700
H	0.56634800	0.58526000	3.31032000
C	-1.39632700	-1.17859800	3.04616400
H	-2.42586600	-1.16475300	2.64734500
H	-1.37790100	-0.49823400	3.91396300
H	-1.19048500	-2.20138900	3.41241900

Molecule 1 – TS2



Energy: -140.00 kcal/mol

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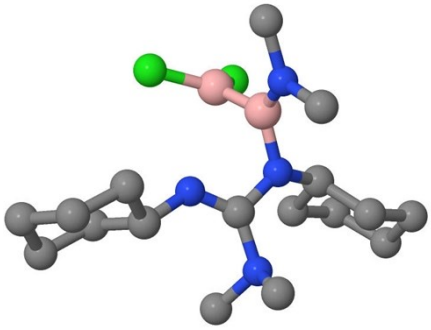
N	1.08772600	-0.88018000	0.51482800
N	-1.02695400	-0.14153300	-0.16685500
C	-1.91886200	-1.27119900	-0.50482600
H	-2.17815800	-1.20439000	-1.59923500
C	-1.25220800	-2.64148200	-0.26416200
H	-0.98417400	-2.76005800	0.80372500
H	-0.30397600	-2.70861900	-0.83035200
C	-3.21738500	-1.17087900	0.32824800
H	-3.69785100	-0.18708500	0.18076500
H	-2.97700600	-1.24891500	1.40622500
C	-4.17700400	-2.29122600	-0.08660600
H	-4.47822500	-2.15967200	-1.14323300
H	-5.10813700	-2.22751100	0.50498500
C	-3.52249800	-3.66534700	0.10687100
H	-4.21598500	-4.46537600	-0.20688900
H	-3.32129500	-3.83765900	1.18100900
C	-2.21374400	-3.75568400	-0.68903200
H	-2.42244000	-3.68855200	-1.77322700
H	-1.73988600	-4.74170000	-0.53069200
C	2.37726900	-1.36562900	0.20601000
H	2.42023600	-2.43939200	0.55192400
C	2.61470400	-1.31570000	-1.32625000
H	2.51605700	-0.27681500	-1.69202100
H	1.82716900	-1.88667600	-1.84743100
H	3.28836000	-0.57250800	2.03352000
H	3.39939300	0.51884500	0.65279000
C	4.00388400	-1.86958000	-1.64816400
H	4.18029700	-1.82911300	-2.73902900
H	4.06700500	-2.93726500	-1.36962100
C	5.08494500	-1.06663200	-0.91181000
H	5.07635100	-0.01736800	-1.26495700
H	6.08645400	-1.46371400	-1.15211900
C	4.84815700	-1.10614100	0.60403200
C	3.46522400	-0.54495800	0.94585100
H	5.62933300	-0.52210100	1.12434300
H	4.94460900	-2.14247600	0.97643600
B	-0.14467200	2.38219400	-0.42962700
B	-1.10869900	1.06648600	-0.79029400
Cl	1.55805100	2.02014400	-0.65144000
Cl	-2.26474700	1.44202200	-2.05762100
N	-0.45502400	-0.22533300	2.19920600
C	-1.32927400	0.92596700	2.48259700
H	-1.69987100	0.84185900	3.51955600
H	-2.21663600	0.90569600	1.82885900
H	-0.82683900	1.89984600	2.37249900
C	0.63558900	-0.31924900	3.19181300
H	1.16736900	-1.27844800	3.06056500

H	0.20257600	-0.31831000	4.20468100
H	1.37010200	0.49804900	3.11408200
N	-0.62858800	3.58488900	-0.03524300
C	0.21847600	4.75286600	0.20590600
H	0.23993400	5.01152000	1.27985600
H	-0.14213800	5.63197100	-0.35809400
H	1.26663200	4.58571300	-0.10875800
C	-2.04970000	3.87814600	0.14852300
H	-2.61200900	2.99869500	0.51369000
H	-2.51166900	4.18572200	-0.81182500
H	-2.21668200	4.68824900	0.87857300

Molecule 1 – TS2i



Energy: -126.41 kcal/mol

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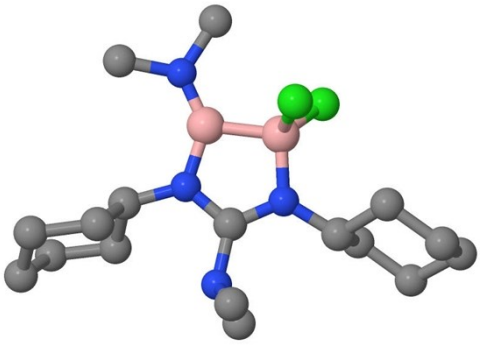
N	1.04461800	0.07590500	0.46633600
C	2.43708400	-0.15120500	0.07764500
H	2.94476500	0.85470000	0.03135000
C	3.17301000	-0.99890300	1.14435100
H	2.72812500	-2.01160800	1.18624600
H	3.03566600	-0.55637100	2.14359900
C	2.58443200	-0.82967100	-1.30326300
H	2.01249500	-0.28563700	-2.07220000
H	2.15998900	-1.85071100	-1.26819200
C	4.07069700	-0.89248800	-1.66998200
H	4.48570100	0.12907600	-1.75430400
H	4.19435000	-1.35556000	-2.66536400
C	4.84409900	-1.69486700	-0.61365300
H	5.91610900	-1.73332000	-0.87358300
H	4.48879700	-2.74263500	-0.60857300
C	4.66000300	-1.08108100	0.78218300
H	5.11534300	-0.07414200	0.81457600
H	5.19760200	-1.68510200	1.53452600
C	-2.43219700	-0.99588900	0.05554300
H	-2.38125100	-2.04602200	0.43574100
C	-3.37662500	-0.18148900	0.97552500
H	-3.39785300	0.87148600	0.63426800
H	-2.97280100	-0.15640700	2.00066600
C	-2.98413200	-0.99888900	-1.39110100
H	-2.30206500	-1.55339800	-2.05651800
H	-3.00176400	0.03969300	-1.77576600
C	-4.78023500	-0.79202600	0.94876500
H	-5.45662100	-0.21090000	1.60124500
H	-4.75906600	-1.81590200	1.36434900
C	-5.32697900	-0.81817700	-0.48564100
H	-5.43659100	0.21699000	-0.86125200
H	-6.33773000	-1.26180600	-0.50009100
C	-4.38887200	-1.60665400	-1.41037500
H	-4.78563600	-1.60501100	-2.44213300
H	-4.35167400	-2.66603400	-1.09809800
B	0.19928500	2.17730000	-0.83675500
B	0.58443100	1.51402100	0.62406900
Cl	-1.43089600	2.59641500	-1.12397700
Cl	1.42996200	2.40794800	-2.01226700
N	0.41043000	2.13095900	1.81878600
C	-0.08072200	3.50033500	1.95829500
H	-1.18714400	3.52747800	1.88317600
H	0.32459500	4.16509500	1.17332900
H	0.19886600	3.94871000	2.92669200
C	0.59313400	1.45524400	3.10145600
H	0.94610600	0.41334700	2.96065300
H	-0.35788100	1.40068200	3.66128700
H	1.34273600	1.97190500	3.72515000

N	0.39167900	-2.23059000	0.42372100
C	-0.13954100	-3.08969400	-0.65135200
H	-0.07510100	-2.56493800	-1.62029800
H	-1.18054200	-3.41650800	-0.50887600
H	0.50273400	-3.98653700	-0.71205700
C	0.06946200	-2.74297400	1.76959500
H	0.55227000	-2.09680700	2.52326800
H	0.49519300	-3.75509900	1.87462300
H	-1.00755800	-2.78756600	1.99273000

Molecule 1 – Product



Energy: -177.98 kcal/mol

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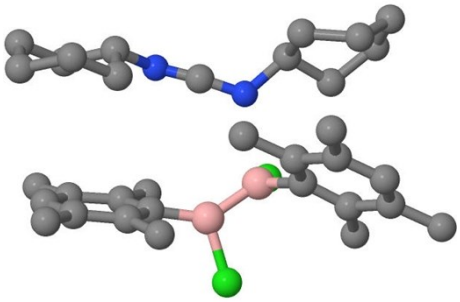
N	1.01544000	-0.14713900	0.09864100
C	2.26443900	-0.91210000	0.13081100
C	3.34410900	-0.20974000	0.97854100
C	2.78792900	-1.12690000	-1.30905900
C	4.02595900	-2.02747000	-1.25779900
C	5.11334900	-1.38057100	-0.38831900
C	4.59024900	-1.10302100	1.02744100
C	-2.65780100	-0.19497700	-0.19964900
C	-3.22922100	-0.65756700	1.15744100
C	-2.92406100	-1.26258700	-1.28320900
C	-4.74210100	-0.85997600	1.01938100
C	-5.05168100	-1.88169600	-0.08449900
C	-4.43976100	-1.44848700	-1.42471900
B	-0.78924000	1.60375200	-0.17775900
B	0.94552000	1.39639100	0.02990100
Cl	1.95302100	2.12937100	-1.25668900
N	-1.34563900	2.83233200	-0.26281900
C	-2.77660900	3.10529300	-0.14829900
C	-0.56380900	4.05007200	-0.48485900
H	2.07604900	-1.91682000	0.59799100
H	2.97162000	-0.00839000	1.99986100
H	3.60897000	0.77931000	0.55295100
H	3.05063900	-0.15514000	-1.77389900
H	2.00526900	-1.55703900	-1.95425900
H	4.41075900	-2.19559100	-2.28084900
H	3.76584800	-3.02572000	-0.86367900
H	5.44669900	-0.43228100	-0.85407900
H	6.00429900	-2.03110100	-0.34517900
H	5.37580900	-0.60903100	1.62991100
H	4.36510900	-2.05269100	1.54447100
H	-3.22028000	0.72936300	-0.52114900
H	-3.00037000	0.08298300	1.94409100
H	-2.74704100	-1.60252700	1.47077100
H	-2.45876100	-2.22567700	-1.00638900
H	-2.47168100	-0.95415700	-2.24167900
H	-5.23982000	0.10146400	0.79620100
H	-5.16465100	-1.20407600	1.98124100
H	-6.14368100	-2.00860600	-0.18888900
H	-4.65382200	-2.87310600	0.20343100
H	-4.91228100	-0.51249600	-1.77481900
H	-4.65491100	-2.20509600	-2.20107900
H	-3.23537900	3.24262300	-1.14451900
H	-2.96718900	4.01780300	0.44659100
H	-3.31417900	2.29028300	0.37101100
H	0.16951100	4.21470100	0.33169100
H	-1.18874800	4.95453200	-0.54606900
H	0.00992100	3.98595100	-1.43146900

N	-0.52964100	-2.06198800	0.39919100
C	-0.18849200	-2.44362800	1.78450100
C	-0.01909200	-3.00884900	-0.60923900
H	-0.73418200	-3.37342800	2.02451100
H	-0.53505100	-1.66146800	2.48544100
H	0.88490800	-2.61048900	1.96704100
H	-0.15935200	-2.59708800	-1.62447900
H	-0.62404200	-3.93192800	-0.53732900
H	1.04075800	-3.28489900	-0.49127900
Cl	1.24202100	2.11853100	1.66946100

Molecule 2 – TS1



Energy: -108.80 kcal/mol

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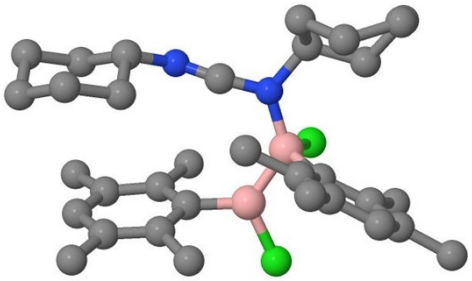
C	1.99922900	-0.30240600	1.50030000
C	3.45095600	-1.54912300	-0.02106900
C	4.49735700	-1.47252200	0.92397300
C	4.28732900	-0.80748000	2.13870700
C	3.05014900	-0.23436900	2.44425900
C	0.67992300	0.30439100	1.86147000
C	2.86664600	0.44463700	3.76635300
C	5.84060200	-2.08070000	0.66186400
C	3.65818700	-2.32120700	-1.28548000
Cl	1.34133600	-0.85276300	-2.54522000
Cl	0.25599500	-3.57027100	-0.50069700
C	-1.77249700	-1.66776700	-0.26684500
C	-2.56151900	-1.40884100	-1.39692600
C	-2.32815300	-1.85358100	1.00281500
C	-3.72630900	-1.72208500	1.15866200
C	-4.52036100	-1.45654500	0.03681400
C	-3.96034900	-1.31174000	-1.24061100
C	-4.37116300	-1.87838500	2.49984300
C	-1.47527700	-2.22802000	2.17292700
C	-1.90451800	-1.25754200	-2.72976000
C	-4.86553100	-1.07412300	-2.40906200
N	0.72480300	1.41436000	-0.96380800
C	-0.46729200	1.81963200	-0.94786400
N	-1.65038700	2.11335200	-1.14739300
C	1.84288800	2.40840300	-1.11401800
C	2.20902000	2.99625900	0.27171100
C	3.03332000	1.72888800	-1.80943500
C	4.22480400	2.69025900	-1.91356200
C	3.70550200	2.87898400	0.57936100
C	4.56162200	3.38997300	-0.58484700
C	-2.69453500	2.55367700	-0.19451300
C	-4.06164100	2.26892400	-0.84794400
C	-5.19701600	2.71993400	0.07814400
C	-5.08949900	2.04795900	1.45419700
C	-3.72277900	2.31872400	2.09871800
C	-2.58012700	1.86599600	1.18127800
H	5.09971000	-0.74602300	2.86087600
H	-0.13392200	0.02073100	1.17926000
H	0.75510500	1.40800100	1.83155500
H	0.36389500	0.01738300	2.87264700
H	3.78362800	0.44163900	4.36922600
H	2.08941000	-0.05254800	4.36323900
H	2.56799000	1.49363700	3.63770400
H	6.29203400	-1.66729100	-0.25081900
H	5.76456700	-3.16987500	0.53165900
H	6.54919600	-1.90446600	1.48052600
H	2.77381600	-2.91468300	-1.56232400
H	4.47831100	-3.04718100	-1.20915200

H	3.89888600	-1.65526000	-2.12608200
H	-5.59969200	-1.37611800	0.15510700
H	-3.99886700	-1.12772100	3.21007300
H	-4.16055000	-2.86951100	2.92702400
H	-5.46237200	-1.77369300	2.45743800
H	-0.39871800	-2.24549900	1.94955800
H	-1.73001200	-3.24082500	2.52263700
H	-1.61961800	-1.54338500	3.01836300
H	-1.14692600	-2.03518700	-2.91099300
H	-1.40039800	-0.27888700	-2.80529400
H	-2.60563200	-1.31771700	-3.57013400
H	-5.90001300	-0.87067000	-2.10655700
H	-4.88961600	-1.95529800	-3.06710400
H	-4.53067900	-0.22001900	-3.01474600
H	1.50216000	3.25278400	-1.77364800
H	1.63822100	2.48265600	1.07927200
H	1.90006300	4.05673900	0.30621400
H	2.73974400	1.39143400	-2.82178300
H	3.32969300	0.81379900	-1.25590700
H	4.02199300	3.45201600	-2.69005300
H	5.10545100	2.12369300	-2.27236600
H	3.95651800	1.81737200	0.79324400
H	3.94475700	3.43958600	1.50155000
H	4.42190800	4.48191000	-0.69547800
H	5.63164500	3.24513400	-0.34511100
H	-2.57082500	3.66479600	-0.06856500
H	-4.15285200	1.18406100	-1.06350100
H	-4.12880200	2.77780100	-1.82733000
H	-6.17168900	2.47550200	-0.38501700
H	-5.18158000	3.82059100	0.19216000
H	-5.23566000	0.95353400	1.34540200
H	-5.89898000	2.40544600	2.11589700
H	-3.65261100	1.78901200	3.06755400
H	-3.62090900	3.39624100	2.32980000
H	-2.62100300	0.76223200	1.05109200
H	-1.60500900	2.08751800	1.64902100

Molecule 2 – IM1



Energy: -140.10 kcal/mol

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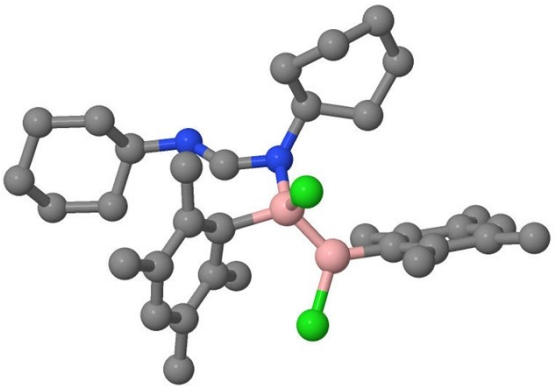
C	2.11683100	-0.63947200	0.12130600
C	1.81904700	-0.30074800	1.45050600
C	3.32183300	-1.29396300	-0.18319000
C	4.20050000	-1.63828600	0.85691500
C	3.90905400	-1.27936200	2.17019100
C	2.73660700	-0.59687000	2.47053200
C	0.56492800	0.40322200	1.87107100
C	2.49583500	-0.19570400	3.89133200
C	5.47559000	-2.38208700	0.61344800
C	3.74600400	-1.61591500	-1.57869100
Cl	1.38907200	-0.38674600	-2.82225500
Cl	0.77647500	-3.09485800	-0.99291700
C	-1.40068800	-1.55714800	-0.42434000
C	-2.30857600	-1.34309000	-1.46662500
C	-1.83149400	-1.94970400	0.84296400
C	-3.20957800	-1.99751700	1.10921300
C	-4.11918600	-1.74339700	0.08628400
C	-3.68198100	-1.44999900	-1.20581200
C	-3.71972000	-2.34283400	2.46918400
C	-0.88426300	-2.40273200	1.90404300
C	-1.82401000	-1.04203500	-2.84487900
C	-4.70452000	-1.28043200	-2.28257500
N	0.66043200	1.33830800	-0.93348100
C	-0.57325800	1.64537200	-0.83519100
N	-1.72980800	1.98972100	-0.97404100
C	1.61212800	2.48346100	-1.11933200
C	1.65323400	3.36031700	0.15788100
C	3.02039800	2.01963100	-1.51901900
C	4.02734900	3.14307900	-1.25175100
C	2.88407300	3.04820400	1.01303200
C	4.17787900	3.38738000	0.25848400
C	-2.79268100	2.34618100	-0.04386800
C	-4.12636000	2.00348900	-0.73681900
C	-5.29811600	2.34385900	0.18648900
C	-5.16756800	1.58851200	1.51482400
C	-3.84880900	1.95291000	2.20687100
C	-2.66100500	1.61215200	1.30335800
H	4.60543400	-1.53191100	2.96560700
H	-0.29951500	0.18224000	1.23484200
H	0.71854300	1.49013300	1.88665200
H	0.24783600	0.10920600	2.88292800
H	3.36930700	-0.37953900	4.53015000
H	1.65840500	-0.75951700	4.32677800
H	2.26217400	0.87443300	3.97366700
H	6.16346000	-1.80248800	-0.01817300
H	5.28439800	-3.34391200	0.11441300
H	6.01282000	-2.61105200	1.54230000
H	3.02404600	-2.25801000	-2.10388500
H	4.69776200	-2.15555700	-1.63850400
H	3.88390800	-0.70300500	-2.17657600

H	-5.18552400	-1.80284400	0.28952800
H	-3.35538500	-1.63421200	3.22608700
H	-3.38886700	-3.34793500	2.77220600
H	-4.81524600	-2.33788200	2.52371100
H	0.17614500	-2.20191300	1.69394100
H	-0.96317000	-3.49483900	2.03425400
H	-1.09708500	-1.93903400	2.87601200
H	-1.01890400	-1.72368500	-3.16433100
H	-1.43814100	-0.01379200	-2.92126400
H	-2.60271900	-1.13823000	-3.61081100
H	-5.72744400	-1.23293900	-1.88945800
H	-4.67124300	-2.12887300	-2.98407800
H	-4.54110000	-0.36390900	-2.86691300
H	1.20202500	3.10147600	-1.96801300
H	0.73442800	3.24385900	0.75802900
H	1.67892800	4.42605500	-0.14345100
H	3.04493500	1.72276900	-2.58474200
H	3.33542200	1.12033500	-0.94647800
H	3.71276700	4.07096500	-1.76209400
H	5.00678400	2.87648000	-1.69096300
H	2.88721200	1.97011900	1.28716800
H	2.84135400	3.60043800	1.96757700
H	4.46586700	4.43727500	0.44194000
H	5.00471500	2.77071400	0.65961800
H	-2.72932200	3.45862200	0.11745800
H	-4.14621700	0.92314400	-0.99392100
H	-4.21011100	2.54330400	-1.69751100
H	-6.25213900	2.08006000	-0.30754500
H	-5.34475300	3.43305700	0.36886300
H	-5.20457100	0.49521900	1.33141400
H	-6.02363100	1.81753800	2.17316500
H	-3.75940600	1.40398200	3.16371400
H	-3.83989700	3.02632600	2.47069600
H	-2.63047500	0.51168700	1.13101700
H	-1.71352000	1.87847000	1.80466500

Molecule 2 – TS2



Energy: -113.86 kcal/mol

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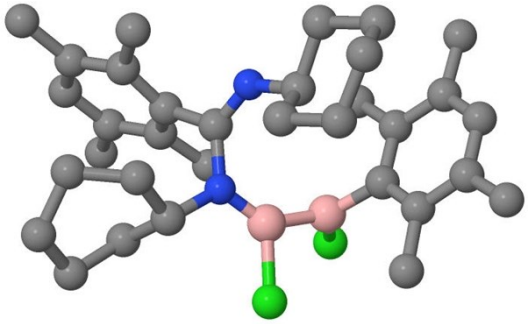
C	1.40343200	0.56630600	0.26568000
C	1.56219500	1.72754300	-0.50665700
C	2.12472700	0.39678500	1.45903700
C	2.86519000	1.47544000	1.96957800
C	2.91743500	2.66489200	1.24781900
C	2.30663800	2.80076200	0.00721400
C	1.01782900	1.80157800	-1.90073300
C	2.43433500	4.08912500	-0.74204600
C	3.59383200	1.37171900	3.27214900
C	2.16927600	-0.91362600	2.17446300
Cl	-0.71542100	-0.32264300	2.11622100
Cl	-0.88263400	2.95459300	0.27711800
C	-2.88482800	1.04393000	-0.21128300
C	-3.81758400	1.06955200	0.83246500
C	-3.27151700	0.82970900	-1.54166400
C	-4.63424000	0.61321400	-1.83384200
C	-5.56713700	0.59843800	-0.78848600
C	-5.17747900	0.81997700	0.53720200
C	-5.10504500	0.39966200	-3.23897800
C	-2.25771300	0.85709300	-2.64149600
C	-3.39758600	1.34705100	2.23976000
C	-6.21136900	0.79346200	1.61936400
N	-0.05933400	-1.13073500	-0.54775300
C	1.29208100	-1.00520000	-0.71695400
N	2.20951500	-1.57669600	-1.34378600
C	-0.74047100	-2.45159800	-0.54655800
C	-0.22680800	-3.35410400	0.60722000
C	-2.26015000	-2.22857700	-0.48979600
C	-3.00519400	-3.56771200	-0.45302500
C	-1.36534200	-3.89090800	1.48017000
C	-2.47680200	-4.52264500	0.63301300
C	3.65849400	-1.41945000	-1.49236800
C	4.12848100	0.04025600	-1.65884900
C	5.64220600	0.07344200	-1.90509700
C	6.40406300	-0.61315400	-0.76224700
C	5.90956000	-2.04992500	-0.54233000
C	4.39427400	-2.09428900	-0.31122700
H	3.47186300	3.51285400	1.66308700
H	0.22955700	1.04956100	-2.10298200
H	1.81946300	1.62934800	-2.63435700
H	0.57223900	2.78250800	-2.12365400
H	3.06392700	4.82120600	-0.22106900
H	1.44467500	4.55682200	-0.87362700
H	2.86865300	3.93992000	-1.73918000
H	4.36013700	0.58529600	3.24510400
H	2.90099900	1.13106000	4.09295200

H	4.09896200	2.30597100	3.54857000
H	1.80346200	-0.81240600	3.21050900
H	3.20145800	-1.29685900	2.22092200
H	1.54980400	-1.70947300	1.71766700
H	-6.61626900	0.41701000	-1.01313400
H	-4.67028200	-0.51287600	-3.66926900
H	-4.81905100	1.24151100	-3.88453100
H	-6.19565600	0.29992200	-3.30478900
H	-2.48487500	0.13143500	-3.43327100
H	-1.23888200	0.61047100	-2.28707100
H	-2.22031800	1.85274400	-3.10469600
H	-2.42465100	1.85366700	2.31248200
H	-3.30875900	0.40993700	2.81042900
H	-4.11635600	1.99019200	2.76365500
H	-7.20189500	0.50376700	1.24835400
H	-6.31645800	1.78190700	2.08861300
H	-5.93954600	0.08036400	2.41024200
H	-0.48384700	-2.94856100	-1.52261900
H	0.48806300	-2.79543900	1.25420400
H	0.34751400	-4.19436000	0.17651400
H	-2.59151500	-1.63130300	-1.36147900
H	-2.53062200	-1.62038800	0.40060000
H	-2.93798700	-4.05928700	-1.44169700
H	-4.08176200	-3.36909700	-0.28783200
H	-1.78218300	-3.05938500	2.08733700
H	-0.97129400	-4.63009400	2.20111300
H	-2.09886600	-5.44807800	0.15926400
H	-3.30689100	-4.83689900	1.29251600
H	3.89227200	-1.98690500	-2.43961300
H	3.89000800	0.62908500	-0.75136300
H	3.58938200	0.52418000	-2.49372600
H	5.98012500	1.12216500	-2.00626500
H	5.88159900	-0.41843800	-2.86752100
H	6.28143500	-0.02898400	0.17035700
H	7.48808600	-0.61723200	-0.98082800
H	6.43214000	-2.49997800	0.32277100
H	6.17534700	-2.67621900	-1.41622300
H	4.13817600	-1.58705100	0.64056300
H	4.05305600	-3.14097700	-0.20303600

Molecule 2 – IM2



Energy: -146.70 kcal/mol

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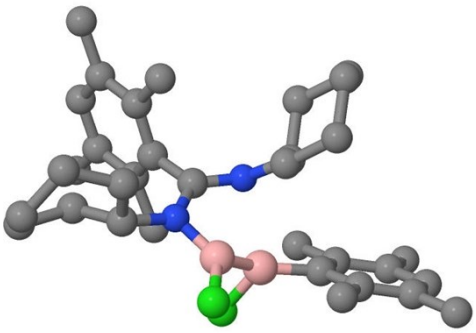
C	-3.04275500	1.47037800	-1.12624200
C	-2.63456400	-0.88836900	-1.56987800
C	-3.96256900	-1.03388900	-1.99506700
C	-4.82319400	0.05933900	-1.95628400
C	-4.36709800	1.31439900	-1.55775400
C	-2.51479000	2.83151800	-0.82061000
C	-5.32076300	2.46307600	-1.59804400
C	-4.48049400	-2.34656200	-2.48137400
C	-1.69391300	-2.03230000	-1.71922300
Cl	0.33792500	-2.51551600	2.26948500
Cl	1.13078100	-3.57781800	-0.79635900
C	2.68661000	-1.26806900	-0.36043400
C	3.64714100	-1.13097600	0.64074600
C	2.87496500	-0.72068600	-1.63591000
C	4.03980200	0.01339000	-1.89455400
C	4.97546900	0.20203800	-0.87674500
C	4.78803200	-0.35425400	0.38633500
C	4.30594800	0.62335000	-3.23154100
C	1.83485500	-0.89512000	-2.69369100
C	3.47923300	-1.79820200	1.96475500
C	5.81093700	-0.09947200	1.44408000
N	-0.73552300	-0.42108000	0.82809000
C	-0.90674000	0.45834400	-0.31911500
N	-0.07649800	1.34986500	-0.69487000
C	-1.69809700	-0.27105200	1.95421000
C	-2.11036100	1.19279200	2.22869600
C	-2.92110200	-1.18150600	1.71877400
C	-3.87643600	-1.08281000	2.91012700
C	-3.63117700	1.36782900	2.24884400
C	-4.28755100	0.37027400	3.20883700
C	1.18288800	1.75244800	-0.10267700
C	1.69837300	2.94408100	-0.94827300
C	3.09309100	3.34341400	-0.45830400
C	3.06302300	3.71398600	1.03041600
C	2.49355100	2.56027100	1.86647100
C	1.09010800	2.18036700	1.37812100
H	-5.86119700	-0.06281100	-2.26188900
H	-1.66060200	3.06093000	-1.48722000
H	-2.13474000	2.91769500	0.20789400
H	-3.24633800	3.63411800	-0.95763200
H	-6.33937700	2.15521200	-1.86860700
H	-5.00865900	3.21327500	-2.34008300
H	-5.39049700	2.96459100	-0.62188600
H	-4.23276000	-3.16281300	-1.78648100
H	-4.05275900	-2.60411500	-3.46200600
H	-5.57183400	-2.35086300	-2.59934400
H	-0.67051800	-1.68753900	-1.92391200

H	-1.95462500	-2.68476700	-2.56563800
H	-1.68803900	-2.67225500	-0.82362600
H	5.86908300	0.79027000	-1.07470500
H	3.54542700	1.37815900	-3.48266100
H	4.30007600	-0.13678200	-4.02612500
H	5.28104300	1.12455400	-3.28025800
H	1.76520000	-1.94159600	-3.02391500
H	2.03621500	-0.30458900	-3.59753000
H	0.84041100	-0.56007900	-2.35517700
H	3.04900400	-2.80667000	1.87753200
H	2.83754600	-1.20549200	2.63358500
H	4.43356700	-1.94107600	2.48999100
H	6.55212700	0.65087400	1.14010200
H	6.36636500	-1.01709100	1.68820700
H	5.34809000	0.26744000	2.37157900
H	-1.18811000	-0.62457600	2.89794100
H	-1.66567900	1.88960300	1.49236700
H	-1.69187500	1.50578400	3.20537900
H	-2.60157200	-2.23085500	1.57468200
H	-3.44858100	-0.89755600	0.78782200
H	-3.40448600	-1.53141800	3.80482200
H	-4.77466300	-1.69583100	2.70853200
H	-4.04358600	1.23716500	1.22736700
H	-3.88805700	2.40218300	2.54287000
H	-4.01974000	0.62715200	4.25053500
H	-5.38671000	0.47104100	3.14835500
H	1.93230800	0.91967500	-0.18265600
H	0.99612000	3.79223400	-0.87868000
H	1.72628200	2.65646900	-2.01551100
H	3.47778000	4.18935500	-1.05422100
H	3.80236200	2.50666900	-0.62349300
H	2.45303200	4.62381900	1.17902300
H	4.08116200	3.96584900	1.37730400
H	2.46132500	2.84137200	2.93376200
H	3.16529900	1.68046600	1.80054800
H	0.40007800	3.03532000	1.48573100
H	0.68689900	1.36422200	2.00133200

Molecule 2 – TS3



Energy: -110.52 kcal/mol

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C	-2.92686100	0.94039100	1.35419700
C	-2.33660600	2.17846100	-0.68304300
C	-3.48540300	2.98527000	-0.51365900
C	-4.32943100	2.76226300	0.57648800
C	-4.05892300	1.76016200	1.51903600
C	-2.59640300	-0.12140300	2.35128400
C	-4.98655000	1.59861700	2.68272100
C	-3.81870200	4.07984200	-1.47791400
C	-1.38256100	2.43037800	-1.79884800
Cl	0.60066300	-2.94754100	-1.78252200
Cl	0.97260400	0.61239500	-2.76864100
C	2.89969100	0.25590500	-0.78943200
C	3.86618700	-0.74605900	-0.60106500
C	3.23599400	1.61921000	-0.71783800
C	4.57799800	1.98163200	-0.46075300
C	5.54097700	0.98334100	-0.28037400
C	5.20485300	-0.37368800	-0.34944800
C	4.99892600	3.41686500	-0.39117700
C	2.22432400	2.70182900	-0.92072400
C	3.49193200	-2.18961900	-0.68583100
C	6.28689200	-1.39239200	-0.16325600
N	-0.98747300	-0.98882600	-0.61210200
C	-0.89651500	0.23978300	0.10996600
N	0.23963500	0.64037400	0.62585900
C	-2.17833000	-1.79606500	-0.99682900
C	-2.47355400	-2.84644300	0.09910900
C	-3.43696600	-0.97760300	-1.33096400
C	-4.48701700	-1.89031000	-1.98705600
C	-3.90626400	-3.39064800	-0.00953700
C	-4.44456500	-3.32987000	-1.44496800
C	1.13651200	0.01250700	1.61858300
C	0.79851300	0.72038000	2.96120900
C	1.70379400	0.21440800	4.08714500
C	1.59903100	-1.30851500	4.24114100
C	1.92255300	-2.01307200	2.91751500
C	1.02591300	-1.51892800	1.77328800
H	-5.21316300	3.38743000	0.70477700
H	-1.63303900	0.10799100	2.85694100
H	-2.48929900	-1.11566000	1.87708500
H	-3.34633900	-0.23272300	3.14160800
H	-5.84036100	2.28730100	2.63719900
H	-4.46853500	1.79665000	3.63227600
H	-5.39960300	0.58156200	2.73074700

H	-3.90160600	3.69748000	-2.50526300
H	-3.04408800	4.86075800	-1.47502600
H	-4.77029500	4.57335100	-1.24235500
H	-0.34189000	2.47955100	-1.41826200
H	-1.55353200	3.37610800	-2.32540500
H	-1.43463400	1.63297800	-2.55483500
H	6.57449100	1.26777400	-0.08791900
H	4.46745900	3.94964800	0.40982900
H	4.78259300	3.93714100	-1.33515800
H	6.07268300	3.53153100	-0.19862800
H	2.24338700	3.04955200	-1.96422300
H	2.41406700	3.56959200	-0.27485300
H	1.18725600	2.39672500	-0.69314300
H	3.24681400	-2.46920700	-1.72170900
H	2.61915300	-2.41764000	-0.04753700
H	4.28901300	-2.86871500	-0.36175400
H	7.25640500	-0.93566200	0.07209500
H	6.42626300	-1.98854600	-1.07651400
H	6.05062100	-2.08482400	0.65603300
H	-1.90469100	-2.34689400	-1.94464700
H	-2.32417400	-2.40346000	1.10971900
H	-1.73833700	-3.66945800	0.01622500
H	-3.18877900	-0.13343800	-2.00065300
H	-3.86977200	-0.52823100	-0.41651700
H	-4.34130500	-1.90728800	-3.08377500
H	-5.49088200	-1.45465300	-1.82298000
H	-4.57592500	-2.81012300	0.65496400
H	-3.93743900	-4.43289700	0.35944800
H	-3.81292200	-3.95910400	-2.10206600
H	-5.45607300	-3.77477800	-1.48520300
H	2.19487400	0.28561200	1.35746600
H	-0.27058500	0.55652200	3.22298000
H	0.90971700	1.81465700	2.83540400
H	1.43357100	0.71223600	5.03702100
H	2.75448500	0.50012200	3.88257200
H	0.58120800	-1.58388000	4.57595200
H	2.28753200	-1.65766100	5.03281700
H	1.80750800	-3.10695100	3.03344300
H	2.98610100	-1.84297700	2.65467000
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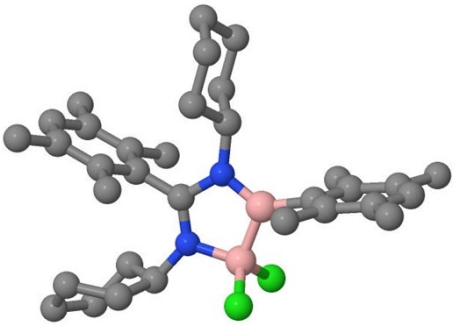
Molecule 2 – Product



Energy:-182.72 kcal/mol

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C	2.06632200	0.56749900	0.04358300
C	2.64789100	0.96970100	1.25437300
C	2.68322900	0.82203900	-1.18662200
C	3.91219400	1.49774100	-1.19985200
C	4.48783000	1.91001100	-0.00015800
C	3.86920800	1.65472700	1.22322800
C	2.00718300	0.66514300	2.56677200
C	4.51876800	2.10936400	2.48534000
C	4.60955800	1.78166300	-2.48632100
C	2.06573800	0.39803000	-2.47616200
Cl	-1.19526700	-2.94467900	-1.27298200
Cl	-1.27100900	-2.68127000	1.74436100
C	-3.07211000	-0.19158300	-0.01245500
C	-3.71345300	-0.22095500	-1.25087300
C	-3.77884600	-0.02622800	1.17851100
C	-5.17729600	0.06413200	1.12782100
C	-5.82986600	0.00915900	-0.10300400
C	-5.11200400	-0.12964100	-1.29028100
C	-5.98398400	0.20788400	2.37679500
C	-3.08142200	0.03795300	2.49831100
C	-2.94526600	-0.36433000	-2.52448100
C	-5.85017100	-0.19028400	-2.58750300
N	0.66241000	-1.47524600	0.16733900
C	0.78459200	-0.16058700	0.07344400
N	-0.45183400	0.51092400	0.01016800
C	1.68576100	-2.52764600	0.19315600
C	2.28120900	-2.76459900	-1.21497300
C	2.77669600	-2.30254700	1.25404600
C	3.82888300	-3.40613200	1.11206200
C	3.77995400	-2.46578200	-1.26257300
C	4.55284300	-3.31578100	-0.24337200
C	-0.66168400	1.96280200	-0.06859900
C	-0.13850200	2.71913000	1.16646900
C	-0.61584400	4.17466200	1.08617000
C	-0.10536300	4.83388700	-0.20288600
C	-0.56570500	4.04693200	-1.43802700
C	-0.08976200	2.59107900	-1.35284800
H	5.44038300	2.43993500	-0.01732100
H	2.65165600	0.01686200	3.18252900
H	1.03772100	0.15136200	2.48543600
H	1.82867100	1.58105700	3.15177000
H	5.47192300	2.62574200	2.31088200
H	4.73325400	1.26233400	3.15504700
H	3.87420900	2.80886300	3.03946100
H	4.01365800	2.45076400	-3.12601800
H	4.79247600	0.85941000	-3.05852900
H	5.58528000	2.26460000	-2.34285000
H	1.05695400	-0.02803800	-2.37004800

H	2.68268500	-0.36490000	-2.97901600
H	1.97416300	1.24286400	-3.17703600
H	-6.91405300	0.07141400	-0.13733200
H	-5.77814400	1.16459900	2.87609300
H	-5.75260800	-0.59649500	3.09107000
H	-7.06376400	0.16737600	2.18790500
H	-3.18792300	-0.92257800	3.03042200
H	-3.50075600	0.82142700	3.14277200
H	-2.00597100	0.23739300	2.42570700
H	-1.87543100	-0.14633700	-2.42755800
H	-3.32878600	0.30148600	-3.30843500
H	-3.02347100	-1.39896300	-2.89947900
H	-6.93866100	-0.20528300	-2.45249800
H	-5.58396700	-1.09701000	-3.15118900
H	-5.61425900	0.67571700	-3.22100100
H	1.13908300	-3.47856200	0.49105900
H	1.74015300	-2.17497900	-1.97740300
H	2.10209900	-3.82110100	-1.50161400
H	2.32788300	-2.31389700	2.26471400
H	3.26637400	-1.32061800	1.13716100
H	3.34976000	-4.39829700	1.22020500
H	4.55993600	-3.33627800	1.93755300
H	3.96005600	-1.39074700	-1.06476900
H	4.17104900	-2.65249000	-2.27948800
H	4.71054300	-4.33288800	-0.64714100
H	5.56230600	-2.88787100	-0.10445900
H	-1.79054200	2.10101200	-0.09776300
H	0.96453000	2.69682200	1.20321300
H	-0.50102400	2.24187300	2.09453600
H	-0.25985500	4.73805500	1.96724300
H	-1.72120900	4.21793200	1.12433900
H	0.99906600	4.89037600	-0.18382400
H	-0.46206500	5.87759200	-0.26285200
H	-0.17352200	4.51906300	-2.35657600
H	-1.66858500	4.08459200	-1.52433100
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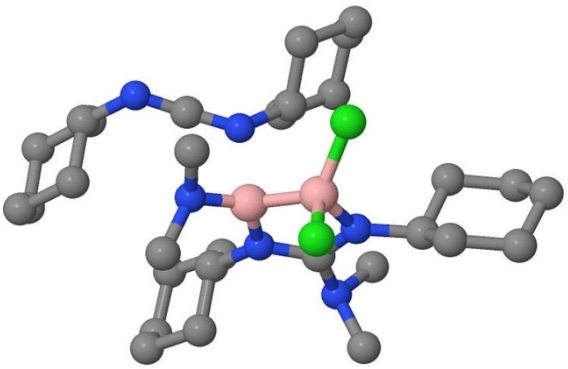
H	-0.41934500	2.02286100	-2.24105800

Molecule 3 – TS1



Energy:-176.96 kcal/mol

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C	3.95729200	0.61650700	-0.88815200
C	5.39303500	0.61841800	-1.42913400
C	6.38189400	0.12193400	-0.36389000
C	5.98818600	-1.26287800	0.16989800
C	-1.43894000	-1.53677600	-0.66725300
C	-1.62337200	-3.06703300	-0.76480300
C	-1.69764000	-0.87955000	-2.03787000
C	-3.04130700	-3.39668000	-1.24807300
C	-3.35304600	-2.71029800	-2.58625800
C	-3.12439200	-1.19373400	-2.50424000
B	0.01616100	-0.55802200	1.31922400
B	1.69196900	-0.41788800	1.48626600
Cl	2.42857200	1.11218900	2.12276400
N	-1.00182100	-0.71459800	2.36394600
C	-1.40938600	-2.11023400	2.64500000
C	-0.61037700	0.01378700	3.59574000
H	3.69528700	-1.51642000	-1.27448900
H	4.27125600	-2.28273200	1.05608000
H	4.46821700	-0.61721400	1.59275700
H	3.87939300	1.33362500	-0.04353700
H	3.24943200	0.97846600	-1.65184400
H	5.66888600	1.64152200	-1.74753000
H	5.46442300	-0.01360800	-2.33368000
H	6.41295100	0.84423400	0.47644400
H	7.40473200	0.09076500	-0.78103400
H	6.67783600	-1.55927900	0.98386900
H	6.11058100	-2.02330700	-0.62350800
H	-2.21637800	-1.12430400	0.05864300
H	-1.43795000	-3.52791400	0.22818200
H	-0.87419800	-3.49653900	-1.45633500
H	-0.98170100	-1.26445700	-2.79051200
H	-1.52879100	0.21676200	-1.97782300
H	-3.78163000	-3.08450900	-0.48570300
H	-3.15433400	-4.49216900	-1.35211600
H	-4.39680900	-2.92031400	-2.88378700
H	-2.71389900	-3.14040800	-3.38157200
H	-3.87308400	-0.74175400	-1.81056900
H	-3.30651100	-0.72984400	-3.49087100
H	-2.31177700	-2.10503000	3.27868200
H	-0.62671600	-2.68805100	3.17292300
H	-1.64959200	-2.65858700	1.71874000
H	0.12514100	-0.52256400	4.22025900
H	-1.50985500	0.21514800	4.19818200
H	-0.15526900	0.98819200	3.33756300

N	1.18640600	-1.87262000	-1.99002700
C	1.94353200	-3.15759000	-1.98318400
C	1.67942000	-0.92161500	-3.02650300
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H	1.55684500	-3.81102900	-1.18116200
H	3.03336500	-3.04532000	-1.83630500
H	1.19312100	0.06076700	-2.90056600
H	1.37956600	-1.31673100	-4.01347300
H	2.77050400	-0.76853600	-3.03828400
Cl	2.10513400	-1.78497100	2.67360500
C	-1.75620700	1.74731000	1.01810200
N	-2.82840900	1.99745400	1.59005200
N	-0.58728400	1.45563600	0.67035200
C	0.27864400	2.26757000	-0.21436900
C	0.64167800	3.61707200	0.44047500
C	-0.38526700	2.49979700	-1.59149700
C	0.56941200	3.27301300	-2.50796900
C	0.98310200	4.60881200	-1.87148300
C	1.58700300	4.40390200	-0.47466300
C	-4.17221100	1.49301900	1.23582200
C	-4.22030100	-0.04248400	1.38860100
C	-4.57986100	1.93705000	-0.18755700
C	-5.59808300	-0.58649300	1.00366300
C	-5.98970400	-0.14993300	-0.41424300
C	-5.96146700	1.37828500	-0.54828900
H	1.21615000	1.65835600	-0.34204400
H	1.12470200	3.43369700	1.42334200
H	-0.26857200	4.20612700	0.65437000
H	-1.32761000	3.06697000	-1.47066200
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H	0.08632700	3.45610600	-3.48592400
H	1.47007200	2.66507800	-2.71774400
H	0.10286400	5.27661300	-1.80129200
H	1.70975700	5.12796600	-2.52333800
H	1.81747700	5.38412400	-0.01590100
H	2.55571900	3.87226900	-0.55455800
H	-4.86190500	1.96720300	1.98622200
H	-3.96299400	-0.32064500	2.43021600
H	-3.42391200	-0.51906800	0.76556500
H	-3.83066600	1.59272700	-0.92525600
H	-4.58642500	3.04159800	-0.24779500
H	-6.35861800	-0.23771900	1.72926400
H	-5.59691900	-1.69067600	1.07369700
H	-6.99154700	-0.53779400	-0.67104300
H	-5.28038300	-0.60036100	-1.14894500
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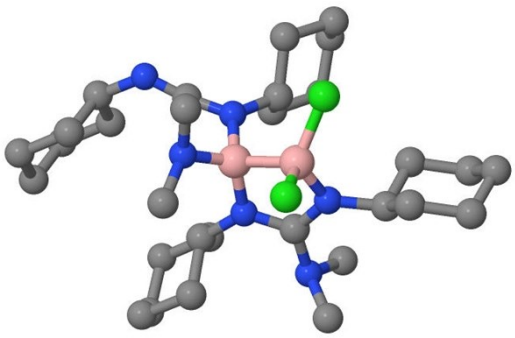
H	-6.22776100	1.67440000	-1.58022500

Molecule 3 – IM1



Energy:-193.80 kcal/mol

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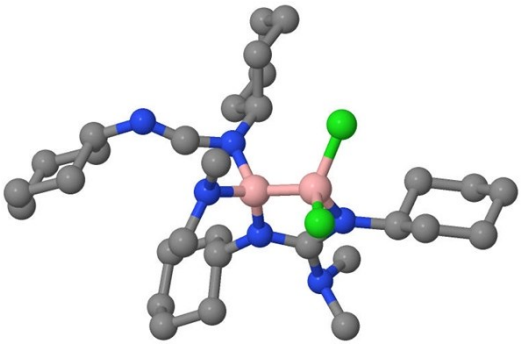
C	3.52528300	0.83259100	0.23266400
C	4.48373900	1.07616500	-0.95064200
C	3.88712300	-0.49590300	0.94311800
C	5.32078700	-0.40432300	1.47566600
C	6.29624200	-0.12814700	0.32258800
C	5.91868200	1.16290900	-0.41669400
C	-1.39874000	1.64445600	0.48575900
C	-1.47623700	3.17828000	0.31587800
C	-1.68175400	1.28449100	1.96287700
C	-2.89193000	3.64500600	0.66943900
C	-3.22347700	3.27714800	2.12243600
C	-3.08503300	1.76517000	2.34710600
B	-0.11690200	0.01243800	-1.13104900
B	1.64579000	0.13775200	-1.51605300
Cl	2.35534800	-1.45507900	-1.94145300
N	-1.08534100	0.14320800	-2.32613200
C	-1.33625700	1.50507400	-2.81523300
C	-0.72629100	-0.74472600	-3.44745000
H	3.67786200	1.67312600	0.96197400
H	4.20970500	2.00193900	-1.48905100
H	4.41215200	0.26438900	-1.70241800
H	3.80578800	-1.34363400	0.23423200
H	3.17598300	-0.70722200	1.75765900
H	5.59483600	-1.34630700	1.98472800
H	5.40111300	0.38875000	2.23988200
H	6.28410800	-0.97872100	-0.38709900
H	7.32947800	-0.06099300	0.70447200
H	6.61710900	1.33462500	-1.25713500
H	6.03130700	2.03374500	0.25273900
H	-2.20869700	1.18167700	-0.15241600
H	-1.21381900	3.46585200	-0.71905000
H	-0.73712100	3.67423500	0.97149000
H	-0.92899300	1.76345400	2.61749900
H	-1.58923900	0.19605300	2.11834500
H	-3.62904600	3.18892200	-0.01734800
H	-2.97704300	4.73713100	0.52544500
H	-4.24567400	3.60719800	2.37661800
H	-2.54659800	3.82005500	2.80854300
H	-3.85102300	1.22757100	1.75624300
H	-3.29005500	1.52020400	3.40480800
H	-2.42339100	1.61058700	-2.97890000
H	-0.82493700	1.73460500	-3.76691600
H	-1.01866400	2.28715600	-2.11004900
H	0.12571400	-0.39765500	-4.05657100
H	-1.60276300	-0.83907900	-4.11118100
H	-0.47482300	-1.75577200	-3.09022500
N	1.22899800	2.31992100	1.54551900

C	1.93990400	3.55580300	1.16519700
C	1.74852800	1.69791700	2.77719300
H	1.68421500	4.33602700	1.90307300
H	1.58765000	3.90039200	0.17447800
H	3.03653400	3.46479400	1.11881000
H	1.25641000	0.72387600	2.94322300
H	1.48335200	2.35499600	3.62494900
H	2.83862900	1.54070300	2.79321400
Cl	1.85404800	1.34385300	-2.85542400
C	-1.69149800	-1.77613400	-0.65500500
N	-2.74932600	-2.23614900	-1.05924700
N	-0.49969700	-1.39247100	-0.43136900
C	0.37287600	-2.12323600	0.50559800
C	0.58680500	-3.57058700	0.01811100
C	-0.21530300	-2.12640700	1.93262900
C	0.77991500	-2.81873700	2.87094500
C	1.06693200	-4.25052700	2.39772900
C	1.58629500	-4.25658100	0.95367500
C	-4.10923000	-1.84012100	-0.71384400
C	-4.47373700	-0.61818800	-1.58662600
C	-4.25484300	-1.51209600	0.78691200
C	-5.89418000	-0.15174100	-1.27118900
C	-6.03682500	0.18188700	0.21882900
C	-5.68060600	-1.03632800	1.08049700
H	1.36681000	-1.59278500	0.53044900
H	0.97078000	-3.57278000	-1.02314300
H	-0.36730000	-4.12467300	-0.00917100
H	-1.18923100	-2.64467800	1.95657100
H	-0.40167800	-1.08888300	2.27183000
H	0.38168500	-2.83274800	3.90143600
H	1.72376300	-2.24208200	2.91743400
H	0.15001900	-4.86352700	2.47112100
H	1.80331900	-4.72979800	3.06730200
H	1.76848400	-5.29360600	0.61794900
H	2.56837100	-3.74629800	0.89654900
H	-4.76413500	-2.71277900	-0.98113900
H	-4.37108800	-0.87749400	-2.65880700
H	-3.74208500	0.20167200	-1.42316900
H	-3.52897600	-0.72615200	1.07737700
H	-4.01364200	-2.40001500	1.39827400
H	-6.62697100	-0.92860000	-1.55839300
H	-6.14213300	0.73578800	-1.88399700
H	-7.06735000	0.51377500	0.43869300
H	-5.38282200	1.03784800	0.47664200
H	-6.40203200	-1.85408200	0.89475200
H	-5.78180500	-0.78592400	2.15287500

Molecule 3 – TS2



Energy:-181.88 kcal/mol

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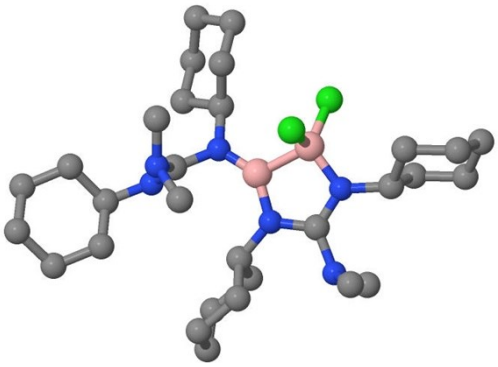
C	3.88213200	-0.70132900	-0.10707800
C	4.74768100	-0.63890100	1.16657000
C	4.26554900	0.44016700	-1.07714400
C	5.74633800	0.32257900	-1.45987200
C	6.63889300	0.34626700	-0.21009300
C	6.23248200	-0.74304700	0.79282300
C	-1.04198400	-1.79967900	-0.52040700
C	-1.08262500	-3.32541700	-0.28184300
C	-1.28911300	-1.50890200	-2.01627700
C	-2.47369000	-3.85701100	-0.65569900
C	-2.84344100	-3.50351500	-2.10514800
C	-2.69314800	-2.00108900	-2.38987800
B	0.12527600	0.07649400	1.00456400
B	1.79079900	0.24302100	1.32612200
Cl	2.41916200	1.96234900	1.35251400
N	-0.94923000	0.05896800	2.14175300
C	-1.45291900	-1.26138700	2.57855300
C	-0.54560000	0.89987300	3.29941800
H	4.10106500	-1.68649300	-0.61031100
H	4.46801100	-1.44726700	1.86824900
H	4.56177600	0.30651700	1.72040300
H	4.08423400	1.42248700	-0.59205500
H	3.62506600	0.43013300	-1.97390500
H	6.02358200	1.15523900	-2.13344400
H	5.92331200	-0.60684700	-2.03208700
H	6.56538200	1.33931500	0.27688600
H	7.69831800	0.22118700	-0.49768900
H	6.84633800	-0.65420600	1.70981200
H	6.45288100	-1.74284100	0.37516300
H	-1.89694200	-1.34355900	0.06435700
H	-0.84139300	-3.56074700	0.76966900
H	-0.30904300	-3.82944200	-0.89359800
H	-0.52904900	-2.02057200	-2.63635800
H	-1.18254700	-0.42251900	-2.22706800
H	-3.23458500	-3.44803000	0.03601800
H	-2.50044200	-4.95482000	-0.52112900
H	-3.87968900	-3.82511900	-2.31708400
H	-2.19603700	-4.07496200	-2.79878400
H	-3.45636700	-1.42521300	-1.82062300
H	-2.89279400	-1.79992000	-3.45837200
H	-2.06910800	-1.17230600	3.48777400
H	-0.62797700	-1.96313900	2.80159300
H	-2.08486100	-1.70256000	1.78854400
H	-0.07924800	0.32941700	4.11921100
H	-1.43395500	1.41916600	3.69446000
H	0.19505500	1.66598200	3.00006200
N	1.69212700	-2.44273300	-1.35917700

C	2.51047200	-3.56013400	-0.80626200
C	2.22728400	-1.92331000	-2.64923000
H	2.45421100	-4.41169000	-1.50362900
H	2.08382100	-3.88645100	0.15857400
H	3.57466300	-3.30743900	-0.64007600
H	1.66932200	-1.02178900	-2.95239400
H	2.05606800	-2.69537800	-3.41980700
H	3.30139100	-1.67743200	-2.64357100
Cl	2.17703700	-0.50952700	2.97375600
C	-1.83625400	1.29413300	0.81804400
N	-2.95242400	1.74655000	1.11066800
N	-0.65014700	1.24875400	0.25530000
C	-0.15994800	2.19128200	-0.77951500
C	-0.16436800	3.63972400	-0.24637800
C	-1.00982100	2.09141100	-2.06503500
C	-0.45530700	3.03882200	-3.13531900
C	-0.41156300	4.48675900	-2.62504500
C	0.38139900	4.59371300	-1.31481600
C	-4.32485400	1.27581100	0.87859400
C	-4.68682200	0.15415200	1.87627200
C	-4.53664600	0.80481800	-0.57927400
C	-6.13665000	-0.29557800	1.66457200
C	-6.37858800	-0.74279700	0.21603200
C	-5.99007100	0.35873200	-0.78024900
H	0.90039900	1.87902400	-0.99537600
H	0.45613200	3.70162700	0.67247400
H	-1.18460100	3.94270100	0.05465700
H	-2.06449900	2.34620300	-1.84921900
H	-1.01382300	1.04177500	-2.43790200
H	-1.07688100	2.97894700	-4.04804000
H	0.56118400	2.71725300	-3.43402900
H	-1.44203400	4.85934900	-2.46808100
H	0.03835700	5.14343200	-3.39244000
H	0.34832700	5.63291500	-0.93635400
H	1.45139400	4.37330000	-1.49963500
H	-4.96960700	2.17677100	1.07815000
H	-4.53805600	0.51263800	2.91311000
H	-3.99761300	-0.70326800	1.75428300
H	-3.85149900	-0.03615700	-0.82542000
H	-4.28710600	1.62098100	-1.28192500
H	-6.82945500	0.52822400	1.92503800
H	-6.37558400	-1.12254000	2.35994800
H	-7.44133500	-1.01690700	0.07893400
H	-5.79621000	-1.66053200	0.00546200
H	-6.66999600	1.22555200	-0.66610200
H	-6.13064800	-0.00251500	-1.81651200

Molecule 3 – IM2



Energy:-198.05 kcal/mol

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N	0.57905100	1.16816600	0.09374800
N	2.73827900	0.40716000	-0.10297800
C	4.19978500	0.47833100	-0.16029100
C	4.75956300	-0.42148900	-1.28148900
C	4.80859500	0.07475900	1.20174300
C	6.32784800	0.26269100	1.13732500
C	6.92016200	-0.59212400	0.00783100
C	6.28096800	-0.23958500	-1.34237000
C	-0.46754400	2.14256900	0.42764600
C	-0.51183700	3.36785600	-0.50808100
C	-0.35100200	2.60874800	1.89572100
C	-1.75983400	4.19404600	-0.17605400
C	-1.72883700	4.64020100	1.29330500
C	-1.59320100	3.43904900	2.23985500
B	0.31208000	-0.28950000	0.05254000
B	1.93167300	-0.89257900	-0.27976500
Cl	2.56541000	-2.31980700	0.57516900
N	-2.40487000	-0.56982600	-1.67073700
C	-2.20930700	-1.83421500	-2.40486800
C	-1.72901300	0.54594300	-2.36188900
H	4.51798000	1.53182700	-0.38916600
H	4.29580700	-0.17073300	-2.25304600
H	4.51841600	-1.48859600	-1.10233000
H	4.57273800	-0.98180000	1.43914600
H	4.36635500	0.66545000	2.02058600
H	6.78268900	-0.02218000	2.10429500
H	6.58278300	1.32631500	0.98451700
H	6.75545500	-1.66522600	0.22812900
H	8.01450000	-0.45338600	-0.04087000
H	6.70028400	-0.88398500	-2.13801400
H	6.53636500	0.79658200	-1.62700300
H	-1.45417400	1.60232200	0.32598800
H	-0.50849400	3.05485700	-1.56500100
H	0.38769700	3.99782300	-0.37019700
H	0.56545700	3.20500200	2.04125600
H	-0.27411400	1.73342300	2.56812000
H	-2.67733800	3.60996500	-0.37839800
H	-1.81316900	5.07738400	-0.83777800
H	-2.64342500	5.21025800	1.53484400
H	-0.88403600	5.33587000	1.45217000
H	-2.49860400	2.80306000	2.18313500
H	-1.53546100	3.78681400	3.28670000
H	-1.14984900	-2.11481700	-2.54158900
H	-2.66934000	-1.73254900	-3.40249300
H	-2.73334500	-2.64961000	-1.87992500
H	-2.17798000	0.65500400	-3.36416600
H	-0.64201700	0.41157100	-2.49114600
H	-1.90791700	1.48566200	-1.81595900

N	2.32059900	2.84268600	0.06988900
C	2.86190700	3.32126100	-1.21715100
C	3.16842800	3.17537800	1.22830500
H	2.87620300	4.42545100	-1.19309300
H	2.18920100	3.01407700	-2.03953300
H	3.87706700	2.96644600	-1.45474700
H	2.80940500	2.64720500	2.12982800
H	3.06389600	4.26025800	1.41680000
H	4.23856200	2.95010800	1.09908400
Cl	1.61195600	-1.18446900	-2.05580600
C	-2.09660500	-0.65240400	-0.25471000
N	-2.92555800	-0.35012800	0.67459400
N	-0.78599800	-1.11206600	0.13747100
C	-0.67727900	-2.46469100	0.73768900
C	-0.44387200	-3.57164600	-0.31012100
C	-1.90617700	-2.84467600	1.59448100
C	-1.60240900	-4.15219900	2.33603800
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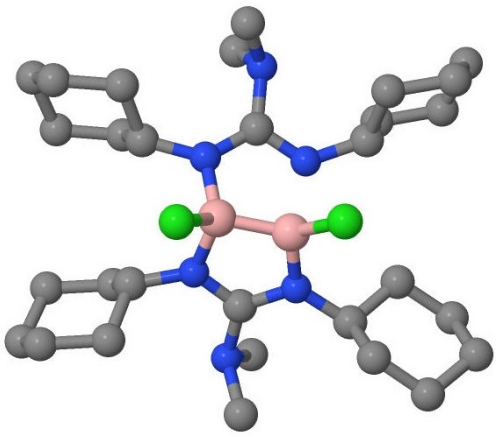
C	-0.10988600	-4.87364600	0.42993400
C	-4.30787300	0.07331700	0.52986800
C	-5.16904400	-0.96695300	-0.22171400
C	-4.43270400	1.45376000	-0.15099500
C	-6.63291700	-0.51721100	-0.22826500
C	-6.76805500	0.86398300	-0.88479700
C	-5.89858900	1.89760300	-0.15501200
H	0.20472600	-2.44205100	1.44307700
H	0.37843000	-3.30851500	-0.99973800
H	-1.33993000	-3.71841400	-0.93467700
H	-2.80796200	-2.95951700	0.96956400
H	-2.13501900	-2.03460200	2.31531300
H	-2.46630600	-4.43695500	2.96238400
H	-0.75617900	-4.00379300	3.03346500
H	-2.16443200	-5.51825800	0.73912200
H	-1.01956200	-6.20285000	1.89486000
H	0.10398700	-5.67618900	-0.29777800
H	0.81878800	-4.74649900	1.01946600
H	-4.68311600	0.15742300	1.59000900
H	-5.06711200	-1.95722800	0.25461000
H	-4.79847900	-1.07925700	-1.26009000
H	-4.05203600	1.39361000	-1.18866400
H	-3.80538600	2.19180100	0.38111500
H	-7.02778400	-0.48649700	0.80396700
H	-7.25182500	-1.25574500	-0.76937100
H	-7.82427700	1.18470300	-0.88393900
H	-6.46498800	0.80339300	-1.94727700
H	-6.25955100	2.03214100	0.88135900
H	-5.99338500	2.88467600	-0.64234200

Molecule 3 – TS3



Energy:-187.45 kcal/mol

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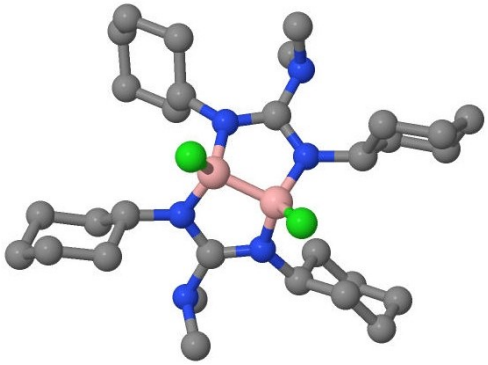
C	2.28343700	-2.41929300	-0.18398100
C	2.78047600	-3.17575600	1.06715800
C	3.38789000	-1.51232700	-0.75747700
C	4.63844300	-2.33635700	-1.08665700
C	5.12697000	-3.13591200	0.12973700
C	4.01139200	-4.01817600	0.70917100
C	-2.69976800	-1.53733600	-0.00935000
C	-3.16980900	-2.79659600	0.74359700
C	-3.13317500	-1.58148200	-1.48856200
C	-4.70020500	-2.88904500	0.66733900
C	-5.19591100	-2.87539800	-0.78674500
C	-4.66381000	-1.66081000	-1.56201700
B	-0.72043000	-0.04278500	0.95781100
B	0.93245400	-0.36812000	0.94783100
Cl	2.10133200	-0.12745700	2.27683500
N	0.28156300	3.40687800	-0.38135000
C	-0.03110400	4.33444000	0.73678500
C	-0.30513400	3.81706300	-1.67910000
H	2.04990000	-3.18519300	-0.97929800
H	1.97844100	-3.80455300	1.49026400
H	3.04599900	-2.46430500	1.87548800
H	3.64047600	-0.70382500	-0.02790300
H	3.02009900	-0.98856700	-1.66005000
H	5.44250600	-1.66144600	-1.43752600
H	4.42989500	-3.02364900	-1.92824200
H	5.48783000	-2.43749100	0.91092800
H	5.99587200	-3.75864000	-0.15097100
H	4.37846100	-4.54093100	1.61305500
H	3.74115200	-4.81072100	-0.01282200
H	-3.20920200	-0.64179100	0.48006100
H	-2.83782400	-2.74174300	1.80021900
H	-2.71459300	-3.70473400	0.30982900
H	-2.68269300	-2.45426800	-1.99764300
H	-2.76616400	-0.67621600	-2.01720000
H	-5.15453100	-2.04954100	1.22908500
H	-5.04270600	-3.81104900	1.17310900
H	-6.30131800	-2.87894200	-0.80603600
H	-4.87539200	-3.80575700	-1.29433600
H	-5.10558200	-0.72427200	-1.15641200
H	-4.98668000	-1.71810300	-2.61775600
H	-1.08906000	4.65839800	0.78149500
H	0.60036700	5.23153000	0.61619600
H	0.22433200	3.86978600	1.70564200

H	0.07721700	4.82046100	-1.93267600
H	-1.41332600	3.85406800	-1.69866900
H	0.03329700	3.12327500	-2.46729900
N	-0.52288500	-3.26014600	-1.00692600
C	-0.19119900	-4.51506000	-0.27521100
C	0.04585200	-3.22361700	-2.38394400
H	-0.78017000	-5.33256500	-0.72742500
H	-0.50213700	-4.42979600	0.78128400
H	0.87198300	-4.80164000	-0.29765600
H	-0.22048700	-2.26871400	-2.86828700
H	-0.41726400	-4.03542200	-2.96999500
H	1.14453100	-3.33981400	-2.42850800
Cl	-1.59734500	-0.13529500	2.68473500
C	0.16376900	1.98501900	-0.04436400
N	1.27988500	1.25093000	-0.10487000
N	-0.99724800	1.33068600	0.33696400
C	-2.42001600	1.71664900	0.22110800
C	-2.89778900	1.86648300	-1.23992400
C	-2.84961900	2.92483000	1.07190400
C	-4.37943100	3.05001400	1.04368800
C	-4.91181000	3.15653400	-0.39311600
C	-4.42685100	1.99389100	-1.27151200
C	2.66795000	1.72316600	-0.26898000
C	3.11575800	2.80851200	0.73338100
C	2.94825300	2.18861900	-1.71658900
C	4.61815700	3.07332400	0.56700200
C	4.95426000	3.49057800	-0.87294800
C	4.44853400	2.45914100	-1.89344600
H	-2.99977500	0.82734100	0.64990900
H	-2.57389000	0.98522300	-1.83436500
H	-2.44325300	2.75726500	-1.71834200
H	-2.39399900	3.86596400	0.70426500
H	-2.49369900	2.78034600	2.11299300
H	-4.69196500	3.93508400	1.62852600
H	-4.83538600	2.17729700	1.55173200
H	-4.58869300	4.11714200	-0.83778200
H	-6.01742200	3.18162200	-0.38140000
H	-4.76869300	2.14228200	-2.31264200
H	-4.88983200	1.04025700	-0.93413200
H	3.29628800	0.79979900	-0.06353800
H	2.88929000	2.48535200	1.76683600
H	2.55237200	3.74450500	0.56723700
H	2.37148600	3.10829500	-1.93117400
H	2.60312100	1.42725700	-2.43656000
H	5.19319100	2.16863100	0.84261500
H	4.93786900	3.86266800	1.27219200
H	6.04581200	3.62441500	-0.98177100
H	4.49844000	4.47637600	-1.08709700
H	5.01678000	1.51572500	-1.78427700
H	4.64566300	2.81920400	-2.91988500

Molecule 3 – Product



Energy: -220.97 kcal/mol

C	0.92696400	1.84337600	-0.10395500
N	1.68901500	0.82196200	0.33594100
N	-0.41377700	1.71872100	0.05624800
C	-1.38923800	2.55657400	-0.63898500
C	-2.59316000	2.89778300	0.26182700
C	-1.86461400	1.84547100	-1.92921800
C	-2.84204500	2.74835100	-2.68583800
C	-4.03430900	3.11740900	-1.79230700
C	-3.55698200	3.80756100	-0.50743000
C	3.14250900	0.83091500	0.51714100
C	3.58906400	1.88330700	1.55508200
C	3.90914900	1.03378800	-0.80796100
C	5.08916700	1.71341300	1.81737400
C	5.88826200	1.85635200	0.51378700
C	5.40691400	0.84670900	-0.53927400
B	0.84364900	-0.27293300	1.03568200
B	-0.78271900	0.49305700	0.93197900
Cl	-1.41088800	1.00990500	2.53469300
N	-1.44262700	-2.97056400	-0.35929500
C	-1.34056100	-4.05700500	0.63191100
C	-1.22249700	-3.39139700	-1.74807700
H	-0.91452400	3.53205000	-0.93193000
H	-2.25021000	3.38341300	1.19451800
H	-3.12752100	1.97812300	0.58207200
H	-2.35207700	0.88487800	-1.67096800
H	-1.00285200	1.57730000	-2.56260700
H	-3.19797600	2.23689700	-3.59893500
H	-2.33095700	3.66449500	-3.03230100
H	-4.60637000	2.20467600	-1.53674500
H	-4.73271900	3.77298300	-2.34101600
H	-4.42321700	4.05945400	0.13220000
H	-3.07129200	4.76965700	-0.74919900
H	3.42428600	-0.18937100	0.91598200
H	3.01300600	1.75995800	2.49293700
H	3.37444900	2.90141800	1.18722400
H	3.72389500	2.04679400	-1.21017600
H	3.55315200	0.32257800	-1.57154200
H	5.28330400	0.72533300	2.27645000
H	5.42992600	2.46204700	2.55471800
H	6.96513600	1.71587100	0.71066500
H	5.78037400	2.88438000	0.12104100
H	5.60978100	-0.18456100	-0.19588100
H	5.97774400	0.97502800	-1.47572000
H	-0.61087100	-4.83979100	0.37802700
H	-2.33862000	-4.53063400	0.70004900
H	-1.08447200	-3.66303100	1.63321000
H	-2.02580300	-4.10119200	-2.01966600
H	-0.25467400	-3.88495800	-1.93674000
H	-1.31187200	-2.51816000	-2.41872600

N	1.59198600	2.98288500	-0.68686200
C	1.32242600	4.24035600	0.03469000
C	1.41985500	3.08847700	-2.14616800
H	2.16713600	4.92564800	-0.15893100
H	1.28580700	4.05180200	1.12452800
H	0.38885000	4.74851900	-0.25206900
H	1.56723200	2.09742200	-2.61095500
H	2.20875300	3.75837100	-2.53363900
H	0.44481300	3.48323500	-2.47149100
Cl	1.41515500	-0.67480400	2.68738200
C	-0.77922200	-1.76186900	0.04494300
N	-1.56745300	-0.69449500	0.30413500
N	0.54818900	-1.58424100	0.25238800
C	1.70397700	-2.27201500	-0.30901600
C	1.85471700	-1.98158700	-1.82121800
C	1.76798600	-3.78548200	-0.03058600
C	3.12626400	-4.31377200	-0.50967900
C	3.30949300	-4.03766500	-2.00857500
C	3.19862100	-2.53581300	-2.30572100
C	-3.02849100	-0.69493200	0.42086500
C	-3.52819500	-1.50982700	1.63302800
C	-3.75191700	-1.17683100	-0.85624900
C	-5.03050800	-1.25784000	1.80460200
C	-5.79765400	-1.64980500	0.53327000
C	-5.25202800	-0.90348700	-0.69362800
H	2.61173500	-1.82539600	0.20945300
H	1.79908000	-0.88988500	-1.99662500
H	1.02705300	-2.41979700	-2.39854100
H	0.96162400	-4.32888900	-0.54841300
H	1.63918800	-3.96849000	1.05345200
H	3.20236800	-5.39762700	-0.31019000
H	3.94483200	-3.84254300	0.06733900
H	2.55212700	-4.59414700	-2.58984800
H	4.28979800	-4.41892900	-2.34668400
H	3.31420200	-2.35416600	-3.38940100
H	4.03130600	-1.99358900	-1.81659400
H	-3.32689300	0.38921200	0.58253400
H	-2.97919300	-1.21938000	2.54949900
H	-3.33069500	-2.58423800	1.48249800
H	-3.58261900	-2.25806700	-1.01403300
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H	-6.87364200	-1.43776000	0.65849500
H	-5.71726200	-2.74056900	0.37085400
H	-5.43578700	0.18193400	-0.58988700
H	-5.79432800	-1.21909300	-1.60218100

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