Electronic Supplementary Material (ESI) for RSC Advances.

Alkylhalovinylboranes: a new class of Diels-Alder dienophiles

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Supporting Information

List of contents:

Experimental procedures

General experimental procedures. All non-aqueous reactions were performed in oven dried glassware, under an inert atmosphere of dry nitrogen or high purity argon. All reagents and solvents were used directly as purchased or purified according to standard procedures. Analytical thin layer chromatography was carried out using commercial silica gel plates (Merck, Silica Gel 60 F254) and visualization was effected with a *p*-anysaldehyde solution (2.5 mL *p*-anysaldehyde + 2.5 mL H_2SO_4 + 0.25 mL AcOH + 95 mL EtOH). Column chromatography was performed with silica gel 60 H (Merck), slurry packed, run under low pressure of nitrogen. The Diels-Alder reactions were monitored using ^{11}B NMR analysis in anhydrous $CDCl_3$. NMR spectra were recorded at 300 MHz for ^{1}H, 75 MHz for ^{13}C and 96 MHz for ^{11}B on a Bruker Avance-300 DPX spectrometer with $CDCl_3$ as solvent and $(CH_3)_4Si$ (^{1}H, 0.00 ppm) and $CDCl_3$ (^{13}C, 76.9 ppm) as internal standards. ^{11}B NMR spectra were externally referenced to $BF_3{\cdot}Et_2O$ (^{11}B, 0.00 ppm). Diastereomeric ratios were determined by ^{1}H NMR integration. Due to the volatility of the 5-norbornen-2-ol (**9**), yields were determined by ^{1}H NMR using α-naphthol as internal standard. Chemical shifts are reported in delta (δ) units in parts per million (ppm) and splitting patterns are designated as s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet and br, broad. Coupling constants are recorded in Hertz (Hz). Infrared spectra were recorded on a Shimadzu IR Prestige-21 spectrometer using sodium chloride plates. Absorbance frequencies are recorded in reciprocal centimeters (cm^{-1}). Low resolution mass spectra (MS) were obtained using a Shimadzu GCMS-QP2010 plus spectrometer.

General procedures for the terpenes reactions under inert atmosphere

Method A (BCl_3)

In a dry Schlenk reaction tube, under an argon atmosphere and magnetic stirring, a 1M solution of BCl_3 in hexanes (1 mL, 1 mmol), Et_3SiH (160 μL, 1 mmol) and the terpene (1.1 mmol) were added on an ice-brine bath at –10 ºC allowing to reach room temperature. After 1 h, the reaction mixture was cooled to 0 ºC and tributylvinylstannane (301 μL, 1 mmol) and cyclopentadiene (411 μL, 5 mmol) were added maintaining the stirring for 3 h allowing to reach room temperature. After that time, the reaction mixture was cooled to 0 ºC and THF (3 mL), Et_3N (1 mL) were added. Finally, a 3N solution of NaOH (3 mL) and 30% H_2O_2 (3 mL) were added in fractions of 0.5 mL alternately, leaving the reaction mixture with stirring at room temperature for 15 h. The organic phase was extracted with Et_2O (3 x 15 mL), washed

with saturated aqueous solutions of KF (15 mL), NH_4Cl (15 mL) and NaCl (15 mL) and dried over Na_2SO_4. The solvent was evaporated under reduced pressure at 0 ºC and the crude reaction was purified by column chromatography (pentane with gradient of Et_2O) to obtain 5-norbornen-2-ol (**9**).

Vinylborane **16'a**

According to Method A, when (+)-α-pinene (175 μL, 1.1 mmol) was used, the compound **9** was obtained with a 51% yield (56.3 mg, *endo/exo* 80:20, *endo R/S* 53:47 and *exo R/S* 50:50).

Vinylborane **17a**

According to Method A, when (+)-2-carene (179 μL, 1.1 mmol) was used, the compound **9** was obtained with a 34% yield (37.2 mg, *endo/exo* 76:24, *endo R/S* 30:70 and *exo R/S* 48:52).

Vinylborane **18a**

According to Method A, when (+)-3-carene (175 μL, 1.1 mmol) was used, the compound **9** was obtained with a 54% yield (59.6 mg, *endo/exo* 79:21, *endo R/S* 62:38 and *exo R/S* 48:52).

Vinylborane **19a**

According to Method A, when (-)-myrtenol (185 μL, 1.1 mmol) was used, the compound **9** was obtained with a 21% yield (22.9 mg, *endo/exo* 76:24, *endo R/S* 48:52 and *exo R/S* 50:50).

Vinylborane **20a**

According to Method A, when the compound **13** (205 μL, 1.1 mmol) was used, the compound **9** was obtained with a 27% yield (30.0 mg, *endo/exo* 78:22, *endo R/S* 47:53 and *exo R/S* 44:56).

Vinylborane **21a**

According to Method A, when the compound **14** (230 μL, 1.1 mmol) was used, the compound **9** was obtained with a 24% yield (26.4 mg, *endo/exo* 79:21, *endo R/S* 45:55 and *exo R/S* 45:55).

Vinylborane **22a**

According to Method A, when the compound **15** (180 μL, 1.1 mmol) was used, the compound **9** was obtained with a 26% yield (28.6 mg, *endo/exo* 78:22, *endo R/S* 47:53 and *exo R/S* 50:50).

Vinylborane **23a**

According to Method A, when (+)-longifolene (240 μL, 1.1 mmol) was used, the compound **9** was obtained with a 42% yield (46.6 mg, *endo/exo* 79:21, *endo R/S* 44:56 and *exo R/S* 50:50).

Vinylborane **24a**

According to Method A, when (-)-camphene (176 μL, 1.1 mmol) was used, the compound **9** was obtained with a 41% yield (44.8 mg, *endo/exo* 78:22, *endo R/S* 48:52 and *exo R/S* 52:48).

Method B (BBr_3)

In a dry Schlenk reaction tube, under an argon atmosphere and magnetic stirring, CH_2Cl_2 (1 mL), BBr_3 (95 μL, 1 mmol), Et_3SiH (160 μL, 1 mmol) and the terpene (1.1 mmol) were added on a ethyl acetate bath cooled with N_2 liquid at –40 ºC allowing to reach room temperature. After 2 h, the reaction mixture was cooled to 0 ºC and tributylvinylstannane (301 μL, 1 mmol) and cyclopentadiene (411 μL, 5 mmol) were added maintaining the stirring for 5 h allowing to reach room temperature. After that time, the reaction mixture was cooled to 0 ºC and THF (3 mL), Et_3N (1 mL) were added. Finally, a 3N solution of NaOH (3 mL) and 30% H_2O_2 (3 mL) were added in fractions of 0.5 mL alternately, leaving the reaction mixture with stirring at room temperature for 15 h. The organic phase was extracted with Et_2O (3 x 15 mL), washed with saturated aqueous solutions of KF (15 mL), NH_4Cl (15 mL) and NaCl (15 mL) and dried over Na_2SO_4. The solvent was evaporated under reduced pressure at 0 ºC and the crude reaction was purified by column chromatography (pentane with gradient of Et_2O) to obtain 5-norbornen-2-ol (**9**).

Vinylborane **16'b**

According to Method B, when (+)-α-pinene (175 μL, 1.1 mmol) was used, the compound **9** was obtained with a 36% yield (39.3 mg, *endo/exo* 90:10, *endo R/S* 50:50 and *exo R/S* 50:50).

Vinylborane **17b**

According to Method B, when (+)-2-carene (179 μL, 1.1 mmol) was used, the compound **9** was obtained with a 35% yield (38.6 mg, *endo/exo* 91:9, *endo R/S* 49:51 and *exo R/S* 50:50).

Vinylborane **18b**

According to Method B, when (+)-3-carene (175 μL, 1.1 mmol) was used, the compound **9** was obtained with a 32% yield (35.3 mg, *endo/exo* 93:7, *endo R/S* 48:52 and *exo R/S* 50:50).

Vinylborane **20b**

According to Method B, when the compound **13** (205 μL, 1.1 mmol) was used, the compound **9** was obtained with a 27% yield (29.8 mg, *endo/exo* 86:14, *endo R/S* 48:52 and *exo R/S* 50:50).

Vinylborane **22b**

According to Method B, when the compound **15** (180 μL, 1.1 mmol) was used, the compound **9** was obtained with a 30% yield (33.2 mg, *endo/exo* 96:4, *endo R/S* 45:55 and *exo R/S* 50:50).

Vinylborane **23b**

According to Method B, when (+)-longifolene (240 μL, 1.1 mmol) was used, the compound **9** was obtained with a 32% yield (35.1 mg, *endo/exo* 91:9, *endo R/S* 47:53 and *exo R/S* 50:50).

Vinylborane **24b**

According to Method B, when (-)-camphene (176 mg, 1.1 mmol) was used, the compound **9** was obtained with a 28% yield (30.7 mg, *endo/exo* 93:7, *endo R/S* 50:50 and *exo R/S* 50:50).

Method C ($HBBr_2 \cdot SMe_2$)

In a dry Schlenk reaction tube, under an argon atmosphere and magnetic stirring, a 1M solution of $HBBr_2 \cdot SMe_2$ in CH_2Cl_2 (1 mL, 1 mmol) and the terpene (1.1 mmol) were added on an ice-brine bath at –10 ºC, leading the reaction mixture to reflux (ca. 50 ºC) for 2 h. After that time, the reaction mixture was cooled to 0 ºC and tributylvinylstannane (301 μL, 1 mmol) and cyclopentadiene (411 μL, 5 mmol) were added leading the reaction mixture to reflux (ca. 50 ºC) for 5 h. Subsequently, the reaction mixture was allowed to reach room temperature maintaining the stirring for 15 h. After that time, the reaction mixture was cooled to 0 ºC and THF (3 mL), Et_3N (1 mL) were added. Finally, a 3N solution of NaOH (3 mL) and 30% H_2O_2 (3 mL) were added in fractions of 0.5 mL alternately, leaving the reaction mixture with stirring at room temperature for 4 h. The organic phase was extracted with Et_2O (3 x 15 mL), washed with saturated aqueous solutions of KF (15 mL), NH_4Cl (15 mL) and NaCl (15 mL) and dried over Na_2SO_4. The solvent was evaporated under reduced pressure at 0 ºC and the crude reaction was purified by column chromatography (pentane with gradient of Et_2O) to obtain 5-norbornen-2-ol (**9**).

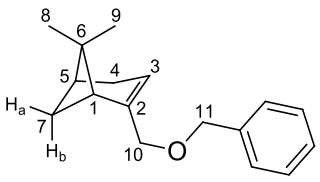
Vinylborane **17b**

According to Method C, when (+)-2-carene (179 μL, 1.1 mmol) was used, the compound **9** was obtained with a 10% yield (10.5 mg, *endo/exo* 60:40, *endo R/S* 45:55 and *exo R/S* 50:50).

Vinylborane **18b**

According to Method C, when (+)-3-carene (175 μL, 1.1 mmol) was used, the compound **9** was obtained with a 23% yield (24.7 mg, *endo/exo* 74:26, *endo R/S* 50:50 and *exo R/S* 49:51).

(*1R,5S*)-2-((benzyloxy)methyl)-6,6-dimethylbicyclo-[3.1.1]-hept-2-ene (13)[1]

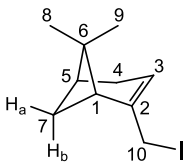


13

[1] Hwu, J. R.; Chua, V.; Schroeder, J. E.; Barrans Jr., R. E.; Khoudary, K. P.; Wang, N.; Wetzel, J. M. *J. Org. Chem.* **1986**, *51*, 4731-4733.

A dispersion of NaH (42%, 1.14 g, 20 mmol) in mineral oil was washed with anhydrous hexane (20 mL) and THF (25 mL) was added on an ice-water bath. A solution of (–)-myrtenol (1.68 mL, 10 mmol) in anhydrous THF (25 mL) was added to the dispersion of NaH, maintaining the reaction mixture with stirring at 0 ºC for 1 h. Subsequently, benzyl bromide (2.38 mL, 20 mmol) was added dropwise maintaining the reaction mixture at 0 ºC for 1.5 h. After that time, a saturated aqueous solution of NH_4Cl was added until the reaction mixture was neutralized. The organic phase was extracted with Et_2O (3 x 40 mL), washed with brine (40 mL), and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and the crude reaction was purified by column chromatography (hexane) to obtain the compound **13** (242 mg, 99%). IR (film) ν_{max} (cm^{-1}): 3088, 3063, 3030, 2982, 2868, 1722, 1703, 1682, 1497, 1456, 1366, 1092, 1070, 1028, 735, 696. ^{1}H NMR (300 MHz; $CDCl_3$) δ: 7.42-7.18 (m, 5H, ArH), 5.56-5.47 (m, 1H, H-3), 4.46 (sa, 2H, H-11), 3.88 (sa, 2H, H-10), 2.41 (ddd, $J_{7a,7b}$= 8.6 and $J_{1,7a}$= $J_{5,7a}$= 5.6 Hz, 1H, H-7a), 2.34-2.24 (m, 2H, H-4), 2.24-2.17 (m, 1H, H-1), 2.15-2.06 (m, 1H, H-5), 1.29 (s, 3H, H-8), 1.20 (d, 1H, $J_{7a,7b}$= 8.6 Hz, H-7b), 0.86 (s, 3H, H-9). ^{13}C NMR (75 MHz; $CDCl_3$) δ: 145.2 (C, C-2), 138.5 (C, Ar), 128.1 (CH x 2, Ar), 127.5 (CH x 2, Ar), 127.3 (CH, Ar), 119.9 (CH, C-3), 72.9 (CH_2, C-10), 71.5 (CH_2, C-11), 43.2 (CH, C-1), 40.8 (CH, C-5), 37.9 (C, C-6), 31.4 (CH_2, C-7), 31.1 (CH_2, C-4), 26.1 (CH_3, C-8), 21.0 (CH_3, C-9). MS-EI m/z (%): 242 (0.1), 169 (0.5), 151 (0.6), 119 (12.7), 91 (100), 65 (12.1), 41 (11.5).

(1*R*,5*S*)-2-(iodomethyl)-6,6-dimethylbicyclo-[3.1.1]-hept-2-ene (14)



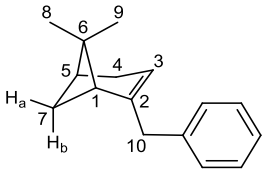
14

To a solution of triphenylphosphine (1.38 g, 5 mmol) and imidazole (0.92 g, 13.4 mmol) in dry CH_2Cl_2 (30 mL) on an ic

e-water bath, iodine (1.27 g, 5 mmol) was added and the mixture was stirred at 0 °C for 10 minutes under argon. After that time, (–)-myrtenol (0.42 mL, 2.5 mmol) was added maintaining the reaction mixture with stirring at 0 ºC for 5 min. The solvent was evaporated under reduced pressure at 0 °C and the crude reaction was purified immediately by column chromatography (pentane with gradient of Et_2O) to obtain the compound **14** (592 mg, 90%).

IR (film) ν_{max} (cm^{-1}): 3022, 2982, 2918, 2884, 2828, 1636, 1468, 1425, 1366, 1146. ^{1}H NMR (300 MHz; $CDCl_3$) δ: 5.71 (sa, 1H, H-3), 3.95-3.86 (m, 2H, H-10), 2.45 (ddd, $J_{7a,7b}$= 8.7 and $J_{1,7a}$= $J_{5,7a}$= 5.6 Hz, 1H, H-7a), 2.30-2.03 (m, 4H, H-1, H-4 and H-5), 1.31 (s, 3H, H-8), 1.16 (d, 1H, $J_{7a,7b}$= 8.7 Hz, H-7b), 0.81 (s, 3H, H-9). ^{13}C NMR (75 MHz; $CDCl_3$) δ: 144.7 (C, C-2), 121.6 (CH, C-3), 45.6 (CH, C-1), 40.2 (CH, C-5), 37.8 (C, C-6), 31.5 (CH_2, C-7), 31.2 (CH_2, C-4), 25.9 (CH_3, C-8), 20.9 (CH_3, C-9), 13.0 (CH_2, C-10). MS-EI m/z (%): 263 (100), 207 (77.7), 135 (62.6), 107 (36.5), 93 (79.6), 69 (85.2), 41 (70.3).

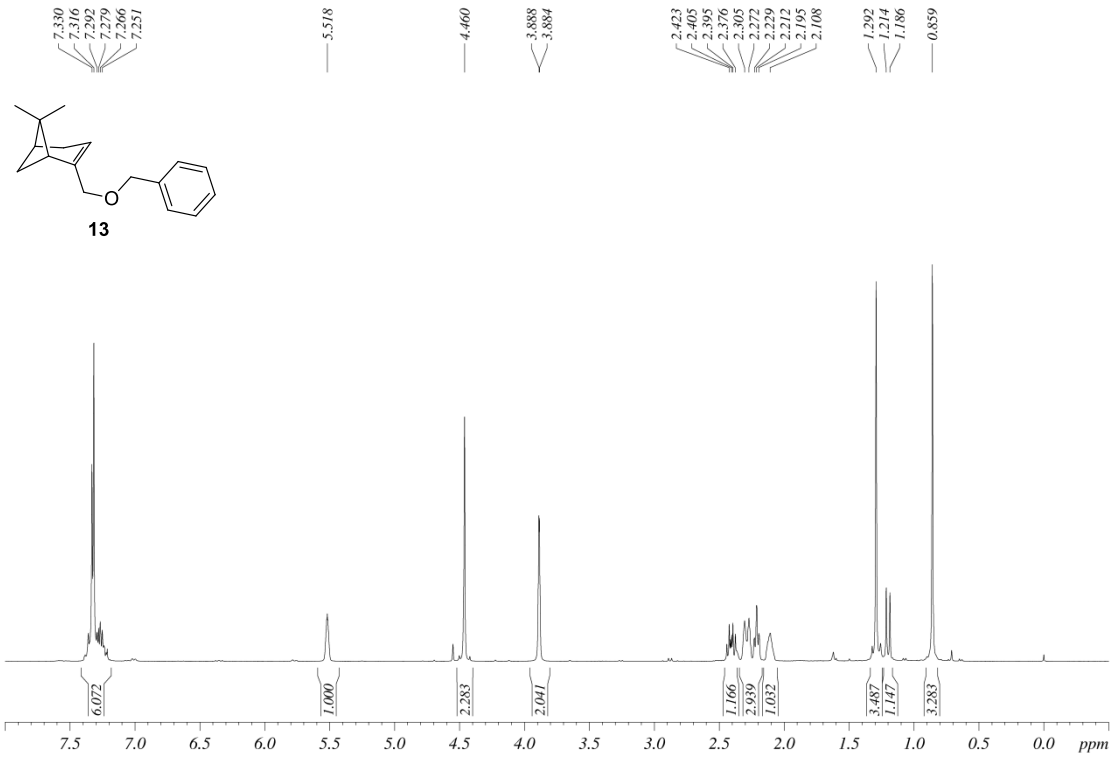
(1*R*,5*S*)-2-benzyl-6,6-dimethylbicyclo-[3.1.1]-hept-2-ene (15)[2]



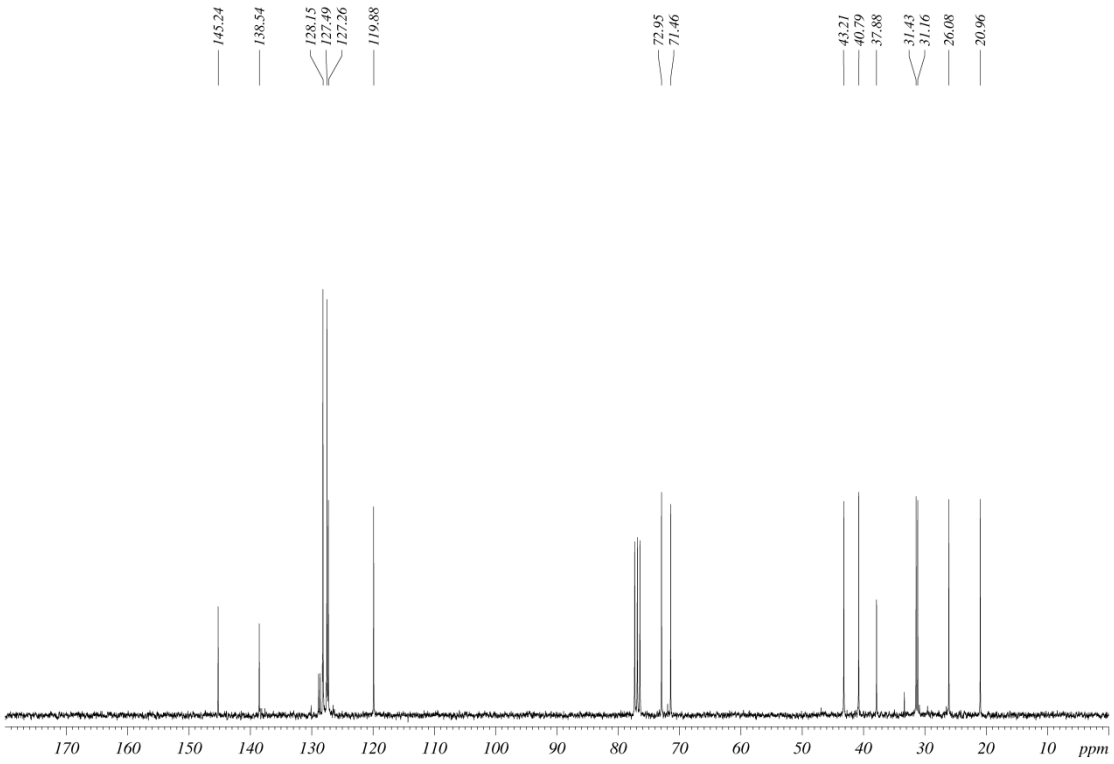
15

To a suspension of magnesium turnings (162 mg, 6.7 mmol) in anhydrous Et_2O (3 mL) on an ice-water bath, bromobenzene (702 μL, 6.7 mmol) was added dropwise maintaining the stirring at room temperature for 1 h. After that time, the reaction mixture was transferred by cannula to a solution of compound **14** (1.05 g, 4 mmol) in anhydrous Et_2O (3 mL) on an ice-water bath maintaining the stirring at room temperature for 2.5 h. Subsequently, a saturated aquepus solution of NH_4Cl (5 mL) was added. The organic phase was extracted with Et_2O (3 x 10 mL), washed with brine (10 mL), and dried over Na_2SO_4. The solvent was evaporated under reduced pressure and the crude reaction was purified by column chromatography (hexane) to obtain the compound **15** (820 mg, 86%). IR (film) ν_{max} (cm^{-1}): 3082, 3061, 3026, 2984, 2913, 2832, 1601, 1493, 1452, 1364, 745, 700. ^{1}H NMR (300 MHz; $CDCl_3$) δ: 7.30-7.10 (m, 5H, ArH); 5.27-5.18 (m, 1H, H-3); 3.36-3.18 (m, 2H, H-10); 2.36-2.13 (m, 3H, H-7a, H-4); 2.11-2.01 (m, 1H, H-5); 2.01-1.94 (m, 1H, H-1); 1.19 (s, 3H, H-8); 1.15 (d, 1H, $J_{7a,7b}$= 8.5 Hz, H-7b); 0.74 (s, 3H, H-9). ^{13}C NMR (75 MHz; $CDCl_3$) δ: 147.2 (C, C-2); 139.4 (C, Ar); 129.1 (CH x 2, Ar); 127.9 (CH x 2, Ar); 125.7 (CH, Ar); 117.6 (CH, C-3); 45.4 (CH, C-1); 43.4 (CH_2, C-10); 40.6 (CH, C-5); 37.8 (C, C-6); 31.7 (CH_2, C-7); 31.3 (CH_2, C-4); 26.1 (CH_3, C-8); 20.9 (CH_3, C-9). MS-EI m/z (%): 210 (3.5), 168 (22.1), 121 (11.6), 91 (100), 65 (10.4), 41 (9.8).

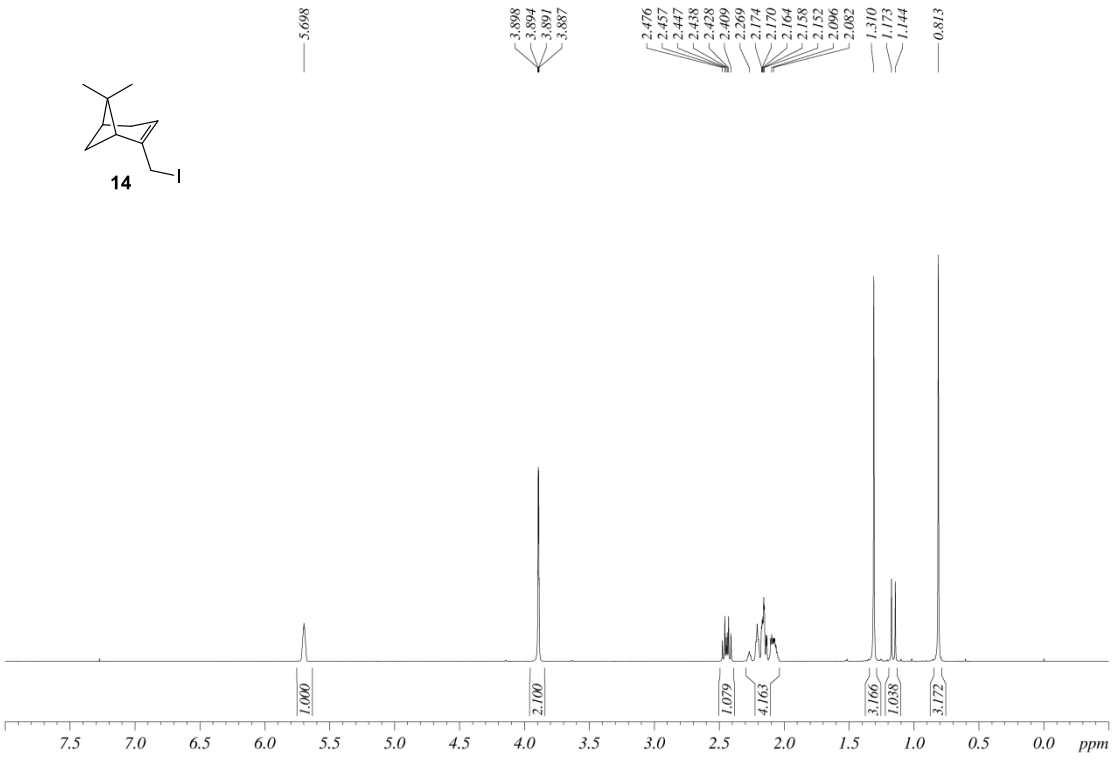
[2] (a) Grigg, R.; Stevenson, P.; Worakun, T. *Tetrahedron* **1988**, *44*, 2033-2048. (b) Bir, G.; Kaufmann, D. *J. Organomet. Chem.* **1990**, *390*, 1-6.



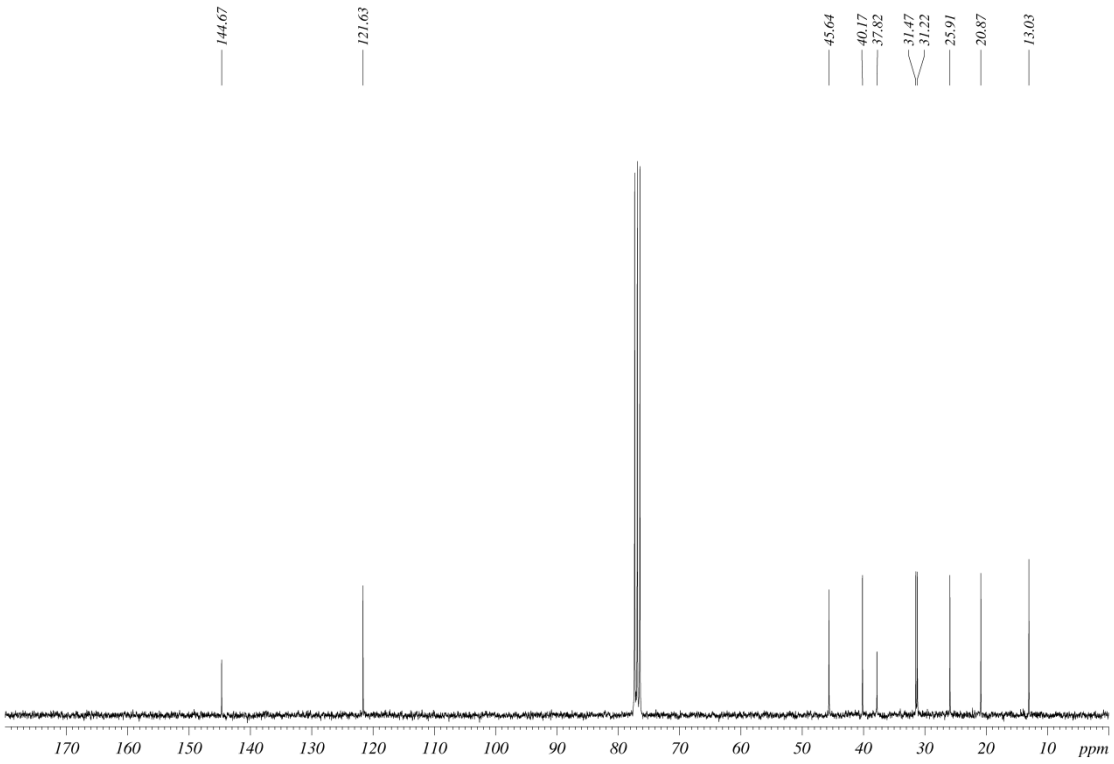
^{1}H NMR spectrum of **13**.



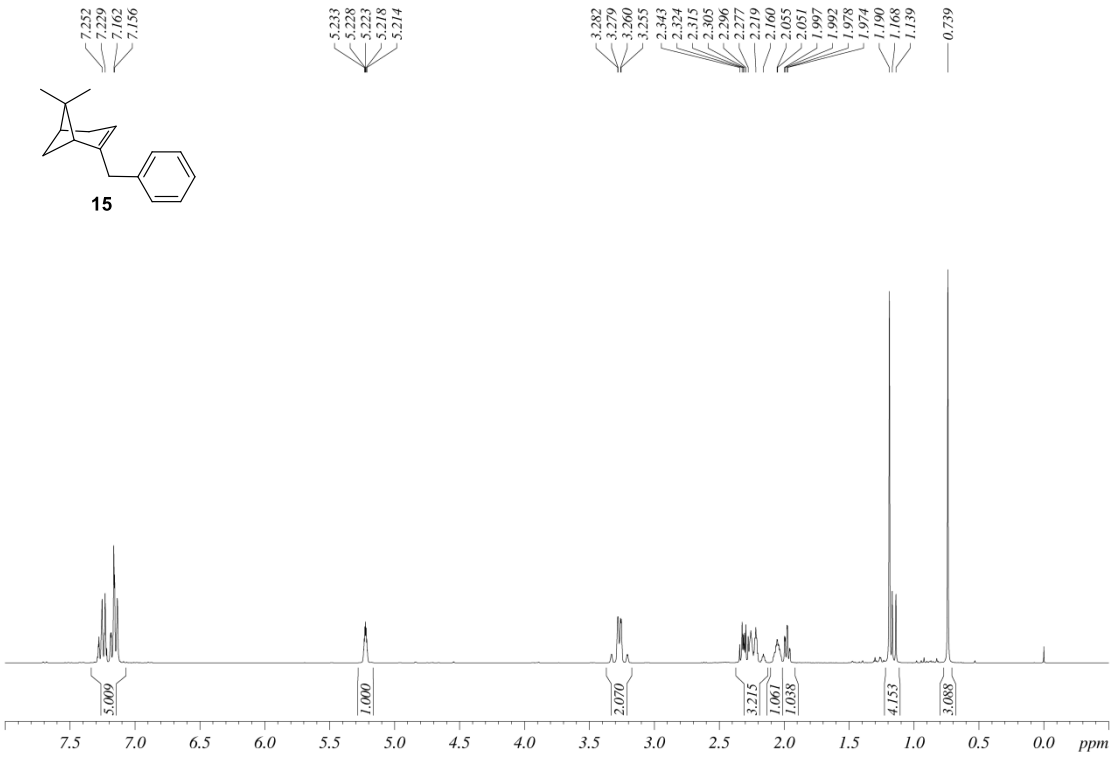
^{13}C NMR spectrum of **13**.



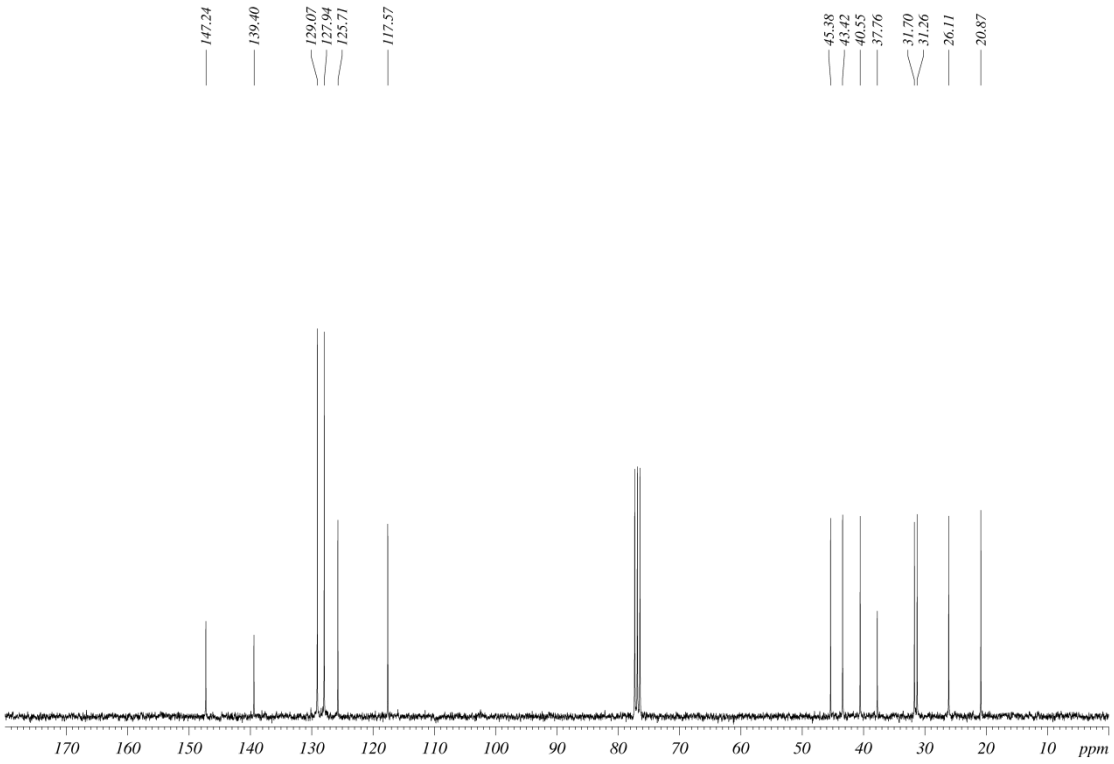
^{1}H NMR spectrum of **14**.



^{13}C NMR spectrum of **14**.



^{1}H NMR spectrum of **15**.



^{13}C NMR spectrum of **15**.

Computational methods

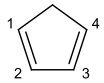
Conformational searches for the reactants, the transition structures (TSs), and the products were run to locate the global minima at the B3LYP/6-31G* level of theory. Initially, a large number of geometries were generated using the conformational search module of Hyperchem with the MM+ method.[3] In the TSs optimizations, the carbon atoms corresponding to the carbon-carbon new bonds formed in the Diels-Alder reaction were fixed during the conformational searches, optimizing the spatial location of the remaining atoms. All selected structures were then successively reoptimized at the RHF/AM1, RHF/3-21G and B3LYP/6-31G* levels of theory (except for compound **21a**, where LANL2DZ[4] was used as the final level of theory).[5] Additionally, solvent effects in dichloromethane (ε= 8.93) and heptane (ε= 1.92) were calculated for the most stable geometries of reagents, TSs, and products using the Polarized Continuum Model of Self-Consistent Reaction Field method (PCM method).[6] Geometries for all structures were fully optimized and normal mode analysis was used to confirm the nature of the stationary points and to evaluate the thermochemical properties. Reported thermochemical properties include zero-point energies (ZPEs) without scaling and were calculated at 1 atm and 298.15 K. The molecular orbitals of the reactants were calculated to analyse the frontier orbital interactions. Intrinsic reaction coordinate (IRCs) calculations were run to verify the connectivity between reactants, TSs and products. To examine the more important interactions in the TSs, we performed natural bond orbital calculations and Wiberg bond indexes (WBIs) were analysed. *Endo/exo* and *Re/Si* ratios were computed using Boltzmann factors based on free energies of activation ($\Delta G^{\neq}$). The global electrophilicity index ω has been given by the following expression, $\omega = \mu^2/2\eta$ (eV), in terms of the electronic chemical potential μ and the chemical hardness η. Both quantities may be approached in terms of the one-electron energies of the frontier molecular orbitals HOMO and LUMO, $\mu \approx (E_{HOMO} + E_{LUMO})/2$ and $\eta \approx (E_{LUMO} - E_{HOMO})$, respectively. The global nucleophilicity index, N, was computed as $N = E_{HOMO(diene)} - E_{HOMO(TCNE)}$ (eV), where TCNE accounts for tetracyanoethylene. The local electrophilic indices, ω_k, were computed according to the

[3] Hyperchem Professional Release 7.52, Hypercube, Inc., 2005.
[4] P. J. Hay and W. R. Wadt, *J. Chem. Phys.*, 1985, **82**, 299-310.
[5] Gaussian 09W, Revision D.01: M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.
[6] J. Tomasi, B. Mennucci and R. Cammi, *Chem. Rev.*, 2005, **105**, 2999-3094.

following expression: $\omega_k = \omega.P^+_k$, where P^+_k is the electrophilic Parr function of atom k, that was computed using the Mulliken atomic spin density (ASD) computed by single-point UB3LYP/6-31G* level of the anion resulting from adding one electron to the optimized neutral B3LYP/6-31G* geometry.[7] In addition, global electron density transfer (GEDT) for the TSs were calculated.[8]

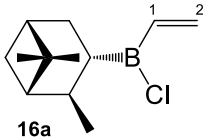
[7] L. R. Domingo, P. Pérez and J. A. Sáez, *RSC Advances*, 2013, **3**, 1486-1494.
[8] L. R. Domingo, *RSC Advances*, 2014, **4**, 32415-32428.

Coefficients of FMOs of reactants



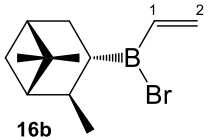
	E (eV)	C-1		C-2		C-3		C-4	
		2pz	3pz	2pz	3pz	2pz	3pz	2pz	3pz
HOMO	-5.76	-0.35	-0.28	-0.24	-0.18	0.24	0.18	0.35	0.28
LUMO	-0.27	0.34	0.42	-0.24	-0.30	-0.24	-0.30	0.34	0.42

	E (eV)	C-1		C-2		B	
		2pz	3pz	2pz	3pz	2pz	3pz
HOMO-3	-7.83	0.35	0.24	0.36	0.26	0.01	0.02
LUMO	-1.78	-0.17	-0.21	0.37	0.42	-0.39	-0.40



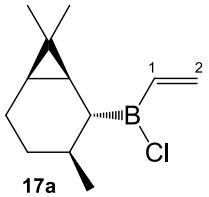
16a

	E (eV)	C-1		C-2		B	
		2pz	3pz	2pz	3pz	2pz	3pz
HOMO-3	-7.63	-0.23	-0.15	-0.25	-0.18	-0.01	-0.01
LUMO	-1.83	-0.17	-0.21	0.36	0.42	-0.39	-0.38



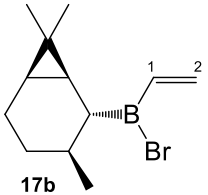
16b

	E (eV)	C-1		C-2		B	
		2pz	3pz	2pz	3pz	2pz	3pz
HOMO-2	-7.74	0.34	0.23	0.35	0.25	0.05	0.03
LUMO	-1.72	-0.18	-0.22	0.37	0.43	-0.39	-0.39



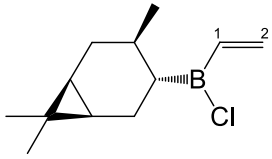
17a

	E (eV)	C-1		C-2		B	
		2pz	3pz	2pz	3pz	2pz	3pz
HOMO-3	-7.57	-0.29	-0.20	-0.31	-0.23	0.00	0.00
LUMO	-1.78	-0.17	-0.22	0.36	0.42	-0.40	-0.37



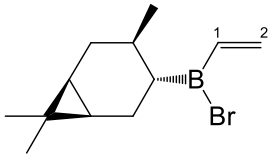
17b

	E (eV)	C-1		C-2		B	
		2pz	3pz	2pz	3pz	2pz	3pz
HOMO-3	-7.79	0.36	0.24	0.37	0.26	0.06	0.04
LUMO	-1.77	-0.18	-0.21	0.37	0.42	-0.39	-0.39



18a

	E (eV)	C-1		C-2		B	
		2pz	3pz	2pz	3pz	2pz	3pz
HOMO-3	-7.60	-0.29	-0.19	-0.31	-0.23	0.01	0.01
LUMO	-1.83	-0.17	-0.21	0.36	0.42	-0.40	-0.37



18b

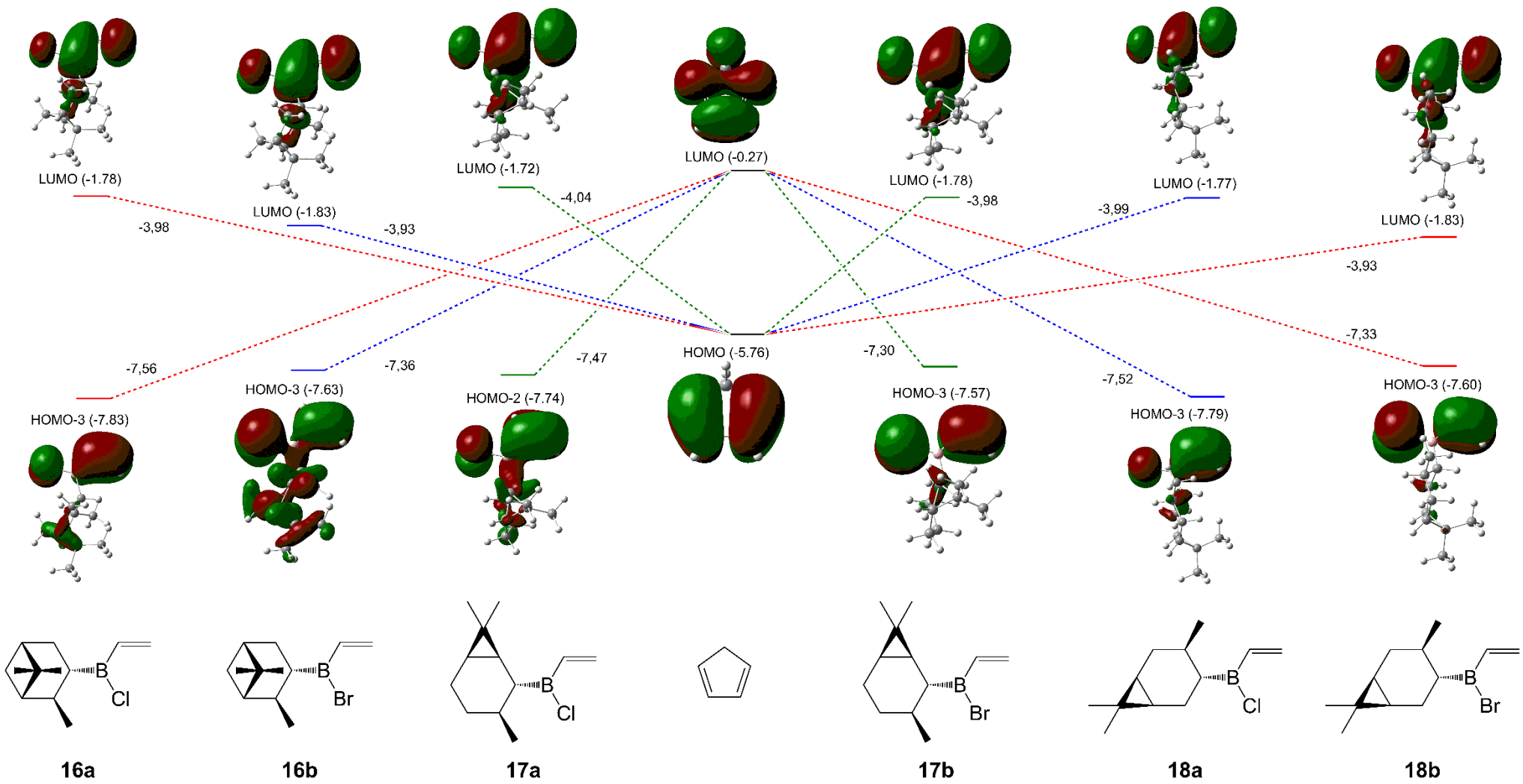


Figure S1. Shapes and energies (in eV) of FMOs of reactants (top: LUMOs, bottom: HOMOs).

Table S1. Global reactivity indices and FMO energies for reactants **10-18** calculated at the B3LYP/6-31G* level.

	HOMO (eV)	LUMO (eV)	ω (eV)	N (eV)
CP	-5.76	-0.27	0.83	**3.36**
10	-7.42	-1.32	**1.57**	1.70
11ª	-7.77	-1.76	**1.89**	1.35
11b	-7.57	-1.81	**1.91**	1.55
16ª	-7.83	-1.78	**1.91**	1.29
16b	-7.63	-1.83	**1.93**	1.49
17ª	-7.74	-1.72	**1.86**	1.38
17b	-7.57	-1.78	**1.89**	1.55
18ª	-7.79	-1.77	**1.90**	1.33
18b	-7.60	-1.83	**1.93**	1.52

Table S2. Local reactivity indices for reactants **10-18** calculated at the B3LYP/6-31G* level.

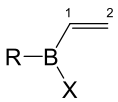
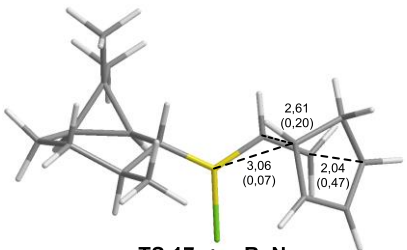
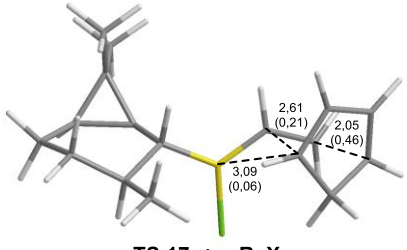
					
	ω_B	ω_{C1}	ω_{C2}	N_{C1}	N_{C2}
CP				1.59	0.27
10	1.03	-0.16	0.77		
11ª	1.23	-0.20	0.95		
11b	1.25	-0.22	0.96		
16ª	1.24	-0.20	0.96		
16b	1.26	-0.21	0.97		
17ª	1.20	-0.20	0.94		
17b	1.22	-0.22	0.95		
18ª	1.23	-0.20	0.95		
18b	1.25	-0.22	0.97		

Table S3. Global electron density transfer (GEDT) for transition structures computed for the Diels-Alder reactions between **10-18** and cyclopentadiene (**cp**) at the B3LYP/6-31G* level (in e).

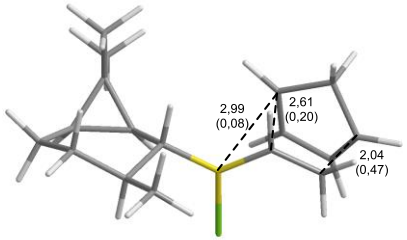
	Endo		***exo***	
TS10+cp	0.132		0.130	
TS11a+cp	0.176		0.169	
TS11b+cp	0.187		0.177	
	Re endo	***Re exo***	***Si endo***	***Si exo***
TS16a+cp	0.178	0.166	0.183	0.174
TS16b+cp	0.187	0.181	0.192	0.181
TS17a+cp	0.173	0.167	0.182	0.175
TS17b+cp	0.182	0.173	0.191	0.180
TS18a+cp	0.180	0.174	0.176	0.172
TS18b+cp	0.197	0.187	0.192	0.183



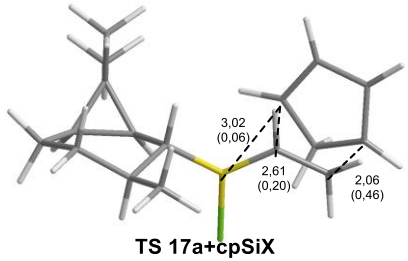
TS 17a+cpReN
ΔG*= 13.56 (0.23)



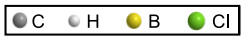
TS 17a+cpReX
ΔG*= 13.97 (0.63)

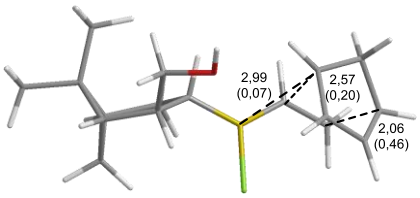


TS 17a+cpSiN
ΔG*= 13.34 (0.00)

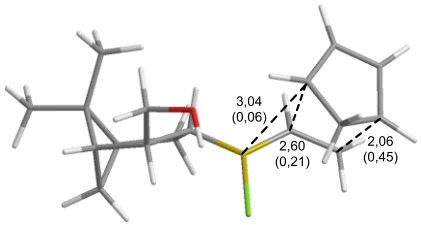


TS 17a+cpSiX
ΔG*= 13.72 (0.38)

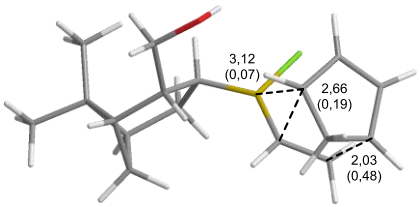




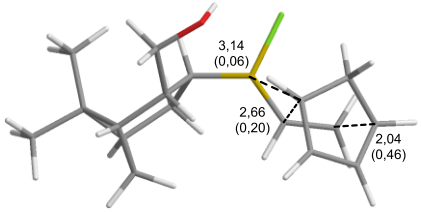
TS 19a+cpReN
ΔG*= 13.71 (0.83)



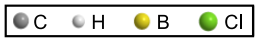
TS 19a+cpReX
ΔG*= 12.88 (0.00)

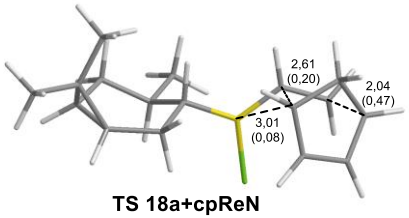


TS 19a+cpSiN
ΔG*= 13.79 (0.91)

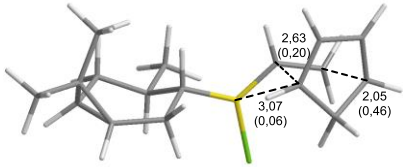


TS 19a+cpSiX
ΔG*= 13.82 (0.93)

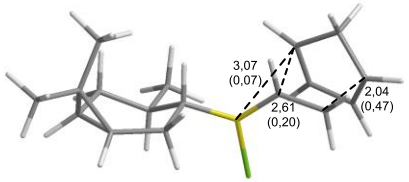




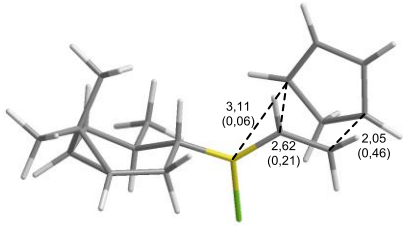
TS 18a+cpReN
ΔG*= 12.99 (0.00)



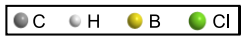
TS 18a+cpReX
ΔG*= 13.50 (0.51)

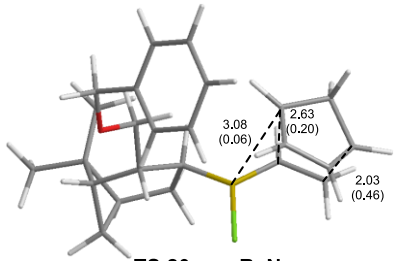


TS 18a+cpSiN
ΔG*= 13.16 (0.16)

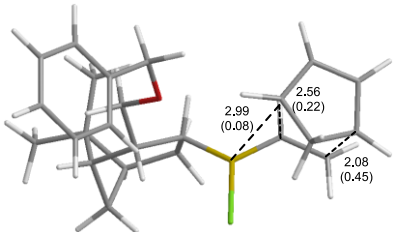


TS 18a+cpSiX
ΔG*= 13.57 (0.58)

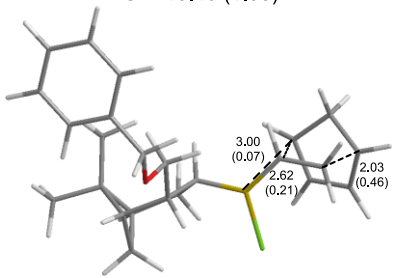




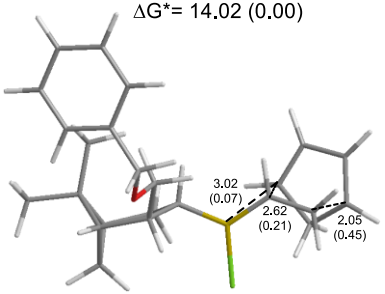
TS 20a+cpReN
ΔG*= 15.40 (1.38)



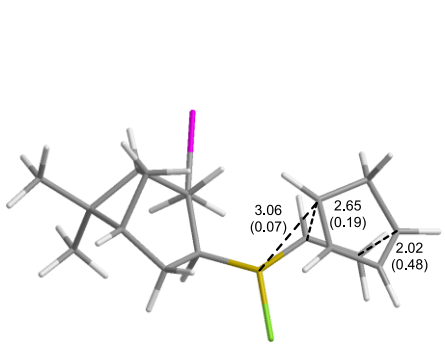
TS 20a+cpReX
ΔG*= 14.02 (0.00)



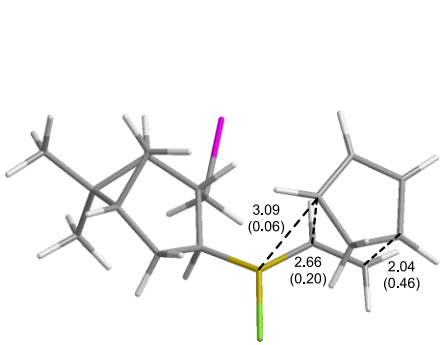
TS 20a+cpSiN
ΔG*= 14.02 (0.00)



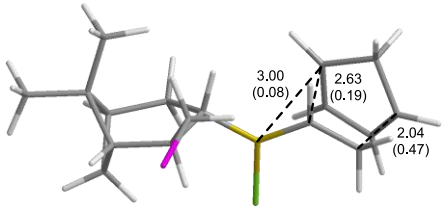
TS 20a+cpSiX
ΔG*= 14.48 (0.46)



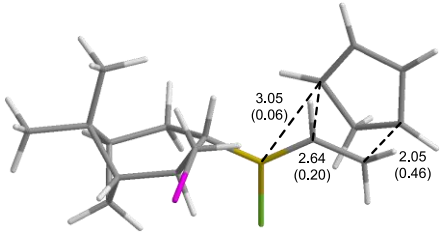
TS 21a+cpReN
ΔG*= 16.00 (0.92)



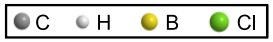
TS 21a+cpReX
ΔG*= 16.54 (1.47)

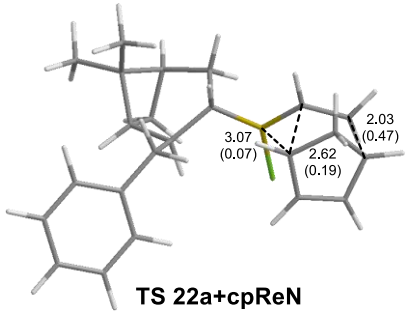


TS 21a+cpSiN
ΔG*= 15.08 (0.00)

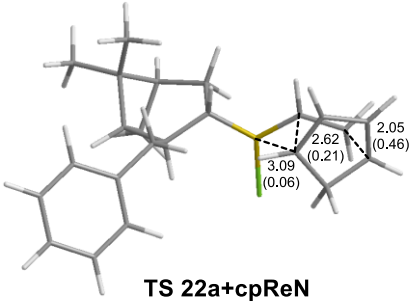


TS 21a+cpSiX
ΔG*= 15.69 (0.61)

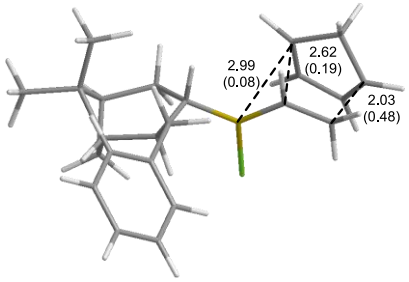




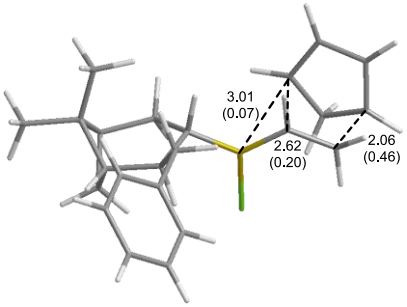
TS 22a+cpReN
ΔG*= 14.67 (1.10)



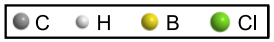
TS 22a+cpReN
ΔG*= 15.15 (1.59)



TS 22a+cpReN
ΔG*= 13.56 (0.00)



TS 22a+cpReN
ΔG*= 14.07 (0.51)



Cartesian coordinates of reactants, TSs and products

Reactants

Cyclopentadiene

C	0	-1.110428	-0.484303	0.948296
C	0	-1.359052	0.048076	-0.439189
C	0	0.027097	0.157511	-1.019681
C	0	0.924160	-0.251366	-0.099150
C	0	0.216283	-0.650763	1.125513
H	0	-1.895359	-0.690610	1.667047
H	0	-1.876913	1.019698	-0.421645
H	0	-2.001834	-0.623264	-1.029671
H	0	0.237109	0.512567	-2.022233
H	0	2.001834	-0.287417	-0.223145
H	0	0.703966	-1.019698	2.022233

Energy + ZPE = -194.008161
Free energy = -194.034758
Free energy in DCM = -194.101477
Free energy in heptane = -194.101511
Number of imaginary frequencies = 0

Vinylborane 10

C	0	-1.195671	-1.166359	-0.486404
C	0	-1.195671	0.386681	-0.486404
C	0	-2.619500	-1.746498	-0.486404
B	0	0.284050	0.968102	-0.443466
C	0	-2.046273	0.910958	0.702500
C	0	-3.448540	-1.208413	0.688812
C	0	0.851356	1.861230	-1.597839
C	0	1.236961	0.650506	0.793045
C	0	-3.468514	0.326943	0.700317
C	0	0.177894	2.218743	-2.704590
C	0	1.654640	1.944420	1.544189
C	0	2.504722	-0.133095	0.355240
C	0	3.445152	-0.421975	1.537018
C	0	2.596534	1.652001	2.723938
C	0	3.837104	0.865593	2.276230
H	0	-0.661446	-1.533913	0.401900
H	0	-0.643608	-1.544213	-1.357697
H	0	-1.714791	0.700326	-1.405853
H	0	-3.117073	-1.481926	-1.431274
H	0	-2.578179	-2.843331	-0.452133
H	0	-2.098108	2.007897	0.675262
H	0	-1.554665	0.647607	1.650436
H	0	-4.471962	-1.603188	0.646408
H	0	-3.012780	-1.570031	1.632370
H	0	1.875282	2.236947	-1.521454
H	0	0.711097	0.016502	1.524872
H	0	-4.026436	0.693581	1.572220
H	0	-4.005806	0.688470	-0.189056
H	0	0.615547	2.843331	-3.482681
H	0	-0.847313	1.901513	-2.884155
H	0	0.764549	2.476174	1.906769
H	0	2.158058	2.630517	0.847351
H	0	2.218696	-1.077599	-0.127060
H	0	3.052665	0.444237	-0.403824
H	0	4.343055	-0.945671	1.182800
H	0	2.942344	-1.103447	2.239182
H	0	2.053292	1.069375	3.482681
H	0	2.895668	2.591637	3.207184
H	0	4.441688	1.496056	1.606842
H	0	4.471962	0.630791	3.140396

Energy + ZPE = -573.035437
Free energy = -573.078945
Free energy in DCM = -573.396396
Free energy in heptane = -573.400542
Number of imaginary frequencies = 0

Vinylborane 11a

C	0	1.123192	0.471101	0.432107
C	0	1.123192	2.007988	0.432107
C	0	-0.319081	-0.106440	0.432107
C	0	0.314254	2.575274	1.607542
C	0	-1.121199	0.477026	1.627895
B	0	-0.330499	-1.683010	0.418743
C	0	-1.114877	2.013897	1.624525
Cl	0	0.409310	-2.545869	1.810851
C	0	-0.923993	-2.588803	-0.689688
C	0	-1.515502	-2.119878	-1.802041
H	0	1.655207	0.106622	1.321179
H	0	1.680382	0.099241	-0.438056
H	0	2.155736	2.379488	0.466326
H	0	0.692224	2.370808	-0.513103
H	0	-0.807964	0.253524	-0.487241
H	0	0.816145	2.313566	2.550848
H	0	0.291752	3.671660	1.559875
H	0	-0.681552	0.112796	2.566182
H	0	-2.155736	0.109372	1.605781
H	0	-1.657486	2.377008	0.738795
H	0	-1.660892	2.389566	2.499779
H	0	-0.863818	-3.671660	-0.570830
H	0	-1.924729	-2.778737	-2.566182
H	0	-1.616743	-1.054678	-1.997895

Energy + ZPE = -798.164932
Free energy = -798.203580
Free energy in DCM = -798.369611
Free energy in heptane = -798.371598
Number of imaginary frequencies = 0

Vinylborane 11b

C	0	1.119101	0.482404	0.416600
C	0	1.129784	2.018388	0.440108

C	0	-0.326710	-0.088627	0.412851
C	0	0.327162	2.571660	1.626415
C	0	-1.127472	0.488468	1.613769
B	0	-0.336306	-1.663270	0.402821
C	0	-1.107458	2.024426	1.632305
Br	0	0.473654	-2.566735	1.927343
C	0	-0.920832	-2.588836	-0.689384
C	0	-1.515328	-2.135918	-1.807274
H	0	1.650232	0.096417	1.296788
H	0	1.669948	0.119829	-0.461522
H	0	2.165075	2.381741	0.478165
H	0	0.699674	2.399201	-0.498327
H	0	-0.815105	0.274864	-0.505494
H	0	0.826003	2.284894	2.563977
H	0	0.316376	3.668910	1.600617
H	0	-0.694682	0.102746	2.546362
H	0	-2.165075	0.130180	1.582110
H	0	-1.644955	2.405527	0.751093
H	0	-1.651685	2.392044	2.512063
H	0	-0.852036	-3.668910	-0.554812
H	0	-1.920379	-2.805821	-2.563977
H	0	-1.623040	-1.073524	-2.014783

Energy + ZPE = -2909.672434
Free energy = -2909.711097
Free energy in DCM = -2909.876764
Free energy in heptane = -2909.878892
Number of imaginary frequencies = 0

Vinylborane 16a

Cl	0	-3.069293	-1.508824	-0.510834
C	0	-3.065748	1.321767	-0.551785
C	0	-2.613062	2.578822	-0.401179
B	0	-2.220621	0.056554	-0.252611
C	0	-0.717484	0.028602	0.224740
C	0	0.231917	-0.497770	-0.929057
C	0	1.349046	-1.403036	-0.369876
C	0	1.974514	-0.938112	0.999977
C	0	0.716169	-1.617585	1.640758
C	0	-0.528144	-0.716339	1.600620
C	0	0.752677	0.657987	-1.796181
C	0	3.265731	-1.722161	1.303244
C	0	0.667644	-2.561208	0.411219
C	0	2.270497	0.536721	1.302261
H	0	-4.091065	1.196668	-0.902883
H	0	-3.229854	3.449665	-0.616971
H	0	-1.604696	2.792636	-0.053964
H	0	-0.420768	1.068994	0.395570
H	0	-0.351390	-1.150215	-1.594450
H	0	2.055167	-1.666635	-1.168707
H	0	0.836397	-2.064353	2.636277
H	0	-1.395905	-1.348061	1.826889
H	0	-0.480707	0.036062	2.398084
H	0	-0.076227	1.242199	-2.214415
H	0	1.389064	1.344288	-1.227173
H	0	1.344124	0.274209	-2.636277
H	0	3.558760	-1.586495	2.352230
H	0	3.174700	-2.796904	1.123659
H	0	4.091065	-1.353686	0.680526
H	0	-0.324718	-2.869760	0.065588
H	0	1.293700	-3.449665	0.515757
H	0	3.082933	0.907959	0.664570
H	0	1.416219	1.201872	1.169018
H	0	2.606306	0.642128	2.342465

Energy + ZPE = -954.072615
Free energy = -954.115140
Free energy in DCM = -954.363646
Free energy in heptane = -954.366543
Number of imaginary frequencies = 0

Vinylborane 16b

Br	0	-3.137244	-1.641128	-0.330880
C	0	-3.071833	1.295916	-0.698250
C	0	-2.656307	2.572137	-0.612188
B	0	-2.234458	0.085349	-0.218974
C	0	-0.741507	0.103623	0.281636
C	0	0.189322	-0.390353	-0.909921
C	0	1.293105	-1.339469	-0.402247
C	0	1.964376	-0.924803	0.961398
C	0	0.709481	-1.593716	1.618666
C	0	-0.507610	-0.656567	1.640153
C	0	0.719211	0.786801	-1.740795
C	0	3.246289	-1.741127	1.210819
C	0	0.602074	-2.501300	0.365654
C	0	2.291615	0.537065	1.290524
H	0	-4.063316	1.114751	-1.114828
H	0	-3.270049	3.407819	-0.944411
H	0	-1.685143	2.837184	-0.200260
H	0	-0.467672	1.150909	0.453416
H	0	-0.415120	-1.006134	-1.592374
H	0	1.972063	-1.598517	-1.225691
H	0	0.848014	-2.069834	2.597932
H	0	-1.385827	-1.260427	1.896518
H	0	-0.399364	0.085971	2.441016
H	0	-0.105786	1.393659	-2.132548
H	0	1.369225	1.445024	-1.154948
H	0	1.298621	0.422478	-2.597932
H	0	3.568375	-1.638598	2.255040
H	0	3.126783	-2.808942	1.007284
H	0	4.063316	-1.374306	0.576261
H	0	-0.408314	-2.771023	0.042166
H	0	1.207671	-3.407819	0.427572
H	0	3.087294	0.914495	0.635619
H	0	1.440863	1.214612	1.201725
H	0	2.661777	0.613065	2.321629

Energy + ZPE = -3065.581406
Free energy = -3065.624032
Free energy in DCM = -3065.872541
Free energy in heptane = -3065.875542
Number of imaginary frequencies = 0

Vinylborane 17a

Cl	0	-1.398275	-2.626328	-0.517022
B	0	-1.367266	-0.836936	-0.337843
C	0	0.034100	-0.108733	-0.365883
C	0	-2.745559	-0.165262	-0.114323
C	0	0.916942	-0.468957	-1.595334
C	0	0.753218	-0.416149	0.967969
C	0	-2.916460	1.159767	0.033578
C	0	2.278097	0.236160	-1.490318
C	0	2.273916	-0.426573	1.019045
C	0	0.219719	-0.110369	-2.914434
C	0	1.499727	0.632164	1.783181
C	0	3.088935	-0.189102	-0.249126
C	0	1.539450	2.093472	1.370805
C	0	1.445796	0.462132	3.295520
H	0	-0.151370	0.973924	-0.426350
H	0	-3.635204	-0.795426	-0.072080
H	0	1.089538	-1.554392	-1.578841
H	0	0.278581	-1.188024	1.572798
H	0	-2.081909	1.856598	0.004356
H	0	-3.896743	1.606487	0.191336
H	0	2.112213	1.322437	-1.499322
H	0	2.873544	0.020061	-2.387468
H	0	2.707279	-1.199252	1.653446
H	0	0.003039	0.965015	-2.966046
H	0	0.850561	-0.361906	-3.775276
H	0	-0.729174	-0.647207	-3.033886
H	0	3.896743	0.532434	-0.063642
H	0	3.585513	-1.139342	-0.486419
H	0	0.655575	2.626328	1.746922
H	0	2.421538	2.584880	1.801159
H	0	1.580215	2.242516	0.290174
H	0	1.419575	-0.595333	3.581985
H	0	2.323603	0.915243	3.775276
H	0	0.552539	0.943279	3.715762

Energy + ZPE = -954.082390
Free energy = -954.125854
Free energy in DCM = -954.371070
Free energy in heptane = -954.374051
Number of imaginary frequencies = 0

Vinylborane 17b

Br	0	-1.330705	-2.790592	-0.440174
B	0	-1.330705	-0.841446	-0.440174
C	0	0.071745	-0.120882	-0.440174
C	0	-2.723086	-0.170900	-0.386487
C	0	1.035258	-0.602967	-1.563857
C	0	0.701277	-0.307327	0.959500
C	0	-2.903017	1.161490	-0.369726
C	0	2.380767	0.128363	-1.444828
C	0	2.215446	-0.297663	1.110497
C	0	0.423308	-0.409230	-2.957107
C	0	1.386080	0.812583	1.730323
C	0	3.112016	-0.158310	-0.116756
C	0	1.450854	2.232914	1.195925
C	0	1.230536	0.772127	3.244529
H	0	-0.097012	0.952056	-0.615746
H	0	-3.611038	-0.803282	-0.357121
H	0	1.208945	-1.677732	-1.412871
H	0	0.192759	-1.036241	1.589104
H	0	-2.066404	1.856067	-0.395336
H	0	-3.891578	1.615810	-0.327756
H	0	2.207691	1.205998	-1.574216
H	0	3.035560	-0.168370	-2.275018
H	0	2.608120	-1.010815	1.834713
H	0	0.175572	0.644833	-3.139965
H	0	1.119879	-0.726533	-3.742280
H	0	-0.495965	-0.995481	-3.075565
H	0	3.891578	0.597353	0.053015
H	0	3.641235	-1.113797	-0.228900
H	0	0.543100	2.790592	1.463681
H	0	2.301367	2.766459	1.639680
H	0	1.564595	2.287238	0.111404
H	0	1.191375	-0.257209	3.618316
H	0	2.069978	1.275655	3.742280
H	0	0.307122	1.275941	3.560098

Energy + ZPE = -3065.590421
Free energy = -3065.634796
Free energy in DCM = -3065.878492
Free energy in heptane = -3065.881694
Number of imaginary frequencies = 0

Vinylborane 18a

C	0	-1.119415	-1.162933	0.076510
C	0	-1.130475	0.378409	0.120860
C	0	0.323861	0.921208	0.095436
C	0	1.079565	0.481649	-1.203417
C	0	0.752866	-0.910501	-1.740110
C	0	-0.366670	-1.732771	-1.122196
C	0	-1.907623	0.868180	1.350956
C	0	1.073532	-2.223103	-1.052497
C	0	1.836617	-2.269175	0.259776
C	0	1.430044	-3.385777	-1.968819
Cl	0	-0.488554	3.517792	-0.914527
B	0	0.431780	2.490574	0.240259
C	0	1.303156	3.258359	1.266210
C	0	2.058915	2.658950	2.202563
H	0	-0.701932	-1.536353	1.022774
H	0	-2.155255	-1.523409	0.047446
H	0	-1.643255	0.743569	-0.780446
H	0	0.835211	0.471295	0.958805
H	0	2.161480	0.587918	-1.043337
H	0	0.823038	1.188526	-2.002002
H	0	0.817783	-0.953654	-2.827005
H	0	-0.996667	-2.273952	-1.826331
H	0	-1.403636	0.569865	2.279851
H	0	-2.012537	1.959413	1.363302
H	0	-2.917677	0.441404	1.372186
H	0	1.641326	-3.212267	0.787456

H	0	2.917677	-2.216412	0.075857
H	0	1.581390	-1.454614	0.940958
H	0	0.867951	-3.345620	-2.908774
H	0	2.499127	-3.378468	-2.220166
H	0	1.208658	-4.348769	-1.489504
H	0	1.315038	4.348769	1.233253
H	0	2.666780	3.222068	2.908774
H	0	2.103262	1.576949	2.304425

Energy + ZPE = -954.081976
Free energy = -954.125302
Free energy in DCM = -954.371210
Free energy in heptane = -954.374219
Number of imaginary frequencies = 0

Vinylborane 18b

C	0	-1.116433	-1.168420	0.087917
C	0	-1.121185	0.372149	0.140481
C	0	0.335845	0.909328	0.130874
C	0	1.090029	0.479922	-1.172050
C	0	0.764177	-0.908001	-1.718830
C	0	-0.358480	-1.732765	-1.110306
C	0	-1.912872	0.865506	1.359338
C	0	1.080711	-2.225369	-1.038280
C	0	1.839999	-2.280487	0.275866
C	0	1.437433	-3.383350	-1.960319
Br	0	-0.581919	3.568364	-0.967373
B	0	0.446442	2.475894	0.278083
C	0	1.323606	3.258679	1.282766
C	0	2.098636	2.668128	2.209603
H	0	-0.707325	-1.550256	1.034453
H	0	-2.153690	-1.524034	0.049264
H	0	-1.618221	0.747337	-0.765396
H	0	0.843745	0.454202	0.993980
H	0	2.172423	0.588437	-1.016362
H	0	0.824691	1.195525	-1.959962
H	0	0.833739	-0.944135	-2.805744
H	0	-0.986204	-2.269103	-1.820242
H	0	-1.418317	0.577912	2.296562
H	0	-2.021175	1.956258	1.355163
H	0	-2.921378	0.434773	1.372338
H	0	1.647518	-3.229549	0.793782
H	0	2.921378	-2.220862	0.095761
H	0	1.578814	-1.473783	0.963894
H	0	0.881978	-3.332949	-2.903746
H	0	2.508223	-3.380765	-2.204496
H	0	1.206868	-4.348410	-1.489592
H	0	1.324676	4.348410	1.241526
H	0	2.713962	3.238138	2.903746
H	0	2.151104	1.586779	2.314644

Energy + ZPE = -3065.590106
Free energy = -3065.634015
Free energy in DCM = -3065.879002
Free energy in heptane = -3065.882207
Number of imaginary frequencies = 0

Vinylborane 19a

C	0	1.408487	3.279371	-0.716203
C	0	1.400700	4.601564	-0.949809
B	0	0.159818	2.362449	-0.654930
C	0	0.235477	0.860113	-0.187851
O	0	0.374310	0.634875	-3.053997
C	0	-0.668764	-0.135387	-0.979194
C	0	0.070039	0.741400	1.374797
C	0	0.022094	-0.522121	-2.289952
C	0	-1.131765	-1.323105	-0.109483
C	0	-0.580661	-0.587867	1.803523
C	0	-0.088865	-1.820903	0.963882
C	0	-1.942034	-0.711847	1.069707
C	0	-0.550741	-3.151223	1.592867
C	0	1.400103	-1.994439	0.633622
Cl	0	-1.453044	3.094476	-1.011242
H	0	2.378780	2.807864	-0.544058
H	0	2.312806	5.195467	-0.969546
H	0	0.473806	5.140713	-1.131655
H	0	1.269496	0.569424	-0.404781
H	0	-0.451215	1.078775	-3.307580
H	0	-1.595333	0.381248	-1.271900
H	0	-0.555595	1.552474	1.771828
H	0	1.055764	0.859694	1.841390
H	0	0.966232	-1.044746	-2.106010
H	0	-0.621527	-1.196667	-2.876789
H	0	-1.616549	-2.094964	-0.722554
H	0	-0.569408	-0.687747	2.896492
H	0	-2.634064	-1.411590	1.541884
H	0	-2.476196	0.222251	0.862597
H	0	-0.371447	-3.982403	0.898953
H	0	0.018719	-3.358493	2.507711
H	0	-1.611815	-3.167777	1.855208
H	0	1.885940	-1.099942	0.244006
H	0	1.949633	-2.296416	1.534784
H	0	1.536807	-2.794515	-0.105709

Energy + ZPE = -1029.275086
Free energy = -1029.318857
Free energy in DCM = -1029.576889
Free energy in heptane = -1029.576554
Number of imaginary frequencies = 0

Vinylborane 20a

C	0	-1.604453	2.284903	2.359076
C	0	-1.604453	3.683405	2.359076
C	0	-2.830807	1.606997	2.359076
C	0	-0.302109	1.505206	2.399988
C	0	-4.031128	2.316227	2.363242
C	0	-2.805402	4.396394	2.372871
O	0	-0.302283	0.343820	1.584438
C	0	-4.022146	3.713687	2.373895
C	0	-0.232618	0.603524	0.184386
C	0	-0.214850	-0.748980	-0.523598
C	0	0.988683	-1.618427	-0.019877

C	0	-0.259109	-0.650838	-2.062928
B	0	0.682180	-2.478229	1.265899
C	0	1.621984	-2.526616	-1.144432
C	0	1.143377	-0.575210	-2.778282
C	0	-0.372990	-2.108236	-2.593489
C	0	1.625550	-2.644518	2.486768
C	0	1.177679	-2.128663	-2.562612
C	0	0.976727	-0.211480	-4.266839
C	0	2.283363	0.297772	-2.237616
Cl	0	-0.805785	-3.490321	1.300962
C	0	2.826386	-2.052128	2.592792
H	0	-0.657816	4.220339	2.348288
H	0	-2.833541	0.520563	2.345785
H	0	0.539262	2.164800	2.131277
H	0	-0.116384	1.134876	3.415457
H	0	-4.975820	1.778470	2.360135
H	0	-2.789134	5.483242	2.373559
H	0	-4.958297	4.265727	2.379023
H	0	0.672269	1.192625	-0.037308
H	0	-1.103389	1.192371	-0.140216
H	0	-1.153603	-1.239389	-0.235112
H	0	1.767554	-0.908682	0.277624
H	0	-1.016760	0.075555	-2.385735
H	0	1.349317	-3.581164	-1.002706
H	0	2.714541	-2.480892	-1.053741
H	0	-0.793850	-2.181053	-3.598133
H	0	-0.888715	-2.823902	-1.944150
H	0	1.313945	-3.297331	3.303482
H	0	1.705034	-2.729213	-3.315048
H	0	0.743864	0.855689	-4.374827
H	0	1.909011	-0.402003	-4.813661
H	0	0.182245	-0.772008	-4.766885
H	0	2.544723	0.101466	-1.197245
H	0	3.189989	0.141878	-2.837091
H	0	2.025861	1.361829	-2.319883
H	0	3.478728	-2.204856	3.451065
H	0	3.213193	-1.387227	1.823242

Energy + ZPE = -1299.527344
Free energy = -1299.581789
Free energy in DCM = -1299.932490
Free energy in heptane = -1299.935060
Number of imaginary frequencies = 0

Vinylborane 21a

Cl	0	2.316796	-2.615442	0.473216
B	0	2.316796	-0.818333	0.473216
C	0	3.677039	-0.074502	0.473216
C	0	0.944080	-0.053077	0.310758
C	0	4.885071	-0.659819	0.425502
C	0	-0.277561	-0.608403	1.117372
C	0	0.688056	0.063721	-1.252059
C	0	-1.571177	-0.646599	0.262630
C	0	-0.778738	-0.168339	-1.644237
C	0	-0.530397	0.153115	2.413577
C	0	-1.777275	0.582695	-0.699143
C	0	-1.249115	-1.497380	-0.999153
I	0	1.169234	0.038719	3.847219
C	0	-3.208215	0.593798	-1.269804
C	0	-1.460092	2.017308	-0.258391
H	0	3.650090	1.017006	0.507164
H	0	1.123069	0.968423	0.665067
H	0	5.810674	-0.086951	0.419623
H	0	4.990141	-1.741812	0.392883
H	0	-0.083753	-1.652169	1.391466
H	0	1.290662	-0.667880	-1.807558
H	0	1.026931	1.051203	-1.586917
H	0	-2.431628	-0.944829	0.875336
H	0	-0.913087	-0.038062	-2.725555
H	0	-0.680144	1.222845	2.276148
H	0	-1.362335	-0.267333	2.978658
H	0	-0.498570	-2.286152	-0.882556
H	0	-2.136262	-1.923626	-1.471592
H	0	-3.275157	1.284960	-2.119446
H	0	-3.546588	-0.386977	-1.615858
H	0	-3.919956	0.937498	-0.508354
H	0	-2.153974	2.344842	0.526704
H	0	-0.444250	2.157325	0.115686
H	0	-1.590367	2.704228	-1.104820

Energy + ZPE = -964.852523
Free energy = -964.898607
Free energy in DCM = -965.146774
Free energy in heptane = -965.144437
Number of imaginary frequencies = 0

Vinylborane 22a

Cl	0	1.445446	-2.486408	-0.906736
B	0	1.551525	-0.702601	-0.669514
C	0	2.983006	-0.150917	-0.447831
C	0	0.244378	0.166207	-0.831883
C	0	3.261076	1.144484	-0.225022
C	0	-1.034438	-0.367529	-0.090662
C	0	0.036403	0.404576	-2.385894
C	0	-2.295489	-0.261842	-0.972927
C	0	-1.432452	0.302210	-2.824332
C	0	-1.228056	0.295339	1.296513
C	0	-2.401784	1.047613	-1.844745
C	0	-2.007030	-1.035013	-2.289999
C	0	-0.045390	0.161847	2.235905
C	0	-3.814596	1.195026	-2.440197
C	0	-2.000780	2.424007	-1.299352
C	0	0.632447	1.295174	2.704941
C	0	0.400707	-1.098292	2.665089
C	0	1.492031	-1.219541	3.525876
C	0	1.723916	1.179570	3.568091
C	0	2.159175	-0.080046	3.980391
H	0	3.821363	-0.848567	-0.467492
H	0	0.464293	1.148544	-0.400628
H	0	4.277231	1.504317	-0.072381
H	0	2.483254	1.902998	-0.177099
H	0	-0.905520	-1.442052	0.092988

H	0	0.602396	-0.327035	-2.978657
H	0	0.450906	1.386592	-2.644231
H	0	-3.188691	-0.542131	-0.398819
H	0	-1.530085	0.521640	-3.895564
H	0	-1.465733	1.357815	1.172981
H	0	-2.112866	-0.163958	1.760587
H	0	-1.313247	-1.879494	-2.220568
H	0	-2.907400	-1.363454	-2.813408
H	0	-3.818251	1.949598	-3.237233
H	0	-4.205180	0.266196	-2.864981
H	0	-4.521644	1.526924	-1.669071
H	0	-2.696094	2.749724	-0.515079
H	0	-0.992097	2.463383	-0.885407
H	0	-2.052810	3.171363	-2.102350
H	0	0.295391	2.282032	2.394309
H	0	-0.113315	-1.994155	2.324679
H	0	1.819513	-2.205937	3.844036
H	0	2.231327	2.074498	3.919624
H	0	3.008298	-0.174146	4.652076

Energy + ZPE = -1185.040509
Free energy = -1185.089684
Free energy in DCM = -1185.414037
Free energy in heptane = -1185.416246
Number of imaginary frequencies = 0

Diels-Alder reaction with Vinylborane (10)

TS 10+cpN

C	0	-0.915637	-0.507129	2.626091
C	0	-0.985131	0.880636	2.577049
C	0	-2.326612	-1.030609	2.567725
C	0	-2.264660	1.262568	2.140424
C	0	-3.011102	0.106919	1.832245
H	0	-0.071912	-1.083591	2.984584
H	0	-0.157602	1.557840	2.757523
H	0	-2.455824	-2.026215	2.141694
H	0	-2.723552	-1.051976	3.597620
H	0	-2.577985	2.281267	1.936339
H	0	-4.089159	0.131712	1.697842
C	0	-1.076502	-1.000110	0.125176
B	0	0.290365	-0.359923	-0.184042
C	0	-2.340477	-0.401443	-0.032699
C	0	0.395278	1.196002	-0.537811
C	0	1.581426	-1.307073	-0.307486
C	0	0.367901	1.372154	-2.084461
C	0	1.628434	1.932576	0.035776
C	0	1.980805	-1.995225	1.023395
C	0	1.392096	-2.386724	-1.407659
C	0	0.411912	2.851573	-2.502280
C	0	1.669248	3.414002	-0.373077
C	0	2.630520	-3.284695	-1.563872
C	0	3.218204	-2.895282	0.871319
C	0	1.623428	3.577437	-1.899526
C	0	3.021162	-3.943698	-0.232958
H	0	-1.105830	-2.073135	0.325846
H	0	-3.198194	-1.041376	-0.238873
H	0	-2.410401	0.569055	-0.516652
H	0	-0.495411	1.720588	-0.153662
H	0	2.450384	-0.703268	-0.615552
H	0	1.231018	0.851075	-2.526470
H	0	-0.526838	0.894776	-2.505742
H	0	1.644555	1.852784	1.131546
H	0	2.548786	1.445071	-0.316630
H	0	2.170557	-1.239876	1.798626
H	0	1.139311	-2.604877	1.385686
H	0	1.157476	-1.911153	-2.369662
H	0	0.524368	-3.015363	-1.159853
H	0	0.426227	2.933740	-3.597620
H	0	-0.510827	3.346575	-2.163924
H	0	2.569121	3.895791	0.032687
H	0	0.808626	3.93658	0.071546
H	0	3.473328	-2.677458	-1.926845
H	0	2.447795	-4.052225	-2.328177
H	0	4.089159	-2.270052	0.624355
H	0	3.448576	-3.387294	1.826218
H	0	2.544843	3.160817	-2.333754
H	0	1.604699	4.641195	-2.17103
H	0	2.225598	-4.641195	0.070672
H	0	3.931776	-4.544762	-0.355961

Energy + ZPE = -767.013956
Free energy = -767.062266
Free energy in DCM = -767.471641
Free energy in heptane = -767.475698
Number of imaginary frequencies = 1 (-426.56)

TS 10+cpX

C	0	3.712156	1.006260	2.588110
C	0	3.712156	2.412362	2.588110
C	0	2.398621	0.549769	2.588110
C	0	2.384036	2.871534	2.495167
C	0	1.513950	1.712052	2.940005
H	0	4.594864	0.379646	2.513430
H	0	4.596855	3.037770	2.524372
H	0	2.094904	-0.487496	2.657954
H	0	2.105002	3.903817	2.688197
H	0	0.504957	1.685426	2.530761
H	0	1.431430	1.758894	4.039861
C	0	2.070111	1.314982	0.168283
C	0	1.950913	2.678573	0.485294
B	0	0.927773	0.315666	-0.089827
C	0	1.272167	-1.064759	-0.835273
C	0	-0.603158	0.669428	0.218754
C	0	2.287066	-1.964359	-0.085416
C	0	1.794101	-0.788580	-2.273537
C	0	-1.312652	-0.372706	1.120483
C	0	-1.395698	0.829212	-1.108990
C	0	2.603940	-3.258650	-0.853460
C	0	2.107131	-2.082767	-3.042292
C	0	-2.792501	-0.029519	1.359914

C	0	-2.875364	1.172199	-0.870771
C	0	3.102021	-2.965993	-2.276137
C	0	-3.554785	0.137292	0.037345
H	0	3.079248	1.004516	-0.107061
H	0	2.708997	3.375038	0.134865
H	0	0.957135	3.120737	0.54244
H	0	0.352346	-1.661759	-0.949987
H	0	-0.679111	1.641203	0.735169
H	0	1.902143	-2.218842	0.911883
H	0	3.221496	-1.407857	0.078740
H	0	1.062114	-0.193681	-2.836127
H	0	2.705675	-0.175857	-2.217610
H	0	-0.795200	-0.457751	2.086489
H	0	-1.249496	-1.366153	0.652996
H	0	-1.336488	-0.106675	-1.683889
H	0	-0.932309	1.604648	-1.733814
H	0	1.694310	-3.875080	-0.910346
H	0	3.348061	-3.851821	-0.304530
H	0	1.173653	-2.643429	-3.200390
H	0	2.500298	-1.844103	-4.039861
H	0	-2.857758	0.907289	1.933902
H	0	-3.266242	-0.805608	1.976079
H	0	-3.405469	1.242364	-1.830202
H	0	-2.945141	2.165415	-0.402390
H	0	3.278948	-3.903817	-2.819121
H	0	4.072626	-2.450206	-2.219679
H	0	-4.596855	0.423763	0.230909
H	0	-3.588967	-0.831704	-0.482997

Energy + ZPE = -767.013791
Free energy = -767.062128
Free energy in DCM = -767.471297
Free energy in heptane = -767.475368
Number of imaginary frequencies = 1 (-422.46)

Product 10+cpN

C	0	0.000000	0.000000	0.000000
C	0	0.000000	1.519837	0.000000
C	0	-1.525070	-0.267578	0.000000
C	0	0.355972	-0.513595	-1.477035
C	0	-1.068329	1.924958	-0.701950
C	0	-1.790909	0.679535	-1.191131
B	0	1.825470	-0.144638	-1.955795
C	0	-0.867767	0.037293	-2.289810
C	0	2.168838	1.278031	-2.583709
C	0	2.969604	-1.253326	-1.843399
C	0	2.516113	1.122895	-4.092208
C	0	3.326004	2.015473	-1.861068
C	0	3.109695	-1.869995	-0.427688
C	0	2.727051	-2.390152	-2.878524
C	0	2.842300	2.473862	-4.750656
C	0	3.652542	3.366288	-2.519546
C	0	3.824234	-3.466003	-2.821151
C	0	4.207428	-2.944580	-0.368591
C	0	3.973724	3.203431	-4.012176
C	0	3.972809	-4.049804	-1.408752
H	0	0.588882	-0.482971	0.782898
H	0	0.789535	2.141999	0.410523
H	0	-1.785034	-1.314254	-0.199020
H	0	-2.012009	0.066635	0.922120
H	0	0.258392	-1.606155	-1.418228
H	0	-1.321579	2.941925	-0.986007
H	0	-2.829788	0.815323	-1.502731
H	0	-1.388718	-0.779907	-2.802627
H	0	-0.590973	0.774231	-3.050476
H	0	1.288589	1.934754	-2.527511
H	0	3.947052	-0.810867	-2.095016
H	0	3.382538	0.454514	-4.203201
H	0	1.685898	0.644013	-4.629791
H	0	3.072372	2.175507	-0.804092
H	0	4.229295	1.388672	-1.868805
H	0	3.325638	-1.084655	0.309739
H	0	2.153717	-2.322067	-0.125381
H	0	2.670776	-1.978317	-3.895004
H	0	1.753448	-2.863144	-2.683334
H	0	3.111511	2.322800	-5.804596
H	0	1.940414	3.103577	-4.744538
H	0	4.493500	3.844788	-2.000045
H	0	2.790634	4.040467	-2.406540
H	0	4.780899	-3.021164	-3.132415
H	0	3.602936	-4.265091	-3.541336
H	0	5.183578	-2.472885	-0.555496
H	0	4.258133	-3.376892	0.639634
H	0	4.904663	2.626633	-4.119644
H	0	4.159317	4.182953	-4.471679
H	0	3.056366	-4.600799	-1.148666
H	0	4.792450	-4.779586	-1.382476

Energy + ZPE = -767.059079
Free energy = -767.106476
Free energy in DCM = -767.520853
Free energy in heptane = -767.525416
Number of imaginary frequencies = 0

Product 10+cpX

C	0	0.000000	0.000000	0.000000
C	0	0.000000	1.341445	0.000000
C	0	-1.449883	-0.457480	0.000000
C	0	-1.449648	1.797722	0.001996
C	0	-1.993218	-0.108236	-1.475859
C	0	-2.089353	0.669471	0.841366
C	0	-2.040670	1.455491	-1.412827
B	0	-3.330124	-0.902024	-1.805100
C	0	-3.232400	-2.206311	-2.720467
C	0	-4.755177	-0.462209	-1.240867
C	0	-2.139144	-3.217019	-2.290780
C	0	-2.996453	-1.783333	-4.200604
C	0	-5.258396	-1.490845	-0.188173
C	0	-5.823072	-0.293167	-2.354432
C	0	-2.065435	-4.429059	-3.233392
C	0	-2.921493	-2.996552	-5.142485
C	0	-6.639259	-1.116313	0.375900

C	0	-7.200893	0.083048	-1.785279
C	0	-1.849316	-3.998687	-4.691423
C	0	-7.677412	-0.936293	-0.740804
H	0	0.854554	-0.660313	-0.113949
H	0	0.857793	1.998595	-0.106285
H	0	-1.626327	-1.485509	0.325685
H	0	-1.632787	2.826081	0.324462
H	0	-1.211181	-0.416856	-2.178812
H	0	-3.183738	0.675212	0.824095
H	0	-1.738222	0.662364	1.878269
H	0	-1.462675	1.915791	-2.220673
H	0	-3.064390	1.841432	-1.483187
H	0	-4.191660	-2.749112	-2.703715
H	0	-4.687936	0.508710	-0.726063
H	0	-2.325307	-3.562611	-1.264664
H	0	-1.158900	-2.718943	-2.274787
H	0	-3.792574	-1.106294	-4.538298
H	0	-2.056833	-1.216104	-4.274357
H	0	-4.537892	-1.576747	0.636760
H	0	-5.319966	-2.487552	-0.649080
H	0	-5.916532	-1.229696	-2.922684
H	0	-5.501523	0.472620	-3.073523
H	0	-3.003025	-5.000126	-3.160304
H	0	-1.262294	-5.106631	-2.914358
H	0	-3.900710	-3.497459	-5.161824
H	0	-2.721539	-2.661599	-6.169084
H	0	-6.553690	-0.179000	0.945440
H	0	-6.973748	-1.883717	1.086679
H	0	-7.933871	0.164917	-2.598875
H	0	-7.139695	1.077556	-1.318835
H	0	-1.845881	-4.875439	-5.352041
H	0	-0.857042	-3.532353	-4.787212
H	0	-8.642267	-0.627577	-0.318042
H	0	-7.848011	-1.905087	-1.234135

Energy + ZPE = -767.058909
Free energy = -767.106350
Free energy in DCM = -767.520813
Free energy in heptane = -767.525343
Number of imaginary frequencies = 0

Diels-Alder reaction with Vinylborane (11a)

TS 11a+cpN

C	0	2.074846	1.437986	-0.362010
C	0	2.074846	2.975005	-0.362010
C	0	0.633990	0.854261	-0.362010
C	0	1.262768	3.540620	-1.536107
C	0	-0.166766	1.439569	-1.549511
B	0	0.675658	-0.728914	-0.296493
C	0	-0.165540	2.976398	-1.550224
Cl	0	1.165702	-1.622884	-1.805285
C	0	0.438121	-1.532228	0.969477
C	0	0.551129	-2.924114	1.122105
H	0	2.607562	1.075229	-1.252458
H	0	2.634052	1.065739	0.506658
H	0	3.106384	3.350081	-0.397829
H	0	1.643608	3.336444	0.583717
H	0	0.150405	1.203384	0.566780
H	0	1.763550	3.277828	-2.479933
H	0	1.239285	4.637346	-1.490301
H	0	0.268376	1.074984	-2.489961
H	0	-1.201483	1.070094	-1.526696
H	0	-0.705828	3.340616	-0.663193
H	0	-0.713478	3.353019	-2.424238
H	0	0.217078	-0.962025	1.873148
H	0	0.704683	-3.329712	2.121318
H	0	1.048766	-3.490333	0.340391
C	0	-2.006394	-2.327285	-0.770191
C	0	-1.584196	-3.625708	-0.436127
C	0	-2.098280	-1.568913	0.388753
C	0	-1.328657	-3.691051	0.948788
C	0	-2.070366	-2.514111	1.559332
H	0	-2.139649	-1.954996	-1.779313
H	0	-1.355013	-4.408709	-1.150891
H	0	-2.438375	-0.541488	0.447428
H	0	-1.231366	-4.637346	1.474001
H	0	-3.106384	-2.837677	1.759962
H	0	-1.662634	-2.117743	2.489961

Energy + ZPE = -992.147909
Free energy = -992.190370
Free energy in DCM = -992.451907
Free energy in heptane = -992.452819
Number of imaginary frequencies = 1 (-404.86)

TS 11a+cpX

C	0	-1.094232	0.174633	0.430982
C	0	-1.094232	1.722814	0.430982
C	0	-2.557899	-0.349499	0.430982
B	0	-0.260151	-0.491810	-0.739929
C	0	-3.379035	0.231725	1.593306
C	0	-1.915820	2.302291	1.593625
C	0	0.743027	-1.610862	-0.524162
Cl	0	-0.634435	0.053461	-2.439895
C	0	-3.355255	1.766993	1.590141
C	0	1.406964	-2.384965	-1.488387
H	0	-0.638861	-0.153813	1.380654
H	0	-1.506081	2.083994	-0.521080
H	0	-0.063871	2.101771	0.482922
H	0	-2.566594	-1.446446	0.481129
H	0	-3.034920	-0.078318	-0.521346
H	0	-2.967247	-0.134855	2.545653
H	0	-4.413607	-0.132673	1.539938
H	0	-1.434085	2.035686	2.546544
H	0	-1.918437	3.399266	1.542205
H	0	0.875547	-1.927548	0.510968
H	0	-3.910063	2.158927	2.452667
H	0	-3.873916	2.133471	0.691769
H	0	1.708001	-3.399266	-1.239129
H	0	1.130274	-2.254141	-2.532717

C	0	2.657434	0.145803	-0.299488
C	0	3.408675	-0.752594	0.448636
C	0	2.882392	-0.159062	-1.75118
C	0	3.302859	-1.613811	-1.674715
C	0	3.853204	-1.790871	-0.389508
H	0	2.235292	1.074081	0.067529
H	0	3.562934	-0.703442	1.521507
H	0	2.052221	0.069245	-2.419249
H	0	3.757035	0.422555	-2.090613
H	0	3.666400	-2.150676	-2.546544
H	0	4.413607	-2.661099	-0.063086

Energy + ZPE = -992.147619
Free energy = -992.190174
Free energy in DCM = -992.450514
Free energy in heptane = -992.451956
Number of imaginary frequencies = 1 (-405.55)

Product 11a+cpN

C	0	1.880995	0.829451	-0.982607
C	0	1.880995	2.366130	-0.982607
C	0	0.446285	0.254066	-0.982607
C	0	1.077098	2.931758	-2.162511
C	0	-0.359056	0.834209	-2.187065
B	0	0.314408	-1.313910	-1.018212
C	0	-0.352304	2.371479	-2.184894
Cl	0	1.445345	-2.234845	-2.078167
C	0	-0.735350	-2.186624	-0.237659
C	0	-0.083393	-2.880188	1.050824
C	0	-2.000104	-1.501308	0.380644
C	0	0.357428	-1.770081	1.993343
C	0	-1.947042	-1.924548	1.891859
C	0	-1.369108	-3.352649	1.768618
C	0	-0.749993	-1.204093	2.495494
H	0	2.419049	0.464686	-1.867384
H	0	2.434590	0.456617	-0.110686
H	0	2.912699	2.740081	-1.013029
H	0	1.445290	2.730006	-0.039917
H	0	-0.056203	0.606779	-0.068422
H	0	1.582525	2.667067	-3.103140
H	0	1.054176	4.028284	-2.118386
H	0	0.086084	0.471128	-3.124244
H	0	-1.394474	0.468197	-2.171580
H	0	-0.898321	2.732367	-1.300747
H	0	-0.895265	2.746035	-3.062669
H	0	-1.050597	-3.013073	-0.888106
H	0	0.664133	-3.635221	0.800827
H	0	-2.912699	-1.880913	-0.093287
H	0	-2.007517	-0.412409	0.274035
H	0	1.384336	-1.445371	2.133141
H	0	-2.896147	-1.811051	2.421590
H	0	-1.162360	-3.811294	2.741024
H	0	-1.984358	-4.028284	1.162440
H	0	-0.810038	-0.320887	3.124244

Energy + ZPE = -992.191002
Free energy = -992.233115
Free energy in DCM = -992.506733
Free energy in heptane = -992.499680
Number of imaginary frequencies = 0

Product 11a+cpX

C	0	0.000000	0.000000	0.000000
C	0	0.000000	1.544387	0.000000
C	0	-1.467556	-0.530311	0.000000
B	0	0.780386	-0.719060	-1.167276
C	0	-2.279112	0.049250	1.170429
C	0	-0.811794	2.118359	1.171990
C	0	1.560580	-2.061196	-0.924430
Cl	0	0.745953	0.028775	-2.800986
C	0	-2.251754	1.584618	1.175300
C	0	3.065156	-1.740339	-0.441128
C	0	1.819757	-3.056186	-2.098870
C	0	3.559573	-3.029340	0.194666
C	0	3.379604	-3.235394	-2.099657
C	0	3.818279	-1.785840	-1.788544
C	0	3.748260	-3.917639	-0.791928
H	0	0.449520	-0.339508	0.948939
H	0	-0.422450	1.905615	-0.946928
H	0	1.030271	1.922051	0.039108
H	0	-1.480945	-1.627544	0.046436
H	0	-1.950137	-0.250887	-0.947480
H	0	-3.314059	-0.313641	1.118973
H	0	-1.862236	-0.325240	2.116919
H	0	-0.322854	1.847590	2.119913
H	0	-0.813652	3.215054	1.125300
H	0	1.059386	-2.568426	-0.089729
H	0	-2.776219	1.956957	0.282768
H	0	-2.800800	1.970432	2.043759
H	0	3.169237	-0.835451	0.163115
H	0	1.296932	-4.006723	-1.953856
H	0	1.495847	-2.640060	-3.057879
H	0	3.618510	-3.205243	1.264490
H	0	3.773009	-3.691827	-3.011315
H	0	3.462864	-1.054114	-2.521483
H	0	4.900933	-1.688323	-1.660850
H	0	4.001451	-4.968436	-0.689418

Energy + ZPE = -992.191066
Free energy = -992.233223
Free energy in DCM = -992.497432
Free energy in heptane = -992.499930
Number of imaginary frequencies = 0

Diels-Alder reaction with Vinylborane (11b)

TS 11b+cpN

C	0	2.098968	1.480191	-0.329394
C	0	2.128553	3.014505	-0.410418

C	0	0.652579	0.924131	-0.208832
C	0	1.252329	3.537903	-1.557485
C	0	-0.219654	1.476899	-1.363766
B	0	0.665585	-0.654516	-0.111167
C	0	-0.185214	3.010821	-1.442854
Br	0	1.194491	-1.638029	-1.746609
C	0	0.388367	-1.473987	1.128693
C	0	0.511576	-2.869772	1.250105
H	0	2.565878	1.056358	-1.229343
H	0	2.704871	1.140873	0.521419
H	0	3.163030	3.362315	-0.532712
H	0	1.768380	3.435040	0.540567
H	0	0.235014	1.309627	0.737237
H	0	1.680820	3.210873	-2.516522
H	0	1.256837	4.635733	-1.570849
H	0	0.137217	1.051483	-2.311432
H	0	-1.257816	1.135807	-1.246626
H	0	-0.653083	3.432223	-0.540206
H	0	-0.785952	3.356347	-2.294856
H	0	0.116524	-0.927438	2.033552
H	0	0.616778	-3.298366	2.246197
H	0	1.070291	-3.398930	0.483761
C	0	-1.978373	-2.263668	-0.757911
C	0	-1.510947	-3.555698	-0.456497
C	0	-2.165312	-1.563536	0.423308
C	0	-1.316759	-3.669588	0.935857
C	0	-2.136920	-2.550352	1.557829
H	0	-2.075417	-1.855208	-1.756801
H	0	-1.213345	-4.295439	-1.191525
H	0	-2.544983	-0.551874	0.507361
H	0	-1.215676	-4.635733	1.423151
H	0	-3.163030	-2.927631	1.708708
H	0	-1.782181	-2.169604	2.516522

Energy + ZPE = -3103.658833
Free energy = -3103.702473
Free energy in DCM = -3103.962277
Free energy in heptane = -3103.963437
Number of imaginary frequencies = 1 (-394.40)

TS 11b+cpX

C	0	-1.112507	0.117410	0.516418
C	0	-1.045373	1.665884	0.506949
C	0	-2.595242	-0.344636	0.461565
B	0	-0.262160	-0.563694	-0.630149
C	0	-3.444694	0.289570	1.573715
C	0	-1.897836	2.295581	1.619099
C	0	0.784032	-1.637356	-0.429378
Br	0	-0.704203	-0.012281	-2.483405
C	0	-3.356730	1.822271	1.549153
C	0	1.441066	-2.385366	-1.421415
H	0	-0.698838	-0.227312	1.479498
H	0	-1.387561	2.029519	-0.471250
H	0	-0.002781	1.998163	0.609921
H	0	-2.651226	-1.439338	0.528957
H	0	-3.012918	-0.073803	-0.518066
H	0	-3.095535	-0.076948	2.550781
H	0	-4.489779	-0.033110	1.475320
H	0	-1.476460	2.022380	2.598443
H	0	-1.849670	3.390783	1.553949
H	0	0.961948	-1.945309	0.601763
H	0	-3.937380	2.251184	2.376355
H	0	-3.812561	2.195283	0.619901
H	0	1.783070	-3.390783	-1.189061
H	0	1.104429	-2.263557	-2.449430
C	0	2.715165	0.173323	-0.255821
C	0	3.504190	-0.737035	0.433811
C	0	2.848374	-0.106714	-1.722047
C	0	3.283135	-1.560228	-1.697731
C	0	3.907455	-1.756070	-0.448510
H	0	2.297453	1.085921	0.153060
H	0	3.716420	-0.708460	1.497460
H	0	1.973245	0.130730	-2.327218
H	0	3.695335	0.485642	-2.109846
H	0	3.611202	-2.071993	-2.598443
H	0	4.489779	-2.628857	-0.170733

Energy + ZPE = -3103.658734
Free energy = -3103.702282
Free energy in DCM = -3103.961258
Free energy in heptane = -3103.962831
Number of imaginary frequencies = 1 (-401.21)

Product 11b+cpN

C	0	1.944383	1.563171	-0.040738
C	0	1.995955	3.099015	-0.022509
C	0	0.495115	1.033996	-0.257022
C	0	1.380581	3.701714	-1.293572
C	0	-0.107238	1.658374	-1.540374
B	0	0.496466	-0.542548	-0.228042
C	0	-0.051276	3.193327	-1.515988
Br	0	1.251323	-1.456406	-1.771925
C	0	-0.078210	-1.377222	0.966865
C	0	0.294122	-2.880047	1.168230
C	0	-2.053208	-2.225950	-0.352195
C	0	-1.708534	-3.504707	-0.145858
C	0	-1.682514	-1.446526	0.899923
C	0	-1.099722	-3.598608	1.244987
C	0	-1.934944	-2.525091	1.978991
H	0	2.582322	1.182786	-0.850398
H	0	2.360868	1.167156	0.895557
H	0	3.035411	3.433226	0.093009
H	0	1.448830	3.468954	0.857252
H	0	-0.105190	1.384477	0.599688
H	0	1.999844	3.425000	-2.159653
H	0	1.392643	4.797823	-1.237875
H	0	0.444539	1.282947	-2.412014
H	0	-1.146480	1.326488	-1.668299
H	0	-0.698422	3.568526	-0.709049
H	0	-0.456551	3.596618	-2.453129
H	0	0.150162	-0.813574	1.884488
H	0	0.847111	-3.018575	2.104676

H	0	0.909795	-3.274843	0.356115
H	0	-2.412433	-1.783616	-1.276136
H	0	-1.729195	-4.313825	-0.869137
H	0	-2.167611	-0.476921	1.034927
H	0	-1.064788	-4.596035	1.690186
H	0	-2.993113	-2.793367	2.062911
H	0	-1.540027	-2.255735	2.966125

Energy + ZPE = -3103.699526
Free energy = -3103.742661
Free energy in DCM = -3104.005536
Free energy in heptane = -3104.008024
Number of imaginary frequencies = 0

Product 11b+cpX

C	0	-0.758240	0.631797	0.470650
C	0	-0.472117	2.153817	0.543246
C	0	-2.291019	0.385662	0.345236
B	0	0.008983	-0.114822	-0.686243
C	0	-3.077055	1.077083	1.470259
C	0	-1.262872	2.836762	1.668991
C	0	0.935405	-1.357088	-0.450574
Br	0	-0.201215	0.612237	-2.486965
C	0	-2.770818	2.580046	1.534735
C	0	2.409800	-0.839233	-0.043906
C	0	1.264077	-2.335578	-1.620671
C	0	3.102618	-2.044171	0.569555
C	0	2.831207	-2.297839	-1.711151
C	0	3.087807	-0.798927	-1.431360
C	0	3.358492	-2.909149	-0.422852
H	0	-0.437066	0.185698	1.426913
H	0	-0.732061	2.611634	-0.420108
H	0	0.603017	2.328330	0.685888
H	0	-2.506114	-0.691624	0.350297
H	0	-2.630281	0.765714	-0.628201
H	0	-4.152864	0.913193	1.324586
H	0	-2.817616	0.611593	2.432669
H	0	-0.915451	2.456360	2.641223
H	0	-1.059153	3.915519	1.666124
H	0	0.532281	-1.898092	0.415397
H	0	-3.138376	3.062491	0.616965
H	0	-3.312708	3.042428	2.369760
H	0	2.425112	0.078019	0.550383
H	0	0.889811	-3.345752	-1.427282
H	0	0.825782	-1.990116	-2.562028
H	0	3.239140	-2.199496	1.635444
H	0	3.231911	-2.708374	-2.641223
H	0	2.594083	-0.128723	-2.142322
H	0	4.152864	-0.555583	-1.365466
H	0	3.755301	-3.915519	-0.329829

Energy + ZPE = -3103.700722
Free energy = -3103.743630
Free energy in DCM = -3104.006578
Free energy in heptane = -3104.009330
Number of imaginary frequencies = 0

Diels-Alder reaction with Vinylborane (16a)

TS 16a+cpReN

C	0	-2.794353	1.195825	0.641502
C	0	-2.898677	1.912734	-0.541722
C	0	-4.059651	0.399514	0.810585
C	0	-3.961735	1.392546	-1.300889
C	0	-4.506168	0.275647	-0.635956
H	0	-2.092713	1.394001	1.443088
H	0	-2.213269	2.683484	-0.875082
H	0	-4.793272	1.034486	1.336629
H	0	-3.970374	-0.532991	1.369416
H	0	-4.225217	1.712241	-2.303337
H	0	-5.476273	-0.137205	-0.899138
Cl	0	-0.751329	0.231914	-2.616338
C	0	-2.062972	-1.067194	-0.421932
C	0	-3.253090	-1.244849	-1.147959
B	0	-0.768355	-0.454237	-0.929889
C	0	0.602132	-0.525110	-0.134245
C	0	1.524917	0.742901	-0.190542
C	0	3.015361	0.366025	-0.331610
C	0	3.474371	-0.892814	0.498754
C	0	2.855831	-1.717153	-0.681864
C	0	1.329967	-1.863652	-0.566004
C	0	1.252683	1.692561	0.985977
C	0	5.010966	-0.999778	0.527433
C	0	3.153005	-0.509806	-1.608142
C	0	2.984969	-1.144522	1.930899
H	0	-2.033924	-1.509953	0.574983
H	0	-3.948608	-2.019167	-0.826677
H	0	-3.229099	-1.101381	-2.224182
H	0	0.323188	-0.660157	0.918640
H	0	1.286828	1.302838	-1.104782
H	0	3.646030	1.261899	-0.252869
H	0	3.320117	-2.683484	-0.919684
H	0	1.070346	-2.651480	0.152149
H	0	0.965331	-2.212009	-1.541991
H	0	1.477775	1.228853	1.952717
H	0	1.861612	2.601390	0.902626
H	0	0.200543	2.003141	1.003609
H	0	5.476273	-0.837733	-0.448694
H	0	5.432092	-0.259087	1.219545
H	0	5.319911	-1.992500	0.879698
H	0	2.434844	-0.317409	-2.412703
H	0	4.159790	-0.519484	-2.031486
H	0	3.384734	-0.386018	2.616338
H	0	1.899491	-1.147274	2.036618
H	0	3.350191	-2.118555	2.283468

Energy + ZPE = -1148.055228
Free energy = -1148.102263
Free energy in DCM = -1148.444469
Free energy in heptane = -1148.446623
Number of imaginary frequencies = 1 (-408.09)

TS 16a+cpReX

C	0	-0.461590	2.380728	4.025915
C	0	0.885909	2.775345	3.911077
C	0	-1.136259	2.820657	2.741014
C	0	1.188893	2.990701	2.554199
C	0	0.032406	2.835797	1.800646
H	0	-0.989690	2.371607	4.975453
H	0	1.608954	2.776124	4.720500
H	0	-1.475085	3.861711	2.882474
H	0	-1.995694	2.231855	2.421225
H	0	2.181231	3.171644	2.154435
H	0	-0.049989	2.996473	0.732286
Cl	0	-2.593738	-0.052984	1.134747
C	0	0.047649	0.263053	2.250830
C	0	-0.400482	0.379395	3.576157
B	0	-0.775320	-0.032290	1.006975
C	0	-0.117907	-0.493378	-0.359961
C	0	-0.793303	-0.010022	-1.691414
C	0	-0.836933	-1.127962	-2.754917
C	0	0.443948	-2.043945	-2.824060
C	0	-0.197217	-2.785976	-1.601601
C	0	0.065402	-2.065453	-0.269996
C	0	-0.154880	1.288054	-2.209179
C	0	0.428011	-2.915117	-4.094457
C	0	-1.585278	-2.336583	-2.126853
C	0	1.859862	-1.468313	-2.695445
H	0	1.129543	0.223548	2.118274
H	0	0.263061	0.090519	4.387146
H	0	-1.451672	0.186758	3.781970
H	0	0.895242	-0.072266	-0.352898
H	0	-1.845858	0.221911	-1.481166
H	0	-1.209721	-0.733781	-3.709985
H	0	0.000698	-3.861711	-1.504735
H	0	1.078129	-2.279895	0.093195
H	0	-0.619256	-2.499836	0.471484
H	0	0.899827	1.154035	-2.473068
H	0	-0.678957	1.650686	-3.102041
H	0	-0.207910	2.081685	-1.452966
H	0	-0.539772	-3.386933	-4.285657
H	0	0.678660	-2.310113	-4.975453
H	0	1.176315	-3.714915	-4.020729
H	0	-2.346013	-2.102188	-1.374057
H	0	-2.018049	-3.019251	-2.861423
H	0	2.105936	-0.845079	-3.564899
H	0	2.013175	-0.863762	-1.800798
H	0	2.593738	-2.285099	-2.668800

Energy + ZPE = -1148.055157
Free energy = -1148.102421
Free energy in DCM = -1148.442985
Free energy in heptane = -1148.445593
Number of imaginary frequencies = 1 (-407.95)

TS 16a+cpSiN

C	0	1.605870	-1.592881	3.707809
C	0	2.566864	-0.670248	3.245462
C	0	0.316028	-0.803303	3.854212
C	0	1.913080	0.440224	2.683727
C	0	0.543013	0.287366	2.842772
H	0	1.861715	-2.396006	4.393638
H	0	3.635390	-0.851359	3.201016
H	0	0.317120	-0.342338	4.857046
H	0	-0.610295	-1.369907	3.752885
H	0	2.398646	1.236340	2.131348
H	0	-0.212132	1.004451	2.542527
Cl	0	2.425274	-0.910911	-0.395543
C	0	0.263053	-1.788222	1.272790
C	0	1.093072	-2.627226	2.035666
B	0	0.673046	-0.904559	0.109256
C	0	-0.339521	-0.049189	-0.762379
C	0	-0.597540	-0.735386	-2.162686
C	0	-0.754272	0.309061	-3.288633
C	0	-1.552911	1.610477	-2.895942
C	0	-0.197806	2.075518	-2.259661
C	0	0.038092	1.472572	-0.864894
C	0	-1.758250	-1.738380	-2.089808
C	0	-1.909492	2.432615	-4.149313
C	0	0.531533	1.182247	-3.296491
C	0	-2.815394	1.558308	-2.026053
H	0	-0.801474	-1.816232	1.510779
H	0	0.637609	-3.446760	2.590273
H	0	2.084485	-2.857035	1.656424
H	0	-1.296617	-0.099921	-0.228239
H	0	0.296672	-1.312973	-2.438497
H	0	-1.047692	-0.182905	-4.225976
H	0	0.014377	3.152967	-2.259475
H	0	-0.536841	2.028099	-0.111318
H	0	1.096615	1.625995	-0.619791
H	0	-1.575256	-2.492248	-1.314075
H	0	-2.710922	-1.248726	-1.859488
H	0	-1.876664	-2.266551	-3.044067
H	0	-2.747697	1.968329	-4.684933
H	0	-2.220914	3.446760	-3.867001
H	0	-1.081408	2.527620	-4.857046
H	0	1.454917	0.696201	-2.963544
H	0	0.721150	1.681329	-4.249405
H	0	-3.635390	1.063115	-2.561980
H	0	-2.680072	1.039744	-1.076384
H	0	-3.152548	2.578461	-1.797590

Energy + ZPE = -1148.056005
Free energy = -1148.103312
Free energy in DCM = -1148.445431
Free energy in heptane = -1148.447364
Number of imaginary frequencies = 1 (-401.79)

TS 16a+cpSiX

C	0	0.114402	2.362720	1.729414
C	0	-0.506619	3.432889	1.096480
C	0	-0.511536	2.198946	3.083024
C	0	-1.672949	3.772912	1.805124

C	0	-1.861496	2.850438	2.853830
H	0	1.061421	1.921535	1.440930
H	0	-0.186286	3.884214	0.163226
H	0	0.046375	2.831186	3.795395
H	0	-0.525947	1.184379	3.480549
H	0	-2.384896	4.536051	1.507416
H	0	-2.557457	3.026327	3.669455
Cl	0	-0.788492	-1.346790	2.631105
C	0	-1.816231	0.774785	0.968277
C	0	-2.734896	1.242142	1.920982
B	0	-0.866784	-0.405325	1.068138
C	0	0.010992	-0.934958	-0.141573
C	0	-0.599875	-2.263882	-0.743006
C	0	0.503639	-3.247191	-1.187794
C	0	1.760411	-2.585866	-1.872014
C	0	2.221128	-2.285522	-0.404058
C	0	1.546591	-1.035225	0.183390
C	0	-1.629576	-1.960282	-1.841400
C	0	2.644816	-3.654654	-2.542037
C	0	1.405308	-3.524732	0.047407
C	0	1.625485	-1.429534	-2.870861
H	0	-1.860504	1.258412	-0.008121
H	0	-3.628864	1.761776	1.585712
H	0	-2.882868	0.654769	2.825163
H	0	-0.092678	-0.178429	-0.929035
H	0	-1.141048	-2.792327	0.055293
H	0	0.059438	-4.108735	-1.704594
H	0	3.301552	-2.273552	-0.208206
H	0	1.713489	-1.055977	1.267766
H	0	2.042783	-0.128318	-0.188695
H	0	-2.105730	-2.883686	-2.193778
H	0	-2.421475	-1.301447	-1.464402
H	0	-1.172396	-1.469556	-2.707503
H	0	3.628864	-3.236824	-2.791327
H	0	2.810528	-4.536051	-1.916388
H	0	2.186214	-3.997917	-3.478431
H	0	0.922320	-3.463646	1.028577
H	0	1.961323	-4.462919	-0.012852
H	0	1.141139	-1.769534	-3.795395
H	0	1.055338	-0.580521	-2.492322
H	0	2.621250	-1.058541	-3.148862

Energy + ZPE = -1148.055828
Free energy = -1148.103507
Free energy in DCM = -1148.444230
Free energy in heptane = -1148.446532
Number of imaginary frequencies = 1 (-404.95)

Product 16a+cpReN

C	0	-2.982818	0.654683	0.643200
C	0	-3.283755	1.885578	-0.198574
C	0	-4.415137	0.111896	0.855498
C	0	-4.344946	1.597580	-0.965490
C	0	-4.767797	0.171146	-0.648456
Cl	0	-0.911817	0.442344	-2.676643
C	0	-2.412912	-0.472382	-0.345350
C	0	-3.654510	-0.760650	-1.246603
B	0	-1.024554	-0.058491	-0.956120
C	0	0.300488	-0.134449	-0.100649
C	0	1.328502	1.040650	-0.260622
C	0	2.780382	0.525701	-0.346853
C	0	3.126913	-0.676534	0.611246
C	0	2.446080	-1.562319	-0.487478
C	0	0.913797	-1.575212	-0.366671
C	0	1.123861	2.112297	0.821322
C	0	4.648498	-0.910225	0.670283
C	0	2.845157	-0.483680	-1.527308
C	0	2.608955	-0.740111	2.053621
H	0	-2.368251	0.809958	1.532912
H	0	-2.664815	2.776744	-0.241306
H	0	-5.031498	0.782195	1.463340
H	0	-4.441188	-0.900626	1.276499
H	0	-4.763076	2.205349	-1.761847
H	0	-5.785120	-0.105886	-0.935939
H	0	-2.215259	-1.346304	0.295523
H	0	-3.953999	-1.812440	-1.169403
H	0	-3.473973	-0.544039	-2.302333
H	0	-0.015367	-0.136168	0.949835
H	0	1.144973	1.532867	-1.224775
H	0	3.484362	1.368336	-0.351685
H	0	2.827446	-2.583099	-0.621224
H	0	0.595923	-2.245128	0.441586
H	0	0.521050	-2.013176	-1.295547
H	0	1.315396	1.726327	1.828389
H	0	1.796330	2.962993	0.656609
H	0	0.096259	2.497693	0.804435
H	0	5.129190	-0.896268	-0.311817
H	0	5.129087	-0.136574	1.282707
H	0	4.870078	-1.880821	1.132456
H	0	2.149717	-0.313722	-2.356312
H	0	3.848277	-0.622779	-1.935659
H	0	3.078653	0.037853	2.668923
H	0	1.528084	-0.624214	2.143876
H	0	2.873335	-1.706909	2.502391

Energy + ZPE = -1148.098870
Free energy = -1148.146106
Free energy in DCM = -1148.490336
Free energy in heptane = -1148.493654
Number of imaginary frequencies = 0

Product 16a+cpReX

C	0	2.500135	0.316342	4.083265
C	0	3.309379	1.507801	3.596102
C	0	1.073297	0.907986	4.022142
C	0	2.561532	2.163491	2.696644
C	0	1.240276	1.421818	2.575010
Cl	0	-0.618740	-1.830498	2.152310
C	0	1.593809	0.049598	1.808118
C	0	2.427369	-0.703708	2.891955
B	0	0.280544	-0.584086	1.217614
C	0	-0.247223	-0.173154	-0.210768

C	0	-1.796616	-0.093548	-0.431485
C	0	-2.217084	-0.716819	-1.779249
C	0	-1.246485	-0.427998	-2.987161
C	0	-0.386483	-1.594059	-2.389521
C	0	0.506976	-1.133813	-1.226706
C	0	-2.316740	1.338144	-0.230357
C	0	-1.897857	-0.830358	-4.323948
C	0	-1.693418	-2.180390	-1.795518
C	0	-0.604243	0.948757	-3.198976
H	0	2.815828	-0.128917	5.030012
H	0	4.345949	1.701853	3.854406
H	0	0.920729	1.723045	4.736560
H	0	0.283384	0.158591	4.139232
H	0	2.861354	2.994981	2.065994
H	0	0.410390	1.987181	2.143083
H	0	2.225357	0.315714	0.950380
H	0	3.421817	-0.977981	2.526150
H	0	1.928216	-1.620654	3.220127
H	0	0.154286	0.829965	-0.400647
H	0	-2.286380	-0.712081	0.331792
H	0	-3.287430	-0.551740	-1.959749
H	0	0.189245	-2.208872	-3.093735
H	0	1.398445	-0.617384	-1.602500
H	0	0.872788	-2.041692	-0.724964
H	0	-3.409511	1.369443	-0.318654
H	0	-2.057457	1.714261	0.767768
H	0	-1.902910	2.037077	-0.965332
H	0	-2.390125	-1.806175	-4.290509
H	0	-2.653438	-0.090682	-4.617930
H	0	-1.144848	-0.867455	-5.121628
H	0	-1.613482	-2.682501	-0.825118
H	0	-2.230437	-2.835729	-2.484202
H	0	0.115849	0.901602	-4.026802
H	0	-1.363110	1.691402	-3.476573
H	0	-0.072938	1.331250	-2.326643

Energy + ZPE = -1148.099114
Free energy = -1148.145844
Free energy in DCM = -1148.490314
Free energy in heptane = -1148.494002
Number of imaginary frequencies = 0

Product 16a+cpSiN

C	0	-0.737634	-1.141656	3.834518
C	0	0.204362	0.049450	3.732046
C	0	-2.034030	-0.424886	4.276207
C	0	-0.519208	1.102564	3.324176
C	0	-1.955349	0.630001	3.148743
Cl	0	-2.866911	1.561411	-0.064714
C	0	-1.987482	-0.333493	1.871664
C	0	-1.112626	-1.535674	2.362502
B	0	-1.605353	0.422348	0.542617
C	0	-0.294205	0.214038	-0.301795
C	0	0.282544	1.438448	-1.092039
C	0	0.738704	1.041218	-2.510931
C	0	1.452040	-0.360599	-2.622476
C	0	-0.003449	-0.941207	-2.619791
C	0	-0.585976	-1.063736	-1.202645
C	0	1.371384	2.160997	-0.283735
C	0	2.128762	-0.522177	-3.997213
C	0	-0.482071	0.401181	-3.229616
C	0	2.456887	-0.846885	-1.570521
H	0	-0.392470	-1.978069	4.447403
H	0	1.281284	0.001610	3.861989
H	0	-1.953702	0.019536	5.273565
H	0	-2.928919	-1.056562	4.222161
H	0	-0.154371	2.091124	3.061549
H	0	-2.724409	1.403859	3.123583
H	0	-3.031911	-0.662053	1.778474
H	0	-1.693274	-2.465294	2.349814
H	0	-0.217119	-1.705773	1.757876
H	0	0.477641	-0.093168	0.412702
H	0	-0.525846	2.164742	-1.245400
H	0	1.239141	1.885670	-3.002697
H	0	-0.180973	-1.864816	-3.186242
H	0	-0.188464	-1.950142	-0.694441
H	0	-1.665832	-1.240431	-1.314615
H	0	0.988768	2.477587	0.694417
H	0	2.245063	1.524796	-0.105409
H	0	1.714246	3.059144	-0.811672
H	0	3.056874	0.062432	-4.034820
H	0	2.393720	-1.572541	-4.174220
H	0	1.502236	-0.194881	-4.831471
H	0	-0.420438	0.430424	-4.319466
H	0	-1.472584	0.757793	-2.925951
H	0	2.762230	-1.877607	-1.795101
H	0	3.365789	-0.232171	-1.589289
H	0	2.072947	-0.836562	-0.549740

Energy + ZPE = -1148.099105
Free energy = -1148.145786
Free energy in DCM = -1148.490965
Free energy in heptane = -1148.494252
Number of imaginary frequencies = 0

Product 16a+cpSiX

C	0	-0.264513	1.845866	2.521993
C	0	-0.279768	3.327651	2.169003
C	0	-1.682692	1.696556	3.121125
C	0	-1.530636	3.643203	1.802778
C	0	-2.370346	2.380278	1.917933
Cl	0	-0.104371	-1.445543	2.553055
C	0	-0.418658	1.091294	1.144027
C	0	-1.920234	1.421640	0.762089
B	0	-0.150192	-0.455606	1.053018
C	0	0.159145	-1.146105	-0.331116
C	0	-0.369794	-2.603226	-0.564327
C	0	0.692745	-3.499466	-1.234376
C	0	1.552850	-2.802035	-2.355938
C	0	2.382364	-2.221657	-1.159441
C	0	1.726068	-0.979462	-0.537274
C	0	-1.719044	-2.594368	-1.299599

C	0	2.358472	-3.842664	-3.156619
C	0	1.959531	-3.464414	-0.334358
C	0	0.929437	-1.839364	-3.374271
H	0	0.570931	1.500214	3.133973
H	0	0.601884	3.959248	2.111812
H	0	-1.805139	2.256503	4.053324
H	0	-1.990482	0.656855	3.272790
H	0	-1.879474	4.584713	1.389655
H	0	-3.453174	2.519998	1.972029
H	0	0.234669	1.565116	0.397767
H	0	-2.002452	1.881182	-0.227081
H	0	-2.558919	0.528541	0.761709
H	0	-0.308558	-0.512011	-1.094356
H	0	-0.553314	-3.065463	0.414416
H	0	0.265848	-4.480306	-1.481867
H	0	3.453174	-2.045401	-1.325634
H	0	2.239203	-0.787846	0.416579
H	0	1.905504	-0.094213	-1.159114
H	0	-2.117454	-3.611986	-1.392224
H	0	-2.460626	-1.999675	-0.750785
H	0	-1.640153	-2.174180	-2.308103
H	0	3.130729	-3.348730	-3.760223
H	0	2.857298	-4.584713	-2.527011
H	0	1.699299	-4.385956	-3.845750
H	0	1.793850	-3.314694	0.738180
H	0	2.621952	-4.321838	-0.468821
H	0	0.255416	-2.376853	-4.053324
H	0	0.363197	-1.021611	-2.926515
H	0	1.717295	-1.390471	-3.993767

Energy + ZPE = -1148.098937
Free energy = -1148.145511
Free energy in DCM = -1148.490882
Free energy in heptane = -1148.494321
Number of imaginary frequencies = 0

C	0	1.435164	0.727509	-0.024124
C	0	2.922814	0.411362	-0.281476
C	0	3.483772	-0.846438	0.484046
C	0	2.820744	-1.668145	-0.672620
C	0	1.315832	-1.882753	-0.451407
C	0	1.211332	1.613490	1.210923
C	0	5.021316	-0.893388	0.411362
C	0	3.001252	-0.428936	-1.587781
C	0	3.090691	-1.152049	1.934606
H	0	-2.172305	-1.455963	0.740905
H	0	-4.042457	-1.967544	-0.724288
H	0	-3.203447	-1.178050	-2.135528
H	0	0.293948	-0.740239	1.077786
H	0	1.116100	1.318355	-0.893175
H	0	3.524567	1.328530	-0.223875
H	0	3.306633	-2.608615	-0.964668
H	0	1.143112	-2.677884	0.284539
H	0	0.899653	-2.250926	-1.398750
H	0	1.525038	1.122281	2.138106
H	0	1.774268	2.551110	1.123688
H	0	0.151306	1.875793	1.318365
H	0	5.413528	-0.692783	-0.589651
H	0	5.459768	-0.151233	1.091158
H	0	5.390244	-1.880469	0.719121
H	0	2.215813	-0.249821	-2.329292
H	0	3.973769	-0.387070	-2.083282
H	0	3.506843	-0.400445	2.617782
H	0	2.013171	-1.191272	2.101174
H	0	3.504564	-2.123674	2.236492

Energy + ZPE = -3259.567511
Free energy = -3259.615248
Free energy in DCM = -3259.956520
Free energy in heptane = -3259.958756
Number of imaginary frequencies = 1 (-394.92)

Diels-Alder reaction with Vinylborane (16b)

TS 16b+cpReN

C	0	-2.869999	1.322500	0.615486
C	0	-2.852701	1.951901	-0.618323
C	0	-4.158996	0.557661	0.731217
C	0	-3.865037	1.403754	-1.427177
C	0	-4.493995	0.346749	-0.736994
H	0	-2.224928	1.553068	1.455038
H	0	-2.118768	2.677884	-0.947759
H	0	-4.920377	1.232494	1.158774
H	0	-4.129372	-0.339399	1.351393
H	0	-4.036287	1.660239	-2.466811
H	0	-5.459768	-0.044257	-1.046211
Br	0	-0.761709	0.179172	-2.617782
C	0	-2.136972	-1.074109	-0.280974
C	0	-3.299624	-1.242671	-1.055676
B	0	-0.815110	-0.518020	-0.763648
C	0	0.556384	-0.575631	0.024500

TS 16b+cpReX

C	0	-0.620545	2.513931	4.041620
C	0	0.648340	3.120680	3.933534
C	0	-1.340756	2.822599	2.742075
C	0	0.929834	3.365058	2.576496
C	0	-0.181196	3.029369	1.816719
H	0	-1.153931	2.450207	4.986323
H	0	1.352152	3.246990	4.750071
H	0	-1.855795	3.790562	2.870332
H	0	-2.081271	2.094802	2.409796
H	0	1.885363	3.696786	2.184048
H	0	-0.275653	3.152137	0.744616
Br	0	-2.485528	-0.332881	1.362963
C	0	0.247107	0.440827	2.361001
C	0	-0.222747	0.561969	3.681841
B	0	-0.527902	-0.057703	1.161159
C	0	0.101355	-0.516714	-0.216914
C	0	-0.558126	0.131324	-1.492964
C	0	-0.791267	-0.905731	-2.611099
C	0	0.373533	-1.948064	-2.812808

C	0	-0.278736	-2.695652	-1.601684
C	0	0.143713	-2.098888	-0.249901
C	0	0.224077	1.364222	-1.970556
C	0	0.193896	-2.724265	-4.130866
C	0	-1.635415	-2.064080	-2.008540
C	0	1.850322	-1.542389	-2.726577
H	0	1.320814	0.572091	2.219888
H	0	0.472927	0.417473	4.504770
H	0	-1.226625	0.195925	3.889787
H	0	1.145715	-0.179251	-0.200790
H	0	-1.561339	0.483704	-1.215918
H	0	-1.168400	-0.411120	-3.516452
H	0	-0.197140	-3.790562	-1.582479
H	0	1.155761	-2.429070	0.015575
H	0	-0.523838	-2.520391	0.513013
H	0	1.229365	1.107349	-2.320354
H	0	-0.299359	1.861977	-2.796364
H	0	0.337609	2.095494	-1.160809
H	0	-0.832213	-3.064272	-4.297141
H	0	0.475205	-2.096448	-4.986323
H	0	0.841930	-3.610243	-4.145493
H	0	-2.316774	-1.800088	-1.193851
H	0	-2.182549	-2.645192	-2.754081
H	0	2.127051	-0.894511	-3.568280
H	0	2.112475	-1.020193	-1.805020
H	0	2.485528	-2.436372	-2.787946

Energy + ZPE = -3259.567397
Free energy = -3259.615082
Free energy in DCM = -3259.955857
Free energy in heptane = -3259.958424
Number of imaginary frequencies = 1 (-399.33)

TS 16b+cpSiN

C	0	1.679633	-1.606597	3.620866
C	0	2.600475	-0.664866	3.116596
C	0	0.399331	-0.829124	3.883760
C	0	1.903282	0.461300	2.641744
C	0	0.552257	0.299964	2.902257
H	0	1.991045	-2.420256	4.270558
H	0	3.663047	-0.837861	2.986174
H	0	0.463796	-0.408026	4.901818
H	0	-0.529896	-1.397049	3.821369
H	0	2.345364	1.274419	2.078358
H	0	-0.227446	1.017538	2.674817
Br	0	2.453406	-0.845678	-0.430995
C	0	0.183044	-1.776948	1.277605
C	0	1.055118	-2.619477	1.990422
B	0	0.547197	-0.886825	0.111690
C	0	-0.458778	-0.043871	-0.772363
C	0	-0.664988	-0.733823	-2.181056
C	0	-0.754100	0.306241	-3.317761
C	0	-1.564897	1.612120	-2.973536
C	0	-0.243635	2.074805	-2.269656
C	0	-0.087014	1.481563	-0.860786
C	0	-1.838334	-1.723956	-2.156093
C	0	-1.851937	2.429778	-4.246999
C	0	0.537781	1.169679	-3.257800
C	0	-2.869167	1.563810	-2.167949
H	0	-0.868751	-1.807153	1.567571
H	0	0.629690	-3.441560	2.565011
H	0	2.018032	-2.850122	1.543918
H	0	-1.429003	-0.105938	-0.262726
H	0	0.234889	-1.322451	-2.410261
H	0	-1.000315	-0.188425	-4.267175
H	0	-0.026708	3.151304	-2.265239
H	0	-0.705412	2.038272	-0.143687
H	0	0.955891	1.636656	-0.557686
H	0	-1.696881	-2.476001	-1.369918
H	0	-2.795281	-1.224303	-1.970702
H	0	-1.918915	-2.255178	-3.112647
H	0	-2.651078	1.957378	-4.832926
H	0	-2.188857	3.441560	-3.986234
H	0	-0.981943	2.531424	-4.901818
H	0	1.433772	0.678749	-2.863836
H	0	0.787355	1.659618	-4.201595
H	0	-3.663047	1.070127	-2.743313
H	0	-2.780854	1.043606	-1.213246
H	0	-3.215229	2.584369	-1.955258

Energy + ZPE = -3259.568130
Free energy = -3259.615921
Free energy in DCM = -3259.957418
Free energy in heptane = -3259.959554
Number of imaginary frequencies = 1 (-390.52)

TS 16b+cpSiX

C	0	0.102064	2.497255	1.730668
C	0	-0.586985	3.561061	1.164095
C	0	-0.480043	2.231149	3.086014
C	0	-1.746155	3.812892	1.920820
C	0	-1.863893	2.832298	2.927174
H	0	1.053585	2.105923	1.390005
H	0	-0.315742	4.069531	0.244817
H	0	0.066219	2.846555	3.821773
H	0	-0.434356	1.194998	3.421565
H	0	-2.500202	4.555481	1.680087
H	0	-2.538039	2.943044	3.772126
Br	0	-0.738286	-1.363375	2.687486
C	0	-1.816908	0.847415	0.948140
C	0	-2.719575	1.263403	1.941398
B	0	-0.860442	-0.323047	1.000190
C	0	0.008609	-0.855203	-0.209827
C	0	-0.611178	-2.191214	-0.788519
C	0	0.484147	-3.206312	-1.175066
C	0	1.760477	-2.589879	-1.863788
C	0	2.204634	-2.240682	-0.402285
C	0	1.543628	-0.955769	0.121354
C	0	-1.612905	-1.903402	-1.916316
C	0	2.637436	-3.695798	-2.480688
C	0	1.361917	-3.447761	0.085514
C	0	1.655206	-1.468232	-2.904612
H	0	-1.887106	1.363260	-0.010320

H	0	-3.631815	1.777189	1.648885
H	0	-2.835256	0.626396	2.816464
H	0	-0.097091	-0.105180	-1.004152
H	0	-1.178902	-2.683617	0.014263
H	0	0.036149	-4.081097	-1.665590
H	0	3.282181	-2.237730	-0.190911
H	0	1.701382	-0.925671	1.206727
H	0	2.051773	-0.073773	-0.291537
H	0	-2.096182	-2.829147	-2.252521
H	0	-2.402195	-1.223497	-1.572339
H	0	-1.132949	-1.442802	-2.786448
H	0	3.631815	-3.303015	-2.729895
H	0	2.779288	-4.555481	-1.819865
H	0	2.187303	-4.066549	-3.410733
H	0	0.866577	-3.337026	1.055665
H	0	1.904127	-4.395844	0.070689
H	0	1.175019	-1.832954	-3.821773
H	0	1.095084	-0.597463	-2.561609
H	0	2.659725	-1.122950	-3.184203

Energy + ZPE = -3259.568345
Free energy = -3259.615914
Free energy in DCM = -3259.956681
Free energy in heptane = -3259.959174
Number of imaginary frequencies = 1 (-398.70)

Product 16b+cpReN

C	0	-2.773596	0.666749	1.161045
C	0	-3.085089	1.762178	0.153532
C	0	-4.187551	0.074830	1.367866
C	0	-4.088485	1.323916	-0.619605
C	0	-4.456820	-0.073484	-0.146581
Br	0	-0.576229	0.461668	-2.067880
C	0	-2.096601	-0.553584	0.363397
C	0	-3.266699	-1.008680	-0.565797
B	0	-0.698658	-0.147928	-0.220400
C	0	0.632969	-0.254576	0.613548
C	0	1.668239	0.917139	0.471087
C	0	3.105021	0.392944	0.274898
C	0	3.490412	-0.855696	1.155047
C	0	2.740385	-1.683659	0.057368
C	0	1.218562	-1.692047	0.267605
C	0	1.533309	1.928274	1.620151
C	0	5.009604	-1.104514	1.119511
C	0	3.086953	-0.560272	-0.954170
C	0	3.047265	-0.982436	2.617620
H	0	-2.218635	0.965502	2.053584
H	0	-2.504963	2.670145	0.023060
H	0	-4.869556	0.780496	1.853251
H	0	-4.187541	-0.876626	1.913524
H	0	-4.487787	1.802891	-1.508051
H	0	-5.441364	-0.441524	-0.445835
H	0	-1.911371	-1.327521	1.123438
H	0	-3.520053	-2.059083	-0.380055
H	0	-3.026676	-0.905910	-1.627116
H	0	0.337109	-0.295873	1.669443
H	0	1.436187	1.464858	-0.451581
H	0	3.818875	1.227275	0.268018
H	0	3.103398	-2.699892	-0.144864
H	0	0.940443	-2.387313	1.068808
H	0	0.769873	-2.093893	-0.652254
H	0	1.771752	1.487841	2.594070
H	0	2.205926	2.780842	1.466145
H	0	0.510602	2.323038	1.677019
H	0	5.435987	-1.040768	0.114435
H	0	5.531022	-0.368617	1.744956
H	0	5.245630	-2.100423	1.516066
H	0	2.340716	-0.346743	-1.726612
H	0	4.061548	-0.687563	-1.430050
H	0	3.562626	-0.244204	3.245160
H	0	1.974638	-0.853372	2.769948
H	0	3.315586	-1.974820	3.004108

Energy + ZPE = -3259.609069
Free energy = -3259.656895
Free energy in DCM = -3260.000166
Free energy in heptane = -3260.003603
Number of imaginary frequencies = 0

Product 16b+cpReX

C	0	2.527200	0.611134	3.543427
C	0	3.288855	1.873307	3.170787
C	0	1.076279	1.144566	3.511093
C	0	2.524027	2.570100	2.317519
C	0	1.237809	1.786344	2.114928
Br	0	-0.575898	-1.552998	1.559478
C	0	1.660269	0.499007	1.240514
C	0	2.516702	-0.304671	2.268503
B	0	0.377422	-0.141311	0.600982
C	0	-0.159341	0.282256	-0.816162
C	0	-1.713635	0.383733	-1.008382
C	0	-2.177861	-0.312979	-2.302563
C	0	-1.246979	-0.092363	-3.554688
C	0	-0.371646	-1.229668	-2.927811
C	0	0.565706	-0.707536	-1.828996
C	0	-2.202304	1.835134	-0.883066
C	0	-1.945109	-0.556843	-4.846532
C	0	-1.656663	-1.777509	-2.254503
C	0	-0.603200	1.266976	-3.854385
H	0	2.851725	0.100964	4.453699
H	0	4.312925	2.089052	3.459992
H	0	0.880460	1.889280	4.288858
H	0	0.316655	0.357266	3.547055
H	0	2.794864	3.463635	1.763256
H	0	0.389008	2.350054	1.718984
H	0	2.283092	0.861445	0.412358
H	0	3.527138	-0.499903	1.895776
H	0	2.054237	-1.268271	2.503544
H	0	0.256366	1.277199	-1.019360
H	0	-2.193735	-0.174377	-0.194009
H	0	-3.253316	-0.154731	-2.457070
H	0	0.176419	-1.884076	-3.618283

H	0	1.429010	-0.192018	-2.266140
H	0	0.970772	-1.586807	-1.307130
H	0	-3.296161	1.881560	-0.948811
H	0	-1.913780	2.264273	0.085235
H	0	-1.793896	2.482281	-1.666373
H	0	-2.443996	-1.524858	-4.745910
H	0	-2.704584	0.173793	-5.152999
H	0	-1.219876	-0.642022	-5.666029
H	0	-1.540052	-2.222298	-1.260446
H	0	-2.218688	-2.468567	-2.886125
H	0	0.085484	1.173922	-4.704802
H	0	-1.365758	2.003182	-4.138732
H	0	-0.035681	1.685499	-3.021288

Energy + ZPE = -3259.610200
Free energy = -3259.657484
Free energy in DCM = -3260.001335
Free energy in heptane = -3260.005050
Number of imaginary frequencies = 0

Product 16b+cpSiN

C	0	-0.105194	-1.327717	3.871428
C	0	0.747630	-0.073012	3.744866
C	0	-1.474745	-0.692323	4.206274
C	0	-0.031662	0.896546	3.243081
C	0	-1.416278	0.302416	3.025324
Br	0	-2.251829	1.186319	-0.267039
C	0	-1.297148	-0.723315	1.804501
C	0	-0.373305	-1.832297	2.410047
B	0	-0.875531	0.000562	0.472985
C	0	0.452649	-0.190764	-0.342554
C	0	1.048494	1.060724	-1.080413
C	0	1.417637	0.742505	-2.542838
C	0	2.103695	-0.657183	-2.772455
C	0	0.643556	-1.221601	-2.729084
C	0	0.142458	-1.431369	-1.292636
C	0	2.197807	1.691146	-0.278248
C	0	2.709766	-0.748404	-4.184710
C	0	0.147203	0.161127	-3.226318
C	0	3.143382	-1.215575	-1.793396
H	0	0.269435	-2.098889	4.549209
H	0	1.816751	-0.028887	3.928947
H	0	-1.482185	-0.189879	5.178947
H	0	-2.314117	-1.395625	4.144949
H	0	0.268726	1.895708	2.941837
H	0	-2.238591	1.009802	2.908417
H	0	-2.307820	-1.128868	1.657804
H	0	-0.891180	-2.798238	2.428444
H	0	0.561233	-1.977205	1.860011
H	0	1.213251	-0.534946	0.367310
H	0	0.262660	1.824054	-1.143478
H	0	1.903144	1.608674	-3.011426
H	0	0.425927	-2.106732	-3.341200
H	0	0.586584	-2.331870	-0.852204
H	0	-0.937788	-1.628560	-1.356489
H	0	1.867695	1.953449	0.734508
H	0	3.057133	1.019573	-0.180184
H	0	2.547071	2.611346	-0.762331
H	0	3.635617	-0.161785	-4.241602
H	0	2.962654	-1.788361	-4.428340
H	0	2.039530	-0.380445	-4.966673
H	0	0.145940	0.258244	-4.313972
H	0	-0.816412	0.507635	-2.838591
H	0	3.405927	-2.244622	-2.073383
H	0	4.068981	-0.627235	-1.830280
H	0	2.805854	-1.235820	-0.756026

Energy + ZPE = -3259.608204
Free energy = -3259.655452
Free energy in DCM = -3259.999827
Free energy in heptane = -3260.003224
Number of imaginary frequencies = 0

Product 16b+cpSiX

C	0	-0.315420	2.673818	2.041621
C	0	-0.407606	4.160106	1.724122
C	0	-1.703332	2.446854	2.685492
C	0	-1.683679	4.427520	1.409832
C	0	-2.463003	3.126265	1.524039
Br	0	0.005499	-0.672035	2.144377
C	0	-0.486742	1.940471	0.654460
C	0	-2.013217	2.215219	0.329872
B	0	-0.165766	0.409392	0.528152
C	0	0.112872	-0.282537	-0.858542
C	0	-0.455260	-1.730565	-1.071835
C	0	0.597568	-2.674078	-1.686614
C	0	1.491274	-2.037626	-2.817667
C	0	2.317725	-1.436615	-1.630745
C	0	1.684177	-0.156144	-1.066561
C	0	-1.783125	-1.702830	-1.844456
C	0	2.281058	-3.125155	-3.569573
C	0	1.849636	-2.634950	-0.764992
C	0	0.906403	-1.092281	-3.874540
H	0	0.553458	2.346667	2.615901
H	0	0.442518	4.831990	1.651095
H	0	-1.817721	2.978087	3.635327
H	0	-1.950329	1.389089	2.820988
H	0	-2.087801	5.361454	1.031253
H	0	-3.548311	3.216774	1.618301
H	0	0.121633	2.451792	-0.105419
H	0	-2.146937	2.693807	-0.644461
H	0	-2.613699	1.296043	0.328139
H	0	-0.345308	0.357676	-1.622572
H	0	-0.679770	-2.157295	-0.085442
H	0	0.151475	-3.652986	-1.906312
H	0	3.395029	-1.293336	-1.786471
H	0	2.195897	0.064250	-0.118393
H	0	1.884062	0.698397	-1.724009
H	0	-2.206124	-2.711666	-1.923708
H	0	-2.522642	-1.075388	-1.330478
H	0	-1.665759	-1.309828	-2.859824
H	0	3.076488	-2.672797	-4.175703
H	0	2.748807	-3.857912	-2.905999

H	0	1.619032	-3.674316	-4.251294
H	0	1.668353	-2.433679	0.296214
H	0	2.491490	-3.514028	-0.852797
H	0	0.228764	-1.633663	-4.546855
H	0	0.353834	-0.247798	-3.459295
H	0	1.713887	-0.681824	-4.495536

Energy + ZPE = -3259.609639
Free energy = -3259.657255
Free energy in DCM = -3260.001307
Free energy in heptane = -3260.004850
Number of imaginary frequencies = 0

Diels-Alder reaction with Vinylborane (17a)

TS 17a+cpReN

C	0	-2.245410	2.419605	0.338633
C	0	-2.333705	2.997826	-0.919435
C	0	-3.514638	1.648196	0.579624
C	0	-3.388101	2.396414	-1.628966
C	0	-3.942670	1.362189	-0.849332
H	0	-1.550827	2.706854	1.119031
H	0	-1.644898	3.727781	-1.328547
H	0	-3.435454	0.784528	1.241127
H	0	-4.254725	2.338758	1.019673
H	0	-3.638834	2.601228	-2.664271
H	0	-4.909245	0.921005	-1.077038
C	0	-2.677799	-0.200333	-1.178438
Cl	0	-0.085098	1.071628	-2.711044
B	0	-0.183513	0.567331	-0.966293
C	0	1.161858	0.524507	-0.121997
C	0	2.183140	1.669681	-0.347520
C	0	3.457191	1.419417	0.477057
C	0	4.193770	0.122849	0.085702
C	0	3.294907	-1.056094	-0.272012
C	0	1.791614	-0.861219	-0.404879
C	0	1.589891	3.041838	-0.004371
C	0	2.353507	-1.772865	0.678751
C	0	2.282451	-1.406425	2.151080
C	0	2.181094	-3.268563	0.450541
C	0	-1.508495	0.043549	-0.438322
H	0	-2.620559	-0.163616	-2.262329
H	0	-3.386576	-0.937590	-0.803618
H	0	0.867181	0.563189	0.939105
H	0	2.457543	1.672937	-1.412292
H	0	3.188186	1.410766	1.542681
H	0	4.148460	2.264138	0.353599
H	0	4.909245	-0.155257	0.872408
H	0	4.798209	0.339739	-0.805325
H	0	3.743121	-1.708510	-1.021183
H	0	1.342906	-1.399292	-1.239769
H	0	1.283733	3.085242	1.050187
H	0	2.322933	3.841696	-0.165812
H	0	0.712873	3.266394	-0.620646
H	0	1.321705	-1.720328	2.581640
H	0	3.073332	-1.922515	2.711044
H	0	2.393717	-0.337300	2.341346
H	0	2.234992	-3.523046	-0.614031
H	0	2.961264	-3.841696	0.969667
H	0	1.209281	-3.615718	0.826629
H	0	-1.515729	-0.293006	0.599594

Energy + ZPE = -1148.064264
Free energy = -1148.112657
Free energy in DCM = -1148.451777
Free energy in heptane = -1148.453913
Number of imaginary frequencies = 1 (-408.84)

TS 17a+cpReX

C	0	-1.125265	2.090295	3.375765
C	0	-0.324090	3.122354	2.849035
C	0	-2.267341	1.906552	2.395287
C	0	-0.599322	3.264199	1.476643
C	0	-1.634877	2.406182	1.129760
H	0	-1.257954	1.939480	4.443572
H	0	0.474281	3.628730	3.382109
H	0	-2.704520	0.909267	2.347133
H	0	-3.067453	2.611748	2.680161
H	0	-0.039766	3.886644	0.786156
H	0	-2.094857	2.335222	0.151757
Cl	0	-2.269047	-1.526106	1.245320
B	0	-0.917112	-0.533479	0.529908
C	0	-0.570610	-0.757738	-1.003267
C	0	-1.761798	-0.944046	-1.979750
C	0	-1.243933	-1.217239	-3.401441
C	0	-0.416913	-2.514198	-3.508389
C	0	0.482301	-2.816889	-2.313489
C	0	0.394739	-1.966970	-1.054033
C	0	-2.702492	0.267741	-1.976943
C	0	1.677898	-1.991113	-1.874839
C	0	2.140568	-0.784719	-2.673392
C	0	2.843567	-2.763860	-1.272387
C	0	-0.074199	0.337752	1.445903
C	0	-0.100720	0.391358	2.848699
H	0	-0.023737	0.139496	-1.334619
H	0	-2.335945	-1.821687	-1.649564
H	0	-0.657109	-0.349095	-3.733500
H	0	-2.091212	-1.285560	-4.097198
H	0	-1.122468	-3.351822	-3.591138
H	0	0.160592	-2.516146	-4.443572
H	0	0.598923	-3.886644	-2.140745
H	0	0.457410	-2.534296	-0.125587
H	0	-2.165617	1.183362	-2.261796
H	0	-3.523229	0.133244	-2.692099
H	0	-3.149946	0.427812	-0.989547
H	0	2.712237	-0.094981	-2.037631
H	0	2.803622	-1.100354	-3.489485
H	0	1.321512	-0.218610	-3.120516
H	0	2.499068	-3.632163	-0.699284
H	0	3.523229	-3.129250	-2.054094
H	0	3.429427	-2.129015	-0.594085
H	0	0.751929	0.862493	0.965098

H	0	-0.754392	-0.300595	3.376272
H	0	0.813505	0.625547	3.387869

Energy + ZPE = -1148.064286
Free energy = -1148.112219
Free energy in DCM = -1148.450574
Free energy in heptane = -1148.453270
Number of imaginary frequencies = 1 (-408.54)

TS 17a+cpSiN

C	0	2.859485	-1.579050	3.126579
C	0	2.959813	-0.173731	3.164725
C	0	1.375537	-1.888159	3.229397
C	0	1.715589	0.390102	2.832805
C	0	0.790035	-0.627982	2.651943
H	0	3.608114	-2.224287	3.578221
H	0	3.882199	0.383130	3.289868
H	0	1.045258	-2.824445	2.778201
H	0	1.114138	-1.923854	4.301110
H	0	1.536532	1.443605	2.652025
H	0	-0.260330	-0.494087	2.421824
Cl	0	2.851257	0.874502	-0.347815
B	0	1.548938	-0.394716	-0.227351
C	0	0.181763	-0.103869	-0.983730
C	0	1.863729	-1.676755	0.520275
C	0	0.362509	-0.038712	-2.531845
C	0	-0.499749	1.170851	-0.448290
C	0	3.074759	-2.015534	1.147034
C	0	-0.990255	0.230884	-3.209755
C	0	-1.413968	1.987133	-1.350008
C	0	0.998964	-1.317610	-3.092878
C	0	-1.991407	1.268123	-0.145775
C	0	-1.615449	1.581623	-2.807494
C	0	-2.922462	0.078808	-0.307247
C	0	-2.380765	2.146495	1.035791
H	0	-0.470193	-0.970200	-0.787859
H	0	1.090476	-2.446469	0.514176
H	0	1.032739	0.804884	-2.753265
H	0	0.126939	1.768494	0.211502
H	0	3.955239	-1.419301	0.926304
H	0	3.293013	-3.067354	1.327418
H	0	-1.669416	-0.601262	-2.976954
H	0	-0.865429	0.215035	-4.301110
H	0	-1.341748	3.067354	-1.224627
H	0	0.376428	-2.195514	-2.873520
H	0	1.110745	-1.255532	-4.182279
H	0	1.991757	-1.501959	-2.666559
H	0	-2.681446	1.597452	-3.075177
H	0	-1.142126	2.361631	-3.418806
H	0	-2.914116	-0.548149	0.595177
H	0	-3.955239	0.420972	-0.454536
H	0	-2.667333	-0.561531	-1.153269
H	0	-1.704738	3.002442	1.142583
H	0	-3.399495	2.540337	0.919079
H	0	-2.353315	1.581378	1.978110

Energy + ZPE = -1148.065334
Free energy = -1148.113469
Free energy in DCM = -1148.452058
Free energy in heptane = -1148.454274
Number of imaginary frequencies = 1 (-399.87)

TS 17a+cpSiX

C	0	-1.282182	0.912134	2.330620
C	0	-1.209973	2.299737	2.328872
C	0	-2.725440	0.524089	2.195664
C	0	-2.443855	2.825000	1.904371
C	0	-3.293757	1.764100	1.533362
H	0	-0.498524	0.238763	2.657572
H	0	-0.321283	2.883587	2.544808
H	0	-2.918502	-0.423076	1.692524
H	0	-3.158047	0.460776	3.209248
H	0	-2.656189	3.878708	1.754242
H	0	-4.362042	1.894477	1.384039
Cl	0	-1.948702	-1.928250	-0.311602
B	0	-0.784107	-0.522409	-0.274293
C	0	0.763583	-0.878382	-0.302541
C	0	-1.333909	0.891484	-0.277886
C	0	1.193709	-1.579889	-1.627217
C	0	1.162891	-1.715485	0.929350
C	0	-2.671845	1.305303	-0.372383
C	0	2.698469	-1.891613	-1.595364
C	0	2.342377	-2.673720	0.851552
C	0	0.844912	-0.737329	-2.861766
C	0	2.420118	-1.457281	1.753751
C	0	3.097823	-2.857488	-0.461126
C	0	3.356982	-0.301555	1.447204
C	0	2.308756	-1.725565	3.248775
H	0	1.302362	0.081921	-0.274775
H	0	-0.587582	1.685058	-0.323946
H	0	0.646314	-2.531614	-1.693752
H	0	0.320332	-2.091230	1.508074
H	0	-3.432900	0.549506	-0.556767
H	0	-2.898453	2.271730	-0.815394
H	0	3.249614	-0.944040	-1.517295
H	0	3.003011	-2.333472	-2.553832
H	0	2.209979	-3.612115	1.389673
H	0	1.157798	-1.241646	-3.784185
H	0	-0.231998	-0.546525	-2.935737
H	0	1.351592	0.236560	-2.828946
H	0	4.183911	-2.815995	-0.297474
H	0	2.886348	-3.878708	-0.805294
H	0	4.362042	-0.512774	1.835423
H	0	3.457151	-0.092271	0.380605
H	0	3.008128	0.620127	1.932822
H	0	1.627143	-2.557324	3.459781
H	0	3.286444	-1.979362	3.680310
H	0	1.933441	-0.842150	3.784185

Energy + ZPE = -1148.065229
Free energy = -1148.113310
Free energy in DCM = -1148.451055

Free energy in heptane = -1148.453662
Number of imaginary frequencies = 1 (-401.20)

Product 17a+cpReN

C	0	-1.444175	-0.993275	2.792183
C	0	-1.471031	0.520151	2.971910
C	0	-2.961155	-1.287369	2.729358
C	0	-1.038052	-1.258868	1.291411
C	0	-2.531018	0.985944	2.295345
C	0	-3.226317	-0.207821	1.654436
C	0	-2.281521	-0.701243	0.504727
B	0	0.386296	-0.817153	0.796166
Cl	0	1.708642	-0.718823	2.015158
C	0	0.735117	-0.475246	-0.706237
C	0	2.076262	-1.038999	-1.246784
C	0	0.671587	1.069742	-0.802623
C	0	2.331970	-0.526700	-2.672671
C	0	1.515309	1.792085	-1.842666
C	0	2.093847	-2.573028	-1.211544
C	0	0.001357	1.818410	-1.948677
C	0	2.456818	1.008327	-2.752145
C	0	-0.728766	1.090964	-3.064693
C	0	-0.671616	3.134770	-1.582812
H	0	-0.851908	-1.554275	3.516946
H	0	-0.698846	1.097086	3.469924
H	0	-3.196541	-2.305884	2.395629
H	0	-3.474838	-1.081113	3.673594
H	0	-1.012021	-2.356427	1.146774
H	0	-2.798925	2.024072	2.123212
H	0	-4.262396	-0.053780	1.341902
H	0	-2.028519	0.113315	-0.179703
H	0	-2.767681	-1.487861	-0.083753
H	0	-0.066974	-0.899073	-1.329927
H	0	2.884583	-0.669433	-0.600318
H	0	0.603728	1.585869	0.155426
H	0	1.528313	-0.890707	-3.327502
H	0	3.256655	-0.972510	-3.062918
H	0	1.948573	2.734243	-1.508039
H	0	3.041422	-2.965722	-1.599156
H	0	1.971265	-2.958757	-0.192396
H	0	1.286498	-2.990130	-1.828416
H	0	2.355394	1.340576	-3.794678
H	0	3.478869	1.274508	-2.451154
H	0	-1.764555	0.872842	-2.771791
H	0	-0.770319	1.719873	-3.963302
H	0	-0.262341	0.146409	-3.350149
H	0	-0.137465	3.651862	-0.777667
H	0	-0.707943	3.812028	-2.446420
H	0	-1.704105	2.971670	-1.245741

Energy + ZPE = -1148.108772
Free energy = -1148.156737
Free energy in DCM = -1148.498333
Free energy in heptane = -1148.501645
Number of imaginary frequencies = 0

Product 17a+cpReX

C	0	1.908410	0.445181	3.694019
C	0	1.931916	1.963977	3.627066
C	0	0.383924	0.195754	3.759372
C	0	2.211287	-0.082070	2.246763
C	0	0.847401	2.355121	2.942072
C	0	0.082229	1.102934	2.545703
C	0	0.983858	0.399122	1.410949
B	0	0.115394	-0.627404	0.597618
Cl	0	0.070373	-2.360820	1.078179
C	0	-0.695537	-0.182159	-0.683056
C	0	-2.071944	-0.849314	-0.928556
C	0	0.286337	-0.417464	-1.859283
C	0	-2.651026	-0.395675	-2.278523
C	0	-0.263561	-0.689420	-3.251779
C	0	-3.054402	-0.542104	0.209581
C	0	0.513795	0.586529	-2.982366
C	0	-1.768508	-0.786108	-3.481442
C	0	-0.163658	1.945934	-2.987737
C	0	1.925159	0.643674	-3.551686
H	0	2.523364	-0.014801	4.471565
H	0	2.750002	2.588310	3.973250
H	0	0.105410	-0.853010	3.611791
H	0	-0.068978	0.573567	4.681441
H	0	2.286582	-1.173868	2.260597
H	0	3.153860	0.312335	1.854417
H	0	0.601494	3.358610	2.608076
H	0	-0.966674	1.246491	2.274173
H	0	1.280878	1.184165	0.703943
H	0	-0.871769	0.901281	-0.589747
H	0	-1.920225	-1.937353	-0.968787
H	0	1.172459	-1.002484	-1.608603
H	0	-2.811071	0.690905	-2.245513
H	0	-3.646866	-0.836887	-2.418282
H	0	0.292832	-1.427775	-3.828453
H	0	-3.231915	0.538665	0.294298
H	0	-4.024964	-1.021700	0.034960
H	0	-2.680242	-0.898143	1.176549
H	0	-2.063825	-0.207237	-4.367572
H	0	-1.982651	-1.835394	-3.724706
H	0	-1.171415	1.933475	-2.568706
H	0	0.425146	2.672252	-2.411475
H	0	-0.239768	2.329345	-4.013365
H	0	2.405363	-0.341419	-3.541758
H	0	1.918106	0.999488	-4.590537
H	0	2.557428	1.328677	-2.971199

Energy + ZPE = -1148.108778
Free energy = -1148.156389
Free energy in DCM = -1148.497758
Free energy in heptane = -1148.501518
Number of imaginary frequencies = 0

Product 17a+cpSiN

C	0	-0.535877	-1.254243	3.336436

C	0	-0.506400	0.266278	3.389308
C	0	-2.062856	-1.494691	3.323965
C	0	-0.167061	-1.651459	1.863167
C	0	-1.560907	0.715213	2.692612
C	0	-2.311924	-0.499520	2.166887
C	0	-1.404009	-1.171532	1.033199
B	0	-1.189427	-0.222587	-0.203975
Cl	0	-2.615609	-0.067801	-1.299926
C	0	0.146900	0.512024	-0.606589
C	0	0.026021	1.874431	-1.335725
C	0	0.900493	-0.541624	-1.461526
C	0	1.411801	2.359709	-1.790466
C	0	1.878437	-0.080382	-2.532715
C	0	-0.649805	2.931087	-0.451919
C	0	2.387765	-0.844001	-1.323285
C	0	2.087740	1.407782	-2.796245
C	0	3.248472	-0.171014	-0.268332
C	0	2.800848	-2.289010	-1.568944
H	0	0.047806	-1.775065	4.099659
H	0	0.296497	0.856501	3.820582
H	0	-2.346712	-2.526089	3.082244
H	0	-2.548135	-1.185360	4.255347
H	0	0.774617	-1.192585	1.549809
H	0	-0.043979	-2.737346	1.777007
H	0	-1.795683	1.745643	2.444716
H	0	-3.344095	-0.337029	1.851457
H	0	-1.969706	-2.047361	0.686874
H	0	0.716012	0.685963	0.318959
H	0	-0.595023	1.727331	-2.230603
H	0	0.305614	-1.409461	-1.750814
H	0	2.043142	2.508331	-0.903516
H	0	1.319077	3.350019	-2.256028
H	0	1.865142	-0.668421	-3.449953
H	0	-0.074541	3.101292	0.467829
H	0	-0.727428	3.891149	-0.976166
H	0	-1.663307	2.629648	-0.164202
H	0	3.158775	1.640868	-2.874548
H	0	1.662923	1.614607	-3.787581
H	0	3.217342	-0.735467	0.673240
H	0	4.296076	-0.140736	-0.594530
H	0	2.945329	0.853801	-0.047254
H	0	2.181270	-2.761101	-2.339916
H	0	3.846191	-2.349866	-1.899749
H	0	2.707459	-2.888001	-0.653217

Energy + ZPE = -1148.108229
Free energy = -1148.155655
Free energy in DCM = -1148.499266
Free energy in heptane = -1148.502439
Number of imaginary frequencies = 0

Product 17a+cpSiX

C	0	-1.151187	1.677072	2.407508
C	0	-1.119495	3.199853	2.378894
C	0	-2.677437	1.439790	2.489219
C	0	-0.839518	1.225916	0.928031
C	0	-2.207651	3.614572	1.713828
C	0	-2.986164	2.375734	1.298981
B	0	-0.493643	-0.276401	0.621503
C	0	-2.158423	1.668861	0.170681
Cl	0	-0.826961	-1.546172	1.850587
C	0	0.225949	-0.704781	-0.719206
C	0	-0.223343	-2.040801	-1.365312
C	0	1.737963	-0.704465	-0.379884
C	0	0.649455	-2.356202	-2.590639
C	0	2.683267	-1.601035	-1.166755
C	0	-1.707404	-2.007925	-1.753986
C	0	2.803662	-0.091864	-1.279851
C	0	2.141104	-2.536024	-2.244055
C	0	2.442393	0.638550	-2.561457
C	0	3.994006	0.540232	-0.571022
H	0	-0.533158	1.192202	3.165652
H	0	-0.291521	3.808308	2.730669
H	0	-2.970851	0.398599	2.319010
H	0	-3.108212	1.794298	3.430700
H	0	-0.002761	1.820286	0.534386
H	0	-2.451494	4.629523	1.415009
H	0	-4.037196	2.526833	1.039053
H	0	-2.726873	0.813418	-0.216020
H	0	-1.945579	2.328101	-0.675786
H	0	0.034642	0.091022	-1.456002
H	0	-0.078719	-2.840924	-0.625457
H	0	1.970263	-0.637840	0.683817
H	0	0.511943	-1.559621	-3.335009
H	0	0.289778	-3.275589	-3.071632
H	0	3.475377	-2.061607	-0.577008
H	0	-2.016379	-2.953813	-2.214821
H	0	-2.351590	-1.841488	-0.882523
H	0	-1.907472	-1.206989	-2.478371
H	0	2.749554	-2.471408	-3.156772
H	0	2.273766	-3.559024	-1.867594
H	0	3.290728	0.627628	-3.257778
H	0	1.586828	0.205881	-3.083034
H	0	2.205528	1.690502	-2.352747
H	0	4.244411	0.006454	0.352875
H	0	4.885758	0.531570	-1.211788
H	0	3.786705	1.585694	-0.306183

Energy + ZPE = -1148.108402
Free energy = -1148.155842
Free energy in DCM = -1148.498100
Free energy in heptane = -1148.501719
Number of imaginary frequencies = 0

Diels-Alder reaction with Vinylborane (17b)

TS 17b+cpReN

C	0	-1.233954	0.554967	3.172652
C	0	-1.233954	1.940375	3.172652
C	0	-2.664615	0.091136	3.172652
C	0	-2.523463	2.400860	2.849611

C	0	-3.352360	1.299172	2.557438
H	0	-0.388130	-0.078333	3.412642
H	0	-0.364633	2.572562	3.308355
H	0	-2.857905	-0.868536	2.691411
H	0	-2.999181	0.010790	4.221326
H	0	-2.794781	3.441532	2.709610
H	0	-4.435486	1.384819	2.534985
C	0	-2.936988	0.882822	0.622321
C	0	-1.682473	0.249348	0.577481
B	0	-0.360570	0.897159	0.225358
Br	0	-0.342716	2.859061	-0.009851
C	0	0.963330	0.106645	-0.140931
C	0	2.317275	0.750729	0.257471
C	0	0.890778	-0.136109	-1.667973
C	0	3.482026	-0.121059	-0.240029
C	0	2.169737	-0.342306	-2.465903
C	0	2.423070	0.982875	1.769380
C	0	1.174783	-1.480041	-2.324812
C	0	3.527741	-0.255433	-1.776260
C	0	1.501465	-2.716061	-1.504884
C	0	0.351216	-1.809627	-3.562315
H	0	-3.018243	1.881040	0.202213
H	0	-3.830746	0.274966	0.486757
H	0	-1.680748	-0.834954	0.703055
H	0	0.905580	-0.866007	0.373923
H	0	2.379014	1.729722	-0.239125
H	0	0.134132	0.456882	-2.181156
H	0	3.409068	-1.108334	0.238055
H	0	4.435486	0.304019	0.101609
H	0	2.174348	0.116618	-3.454307
H	0	2.306104	0.042157	2.325163
H	0	3.399565	1.404391	2.037731
H	0	1.653658	1.681455	2.114074
H	0	4.167241	-1.102891	-2.061097
H	0	4.024570	0.640151	-2.172732
H	0	0.581191	-3.211605	-1.166651
H	0	2.056786	-3.441532	-2.113757
H	0	2.105328	-2.504044	-0.620629
H	0	0.121981	-0.910377	-4.145243
H	0	0.887336	-2.505909	-4.221326
H	0	-0.602660	-2.280279	-3.288437

Energy + ZPE = -3259.575356
Free energy = -3259.624288
Free energy in DCM = -3259.962387
Free energy in heptane = -3259.964607
Number of imaginary frequencies = 1 (-398.72)

TS 17b+cpReX

C	0	2.390770	-0.116459	3.877037
C	0	2.390770	1.292886	3.877037
C	0	0.932217	-0.533521	3.877037
C	0	1.137639	1.754200	3.433631
C	0	0.295506	0.666968	3.244001
H	0	3.152432	-0.700317	4.386564
H	0	3.260202	1.918240	4.053397
H	0	0.701783	-1.491676	3.410818
H	0	0.601067	-0.583592	4.928918
H	0	0.895162	2.786561	3.204022
H	0	-0.744899	0.716624	2.946731
Br	0	0.387738	-2.786561	1.061715
B	0	0.563023	-0.878388	0.561625
C	0	-0.424688	-0.338513	-0.552695
C	0	1.707228	-0.080222	1.151590
C	0	-1.892468	-0.839787	-0.504015
C	0	0.229724	-0.676696	-1.914053
C	0	2.776984	-0.569478	1.920099
C	0	-2.687521	-0.240355	-1.674787
C	0	-0.637845	-0.814884	-3.156975
C	0	-2.568874	-0.523512	0.835473
C	0	0.363996	0.321272	-3.055584
C	0	-2.154592	-0.678538	-3.054347
C	0	-0.090208	1.763578	-2.913387
C	0	1.614742	0.192972	-3.914459
H	0	-0.455559	0.756840	-0.436625
H	0	1.789396	0.954493	0.816605
H	0	-1.875159	-1.932993	-0.620073
H	0	1.045989	-1.396249	-1.854104
H	0	2.844346	-1.646500	2.061834
H	0	3.742199	-0.072803	1.863956
H	0	-2.679906	0.854776	-1.580074
H	0	-3.742199	-0.537414	-1.598035
H	0	-0.336370	-1.606292	-3.842910
H	0	-2.556364	0.555592	1.043186
H	0	-3.617274	-0.846019	0.835929
H	0	-2.063990	-1.039871	1.659333
H	0	-2.573883	-1.670019	-3.271437
H	0	-2.542457	-0.012059	-3.837596
H	0	0.693810	2.372045	-2.442503
H	0	-0.290375	2.198350	-3.901399
H	0	-0.998105	1.877673	-2.317992
H	0	1.937036	-0.850605	-4.004002
H	0	1.440218	0.576146	-4.928918
H	0	2.449027	0.762741	-3.483678

Energy + ZPE = -3259.576256
Free energy = -3259.625383
Free energy in DCM = -3259.961937
Free energy in heptane = -3259.964800
Number of imaginary frequencies = 1 (-403.70)

TS 17b+cpSiN

C	0	2.953415	-1.550556	3.063486
C	0	3.044071	-0.143716	3.077123
C	0	1.480246	-1.870036	3.262765
C	0	1.774727	0.407786	2.823366
C	0	0.847528	-0.616548	2.723450
H	0	3.731927	-2.179543	3.486961
H	0	3.967307	0.422502	3.133211
H	0	1.129039	-2.808564	2.831822
H	0	1.288071	-1.910349	4.348819
H	0	1.578143	1.457737	2.642064

H	0	-0.215571	-0.494395	2.552450
Br	0	2.921114	0.954760	-0.322855
B	0	1.511229	-0.431562	-0.231595
C	0	0.167463	-0.112927	-1.008803
C	0	1.839764	-1.706053	0.510826
C	0	0.393246	-0.023612	-2.550615
C	0	-0.503180	1.166797	-0.474110
C	0	3.072075	-2.033971	1.103654
C	0	-0.937579	0.270182	-3.261294
C	0	-1.384262	2.005887	-1.386858
C	0	1.038625	-1.296390	-3.114943
C	0	-1.997798	1.285389	-0.201526
C	0	-1.562064	1.620503	-2.852136
C	0	-2.943924	0.112964	-0.395973
C	0	-2.398357	2.158983	0.979596
H	0	-0.502401	-0.972042	-0.843116
H	0	1.065000	-2.474009	0.542721
H	0	1.078797	0.817059	-2.732568
H	0	0.124515	1.748609	0.198228
H	0	3.942799	-1.445375	0.830073
H	0	3.293820	-3.083190	1.295441
H	0	-1.630052	-0.559698	-3.061410
H	0	-0.782781	0.271972	-4.348819
H	0	-1.295847	3.083190	-1.247934
H	0	0.414575	-2.177821	-2.914986
H	0	1.168516	-1.222747	-4.201606
H	0	2.024547	-1.481691	-2.673428
H	0	-2.622687	1.646322	-3.139699
H	0	-1.072510	2.404985	-3.444453
H	0	-2.967318	-0.522181	0.500428
H	0	-3.967307	0.472870	-0.565169
H	0	-2.678973	-0.524055	-1.242000
H	0	-1.710597	3.002358	1.109469
H	0	-3.407568	2.571184	0.844464
H	0	-2.401125	1.584422	1.916541

Energy + ZPE = -3259.576642
Free energy = -3259.625723
Free energy in DCM = -3259.962560
Free energy in heptane = -3259.965002
Number of imaginary frequencies = 1 (-392.48)

TS 17b+cpSiX

C	0	-1.271218	0.994968	2.357763
C	0	-1.258741	2.382808	2.321853
C	0	-2.691345	0.536876	2.212799
C	0	-2.512097	2.842704	1.876818
C	0	-3.310524	1.737028	1.521664
H	0	-0.458872	0.362650	2.696624
H	0	-0.398481	3.010453	2.529719
H	0	-2.827218	-0.428931	1.725816
H	0	-3.135349	0.469333	3.221167
H	0	-2.769707	3.882370	1.701379
H	0	-4.382961	1.817099	1.366485
Br	0	-2.002865	-2.008207	-0.284336
B	0	-0.744340	-0.475003	-0.270752
C	0	0.793041	-0.855289	-0.303707
C	0	-1.313839	0.925737	-0.278078
C	0	1.200961	-1.567101	-1.630347
C	0	1.175998	-1.711414	0.919525
C	0	-2.664476	1.298781	-0.373042
C	0	2.703022	-1.890355	-1.608162
C	0	2.341212	-2.686103	0.833915
C	0	0.841473	-0.733953	-2.867507
C	0	2.431787	-1.482227	1.751981
C	0	3.098894	-2.864071	-0.479186
C	0	3.389240	-0.339194	1.461249
C	0	2.309992	-1.765684	3.243217
H	0	1.351784	0.093785	-0.274248
H	0	-0.586657	1.737025	-0.326759
H	0	0.641487	-2.512846	-1.679196
H	0	0.322468	-2.085349	1.482330
H	0	-3.393640	0.513294	-0.562653
H	0	-2.922380	2.255619	-0.819638
H	0	3.261136	-0.946940	-1.528066
H	0	3.000684	-2.330652	-2.569598
H	0	2.191035	-3.629383	1.358728
H	0	1.158920	-1.239482	-3.787605
H	0	-0.238387	-0.559675	-2.938834
H	0	1.334952	0.246804	-2.840514
H	0	4.185087	-2.827330	-0.314734
H	0	2.883987	-3.882370	-0.829459
H	0	4.382961	-0.562854	1.871095
H	0	3.515394	-0.136454	0.396073
H	0	3.043714	0.589580	1.935643
H	0	1.612519	-2.587126	3.442146
H	0	3.281519	-2.041636	3.674948
H	0	1.948305	-0.881937	3.787605

Energy + ZPE = -3259.577057
Free energy = -3259.625938
Free energy in DCM = -3259.962217
Free energy in heptane = -3259.965040
Number of imaginary frequencies = 1 (-398.24)

Product 17b+cpReN

C	0	-1.550612	-0.473474	2.319234
C	0	-1.508283	0.902391	2.965217
C	0	-3.023095	-0.859427	2.594997
C	0	-2.715934	1.460698	2.801910
C	0	-3.580694	0.469937	2.037994
C	0	-3.018019	0.432628	0.571757
C	0	-1.630693	-0.268030	0.728514
B	0	-0.321933	0.384053	0.163457
Br	0	-0.257205	2.306786	-0.135214
C	0	0.945724	-0.467931	-0.229719
C	0	2.341758	0.157768	0.012987
C	0	0.723429	-0.808896	-1.725453
C	0	3.435197	-0.777914	-0.525484
C	0	1.925280	-1.102787	-2.611755
C	0	2.570495	0.471352	1.497183
C	0	0.920217	-2.200571	-2.311311

C	0	3.340517	-1.008420	-2.047500
C	0	1.284937	-3.389067	-1.438613
C	0	-0.014493	-2.585912	-3.449982
H	0	-0.779057	-1.182341	2.628830
H	0	-0.617559	1.370791	3.371584
H	0	-3.353619	-1.745636	2.039730
H	0	-3.228032	-0.991911	3.662265
H	0	-3.005432	2.478648	3.043240
H	0	-4.660918	0.624200	2.098487
H	0	-2.937760	1.435675	0.144785
H	0	-3.676440	-0.155755	-0.078054
H	0	-1.683476	-1.283445	0.308213
H	0	0.900146	-1.402308	0.352510
H	0	2.386069	1.103611	-0.545409
H	0	-0.058647	-0.227051	-2.215289
H	0	3.382808	-1.730258	0.020476
H	0	4.424630	-0.359955	-0.296949
H	0	1.854059	-0.708767	-3.625149
H	0	2.485775	-0.434992	2.111864
H	0	3.569914	0.890864	1.663818
H	0	1.840529	1.201706	1.864451
H	0	3.932473	-1.889204	-2.332695
H	0	3.818998	-0.153542	-2.543469
H	0	0.384527	-3.833526	-0.993433
H	0	1.768132	-4.168316	-2.041964
H	0	1.966697	-3.139608	-0.623503
H	0	-0.275018	-1.720480	-4.069717
H	0	0.448488	-3.336583	-4.104099
H	0	-0.949909	-3.013693	-3.065148

Energy + ZPE = -3259.617788
Free energy = -3259.666090
Free energy in DCM = -3260.006708
Free energy in heptane = -3260.010376
Number of imaginary frequencies = 0

Product 17b+cpReX

C	0	2.230129	-0.036534	3.666602
C	0	2.230129	1.484014	3.666602
C	0	0.708927	-0.313329	3.666602
C	0	2.595465	-0.489428	2.208128
C	0	1.164443	1.888286	2.960022
C	0	0.434244	0.643195	2.485131
C	0	1.385074	0.000392	1.352597
B	0	0.559076	-1.020183	0.493604
Br	0	0.501446	-2.901485	1.013675
C	0	-0.214132	-0.595908	-0.812135
C	0	-1.557457	-1.303688	-1.122586
C	0	0.818316	-0.803509	-1.949780
C	0	-2.100105	-0.823611	-2.477352
C	0	0.326729	-1.058793	-3.367461
C	0	-2.585876	-1.078415	-0.006807
C	0	1.080733	0.219622	-3.046025
C	0	-1.168012	-1.164101	-3.658168
C	0	0.385960	1.570132	-3.058962
C	0	2.513213	0.301819	-3.555978
H	0	2.826612	-0.520637	4.443851
H	0	3.025050	2.105085	4.068258
H	0	0.452784	-1.356457	3.455608
H	0	0.217412	0.013756	4.588264
H	0	2.694266	-1.578726	2.169278
H	0	3.540318	-0.054098	1.867953
H	0	0.913795	2.901485	2.660716
H	0	-0.606833	0.782345	2.182960
H	0	1.684231	0.813766	0.679152
H	0	-0.425876	0.481656	-0.723451
H	0	-1.360759	-2.383193	-1.189962
H	0	1.695414	-1.389155	-1.670494
H	0	-2.281869	0.258826	-2.419409
H	0	-3.081433	-1.279214	-2.664863
H	0	0.912813	-1.783568	-3.931829
H	0	-2.786889	-0.008207	0.138259
H	0	-3.540318	-1.563647	-0.243779
H	0	-2.232659	-1.491155	0.944896
H	0	-1.436832	-0.560825	-4.536370
H	0	-1.359418	-2.207471	-3.941921
H	0	-0.647831	1.532239	-2.710630
H	0	0.923548	2.288273	-2.425201
H	0	0.373009	1.980299	-4.076928
H	0	3.003981	-0.678002	-3.541888
H	0	2.544272	0.674828	-4.588264
H	0	3.112886	0.983924	-2.938651

Energy + ZPE = -3259.619242
Free energy = -3259.667519
Free energy in DCM = -3260.007876
Free energy in heptane = -3260.011829
Number of imaginary frequencies = 0

Product 17b+cpSiN

C	0	2.295129	-1.508653	3.613957
C	0	2.295129	0.012059	3.613957
C	0	0.773414	-1.778351	3.613957
C	0	2.671782	-1.948952	2.154205
C	0	1.233923	0.416820	2.902174
C	0	0.502655	-0.827554	2.424504
C	0	1.421173	-1.538755	1.312736
B	0	1.559753	-0.652809	0.028550
Br	0	3.126265	0.486825	-0.186272
C	0	0.464204	-0.563873	-1.106082
C	0	1.018764	-0.948868	-2.511379
C	0	-0.167753	0.844711	-1.123179
C	0	-0.099096	-0.844748	-3.559005
C	0	-0.750537	1.393724	-2.417864
C	0	1.645527	-2.349663	-2.513450
C	0	-1.666001	1.088687	-1.246978
C	0	-0.658199	0.585209	-3.709488
C	0	-2.661018	-0.057718	-1.302165
C	0	-2.212615	2.291059	-0.489160
H	0	2.888856	-1.992068	4.393775
H	0	3.092750	0.631892	4.011297
H	0	0.508292	-2.822356	3.407414

H	0	0.283317	-1.446321	4.534990
H	0	3.588278	-1.463012	1.810250
H	0	2.829312	-3.032846	2.107782
H	0	0.990173	1.432042	2.605897
H	0	-0.535490	-0.695082	2.111525
H	0	0.866892	-2.441611	1.016404
H	0	-0.312491	-1.305622	-0.862547
H	0	1.804226	-0.222086	-2.763248
H	0	0.359971	1.582327	-0.520818
H	0	-0.895766	-1.553867	-3.293811
H	0	0.280377	-1.176110	-4.534990
H	0	-0.583096	2.458075	-2.580527
H	0	0.916169	-3.111824	-2.208352
H	0	2.007288	-2.619480	-3.512841
H	0	2.500674	-2.410412	-1.828584
H	0	-1.629221	0.556406	-4.222954
H	0	0.017065	1.136195	-4.377312
H	0	-2.927247	-0.389568	-0.289363
H	0	-3.588278	0.266665	-1.791862
H	0	-2.292694	-0.928949	-1.847302
H	0	-1.487106	3.111824	-0.456790
H	0	-3.127302	2.674165	-0.961071
H	0	-2.461464	2.025183	0.547094

Energy + ZPE = -3259.617584
Free energy = -3259.666349
Free energy in DCM = -3260.005935
Free energy in heptane = -3260.009746
Number of imaginary frequencies = 0

Product 17b+cpSiX

C	0	-1.287300	1.336266	0.632412
C	0	-1.287300	2.855437	0.632412
C	0	-2.806090	1.053283	0.632412
C	0	-0.907418	0.913114	-0.879532
C	0	-2.360375	3.258076	-0.063946
C	0	-3.086457	2.012990	-0.547465
B	0	-0.459616	-0.588499	-0.899122
C	0	-2.183516	1.364736	-1.655808
Br	0	-1.776957	-1.989377	-1.252994
C	0	1.004734	-1.081634	-0.573963
C	0	1.646783	-1.852663	-1.770176
C	0	1.016909	-1.937135	0.709839
C	0	3.069960	-2.294232	-1.398537
C	0	2.088668	-3.000999	0.898629
C	0	1.648779	-1.014966	-3.055862
C	0	2.063179	-1.786048	1.806418
C	0	3.111649	-3.268041	-0.202059
C	0	3.150382	-0.727453	1.735545
C	0	1.577343	-2.021204	3.230254
H	0	-0.684757	0.853917	1.406016
H	0	-0.484715	3.471249	1.026802
H	0	-3.057670	0.009561	0.418708
H	0	-3.287187	1.371945	1.562372
H	0	-0.035750	1.511602	-1.173080
H	0	-2.614634	4.274892	-0.347385
H	0	-4.129077	2.146047	-0.846477
H	0	-2.698227	0.509786	-2.104862
H	0	-1.946704	2.072405	-2.456490
H	0	1.619730	-0.181692	-0.417693
H	0	1.036474	-2.750034	-1.946358
H	0	0.029724	-2.226248	1.065548
H	0	3.672747	-1.397329	-1.198226
H	0	3.540434	-2.781999	-2.262841
H	0	1.745088	-3.916654	1.378907
H	0	2.133287	-1.555410	-3.877725
H	0	0.630060	-0.769355	-3.381682
H	0	2.191744	-0.071197	-2.914095
H	0	4.129077	-3.310365	0.210780
H	0	2.902884	-4.274892	-0.586995
H	0	4.001613	-1.016091	2.365560
H	0	3.534284	-0.562869	0.726847
H	0	2.780244	0.236378	2.110499
H	0	0.791639	-2.784224	3.267288
H	0	2.398385	-2.356865	3.877725
H	0	1.167631	-1.100129	3.666463

Energy + ZPE = -3259.619004
Free energy = -3259.669780
Free energy in DCM = -3260.007197
Free energy in heptane = -3260.011131
Number of imaginary frequencies = 0

Diels-Alder reaction with Vinylborane (18a)

TS 18a+cpReN

C	0	0.020401	2.399638	1.636553
C	0	0.183805	3.792885	1.092211
C	0	1.661288	4.025003	1.357883
C	0	1.986680	3.200418	2.453660
C	0	1.012759	2.194500	2.584124
H	0	-0.878873	1.805633	1.523019
H	0	-0.386524	4.480117	1.740751
H	0	-0.152380	3.951737	0.066892
H	0	2.119452	4.999484	1.212236
H	0	2.912472	3.247013	3.016925
H	0	1.079870	1.344024	3.252715
C	0	0.273401	-2.774486	-1.817001
C	0	1.320142	-1.737888	-1.358590
C	0	0.667678	-0.701003	-0.400135
C	0	0.090950	-1.399544	0.868031
C	0	-0.535973	-2.778573	0.674419
C	0	-0.423761	-3.490576	-0.663404
C	0	1.976688	-1.078866	-2.579877
C	0	-1.788349	-3.080476	-0.125735
C	0	-2.601748	-1.977851	-0.780764
C	0	-2.664354	-4.207567	0.404045
Cl	0	3.140036	0.058252	0.948170
B	0	1.655879	0.485111	-0.019991
C	0	1.488080	1.923562	-0.473755
C	0	2.372616	2.991010	-0.245189

H	0	-0.454343	-2.269579	-2.468829
H	0	0.768202	-3.522420	-2.449624
H	0	2.100449	-2.268898	-0.793642
H	0	-0.161695	-0.240422	-0.960002
H	0	-0.624542	-0.724065	1.359525
H	0	0.915106	-1.531297	1.579747
H	0	-0.412408	-3.413012	1.552090
H	0	-0.219398	-4.559192	-0.614661
H	0	1.243359	-0.497828	-3.154991
H	0	2.787444	-0.399152	-2.294816
H	0	2.398571	-1.835768	-3.252715
H	0	-3.193489	-2.377072	-1.615614
H	0	-3.307791	-1.543081	-0.060719
H	0	-1.990068	-1.162693	-1.172288
H	0	-2.065906	-4.999484	0.868965
H	0	-3.371570	-3.839023	1.159507
H	0	-3.251463	-4.665340	-0.403583
H	0	0.627294	2.137086	-1.109318
H	0	2.332399	3.852863	-0.910112
H	0	3.371570	2.767195	0.117012

Energy + ZPE = -1148.065188
Free energy = -1148.113559
Free energy in DCM = -1148.452918
Free energy in heptane = -1148.454991
Number of imaginary frequencies = 1 (-402.78)

TS 18a+cpReX

C	0	0.591771	4.443646	0.236330
C	0	-0.740892	3.720412	0.275010
C	0	-0.561862	2.737969	-0.844213
C	0	0.402534	3.240101	-1.707955
C	0	1.065193	4.313222	-1.084233
H	0	0.781342	5.326150	0.841122
H	0	-1.520300	4.442264	-0.024903
H	0	-1.032615	3.296961	1.235957
H	0	-1.262844	1.943884	-1.072471
H	0	0.656838	2.824743	-2.677508
H	0	1.902408	4.860463	-1.505585
C	0	0.641211	-3.220825	1.017971
C	0	0.691381	-1.833580	1.690792
C	0	0.201073	-0.736517	0.704111
C	0	-1.266679	-1.004859	0.248877
C	0	-1.677557	-2.463814	0.061546
C	0	-0.735450	-3.584550	0.470518
C	0	2.105568	-1.556701	2.220294
C	0	-1.130582	-3.410353	-0.989584
C	0	-0.130986	-2.946703	-2.034691
C	0	-2.112309	-4.434030	-1.543209
Cl	0	-0.599027	1.142723	2.779650
B	0	0.366932	0.733696	1.284475
C	0	1.316421	1.772044	0.715818
C	0	1.658787	3.021382	1.257600
H	0	1.405002	-3.253756	0.227524
H	0	0.941749	-3.980472	1.750772
H	0	0.000706	-1.845337	2.546811
H	0	0.858653	-0.794068	-0.177470
H	0	-1.467364	-0.435647	-0.670571
H	0	-1.936573	-0.590349	1.012026
H	0	-2.728569	-2.628917	0.298348
H	0	-1.201786	-4.433934	0.967600
H	0	2.827380	-1.485145	1.395809
H	0	2.156668	-0.620756	2.788071
H	0	2.439651	-2.364905	2.882600
H	0	0.439242	-3.798320	-2.429790
H	0	-0.651831	-2.482360	-2.882600
H	0	0.588459	-2.218167	-1.655382
H	0	-2.827380	-4.760477	-0.779472
H	0	-2.687877	-4.018930	-2.381656
H	0	-1.587647	-5.326150	-1.911017
H	0	1.903340	1.452042	-0.145691
H	0	2.643577	3.434589	1.055146
H	0	1.270890	3.278334	2.241386

Energy + ZPE = -1148.064818
Free energy = -1148.113137
Free energy in DCM = -1148.451764
Free energy in heptane = -1148.454185
Number of imaginary frequencies = 1 (-400.99)

TS 18a+cpSiN

C	0	2.343493	2.570336	0.330433
C	0	3.314164	2.485928	1.477238
C	0	4.427564	1.671839	0.841356
C	0	4.341708	1.920903	-0.542303
C	0	3.062885	2.421057	-0.845822
H	0	1.340496	2.972033	0.411393
H	0	2.915848	2.105108	2.418456
H	0	3.705646	3.500181	1.667244
H	0	5.378357	1.515790	1.343643
H	0	5.090335	1.639347	-1.275077
H	0	2.675616	2.573683	-1.846398
C	0	-2.606954	0.074323	-1.208193
C	0	-1.088138	0.186946	-1.459918
C	0	-0.297005	-0.316344	-0.229702
C	0	-0.636917	-1.812796	0.093878
C	0	-2.074485	-2.263591	-0.156625
C	0	-3.064572	-1.332586	-0.835795
C	0	-0.730851	1.631157	-1.834293
C	0	-3.297654	-1.783148	0.600078
C	0	-3.181603	-0.815608	1.764866
C	0	-4.401209	-2.811072	0.808159
Cl	0	2.105261	-0.735096	-1.841906
B	0	1.288766	-0.243343	-0.290926
C	0	2.155273	0.036839	0.924749
C	0	3.542533	-0.155017	1.038300
H	0	-2.886142	0.800215	-0.430493
H	0	-3.141278	0.391529	-2.112686
H	0	-0.835515	-0.459233	-2.313122
H	0	-0.610360	0.299620	0.628463
H	0	-0.337799	-2.034118	1.127478
H	0	-0.003716	-2.446473	-0.541079

H	0	-2.128787	-3.307733	-0.464292
H	0	-3.721861	-1.796307	-1.569916
H	0	-0.940419	2.316167	-1.000919
H	0	0.326902	1.730972	-2.097837
H	0	-1.321345	1.972513	-2.693634
H	0	-4.126029	-0.275387	1.915969
H	0	-2.965456	-1.359853	2.693634
H	0	-2.394335	-0.070794	1.632730
H	0	-4.475310	-3.500181	-0.040936
H	0	-4.218466	-3.412324	1.709027
H	0	-5.378357	-2.323726	0.927272
H	0	1.628190	0.296195	1.844597
H	0	3.965566	-0.325017	2.027499
H	0	4.056247	-0.693333	0.247208

Energy + ZPE = -1148.064013
Free energy = -1148.111679
Free energy in DCM = -1148.452749
Free energy in heptane = -1148.454730
Number of imaginary frequencies = 1 (-403.87)

TS 18a+cpSiX

C	0	-1.474000	4.534000	-1.308500
C	0	-0.039000	4.044000	-1.337500
C	0	-0.202000	2.735000	-2.052500
C	0	-1.367000	2.798000	-2.804500
C	0	-2.115000	3.920000	-2.401500
H	0	-1.730000	5.533000	-0.964500
H	0	0.475000	4.000000	-0.376500
H	0	0.532000	4.724000	-1.993500
H	0	0.590000	2.007000	-2.173500
H	0	-1.688000	2.060000	-3.531500
H	0	-3.097000	4.186000	-2.780500
C	0	1.416000	-2.132000	0.622500
C	0	1.354000	-0.592000	0.690500
C	0	-0.117000	-0.117000	0.749500
C	0	-0.852000	-0.694000	2.009500
C	0	-0.459000	-2.102000	2.450500
C	0	0.697000	-2.823000	1.776500
C	0	2.117000	0.013000	-0.495500
C	0	-0.717000	-3.377000	1.671500
C	0	-1.481000	-3.363000	0.358500
C	0	-1.013000	-4.619000	2.500500
Cl	0	0.694000	2.470000	1.832500
B	0	-0.381000	1.449000	0.768500
C	0	-1.574000	2.095000	0.085500
C	0	-2.079000	3.390000	0.281500
H	0	1.012000	-2.456000	-0.348500
H	0	2.467000	-2.446000	0.622500
H	0	1.853000	-0.272000	1.616500
H	0	-0.618000	-0.507000	-0.150500
H	0	-1.938000	-0.626000	1.853500
H	0	-0.632000	-0.034000	2.859500
H	0	-0.520000	-2.226000	3.531500
H	0	1.355000	-3.382000	2.440500
H	0	1.632000	-0.248000	-1.446500
H	0	2.175000	1.104000	-0.427500
H	0	3.145000	-0.369000	-0.538500
H	0	-1.224000	-4.241000	-0.248500
H	0	-2.562000	-3.401000	0.546500
H	0	-1.286000	-2.475000	-0.246500
H	0	-0.455000	-4.616000	3.443500
H	0	-2.081000	-4.688000	2.744500
H	0	-0.738000	-5.533000	1.954500
H	0	-2.203000	1.423000	-0.499500
H	0	-3.145000	3.567000	0.165500
H	0	-1.616000	4.011000	1.046500

Energy + ZPE = -1148.064248
Free energy = -1148.112172
Free energy in DCM = -1148.451500
Free energy in heptane = -1148.454073
Number of imaginary frequencies = 1 (-403.90)

Product 18a+cpReN

C	0	-0.407230	2.581379	0.738173
C	0	-0.299651	4.110537	0.536639
C	0	1.169348	4.171077	1.013804
C	0	1.057029	3.404493	2.323495
C	0	0.121002	2.458798	2.160048
C	0	-0.497511	-2.508789	-2.014857
C	0	0.601298	-1.523555	-1.569016
C	0	0.048327	-0.561193	-0.480860
C	0	-0.435892	-1.345758	0.780602
C	0	-1.089750	-2.703674	0.530566
C	0	-1.099848	-3.309035	-0.864147
C	0	1.159996	-0.767165	-2.783091
C	0	-2.408484	-2.937783	-0.180243
C	0	-3.264762	-1.784134	-0.672889
C	0	-3.246728	-4.100272	0.334111
Cl	0	2.650406	0.044018	0.628712
B	0	1.080999	0.568581	-0.070197
C	0	0.763427	2.097099	-0.242498
C	0	1.849592	3.194037	-0.009056
H	0	-1.373966	2.115130	0.534468
H	0	-0.981401	4.668528	1.186723
H	0	-0.439146	4.424881	-0.504826
H	0	1.637259	5.157045	1.070311
H	0	1.714743	3.536097	3.177015
H	0	-0.141303	1.665527	2.853614
H	0	-1.271523	-1.947909	-2.558174
H	0	-0.069943	-3.206793	-2.745627
H	0	1.419405	-2.103827	-1.118522
H	0	-0.817590	-0.049324	-0.928555
H	0	-1.105314	-0.703594	1.370484
H	0	0.436934	-1.535804	1.416696
H	0	-0.895697	-3.405292	1.341478
H	0	-0.900718	-4.378333	-0.914899
H	0	0.391477	-0.127617	-3.237451
H	0	2.011739	-0.129758	-2.515848
H	0	1.505413	-1.465025	-3.555399
H	0	-3.932370	-2.115430	-1.479569

H	0	-3.898896	-1.404690	0.139074
H	0	-2.684987	-0.940779	-1.054066
H	0	-2.617681	-4.926417	0.684578
H	0	-3.884201	-3.788562	1.172264
H	0	-3.903115	-4.492609	-0.454113
H	0	0.352350	2.198640	-1.259878
H	0	2.079326	3.718503	-0.943923
H	0	2.786358	2.789844	0.382405

Energy + ZPE = -1148.107985
Free energy = -1148.156062
Free energy in DCM = -1148.498025
Free energy in heptane = -1148.501377
Number of imaginary frequencies = 0

Product 18a+cpReX

C	0	-2.921274	-2.490627	2.238594
C	0	-2.726865	-0.974261	2.470907
C	0	-1.197825	-1.036001	2.257886
C	0	-0.836283	-2.183482	3.186552
C	0	-1.862289	-3.046853	3.177080
C	0	2.203790	0.566377	-2.319347
C	0	0.788571	-0.002069	-2.091298
C	0	0.355204	0.219440	-0.612603
C	0	0.320206	1.737939	-0.257220
C	0	1.409502	2.608189	-0.880113
C	0	2.339666	2.037762	-1.938686
C	0	0.739271	-1.481436	-2.500395
C	0	2.896677	2.509663	-0.601789
C	0	3.458417	1.533677	0.417705
C	0	3.665988	3.823627	-0.625640
Cl	0	-2.494036	0.115670	-1.112933
B	0	-1.019680	-0.493600	-0.278825
C	0	-1.128294	-1.656776	0.770780
C	0	-2.355055	-2.620189	0.780239
H	0	-3.931971	-2.888315	2.359131
H	0	-2.991192	-0.662849	3.486274
H	0	-3.252901	-0.348845	1.741535
H	0	-0.632958	-0.110581	2.396108
H	0	0.133523	-2.312072	3.657547
H	0	-1.901929	-4.024187	3.648310
H	0	2.922935	-0.055294	-1.766854
H	0	2.463611	0.449201	-3.378980
H	0	0.088269	0.555714	-2.729982
H	0	1.118627	-0.270496	0.010656
H	0	0.319823	1.854567	0.836192
H	0	-0.637562	2.144538	-0.602868
H	0	1.062973	3.624950	-1.063802
H	0	2.557702	2.695280	-2.778789
H	0	1.382572	-2.091858	-1.853000
H	0	-0.276343	-1.892759	-2.446071
H	0	1.089337	-1.613783	-3.531213
H	0	4.519005	1.333294	0.215082
H	0	3.394613	1.957225	1.428545
H	0	2.941875	0.571677	0.434035
H	0	3.254389	4.518625	-1.366373
H	0	3.630297	4.321380	0.352699
H	0	4.722617	3.658113	-0.875061
H	0	-0.190336	-2.222740	0.705398
H	0	-2.069163	-3.649203	0.540856
H	0	-3.117199	-2.309844	0.058770

Energy + ZPE = -1148.107858
Free energy = -1148.155638
Free energy in DCM = -1148.497879
Free energy in heptane = -1148.501516
Number of imaginary frequencies = 0

Product 18a+cpSiN

C	0	-2.263284	1.797704	-2.119777
C	0	-2.090502	3.331898	-2.208319
C	0	-0.548555	3.262779	-2.116636
C	0	-0.260497	2.225333	-3.193496
C	0	-1.279223	1.353386	-3.195830
C	0	0.630385	-1.630686	2.760355
C	0	-0.560833	-1.340611	1.824235
C	0	-0.110212	-0.425181	0.656222
C	0	1.020544	-1.094527	-0.196702
C	0	2.037187	-1.938044	0.569940
C	0	1.834410	-2.237690	2.046295
C	0	-1.721490	-0.727909	2.620562
C	0	3.035227	-1.421346	1.587618
C	0	3.160136	0.059054	1.903102
C	0	4.380453	-2.133980	1.622556
Cl	0	-2.324237	-1.264538	-1.009477
B	0	-1.258262	0.022021	-0.333772
C	0	-1.568646	1.510100	-0.732708
C	0	-0.369605	2.528634	-0.743066
H	0	-3.275951	1.399224	-2.198821
H	0	-2.556040	3.873945	-1.375589
H	0	-2.440570	3.746012	-3.159067
H	0	0.002102	4.204000	-2.191784
H	0	0.663678	2.161174	-3.759923
H	0	-1.361946	0.434380	-3.766561
H	0	0.903543	-0.699636	3.277535
H	0	0.301063	-2.320554	3.547353
H	0	-0.900475	-2.294656	1.396765
H	0	0.296318	0.490858	1.109693
H	0	1.531074	-0.325441	-0.793168
H	0	0.546101	-1.768834	-0.920664
H	0	2.407405	-2.770151	-0.028395
H	0	2.068854	-3.254898	2.356108
H	0	-1.445192	0.255054	3.025095
H	0	-2.619253	-0.599405	2.004537
H	0	-1.995965	-1.366837	3.468584
H	0	3.812841	0.552314	1.170965
H	0	2.205740	0.589626	1.897844
H	0	3.612094	0.206017	2.893209
H	0	4.277391	-3.200932	1.394526
H	0	5.076697	-1.702970	0.890732
H	0	4.846180	-2.048672	2.613468
H	0	-2.273991	1.827605	0.059789

H	0	-0.442054	3.239130	0.088341
H	0	0.610755	2.047206	-0.676689

Energy + ZPE = -1148.107866
Free energy = -1148.155348
Free energy in DCM = -1148.498022
Free energy in heptane = -1148.501481
Number of imaginary frequencies = 0

Product 18a+cpSiX

C	0	-2.817803	-2.291929	-2.572510
C	0	-2.870616	-0.748417	-2.629770
C	0	-1.337690	-0.591248	-2.516867
C	0	-0.881311	-1.557324	-3.597616
C	0	-1.762793	-2.567333	-3.632221
C	0	1.551372	2.525018	1.147864
C	0	0.161964	1.941990	0.814382
C	0	0.281216	0.436563	0.477670
C	0	0.875916	-0.381164	1.677660
C	0	1.948586	0.319918	2.509076
C	0	2.275528	1.784436	2.268282
C	0	-0.478878	2.738893	-0.330280
C	0	3.329098	0.712552	2.020694
C	0	3.804845	0.367365	0.620351
C	0	4.448517	0.626436	3.049278
Cl	0	-2.537872	0.002808	1.005085
B	0	-1.042165	-0.319147	0.057173
C	0	-1.059216	-1.354757	-1.124294
C	0	-2.126734	-2.492019	-1.176705
H	0	-3.763778	-2.828322	-2.680129
H	0	-3.426234	-0.298355	-1.800343
H	0	-3.255435	-0.371325	-3.582460
H	0	-0.930695	0.421174	-2.574101
H	0	0.057814	-1.479229	-4.136982
H	0	-1.691678	-3.480882	-4.214643
H	0	2.153799	2.537586	0.227955
H	0	1.433524	3.576423	1.438014
H	0	-0.475196	2.042736	1.704674
H	0	0.977562	0.349032	-0.370846
H	0	1.246365	-1.348208	1.309726
H	0	0.057343	-0.616214	2.370653
H	0	1.918746	0.012512	3.554070
H	0	2.439723	2.382292	3.163463
H	0	0.109002	2.640495	-1.252970
H	0	-1.500264	2.403534	-0.542335
H	0	-0.528032	3.807069	-0.086217
H	0	4.628705	1.027649	0.318233
H	0	4.184385	-0.662344	0.588830
H	0	3.024022	0.450270	-0.138249
H	0	4.090663	0.871007	4.055901
H	0	4.877276	-0.384001	3.085209
H	0	5.261680	1.323414	2.806415
H	0	-0.045526	-1.771846	-1.186554
H	0	-1.673323	-3.483627	-1.081532
H	0	-2.867759	-2.386717	-0.378100

Energy + ZPE = -1148.108038
Free energy = -1148.155677
Free energy in DCM = -1148.498353
Free energy in heptane = -1148.501954
Number of imaginary frequencies = 0

Diels-Alder reaction with Vinylborane (18b)

TS 18b+cpReN

C	0	0.073801	2.458991	1.716705
C	0	0.265975	3.850632	1.181244
C	0	1.768399	4.013462	1.350703
C	0	2.129087	3.147561	2.403818
C	0	1.119873	2.183225	2.581533
H	0	-0.853974	1.903550	1.645674
H	0	-0.229830	4.554637	1.871563
H	0	-0.128418	4.038245	0.181632
H	0	2.252650	4.976154	1.209781
H	0	3.091896	3.137737	2.902770
H	0	1.196493	1.313484	3.223116
C	0	0.352485	-2.808765	-1.821363
C	0	1.361842	-1.733780	-1.371375
C	0	0.655286	-0.671086	-0.482194
C	0	0.059614	-1.330752	0.798841
C	0	-0.526708	-2.732051	0.645744
C	0	-0.363023	-3.493196	-0.660009
C	0	2.059770	-1.111313	-2.588459
C	0	-1.749996	-3.093889	-0.174630
C	0	-2.568853	-2.034278	-0.891152
C	0	-2.615177	-4.219362	0.375604
Br	0	3.231601	0.103102	0.928233
B	0	1.605389	0.543719	-0.114285
C	0	1.426175	1.984729	-0.532201
C	0	2.339045	3.033473	-0.316276
H	0	-0.364966	-2.346550	-2.514876
H	0	0.882341	-3.570240	-2.407709
H	0	2.129306	-2.220708	-0.752050
H	0	-0.166384	-0.251567	-1.084475
H	0	-0.685110	-0.654174	1.242775
H	0	0.871730	-1.408728	1.532248
H	0	-0.411119	-3.328071	1.551068
H	0	-0.137384	-4.554122	-0.562283
H	0	1.349767	-0.545256	-3.206090
H	0	2.860916	-0.427033	-2.287577
H	0	2.505887	-1.887050	-3.223116
H	0	-3.143835	-2.480205	-1.713940
H	0	-3.289854	-1.575946	-0.201221
H	0	-1.962217	-1.230263	-1.312346
H	0	-2.012848	-4.976154	0.891308
H	0	-3.353924	-3.837549	1.093360
H	0	-3.165830	-4.724762	-0.429280
H	0	0.535856	2.225702	-1.115630
H	0	2.276026	3.915458	-0.952778
H	0	3.353924	2.771461	-0.031011

Energy + ZPE = -3259.576541
Free energy = -3259.625245
Free energy in DCM = -3259.964199
Free energy in heptane = -3259.966381
Number of imaginary frequencies = 1 (-391.55)

TS 18b+cpReX

C	0	0.556528	4.456333	0.258303
C	0	-0.759291	3.701143	0.265927
C	0	-0.563174	2.778362	-0.898470
C	0	0.392430	3.333775	-1.737648
C	0	1.030265	4.394727	-1.068382
H	0	0.720988	5.321440	0.894945
H	0	-1.555389	4.419814	0.004671
H	0	-1.040787	3.221307	1.203494
H	0	-1.240579	1.972815	-1.155868
H	0	0.656463	2.965362	-2.723394
H	0	1.854654	4.978360	-1.465578
C	0	0.639187	-3.222667	1.015353
C	0	0.710763	-1.829446	1.670459
C	0	0.274482	-0.736610	0.655287
C	0	-1.195589	-0.969617	0.182787
C	0	-1.651774	-2.419312	0.031563
C	0	-0.743942	-3.558849	0.465730
C	0	2.113427	-1.572996	2.238094
C	0	-1.129033	-3.402064	-0.998688
C	0	-0.113952	-2.981339	-2.046740
C	0	-2.135461	-4.409638	-1.536758
Br	0	-0.565383	1.164180	2.861546
B	0	0.456238	0.735891	1.214041
C	0	1.368595	1.797251	0.642615
C	0	1.678788	3.047354	1.206593
H	0	1.406768	-3.281924	0.230198
H	0	0.917354	-3.980171	1.759185
H	0	-0.003600	-1.807088	2.506233
H	0	0.947689	-0.825354	-0.212411
H	0	-1.364771	-0.420937	-0.755152
H	0	-1.855676	-0.507781	0.927263
H	0	-2.707851	-2.546539	0.269155
H	0	-1.237095	-4.384297	0.977137
H	0	2.860320	-1.507403	1.435709
H	0	2.152168	-0.638199	2.808643
H	0	2.419441	-2.384591	2.909871
H	0	0.446588	-3.850503	-2.416554
H	0	-0.620801	-2.529650	-2.909871
H	0	0.611693	-2.254096	-1.677285
H	0	-2.860320	-4.704545	-0.769318
H	0	-2.698492	-3.995118	-2.384010
H	0	-1.633335	-5.321440	-1.887489
H	0	1.946592	1.511240	-0.237002
H	0	2.648381	3.494504	1.002155
H	0	1.303130	3.254310	2.207114

Energy + ZPE = -3259.576745
Free energy = -3259.625717
Free energy in DCM = -3259.963395
Free energy in heptane = -3259.965932
Number of imaginary frequencies = 1 (-398.97)

TS 18b+cpSiN

C	0	2.398487	2.655207	0.297731
C	0	3.402184	2.536511	1.411077
C	0	4.443480	1.641187	0.758682
C	0	4.314282	1.852468	-0.628497
C	0	3.055670	2.421426	-0.898225
H	0	1.420005	3.107928	0.405779
H	0	3.013766	2.200328	2.373589
H	0	3.859937	3.528652	1.566390
H	0	5.408839	1.462278	1.224631
H	0	5.013774	1.505780	-1.381219
H	0	2.638557	2.566680	-1.887415
C	0	-2.619521	0.080296	-1.210757
C	0	-1.098163	0.198564	-1.436563
C	0	-0.331181	-0.303739	-0.189692
C	0	-0.658645	-1.809651	0.098878
C	0	-2.086669	-2.270474	-0.186543
C	0	-3.073365	-1.335167	-0.866012
C	0	-0.729505	1.638439	-1.814035
C	0	-3.327035	-1.814410	0.556882
C	0	-3.239212	-0.869416	1.742239
C	0	-4.425641	-2.854928	0.725393
Br	0	2.159811	-0.730939	-1.890421
B	0	1.250649	-0.206219	-0.213720
C	0	2.125054	0.092987	0.984037
C	0	3.512410	-0.121817	1.075423
H	0	-2.914601	0.795705	-0.429072
H	0	-3.140501	0.405636	-2.120182
H	0	-0.825253	-0.451807	-2.280296
H	0	-0.674147	0.297857	0.667495
H	0	-0.373463	-2.050779	1.132066
H	0	-0.004952	-2.416391	-0.541590
H	0	-2.124792	-3.309072	-0.514896
H	0	-3.713943	-1.792173	-1.618982
H	0	-0.910050	2.326486	-0.976623
H	0	0.324571	1.713085	-2.098759
H	0	-1.330090	1.988993	-2.662630
H	0	-4.192205	-0.343857	1.890952
H	0	-3.028813	-1.429937	2.662630
H	0	-2.459301	-0.113021	1.635353
H	0	-4.478088	-3.528652	-0.137529
H	0	-4.255033	-3.471314	1.618349
H	0	-5.408839	-2.377608	0.834875
H	0	1.619782	0.398464	1.902232
H	0	3.951478	-0.257842	2.063097
H	0	3.987574	-0.716219	0.300473

Energy + ZPE = -3259.575524
Free energy = -3259.624611
Free energy in DCM = -3259.963658
Free energy in heptane = -3259.965747
Number of imaginary frequencies = 1 (-395.53)

TS 18b+cpSiX

C	0	-1.451394	4.536204	-1.296635
C	0	-0.024494	4.023802	-1.344079
C	0	-0.212436	2.729651	-2.077068
C	0	-1.386045	2.813930	-2.812652
C	0	-2.113039	3.942709	-2.390466
H	0	-1.687442	5.537381	-0.946371
H	0	0.497315	3.953345	-0.389322
H	0	0.552443	4.705922	-1.992476
H	0	0.565337	1.987119	-2.206862
H	0	-1.725452	2.087214	-3.543348
H	0	-3.094906	4.226174	-2.756053
C	0	1.416737	-2.121786	0.634065
C	0	1.336496	-0.582947	0.705258
C	0	-0.141806	-0.126437	0.756312
C	0	-0.858534	-0.698837	2.026500
C	0	-0.459005	-2.106988	2.462500
C	0	0.699283	-2.821054	1.785321
C	0	2.108690	0.043896	-0.462564
C	0	-0.712979	-3.380833	1.679864
C	0	-1.478666	-3.371940	0.368201
C	0	-1.002154	-4.625828	2.507585
Br	0	0.763824	2.548098	1.887442
B	0	-0.421484	1.433111	0.755642
C	0	-1.605983	2.094087	0.084231
C	0	-2.075272	3.403925	0.282595
H	0	1.021808	-2.448820	-0.339037
H	0	2.471786	-2.423582	0.641154
H	0	1.817836	-0.257074	1.638704
H	0	-0.639891	-0.533299	-0.137868
H	0	-1.946619	-0.630466	1.891165
H	0	-0.618735	-0.034648	2.867651
H	0	-0.519157	-2.233742	3.543348
H	0	1.360041	-3.380166	2.446178
H	0	1.633461	-0.192648	-1.424717
H	0	2.161253	1.132751	-0.359614
H	0	3.137199	-0.335714	-0.503483
H	0	-1.229541	-4.258362	-0.230711
H	0	-2.559956	-3.399636	0.556764
H	0	-1.277412	-2.492780	-0.246826
H	0	-0.441560	-4.624028	3.449492
H	0	-2.069620	-4.697022	2.756334
H	0	-0.728404	-5.537381	1.959251
H	0	-2.249356	1.438358	-0.504223
H	0	-3.137199	3.609056	0.173869
H	0	-1.589517	4.001616	1.051769

Energy + ZPE = -3259.576285
Free energy = -3259.624879
Free energy in DCM = -3259.963375
Free energy in heptane = -3259.966053
Number of imaginary frequencies = 1 (-400.68)

Product 18b+cpReN

C	0	-0.659904	2.615967	0.839608
C	0	-0.579125	4.141359	0.599001
C	0	0.944680	4.201969	0.848194
C	0	1.027900	3.457265	2.171641
C	0	0.077655	2.511877	2.165291
C	0	-0.723535	-2.570824	-2.092966
C	0	0.327631	-1.550612	-1.614154
C	0	-0.309235	-0.567471	-0.590690
C	0	-0.836551	-1.329129	0.667654
C	0	-1.444678	-2.708468	0.423622
C	0	-1.371113	-3.350883	-0.952240
C	0	0.953879	-0.819064	-2.809507
C	0	-2.720464	-2.990071	-0.345802
C	0	-3.572073	-1.866573	-0.910725
C	0	-3.560996	-4.155938	0.156840
Br	0	2.353784	0.054711	0.669845
B	0	0.674230	0.593381	-0.159537
C	0	0.343060	2.117078	-0.313701
C	0	1.460701	3.206052	-0.250611
H	0	-1.647831	2.151949	0.791047
H	0	-1.153411	4.712163	1.336026
H	0	-0.874544	4.439927	-0.414142
H	0	1.417898	5.186530	0.816847
H	0	1.807974	3.597188	2.913339
H	0	-0.074533	1.728793	2.901339
H	0	-1.477413	-2.042158	-2.693990
H	0	-0.241913	-3.279874	-2.778065
H	0	1.126024	-2.096787	-1.091645
H	0	-1.161536	-0.090491	-1.099346
H	0	-1.548618	-0.688699	1.207593
H	0	0.012369	-1.476842	1.345979
H	0	-1.276443	-3.382558	1.263130
H	0	-1.149130	-4.416856	-0.961889
H	0	0.212338	-0.196538	-3.327753
H	0	1.781887	-0.170922	-2.497678
H	0	1.354035	-1.532363	-3.540119
H	0	-4.198266	-2.232726	-1.735328
H	0	-4.247091	-1.473143	-0.139369
H	0	-2.987555	-1.026613	-1.291586
H	0	-2.935141	-4.958768	0.562890
H	0	-4.247993	-3.835655	0.951601
H	0	-4.167097	-4.583667	-0.652969
H	0	-0.220532	2.223181	-1.252823
H	0	1.557406	3.716001	-1.216244
H	0	2.438487	2.791906	0.007452

Energy + ZPE = -3259.617370
Free energy = -3259.666145
Free energy in DCM = -3260.007146
Free energy in heptane = -3260.010718
Number of imaginary frequencies = 0

Product 18b+cpReX

C	0	-2.697861	-2.473301	2.343052
C	0	-2.524456	-0.946722	2.516078
C	0	-0.983546	-1.010946	2.428870
C	0	-0.693420	-2.112689	3.434056

C	0	-1.716158	-2.978983	3.387949
C	0	2.459731	0.621466	-2.245850
C	0	1.069541	0.012429	-1.982169
C	0	0.708268	0.136966	-0.474873
C	0	0.666094	1.634706	-0.026284
C	0	1.682071	2.570991	-0.677327
C	0	2.570150	2.079229	-1.809407
C	0	1.014822	-1.441284	-2.472922
C	0	3.185424	2.515953	-0.487440
C	0	3.831586	1.516753	0.456561
C	0	3.910993	3.854504	-0.498021
Br	0	-2.241979	0.055277	-1.057046
B	0	-0.651806	-0.583144	-0.112609
C	0	-0.797529	-1.698747	0.979317
C	0	-2.012871	-2.678078	0.945528
H	0	-3.714252	-2.870414	2.401377
H	0	-2.869735	-0.588081	3.490811
H	0	-2.985208	-0.358383	1.716206
H	0	-0.432389	-0.077368	2.567041
H	0	0.237310	-2.215213	3.983706
H	0	-1.791504	-3.932979	3.900858
H	0	3.217243	-0.003386	-1.751629
H	0	2.676229	0.556036	-3.319628
H	0	0.326257	0.592504	-2.547361
H	0	1.503909	-0.378255	0.085298
H	0	0.746715	1.688363	1.068780
H	0	-0.326383	2.028625	-0.275398
H	0	1.288160	3.579743	-0.798320
H	0	2.714997	2.778952	-2.631038
H	0	1.688664	-2.082521	-1.889461
H	0	0.002325	-1.856287	-2.396525
H	0	1.318861	-1.512883	-3.524190
H	0	4.872773	1.325423	0.164334
H	0	3.848266	1.914504	1.479683
H	0	3.317918	0.553632	0.490326
H	0	3.439237	4.563593	-1.187744
H	0	3.912907	4.312358	0.500212
H	0	4.957172	3.733541	-0.809424
H	0	0.150655	-2.250674	1.002433
H	0	-1.698096	-3.715140	0.792761
H	0	-2.710722	-2.418174	0.143756

Energy + ZPE = -3259.618390
Free energy = -3259.666635
Free energy in DCM = -3260.008247
Free energy in heptane = -3260.012041
Number of imaginary frequencies = 0

Product 18b+cpSiN

C	0	-2.115955	1.995618	-1.882081
C	0	-1.940235	3.529095	-1.972566
C	0	-0.398429	3.446222	-2.057039
C	0	-0.243934	2.419589	-3.170824
C	0	-1.264343	1.555919	-3.067674
C	0	0.845916	-1.468536	2.903060
C	0	-0.301529	-1.173734	1.917128
C	0	0.206417	-0.254933	0.771613
C	0	1.357662	-0.942513	-0.035986
C	0	2.327622	-1.805360	0.768026
C	0	2.066152	-2.097794	2.236475
C	0	-1.505089	-0.569922	2.653300
C	0	3.297734	-1.305213	1.820628
C	0	3.434006	0.173308	2.140003
C	0	4.627965	-2.040898	1.906720
Br	0	-1.985774	-1.219951	-1.054326
B	0	-0.917216	0.200396	-0.239258
C	0	-1.274710	1.686332	-0.586893
C	0	-0.070060	2.694425	-0.720546
H	0	-3.133193	1.601627	-1.849241
H	0	-2.303219	4.065185	-1.086541
H	0	-2.391057	3.958109	-2.872834
H	0	0.149194	4.383899	-2.182564
H	0	0.610747	2.353815	-3.837335
H	0	-1.416464	0.639591	-3.627131
H	0	1.110608	-0.535657	3.421447
H	0	0.478339	-2.147503	3.682639
H	0	-0.619772	-2.123170	1.463953
H	0	0.603895	0.656219	1.243968
H	0	1.906084	-0.182381	-0.610019
H	0	0.893214	-1.603437	-0.778122
H	0	2.703172	-2.645680	0.184677
H	0	2.269011	-3.118913	2.555565
H	0	-1.262708	0.417032	3.069738
H	0	-2.367896	-0.455740	1.986416
H	0	-1.817881	-1.210995	3.486272
H	0	4.136545	0.651880	1.445294
H	0	2.491053	0.720255	2.078086
H	0	3.830972	0.314630	3.154197
H	0	4.514490	-3.107247	1.680604
H	0	5.356715	-1.626160	1.197479
H	0	5.060244	-1.958332	2.912912
H	0	-1.875284	2.003587	0.287395
H	0	-0.039829	3.393979	0.122538
H	0	0.906116	2.202052	-0.771776

Energy + ZPE = -3259.617645
Free energy = -3259.666006
Free energy in DCM = -3260.007207
Free energy in heptane = -3260.010786
Number of imaginary frequencies = 0

Product 18b+cpSiX

C	0	-2.550008	-2.323495	-2.638849
C	0	-2.611465	-0.780006	-2.705796
C	0	-1.075981	-0.617109	-2.668331
C	0	-0.666202	-1.592747	-3.758871
C	0	-1.546116	-2.604690	-3.745169
C	0	1.855034	2.519100	1.055782
C	0	0.474821	1.931996	0.698049
C	0	0.610031	0.432188	0.340405
C	0	1.175783	-0.392526	1.550656

C	0	2.231953	0.304014	2.406383
C	0	2.561593	1.770714	2.182557
C	0	-0.173017	2.741722	-0.433225
C	0	3.621130	0.702527	1.947606
C	0	4.125906	0.370011	0.554119
C	0	4.721391	0.610583	2.996371
Br	0	-2.336210	0.059303	0.888345
B	0	-0.699300	-0.322851	-0.109840
C	0	-0.730431	-1.365780	-1.280459
C	0	-1.789791	-2.513098	-1.278456
H	0	-3.497726	-2.864591	-2.696071
H	0	-3.122427	-0.324151	-1.852016
H	0	-3.044709	-0.412302	-3.641251
H	0	-0.675691	0.396125	-2.753615
H	0	0.246483	-1.516515	-4.342097
H	0	-1.499440	-3.522494	-4.323383
H	0	2.472463	2.544642	0.146238
H	0	1.726603	3.566754	1.355095
H	0	-0.171468	2.007967	1.584177
H	0	1.327218	0.356161	-0.491751
H	0	1.549599	-1.361636	1.191748
H	0	0.336786	-0.620806	2.221462
H	0	2.182720	-0.011803	3.448225
H	0	2.707129	2.362178	3.085148
H	0	0.400914	2.649781	-1.365349
H	0	-1.197699	2.406743	-0.627169
H	0	-0.216911	3.807592	-0.178428
H	0	4.960951	1.028116	0.279266
H	0	4.499319	-0.661772	0.518724
H	0	3.363534	0.467717	-0.221212
H	0	4.344686	0.844568	3.998601
H	0	5.153207	-0.398612	3.030493
H	0	5.536274	1.312619	2.774758
H	0	0.285544	-1.770616	-1.375533
H	0	-1.323209	-3.500306	-1.203107
H	0	-2.488044	-2.407074	-0.442421

Energy + ZPE = -3259.618874
Free energy = -3259.667160
Free energy in DCM = -3260.008822
Free energy in heptane = -3260.012630
Number of imaginary frequencies = 0

C	0	-2.083866	0.106605	1.700035
C	0	-3.132546	0.593923	-1.495525
C	0	-2.488527	-1.447309	-1.832288
O	0	-1.013676	-0.077435	2.634290
C	0	-4.516012	0.570486	-2.170981
C	0	-2.903750	2.019219	-0.978788
H	0	2.240928	1.059761	-0.166277
H	0	-0.314371	1.014178	0.118855
H	0	4.382853	-0.039830	-0.484431
H	0	3.609601	-1.683863	-0.355838
H	0	-1.512749	-1.635547	0.668886
H	0	-0.301243	1.222725	-2.134108
H	0	0.063835	-0.465903	-2.415555
H	0	-3.830879	-1.023932	-0.035948
H	0	-2.091109	0.096308	-3.471408
H	0	-3.012038	-0.334116	2.098208
H	0	-2.267874	1.178908	1.540028
H	0	-1.712459	-2.206196	-1.689014
H	0	-3.316779	-1.891114	-2.389040
H	0	-1.280716	0.331257	3.471408
H	0	-4.781297	-0.408497	-2.579860
H	0	-5.297792	0.850040	-1.452699
H	0	-4.552728	1.293788	-2.995787
H	0	-3.665885	2.292572	-0.237224
H	0	-1.924141	2.169235	-0.521961
H	0	-2.992036	2.735482	-1.806599
C	0	4.223944	-0.669564	1.814653
C	0	3.578826	0.637396	2.242048
C	0	3.453095	-1.688187	2.406969
C	0	2.162195	0.183613	2.466978
C	0	2.191353	-1.173443	2.754571
H	0	5.297792	-0.758746	1.673638
H	0	4.006590	0.919974	3.219605
H	0	3.712598	1.484318	1.567273
H	0	3.732908	-2.735482	2.451664
H	0	1.316211	0.835345	2.640293
H	0	1.338133	-1.753124	3.085162

Energy + ZPE = -1223.256574
Free energy = -1223.304539
Free energy in DCM = -1223.657144
Free energy in heptane = -1223.656179
Number of imaginary frequencies = 1 (-405.60)

Diels-Alder reaction with Vinylborane (19a)

TS 19a+cpReN

Cl	0	0.924526	-2.563618	-0.093077
B	0	0.924526	-0.742426	-0.093077
C	0	2.266655	-0.028861	-0.093077
C	0	-0.457469	0.011304	-0.303217
C	0	3.537013	-0.625119	-0.126481
C	0	-1.727918	-0.596051	0.388992
C	0	-0.614352	0.204933	-1.870518
C	0	-2.938480	-0.665503	-0.566846
C	0	-2.032693	-0.073554	-2.388115

TS 19a+cpReX

C	0	-1.043477	1.255952	2.550812
C	0	-1.043477	2.756767	2.550812
C	0	-2.366823	0.832570	2.550812
C	0	-2.407496	3.048069	1.956128
C	0	-3.202974	1.923926	2.249977
H	0	-0.168758	0.652958	2.767609
H	0	-1.057901	3.095995	3.601149
H	0	-0.192912	3.230845	2.061199
H	0	-2.698457	-0.192381	2.681606
H	0	-2.811403	4.055813	1.909585
H	0	-4.280384	1.871170	2.128293

Cl	0	1.469483	2.831186	-0.038497
B	0	0.391072	1.355749	-0.127760
C	0	-1.112493	1.538220	-0.035675
C	0	1.044914	-0.057816	-0.439269
C	0	-1.850989	2.731174	-0.005750
C	0	2.537250	-0.284167	-0.039589
C	0	0.737728	-0.439711	-1.940965
C	0	3.282030	-1.200219	-1.036290
C	0	1.846480	-1.282959	-2.593334
C	0	2.668479	-0.746639	1.415957
C	0	2.425794	-2.380875	-1.633825
C	0	3.186015	-0.518427	-2.429835
O	0	2.086097	0.175440	2.341374
C	0	3.323625	-3.381402	-2.387747
C	0	1.477800	-3.213738	-0.761192
H	0	-1.698781	0.625020	-0.146972
H	0	0.455218	-0.751763	0.172580
H	0	-2.855623	2.743615	-0.420210
H	0	-1.318463	3.672946	-0.123002
H	0	3.067757	0.678720	-0.093482
H	0	-0.223389	-0.967271	-1.979068
H	0	0.610086	0.460519	-2.557648
H	0	4.280384	-1.458610	-0.657884
H	0	1.549911	-1.601853	-3.601149
H	0	3.732047	-0.907433	1.657111
H	0	2.147322	-1.694167	1.585761
H	0	3.132815	0.576259	-2.435205
H	0	3.961760	-0.833675	-3.130585
H	0	2.449247	1.053496	2.139853
H	0	4.051323	-2.904511	-3.050043
H	0	3.884052	-4.001525	-1.676242
H	0	2.712332	-4.055813	-3.000932
H	0	2.046402	-3.807851	-0.033732
H	0	0.746346	-2.625166	-0.207119
H	0	0.920138	-3.923552	-1.386383

Energy + ZPE = -1223.259775
Free energy = -1223.307780
Free energy in DCM = -1223.656787
Free energy in heptane = -1223.657499
Number of imaginary frequencies = 1 (-403.57)

TS 19a+cpSiN

C	0	2.235243	-0.202144	3.981116
C	0	2.235243	1.207027	3.981116
C	0	0.771581	-0.612138	3.981116
C	0	0.982922	1.671950	3.540279
C	0	0.139385	0.591165	3.338290
H	0	2.987317	-0.777295	4.514841
H	0	3.105390	1.830532	4.157487
H	0	0.435479	-0.652584	5.031586
H	0	0.540413	-1.576344	3.526440
H	0	0.748491	2.705473	3.312160
H	0	-0.886276	0.654500	2.995880
C	0	2.646169	-0.659756	2.051418
C	0	1.477793	-0.453988	1.294807
B	0	1.172871	0.730949	0.403150
Cl	0	2.320631	2.150674	0.422776
C	0	0.045700	0.799867	-0.716117
C	0	-1.319194	0.099482	-0.379018
C	0	0.728119	0.267986	-2.048285
C	0	-1.817309	-0.797454	-1.530938
C	0	-0.152305	-0.709235	-2.839869
C	0	-2.383659	1.110843	0.073555
C	0	-1.626753	-0.201263	-2.978565
C	0	-0.674524	-1.796842	-1.866276
O	0	-2.016602	1.832380	1.251821
C	0	-2.423937	-1.016774	-4.013745
C	0	-1.873336	1.281259	-3.282007
H	0	2.933490	-1.683620	2.287759
H	0	3.493502	-0.002151	1.880537
H	0	0.780305	-1.291715	1.263386
H	0	-0.175174	1.859117	-0.904664
H	0	-1.175436	-0.572960	0.478079
H	0	1.007512	1.127487	-2.668350
H	0	1.667807	-0.253335	-1.820270
H	0	-2.807945	-1.211769	-1.299176
H	0	0.357252	-1.033110	-3.756747
H	0	-2.630645	1.811447	-0.736513
H	0	-3.304508	0.579860	0.338994
H	0	-0.010765	-2.081070	-1.041834
H	0	-1.016794	-2.705473	-2.366241
H	0	-1.250002	2.383179	1.027731
H	0	-3.493502	-0.780019	-3.945041
H	0	-2.096480	-0.769359	-5.031586
H	0	-2.319016	-2.098048	-3.887837
H	0	-2.936352	1.531363	-3.172035
H	0	-1.303682	1.962308	-2.647849
H	0	-1.598678	1.499031	-4.322607

Energy + ZPE = -1223.257460
Free energy = -1223.305401
Free energy in DCM = -1223.656166
Free energy in heptane = -1223.656056
Number of imaginary frequencies = 1 (-396.69)

TS 19a+cpSiX

C	0	-1.713398	0.222240	2.572411
C	0	-1.713398	1.610268	2.572411
C	0	-3.138689	-0.240548	2.572411
C	0	-3.012125	2.073073	2.287268
C	0	-3.841843	0.972525	1.993527
H	0	-0.868750	-0.429241	2.766551
H	0	-0.838377	2.239632	2.697991
H	0	-3.461517	-0.344836	3.622911
H	0	-3.325660	-1.191663	2.074706
H	0	-3.293796	3.115478	2.175372
H	0	-4.925647	1.050387	1.971404
C	0	-2.060397	0.229578	-0.060603
C	0	-3.421499	0.570102	0.039419
B	0	-1.455558	-1.145875	-0.239242
Cl	0	-2.513878	-2.627564	-0.034007

C	0	0.031632	-1.434407	-0.728994
C	0	1.145757	-0.846109	0.212130
C	0	0.191410	-0.993990	-2.237137
C	0	2.346774	-0.291867	-0.583885
C	0	1.557325	-0.360842	-2.550573
C	0	1.559335	-1.866767	1.282245
C	0	2.748229	-1.116649	-1.866897
C	0	1.792968	0.796814	-1.545827
O	0	0.480630	-2.252432	2.137410
C	0	4.112519	-0.648110	-2.409717
C	0	2.775378	-2.650568	-1.872013
H	0	-1.376508	1.069157	-0.193622
H	0	-3.753744	1.525635	-0.358560
H	0	-4.157226	-0.224215	-0.072199
H	0	0.170361	-2.521613	-0.721524
H	0	0.735485	0.011176	0.763568
H	0	-0.579355	-0.261717	-2.511566
H	0	0.017002	-1.869457	-2.874921
H	0	3.164232	-0.009128	0.093414
H	0	1.648086	-0.144332	-3.622911
H	0	2.017062	-2.754103	0.821225
H	0	2.307455	-1.420900	1.947250
H	0	0.905979	1.345078	-1.207698
H	0	2.542857	1.519281	-1.874411
H	0	-0.149533	-2.772895	1.612706
H	0	4.269823	-1.027539	-3.427388
H	0	4.219525	0.439623	-2.444312
H	0	4.925647	-1.038182	-1.784046
H	0	3.558679	-3.025584	-1.200640
H	0	1.834390	-3.115478	-1.576840
H	0	3.016272	-3.015207	-2.879266

Energy + ZPE = -1223.258382
Free energy = -1223.306158
Free energy in DCM = -1223.654777
Free energy in heptane = -1223.656010
Number of imaginary frequencies = 1 (-398.45)

Product 19a+cpReN

Cl	0	1.187782	-2.617538	-0.375084
B	0	0.887771	-0.807913	0.014110
C	0	2.270687	0.002038	0.108627
C	0	-0.438706	-0.194864	-0.649549
C	0	3.328773	-0.520835	1.146914
C	0	-1.584434	-0.849771	0.160518
C	0	-0.756636	-0.169708	-2.160201
C	0	2.235466	1.550429	0.440154
C	0	-2.969612	-0.524675	-0.438055
C	0	-2.285261	-0.049048	-2.402457
C	0	-1.220711	-0.516449	1.599460
C	0	1.671428	1.731888	1.846755
C	0	3.735200	1.806276	0.735516
C	0	3.781162	0.780281	1.894382
C	0	-3.026678	0.802698	-1.298748
C	0	-2.977810	-1.297700	-1.793968
C	0	2.588895	1.260119	2.712399
O	0	0.225565	-0.824262	1.634233
C	0	-4.486065	1.106294	-1.698617
C	0	-2.418540	2.135148	-0.795858
H	0	2.713116	-0.081199	-0.894425
H	0	-0.427588	0.854247	-0.327228
H	0	4.182994	-0.986624	0.644989
H	0	2.924567	-1.268444	1.836889
H	0	-1.478320	-1.940825	0.095986
H	0	-0.223690	0.666141	-2.632946
H	0	-0.401463	-1.082731	-2.655394
H	0	1.771434	2.163175	-0.336204
H	0	-3.795667	-0.700006	0.264611
H	0	-2.504467	0.196855	-3.448974
H	0	-1.702572	-1.144101	2.353443
H	0	-1.361330	0.539984	1.852386
H	0	0.692432	2.142278	2.083845
H	0	3.941767	2.830864	1.063469
H	0	4.393145	1.547330	-0.102223
H	0	4.720361	0.683135	2.444399
H	0	-2.411849	-2.234921	-1.822429
H	0	-3.976807	-1.482854	-2.191984
H	0	2.498652	1.175912	3.791943
H	0	0.724113	-0.149332	2.149252
H	0	-5.045671	0.230914	-2.037534
H	0	-5.029361	1.532858	-0.845311
H	0	-4.510084	1.848350	-2.506498
H	0	-2.315608	2.152401	0.295939
H	0	-1.434958	2.343870	-1.225514
H	0	-3.061782	2.981808	-1.062111

Energy + ZPE = -1223.301406
Free energy = -1223.346565
Free energy in DCM = -1223.707571
Free energy in heptane = -1223.706948
Number of imaginary frequencies = 0

Product 19a+cpReX

Cl	0	0.703825	-2.787626	0.143530
B	0	0.854202	-0.983740	0.032336
C	0	2.315998	-0.429799	0.207612
C	0	-0.428437	-0.149567	-0.343979
O	0	-0.707329	-0.346182	2.536832
C	0	2.910522	-0.668339	1.653310
C	0	-1.759006	-0.598630	0.339030
C	0	-0.549175	-0.012987	-1.911516
C	0	2.534898	1.124614	0.023862
C	0	-1.848672	0.002394	1.744408
C	0	-2.990667	-0.343539	-0.555677
C	0	-2.010662	0.074553	-2.390082
C	0	3.440888	0.749661	2.052398
C	0	2.314253	1.633402	1.468356
C	0	4.040940	1.314702	-0.103931
C	0	-2.918395	0.949947	-1.454067
C	0	-2.765949	-1.169732	-1.854610
C	0	4.579703	1.086175	1.102035
C	0	-4.287316	1.238007	-2.103155

C	0	-2.406440	2.290551	-0.910008
H	0	2.939638	-0.972193	-0.517602
H	0	-0.220570	0.858466	0.029021
H	0	-0.705200	-1.312439	2.632893
H	0	3.694027	-1.430940	1.655441
H	0	2.138836	-0.980538	2.364906
H	0	-1.735476	-1.689202	0.482963
H	0	0.015629	0.871815	-2.230321
H	0	-0.091025	-0.869938	-2.424321
H	0	1.930732	1.581246	-0.764252
H	0	-2.776682	-0.322811	2.240353
H	0	-1.855383	1.096354	1.715459
H	0	-3.922496	-0.505377	0.002902
H	0	-2.050601	0.282913	-3.466933
H	0	3.651702	0.853389	3.119904
H	0	2.514896	2.704227	1.574340
H	0	1.327587	1.392888	1.879749
H	0	4.565622	1.478395	-1.040634
H	0	-2.184466	-2.092723	-1.752327
H	0	-3.684007	-1.394539	-2.400480
H	0	5.634771	1.029423	1.352143
H	0	-4.773399	0.349417	-2.514414
H	0	-4.972806	1.676095	-1.366482
H	0	-4.177007	1.961898	-2.920406
H	0	-3.080829	2.670458	-0.131525
H	0	-1.402285	2.254031	-0.487600
H	0	-2.393501	3.039015	-1.713038

Energy + ZPE = -1223.302205
Free energy = -1223.349666
Free energy in DCM = -1223.705175
Free energy in heptane = -1223.705481
Number of imaginary frequencies = 0

Product 19a+cpSiN

C	0	0.000000	0.000000	0.000000
C	0	0.000000	1.524461	0.000000
C	0	-1.524507	-0.266241	0.000000
C	0	0.368821	-0.446812	-1.457113
C	0	-1.071914	1.924915	-0.709348
C	0	-1.788123	0.672761	-1.202908
C	0	-0.878407	-0.002750	-2.305467
B	0	-0.595116	0.797814	-3.669979
C	0	0.482768	0.256309	-4.731590
O	0	0.344905	2.198738	-3.240939
Cl	0	-2.154249	1.510243	-4.427424
C	0	1.117588	1.543377	-5.314387
C	0	0.208525	-0.788087	-5.834906
C	0	1.559872	2.298243	-4.069882
C	0	2.078831	1.229372	-6.480549
C	0	1.255420	-0.675977	-6.975802
C	0	2.684108	-0.233490	-6.470758
C	0	1.131501	0.731990	-7.616978
C	0	3.748843	-0.365261	-7.580656
C	0	3.297704	-0.864163	-5.196962
H	0	0.596556	-0.475177	0.782890
H	0	0.767021	2.147270	0.453169
H	0	-2.012901	0.065463	0.922547
H	0	-1.785663	-1.312555	-0.199037
H	0	0.517724	-1.531745	-1.499877
H	0	1.312031	0.010367	-1.781639
H	0	-1.358265	2.942644	-0.959350
H	0	-2.822129	0.814902	-1.518255
H	0	-1.412431	-0.911042	-2.621920
H	0	1.265215	-0.176656	-4.097087
H	0	0.499373	2.229470	-2.272597
H	0	0.320404	2.167798	-5.740804
H	0	0.222143	-1.795027	-5.396704
H	0	-0.790080	-0.653149	-6.270398
H	0	2.395670	1.825216	-3.542985
H	0	1.766499	3.360969	-4.224022
H	0	2.769836	2.053503	-6.704525
H	0	1.212161	-1.545999	-7.642878
H	0	0.129194	1.172738	-7.642242
H	0	1.565805	0.799460	-8.615751
H	0	4.686505	0.107202	-7.259984
H	0	3.964575	-1.423574	-7.773812
H	0	3.461937	0.091588	-8.531152
H	0	3.643649	-0.100627	-4.489229
H	0	2.603881	-1.519926	-4.664922
H	0	4.172286	-1.474782	-5.449945

Energy + ZPE = -1223.301566
Free energy = -1223.346652
Free energy in DCM = -1223.707566
Free energy in heptane = -1223.707182
Number of imaginary frequencies = 0

Product 19a+cpSiX

C	0	0.000000	0.000000	0.000000
C	0	0.000000	1.523407	0.000000
C	0	-1.522189	-0.271863	0.000000
C	0	0.384980	-0.426688	-1.469244
C	0	-1.064495	1.928670	-0.707098
C	0	-1.793161	0.681730	-1.186064
C	0	-0.896099	0.020412	-2.286398
B	0	0.796243	-1.915483	-1.766902
C	0	1.360482	-2.353963	-3.174663
Cl	0	0.765900	-3.130813	-0.431469
C	0	0.989986	-3.790824	-3.660049
C	0	2.908822	-2.051760	-3.237637
C	0	2.111268	-4.429256	-4.508577
C	0	3.676940	-3.051450	-4.121763
C	0	-0.389333	-3.787074	-4.327008
C	0	2.906222	-3.432851	-5.435513
C	0	3.373820	-4.481108	-3.601937
O	0	-1.403025	-3.287195	-3.448654
C	0	3.808747	-4.206985	-6.417201
C	0	2.196887	-2.349097	-6.257573
H	0	0.591111	-0.484605	0.778980
H	0	0.796639	2.141391	0.403826
H	0	-2.008972	0.051321	0.925418

H	0	-1.782672	-1.315390	-0.208876
H	0	1.239628	0.180339	-1.808278
H	0	-1.315922	2.944367	-0.997088
H	0	-2.833988	0.815194	-1.492349
H	0	-0.646509	0.715631	-3.093666
H	0	-1.415614	-0.833508	-2.733159
H	0	0.891342	-1.661345	-3.882110
H	0	0.892783	-4.447043	-2.781998
H	0	3.364502	-2.089100	-2.238049
H	0	3.050064	-1.025774	-3.599130
H	0	1.769237	-5.365750	-4.969308
H	0	4.726477	-2.747476	-4.224450
H	0	-0.414469	-3.125806	-5.198500
H	0	-0.643985	-4.801611	-4.672585
H	0	3.198484	-4.587114	-2.525612
H	0	4.109618	-5.226228	-3.909857
H	0	-1.438015	-3.880714	-2.681036
H	0	4.547380	-3.533087	-6.869261
H	0	4.356060	-5.031041	-5.951893
H	0	3.208001	-4.630553	-7.232157
H	0	1.553672	-2.806433	-7.020454
H	0	1.580351	-1.669321	-5.669400
H	0	2.938027	-1.738173	-6.789229

Energy + ZPE = -1223.302507
Free energy = -1223.350806
Free energy in DCM = -1223.704945
Free energy in heptane = -1223.705414
Number of imaginary frequencies = 0

Diels-Alder reaction with Vinylborane (20a)

TS 20a+cpReN

C	0	-1.836586	-0.165379	0.903077
C	0	-1.836586	1.221311	0.903077
C	0	-3.266812	-0.629764	0.903077
C	0	-3.951982	0.574701	0.279495
C	0	-3.125548	1.678264	0.574421
H	0	-0.994172	-0.795895	1.162119
H	0	-0.965237	1.848294	1.052008
H	0	-3.600291	-0.700565	1.952750
H	0	-3.460677	-1.593489	0.430188
H	0	-5.035020	0.658782	0.247918
H	0	-3.400211	2.718196	0.433696
Cl	0	-0.925611	1.979763	-2.343327
B	0	-0.931327	0.189364	-2.022614
C	0	-2.253586	-0.471861	-1.676581
C	0	0.404836	-0.629422	-2.278212
C	0	-3.518364	0.141320	-1.651892
C	0	1.750968	0.035433	-1.834514
C	0	0.400074	-1.082721	-3.795091
C	0	2.893097	-0.216828	-2.840751
C	0	1.793818	-1.062348	-4.444478
C	0	2.095343	-0.367718	-0.399464
C	0	2.903185	-1.646981	-3.505073
C	0	2.413420	0.339686	-4.210619
O	0	3.229347	0.380947	0.027794
C	0	4.225176	-1.887083	-4.259474
C	0	2.615049	-2.922222	-2.701661
C	0	3.586504	0.159805	1.379984
C	0	2.669175	0.847938	2.377736
C	0	2.175277	2.131418	2.107877
C	0	2.340553	0.239419	3.593240
C	0	1.374801	2.792743	3.039487
C	0	1.544695	0.901889	4.531014
C	0	1.059104	2.180573	4.255940
H	0	-2.237281	-1.553396	-1.531867
H	0	0.297370	-1.550950	-1.690609
H	0	-4.401411	-0.482676	-1.784505
H	0	-3.618736	1.132165	-2.085097
H	0	1.619991	1.124656	-1.807810
H	0	-0.042755	-2.084455	-3.860109
H	0	-0.246078	-0.427810	-4.395539
H	0	3.842611	0.148310	-2.436039
H	0	1.745824	-1.447717	-5.471780
H	0	2.317189	-1.444455	-0.323616
H	0	1.235931	-0.160962	0.257554
H	0	1.719189	1.186769	-4.179353
H	0	3.226347	0.579903	-4.899379
H	0	4.539782	-1.034225	-4.867124
H	0	5.035020	-2.100819	-3.550044
H	0	4.134396	-2.753577	-4.927473
H	0	1.665727	-2.905884	-2.164792
H	0	2.593236	-3.789891	-3.374732
H	0	3.410890	-3.106406	-1.968395
H	0	4.604029	0.559238	1.475868
H	0	3.637964	-0.919405	1.600413
H	0	2.420004	2.600219	1.158918
H	0	2.711436	-0.760611	3.810168
H	0	1.001552	3.789891	2.819360
H	0	1.299183	0.415729	5.471780
H	0	0.437426	2.697160	4.982439

Energy + ZPE = -1493.508717
Free energy = -1493.568781
Free energy in DCM = -1494.010333
Free energy in heptane = -1494.012000
Number of imaginary frequencies = 1 (-405.51)

TS 20a+cpReX

C	0	-2.107428	1.131230	1.088712
C	0	-2.107428	2.632375	1.088712
C	0	-3.432192	0.708557	1.088712
C	0	-3.466214	2.918726	0.481964
C	0	-4.265355	1.798414	0.775964
H	0	-1.237921	0.522848	1.306152
H	0	-2.131808	2.972691	2.138625
H	0	-1.253171	3.106280	0.606303
H	0	-3.765014	-0.316185	1.218949
H	0	-3.866637	3.926388	0.412180
H	0	-5.341709	1.745581	0.645521

Cl	0	0.444897	2.661121	-1.424543
B	0	-0.621644	1.184311	-1.499528
C	0	-2.131397	1.363260	-1.458340
C	0	0.058948	-0.215945	-1.807091
C	0	-2.867593	2.556354	-1.481234
C	0	1.468704	-0.499817	-1.178284
C	0	0.017926	-0.370951	-3.387467
C	0	1.405164	-1.378196	0.073089
C	0	2.464189	-1.072039	-2.211336
C	0	1.320149	-0.918463	-3.987769
O	0	0.697730	-0.694351	1.110615
C	0	1.865867	-2.151315	-3.192195
C	0	2.502008	-0.092695	-3.417671
C	0	0.672769	-1.407583	2.338998
C	0	2.986229	-2.880730	-3.955931
C	0	0.876332	-3.218800	-2.709923
C	0	1.999360	-1.410869	3.078473
C	0	2.792439	-0.256268	3.109140
C	0	2.429975	-2.546704	3.771650
C	0	3.990514	-0.239939	3.822163
C	0	3.624712	-2.529882	4.494644
C	0	4.408501	-1.375829	4.520590
H	0	-2.712989	0.447242	-1.569759
H	0	-0.627044	-0.972858	-1.406444
H	0	-3.864886	2.559191	-1.912834
H	0	-2.331837	3.495407	-1.603688
H	0	1.905516	0.450394	-0.844729
H	0	-0.829975	-1.012288	-3.657375
H	0	-0.176202	0.597518	-3.868738
H	0	2.427833	-1.599213	0.412437
H	0	0.906202	-2.338990	-0.124907
H	0	3.417939	-1.324611	-1.729294
H	0	1.231952	-1.020970	-5.077425
H	0	2.310231	0.962900	-3.199491
H	0	3.414855	-0.168799	-4.012278
H	0	-0.090770	-0.903709	2.945292
H	0	0.330034	-2.442616	2.177255
H	0	3.753930	-2.206585	-4.346079
H	0	3.487257	-3.605556	-3.301284
H	0	2.571709	-3.436527	-4.806817
H	0	0.004248	-2.811877	-2.194939
H	0	0.508490	-3.801158	-3.565336
H	0	1.367021	-3.926388	-2.028912
H	0	2.466844	0.622082	2.558729
H	0	1.827185	-3.452510	3.745627
H	0	4.599178	0.660602	3.834261
H	0	3.946433	-3.420457	5.028383
H	0	5.341709	-1.361879	5.077425

Energy + ZPE = -1493.509520
Free energy = -1493.567718
Free energy in DCM = -1494.011516
Free energy in heptane = -1494.014195
Number of imaginary frequencies = 1 (-404.99)

TS 20a+cpSiN

C	0	2.590427	0.684931	4.411255
C	0	2.590427	2.094834	4.411255
C	0	1.127517	0.274060	4.411255
C	0	1.339779	2.560320	3.968585
C	0	0.502632	1.474987	3.754470
H	0	3.342635	0.108713	4.943168
H	0	3.459597	2.719028	4.588597
H	0	0.786782	0.244610	5.460609
H	0	0.898365	-0.693554	3.963136
H	0	1.103686	3.593232	3.740358
H	0	-0.534845	1.527021	3.445520
C	0	2.995423	0.204250	2.478829
C	0	1.823256	0.443694	1.741443
B	0	1.490932	1.681818	0.929638
Cl	0	2.711999	3.032942	0.886784
C	0	0.189530	1.835895	0.033953
C	0	0.533798	1.661294	-1.496649
C	0	-0.648578	3.129345	0.341314
C	0	-0.309320	2.593821	-2.390697
C	0	-1.219485	3.811180	-0.913026
C	0	0.453192	0.183268	-1.885784
C	0	-1.808489	2.784383	-1.940202
C	0	-0.049229	4.046974	-1.902804
O	0	0.951382	0.030286	-3.211604
C	0	-2.623732	3.482315	-3.045216
C	0	-2.661232	1.613494	-1.432970
C	0	0.983001	-1.312990	-3.659830
C	0	-0.384173	-1.901111	-3.967900
C	0	-1.351014	-1.130592	-4.627812
C	0	-0.688368	-3.225092	-3.635984
C	0	-2.593530	-1.675673	-4.949824
C	0	-1.928681	-3.777117	-3.965127
C	0	-2.885226	-3.002663	-4.621968
H	0	3.262829	-0.825360	2.713337
H	0	3.852983	0.848479	2.308779
H	0	1.101269	-0.373541	1.703070
H	0	-0.447517	0.981561	0.298591
H	0	1.577255	1.957179	-1.672514
H	0	-1.461634	2.865283	1.031089
H	0	-0.031056	3.872234	0.861588
H	0	-0.131934	2.363473	-3.446698
H	0	-1.849809	4.667049	-0.636810
H	0	1.068423	-0.416807	-1.192930
H	0	-0.577671	-0.191310	-1.819005
H	0	0.933635	4.248131	-1.463088
H	0	-0.258589	4.808187	-2.657585
H	0	-2.854982	2.775934	-3.852909
H	0	-3.578138	3.847987	-2.644583
H	0	-2.106317	4.334891	-3.493715
H	0	-2.841381	0.887045	-2.235607
H	0	-2.222375	1.073899	-0.592635
H	0	-3.642993	1.981946	-1.105729
H	0	1.593315	-1.292541	-4.571365
H	0	1.506708	-1.952450	-2.929640
H	0	-1.121413	-0.098664	-4.878448
H	0	0.050988	-3.830529	-3.115081
H	0	-3.334898	-1.066322	-5.460609
H	0	-2.149143	-4.808187	-3.700571
H	0	-3.852983	-3.427776	-4.874857

Energy + ZPE = -1493.508652
Free energy = -1493.567807
Free energy in DCM = -1494.013304
Free energy in heptane = -1494.014200
Number of imaginary frequencies = 1 (-401.37)

TS 20a+cpSiX

C	0	-2.227418	1.208431	3.747646
C	0	-2.227418	2.597766	3.747646
C	0	-3.653914	0.744705	3.747646
C	0	-3.522310	3.058203	3.447915
C	0	-4.347833	1.954685	3.152451
H	0	-1.383028	0.576577	3.997069
H	0	-1.353857	3.227031	3.882301
H	0	-3.983603	0.656084	4.797365
H	0	-3.843804	-0.210612	3.258861
H	0	-3.803089	4.099640	3.327781
H	0	-5.431009	2.029675	3.111700
C	0	-2.541730	1.196820	1.144407
C	0	-3.901761	1.541824	1.193431
B	0	-1.921375	-0.186667	1.083463
Cl	0	-3.010662	-1.648847	1.161000
C	0	-0.369252	-0.452160	0.884532
C	0	-0.050725	-1.040745	-0.544242
C	0	0.266694	-1.283498	2.060217
C	0	1.071985	-2.096477	-0.501054
C	0	1.289546	-2.332487	1.594707
C	0	0.202070	0.102152	-1.530633
C	0	2.255429	-1.780718	0.491616
C	0	0.620123	-3.199599	0.497198
O	0	0.292769	-0.436438	-2.845982
C	0	3.441043	-2.732980	0.240825
C	0	2.844505	-0.371468	0.637100
C	0	0.476996	0.543202	-3.852986
C	0	1.862611	1.167114	-3.869929
C	0	2.998371	0.365626	-3.691559
C	0	2.032607	2.536174	-4.098453
C	0	4.275343	0.923445	-3.743878
C	0	3.310654	3.096885	-4.160328
C	0	4.435540	2.291470	-3.981630
H	0	-1.846055	2.029556	1.034921
H	0	-4.221182	2.497696	0.786103
H	0	-4.638142	0.748971	1.076922
H	0	0.102763	0.538512	0.916516
H	0	-0.933947	-1.571259	-0.925398
H	0	-0.511613	-1.817284	2.620549
H	0	0.734832	-0.586214	2.768223
H	0	1.343485	-2.399538	-1.517894
H	0	1.743899	-2.839784	2.456261
H	0	-0.634885	0.821008	-1.486880
H	0	1.119800	0.651004	-1.278052
H	0	-0.458601	-3.364659	0.590768
H	0	1.109829	-4.162934	0.339376
H	0	4.145515	-2.698588	1.082098
H	0	3.140976	-3.775815	0.104829
H	0	3.989422	-2.429323	-0.660249
H	0	3.339642	-0.060023	-0.291397
H	0	2.112691	0.396524	0.892930
H	0	3.608456	-0.367389	1.426365
H	0	0.294316	0.015550	-4.797365
H	0	-0.286145	1.334704	-3.766888
H	0	2.869683	-0.696795	-3.503996
H	0	1.157896	3.170433	-4.229077
H	0	5.147791	0.290432	-3.602631
H	0	3.425467	4.162934	-4.339351
H	0	5.431009	2.725597	-4.024149

Energy + ZPE = -1493.508282
Free energy = -1493.567501
Free energy in DCM = -1494.012227
Free energy in heptane = -1494.013464
Number of imaginary frequencies = 1 (-401.87)

Product 20a+cpReN

C	0	-1.386116	2.269857	-1.293928
C	0	-2.418936	1.915214	-0.234308
C	0	-2.018436	3.555579	-1.875285
C	0	-2.215335	4.205521	-0.486820
C	0	-2.911448	3.066868	0.243769
Cl	0	0.467448	1.990626	2.165690
B	0	0.604768	1.867262	0.380992
C	0	-0.124285	2.911425	-0.540656
C	0	1.524160	0.735886	-0.230587
C	0	-0.735648	4.227284	0.037529
C	0	1.442756	-0.682482	0.427160
C	0	2.993789	1.331980	-0.286332
C	0	2.829283	-1.339064	0.579725
C	0	4.076232	0.299042	0.068152
C	0	0.421166	-1.550657	-0.312125
C	0	3.826850	-1.088551	-0.615714
C	0	3.698908	-0.361351	1.419272
O	0	0.201105	-2.731924	0.449693
C	0	5.055580	-2.011332	-0.502215
C	0	3.372570	-1.131995	-2.080528
C	0	-0.764087	-3.606795	-0.108874
C	0	-2.193965	-3.105914	0.011255
C	0	-2.606411	-2.418617	1.160576
C	0	-3.127781	-3.353539	-0.999999
C	0	-3.927328	-1.989840	1.293545
C	0	-4.453360	-2.935061	-0.864940
C	0	-4.855985	-2.249703	0.281828
H	0	-1.121068	1.479599	-2.000198
H	0	-2.620262	0.911347	0.127825
H	0	-2.964056	3.361084	-2.391700
H	0	-1.343532	4.115399	-2.534371
H	0	-2.715280	5.176862	-0.454807
H	0	-3.589479	3.192270	1.082257
H	0	0.592032	3.161958	-1.339526
H	0	1.211127	0.623254	-1.276546
H	0	-0.204598	5.104938	-0.349296
H	0	-0.697059	4.270559	1.128684

H	0	1.051910	-0.582463	1.447551
H	0	3.166023	1.745201	-1.287621
H	0	3.108403	2.172586	0.412747
H	0	2.721767	-2.370863	0.929805
H	0	5.075085	0.742842	-0.036040
H	0	0.772558	-1.820400	-1.320972
H	0	-0.522370	-0.994687	-0.431953
H	0	3.170671	0.264889	2.146493
H	0	4.542691	-0.839626	1.920599
H	0	5.467594	-2.065223	0.509182
H	0	4.792119	-3.033055	-0.803857
H	0	5.857323	-1.666964	-1.168209
H	0	2.532961	-0.473440	-2.307664
H	0	4.202783	-0.838502	-2.736809
H	0	3.083272	-2.151085	-2.367364
H	0	-0.649109	-4.545844	0.446597
H	0	-0.530743	-3.821038	-1.165115
H	0	-1.880086	-2.216723	1.942914
H	0	-2.816445	-3.877770	-1.901583
H	0	-4.233920	-1.456406	2.189744
H	0	-5.167389	-3.135720	-1.659546
H	0	-5.885256	-1.917077	0.386567

Energy + ZPE = -1493.551703
Free energy = -1493.609759
Free energy in DCM = -1494.056435
Free energy in heptane = -1494.059181
Number of imaginary frequencies = 0

Product 20a+cpReX

C	0	-2.116579	-2.216785	-0.830997
C	0	-2.361706	-3.274886	0.268063
C	0	-3.039979	-2.735772	-1.920796
C	0	-3.900764	-3.157400	0.181605
C	0	-4.099652	-3.296529	-1.319338
Cl	0	-1.621112	-0.310957	2.358640
B	0	-1.869641	-0.046281	0.594906
C	0	-2.883357	-0.947407	-0.201596
C	0	-1.115183	1.148083	-0.107559
C	0	-4.078352	-1.636737	0.529261
C	0	0.354448	1.439332	0.343438
C	0	-2.077631	2.403751	-0.007963
C	0	1.366770	0.718320	-0.545973
C	0	0.636967	2.950763	0.474827
C	0	-1.327477	3.718792	0.256025
O	0	1.093811	-0.681807	-0.488561
C	0	-0.036466	3.860995	-0.622367
C	0	-0.402669	3.515341	1.483903
C	0	2.040136	-1.482227	-1.183213
C	0	0.535377	5.290404	-0.573305
C	0	-0.083516	3.447366	-2.098232
C	0	3.380038	-1.599232	-0.478529
C	0	3.432761	-1.743872	0.914211
C	0	4.574589	-1.606485	-1.205878
C	0	4.657281	-1.895604	1.563427
C	0	5.801736	-1.767931	-0.558893
C	0	5.845598	-1.911952	0.828236
H	0	-1.082612	-2.016635	-1.116191
H	0	-1.995027	-4.264997	-0.021213
H	0	-1.955577	-3.000033	1.246931
H	0	-2.901678	-2.557158	-2.983110
H	0	-4.490164	-3.827981	0.812142
H	0	-4.999709	-3.675869	-1.793859
H	0	-3.245713	-0.343051	-1.043404
H	0	-1.074168	0.880392	-1.170225
H	0	-5.044527	-1.247619	0.192449
H	0	-4.022700	-1.497641	1.613489
H	0	0.505271	1.024309	1.348172
H	0	-2.663252	2.472184	-0.932655
H	0	-2.809118	2.283379	0.804186
H	0	2.386189	0.919032	-0.184717
H	0	1.310011	1.057469	-1.592656
H	0	1.700562	3.131853	0.679133
H	0	-2.027099	4.564782	0.265485
H	0	-0.753847	2.827844	2.261048
H	0	-0.093951	4.449646	1.956897
H	0	1.570280	-2.470295	-1.261884
H	0	2.185349	-1.105733	-2.208863
H	0	0.621403	5.689750	0.440975
H	0	1.536447	5.316058	-1.022575
H	0	-0.100282	5.977520	-1.146209
H	0	-0.528986	2.466634	-2.270683
H	0	-0.669337	4.177559	-2.672162
H	0	0.925439	3.436764	-2.530562
H	0	2.506652	-1.725178	1.482022
H	0	4.545984	-1.484943	-2.287050
H	0	4.685172	-2.003431	2.644719
H	0	6.721856	-1.772039	-1.137563
H	0	6.799521	-2.032432	1.334865

Energy + ZPE = -1493.554210
Free energy = -1493.612567
Free energy in DCM = -1494.059556
Free energy in heptane = -1494.063105
Number of imaginary frequencies = 0

Product 20a+cpSiN

C	0	-5.236459	-2.111344	-0.419062
C	0	-5.605459	-0.697428	-0.844194
C	0	-4.278375	-2.500107	-1.568050
C	0	-4.533652	-0.163101	-1.446673
C	0	-3.431690	-1.213669	-1.430847
C	0	-4.222297	-1.961953	0.768412
C	0	-2.953319	-1.358283	0.086652
B	0	-2.257686	-0.060985	0.642498
Cl	0	-2.916203	0.752308	2.100982
C	0	-0.982916	0.575492	-0.046031
C	0	0.252462	0.761513	0.912558
C	0	-1.398977	1.897722	-0.809239
C	0	0.983936	2.095026	0.665703
C	0	-0.369765	3.031223	-0.670444
C	0	1.158587	-0.471050	0.834183

C	0	1.102980	2.528188	-0.845394
C	0	-0.066379	3.228554	0.837076
O	0	2.155811	-0.369772	1.842832
C	0	2.092800	3.699741	-0.995995
C	0	1.432414	1.525393	-1.958926
C	0	3.035938	-1.480962	1.892311
C	0	4.015075	-1.551351	0.732871
C	0	4.666978	-0.392019	0.290612
C	0	4.309100	-2.769192	0.111776
C	0	5.594523	-0.452908	-0.748775
C	0	5.244402	-2.835258	-0.923908
C	0	5.888252	-1.676350	-1.357704
H	0	-6.070804	-2.786371	-0.213039
H	0	-6.532086	-0.194636	-0.585280
H	0	-4.782406	-2.570508	-2.537398
H	0	-3.711222	-3.419433	-1.377167
H	0	-4.409375	0.861565	-1.783396
H	0	-2.614563	-1.073932	-2.142366
H	0	-4.001904	-2.941644	1.208114
H	0	-4.620796	-1.326422	1.562752
H	0	-2.151572	-2.117316	0.073238
H	0	-0.668228	-0.135939	-0.819857
H	0	-0.096252	0.807707	1.952277
H	0	-1.559661	1.653539	-1.866744
H	0	-2.356887	2.282132	-0.434639
H	0	1.896203	2.140193	1.269418
H	0	-0.680598	3.903777	-1.259960
H	0	0.560568	-1.385445	1.001936
H	0	1.622366	-0.563706	-0.157442
H	0	-0.887650	3.036568	1.535828
H	0	0.371290	4.201133	1.071125
H	0	3.125725	3.336756	-0.919358
H	0	1.981708	4.172039	-1.980601
H	0	1.963386	4.479201	-0.239915
H	0	2.448080	1.128848	-1.835923
H	0	0.751785	0.673968	-2.013971
H	0	1.399347	2.029222	-2.934208
H	0	3.581392	-1.365379	2.836841
H	0	2.465236	-2.422391	1.955813
H	0	4.434937	0.557650	0.764850
H	0	3.802840	-3.674751	0.440480
H	0	6.092719	0.453836	-1.082470
H	0	5.462202	-3.789932	-1.395792
H	0	6.612661	-1.723712	-2.166468

Energy + ZPE = -1493.550551
Free energy = -1493.608531
Free energy in DCM = -1494.058039
Free energy in heptane = -1494.060282
Number of imaginary frequencies = 0

Product 20a+cpSiX

C	0	3.733464	-1.001611	1.315756
C	0	3.825513	-2.459001	1.737830
C	0	5.147611	-0.789896	0.731399
C	0	4.627408	-3.081589	0.861470
C	0	5.077403	-2.050330	-0.161067
C	0	2.848317	-1.009842	-0.033628
C	0	3.823588	-1.698741	-1.037997
B	0	2.299067	0.437102	-0.309264
Cl	0	3.218110	1.552747	-1.381848
C	0	0.959467	0.973611	0.338425
C	0	-0.190933	0.935388	-0.754977
C	0	1.090656	2.359034	1.072381
C	0	-1.106496	2.171507	-0.664423
C	0	-0.052526	3.337164	0.757905
C	0	-0.943123	-0.397619	-0.694464
C	0	-1.456090	2.643681	0.797979
C	0	-0.200832	3.429177	-0.782687
O	0	-1.825550	-0.467765	-1.808096
C	0	-2.605203	3.669527	0.773593
C	0	-1.771533	1.649106	1.922608
C	0	-2.552062	-1.684299	-1.888075
C	0	-3.628480	-1.837267	-0.827414
C	0	-4.485755	-0.767475	-0.534587
C	0	-3.804211	-3.047404	-0.149285
C	0	-5.496728	-0.908565	0.415169
C	0	-4.821894	-3.195184	0.796410
C	0	-5.669478	-2.124898	1.082071
H	0	3.395681	-0.299247	2.082120
H	0	3.238524	-2.907921	2.533382
H	0	5.925391	-0.856111	1.498595
H	0	5.261083	0.141311	0.166877
H	0	4.833992	-4.145863	0.802463
H	0	5.968587	-2.301150	-0.741614
H	0	1.978447	-1.649372	0.162786
H	0	3.379583	-2.588937	-1.494486
H	0	4.115073	-1.020465	-1.845712
H	0	0.673310	0.236290	1.099620
H	0	0.251814	0.978273	-1.760608
H	0	2.030015	2.852599	0.796881
H	0	1.144522	2.175956	2.153224
H	0	-1.940422	2.065197	-1.365991
H	0	0.068113	4.267422	1.328095
H	0	-0.228072	-1.237418	-0.742639
H	0	-1.501275	-0.497360	0.245930
H	0	0.714648	3.323484	-1.374239
H	0	-0.733417	4.321078	-1.119313
H	0	-2.675499	4.189495	1.737661
H	0	-2.492753	4.430650	-0.003744
H	0	-3.563770	3.163367	0.601442
H	0	-2.701232	1.105551	1.712353
H	0	-0.989160	0.908818	2.099354
H	0	-1.921092	2.191067	2.866012
H	0	-3.006627	-1.673651	-2.886075
H	0	-1.865133	-2.546001	-1.848459
H	0	-4.348698	0.177334	-1.053544
H	0	-3.139669	-3.882453	-0.362138
H	0	-6.154432	-0.070955	0.633189
H	0	-4.945656	-4.142842	1.314179
H	0	-6.459168	-2.235093	1.820550

Energy + ZPE = -1493.550382
Free energy = -1493.608167

Free energy in DCM = -1494.057252
Free energy in heptane = -1494.060024
Number of imaginary frequencies = 0

Diels-Alder reaction with Vinylborane (21a)

TS 21a+cpReN

C	0	-1.918278	0.930792	2.021681
C	0	-1.918278	2.317049	2.021681
C	0	-3.348374	0.465504	2.021681
C	0	-3.209281	2.775773	1.700699
C	0	-4.038140	1.673143	1.409269
H	0	-1.075595	0.296318	2.269714
H	0	-1.048184	2.949082	2.156620
H	0	-3.679624	0.386701	3.071501
H	0	-3.541202	-0.495715	1.543825
H	0	-3.484075	3.816232	1.565565
H	0	-5.121183	1.757714	1.387212
C	0	-3.625954	1.270561	-0.530629
C	0	-2.373180	0.631365	-0.575252
B	0	-1.042259	1.286564	-0.885032
Cl	0	-1.028303	3.084392	-1.179209
C	0	0.350268	0.555624	-1.128592
C	0	0.326463	-1.001215	-0.880950
C	0	1.578474	1.280659	-0.460488
C	0	1.677693	-1.524130	-0.354081
C	0	2.665553	0.313358	0.032857
C	0	-0.174211	-1.673326	-2.156590
C	0	2.954710	-0.845251	-0.982929
C	0	1.989333	-0.737531	0.949153
I	0	-0.729054	-3.816232	-1.891985
C	0	4.226224	-1.631350	-0.607781
C	0	3.055049	-0.530292	-2.481536
H	0	-4.520106	0.663874	-0.668185
H	0	-3.710926	2.270350	-0.945951
H	0	-2.389444	-0.449912	-0.441385
H	0	0.489362	0.690256	-2.213069
H	0	-0.402605	-1.220821	-0.091644
H	0	1.995017	2.000596	-1.173714
H	0	1.248031	1.874133	0.401790
H	0	1.675616	-2.618488	-0.302570
H	0	3.528994	0.866561	0.424453
H	0	0.563112	-1.693338	-2.957691
H	0	-1.100847	-1.226900	-2.516463
H	0	1.127472	-0.395573	1.535258
H	0	2.679492	-1.253631	1.619241
H	0	4.266896	-1.916321	0.447209
H	0	4.294057	-2.552777	-1.199849
H	0	5.121183	-1.033658	-0.822940
H	0	3.084734	-1.455773	-3.071501
H	0	2.240794	0.085169	-2.866350
H	0	3.990176	0.007376	-2.686123

Energy + ZPE = -1158.831822
Free energy = -1158.882944
Free energy in DCM = -1159.224071
Free energy in heptane = -1159.220745
Number of imaginary frequencies = 1 (-393.94)

TS 21a+cpReX

Cl	0	0.922025	-3.329490	-0.612926
B	0	0.922025	-1.503200	-0.612926
C	0	2.251788	-0.777672	-0.612926
C	0	-0.522126	-0.848993	-0.742900
C	0	3.534959	-1.343320	-0.708937
C	0	-0.537420	0.727704	-0.785510
C	0	-1.577269	-1.463256	0.254805
C	0	-1.798711	1.311275	-0.118225
C	0	-2.604181	-0.441679	0.764515
C	0	-0.311180	1.157647	-2.232330
C	0	-3.130171	0.505516	-0.368755
C	0	-1.828635	0.771316	1.338269
I	0	0.126425	3.329490	-2.479111
C	0	-4.351665	1.326041	0.090007
C	0	-3.482697	-0.081721	-1.742040
H	0	2.221042	0.309967	-0.659106
H	0	-0.840094	-1.184794	-1.742420
H	0	4.332974	-0.763658	-1.165784
H	0	3.612417	-2.413374	-0.891228
H	0	0.308193	1.105624	-0.198510
H	0	-2.079267	-2.304855	-0.234982
H	0	-1.072428	-1.889292	1.131632
H	0	-1.844672	2.396453	-0.261233
H	0	-3.353399	-0.929260	1.401566
H	0	-1.174237	0.993522	-2.875648
H	0	0.569274	0.683867	-2.665946
H	0	-0.857513	0.561649	1.803711
H	0	-2.412835	1.388438	2.023419
H	0	-4.215749	1.800614	1.065800
H	0	-4.569906	2.121262	-0.634008
H	0	-5.240048	0.684965	0.155183
H	0	-3.666315	0.718824	-2.470540
H	0	-2.721453	-0.743277	-2.157981
H	0	-4.410512	-0.664172	-1.669077
C	0	4.331520	-1.393297	1.170846
C	0	4.395078	-0.032610	1.532611
C	0	3.110136	-1.955114	1.873738
C	0	3.133235	0.381515	1.999746
C	0	2.283526	-0.715459	2.042237
H	0	5.220922	-1.994661	1.004132
H	0	5.240048	0.623948	1.352090
H	0	3.429076	-2.291143	2.875648
H	0	2.614923	-2.793876	1.385021
H	0	2.852034	1.405631	2.220828
H	0	1.263066	-0.710523	2.407092

Energy + ZPE = -1158.831670
Free energy = -1158.883076
Free energy in DCM = -1159.223434
Free energy in heptane = -1159.220291
Number of imaginary frequencies = 1 (-398.47)

TS 21a+cpSiN

C	0	2.448615	-1.252395	3.716462
C	0	2.448615	0.157033	3.716462
C	0	0.986100	-1.664557	3.716462
C	0	1.195018	0.623664	3.279680
C	0	0.357270	-0.461191	3.068077
H	0	3.203050	-1.829467	4.243938
H	0	3.317864	0.781339	3.892642
H	0	0.648064	-1.699892	4.766483
H	0	0.757285	-2.630527	3.264736
H	0	0.958136	1.657366	3.056348
H	0	-0.681533	-0.409053	2.763507
C	0	2.857164	-1.727119	1.779561
C	0	1.682501	-1.495275	1.043748
B	0	1.344462	-0.255574	0.240364
Cl	0	2.548925	1.107559	0.210720
C	0	0.056545	-0.117059	-0.680712
C	0	0.457996	-0.377572	-2.198510
C	0	-0.769069	1.203139	-0.467000
C	0	-0.299636	0.558497	-3.158759
C	0	-1.240392	1.860666	-1.773720
C	0	0.297963	-1.870959	-2.468876
C	0	-1.811023	0.818318	-2.794955
C	0	-0.007926	2.015270	-2.701144
I	0	1.162072	-2.546501	-4.407648
C	0	-2.540791	1.501592	-3.967080
C	0	-2.729564	-0.302573	-2.289661
H	0	3.132617	-2.754496	2.013813
H	0	3.709067	-1.075242	1.610535
H	0	0.964457	-2.316280	1.008669
H	0	-0.601627	-0.947809	-0.394337
H	0	1.521257	-0.138717	-2.327125
H	0	-1.630368	0.976118	0.175361
H	0	-0.166893	1.944231	0.072597
H	0	-0.081416	0.296001	-4.199921
H	0	-1.851809	2.747975	-1.563962
H	0	0.839181	-2.474068	-1.740181
H	0	-0.739475	-2.195683	-2.522279
H	0	0.955622	2.194712	-2.212665
H	0	-0.142578	2.754496	-3.493242
H	0	-2.741652	0.777078	-4.766483
H	0	-3.506499	1.903293	-3.634066
H	0	-1.975022	2.327154	-4.407701
H	0	-2.906917	-1.045659	-3.078114
H	0	-2.349710	-0.829954	-1.412852
H	0	-3.709067	0.113164	-2.018110

Energy + ZPE = -1158.832248
Free energy = -1158.883686
Free energy in DCM = -1159.224911
Free energy in heptane = -1159.221371
Number of imaginary frequencies = 1 (-396.52)

TS 21a+cpSiX

C	0	-1.534955	1.191533	3.242848
C	0	-1.534955	2.580203	3.242848
C	0	-2.960398	0.725211	3.242848
C	0	-2.832858	3.040444	2.950164
C	0	-3.660353	1.937835	2.659360
H	0	-0.688256	0.559346	3.483959
H	0	-0.661742	3.210387	3.374568
H	0	-3.287398	0.626169	4.292475
H	0	-3.148750	-0.226279	2.746296
H	0	-3.115036	4.081995	2.835010
H	0	-4.743727	2.012364	2.626913
Cl	0	-2.334563	-1.653254	0.647717
B	0	-1.259142	-0.186840	0.537505
C	0	-1.875580	1.194623	0.623394
C	0	0.281828	-0.440130	0.242078
C	0	-3.235576	1.537369	0.693404
C	0	0.479725	-0.856937	-1.281344
C	0	0.992675	-1.409243	1.255739
C	0	1.567670	-1.935127	-1.441999
C	0	1.941785	-2.417845	0.589520
C	0	0.693422	0.423187	-2.084358
C	0	2.833094	-1.759453	-0.518586
C	0	1.158540	-3.133605	-0.540416
I	0	0.618777	0.139687	-4.292475
C	0	3.969723	-2.694005	-0.974307
C	0	3.462100	-0.384611	-0.257355
H	0	-1.182534	2.029840	0.514855
H	0	0.765943	0.538638	0.354716
H	0	-3.561813	2.495440	0.297090
H	0	-3.971960	0.743869	0.581207
H	0	-0.448607	-1.315745	-1.644534
H	0	0.247666	-1.985691	1.817920
H	0	1.537943	-0.803661	1.991930
H	0	1.755002	-2.133569	-2.503074
H	0	2.448217	-3.032304	1.345216
H	0	-0.099666	1.149196	-1.906427
H	0	1.663968	0.886653	-1.916705
H	0	0.086071	-3.283214	-0.376862
H	0	1.602135	-4.081995	-0.850310
H	0	4.743727	-2.761229	-0.198917
H	0	3.632962	-3.711017	-1.193274
H	0	4.444615	-2.302352	-1.882868
H	0	3.904807	0.021544	-1.176175
H	0	2.763661	0.357009	0.133845
H	0	4.276329	-0.480044	0.473316

Energy + ZPE = -1158.832170
Free energy = -1158.884040
Free energy in DCM = -1159.224016
Free energy in heptane = -1159.220738
Number of imaginary frequencies = 1 (-395.45)

Product 21a+cpReN

C	0	-1.749479	1.369039	2.139626

C	0	-1.668948	2.825130	2.569007
C	0	-3.194723	1.032656	2.575868
C	0	-2.889308	3.357856	2.412857
C	0	-3.801155	2.267205	1.872273
C	0	-3.350531	2.011901	0.389969
C	0	-1.945665	1.341485	0.543343
B	0	-0.696530	1.905777	-0.223203
Cl	0	-0.733561	3.587058	-0.855977
C	0	0.660918	1.131467	-0.497509
C	0	0.646913	-0.417173	-0.207922
C	0	1.880153	1.891499	0.167986
C	0	1.997273	-0.911294	0.348137
C	0	2.966318	0.943498	0.698246
C	0	0.167235	-1.123604	-1.474579
C	0	3.275276	-0.237868	-0.284493
C	0	2.286061	-0.087164	1.633582
I	0	-0.324937	-3.272714	-1.185099
C	0	4.548407	-1.003786	0.125256
C	0	3.391006	0.039977	-1.789491
H	0	-0.954929	0.709716	2.495973
H	0	-0.754316	3.345588	2.835685
H	0	-3.318785	1.059666	3.663176
H	0	-3.558082	0.075085	2.184038
H	0	-3.168439	4.400867	2.523730
H	0	-4.874892	2.432819	1.989131
H	0	-4.047784	1.330195	-0.110722
H	0	-3.322030	2.940182	-0.185433
H	0	-2.033179	0.276342	0.286667
H	0	0.809559	1.246651	-1.580364
H	0	-0.089342	-0.628405	0.576052
H	0	2.292392	2.594193	-0.563830
H	0	1.541330	2.505418	1.013368
H	0	2.004480	-2.003462	0.429789
H	0	3.819463	1.515576	1.084702
H	0	0.905367	-1.127860	-2.275259
H	0	-0.770150	-0.707832	-1.845915
H	0	1.416265	0.262207	2.202879
H	0	2.973082	-0.579635	2.323913
H	0	4.577928	-1.263577	1.186986
H	0	4.630329	-1.938195	-0.443971
H	0	5.441110	-0.404073	-0.093052
H	0	3.431066	-0.899897	-2.355316
H	0	2.579584	0.642496	-2.200431
H	0	4.326335	0.575950	-1.996878

Energy + ZPE = -1158.872912
Free energy = -1158.923506
Free energy in DCM = -1159.258328
Free energy in heptane = -1159.260912
Number of imaginary frequencies = 0

Product 21a+cpReX

C	0	2.462224	-1.341380	3.917963
C	0	2.569107	0.168126	4.065993
C	0	0.943094	-1.533165	4.130696
C	0	1.438492	0.704206	3.582982
C	0	0.559998	-0.441191	3.107408
Cl	0	0.162923	-3.629371	1.233136
B	0	0.282918	-1.856965	0.932813
C	0	1.290081	-0.998963	1.777029
C	0	-0.701756	-1.314860	-0.185318
C	0	2.568081	-1.661201	2.384982
C	0	-0.541986	0.205221	-0.570679
C	0	-2.198107	-1.748356	0.083958
C	0	-1.891504	0.846387	-0.950650
C	0	-3.223272	-0.702137	-0.376069
C	0	0.542770	0.300708	-1.642422
C	0	-2.871176	-0.078323	-1.770213
C	0	-2.841403	0.656758	0.264744
I	0	1.227508	2.372609	-2.069401
C	0	-4.040418	0.748374	-2.340473
C	0	-2.379752	-0.988741	-2.904231
H	0	3.132810	-1.938039	4.541094
H	0	3.457009	0.698190	4.396378
H	0	0.621330	-1.277121	5.144938
H	0	0.586775	-2.534598	3.869250
H	0	1.216829	1.755643	3.428800
H	0	-0.502982	-0.215359	2.989858
H	0	1.570104	-0.123345	1.181231
H	0	-0.392786	-1.891425	-1.070499
H	0	3.483843	-1.256544	1.943006
H	0	2.573921	-2.744825	2.233296
H	0	-0.184826	0.761767	0.304206
H	0	-2.376470	-2.712379	-0.404140
H	0	-2.363486	-1.921442	1.155241
H	0	-1.740582	1.863233	-1.328406
H	0	-4.244758	-1.077097	-0.233406
H	0	0.222206	-0.075476	-2.612667
H	0	1.462424	-0.202144	-1.341882
H	0	-2.372499	0.620585	1.255889
H	0	-3.661048	1.376565	0.298121
H	0	-4.466480	1.453322	-1.621405
H	0	-3.707464	1.328468	-3.210281
H	0	-4.849480	0.086482	-2.674449
H	0	-1.992772	-0.392368	-3.740623
H	0	-1.602134	-1.696144	-2.611286
H	0	-3.218540	-1.578899	-3.295585

Energy + ZPE = -1158.873394
Free energy = -1158.924547
Free energy in DCM = -1159.258148
Free energy in heptane = -1159.260909
Number of imaginary frequencies = 0

Product 21a+cpSiN

C	0	2.002751	-0.686912	4.807272
C	0	1.668777	0.775026	5.064176
C	0	0.583265	-1.298592	4.833460
C	0	0.484767	1.028088	4.488053
C	0	0.009712	-0.262691	3.838693
C	0	2.341032	-0.797046	3.278046
C	0	0.967097	-0.543625	2.581587

B	0	0.796252	0.549931	1.468216
Cl	0	2.090266	1.756312	1.183391
C	0	-0.506372	0.639604	0.568090
C	0	-0.180368	0.254852	-0.942367
C	0	-1.266830	2.012215	0.724701
C	0	-0.924537	1.169133	-1.933731
C	0	-1.747353	2.605955	-0.608045
C	0	-0.439301	-1.241521	-1.111312
C	0	-2.406779	1.529947	-1.536241
C	0	-0.543391	2.634748	-1.583486
I	0	0.317052	-2.081888	-3.025843
C	0	-3.145400	2.170881	-2.726355
C	0	-3.358523	0.494213	-0.923359
H	0	2.752759	-1.133682	5.464358
H	0	2.340633	1.492207	5.525087
H	0	0.111813	-1.237189	5.819576
H	0	0.539651	-2.330473	4.464271
H	0	-0.005222	1.991689	4.387081
H	0	-1.055178	-0.328657	3.603476
H	0	2.717320	-1.798464	3.039087
H	0	3.107460	-0.076231	2.982913
H	0	0.597861	-1.485980	2.145693
H	0	-1.186548	-0.136954	0.940382
H	0	0.887723	0.422681	-1.128221
H	0	-2.115262	1.861342	1.403871
H	0	-0.619241	2.758874	1.200512
H	0	-0.758161	0.828959	-2.961588
H	0	-2.304793	3.535620	-0.436391
H	0	0.084269	-1.836659	-0.362869
H	0	-1.496032	-1.501972	-1.110317
H	0	0.445658	2.796038	-1.142128
H	0	-0.671455	3.326972	-2.417921
H	0	-3.415974	1.405344	-3.464516
H	0	-4.074265	2.647319	-2.387667
H	0	-2.554671	2.931256	-3.244519
H	0	-3.603302	-0.289096	-1.652359
H	0	-2.971280	0.007332	-0.026518
H	0	-4.304593	0.977163	-0.645457

Energy + ZPE = -1158.873871
Free energy = -1158.925441
Free energy in DCM = -1159.259599
Free energy in heptane = -1159.262051
Number of imaginary frequencies = 0

Product 21a+cpSiX

C	0	-1.525265	1.537837	3.224533
C	0	-1.696851	3.039985	3.381098
C	0	-2.843736	1.037067	3.855526
C	0	-3.005170	3.309449	3.261121
C	0	-3.724872	1.992352	3.017934
Cl	0	-2.296353	-1.612082	1.252435
B	0	-1.226318	-0.170268	1.292518
C	0	-1.810874	1.238748	1.664235
C	0	0.311180	-0.388152	0.975436
C	0	-3.341558	1.523877	1.569249
C	0	0.515208	-0.658841	-0.582487
C	0	1.006628	-1.455669	1.901513
C	0	1.582744	-1.740331	-0.833155
C	0	1.936805	-2.416556	1.145670
C	0	0.774865	0.684599	-1.262630
C	0	2.845513	-1.673975	0.108123
C	0	1.146930	-3.009422	-0.048751
I	0	0.718081	0.601021	-3.484521
C	0	3.967627	-2.583443	-0.427970
C	0	3.498153	-0.341325	0.499625
H	0	-0.592317	1.117977	3.609457
H	0	-0.877879	3.749226	3.451736
H	0	-2.893256	1.244633	4.928912
H	0	-3.050943	-0.022791	3.672246
H	0	-3.472660	4.288490	3.222725
H	0	-4.799178	1.983595	3.216959
H	0	-1.239329	1.981229	1.091431
H	0	0.800278	0.571801	1.183191
H	0	-3.570417	2.285666	0.817695
H	0	-3.903051	0.621083	1.310507
H	0	-0.417388	-1.059977	-0.999742
H	0	0.254559	-2.065075	2.416795
H	0	1.562502	-0.923690	2.683962
H	0	1.772793	-1.842280	-1.906853
H	0	2.426793	-3.107218	1.843701
H	0	0.005527	1.420738	-1.029223
H	0	1.756609	1.099146	-1.040998
H	0	0.071209	-3.155046	0.094781
H	0	1.574868	-3.931949	-0.445033
H	0	4.735412	-2.736445	0.341193
H	0	3.614302	-3.569850	-0.740945
H	0	4.454886	-2.118742	-1.294368
H	0	3.958274	0.138031	-0.374142
H	0	2.812944	0.377626	0.952491
H	0	4.302798	-0.520742	1.224747

Energy + ZPE = -1158.873849
Free energy = -1158.924945
Free energy in DCM = -1159.259430
Free energy in heptane = -1159.262267
Number of imaginary frequencies = 0

Diels-Alder reaction with Vinylborane (22a)

TS 22a+cpReN

C	0	-2.550232	-0.314699	2.183366
C	0	-2.642771	1.066886	2.103442
C	0	-3.941181	-0.877216	2.075892
C	0	-3.918973	1.414426	1.625558
C	0	-4.636730	0.241045	1.318098
H	0	-1.698684	-0.872271	2.555435
H	0	-1.834664	1.765372	2.288461
H	0	-4.372033	-0.914938	3.091224
H	0	-4.024370	-1.875819	1.645029
H	0	-4.244512	2.423481	1.396895

H	0	-5.713656	0.245337	1.173000
Cl	0	-1.448258	1.716762	-1.059013
B	0	-1.368577	-0.051616	-0.635517
C	0	-2.676345	-0.785346	-0.389690
C	0	0.037790	-0.783648	-0.702269
C	0	-3.972945	-0.262497	-0.533481
C	0	1.283782	0.003634	-0.168817
C	0	0.211463	-1.326225	-2.179852
C	0	2.528018	-0.212609	-1.054714
C	0	1.656134	-1.233708	-2.696690
C	0	1.516294	-0.298027	1.334735
C	0	2.709005	-1.673566	-1.623204
C	0	2.143527	0.224223	-2.496908
C	0	2.544171	0.593779	2.001477
C	0	4.111459	-1.849994	-2.236326
C	0	2.437719	-2.919733	-0.770106
C	0	2.264088	1.946418	2.248547
C	0	3.799154	0.100644	2.381835
C	0	4.746996	0.928760	2.987317
C	0	3.206176	2.778345	2.852545
C	0	4.453741	2.271720	3.224615
H	0	-2.606158	-1.854098	-0.180419
H	0	-0.066455	-1.672782	-0.067484
H	0	-4.795349	-0.952995	-0.716284
H	0	-4.090551	0.694904	-1.032442
H	0	1.069952	1.078221	-0.235023
H	0	-0.148528	-2.361997	-2.217338
H	0	-0.419033	-0.762781	-2.881415
H	0	3.412594	0.248848	-0.600942
H	0	1.738087	-1.679649	-3.696928
H	0	1.804901	-1.347383	1.464479
H	0	0.553112	-0.177245	1.850821
H	0	1.388787	1.013313	-2.586230
H	0	3.000530	0.488752	-3.119997
H	0	4.415672	-1.013405	-2.871174
H	0	4.864555	-1.951148	-1.444230
H	0	4.151461	-2.760807	-2.847782
H	0	3.178348	-3.008406	0.035489
H	0	1.447500	-2.940769	-0.313261
H	0	2.530719	-3.822692	-1.388541
H	0	1.295155	2.350939	1.962511
H	0	4.035076	-0.946277	2.202985
H	0	5.713656	0.522406	3.274378
H	0	2.965842	3.822692	3.035650
H	0	5.188683	2.918233	3.696928

Energy + ZPE = -1379.023033
Free energy = -1379.077754
Free energy in DCM = -1379.492596
Free energy in heptane = -1379.494386
Number of imaginary frequencies = 1 (-406.69)

TS 22a+cpReX

Cl	0	1.251415	-2.253720	-0.994293
B	0	1.215765	-0.433057	-1.074382
C	0	2.529632	0.328622	-1.136241
C	0	-0.188488	0.284876	-1.246064
C	0	3.823851	-0.190030	-1.302303
C	0	-1.409180	-0.307260	-0.460377
C	0	-0.441651	0.434817	-2.802440
C	0	-2.699807	-0.298532	-1.306781
C	0	-1.913580	0.244059	-3.200038
C	0	-1.553063	0.384124	0.920823
C	0	-2.899123	0.969777	-2.222676
C	0	-2.399755	-1.101916	-2.603997
C	0	-2.533227	-0.287657	1.860878
C	0	-4.332174	1.015444	-2.787225
C	0	-2.568385	2.387370	-1.737638
C	0	-2.219319	-1.517260	2.459749
C	0	-3.774657	0.291359	2.154884
C	0	-4.677312	-0.335749	3.016633
C	0	-3.116402	-2.148206	3.320892
C	0	-4.351173	-1.558786	3.602902
H	0	2.440351	1.412577	-1.219291
H	0	-0.037668	1.304218	-0.868996
H	0	4.570132	0.405682	-1.821590
H	0	3.931729	-1.261090	-1.462623
H	0	-1.209948	-1.366368	-0.252686
H	0	-0.077765	1.418712	-3.123536
H	0	0.143402	-0.302578	-3.369263
H	0	-3.560837	-0.607439	-0.702839
H	0	-2.048994	0.418819	-4.275739
H	0	-1.837622	1.433665	0.784741
H	0	-0.560208	0.394749	1.393180
H	0	-1.655970	-1.902480	-2.524117
H	0	-3.291554	-1.502228	-3.090910
H	0	-4.678867	0.052002	-3.171054
H	0	-5.039078	1.332078	-2.009550
H	0	-4.398262	1.741306	-3.608187
H	0	-3.268952	2.703488	-0.953676
H	0	-1.557787	2.500233	-1.343043
H	0	-2.676906	3.099313	-2.566953
H	0	-1.258867	-1.983045	2.248347
H	0	-4.035181	1.247388	1.705635
H	0	-5.633988	0.134146	3.230949
H	0	-2.850337	-3.099313	3.775327
H	0	-5.050605	-2.047951	4.275739
C	0	4.736323	-0.157080	0.533882
C	0	4.773583	1.215977	0.848270
C	0	3.568399	-0.731274	1.312447
C	0	3.521659	1.606572	1.357326
C	0	2.707134	0.486937	1.467509
H	0	5.633988	-0.737070	0.338123
H	0	5.588194	1.891270	0.606750
H	0	3.941888	-1.014820	2.311757
H	0	3.082572	-1.605011	0.878851
H	0	3.217699	2.628484	1.558593
H	0	1.707551	0.474057	1.885469

Energy + ZPE = -1379.022581
Free energy = -1379.077637
Free energy in DCM = -1379.491427
Free energy in heptane = -1379.493612
Number of imaginary frequencies = 1 (-408.80)

TS 22a+cpSiN

Cl	0	2.034971	-1.757138	-2.034696
C	0	1.964765	0.964697	-1.134156
C	0	3.326741	0.960061	-0.786746
B	0	1.166767	-0.185078	-1.719964
C	0	-0.398406	-0.145057	-1.977957
C	0	-1.166498	-0.960454	-0.862132
C	0	-2.390101	-1.702401	-1.438201
C	0	-3.203776	-0.915161	-2.536827
C	0	-2.081213	-1.401973	-3.514862
C	0	-0.817597	-0.529228	-3.443039
C	0	-1.478901	-0.048299	0.353448
C	0	-4.549959	-1.609202	-2.819407
C	0	-1.872109	-2.621618	-2.581319
C	0	-3.495356	0.586039	-2.414748
C	0	-1.983799	-0.786731	1.575944
C	0	-1.107405	-1.553540	2.358779
C	0	-3.330961	-0.730876	1.957088
C	0	-3.792470	-1.419985	3.080771
C	0	-2.909111	-2.180838	3.846824
C	0	-1.562323	-2.244505	3.481411
H	0	1.411012	1.876555	-0.904993
H	0	3.684661	1.700491	-0.072379
H	0	3.838953	0.004995	-0.716553
H	0	-0.690528	0.902948	-1.833990
H	0	-0.505163	-1.754755	-0.487628
H	0	-2.972974	-2.166228	-0.633852
H	0	-2.368363	-1.586683	-4.558633
H	0	-0.961868	0.394327	-4.020157
H	0	-0.012196	-1.082266	-3.942408
H	0	-0.554333	0.484626	0.615836
H	0	-2.206422	0.718225	0.062921
H	0	-5.256839	-1.420329	-2.001259
H	0	-4.998799	-1.215125	-3.740590
H	0	-4.463770	-2.693276	-2.932952
H	0	-0.847287	-2.995580	-2.483399
H	0	-2.532953	-3.462969	-2.801422
H	0	-4.202257	0.779968	-1.597396
H	0	-2.610375	1.198559	-2.238552
H	0	-3.967799	0.950064	-3.337167
H	0	-0.055097	-1.603532	2.086235
H	0	-4.025727	-0.135928	1.367957
H	0	-4.842088	-1.359304	3.357615
H	0	-3.264747	-2.716504	4.723095
H	0	-0.864133	-2.829569	4.074858
C	0	4.342550	1.770956	-2.348404
C	0	4.339577	0.745724	-3.316104
C	0	3.272210	2.755144	-2.789058
C	0	3.121731	0.771654	-4.018409
C	0	2.365188	1.845729	-3.573135
H	0	5.256839	2.104337	-1.864971
H	0	5.095195	-0.026845	-3.409248
H	0	3.737663	3.462969	-3.496437
H	0	2.800784	3.340838	-1.999010
H	0	2.792080	0.017068	-4.723095
H	0	1.394877	2.138566	-3.956820

Energy + ZPE = -1379.023709
Free energy = -1379.078927
Free energy in DCM = -1379.494735
Free energy in heptane = -1379.496142
Number of imaginary frequencies = 1 (-398.97)

TS 22a+cpSiX

Cl	0	2.336681	-1.673276	-2.089099
C	0	2.013670	1.187604	-2.275050
C	0	3.385944	1.459613	-2.389759
B	0	1.326119	-0.152337	-2.087573
C	0	-0.225693	-0.314726	-1.800589
C	0	-0.491722	-0.733637	-0.300418
C	0	-1.674064	-1.717381	-0.183671
C	0	-2.891155	-1.430454	-1.145445
C	0	-2.020820	-2.150567	-2.230725
C	0	-0.965890	-1.220674	-2.852413
C	0	-0.609195	0.525192	0.598331
C	0	-4.115222	-2.274545	-0.741564
C	0	-1.341641	-2.941594	-1.083780
C	0	-3.401013	-0.008340	-1.412675
C	0	-0.622026	0.232403	2.084623
C	0	0.549588	-0.169690	2.743930
C	0	0.546389	-0.451296	4.109705
C	0	-0.633649	-0.333813	4.848048
C	0	-1.805993	0.068562	4.207947
C	0	-1.796584	0.348374	2.839692
H	0	1.363317	2.060744	-2.210833
H	0	3.763867	2.426197	-2.066540
H	0	4.087579	0.641584	-2.238208
H	0	-0.646010	0.692852	-1.908954
H	0	0.379011	-1.293823	0.068718
H	0	-1.914631	-1.907334	0.868796
H	0	-2.551418	-2.712975	-3.010547
H	0	-0.250192	-1.856361	-3.389426
H	0	-1.430601	-0.571561	-3.606952
H	0	0.244494	1.178840	0.370093
H	0	-1.509690	1.088961	0.329288
H	0	-4.868338	-2.264244	-1.540241
H	0	-3.871802	-3.319846	-0.532639
H	0	-4.584860	-1.860381	0.159900
H	0	-0.280783	-3.181039	-1.213777
H	0	-1.874237	-3.852170	-0.801132
H	0	-3.862863	0.415158	-0.511225
H	0	-2.629500	0.686683	-1.746128
H	0	-4.178673	-0.030960	-2.188097
H	0	1.475565	-0.257531	2.179180
H	0	1.467025	-0.758390	4.599654
H	0	-0.637234	-0.550581	5.913056
H	0	-2.729747	0.167531	4.772647
H	0	-2.714362	0.666091	2.349268
C	0	1.615515	1.002488	-4.854450
C	0	1.667917	2.386350	-4.967431
C	0	3.023020	0.483210	-4.863694
C	0	2.988837	2.816601	-4.746641
C	0	3.782383	1.707647	-4.390967

H	0	0.740224	0.387181	-5.026901
H	0	0.814539	3.037719	-5.124491
H	0	3.310742	0.297725	-5.913056
H	0	3.194692	-0.436607	-4.305090
H	0	3.312449	3.852170	-4.719510
H	0	4.868338	1.741955	-4.388714

Energy + ZPE = -1379.023454
Free energy = -1379.078439
Free energy in DCM = -1379.493399
Free energy in heptane = -1379.495331
Number of imaginary frequencies = 1 (-402.92)

Product 22a+cpReN

C	0	-3.425639	-0.335220	0.923807
C	0	-3.628479	1.166890	0.798797
C	0	-4.897484	-0.809151	0.944749
C	0	-2.990851	-0.886905	-0.518432
C	0	-4.730909	1.363229	0.061831
C	0	-5.279123	-0.004015	-0.318025
B	0	-1.580947	-0.344216	-0.956471
C	0	-4.273579	-0.605813	-1.363722
Cl	0	-1.463649	0.974479	-2.167506
C	0	-0.256810	-0.990884	-0.390422
C	0	0.988076	-0.065757	-0.176145
C	0	0.023284	-2.252295	-1.314820
C	0	2.296327	-0.752521	-0.618955
C	0	1.519718	-2.474991	-1.584168
C	0	1.008808	0.477777	1.277339
C	0	2.394523	-2.293552	-0.296968
C	0	2.119313	-1.146924	-2.112723
C	0	2.034330	1.565776	1.521873
C	0	3.832930	-2.803675	-0.509316
C	0	1.907131	-2.881431	1.033548
C	0	1.839985	2.857693	1.010006
C	0	3.201438	1.314690	2.255084
C	0	4.148969	2.318097	2.468950
C	0	2.782605	3.863598	1.220220
C	0	3.942755	3.596944	1.951216
H	0	-2.778195	-0.674291	1.735897
H	0	-2.929353	1.920232	1.148942
H	0	-5.432624	-0.475342	1.839604
H	0	-5.008918	-1.894087	0.828348
H	0	-2.874427	-1.973733	-0.385467
H	0	-5.109273	2.308815	-0.313701
H	0	-6.324692	-0.034250	-0.634425
H	0	-4.670585	-1.536372	-1.785977
H	0	-4.095105	0.084528	-2.191855
H	0	-0.520738	-1.401209	0.592317
H	0	0.889200	0.811157	-0.828683
H	0	-0.423032	-3.136992	-0.844722
H	0	-0.468401	-2.149225	-2.293244
H	0	3.164729	-0.139638	-0.352655
H	0	1.670271	-3.388627	-2.174167
H	0	1.175290	-0.346647	1.980212
H	0	0.008074	0.875344	1.501345
H	0	1.459239	-0.510675	-2.712925
H	0	3.061484	-1.275457	-2.649652
H	0	4.289832	-2.442547	-1.434713
H	0	4.476303	-2.483787	0.320243
H	0	3.851893	-3.900870	-0.537150
H	0	2.539062	-2.539064	1.863100
H	0	0.874567	-2.632402	1.281161
H	0	1.981323	-3.976755	1.006790
H	0	0.937022	3.077199	0.443755
H	0	3.367508	0.321601	2.667242
H	0	5.046034	2.099713	3.042891
H	0	2.609505	4.858219	0.817037
H	0	4.676868	4.380747	2.118070

Energy + ZPE = -1379.066402
Free energy = -1379.120376
Free energy in DCM = -1379.538867
Free energy in heptane = -1379.541766
Number of imaginary frequencies = 0

Product 22a+cpReX

C	0	3.348680	0.994058	3.949037
C	0	3.313954	2.513200	3.897145
C	0	1.835117	0.684971	4.003913
C	0	3.679044	0.493874	2.498029
C	0	2.218139	2.869431	3.211190
C	0	1.504062	1.592473	2.798281
C	0	2.439045	0.938793	1.660214
B	0	1.616215	-0.110179	0.825448
Cl	0	1.607588	-1.841832	1.311862
C	0	0.822968	0.328925	-0.465210
C	0	-0.509890	-0.416895	-0.811936
C	0	1.901861	0.314644	-1.632307
C	0	-0.617697	-0.729814	-2.318038
C	0	1.333496	-0.201562	-2.963197
C	0	-1.725020	0.350503	-0.226430
C	0	-0.079235	0.396159	-3.282519
C	0	0.638803	-1.561944	-2.700370
C	0	-3.032850	-0.411513	-0.292282
C	0	-0.500473	0.116842	-4.737862
C	0	-0.340216	1.885007	-3.020362
C	0	-3.267693	-1.500068	0.561335
C	0	-4.035789	-0.059328	-1.204896
C	0	-5.235139	-0.772030	-1.269040
C	0	-4.463106	-2.215562	0.501666
C	0	-5.452615	-1.853932	-0.415683
H	0	3.977215	0.550465	4.725187
H	0	4.105647	3.164899	4.253955
H	0	1.363388	1.035796	4.927130
H	0	1.597575	-0.371860	3.843913
H	0	4.608390	0.927369	2.115563
H	0	3.794746	-0.594496	2.499972
H	0	1.934749	3.866050	2.886516
H	0	0.451258	1.698862	2.523405
H	0	2.711455	1.746326	0.968476
H	0	0.569090	1.385637	-0.313103

H	0	-0.501231	-1.396046	-0.316350
H	0	2.306559	1.327111	-1.748578
H	0	2.759633	-0.325388	-1.378070
H	0	-1.600777	-1.150808	-2.556525
H	0	2.096060	-0.146866	-3.751213
H	0	-1.836862	1.314976	-0.734823
H	0	-1.501134	0.581302	0.825438
H	0	1.067395	-2.192694	-1.913575
H	0	0.509515	-2.167650	-3.599772
H	0	-0.356548	-0.924203	-5.039745
H	0	-1.562257	0.355506	-4.879552
H	0	0.074089	0.744608	-5.431172
H	0	-1.404968	2.120170	-3.145769
H	0	-0.043051	2.222054	-2.026414
H	0	0.209352	2.494321	-3.750248
H	0	-2.505455	-1.786001	1.283324
H	0	-3.876370	0.786483	-1.870380
H	0	-5.999566	-0.478750	-1.984206
H	0	-4.624827	-3.053497	1.175087
H	0	-6.385825	-2.409043	-0.461433

Energy + ZPE = -1379.066823
Free energy = -1379.121155
Free energy in DCM = -1379.539289
Free energy in heptane = -1379.542491
Number of imaginary frequencies = 0

Product 22a+cpSiN

C	0	1.507393	-1.003003	4.972125
C	0	1.646810	0.510712	5.041528
C	0	-0.032728	-1.133775	4.949351
C	0	1.855277	-1.409979	3.497025
C	0	0.630711	1.043587	4.348161
C	0	-0.203220	-0.107618	3.805562
C	0	0.670715	-0.820614	2.668003
B	0	0.911758	0.120437	1.432205
Cl	0	2.573109	0.678457	1.037564
C	0	-0.272068	0.616022	0.506403
C	0	-0.120914	0.144990	-0.993393
C	0	-0.510227	2.168696	0.669437
C	0	-0.560287	1.243817	-1.981952
C	0	-0.818410	2.880238	-0.657825
C	0	-0.821667	-1.223913	-1.200704
C	0	-1.826659	2.078559	-1.548616
C	0	0.292210	2.507604	-1.672545
C	0	-0.546580	-1.870410	-2.543167
C	0	-2.348259	2.925734	-2.725128
C	0	-3.050772	1.423950	-0.895158
C	0	0.709301	-2.429374	-2.823862
C	0	-1.531363	-1.926434	-3.538050
C	0	-1.272597	-2.517373	-4.776630
C	0	0.973899	-3.020106	-4.058999
C	0	-0.017618	-3.065674	-5.041843
H	0	2.046960	-1.572949	5.732507
H	0	2.493352	1.035640	5.473006
H	0	-0.501859	-0.804422	5.882152
H	0	-0.386362	-2.139272	4.690730
H	0	1.891398	-2.501478	3.401644
H	0	2.827864	-1.019208	3.188377
H	0	0.478292	2.090135	4.102261
H	0	-1.222692	0.132108	3.494688
H	0	0.042598	-1.644230	2.289768
H	0	-1.175513	0.124764	0.887311
H	0	0.944149	-0.018542	-1.207123
H	0	-1.328341	2.321779	1.384550
H	0	0.371915	2.658182	1.102027
H	0	-0.552373	0.860544	-3.008593
H	0	-1.032590	3.942787	-0.483494
H	0	-0.482763	-1.901829	-0.403809
H	0	-1.902888	-1.110076	-1.064664
H	0	1.294288	2.336312	-1.265124
H	0	0.369977	3.200549	-2.512675
H	0	-2.874854	2.290977	-3.449104
H	0	-3.060983	3.680026	-2.367642
H	0	-1.556765	3.451358	-3.266100
H	0	-3.575707	0.778980	-1.611668
H	0	-2.820475	0.821028	-0.015747
H	0	-3.763967	2.198111	-0.582014
H	0	1.486705	-2.405923	-2.062760
H	0	-2.514614	-1.506188	-3.337500
H	0	-2.053499	-2.550804	-5.532126
H	0	1.953333	-3.449872	-4.252983
H	0	0.186088	-3.528266	-6.003864

Energy + ZPE = -1379.065829
Free energy = -1379.118593
Free energy in DCM = -1379.539067
Free energy in heptane = -1379.541865
Number of imaginary frequencies = 0

Product 22a+cpSiX

C	0	-2.283110	2.254350	2.189029
C	0	-2.192613	3.771487	2.186959
C	0	-3.816156	2.064798	2.201596
C	0	-1.940043	1.808545	0.676103
C	0	-3.243865	4.236528	1.496511
C	0	-4.047471	3.036305	1.021662
C	0	-3.195495	2.328231	-0.090807
B	0	-1.551342	0.286088	0.657745
Cl	0	-2.794431	-0.954885	0.261398
C	0	-0.095523	-0.220280	1.011863
C	0	0.640285	-0.751133	-0.288302
C	0	-0.057469	-1.226402	2.223277
C	0	1.502501	-1.991812	0.019720
C	0	0.905153	-2.405531	2.011817
C	0	1.405228	0.401498	-0.992440
C	0	2.273429	-1.956620	1.395071
C	0	0.567589	-3.062616	0.649276
C	0	1.941178	0.043613	-2.363836
C	0	3.326354	-3.079780	1.455617
C	0	2.950488	-0.683562	1.919668
C	0	1.076536	-0.057417	-3.464107
C	0	3.304916	-0.202126	-2.571073

C	0	1.557271	-0.398173	-4.728065
C	0	3.792340	-0.543251	-3.834433
C	0	2.919183	-0.643415	-4.917891
H	0	-1.706300	1.739335	2.961480
H	0	-1.351997	4.338423	2.575394
H	0	-4.268304	2.415159	3.134683
H	0	-4.139196	1.039102	1.994403
H	0	-1.043152	2.366450	0.377659
H	0	-3.438987	5.266194	1.212824
H	0	-5.082707	3.231106	0.731038
H	0	-2.925969	3.014787	-0.899427
H	0	-3.769306	1.505844	-0.529069
H	0	0.463117	0.669905	1.325733
H	0	-0.113921	-1.102694	-1.006889
H	0	-1.052843	-1.646571	2.412143
H	0	0.217595	-0.668790	3.127916
H	0	2.085238	-2.278644	-0.863004
H	0	0.938491	-3.042136	2.905572
H	0	0.720668	1.255543	-1.091310
H	0	2.228522	0.740528	-0.354142
H	0	-0.482632	-3.042264	0.339006
H	0	0.941908	-4.083608	0.548878
H	0	3.680177	-3.219009	2.485307
H	0	2.952687	-4.044761	1.102519
H	0	4.197144	-2.820189	0.840031
H	0	3.812440	-0.415361	1.295128
H	0	2.293065	0.185606	1.966972
H	0	3.333836	-0.857889	2.933873
H	0	0.014698	0.139217	-3.329047
H	0	3.993519	-0.121016	-1.732755
H	0	0.869191	-0.467347	-5.566800
H	0	4.854946	-0.727440	-3.971108
H	0	3.295872	-0.906296	-5.902797

Energy + ZPE = -1379.065833
Free energy = -1379.120350
Free energy in DCM = -1379.538560
Free energy in heptane = -1379.541748
Number of imaginary frequencies = 0