Electronic Supplementary Material (ESI) for ChemComm.

Electronic supplementary information

Skeletal rearrangement of a boron-containing annulenic molecule into a macrocycle bridged by an electronically stabilized boron cation

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1. Materials and methods

Handling of air- and/or moisture-sensitive compounds were conducted either using standard Schlenk-line techniques or in a glove box under argon. Column chromatography was carried out using Silica Gel 60 N (spherical, neutral, particle size: 63–210 mm, Kanto Chemical Co., Inc.). Anhydrous CH_2Cl_2, *n*-hexane and THF were dried by passing through an activated alumina column and a Q-5 column (Nikko Hansen & Co., Ltd.). Mesitylene, $CDCl_3$ and ODCB-d_4 were dried over CaH_2 and freshly distilled prior to use. Compound $\mathbf{3_{Cl}}$[S1] and $[Et_3Si\text{-}H\text{-}SiEt_3]^+[(C_6F_5)_4B]^-$[S2] were prepared according to previously reported procedures.

Fourier transform infrared (FT-IR) spectra were recorded at 25 °C with a JASCO model FT/IR-6600 Fourier transform infrared spectrometer. Nuclear magnetic resonance (NMR) spectroscopy measurements were carried out on a Bruker model AVANCE-400 spectrometer (400.0 MHz for ^{1}H) or on a Bruker model AVANCE III HD-500 spectrometer (^{1}H: 500.0 MHz, ^{11}B: 160.4 MHz and ^{13}C: 125.7 MHz), where chemical shifts (δ) are expressed relative to the resonances of the residual non-deuterated solvents for ^{1}H ($CDCl_3$: ^{1}H(δ) = 7.26 ppm, ODCB-d_4: ^{1}H(δ) = 7.19 ppm, 6.93 ppm) and for ^{13}C ($CDCl_3$: ^{13}C(δ) = 77.15 ppm、ODCB-d_4: ^{13}C(δ) = 127.1 ppm, 129.9 ppm and 132.3 ppm), and the resonance of external $BF_3{\cdot}Et_2O$ (^{11}B(δ) = 0.0 ppm) for ^{11}B. The absolute values of the coupling constants are given in Hertz (Hz), regardless of their signs. Multiplicities are abbreviated as singlet (s), doublet (d), triplet (t), multiplet (m) and broad (br). Mass spectrometry measurements were carried out on a Bruker micrOTOF II mass spectrometer equipped with an atmospheric pressure chemical ionization (APCI) probe.

2. Synthesis

Preparation of $[Et_3Si(mesitylene)]^+[(C_6F_5)_4B]^-$. This reagent was prepared using a modified procedure reported for the synthesis of silylium salts solvated with aromatic solvent molecules.[S3] Under argon, mesitylene (1.31 g, 11.0 mmol) was added to an ODCB solution (2 mL) of $[Et_3Si\text{-}H\text{-}SiEt_3]^+[(C_6F_5)_4B]^-$ (1.00 g, 1.10 mmol) at 25 °C, and the reaction mixture was stirred at 25 °C for 15 min. The reaction mixture was partially evaporated under reduced pressure, where the amount of the solution was reduced to approximately 1.0 mL and then poured into hexane (10 mL). The precipitate formed was collected by filtration, washed with hexane and dried under reduced pressure to give $[Et_3Si(mesitylene)]^+[(C_6F_5)_4B]^-$ as a colorless powder (0.823 g, 0.900 mmol) in 82% yield. ^{1}H NMR (500 MHz, ODCB-d_4, 25 °C): δ (ppm) 6.56 (s, 3H), 2.19 (s, 9H), 0.74 (t, J = 7.5 Hz, 9H), 0.61 (q, J = 7.5 Hz, 6H). ^{13}C NMR (126 MHz, ODCB-d_4, 25 °C): δ (ppm) 149.6, 147.7, 139.4, 137.5, 135.6, 120.7, 23.3, 6.1, 5.6. ^{29}Si NMR (99 MHz, ODCB-d_4, 25 °C): δ (ppm) 71.4.

Synthesis of $\mathbf{4}^+[(C_6F_5)_4B]^-$. Under argon, $[Et_3Si(mesitylene)]^+[(C_6F_5)_4B]^-$ (1.75 g, 1.91 mmol) was added to an ODCB solution (5 mL) of $\mathbf{3_{Cl}}$ (1.00 g, 1.91 mmol) at 25 °C. The reaction mixture was stirred at 25 °C for 30 min and then evaporated to dryness under reduced pressure. The

residue was dissolved in CH_2Cl_2, and the resultant solution was passed through a plug of silica gel and evaporated to dryness under reduced pressure. The residue was washed with hexane (20 mL) and dried under reduced pressure to give $\mathbf{4}^+[(C_6F_5)_4B]^-$ as a colorless powder (1.36 g, 1.17 mmol) in 61% yield. FT-IR (KBr): ν (cm^{-1}) 3067, 2943, 2864, 1644, 1515, 1464, 1412, 1384, 1373, 1276, 1089, 1033, 980, 922,773, 756, 684, 662, 610, 603, 575. ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C): δ (ppm) 7.79 (d, J = 7.7 Hz, 2H), 7.47 (t, J = 7.3 Hz, 2H), 7.39 (t, J = 7.7 Hz, 2H), 7.32 (d, J = 7.5 Hz, 2H), 3.10 (m, 2H), 2.91 (m, 2H), 2.65 (m, 2H), 2.15 (m, 2H), 1.97(m, 2H), 1.83 (m, 6H), 1.65–1.26 (m, 8H), 1.40–1.19 (m, 6H), 1.09–0.88 (m, 6H). ^{11}B NMR (160 MHz, $CDCl_3$, 25 °C): δ (ppm) –16.6. ^{13}C NMR (126 MHz, $CDCl_3$, 25 °C): δ (ppm) 149.2, 148.5, 147.2, 139.1, 138.8, 137.2, 135.3, 128.6, 127.7, 123.7, 121.0, 119.1, 117.9, 116.0, 34.0, 31.6, 29.0, 27.9, 25.7, 25.3, 25.2, 25.1 (two peaks), 24.9, 24.6, 22.7, 22.4, 20.3, 14.1. APCI-TOF MS: calcd. for $C_{36}H_{44}B$ $[M]^+$ (cation moiety): m/z = 487.3537; found: 487.3538. ^{1}H, ^{11}B and ^{13}C NMR spectra of $\mathbf{4}^+[(C_6F_5)_4B]^-$ are shown in Figs. S2, S3 and S4, respectively.

Synthesis of 5. Under argon, $LiAlH_4$ (3.3 mg, 8.57×10^{-2} mmol) was added to a THF solution (3 mL) of $\mathbf{4}^+[(C_6F_5)_4B]^-$ (100 mg, 8.57×10^{-2} mmol). The reaction mixture was stirred at 25 °C for 12 h and then evaporated to dryness under reduced pressure. Hexane was added to the residue, and the resultant suspension was filtrated off from an insoluble fraction and evaporated to dryness under reduce pressure. The residue was recrystallized from hexane to give **5** as colorless crystals (33.5 mg, 6.86×10^{-2} mmol) in 80% yield. FT-IR (KBr): ν (cm^{-1}) 2953, 2924, 2846, 2767, 1456, 1442, 1353, 1202, 1114, 746, 730. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 7.66 (d, J = 6.7 Hz, 2H) 7.46 (d, J = 6.7 Hz, 2H), 7.25–7.19 (m, 4H), 2.40–2.34 (m, 2H), 2.20–1.94 (m, 5H), 1.82–1.74 (m, 4H), 1.52–1.27 (m, 14H), 1.20–1.12 (m, 2H), 1.10–1.04 (m, 2H), 1.00–0.91 (m, 2H), 0.59–0.47 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$): δ (ppm) 155.1, 139.8, 126.7, 126.2, 125.7, 120.3, 117.1, 59.7, 53.0, 39.0, 32.6, 31.4, 27.9, 27.5, 27.2, 25.2, 24.9, 24.5, 23.7, 22.9, 21.7. ^{11}B NMR (160 MHz, $CDCl_3$): δ (ppm) –23.5. APCI-TOF MS: calcd. for $C_{36}H_{45}B$ $[M]^+$: m/z = 488.3621; found: 488.3629. ^{1}H, ^{11}B and ^{13}C NMR spectra of **5** are shown in Figs. S5, S6 and S7, respectively.

Synthesis of 6. Under argon, a benzene solution (2 mL) of **5** (100 mg, 0.205 mmol) was stirred at 80 °C for 24 h. After allowed to cool to 25 °C, the reaction mixture was evaporated to dryness under reduced pressure. The residue was recrystallized from hexane to give **6** as colorless crystals (60 mg, 0.123 mmol) in 60% yield. FT-IR (KBr): ν (cm^{-1}) 2953, 2924, 2846, 2767, 1456, 1442, 1353, 1202, 1114, 746, 730. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 7.84–7.79 (m, 2H) 7.77 (d, J = 7.4 Hz, 1H), 7.47 (d, J = 7.4 Hz, 1H), 7.36–7.28 (m, 2H), 7.27–7.19 (m, 2H), 2.47–2.39 (m, 1H), 2.29–2.18 (m, 2H), 2.18–2.01 (m, 4H), 1.99–1.88 (m, 2H), 1.87–1.70 (m, 3H), 1.65–1.42 (m, 6H), 1.41–1.18 (m, 7H), 1.13–0.96 (m, 7H), 0.94–0.79 (m, 2H), 0.69–0.60 (m, 1H), 0.52–0.39 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$): δ (ppm) 153.6, 144.8, 142.1, 140.3, 138.4,

137.5, 126.8, 126.6, 126.1, 125.8, 125.4, 124.1, 120.0, 119.3, 58.4, 53.2, 51.8, 46.5, 35.9, 35.2, 34.2, 32.7, 32.5, 31.6, 30.3, 29.9, 28.7, 28.0, 27.3, 26.6, 26.2, 25.6, 25.4, 25.0, 24.2, 23.4. ^{11}B NMR (160 MHz, $CDCl_3$): δ (ppm) 80.2. APCI-TOF MS: calcd. for $C_{36}H_{45}B$ $[M]^+$: m/z = 488.3621; found: 488.3629. ^{1}H, ^{11}B and ^{13}C NMR spectra of **6** are shown in Figs. S8, S9 and S10, respectively.

3. Single-crystal X-ray diffraction analysis

Single crystals of $\mathbf{4}^+[(C_6F_5)_4B]^-$ were obtained by recrystallization from CH_2Cl_2, and those of **5** and **6** were obtained by recrystallization from hexane. Each single crystal was coated with immersion oil (type B: Code 1248, Cargille Laboratories, Inc.) and mounted on a MicroMount (MiTeGen, LLC.). Diffraction data were collected at 90 K under a cold nitrogen gas stream on a RIGAKU model XtaLAB Synergy-DW diffractometer system equipped with a HyPix-6000 detector, using Cu-*K*α radiation (λ = 1.54184 Å).

Crystal data for $C_{61}H_{46}B_2Cl_2F_{20}$ ($\mathbf{4}^+[(C_6F_5)_4B]^-$): colorless prism, 0.04 × 0.07 × 0.08 mm^3, triclinic, *P*-1, a = 12.4793(1) Å, b = 14.1126(2) Å, c = 16.1478(2) Å, V = 2643.86(6) Å^3, Z = 2, ρ_{calcd} = 1.572 g cm^{-3}, T = 93 K, Cu*K*α radiation, λ = 1.54184 Å, μ = 2.121 mm^{-1}, 34697 reflections measured, 10736, unique reflections, 785 parameters, R_{int} = 0.0257, Completeness to theta = 67.68° : 99.9%, Absorption correction: multi-scan, GOF = 1.0419, R_1 = 0.0337 ($I > 2\sigma(I)$), wR_2 = 0.0863 (all data), $\Delta\rho_{max,min}$ = 0.509, –0.598 eÅ^3, CCDC-2297987.

Crystal data for $C_{36}H_{45}B$ (5): colorless prism, 0.13 × 0.09 × 0.05 mm^3, monoclinic, $P2_1/n$, a = 23.31009(11) Å, b = 9.47225(5) Å, c = 24.91264(13) Å, β = 97.6346(5) °, V = 5451.93(5) Å^3, Z = 8, ρ_{calcd} = 1.190 g cm^{-3}, T = 93 K, Cu*K*α radiation, λ = 1.54184 Å, μ = 0.485 mm^{-1}, 108653 reflections measured, 11313 unique reflections, 686 parameters, R_{int} = 0.0262, Completeness to theta = 66.97° : 100%, Absorption correction: multi-scan, GOF = 1.027, R_1 = 0.0393 ($I > 2\sigma(I)$), wR_2 = 0.0992 (all data), $\Delta\rho_{max,min}$ = 0.491, –0.253 eÅ^3, CCDC-2297988.

Crystal data for $C_{36}H_{45}B$ (6): colorless block, 0.30 × 0.22 × 0.20 mm^3, triclinic, *P*–1, a = 12.2748(2) Å, b = 15.6480(2) Å, c = 16.1985(2) Å, α = 103.9700(10) °, β = 97.9440(10) °, γ = 107.094(2) °, V = 2811.60(7) Å^3, Z = 4, ρ_{calcd} = 1.154 g cm^{-3}, T = 93 K, Cu*K*α radiation, λ = 1.54184 Å, μ = 0.471 mm^{-1}, 34513 reflections measured, 11136 unique reflections, 724 parameters, R_{int} = 0.0233, Completeness to theta = 67.68° : 99.8%, Absorption correction: multi-scan, GOF = 1.020, R_1 = 0.0452 ($I > 2\sigma(I)$), wR_2 = 0.1218 (all data), $\Delta\rho_{max,min}$ = 0.292, –0.280 eÅ^3, CCDC-2297989.

4. Computational details

The GRRM program combined with Gaussian 16 and Orca 5 was employed to investigate the reaction mechanism at 298.15 K and 1 atm.[S4–S6] The single-component AFIR (SC-AFIR) method was applied to structures **Int_1** and **Int_2**. In the SC-AFIR calculations, the GFN-XTB2 semiempirical method was employed.[S7] Then, the obtained results were refined with DFT using the RePATH method, in which the B3LYP functional and 6-21G*(C and B)_3-21G*(H) basis set were chosen.[S8] The SMD method was employed to address the solvation effect by specifying *o*-dichlorobenzene (ODCB) as a solvent.[S9] At the final stage, the selected approximate transition states from the RePATH calculations were reoptimized with a higher level of theory [*ω*b97xd/Def2SVPP smd(ODCB) level] to obtain accurate energetics and geometries for the intermediates, products, and transition states.[S10] The intrinsic reaction coordinate (IRC) calculations were performed automatically by the GRRM program for transition states to connect them with equilibrium structures.[S11]

On some selected structures, conformational searches were carried out. First, the GFN-XTB2 semiempirical method was employed, later the energetically lowest conformer was re-optimized at the *ω*b97xd/Def2SVPP smd(ODCB) level. All the energy values shown in this study are relative Gibbs free energies in the unit of kcal/mol, and all the distances are in the unit of Angstrom (Å). It should be noted that all the structures discussed in the manuscript are local minima or first-order saddle points optimized on the potential energy surface (in the absence of artificial force) at the aforementioned computational level, namely higher level of theory, where the number of imaginary frequency modes at each optimized structure was checked by the normal mode analysis. Figure 4 in the main text shows the most energetically favorable pathway, while an unfavorable pathway is shown in Fig. S2. The Cartesian coordinates and energies of intermediates, transition states and the product are shown in Tables S1–S28.

5. Supplementary references

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6. Supplementary figures

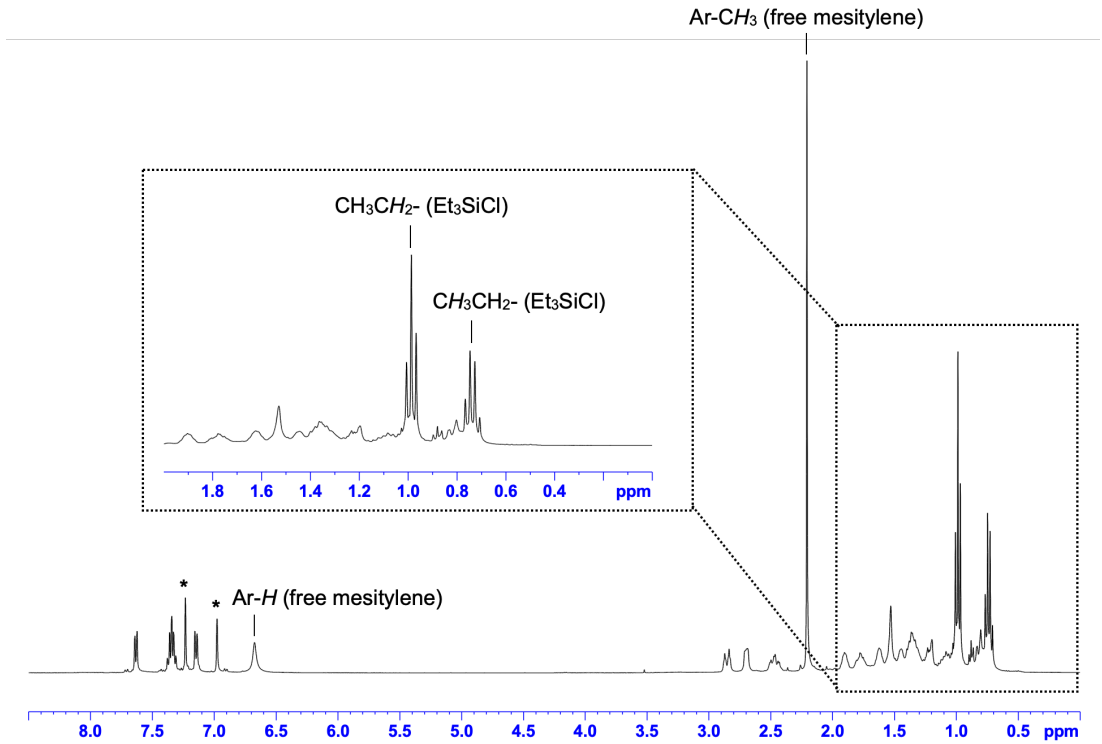

Fig. S1. Expanded region of the ^{1}H NMR spectrum (400 MHz, ODCB-d_4, 25 °C) of a reaction mixture of $\mathbf{3}_{\mathbf{Cl}}$ and $[Et_3Si(mesitylene)]^+[(C_6F_5)_4B]^-$ (1 equiv.) presented in Fig. 2c. Peaks denoted with an asterisk (*) arise from residual non-deuterated solvent.

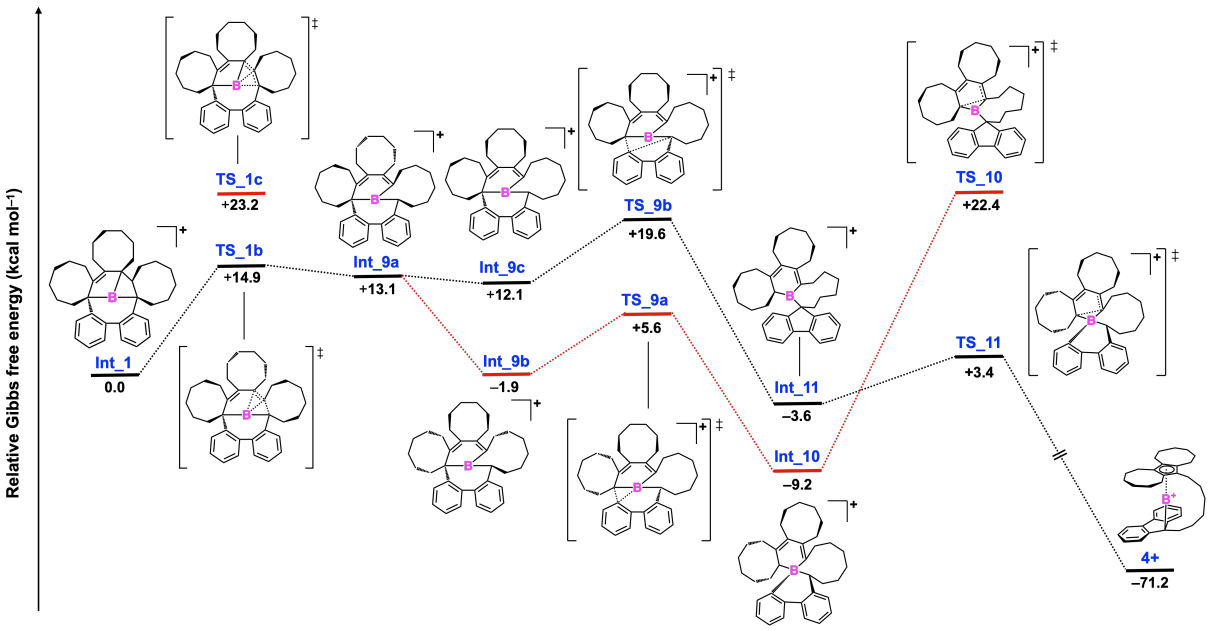

Fig. S2. Energy diagram of an unfavorable pathway [ωB97X-D/Def2-SVPP_scrf=(smd,solvent=*o*-dichlorobenzene) level]. The energy values (in kcal mol^{-1}) are shown relative to that of **Int_1**.

7. Analytical data

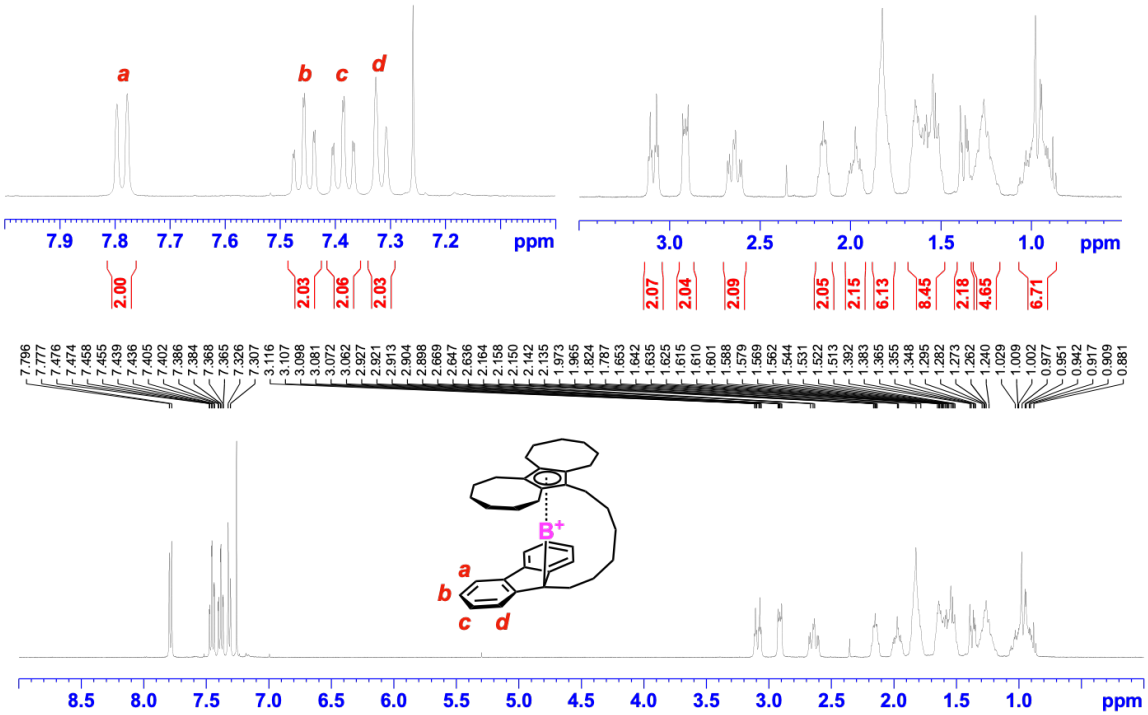

Fig. S3. ^{1}H NMR spectrum (500 MHz) of **4**$^{+}$[$(C_6F_5)_4B]^{-}$ in $CDCl_3$ at 25 °C.

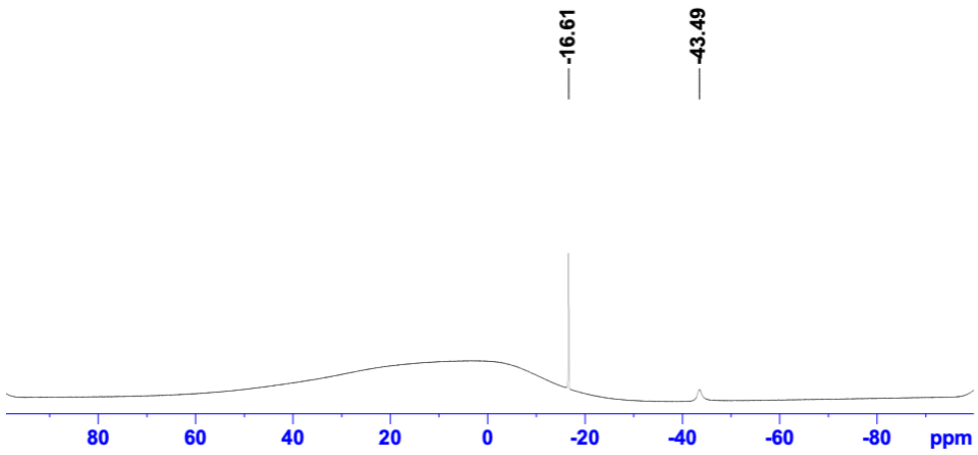

Fig. S4. ^{11}B NMR spectrum (160 MHz) of **4**$^{+}$[$(C_6F_5)_4B]^{-}$ in $CDCl_3$ at 25 °C. The broad peaks in a region from 60 to –40 ppm are the contribution from a borosilicate-glass NMR tube.

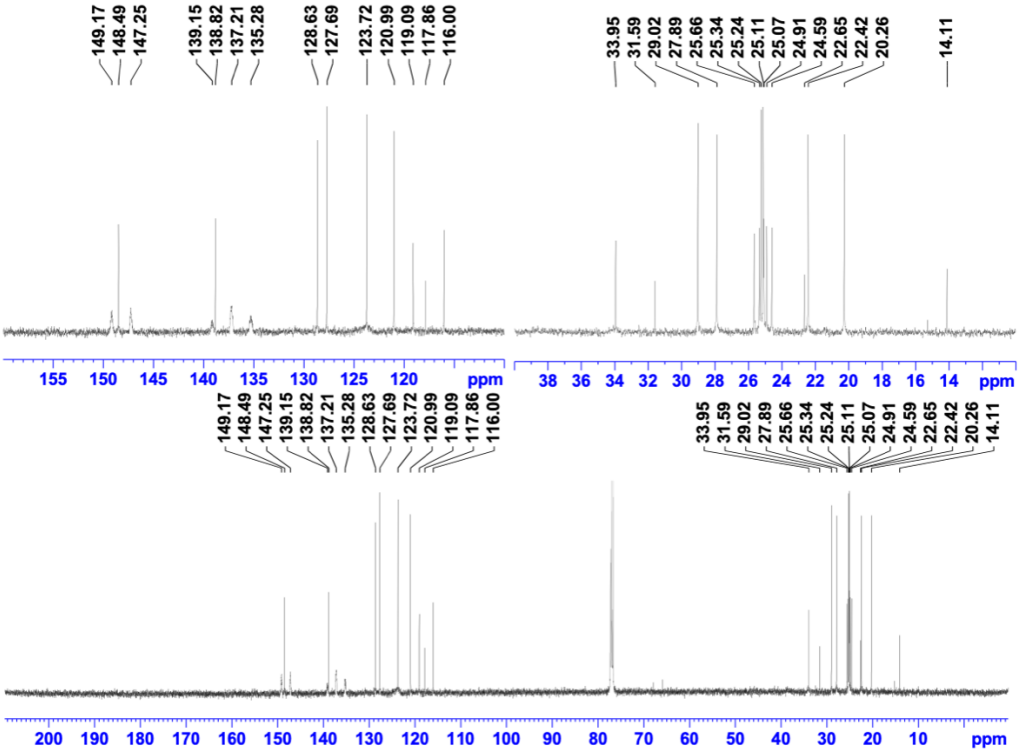

Fig. S5. ^{13}C NMR spectrum (126 MHz) of $\mathbf{4}^{+}[(C_6F_5)_4B]^{-}$ in $CDCl_3$ at 25 °C.

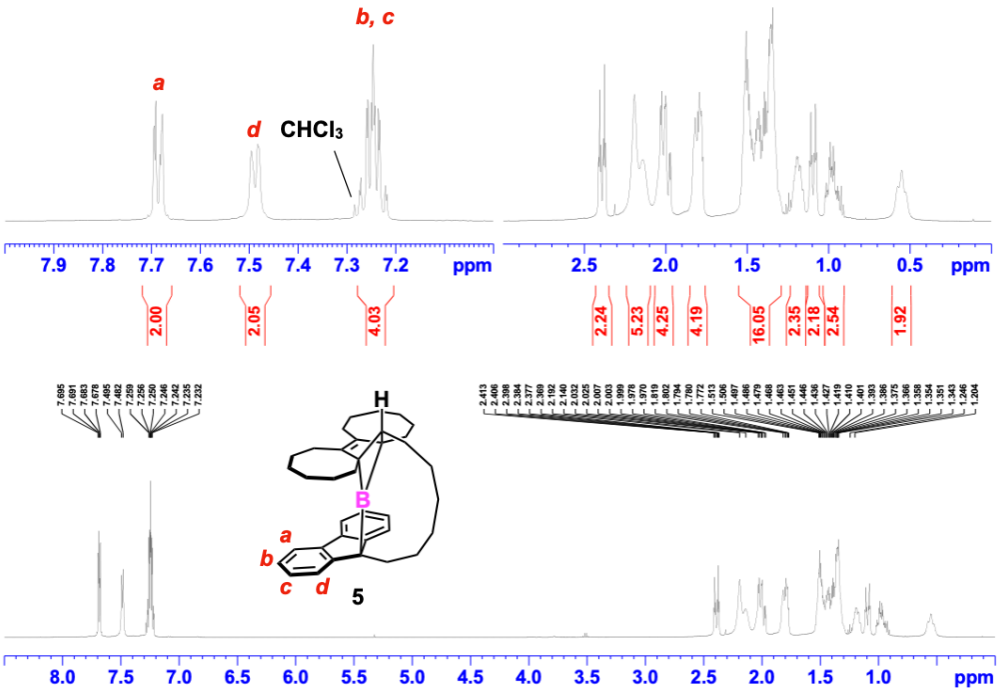

Fig. S6. ^{1}H NMR spectrum (500 MHz) of **5** in $CDCl_3$ at 25 °C.

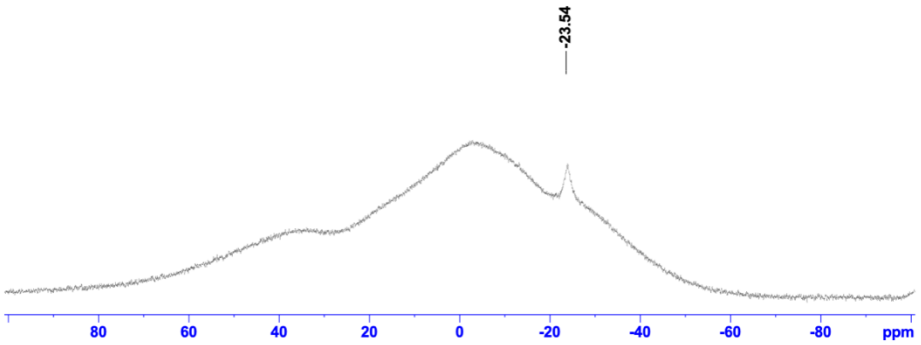

Fig. S7. ^{11}B NMR spectrum (160 MHz) of **5** in $CDCl_3$ at 25 °C. The broad peaks in a region from 60 to –40 ppm are the contribution from a borosilicate-glass NMR tube.

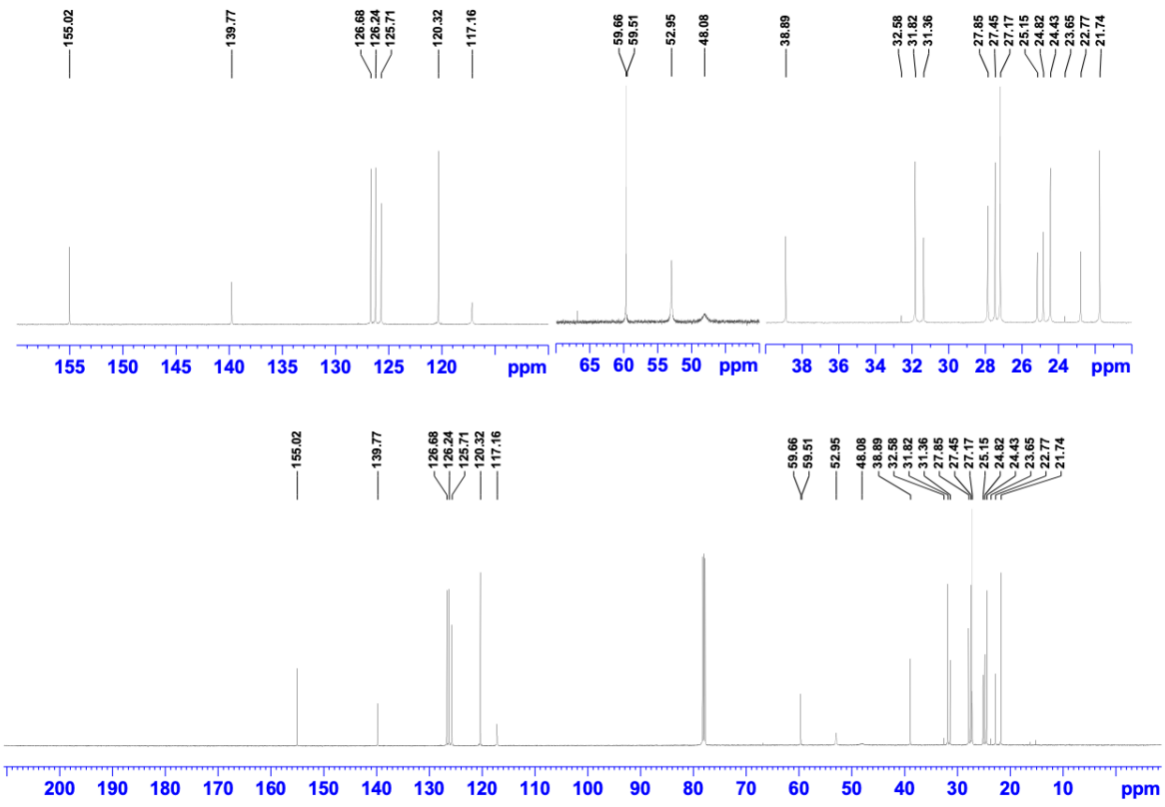

Fig. S8. ^{13}C NMR spectrum (126 MHz) of **5** in $CDCl_3$ at 25 °C.

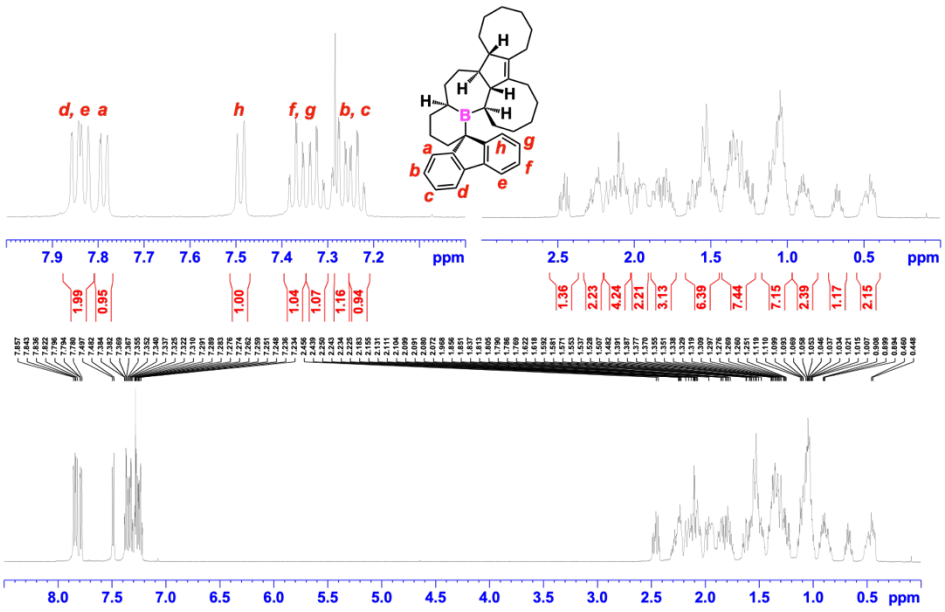

Fig. S9. ^{1}H NMR spectrum (500 MHz) of **6** in $CDCl_3$ at 25 °C.

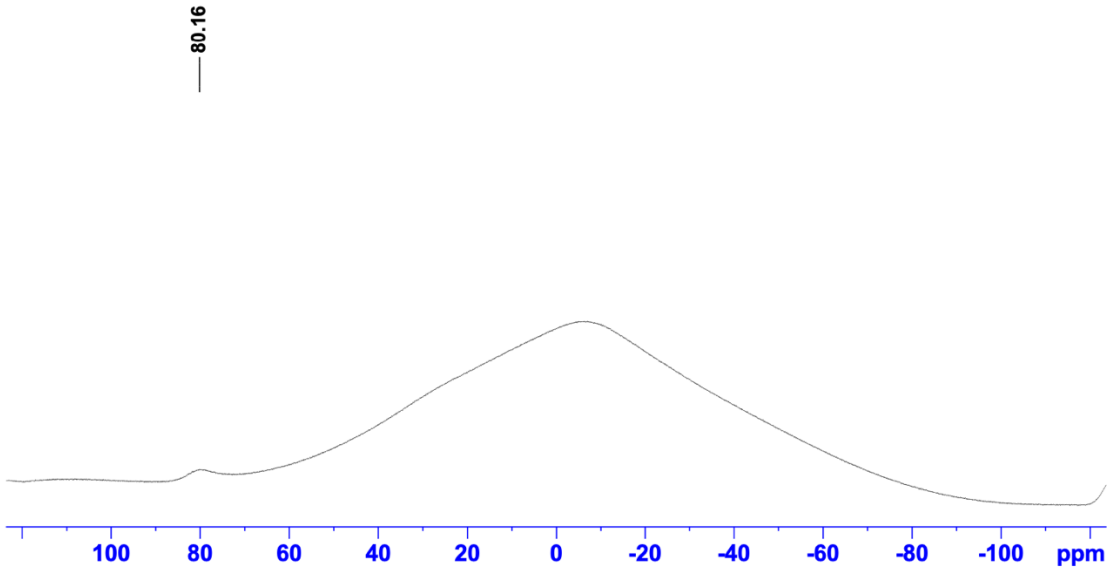

Fig. S10. ^{11}B NMR spectrum (160 MHz) of **6** in $CDCl_3$ at 25 °C. The broad peaks in a region from 60 to –40 ppm are the contribution from a borosilicate-glass NMR tube.

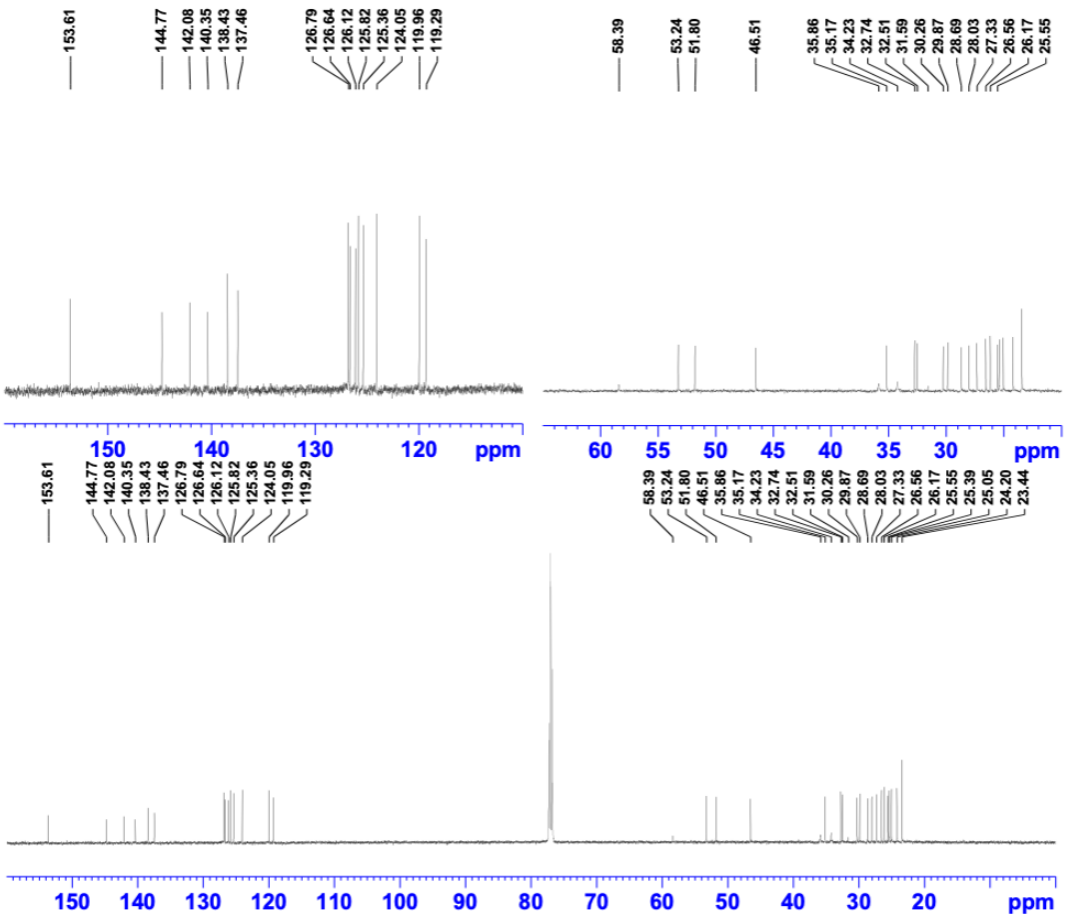

Fig. S11. ^{13}C NMR spectrum (126 MHz) of **6** in $CDCl_3$ at 25 °C.

8. Supplementary tables

Table S1. Cartesian coordinates and energies of Int_1.

C	1.991157210484	1.144551186403	-2.376089423742
C	2.421721155153	0.019054990351	-3.075488067983
C	2.370788907177	1.362137846558	-1.051032399984
C	3.247339754641	-0.904050508548	-2.440026572012
C	3.230545661738	0.447278334070	-0.402414380071
C	3.647936022907	-0.682142227031	-1.123245661181
B	1.217253999697	2.004364914759	1.013321846034
C	3.094282297947	0.920746220088	2.189943612204
C	3.801460076684	0.643798781411	0.981977723462
H	1.331441387415	1.865145500784	-2.863393254448
H	2.103955131748	-0.135587431180	-4.110246702925
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C	5.201880663081	0.532159337544	1.039759139942
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C	5.231431190021	0.958730269046	3.394951465062
H	3.337110032235	1.294270483097	4.304039986808
H	5.747920983791	0.342809917176	0.111930590269
H	7.010908039827	0.597008739349	2.213478608146
H	5.764730455362	1.090171067087	4.340599587069
C	-1.225231305369	0.478852491310	-1.873174447731
C	-0.518817066093	-0.222945405812	-0.705266439081
C	-2.883989854920	1.657249149695	0.664437666643
C	-0.000912801572	0.615111327305	0.452151585720
C	-1.662203072793	2.426312271619	1.171956507809
C	-0.350692651759	2.106704844129	0.482936505280
H	-1.063900475653	-0.162361084319	-2.756025318971
H	0.345788063084	-0.783521530883	-1.099086586991
H	-2.774341907503	0.582338236212	0.897381425262
H	-1.522047040993	2.181292573727	2.237070235102
H	-0.727705488283	1.434399875759	-2.109509840553
H	-1.199621779473	-0.982530612664	-0.277977029017
H	-3.736896189862	2.005905738965	1.270167055921
H	-1.863833891805	3.505836771940	1.126557747038
C	-2.733597278928	0.710525648996	-1.744788831038
H	-3.216052947292	-0.231657575142	-1.421698331632
H	-3.121300336053	0.920237774137	-2.757629617937
C	-3.196032322632	1.845488178708	-0.828455063819
H	-2.763927916991	2.801923344882	-1.181680224747
H	-4.287750256292	1.945317908189	-0.954639567872
C	1.603188122565	-1.934749154887	2.797296152718
C	1.151079474450	-1.370747119005	1.450327353861
C	0.778302731165	0.410658106362	4.655510152869
C	0.801329449965	0.091941741425	1.428428472270
C	0.966104013403	1.519744379889	3.612024243480
C	1.575776125537	1.149469155329	2.250412589191
H	2.450025964258	-1.346548190275	3.187361351588
H	0.276669239062	-1.940748851785	1.094072834972
H	1.748696376945	-0.023041884028	4.952934664248
H	1.562051612516	2.340881168473	4.043027838306
H	2.001272746664	-2.947325415577	2.614046768742
H	1.941644989232	-1.540585224668	0.696542072688
H	0.385866475705	0.905725832774	5.560249033676
H	-0.027719367291	1.954720750160	3.426297209335
C	0.498938706532	-2.033790287727	3.850072917499
H	0.937530804984	-2.480165193610	4.761638326125
H	-0.272268425838	-2.743927203673	3.497937166636
C	-0.184245930083	-0.716103888786	4.232580041587
H	-0.823432467598	-0.366893327804	3.399575822221
H	-0.880907813583	-0.933295042403	5.060501489473
C	0.278131433371	5.031487316971	-1.839572404112
C	0.033629136235	4.453720048431	-0.431658548287
C	3.651030461797	4.125679923018	-1.409098359359
C	0.443050544502	3.017648636771	-0.266619840175

C	2.954572543070	3.669226767812	-0.128788453068
C	1.889066698210	2.572928281371	-0.281132930365
H	-0.458181691823	5.846274820639	-1.941356846282
H	-1.041411841250	4.527322464893	-0.227559826543
H	4.339656649916	4.940957296145	-1.122149391296
H	2.523689763949	4.534374957895	0.397777381684
H	-0.003742930612	4.278178248027	-2.598750045768
H	0.533363953234	5.079450822652	0.327367627499
H	4.288893332219	3.306708776208	-1.787285208880
H	3.727256150317	3.268898408669	0.549731479372
C	1.655314990208	5.614268611876	-2.181230268765
H	1.993624118491	6.276139825399	-1.361472722319
H	1.496091785630	6.273667115423	-3.051743510638
C	2.756086029741	4.610857137295	-2.550888157993
H	2.289319390431	3.749484774641	-3.057721041567
H	3.418298118831	5.070041164403	-3.305383636506

Thermochemistry (use all positive eigenvalues) at 298.15 K, 1.00 Atm
E(el) = -1421.514799010939
ZPVE = 0.727078665307
Enthalpie(0K) = -1420.787720345632
E(tr) = 0.001416276854
E(rot) = 0.001416276854
E(vib) = 0.754738598609
H-E(el) = 0.758515336885
Enthalpie = -1420.756283674054
S(el) = 0.000000000000
S(tr) = 0.000070817727
S(rot) = 0.000058223755 (Symmetry number = 1)
S(vib) = 0.000167584720
G-E(el) = 0.670076234714
Free Energy = -1420.844722776225

Table S2. Cartesian coordinates and energies of TS_1a.

C	2.552172415173	0.738891868699	-2.395822898929
C	2.893305803257	-0.456878518500	-3.019875263198
C	2.772553053368	0.935419625240	-1.028587692075
C	3.462532044026	-1.489558493731	-2.272733440192
C	3.410972770697	-0.078530659704	-0.287797412100
C	3.726521982010	-1.292466136336	-0.922432331922
C	3.812782489346	0.146685547902	1.120407451409
H	2.075885760573	1.534674965839	-2.975672446138
H	2.697172296299	-0.590165357538	-4.087606199855
H	3.705234281911	-2.446550771109	-2.742518807241
H	4.169972677452	-2.105468950937	-0.341975815414
C	3.630955652792	1.293138569481	3.278343266144
C	5.014861690372	-0.410392366500	1.578404835618
C	5.508379056602	-0.135120852404	2.848946748973
C	4.826052890654	0.737334454675	3.700281410156
H	3.103653548054	1.967824224478	3.952428189632
H	5.604385010830	-1.041131982655	0.909834703096
H	6.450552736464	-0.588541347893	3.169180592500
H	5.225444872946	0.979092663725	4.688088961462
C	-1.826996472077	-0.955264968877	-1.239127883224
C	-0.316745514657	-0.794354320774	-0.955086426577
C	-2.116177009757	2.111723232628	-2.196686321352
C	0.146991991659	0.352802043566	-0.073976705652
C	-1.552186425659	2.111694179922	-0.764748398108
C	-0.078722938639	1.749856511182	-0.586585602987
H	-2.417695185300	-0.489086963279	-0.435036357689
H	0.218868714596	-0.681928383349	-1.915324880496
H	-3.217383098862	2.191279085376	-2.131458101688
H	-2.148724777844	1.432773572056	-0.140035748831
H	-2.071855572575	-2.029792843102	-1.188021432470
H	0.060566175541	-1.731308096094	-0.526960962039
H	-1.772425305781	3.023871383561	-2.716127134813
H	-1.722599150619	3.111275795682	-0.329158356492
C	-2.279027931547	-0.446340536068	-2.616781239298

H	-3.384440593076	-0.427692989631	-2.642529429838
H	-1.967362623395	-1.189527706867	-3.374171315365
C	-1.740864094303	0.913770264197	-3.065051963437
H	-0.639350613462	0.867821828847	-3.152702141540
H	-2.111487872544	1.102130141495	-4.088721916442
C	-0.611711987792	-1.794190006796	2.303580071109
C	0.743492034911	-1.277884449776	1.796564723092
C	-0.818984075304	1.632822172274	3.324749421057
C	0.699663070080	0.090311463238	1.141396110103
C	0.704405502838	1.423503063313	3.323348407746
H	-0.453921128564	-2.810245561289	2.708002974423
H	1.168156836861	-2.019108275202	1.097719756404
H	-1.064438697831	1.922057545899	4.362157685204
H	0.958406579257	0.580923654819	3.987626544911
H	-1.298348373178	-1.905745830661	1.444544323365
H	1.448389170490	-1.240438580801	2.645038627650
H	-1.065590084435	2.509367365773	2.698263775253
H	1.144829494077	2.329386361578	3.767140816970
C	-1.311363798016	-0.948396800807	3.375598253558
H	-0.679532670103	-0.891927954332	4.281746847440
H	-2.213482270047	-1.506159813293	3.681310519981
C	-1.737087045206	0.462258181011	2.924660865748
H	-1.884718585206	0.451393453349	1.832986528232
H	-2.728745747270	0.691548315510	3.351863103525
C	1.122207308680	5.254928920895	-0.531633183464
C	0.654870514837	4.025652600752	-1.351589860074
C	3.714365325117	4.208612510311	0.565290239318
C	0.918739613733	2.643165480593	-0.800065212154
C	3.465743775219	3.316981325037	-0.668418714465
C	2.357633096904	2.259872134816	-0.400728741667
H	0.378689019278	6.052655558854	-0.693489311634
H	1.118122853475	4.085920005945	-2.353805164649
H	4.545253566081	3.791150279169	1.156761918561
H	4.404100537579	2.790544740245	-0.898689745382
H	2.062759751230	5.657938223729	-0.939283742552
H	-0.421647567830	4.131558092552	-1.528071711580
H	4.020851069802	5.225189634378	0.267573765737
H	3.228682111238	3.905965270824	-1.566399696318
C	1.277806224418	5.096763938757	0.982579611436
H	0.367695505936	4.659274873597	1.428140185572
H	1.363689390965	6.111594659972	1.406783810120
C	2.511306350962	4.333270654065	1.482820019229
H	2.822083347948	4.717183164349	2.467409588400
H	2.161975992709	3.305595038027	1.921607171619
B	2.141706396946	2.111270964911	1.144865529402
C	3.089215760658	1.002641760311	2.005333020677
C	1.276754924046	1.197418840830	1.938997194263

Thermochemistry (use all positive eigenvalues) at 298.15 K, 1.00 Atm
E(el) = -1421.487170869285
ZPVE = 0.725855843505
Enthalpie(0K) = -1420.761315025780
E(tr) = 0.001416276854
E(rot) = 0.001416276854
E(vib) = 0.753089069779
H-E(el) = 0.756865808055
Enthalpie = -1420.730305061230
S(el) = 0.000000000000
S(tr) = 0.000070817727
S(rot) = 0.000058061498 (Symmetry number = 1)
S(vib) = 0.000165369034
G-E(el) = 0.669135689257
Free Energy = -1420.818035180028

Table S3. Cartesian coordinates and energies of Int_2.

C	2.438311555800	1.476730865137	-2.697570326656
C	2.872287077122	0.607058974939	-3.694509883825
C	2.939315116394	1.390673685085	-1.394581175233

C	3.820002150381	-0.368615558713	-3.392505590037
C	3.969103236919	0.469701604566	-1.111969698804
C	4.370054780164	-0.423069454998	-2.115838875252
B	2.474115103320	1.362319746150	1.170067070846
C	4.004631653616	1.048345483365	1.333256903235
C	4.662615361852	0.516085585306	0.199964815067
H	1.709831394366	2.246184545592	-2.947567285568
H	2.460726665768	0.690977768169	-4.703867841724
H	4.146927473199	-1.079528431348	-4.156185908965
H	5.124049582979	-1.181892323913	-1.894339756383
C	4.733814922083	1.201733733088	2.523364247579
C	6.000233836210	0.113023536744	0.305388595892
C	6.698776701094	0.252199201056	1.501377077773
C	6.068665693505	0.813356126791	2.609728506035
H	4.274250189078	1.650617693957	3.403443868613
H	6.522622204622	-0.281317100120	-0.569121728640
H	7.745716609772	-0.058541548955	1.557851977083
H	6.614133779461	0.952687609944	3.546993096269
C	-2.177983200288	-1.227817045688	-0.468195768982
C	-0.669537050992	-0.985171151469	-0.661538904919
C	-2.045236687294	2.116091533659	-1.556459285713
C	0.006486330332	0.139031815431	0.102113920334
C	-0.551914141290	1.793516163262	-1.752820545010
C	0.170864436032	1.340718265562	-0.496487590872
H	-2.352464260500	-1.864470703799	0.414123242717
H	-0.488703428550	-0.796794244889	-1.731133839383
H	-2.172678340294	2.691856195233	-0.621971942516
H	-0.073810724531	2.712402079013	-2.119151486732
H	-2.526495773403	-1.819616104105	-1.333933128341
H	-0.132373769996	-1.922690170698	-0.438157606566
H	-2.325303993233	2.799135519131	-2.377846635666
H	-0.432773324809	1.045486053407	-2.555231139276
C	-3.046568724807	0.022371379376	-0.345467584697
H	-2.757515312433	0.594058860041	0.557563442049
H	-4.080757146032	-0.320380840728	-0.166321454990
C	-3.044654681868	0.956161726846	-1.565130817933
H	-2.910682294044	0.361295179238	-2.488977162889
H	-4.045431441046	1.415361420563	-1.647322480156
C	-0.349660364081	-1.320739651933	3.746373381994
C	-0.421623301443	-1.075411628914	2.239470963048
C	0.479739890521	1.739058614186	4.284833349508
C	0.415473625373	-0.022490519966	1.529428559738
C	1.615215114892	0.973353242167	3.579214193734
C	1.392069806977	0.754961626358	2.089703942287
H	0.690351582997	-1.447409163806	4.076661350072
H	-1.477340588133	-0.875734681348	1.990409104657
H	0.745952625847	1.793650888620	5.356436248963
H	1.839398526701	0.036384981652	4.107473060258
H	-0.826208436739	-2.300302748320	3.923736089635
H	-0.185503959918	-2.026717653994	1.728729841033
H	0.476964510509	2.779822127413	3.914186861992
H	2.504842642195	1.599333460614	3.719459787040
C	-1.103257285462	-0.277680699155	4.587331080782
H	-0.811351879265	-0.383592619866	5.648463571940
H	-2.181926781959	-0.514745191841	4.539703565945
C	-0.930791450854	1.176529177654	4.149241952839
H	-1.278292042763	1.288709148916	3.105134973704
H	-1.607007144102	1.807443216078	4.753533214149
C	-0.016810635798	4.684089127849	0.192816281265
C	0.502877301410	3.442909303743	0.948615887677
C	3.224446049101	4.579465726933	-1.272302725662
C	1.094890675305	2.358202114639	0.071645827573
C	3.327309708173	3.577638522068	-0.117302543336
C	2.445557192888	2.342434716195	-0.323111946889
H	-0.615720385355	5.240827105497	0.933405444970
H	-0.339657169331	2.986625947800	1.490300622662
H	3.871829623785	5.432600610752	-1.001884785236
H	3.080156156250	4.074694493152	0.833106366596
H	-0.721164870630	4.376426669473	-0.597042619878
H	1.231086763160	3.775436908900	1.703623872502

H	3.664475408879	4.133968413842	-2.181890793043
H	4.373513698074	3.248504855352	-0.034437309693
C	1.020345584708	5.639694913678	-0.403200215733
H	1.707300663905	5.987444578569	0.391169256449
H	0.462348957004	6.534467141344	-0.727789200059
C	1.823121752830	5.097560791463	-1.598037631926
H	1.238285427672	4.306114690581	-2.100587450780
H	1.940863705316	5.894262754488	-2.352062732665

Thermochemistry (use all positive eigenvalues) at 298.15 K, 1.00 Atm
E(el) = -1421.515632316548
ZPVE = 0.727664756890
Enthalpie(0K) = -1420.787967559658
E(tr) = 0.001416276854
E(rot) = 0.001416276854
E(vib) = 0.755905425941
H-E(el) = 0.759682164217
Enthalpie = -1420.755950152331
S(el) = 0.000000000000
S(tr) = 0.000070817727
S(rot) = 0.000058603677 (Symmetry number = 1)
S(vib) = 0.000176610061
G-E(el) = 0.668438882726
Free Energy = -1420.847193433822

Table S4. Cartesian coordinates and energies of TS_2.

C	2.457737904924	1.554021858357	-2.704009345682
C	2.894763083532	0.717279487015	-3.727267067564
C	2.945842308197	1.421404577998	-1.400190688011
C	3.835445468540	-0.272594484783	-3.451504146443
C	3.972270910180	0.489704432310	-1.142799164427
C	4.376507302604	-0.370621181849	-2.173714633314
B	2.484942662845	1.345808960046	1.169687976848
C	4.009067197303	0.999450328333	1.319138072658
C	4.662312813156	0.492045801269	0.171584741664
H	1.736330405801	2.335757253885	-2.933554540163
H	2.490725236702	0.837729377879	-4.735954054157
H	4.164694541633	-0.959489339052	-4.235938049137
H	5.126753683568	-1.138923051113	-1.973761147348
C	4.737621201566	1.102122947654	2.515928607686
C	5.994136798405	0.067010647357	0.268065016743
C	6.691616716672	0.158898044898	1.468910420264
C	6.066217780548	0.692425040094	2.593533434583
H	4.281836738594	1.525876819329	3.410009372908
H	6.513881967962	-0.307515850488	-0.616520615647
H	7.733947606072	-0.168192016700	1.517458177771
H	6.610610597105	0.792931509729	3.536365856142
C	-2.144857178940	-1.280699761220	-0.447395207411
C	-0.638095820724	-1.021508335916	-0.629859549561
C	-2.036126011890	2.044960963663	-1.597969601910
C	0.016748860864	0.122936844106	0.121811815092
C	-0.534497489908	1.746397725709	-1.766358208664
C	0.176555505716	1.315849689192	-0.495357850933
H	-2.321377638354	-1.897069625690	0.448788773785
H	-0.449879610118	-0.847351809239	-1.700715024881
H	-2.188123734818	2.632607181629	-0.674443519832
H	-0.068444481994	2.672946378515	-2.128793748987
H	-2.474384048143	-1.898714219847	-1.302204534893
H	-0.090543650032	-1.948272561228	-0.385986582507
H	-2.313583282032	2.711171932221	-2.433922432816
H	-0.386926240791	0.996693189724	-2.562604072521
C	-3.031021447345	-0.039568410081	-0.367196548873
H	-2.765411075438	0.554173371694	0.528669153242
H	-4.064097957718	-0.391364503896	-0.199518750690
C	-3.016924126060	0.869213564023	-1.605536848084
H	-2.853275115464	0.258577275699	-2.514162405282
H	-4.022613636111	1.310691597654	-1.718451763863
C	-0.392088671907	-1.238755079530	3.797905690214

C	-0.452930926624	-1.026273472673	2.285536811506
C	0.494716008799	1.813141052725	4.280509585075
C	0.411748230430	-0.008331958245	1.557567836287
C	1.617966618981	1.016497721586	3.589588911164
C	1.394777303344	0.768789904916	2.104058052062
H	0.644330465489	-1.374913611378	4.135803688193
H	-1.502957579488	-0.806446824974	2.027459920690
H	0.757771305712	1.876118323001	5.352412702022
H	1.828202703945	0.086731536435	4.136041800537
H	-0.886022611340	-2.205683498473	3.995836011992
H	-0.237290401894	-1.994120662926	1.797704291767
H	0.513988000640	2.848745806932	3.896871318121
H	2.516464114205	1.631962820718	3.718912001258
C	-1.131407491599	-0.163959786360	4.610599484810
H	-0.850632899160	-0.253828267023	5.676160675632
H	-2.214121974319	-0.380600756195	4.558292951793
C	-0.925760871190	1.277323882940	4.145204652044
H	-1.261408658202	1.376961516192	3.095964041845
H	-1.593332785545	1.933667679115	4.731714863156
C	-0.053799723914	4.652738437260	0.185892967962
C	0.473921172832	3.419189243838	0.949032921908
C	3.219679049092	4.601675262234	-1.208010800026
C	1.084122996935	2.346351984544	0.073848368999
C	3.312268570723	3.580242383520	-0.068881342475
C	2.441933824220	2.340369655919	-0.303602851499
H	-0.679238800787	5.195319945228	0.914845505412
H	-0.366586474399	2.952310081311	1.485035927327
H	3.849146856101	5.458502645290	-0.908439246386
H	3.051176549776	4.059988329038	0.886987314883
H	-0.734125249794	4.336293835121	-0.621443118567
H	1.194023130392	3.763130925207	1.706101215717
H	3.686352063521	4.178382411044	-2.114907649864
H	4.359510557121	3.255998008861	0.021722355079
C	0.981964681704	5.628075472027	-0.379633077188
H	1.645455251397	5.978800352135	0.433209316467
H	0.418689578058	6.517307158327	-0.710263282403
C	1.820070213522	5.107818710816	-1.559606244747
H	1.256053756066	4.316834637671	-2.086457254384
H	1.947353815940	5.914777739380	-2.301118326132

Thermochemistry (use all positive eigenvalues) at 298.15 K, 1.00 Atm
E(el) = -1421.515605277817
ZPVE = 0.727350175864
Enthalpie(0K) = -1420.788255101953
E(tr) = 0.001416276854
E(rot) = 0.001416276854
E(vib) = 0.754880817308
H-E(el) = 0.758657555584
Enthalpie = -1420.756947722233
S(el) = 0.000000000000
S(tr) = 0.000070817727
S(rot) = 0.000058608690 (Symmetry number = 1)
S(vib) = 0.000169750659
G-E(el) = 0.669457910218
Free Energy = -1420.846147367599

Table S5. Cartesian coordinates and energies of Int_3.

C	2.512081783663	2.660057306817	-2.764115187001
C	3.123416746650	2.400429881448	-3.985674345727
C	2.922368535769	2.018490742231	-1.587782173187
C	4.163063562324	1.474846427163	-4.043549195108
C	3.967815977137	1.081305012773	-1.639877993590
C	4.567764768975	0.823359048106	-2.884251215084
B	2.036536538728	0.795782228685	0.775967450021
C	3.446214832855	0.092502396223	0.609718971190
C	4.359061986544	0.294203238772	-0.447162836737
H	1.678193222883	3.361761888908	-2.726371929850
H	2.776079634894	2.910351723899	-4.888198209434

H	4.648418007304	1.242007422347	-4.995359172319
H	5.348032760690	0.063357596766	-2.959782564531
C	3.834317972922	-0.754899828868	1.665446857368
C	5.630830177611	-0.298138585510	-0.381500342027
C	5.992972996481	-1.125413297656	0.676098783977
C	5.079568147724	-1.374976105354	1.698425539683
H	3.144805416715	-0.942326488708	2.492601691019
H	6.363462831149	-0.104899369824	-1.168250562232
H	6.991067825839	-1.571890223839	0.700420924257
H	5.341673080227	-2.032452311324	2.532070802183
C	-2.447094146900	-0.642848421276	0.134842745936
C	-1.070128412266	-1.293979530714	0.417902360471
C	-0.427830391040	0.472100789173	-2.572242036941
C	-0.074210360394	-0.252017168048	0.783252668308
C	0.671456821640	-0.078699379308	-1.656925259475
C	0.646492810640	0.459694090865	-0.230644512649
H	-2.838124226903	-0.202842262511	1.068409733523
H	-0.749880845427	-1.836760327360	-0.481845318659
H	-0.401200735835	1.578066615921	-2.530247544183
H	1.637659168800	0.159631678843	-2.113290869042
H	-3.124167781687	-1.474224503812	-0.127931039829
H	-1.189360107289	-2.033582101920	1.220657269045
H	-0.155948370073	0.200874001535	-3.607675841615
H	0.634729867809	-1.178468204240	-1.634728350638
C	-2.488942558730	0.410891604659	-0.976508956973
H	-2.020343504832	1.349603627811	-0.632103845980
H	-3.554029603539	0.654526488905	-1.131485054011
C	-1.864178544118	-0.003862886618	-2.320477337529
H	-1.914041679060	-1.103686556284	-2.434059513947
H	-2.482263318138	0.407288168900	-3.137079977756
C	-0.250066346181	-0.227366951354	4.723012224768
C	-0.690072139609	-0.433510906406	3.270449570934
C	1.314543865079	2.572128452156	4.117001417426
C	0.218970393135	0.066492175253	2.168512496430
C	2.061471177837	1.425031092251	3.405614509876
C	1.386841605571	0.783897589077	2.230947662106
H	0.808124290283	-0.511507351075	4.833033631527
H	-1.700259931258	-0.005473167110	3.125583500957
H	1.855760365449	2.773027497730	5.058345939562
H	2.286148648271	0.632011112840	4.138993573536
H	-0.807726203077	-0.955024974309	5.336889010173
H	-0.812571209425	-1.518604633025	3.115094167211
H	1.419455477081	3.487835960189	3.508396688535
H	3.043274093171	1.806755869711	3.081240279256
C	-0.521702395091	1.166969293545	5.304889173693
H	0.000567031127	1.257193090859	6.275268749689
H	-1.601843192796	1.235536193708	5.530004851927
C	-0.167220965994	2.361404095354	4.419243125958
H	-0.734805109884	2.290841787043	3.474435278405
H	-0.534750521540	3.276845857727	4.916212210619
C	-0.678870238142	3.912487344814	-0.046708365256
C	-0.065017457931	2.779503723375	0.792957077200
C	2.610102375931	5.011268704017	-0.481206686544
C	0.947140748465	1.928902853231	0.029487911477
C	2.714584612090	3.699716811005	0.309306867034
C	2.187764656647	2.438380967070	-0.343805840153
H	-1.689391808419	4.068793006799	0.367258038465
H	-0.873197942407	2.122339319933	1.135791431830
H	3.000153517330	5.794903929365	0.192129477904
H	2.235497139388	3.828479763444	1.291629947186
H	-0.829547094825	3.578690719004	-1.090148554413
H	0.376653289684	3.217479372399	1.696411351764
H	3.301668327127	4.980628786657	-1.341275876908
H	3.785371937842	3.514714845656	0.507755930846
C	0.035556596142	5.272895465300	-0.031983459154
H	0.328175413282	5.526447224106	1.004835335820
H	-0.720425231862	6.022921622710	-0.321960566374
C	1.225621714591	5.438651476643	-0.983792233818
H	0.978135453396	4.917140701814	-1.924134609748
H	1.309367779664	6.504096095708	-1.260207133560

Thermochemistry (use all positive eigenvalues) at 298.15 K, 1.00 Atm
E(el) = -1421.531163508221
ZPVE = 0.728918452631
Enthalpie(0K) = -1420.802245055590
E(tr) = 0.001416276854
E(rot) = 0.001416276854
E(vib) = 0.756719157071
H-E(el) = 0.760495895348
Enthalpie = -1420.770667612873
S(el) = 0.000000000000
S(tr) = 0.000070817727
S(rot) = 0.000058482730 (Symmetry number = 1)
S(vib) = 0.000170459587
G-E(el) = 0.671122438170
Free Energy = -1420.860041070051

Table S6. Cartesian coordinates and energies of TS_3.

C	2.671191327293	2.771675710382	-2.602388423441
C	3.247996849990	2.530596073602	-3.843141347144
C	3.023449246630	2.044550598384	-1.457459383237
C	4.210331849374	1.529565226250	-3.960517153064
C	3.991723629679	1.020522263284	-1.577083146867
C	4.564555934094	0.787726415817	-2.841071876166
B	2.463337752028	1.196814715956	0.890618986855
C	3.549426434078	0.117599449146	0.721698646049
C	4.362725750833	0.141629198497	-0.432443922666
H	1.887973163933	3.524234229000	-2.524102051339
H	2.935935461458	3.112655871835	-4.714608329530
H	4.674398211575	1.311790300094	-4.926489902111
H	5.291360322053	-0.016426094108	-2.967029867689
C	3.835101024176	-0.773378229053	1.768245926428
C	5.472251428151	-0.715916264812	-0.479322856896
C	5.748636824606	-1.589118288947	0.571258516746
C	4.925347958484	-1.633833420348	1.697715751370
H	3.197054591933	-0.780817083585	2.657885318135
H	6.148581061060	-0.711288262328	-1.336111862701
H	6.623102407163	-2.243247662767	0.506844875515
H	5.143474924707	-2.324261187546	2.516960728778
C	-2.270683057425	-1.176887454708	0.295525006738
C	-0.756901242577	-1.453553185628	0.360036705662
C	-0.976502725683	0.701270492734	-2.443363318280
C	0.051543631343	-0.228200281561	0.672819533939
C	0.368198541908	0.327895183386	-1.790760288177
C	0.461468913299	0.647403112826	-0.317588884900
H	-2.652574218455	-0.971782301466	1.311217685873
H	-0.429363313253	-1.858110043866	-0.610659568429
H	-1.195819263987	1.763664372210	-2.235767776410
H	1.149763442016	0.876949829574	-2.327050084264
H	-2.757965308720	-2.111897941637	-0.034337914804
H	-0.571786526723	-2.245663795132	1.100194322030
H	-0.820870291021	0.628354693452	-3.534086800662
H	0.571572179134	-0.742618475673	-1.955287835523
C	-2.699659878608	-0.035133516746	-0.629500882602
H	-2.382961823494	0.934817275804	-0.202449564718
H	-3.803132649050	-0.014847099359	-0.622129337099
C	-2.204494781833	-0.140978111090	-2.083186046937
H	-2.012438810520	-1.200628406887	-2.337923891512
H	-3.014929605122	0.184763871888	-2.758010003709
C	0.119577910581	-0.252610321664	4.615937303241
C	-0.181491957438	-0.632376883759	3.166778667269
C	0.835304044320	2.809067615525	4.043716088368
C	0.437339228729	0.131773080858	2.019566842803
C	1.848164502976	1.955662725819	3.257061256885
C	1.402077137043	1.125638025430	2.069279917731
H	1.204750527511	-0.153644982416	4.771597922256
H	-1.275880038685	-0.663757599612	3.021993244844
H	1.291136288455	3.024669173876	5.026400245985

H	2.337050434845	1.224750561304	3.923752681007
H	-0.182288070569	-1.113092767198	5.236987735693
H	0.157186442843	-1.674412187005	3.016226098101
H	0.734329450450	3.787783934082	3.544580111930
H	2.679775791056	2.610158767925	2.947603328781
C	-0.635306621736	0.978156745538	5.127783725895
H	-0.269797196289	1.221916711604	6.142143419180
H	-1.701298907846	0.707081204884	5.239543347630
C	-0.559301899755	2.225539847653	4.249149473134
H	-1.022811861645	2.017628219372	3.267244237578
H	-1.186327333422	3.009044054400	4.710136228572
C	-0.529041495846	3.978244142565	-0.319666288765
C	-0.096266101942	2.919879178220	0.712668211796
C	2.744555275430	5.056494675247	-0.441257827103
C	0.956694054936	1.954732920633	0.167794067113
C	2.781250507189	3.785620228631	0.420237631529
C	2.355601551705	2.411017535394	-0.142580706493
H	-1.614293798859	4.107083059506	-0.173849945729
H	-0.961618916620	2.311059787140	1.008690943916
H	3.152440354022	5.841409241336	0.220896218429
H	2.213834281011	3.991126801817	1.339523541455
H	-0.409379129385	3.597170308033	-1.349615223080
H	0.252193954776	3.440656633138	1.609871427779
H	3.471087591123	4.967455103777	-1.267482688484
H	3.830055108049	3.667154694447	0.745086310452
C	0.133022105165	5.361578199015	-0.202072868611
H	0.298576788750	5.609423242468	0.863595184495
H	-0.601193553577	6.098912948391	-0.569904157332
C	1.413468758649	5.571728418429	-1.014480851715
H	1.233541933077	5.156536219625	-2.020775443548
H	1.543229941743	6.655784153375	-1.178589786456

Thermochemistry (use all positive eigenvalues) at 298.15 K, 1.00 Atm
E(el) = -1421.520762682298
ZPVE = 0.726775698724
Enthalpie(0K) = -1420.793986983574
E(tr) = 0.001416276854
E(rot) = 0.001416276854
E(vib) = 0.754383467429
H-E(el) = 0.758160205705
Enthalpie = -1420.762602476593
S(el) = 0.000000000000
S(tr) = 0.000070817727
S(rot) = 0.000058516267 (Symmetry number = 1)
S(vib) = 0.000170580359
G-E(el) = 0.668740741263
Free Energy = -1420.852021941035

Table S7. Cartesian coordinates and energies of Int_4.

C	2.579316156344	2.449474314643	-2.524899110685
C	3.063279387845	1.978800539974	-3.742337577415
C	2.869432582148	1.821797732187	-1.306898761738
C	3.874847992779	0.848924605005	-3.759292977174
C	3.757489114651	0.706794060580	-1.316963277286
C	4.216883046552	0.235034718207	-2.559138727892
C	4.233275212565	0.021918837422	-0.065537714239
H	1.942976793664	3.334868039099	-2.529822191081
H	2.796089105493	2.491154241733	-4.670797015917
H	4.249539213266	0.443661024217	-4.703320855598
H	4.852430462147	-0.650708167600	-2.604670570922
C	3.977404685712	-0.476147592578	2.325487879321
C	5.326438508759	-0.860463733084	-0.081972357133
C	5.728424951709	-1.530792337531	1.072028691538
C	5.054013421293	-1.353579576977	2.282558032518
H	3.443803899119	-0.310814901556	3.266823872891
H	5.900792936645	-1.030427391451	-0.994029861063
H	6.588326272227	-2.205292942044	1.022001412600
H	5.374811156508	-1.889944980989	3.179605482061

C	-2.389436436557	-1.095285582681	0.067390628033
C	-0.898965263032	-1.071775816454	-0.306892387711
C	-2.038333494292	1.911025742811	-1.839693262507
C	-0.527662850629	1.573189699735	-1.797391115934
C	-0.008750584001	1.321337463814	-0.421559092309
H	-2.496608700218	-1.355584497896	1.136162195508
H	-0.797612501969	-1.071316449265	-1.403813586294
H	-2.247113596734	2.723586795981	-1.121445271613
H	0.007608978848	2.411509490968	-2.251781330982
H	-2.867478015733	-1.912660059503	-0.501506154048
H	-0.416905480001	-1.998672496377	0.043498570535
H	-2.218824851774	2.334199528293	-2.842577175927
H	-0.341652012584	0.688617651758	-2.430172560781
C	-3.144014766236	0.211971932525	-0.189332262256
H	-2.807606483820	0.982615379347	0.529963384273
H	-4.204631989966	0.026331376254	0.052192776290
C	-3.041485911143	0.773353389706	-1.619426622314
H	-2.835457371127	-0.045098641491	-2.334701442167
H	-4.027127304138	1.178067069102	-1.907066978393
C	0.410385180119	-0.695635466984	3.994213456796
C	0.369333844328	-0.935336707530	2.486216153053
C	-0.374547683972	2.444623310686	3.749846213133
C	1.006513493528	2.222243019833	3.112474619363
H	1.325585535932	-0.154454728013	4.272141279467
H	-0.484231926528	-1.587565954393	2.242303767180
H	-0.203212334910	2.798321799936	4.782820096583
H	1.655816106301	1.663352343524	3.799118173653
H	0.496157701321	-1.684806673353	4.474232603628
H	1.268807737559	-1.509243934769	2.178707800236
H	-0.886579536854	3.267261988149	3.222838016740
H	1.496535121790	3.199915750992	2.994164136546
C	-0.841780898516	0.004096529972	4.541879841456
H	-0.662217015576	0.270483563769	5.599205067023
H	-1.672264718893	-0.725150236042	4.543458485230
C	-1.318180386253	1.243451501834	3.779764469848
H	-1.589517852341	0.959689074796	2.742768875614
H	-2.269143565474	1.575625664518	4.232329921529
C	0.082287100027	4.592903581442	-0.653434921228
C	0.027379075903	3.666229730576	0.571206616059
C	3.056128577283	4.959579658101	-0.209652287327
C	0.743421933356	2.317295758296	0.410648182735
C	3.130001578812	3.590746201569	0.505204458036
H	-0.918823957843	4.693639339523	-1.104576413258
H	-1.017476736085	3.463131772738	0.862100413983
H	4.052491455167	5.410906050617	-0.066828641596
H	2.930630560575	3.769903332863	1.576958835483
H	0.712522717466	4.142470894845	-1.430336205229
H	0.481893438926	4.175199421444	1.432895564156
H	2.949792786945	4.834367636086	-1.300551630404
H	4.182567970830	3.260958585735	0.461897151533
C	0.650851944596	5.978425838869	-0.356507250421
H	-0.054791929006	6.552476219246	0.272227215593
H	0.726081544961	6.525011377578	-1.314209609542
C	2.024830819479	5.969524205780	0.327138104549
H	2.445447534479	6.985950701587	0.233946221360
H	1.906946571402	5.805195709638	1.414062006904
B	2.477732497545	1.268579290505	1.122252482352
C	3.576200304639	0.223770654241	1.176402983299
C	2.329257765699	2.343788299443	0.016143796426
C	0.990550621545	1.519402632101	1.744345270857
C	0.350161276021	0.230620191227	1.557771149861
C	-0.185562338706	0.125777646945	0.246426227293

Thermochemistry (use all positive eigenvalues) at 298.15 K, 1.00 Atm
E(el) = -1421.551425114370
ZPVE = 0.728294335077
Enthalpie(0K) = -1420.823130779293
E(tr) = 0.001416276854
E(rot) = 0.001416276854
E(vib) = 0.756047631279

H-E(el) = 0.759824369555
Enthalpie = -1420.791600744815
S(el) = 0.000000000000
S(tr) = 0.000070817727
S(rot) = 0.000058503640 (Symmetry number = 1)
S(vib) = 0.000172782602
G-E(el) = 0.669752070882
Free Energy = -1420.881673043488

Table S8. Cartesian coordinates and energies of TS_4.

C	2.360923906352	2.618382901399	-2.486954418416
C	2.792728107964	2.187971482735	-3.738629011333
C	2.646775123934	1.903517369357	-1.319328813409
C	3.537149239156	1.015506980017	-3.836813055785
C	3.457199568030	0.739748566874	-1.408398684012
C	3.865070981372	0.310393050593	-2.682938306439
C	3.902252771738	-0.030402368886	-0.199613412987
H	1.753321129953	3.522789662619	-2.421210054685
H	2.532650125883	2.760793893574	-4.633083922845
H	3.866560519415	0.644755652214	-4.811428895086
H	4.441137717221	-0.610841824417	-2.789790640607
C	3.653752662849	-0.661901191642	2.157534232745
C	5.011274175916	-0.888879383878	-0.263228768240
C	5.424438913422	-1.618132026064	0.849536190651
C	4.749276903087	-1.511884409368	2.066908033345
H	3.138272638426	-0.549949098726	3.114817980694
H	5.590569982211	-0.982971115120	-1.183431511969
H	6.297256477245	-2.272059553167	0.764851970525
H	5.085455350161	-2.078624782901	2.939186753555
C	-1.666754281956	-1.667867600318	-0.102130570061
C	-0.217023970424	-1.191967571849	-0.284572685142
C	-1.990774928864	1.309092616870	-2.070590966522
C	-0.463205373107	1.455686309561	-1.886367375256
C	0.008102949184	1.343790915927	-0.473396562225
H	-1.837154965702	-1.964359669456	0.947558846523
H	0.031858376043	-1.195350806347	-1.357957416518
H	-2.508623572771	2.008463457547	-1.389552301947
H	-0.182637358295	2.439869426233	-2.282221106999
H	-1.794378760309	-2.584588346878	-0.705003062997
H	0.467884237363	-1.913059967602	0.191863677141
H	-2.198965816148	1.667453732085	-3.093463796327
H	0.048896494001	0.700725560288	-2.508617342955
C	-2.734024009537	-0.646304151828	-0.498799120828
H	-2.734750835057	0.190481460099	0.225239565932
H	-3.714683615692	-1.139060689470	-0.382484751868
C	-2.617836379027	-0.082611857693	-1.927365438184
H	-2.079924297452	-0.799171477928	-2.576678871909
H	-3.633401269310	-0.002877895072	-2.351951089329
C	0.497475396766	-0.231560188077	4.150128656705
C	0.302597409044	-0.585320459268	2.678192456271
C	-0.488320587028	2.848107833462	3.788867688900
C	0.834953856718	2.653134867326	3.022896066693
H	1.417994787552	0.355006979316	4.285953070737
H	-0.690840249779	-1.051950574017	2.548122835441
H	-0.227499682658	3.290829485885	4.766729024154
H	1.586684832531	2.191762458297	3.676698054828
H	0.673949835621	-1.178449020245	4.687086597441
H	1.015790291469	-1.370046200502	2.372636929614
H	-1.098620970658	3.602252924168	3.263076367334
H	1.223915379917	3.648118355238	2.774991249391
C	-0.710232405460	0.462546341384	4.797192522168
H	-0.415220165574	0.827082607435	5.797906302627
H	-1.491138824558	-0.301363202428	4.964417198575
C	-1.350281515516	1.607296346249	4.008133690251
H	-1.716871177131	1.231003679311	3.034058481091
H	-2.257445227859	1.926451706835	4.550917758519
C	0.398642618707	5.100752921795	-0.240821993143
C	-0.278866109804	3.798427747403	0.192689176020

C	3.426159757493	4.699714626149	-0.098032633201
C	0.557815380120	2.505379236479	0.328764261023
C	3.158103392890	3.382909751445	0.654849404693
H	-0.411790008511	5.786553745722	-0.539764533816
H	-1.086469886603	3.595435063330	-0.527892817323
H	4.513927908489	4.883880689243	-0.092420858473
H	2.901645203048	3.605810408006	1.701625938922
H	0.982018537293	4.924111020984	-1.159595225008
H	-0.791787692711	3.977598751892	1.151812230103
H	3.165440643455	4.584697584519	-1.160500554020
H	4.111321153562	2.829462443770	0.706844182598
C	1.266389269098	5.778730850612	0.834953574925
H	1.191152842139	5.209097731083	1.775763165911
H	0.854982836091	6.774593539942	1.073660695523
C	2.742785322725	5.946163141894	0.473787981355
H	2.853555775365	6.763948296441	-0.262006063909
H	3.282990673078	6.275734787514	1.380345532077
B	2.134164210404	1.143986601847	1.030191922530
C	3.225441440441	0.081888743668	1.046259687383
C	2.147671758588	2.359745246874	0.042231339552
C	0.697264053797	1.856985919777	1.741162171969
C	0.357840226397	0.494109545273	1.637393493629
C	0.050489879784	0.182417100238	0.249787897267

Thermochemistry (use all positive eigenvalues) at 298.15 K, 1.00 Atm
E(el) = -1421.535501643635
ZPVE = 0.728224133008
Enthalpie(0K) = -1420.807277510628
E(tr) = 0.001416276854
E(rot) = 0.001416276854
E(vib) = 0.755333196141
H-E(el) = 0.759109934417
Enthalpie = -1420.776391709218
S(el) = 0.000000000000
S(tr) = 0.000070817727
S(rot) = 0.000058386773 (Symmetry number = 1)
S(vib) = 0.000164043998
G-E(el) = 0.671677894502
Free Energy = -1420.863823749133

Table S9. Cartesian coordinates and energies of Int_5.

C	2.467425314619	2.737062982030	-2.427526293181
C	3.063498625345	2.520929949844	-3.666631573114
C	2.647607409603	1.865281329750	-1.347958297357
C	3.875375084768	1.405142426047	-3.848086624216
C	3.513731735429	0.753390936071	-1.518389566992
C	4.093600277753	0.540639039209	-2.781054989029
C	2.925028950008	-0.379386159906	0.672534530353
C	3.821147046229	-0.208125388382	-0.412570647100
H	1.825928205357	3.609198468963	-2.310538936393
H	2.882414995560	3.220831053900	-4.487114896211
H	4.338933519644	1.202491775974	-4.817649899988
H	4.718368844044	-0.339387954549	-2.947260165776
C	3.191107080639	-1.358009418503	1.639706190405
C	4.989182327253	-0.986215161957	-0.445387287021
C	5.248989077275	-1.937762819387	0.537957425108
C	4.342291986019	-2.139062893882	1.578042012361
H	2.497363565677	-1.509887634491	2.468239302509
H	5.726220720352	-0.844452582285	-1.238662907952
H	6.170410959083	-2.525245258693	0.489175590098
H	4.537770013349	-2.892277856929	2.346307940103
C	-1.598819240762	-1.801484059817	-0.000110536573
C	-0.132325912244	-1.387898076847	-0.180548835927
C	-1.800124453925	0.908218519324	-2.354414362236
C	0.104714688680	0.039740909753	0.210234197587
C	-0.285122773339	1.061841965266	-2.087568065404
C	0.032104213988	1.129220164940	-0.633722842969
H	-1.809667999969	-1.938528821665	1.075534302060

H	0.169012571933	-1.513823338921	-1.232830963169
H	-2.346789143398	1.699472733189	-1.809793370666
H	0.053962040075	1.978954494123	-2.583832894313
H	-1.727348011619	-2.791436299208	-0.472481821654
H	0.517768062280	-2.054351631041	0.408395471744
H	-1.934634397526	1.125581123044	-3.427685007803
H	0.254469802030	0.218751402455	-2.550865513839
C	-2.626008476372	-0.823438774450	-0.576127637632
H	-2.636874242921	0.101194024627	0.030254842224
H	-3.621034093406	-1.278738681934	-0.434337076451
C	-2.444632405860	-0.451837685528	-2.060653616819
H	-1.882136608014	-1.246152639161	-2.586427400662
H	-3.439459380589	-0.427231397227	-2.537375572932
C	-0.994606467757	-0.015926621824	3.807472395217
C	0.156697148667	-0.343414587111	2.836194347321
C	-1.408249127495	2.897860824538	3.097849901567
C	0.273376303758	0.529127377348	1.606050085192
C	0.119871168547	2.731489054283	2.801330655423
C	0.289928840533	1.918447697413	1.569587696512
H	-0.655303811815	0.733056042860	4.541779409205
H	0.062130779918	-1.384539790813	2.494783830561
H	-1.529639845225	2.969289488834	4.191958090464
H	0.619951387152	2.216051868058	3.634056790988
H	-1.177694403465	-0.930990680435	4.395616985369
H	1.097225933698	-0.292074811748	3.407242055577
H	-1.727790183103	3.867719834087	2.687564661288
H	0.572889117947	3.723757563437	2.708245560331
C	-2.327828362832	0.448028563789	3.216832134505
H	-3.044672521836	0.475901423815	4.056266469346
H	-2.714864784757	-0.310216321542	2.512119755805
C	-2.346828268298	1.826256913095	2.527551344524
H	-2.155396990514	1.720485933435	1.444711004061
H	-3.374770597681	2.221246510291	2.594391177259
C	-0.131942847284	5.010859610884	0.436309343847
C	-0.256925942629	3.682085831868	-0.334907954392
C	3.431468007459	4.314309430326	0.287197462766
C	2.941607365261	2.984365227441	0.874829608122
H	-0.787092749802	4.987716306162	1.320945564133
H	0.057234440480	3.851833978894	-1.374735838962
H	4.078729386854	4.765730498094	1.061676338698
H	2.485706264160	3.159769106644	1.861571221477
H	-0.593269641064	5.754751416611	-0.237428248495
H	-1.338761478069	3.464957318040	-0.396337079381
H	4.092697421066	4.111598321671	-0.573644326326
H	3.844353226804	2.380942857655	1.080880633930
C	1.238637600694	5.558297358732	0.868758194457
H	1.531133509075	5.137073009976	1.845279276989
H	1.094332346273	6.634634521876	1.062974840846
C	2.386981958971	5.359796763358	-0.129810344380
H	1.970036689921	5.113645784155	-1.118901249336
H	2.923970524425	6.312390943552	-0.276960728696
B	1.759554106472	0.642204839490	0.655139377485
C	2.007894069010	2.098930526665	0.021712243486
C	0.423538875412	2.392728159211	0.127465404188

Thermochemistry (use all positive eigenvalues) at 298.15 K, 1.00 Atm

E(el) = -1421.542682475513
ZPVE = 0.730158301743
Enthalpie(0K) = -1420.812524173770
E(tr) = 0.001416276854
E(rot) = 0.001416276854
E(vib) = 0.757542151046
H-E(el) = 0.761318889323
Enthalpie = -1420.781363586190
S(el) = 0.000000000000
S(tr) = 0.000070817727
S(rot) = 0.000058241850 (Symmetry number = 1)
S(vib) = 0.000165769975
G-E(el) = 0.673415458263
Free Energy = -1420.869267017250

Table S10. Cartesian coordinates and energies of TS_5.

C	2.638977842081	2.746654104550	-2.415234000820
C	3.365844725836	2.689288272366	-3.600090698898
C	2.789223599188	1.792446897013	-1.403296577622
C	4.286857487399	1.663068038703	-3.787055685806
C	3.743779923981	0.754346856329	-1.583250197516
C	4.468404482234	0.716121194288	-2.784940413588
C	2.973689856418	-0.589187505740	0.393393292756
C	3.984760331613	-0.299838178780	-0.551752094507
H	1.923920862820	3.556680661680	-2.285783788925
H	3.205967571451	3.446518059051	-4.372190146402
H	4.863221372069	1.592855284732	-4.713504844306
H	5.181477451634	-0.092626744977	-2.957087258471
C	3.130188642566	-1.663375743242	1.278810494824
C	5.160951128323	-1.061514073082	-0.531693438805
C	5.319614192829	-2.103528511816	0.381290699420
C	4.300961289833	-2.418707858120	1.280930500054
H	2.333465313265	-1.902443790412	1.987941309484
H	5.977952513258	-0.841983615665	-1.222603344302
H	6.249954127008	-2.678702623738	0.383084098384
H	4.421977716138	-3.246363376935	1.985236325601
C	-1.753358229199	-1.560353986310	0.121125968484
C	-0.237271414826	-1.377625338639	-0.011117571404
C	-1.571900248095	0.886647765919	-2.524069906437
C	0.211995821615	0.030214560864	0.322532862808
C	-0.090876478449	0.971973799522	-2.094046650788
C	0.081058886588	1.138142525895	-0.623557066421
H	-2.029473222930	-1.563830230667	1.190698570815
H	0.089296643056	-1.618251774601	-1.036015815320
H	-2.104247755587	1.786468476096	-2.167997554086
H	0.348585755417	1.832149778972	-2.614523853648
H	-2.015121175597	-2.560068585156	-0.270132329651
H	0.280481699645	-2.097738962863	0.642239880750
H	-1.565641573486	0.946085484438	-3.625538244038
H	0.445360495946	0.070802486452	-2.432598607695
C	-2.597430920175	-0.500415163534	-0.588780975460
H	-2.443017806417	0.480981303249	-0.098146480619
H	-3.657947865169	-0.746425834309	-0.409587551343
C	-2.346706466235	-0.362058483879	-2.102335038418
H	-1.830305237531	-1.261034170113	-2.487240523800
H	-3.315770140874	-0.325558039523	-2.628396728057
C	-0.584155067023	0.273581773501	4.206947036877
C	0.066243797567	-0.219902564095	2.907486908313
C	-1.878037770839	2.934507168370	3.032079730389
C	0.044430610323	0.644490233417	1.665654000068
C	-0.374680821529	2.936183649867	2.670277226749
C	-0.063900418144	2.011377507044	1.529899257243
H	-0.027883310686	1.129973914820	4.614542073999
H	-0.385062939861	-1.191729184680	2.647333269341
H	-1.992779323705	3.451672168675	4.001848949145
H	0.230242731961	2.654991344495	3.541215186036
H	-0.437980754918	-0.535683487748	4.943612954796
H	1.123934596587	-0.442890992819	3.137537409160
H	-2.410289589848	3.551498765051	2.285296183170
H	-0.084686695781	3.962835459879	2.434411078210
C	-2.084070166115	0.587261134030	4.158403512793
H	-2.375136910958	0.969649968302	5.154164527580
H	-2.638929750463	-0.359484854717	4.021115476681
C	-2.568887140163	1.569736286458	3.086915474535
H	-2.504819164207	1.090551700179	2.094056876451
H	-3.645907855677	1.746059221748	3.258223922511
C	-0.266424784601	5.028062146931	0.186324199138
C	-0.347318446354	3.670686003160	-0.533341161955
C	3.262357663774	4.200318799336	0.371524395173
C	2.714240450836	2.859802100782	0.873650541818
H	-1.036596200927	5.075394103922	0.974509467771
H	0.144233052061	3.753240699932	-1.512441892095
H	3.814898656075	4.610944514046	1.236654033460
H	2.096905543877	3.001905703864	1.771388481186

H	-0.592749784163	5.758853214600	-0.575096250580
H	-1.416174034988	3.519615429005	-0.771177212431
H	4.023779635431	4.018280857164	-0.406046557950
H	3.594968868546	2.279891197827	1.214633781340
C	1.068172544949	5.521450338162	0.764776718680
H	1.251528979932	5.075938707123	1.756864127330
H	0.944720270249	6.600711651822	0.957587779800
C	2.299752680872	5.290666761684	-0.120807546843
H	1.976405129145	5.092133006540	-1.154142182603
H	2.889926742440	6.220665277603	-0.184498532019
B	1.778978934438	0.382780112978	0.370767794022
C	2.028674709259	1.873738985332	-0.090341695923
C	0.098851933374	2.374514304673	0.115868050453

Thermochemistry (use all positive eigenvalues) at 298.15 K, 1.00 Atm
E(el) = -1421.522835675099
ZPVE = 0.727533419844
Enthalpie(0K) = -1420.795302255256
E(tr) = 0.001416276854
E(rot) = 0.001416276854
E(vib) = 0.754911674886
H-E(el) = 0.758688413163
Enthalpie = -1420.764147261936
S(el) = 0.000000000000
S(tr) = 0.000070817727
S(rot) = 0.000058429574 (Symmetry number = 1)
S(vib) = 0.000167725008
G-E(el) = 0.670146119261
Free Energy = -1420.852689555838

Table S11. Cartesian coordinates and energies of Int_6.

C	2.850085412874	2.543424427470	-2.539127199936
C	3.607329460028	2.496273537248	-3.705105063468
C	2.962263196710	1.570357733625	-1.537530847904
C	4.517786625389	1.457005038818	-3.882020465972
C	3.916398325809	0.529147973546	-1.699335261031
C	4.667472909480	0.496702375895	-2.887263031145
B	2.058398151951	0.285112526022	0.410898217401
C	3.189355895199	-0.736623461820	0.368616130614
C	4.143424692276	-0.526321992317	-0.658332650043
H	2.138238951470	3.359859599861	-2.403263532266
H	3.480565909751	3.265339744280	-4.472120459666
H	5.114939066108	1.389857247261	-4.795743657744
H	5.380699524196	-0.311784026733	-3.058297828153
C	3.360108900123	-1.769987568067	1.301692909726
C	5.276113627392	-1.354741435183	-0.678827372528
C	5.445365966882	-2.361739386757	0.270789527928
C	4.488200092062	-2.582797377327	1.263454727483
H	2.605000216923	-1.919217148047	2.080469024831
H	6.058227584811	-1.218420589878	-1.428176327866
H	6.343680582954	-2.984945245007	0.231830474701
H	4.627768776527	-3.378868605627	1.999865805598
C	-1.563877884846	-1.404311036176	0.383033363501
C	-0.061593996511	-1.187122091861	0.197616233547
C	-1.469820705290	1.069363329117	-2.199633788965
C	0.467230053213	0.209919381685	0.577929940782
C	0.019604736840	1.206640323544	-1.853764131588
C	0.445321462111	1.434609202077	-0.398820599936
H	-1.797806937730	-1.418644273505	1.463195465798
H	0.230830052487	-1.387544339541	-0.845846815595
H	-2.024606230150	1.939061557458	-1.804801463336
H	0.395919402102	2.056516482004	-2.440043606921
H	-1.796550081871	-2.417648346086	0.007229209053
H	0.476505710511	-1.935706006003	0.802123699433
H	-1.523401445965	1.160942553471	-3.298966967969
H	0.570172573501	0.328958195832	-2.234485643898
C	-2.482172912035	-0.396324009499	-0.307753747300
H	-2.418088581270	0.582347417713	0.202481988992

H	-3.519609665905	-0.739853368741	-0.153128990688
C	-2.220958652083	-0.206195255566	-1.810803901676
H	-1.693145062694	-1.087885276387	-2.220863013206
H	-3.189987596369	-0.170584913832	-2.337920639205
C	1.309096141977	0.603400823085	3.887259470116
C	0.073468363735	0.038681745969	3.120890281753
C	-0.218457372775	3.307683273611	3.977416488440
C	-0.014637509714	0.764372983705	1.831766095603
C	-1.122900988540	2.871838072192	2.798043333637
C	-0.473841070635	2.088243008979	1.691138817240
H	1.862882750597	1.294952522202	3.227966949391
H	-0.849220116687	0.192344974436	3.703656804586
H	0.801143092327	3.529950483203	3.614595062839
H	-1.588787351324	3.762586390541	2.359135854532
H	2.005560108614	-0.226153828617	4.089343707831
H	0.186487145486	-1.040327126858	2.946386700564
H	-0.621287432098	4.266994328139	4.341572720790
H	-1.958594962686	2.270487968474	3.198603976520
C	0.986621431334	1.320234473202	5.199812744402
H	1.911761796689	1.827030792781	5.528245868707
H	0.755687473390	0.568503171634	5.975946257154
C	-0.163270584792	2.336275484279	5.170813075728
H	-1.130707757876	1.806185975484	5.237893200353
H	-0.092480393496	2.924500954023	6.101902245310
C	-0.422465859619	5.135206234050	0.414087437837
C	-0.678817471552	3.776613951301	-0.263954281906
C	3.164552034284	4.092543903098	0.270130897550
C	-0.251763797263	2.495848623822	0.376881829643
C	2.722908965293	2.698601234119	0.730961684876
C	2.132756562628	1.664355344142	-0.273797304512
H	-1.134022253698	5.302963746469	1.237295787979
H	-0.283307701466	3.797577662606	-1.289594733385
H	3.717202529444	4.527355333115	1.123829229430
H	2.053736558028	2.790712624613	1.600356748448
H	-0.656322506551	5.901457362658	-0.346089471878
H	-1.775377954316	3.660708486026	-0.381415397660
H	3.901853963300	3.994406491182	-0.545149528130
H	3.633333993252	2.213912330126	1.129047214676
C	1.002083250388	5.338463053162	0.922492191808
H	1.161158996528	4.679129811780	1.793296087185
H	1.087648999751	6.366074620972	1.314652891970
C	2.078736211013	5.082405669891	-0.147546087645
H	1.601663840288	4.733433835605	-1.077997297499
H	2.572023162176	6.031651743312	-0.418438881619

Thermochemistry (use all positive eigenvalues) at 298.15 K, 1.00 Atm
E(el) = -1421.544057644483
ZPVE = 0.728729832397
Enthalpie(0K) = -1420.815327812086
E(tr) = 0.001416276854
E(rot) = 0.001416276854
E(vib) = 0.756395856206
H-E(el) = 0.760172594482
Enthalpie = -1420.783885050001
S(el) = 0.000000000000
S(tr) = 0.000070817727
S(rot) = 0.000058519035 (Symmetry number = 1)
S(vib) = 0.000169150374
G-E(el) = 0.671178654651
Free Energy = -1420.872878989832

Table S12. Cartesian coordinates and energies of TS_6.

C	3.194897971603	2.716241979548	-2.311441151023
C	3.804425699940	2.586276183107	-3.552363917252
C	3.227928347147	1.679026843978	-1.359299003954
C	4.489594663570	1.412600042156	-3.856807791483
C	3.930463051208	0.474288019440	-1.675489410668
C	4.553582485072	0.379735628903	-2.924566541039

C	3.076279476230	-0.746801950269	0.336500779273
C	4.034463665419	-0.644920057225	-0.697452845383
H	2.632745839035	3.622578341235	-2.101359662205
H	3.735751091448	3.398414890186	-4.280327901100
H	4.973852656041	1.291409034677	-4.829632189809
H	5.087922562194	-0.532360321258	-3.196764695019
C	3.129964063791	-1.831489472880	1.222899642175
C	5.036202004828	-1.619687213749	-0.795955931243
C	5.090703036931	-2.677306161081	0.110546600386
C	4.137152284878	-2.788979830480	1.122143353551
H	2.387425222462	-1.922668788744	2.020186186546
H	5.802032379314	-1.557021976128	-1.571994842671
H	5.888687265202	-3.420160018466	0.023026546207
H	4.179774670065	-3.619170544542	1.832519012623
C	-1.562459180626	-1.353213287305	0.190823672980
C	-0.043778310079	-1.157415102089	0.202150189161
C	-1.242295089670	0.937369724146	-2.578583770302
C	0.452173968847	0.257950642365	0.523764706880
C	0.146117723442	1.161425693564	-1.958687042632
H	-1.944495939565	-1.287203962478	1.222615528982
H	0.379836539844	-1.455237481478	-0.772480921586
H	-1.882925422290	1.808951765248	-2.352347724834
H	0.586870437641	2.050692041764	-2.440908171809
H	-1.749554247946	-2.392369781202	-0.137925129928
H	0.386447842932	-1.855949244150	0.938097909566
H	-1.106664206598	0.929254790723	-3.674544960857
H	0.803422106715	0.315300858149	-2.222334675277
C	-2.389480465916	-0.406580567805	-0.682191991433
H	-2.376815771367	0.608618270515	-0.245113855199
H	-3.439175823986	-0.740360860734	-0.609522360434
C	-1.976195475664	-0.339639246783	-2.165232243033
H	-1.357765910605	-1.219239849366	-2.426169911167
H	-2.878704288884	-0.412687035411	-2.796225427321
C	-0.904713694486	-0.462470125463	3.810093786859
C	0.323616408250	0.193633846885	3.151732851210
C	-2.474175206862	2.648914362687	2.938669964486
C	0.113520005329	0.863406589133	1.822829525501
C	-0.978604288839	2.949068352478	2.747530928936
C	-0.386373410672	2.144719313416	1.627374947191
H	-0.529925265550	-0.996983648330	4.700814369513
H	1.087389431359	-0.589913053261	3.023705244778
H	-2.820417932472	3.223094755719	3.817358964052
H	-0.440509378058	2.715736895163	3.681296480348
H	-1.303804621346	-1.239327039098	3.135952679121
H	0.748475859264	0.927954767625	3.859299578700
H	-3.034860846765	3.037819239420	2.068739847225
H	-0.859303379439	4.027607490756	2.588241612861
C	-2.051784085056	0.452016080726	4.255406146407
H	-1.670570029001	1.192121646907	4.984468543846
H	-2.754815392230	-0.183461362969	4.821336984259
C	-2.825099711655	1.170689775493	3.132046783766
H	-2.679374623437	0.628364045612	2.180202271668
H	-3.907591058623	1.117062789480	3.340513496638
C	-0.678438964069	5.076257415843	0.219973834020
C	-0.870969348391	3.701322164927	-0.446000480704
C	3.052408455573	4.353989678884	0.390445468697
C	-0.349384014443	2.462142894835	0.232610834376
C	2.756611728347	2.929884193133	0.864224542026
H	-1.432298172066	5.223048554974	1.011519031495
H	-0.451893322907	3.728888952012	-1.464601253363
H	3.419373411065	4.903127327570	1.275689537307
H	1.986750833531	2.909178118425	1.653320324101
H	-0.907829462684	5.835047905516	-0.549581960328
H	-1.957275718586	3.546956832080	-0.594013105679
H	3.890675959982	4.344826128557	-0.326580148159
H	3.662385389871	2.554745472860	1.394842686028
C	0.712691123764	5.344312721921	0.797817896503
H	0.861238357113	4.705204281898	1.684154793181
H	0.741844532157	6.379314979184	1.179979400648
C	1.862084312035	5.117566877971	-0.196443017750

H	1.475893937249	4.577327786380	-1.075620026172
H	2.226789224999	6.084593570867	-0.583135782450
B	2.038970770074	0.403733050143	0.423332496411
C	0.161319697614	1.358996490941	-0.468798357768
C	2.539208287502	1.789716305282	-0.070713402118

Thermochemistry (use all positive eigenvalues) at 298.15 K, 1.00 Atm
E(el) = -1421.542006570940
ZPVE = 0.726899434636
Enthalpie(0K) = -1420.815107136304
E(tr) = 0.001416276854
E(rot) = 0.001416276854
E(vib) = 0.754167934066
H-E(el) = 0.757944672342
Enthalpie = -1420.784061898598
S(el) = 0.000000000000
S(tr) = 0.000070817727
S(rot) = 0.000058556611 (Symmetry number = 1)
S(vib) = 0.000164355732
G-E(el) = 0.670369051629
Free Energy = -1420.871637519311

Table S13. Cartesian coordinates and energies of Int_7.

C	3.254662188134	2.712095914969	-2.311782096265
C	3.848946380046	2.561142343237	-3.557012001098
C	3.269041412091	1.674975436464	-1.356181802675
C	4.501310787033	1.368849090250	-3.862409041287
C	3.940536872208	0.450975699458	-1.673900045584
C	4.549671790445	0.337231292716	-2.927261917127
C	3.082471186509	-0.740348443871	0.355182110511
C	4.033315971136	-0.662205083415	-0.687936472607
H	2.715836781013	3.632491036305	-2.102399214024
H	3.794194436982	3.371275492312	-4.288255986646
H	4.973340003606	1.232356394211	-4.839223374334
H	5.060695930889	-0.587628920956	-3.200912751856
C	3.129397268207	-1.818712359926	1.249086299004
C	5.019804646042	-1.651921687476	-0.788001408291
C	5.068522641984	-2.702325393742	0.127203023108
C	4.122708406537	-2.790936101392	1.147813247331
H	2.392281685134	-1.895904030789	2.052479524780
H	5.778384276359	-1.606785786431	-1.572284713012
H	5.855162712798	-3.457060094734	0.039091476177
H	4.159654873983	-3.615091384029	1.865481855014
C	-1.544870298196	-1.329406391593	0.165369905027
C	-0.027849849381	-1.121471649646	0.177298862645
C	-1.249449368985	0.979922669982	-2.593030419081
C	0.465053723358	0.294380975718	0.509507117021
C	0.129397675240	1.223569663413	-1.958985353947
H	-1.927950622082	-1.266275769948	1.197016489358
H	0.395881928717	-1.409670837392	-0.800360246047
H	-1.908127520305	1.837623681711	-2.365262193361
H	0.559413263434	2.128892093686	-2.423104569951
H	-1.720464246369	-2.371178101157	-0.161668586671
H	0.406958755569	-1.824079046427	0.906769584882
H	-1.106723310198	0.980793593266	-3.688227097486
H	0.803828603686	0.393724355551	-2.230689580014
C	-2.383494133898	-0.394729668497	-0.710354494099
H	-2.393113931675	0.618700482462	-0.269888305082
H	-3.426953722812	-0.749403060076	-0.646160115766
C	-1.962493299172	-0.312914985318	-2.190849640731
H	-1.326694832366	-1.179834785436	-2.452618783829
H	-2.859835024108	-0.399240243263	-2.827554415646
C	-0.870122123684	-0.478982258726	3.795452652224
C	0.350887852267	0.198762602850	3.145836624149
C	-2.479646626849	2.625587377988	2.970853397605
C	0.131248296875	0.880228054005	1.823637289869
C	-0.988203424845	2.941577245551	2.772309370648
C	-0.394354283185	2.150872118067	1.643746330972

H	-0.489963394591	-1.024670574449	4.677257164332
H	1.123089766388	-0.574713769383	3.011697615817
H	-2.824996139050	3.186817865747	3.858252865491
H	-0.442515625126	2.709262458291	3.701897506235
H	-1.263589375208	-1.248348218575	3.109284706980
H	0.767536833987	0.929248346970	3.862290257011
H	-3.050748764275	3.018421715650	2.109553358634
H	-0.880968894970	4.022502876945	2.616370830676
C	-2.025132260534	0.417142503990	4.258334700758
H	-1.648025498825	1.152024776724	4.994874192282
H	-2.717788079391	-0.233311031428	4.820117358064
C	-2.814489900669	1.141906989484	3.149986214934
H	-2.671389568657	0.612773050026	2.190453299339
H	-3.894636558319	1.075300005970	3.367023847720
C	-0.723562912596	5.091322019473	0.237581027159
C	-0.967125440241	3.711292595815	-0.404816559182
C	3.033028466627	4.370075587668	0.363950403728
C	-0.393186711750	2.478780944131	0.246450662460
C	2.777995074251	2.945672438363	0.856349315986
H	-1.448689133157	5.264950892574	1.050394174062
H	-0.619978015728	3.732371170945	-1.449858751239
H	3.369040400062	4.952479251630	1.239866813256
H	1.999985925247	2.911243039773	1.637721198443
H	-0.956336455848	5.848834042832	-0.532192393068
H	-2.061059150928	3.557242602907	-0.474576750873
H	3.876490211228	4.380186789841	-0.346353463627
H	3.687139043379	2.593239082987	1.398841510326
C	0.689074519237	5.324541113808	0.774726975064
H	0.840052992979	4.686085216585	1.661228598730
H	0.764177984694	6.360942077226	1.147391811126
C	1.804803724631	5.052485820133	-0.243832055822
H	1.405628814763	4.419981182320	-1.053824996501
H	2.118966817453	5.993920018168	-0.726466334147
B	2.055113807424	0.423465695529	0.422470305376
C	0.126009588761	1.396703442795	-0.466214141648
C	2.594278109422	1.797585992743	-0.068253342262

Thermochemistry (use all positive eigenvalues) at 298.15 K, 1.00 Atm
E(el) = -1421.542025065766
ZPVE = 0.727400107059
Enthalpie(0K) = -1420.814624958707
E(tr) = 0.001416276854
E(rot) = 0.001416276854
E(vib) = 0.755344674285
H-E(el) = 0.759121412561
Enthalpie = -1420.782903653205
S(el) = 0.000000000000
S(tr) = 0.000070817727
S(rot) = 0.000058562832 (Symmetry number = 1)
S(vib) = 0.000170467115
G-E(el) = 0.669721828385
Free Energy = -1420.872303237380

Table S14. Cartesian coordinates and energies of TS_7.

C	3.406778569099	2.614596057716	-2.089742364310
C	3.830569336682	2.414231240865	-3.393980130949
C	3.307992147459	1.544376719597	-1.167218544317
C	4.196593731791	1.134584795344	-3.807450042567
C	3.753053754257	0.242840052702	-1.587260531208
C	4.172160711012	0.071364778473	-2.906747735252
B	2.036593108017	0.336604391842	0.575610349654
C	3.077859551881	-0.846768474135	0.560054579834
C	3.880583323652	-0.861519431777	-0.603334721601
H	3.085348674183	3.612094380781	-1.811918567281
H	3.859219447165	3.255249717031	-4.090609478813
H	4.514379954969	0.959276595717	-4.838887711378
H	4.484128276942	-0.915515192713	-3.253082701924
C	3.292064067857	-1.838764097639	1.525284255945

C	4.828680602868	-1.877571669781	-0.789373620140
C	5.009759635651	-2.865344845203	0.174638304244
C	4.250252948964	-2.835547446406	1.341804429825
H	2.732694748629	-1.831189147411	2.460007708359
H	5.463351546059	-1.886710471421	-1.678402384578
H	5.762183127586	-3.643876972852	0.021626671261
H	4.407126912455	-3.585436900675	2.122250506408
C	-1.389827047177	-1.544225753489	-0.337764070415
C	0.095881026917	-1.171173345529	-0.332188762858
C	-1.504502315891	1.417931018563	-2.397828763318
C	0.445158689529	0.154485723322	0.345546989465
C	-0.118680288119	1.633951398873	-1.765652674719
C	-0.060805890629	1.418932575791	-0.280830955144
H	-1.699911201641	-1.797753711310	0.689787405854
H	0.475147987510	-1.132173307326	-1.368567525869
H	-2.226323476113	2.115601285592	-1.936119393395
H	0.199136927033	2.666907710109	-1.991360097629
H	-1.482942126497	-2.476994118386	-0.924661443953
H	0.653349347170	-1.986093414364	0.156906956742
H	-1.427970786745	1.710765831550	-3.460025405270
H	0.607260863024	0.967015358588	-2.262420629406
C	-2.373576189697	-0.512436760050	-0.896690166329
H	-2.446616016194	0.345397237994	-0.203647349980
H	-3.371960189058	-0.983438858787	-0.884689387060
C	-2.066859726058	-0.003634525419	-2.319493506656
H	-1.373792341147	-0.700284252132	-2.828240749405
H	-2.994775760956	-0.018163194788	-2.917030464942
C	-0.907702907238	-1.217086841122	3.483682752514
C	0.403473754750	-0.676452458881	2.880917587059
C	-1.896095132065	2.199840624030	3.815927654253
C	0.290304822547	0.374932188540	1.802457250940
C	-0.440707737803	2.290905588133	3.325506244523
C	-0.199025781415	1.669468213696	1.981463051042
H	-0.619173482434	-2.107898813717	4.070150616558
H	0.900337121588	-1.552383265181	2.448411412840
H	-1.911513654836	2.527201745050	4.871279986288
H	0.215449804888	1.796813252209	4.060922475985
H	-1.552025484222	-1.588602561467	2.667926674232
H	1.052980870154	-0.319123923204	3.700914342510
H	-2.525713034436	2.916719877883	3.261093849400
H	-0.143261047240	3.353447961941	3.303626464972
C	-1.745681107309	-0.317891551263	4.397462119569
H	-1.107374509939	0.096875002322	5.201105514244
H	-2.466864859633	-0.981150489151	4.905926094407
C	-2.527501427622	0.813010128781	3.706626139036
H	-2.677058849270	0.557842559739	2.640400660930
H	-3.539513180389	0.878827581904	4.142630106953
C	-0.677764836656	4.848149460401	0.026789761515
C	-1.296289261761	3.554634947406	0.574665531202
C	3.048445789055	4.267159255644	0.585030546406
C	-0.486381924127	2.280655634936	0.710349672007
C	2.780942621441	2.839925738507	1.047544556966
C	2.681782651333	1.687357126611	0.128469140866
H	-1.434496270303	5.637441854244	0.176042070813
H	-2.184906298485	3.313897269480	-0.035863295478
H	3.260697949555	4.867403616159	1.486513586495
H	1.945642366171	2.796481296126	1.765569524455
H	-0.534491950031	4.777188967437	-1.066289623041
H	-1.687509295794	3.794126523482	1.575013087483
H	3.966054847365	4.305512139429	-0.024556561700
H	3.645639141470	2.479216044035	1.659113926633
C	0.647474123954	5.243513913000	0.695748510718
H	0.713636262664	4.754432869285	1.685011311902
H	0.664760506979	6.327067079005	0.901329550492
C	1.862220598327	4.870817934634	-0.168471056343
H	1.517362397252	4.148536354597	-0.926054309134
H	2.202533341078	5.756135256484	-0.733323777499

Thermochemistry (use all positive eigenvalues) at 298.15 K, 1.00 Atm
E(el) = -1421.528158527160

ZPVE = 0.725705206760
Enthalpie(0K) = -1420.802453320400
E(tr) = 0.001416276854
E(rot) = 0.001416276854
E(vib) = 0.753488752643
H-E(el) = 0.757265490919
Enthalpie = -1420.770893036241
S(el) = 0.000000000000
S(tr) = 0.000070817727
S(rot) = 0.000058567308 (Symmetry number = 1)
S(vib) = 0.000170555367
G-E(el) = 0.667838259907
Free Energy = -1420.860320267253

Table S15. Cartesian coordinates and energies of Int_8.

C	3.099006048603	2.373917909488	-2.480692956083
C	3.268052184688	1.840906243697	-3.754719563849
C	3.154825350733	1.537441335548	-1.349978113958
C	3.553062437319	0.484227886590	-3.897671934353
C	3.484561893875	0.160503218347	-1.493086618396
C	3.682411338422	-0.341561982502	-2.776275221658
B	2.033542604361	0.991271381026	0.822346004603
C	3.099750921971	-0.193767661710	0.931517751103
C	3.727748580790	-0.625600566936	-0.255896389625
H	2.863913392123	3.434547923968	-2.363617241853
H	3.182820464285	2.486154120803	-4.632322706652
H	3.695566258320	0.058952608655	-4.894929325642
H	3.941044659042	-1.393490813429	-2.917786865199
C	3.418257100971	-0.836372868576	2.132380543229
C	4.600006882085	-1.717113059750	-0.231870348354
C	4.884530339131	-2.364026426794	0.972110647708
C	4.310100118254	-1.911524683809	2.157754980435
H	2.978074874456	-0.490498454210	3.071122546280
H	5.091012033499	-2.055673843708	-1.147809395501
H	5.577391825069	-3.210160537857	0.982461145924
H	4.557135214750	-2.392510841399	3.108507024920
C	-1.044193438106	-1.454947890261	-0.450069144228
C	0.345976824276	-0.800407049880	-0.531771491088
C	-1.807782820130	1.448856482468	-2.438971229739
C	0.414083189532	0.571351807152	0.096306681911
C	-0.385324531138	1.838188112552	-1.996693523370
C	-0.141854718188	1.714073693663	-0.525341263582
H	-1.221603126618	-1.796843558544	0.584110914721
H	0.649102080580	-0.712225640592	-1.589855333778
H	-2.540568936244	2.047121414835	-1.866658150165
H	-0.202732795558	2.882084546201	-2.302363073247
H	-1.013180738541	-2.367527058710	-1.073770524656
H	1.071770234780	-1.483099828894	-0.065754230323
H	-1.914575743124	1.751331635901	-3.495392499638
H	0.343297006918	1.214346465096	-2.541464264401
C	-2.233124420552	-0.594623301476	-0.883426573938
H	-2.368712865276	0.237738377728	-0.167146424633
H	-3.136829077983	-1.220045519908	-0.780042418578
C	-2.165897185507	-0.035253258193	-2.318476644374
H	-1.455294382416	-0.631938678675	-2.921689350503
H	-3.149661683391	-0.166777625831	-2.801375590907
C	0.486062160709	0.098095201377	4.030346580008
C	0.288725547041	-0.224657292954	2.541825831213
C	-1.328594933421	2.850747364772	3.784060656847
C	0.569640712050	0.901410720507	1.542767219300
C	-0.030831205290	3.026141081281	2.973593074171
C	0.006332167158	2.253821329766	1.684171886713
H	1.263548882524	0.869455400807	4.149767135503
H	-0.753176314450	-0.551722652448	2.383746299025
H	-1.183307531546	3.365326761857	4.751208629984
H	0.834922499533	2.745078875794	3.589707352718
H	0.887788089956	-0.798137142505	4.533727254328
H	0.901665900744	-1.091958148497	2.261054236974

H	-2.141676716741	3.388714664217	3.264479066848
H	0.074444433186	4.100800994111	2.769390609622
C	-0.809001776188	0.494665290705	4.766851303101
H	-0.545537384152	0.944229749847	5.742176308190
H	-1.358095701725	-0.436189377209	4.999191485529
C	-1.787118833650	1.416074742655	4.030741107331
H	-2.077642542578	0.957855562808	3.067549224672
H	-2.717821245314	1.461360519526	4.623985609351
C	-0.209990226600	5.275164633849	0.279586832205
C	-1.102116877560	4.034362253979	0.160381433693
C	2.792028201453	4.445886878168	1.158817721503
C	-0.435821077455	2.711569340186	0.449938772693
C	3.450758665782	3.324311233821	0.351039615793
C	2.793093404548	2.076699995072	-0.050666395065
H	0.059656857448	5.424986084196	1.338287459348
H	-1.531748498014	3.998934127903	-0.854350677823
H	1.967968980727	4.053388410021	1.771687989806
H	4.207964992191	2.816037415580	1.006760545217
H	-0.814126941107	6.157708088023	0.007560189439
H	-1.959544893465	4.151821762449	0.846004293406
H	3.547133718654	4.842707774996	1.855687090239
H	4.046125828047	3.745597778910	-0.475152639445
C	1.072351618073	5.234638213904	-0.568966763263
H	0.983753430454	5.924985743875	-1.425001842865
H	1.201889913367	4.227945371175	-1.010524981700
C	2.319441935511	5.581341122468	0.243212533486
H	3.152264412104	5.856071228467	-0.429170734899
H	2.114326380662	6.476167860213	0.858265188148

Thermochemistry (use all positive eigenvalues) at 298.15 K, 1.00 Atm
E(el) = -1421.531232365013
ZPVE = 0.727179240510
Enthalpie(0K) = -1420.804053124503
E(tr) = 0.001416276854
E(rot) = 0.001416276854
E(vib) = 0.755060644890
H-E(el) = 0.758837383167
Enthalpie = -1420.772394981846
S(el) = 0.000000000000
S(tr) = 0.000070817727
S(rot) = 0.000058399864 (Symmetry number = 1)
S(vib) = 0.000171984819
G-E(el) = 0.669033884506
Free Energy = -1420.862198480507

Table S16. Cartesian coordinates and energies of TS_8.

C	3.176651232188	2.546909976178	-2.369134383596
C	3.328075732116	2.094982277718	-3.683129702165
C	3.170616374659	1.628585468770	-1.316722708103
C	3.522570428655	0.740796002078	-3.936400962304
C	3.430213215899	0.261499698735	-1.567122224254
C	3.601587987545	-0.170622210554	-2.876554469917
B	1.896101119278	1.032164969114	0.742478884435
C	3.096487400215	-0.071003604045	0.841145786626
C	3.646378934645	-0.569176075656	-0.354179296249
H	3.037986437944	3.611787277906	-2.174563679484
H	3.305279380966	2.813885620984	-4.506150472005
H	3.648427012233	0.387298348479	-4.963300143787
H	3.814172718866	-1.223260756642	-3.080995590601
C	3.468212690593	-0.639099891291	2.063789201408
C	4.452769296335	-1.705504022455	-0.328219041748
C	4.763500555534	-2.309370427574	0.893903586112
C	4.296949699049	-1.763419287259	2.089071617689
H	3.101759646602	-0.217133091784	3.003350539005
H	4.876550113195	-2.104682244242	-1.253594170557
H	5.407101805634	-3.193469977912	0.910792387047
H	4.579998458728	-2.209953114656	3.046236492535
C	-1.112039640059	-1.504063443618	-0.365853344044

C	0.288355085247	-0.876274838193	-0.442081848024
C	-1.794176522651	1.345509735298	-2.476184115426
C	0.371345533042	0.518832294773	0.136060361847
C	-0.388526276278	1.751874199792	-1.996972168884
C	-0.200509015253	1.650628225499	-0.516156574142
H	-1.322949067031	-1.794847674048	0.677965166201
H	0.618905768795	-0.832962853303	-1.494784982726
H	-2.546364403632	1.962057530331	-1.950018361258
H	-0.201202546199	2.790791075634	-2.315664993530
H	-1.083612015619	-2.444730416003	-0.946507698026
H	0.998055900188	-1.545726074840	0.067483105814
H	-1.862816016182	1.613222744270	-3.545018786034
H	0.362276431346	1.121213692564	-2.502726674801
C	-2.274404736965	-0.643139189040	-0.867469582166
H	-2.420072950510	0.215438591184	-0.185020238758
H	-3.190679331377	-1.250963023630	-0.770032456298
C	-2.154905475382	-0.134682988828	-2.318539310507
H	-1.420867671154	-0.749138474712	-2.873739177961
H	-3.119563222513	-0.285670945750	-2.833109467788
C	0.511610863542	0.160450948103	4.093303085474
C	0.320011701899	-0.229227595645	2.621152023358
C	-1.392210554814	2.848948443550	3.769718101557
C	0.481544169865	0.875621916584	1.580379915110
C	-0.105804126423	3.037671975251	2.944294592533
C	-0.070000227858	2.223594942854	1.683490551141
H	1.264464930127	0.960131383574	4.178237345088
H	-0.690684606692	-0.655645828462	2.495954527178
H	-1.256667735115	3.394535794864	4.720947406767
H	0.772513062667	2.795842960817	3.558905858948
H	0.944326098904	-0.702843348523	4.627358245543
H	1.004992063515	-1.047895993626	2.360577324043
H	-2.224288395388	3.346146982729	3.239802882919
H	-0.026547430447	4.106071015072	2.700367360347
C	-0.792830012848	0.541610233876	4.820510179298
H	-0.540920799587	1.031487391105	5.779339528997
H	-1.311671497688	-0.397819386322	5.085490828431
C	-1.801895247786	1.406891710816	4.058207986063
H	-2.076981355487	0.909766146294	3.109512329375
H	-2.733319527487	1.438357483135	4.651045840013
C	-0.057049967425	5.166176271999	0.172388443258
C	-1.075570844354	4.017784430951	0.107734237013
C	2.908053312362	4.386903214654	1.180335365877
C	-0.504354271283	2.659261526403	0.429244077147
C	3.649200211896	3.118580388737	0.700762762099
C	2.852490912963	2.039320927135	0.067476670381
H	0.224947008601	5.338056264854	1.224671138286
H	-1.524673572179	3.985267289574	-0.898806367365
H	2.038936324367	4.099142888449	1.793386565910
H	4.069423648662	2.639934192898	1.606647713930
H	-0.553424639781	6.097018096098	-0.152105683150
H	-1.903953698603	4.236185608362	0.803660020807
H	3.611628083882	4.903004181455	1.853367956088
H	4.497115927989	3.402621415102	0.056958222627
C	1.208792507132	4.923844346082	-0.661678634470
H	1.133173691998	5.442424571254	-1.633053387497
H	1.273148168697	3.848882014604	-0.906025883354
C	2.493028913719	5.340653652700	0.055551384018
H	3.327113688934	5.428340422041	-0.664189938743
H	2.351676190813	6.349879937363	0.483252791407

Thermochemistry (use all positive eigenvalues) at 298.15 K, 1.00 Atm
E(el) = -1421.529722257748
ZPVE = 0.725710775199
Enthalpie(0K) = -1420.804011482549
E(tr) = 0.001416276854
E(rot) = 0.001416276854
E(vib) = 0.753318044130
H-E(el) = 0.757094782406
Enthalpie = -1420.772627475342
S(el) = 0.000000000000

S(tr) = 0.000070817727
S(rot) = 0.000058333674 (Symmetry number = 1)
S(vib) = 0.000168212792
G-E(el) = 0.668435647835
Free Energy = -1420.861286609913

Table S17. Cartesian coordinates and energies of 4^+.

C	2.594961117040	1.139447723183	-2.633787642142
C	2.746979358785	0.119085230150	-3.576785452659
C	3.112318673387	0.962782597771	-1.351840880028
C	3.399087079895	-1.072559923609	-3.242998740454
C	3.786951434862	-0.228846120416	-1.027516795712
C	3.926452250204	-1.253826092399	-1.964095258340
B	1.525345063067	1.812661074345	0.403800869901
C	3.884329560431	1.115043341781	0.871049019693
C	4.269240225420	-0.132787196973	0.355934438615
H	2.064602390412	2.052952213473	-2.908356079076
H	2.345857589475	0.253691834034	-4.585546890668
H	3.502461949137	-1.863733379265	-3.991285841232
H	4.446601025394	-2.180070463737	-1.703487698720
C	4.284499485890	1.502923012558	2.146357874994
C	5.012159887885	-1.025658513924	1.129967122026
C	5.389104684811	-0.644089406502	2.418507078514
C	5.040009482631	0.615959390635	2.917957572393
H	4.011042618399	2.482843200391	2.546981780613
H	5.305099810120	-2.001422374226	0.731884267100
H	5.974858670183	-1.329361171862	3.038062312097
H	5.359064757532	0.908694963695	3.922549821455
C	-1.113202724555	-1.325686476066	-0.700921083948
C	0.272989941224	-0.664971903279	-0.650621294002
C	-2.208242312544	2.009149107700	-1.561414022913
C	0.292295234773	0.573007405446	0.196357873067
C	-0.678928578415	2.156476007296	-1.594356221149
C	-0.098452217983	1.879557352366	-0.243138059254
H	-1.473977398214	-1.494379116554	0.330667885671
H	0.606572721203	-0.424539134409	-1.672059733059
H	-2.643902732273	2.872589744173	-1.028316068044
H	-0.409073183956	3.166867038456	-1.934256861984
H	-0.969814543727	-2.325313269170	-1.145753873193
H	1.000355382452	-1.384283338110	-0.246271434146
H	-2.568452613029	2.070603283999	-2.603435216977
H	-0.250845570862	1.448518585477	-2.319531380048
C	-2.198241256629	-0.599356794604	-1.507137070023
H	-3.040970024426	-1.304932640552	-1.603589430586
H	-1.832800118662	-0.429776135939	-2.537785620670
C	-2.733767241165	0.721615600547	-0.915866051560
H	-3.832169817923	0.742403181703	-1.017185883570
H	-2.541159772341	0.744739953794	0.173669344602
C	0.339662403087	-0.943116917057	3.414649576047
C	1.346740438465	-0.411646129291	2.382384520000
C	-0.067019047229	2.558452596658	4.235367958010
C	0.773998476381	0.684706537736	1.534635161183
C	1.109493238590	2.594757805553	3.247939233111
C	0.688054286764	2.061656404159	1.914927627973
H	0.765552396758	-1.878798354467	3.815656256997
H	1.665114128217	-1.239268545458	1.732010760749
H	0.330508383514	2.800836989969	5.236594268896
H	1.937695183764	1.980879638340	3.631666228046
H	-0.597134432338	-1.225301561141	2.899401092408
H	2.249884553860	-0.052915062313	2.899890116132
H	-0.780491081160	3.360966877548	3.976925356648
H	1.491376694940	3.623144059573	3.149154629274
C	0.011807540291	-0.026260822792	4.601337255397
H	0.952523261483	0.263423473937	5.107106890659
H	-0.538123241484	-0.645258108591	5.330553103024
C	-0.831433134068	1.230246284979	4.297168525109
H	-1.392591713026	1.079040744565	3.355423419456
H	-1.601691042977	1.344533534562	5.078713934754

C	0.236256520135	5.308984601786	-0.012528499750
C	-0.347029649298	4.238993642309	0.914588409367
C	2.803503739718	4.174649045723	-1.353919538919
C	0.102289311650	2.799505669569	0.835461930067
C	3.567389309308	3.305300377411	-0.344868412577
C	3.028683928159	1.877831626057	-0.132232928031
H	-0.430485507808	6.182588084578	0.074300861466
H	-1.437298056089	4.185862227859	0.746632314444
H	3.319419513481	4.158034447275	-2.328320998752
H	3.574451908741	3.799198528759	0.641450082303
H	0.151789292707	4.984514624988	-1.062555793308
H	-0.217885514221	4.570357814296	1.956961116675
H	1.800794416938	3.752418915337	-1.541301361030
H	4.626078494456	3.222908203954	-0.645997015279
C	1.681171496591	5.730612577196	0.315912682953
H	2.065081313012	5.119821976674	1.154311204173
H	1.689617962478	6.769724111437	0.686417172234
C	2.635132574230	5.616914904385	-0.875418494593
H	2.251712455260	6.238670748749	-1.705090501576
H	3.622347074640	6.032425862942	-0.601123409251

Thermochemistry (use all positive eigenvalues) at 298.15 K, 1.00 Atm
E(el) = -1421.630710103505
ZPVE = 0.729771450363
Enthalpie(0K) = -1420.900938653142
E(tr) = 0.001416276854
E(rot) = 0.001416276854
E(vib) = 0.757237253137
H-E(el) = 0.761013991413
Enthalpie = -1420.869696112092
S(el) = 0.000000000000
S(tr) = 0.000070817727
S(rot) = 0.000058254653 (Symmetry number = 1)
S(vib) = 0.000167590093
G-E(el) = 0.672564075040
Free Energy = -1420.958146028465

Table S18. Cartesian coordinates and energies of TS_1b.

C	3.023661984276	2.100260786855	-2.744113196403
C	3.082204564585	1.149391211566	-3.752979855095
C	3.083889584028	1.722468629880	-1.391820665512
C	3.231499913100	-0.199442317079	-3.415687742567
C	3.320613868279	0.367290209976	-1.048817200062
C	3.377145046787	-0.577227015916	-2.084569526940
C	3.030021723968	0.228903878009	1.512789349053
C	3.751631699208	-0.039476734861	0.326283561794
H	2.894639802827	3.157222994177	-2.992039044848
H	3.001578307727	1.453247126108	-4.799872265954
H	3.260761039763	-0.960442154807	-4.200595905312
H	3.546218015508	-1.628400885988	-1.835456162021
C	3.602738910979	-0.140429237912	2.735058714514
C	4.990386163433	-0.690754792674	0.410337060546
C	5.540707130075	-1.061209764136	1.635399341214
C	4.844533279719	-0.773398664474	2.803458250434
H	3.080520655183	0.059653050868	3.670879031725
H	5.547624163824	-0.889397242490	-0.509281021885
H	6.512366052088	-1.561393756874	1.670620009131
H	5.259150667199	-1.043926892073	3.778765771427
C	-1.367484748636	0.388950882180	-2.858475671903
C	-0.464942615196	-0.068614607698	-1.701339741872
C	-1.287191830845	3.460466459709	-2.467030511634
C	0.139035745369	0.837529375960	-0.624232718655
C	-1.380128671046	2.810383805844	-1.071067645775
C	-0.051483759359	2.289937397549	-0.569625161864
H	-2.334980862152	0.759741626219	-2.485715720578
H	0.410486503019	-0.570313044005	-2.159905883565
H	-2.303450141674	3.531597042029	-2.894879144532
H	-2.102845889460	1.987569562997	-1.066546081356

H	-1.618686482705	-0.542892184585	-3.395433255853
H	-1.022253544080	-0.873472192995	-1.199474422683
H	-0.921611285994	4.495282325789	-2.346821947219
H	-1.775380623813	3.545170233104	-0.352903028873
C	-0.803758715664	1.354377469259	-3.904825408442
H	-1.588624941691	1.491972085830	-4.671636750098
H	0.046045882411	0.867638441164	-4.419794865807
C	-0.343882258353	2.730295440506	-3.421978855095
H	0.635503478939	2.632083455150	-2.925016681382
H	-0.166424343634	3.366031062920	-4.307590036773
C	-0.838282890425	-1.641483850150	1.208114970952
C	0.586569289478	-1.244828354434	0.715387657806
C	-0.528808542958	1.409624139752	2.812755230879
C	0.787788501724	0.221324196731	0.414787394900
C	0.941821867459	0.960413706203	2.808820084616
C	1.671378607445	0.935785694940	1.439330056708
H	-0.714779249316	-2.302033373480	2.084079878330
H	0.835032171936	-1.832969088786	-0.184147405898
H	-0.685021676508	2.018017968592	3.719790389372
H	0.994361980376	-0.049522479870	3.251729705070
H	-1.319931342348	-2.264616034202	0.435726922684
H	1.322664826160	-1.547930560035	1.473717475248
H	-0.742489282343	2.083211277031	1.965605035759
H	1.524962690823	1.612858496848	3.480197306523
C	-1.834881909174	-0.535962796873	1.581287000361
H	-2.804772260101	-1.045042799442	1.725460806172
H	-1.985651323144	0.150912010911	0.729170494707
C	-1.573720521507	0.284767985162	2.851855118284
H	-2.534572479561	0.755108681588	3.128127562216
H	-1.325608023345	-0.403731946268	3.682731599914
C	0.750505410678	5.127501503726	1.670093610925
C	0.608134688324	4.626004806351	0.225729479657
C	4.217903207238	4.214332783267	1.087487996333
C	3.671433539404	4.001770520885	-0.330547707881
H	0.264331949864	4.404471540393	2.351032144163
H	1.245960849997	5.234372339211	-0.440267349816
H	4.946191318960	3.414538084779	1.305469424784
H	4.494786662685	3.937447588064	-1.058578554639
H	0.180851223888	6.068101654966	1.759137367492
H	-0.415712566790	4.847894783149	-0.102006567629
H	4.762373119306	5.172337209123	1.138532476463
H	3.053508173966	4.860009844537	-0.645595804504
C	2.175065267387	5.407202338230	2.151024868563
H	2.112196561955	5.820236130432	3.171076708834
H	2.612321229833	6.204393857752	1.522974053203
C	3.134097410455	4.207468285239	2.157811620670
H	3.600371289975	4.078934589103	3.146532205847
H	2.530348011429	3.239931757690	2.102483648761
B	1.978822989062	2.334557337330	0.797395628016
C	2.896491179474	2.718391724525	-0.337557410756
C	0.861565971347	3.145477172083	0.035476612737

Thermochemistry (use all positive eigenvalues) at 298.15 K, 1.00 Atm
E(el) = -1421.490013930763
ZPVE = 0.725577088574
Enthalpie(0K) = -1420.764436842189
E(tr) = 0.001416276854
E(rot) = 0.001416276854
E(vib) = 0.752806161176
H-E(el) = 0.756582899452
Enthalpie = -1420.733431031311
S(el) = 0.000000000000
S(tr) = 0.000070817727
S(rot) = 0.000058047811 (Symmetry number = 1)
S(vib) = 0.000164715727
G-E(el) = 0.669051645318
Free Energy = -1420.820962285445

Table S19. Cartesian coordinates and energies of TS_1c.

C	2.360799831947	1.319120356698	-2.751959821884
C	2.657441193266	0.126926308087	-3.410231942588
C	2.725034822707	1.493008180824	-1.413337875591
C	3.336008567039	-0.885138994728	-2.734249723706
C	3.367800667893	0.464839741751	-0.706148239063
C	3.681260840892	-0.713719117043	-1.394939701710
C	2.895006854864	0.781773826915	1.828172435404
C	3.777416603898	0.606632102669	0.728007988130
H	1.852653972702	2.129564950491	-3.281961249977
H	2.366534110148	-0.002166425830	-4.456196019263
H	3.586455536130	-1.818675239627	-3.245368064071
H	4.184180076917	-1.521198211556	-0.854984563629
C	3.474011218865	0.874837680275	3.105113610427
C	5.159951628038	0.513646640262	0.961217177763
C	5.704436567238	0.605940708446	2.236667903180
C	4.847308674890	0.792266459980	3.316561019918
H	2.839362902700	1.017183784792	3.979536321475
H	5.822760467573	0.374297037988	0.102272721060
H	6.785842710836	0.535508852587	2.381735866555
H	5.241132523793	0.872170458262	4.333766843414
C	-2.111851812851	-0.110433205944	-1.391647871510
C	-0.700135324463	0.472476423401	-1.576463589685
C	-2.522834982670	2.871923158679	0.572893742643
C	-0.032205760465	0.963351642293	-0.315763474796
C	-1.300769806282	3.254176364912	-0.276801322938
H	-2.059116056702	-0.964507922856	-0.691868921476
H	-0.742086882699	1.299554851529	-2.305903655548
H	-2.315612183366	3.137838986147	1.625085978504
H	-1.103806615080	4.317626047089	-0.094975626748
H	-2.421992379698	-0.529299772536	-2.365450344724
H	-0.062823612543	-0.303483209631	-2.032052922908
H	-3.348911070757	3.526165210713	0.240123818624
H	-1.533857296521	3.154732359877	-1.350327460423
C	-3.203227649592	0.847822636744	-0.905292396501
H	-4.155011193245	0.289890655844	-0.933109246685
H	-3.322400660955	1.673576034274	-1.631975667000
C	-2.995315565954	1.415640268676	0.512333151666
H	-3.945668953769	1.367204671916	1.071289423025
H	-2.292393028594	0.769140551067	1.068064660947
C	1.462540108362	-2.166401179899	1.393712320694
C	0.853894773919	-1.300457101962	0.288438365259
C	0.472974857883	-0.461005298419	3.782702388927
C	0.676626905707	0.178287094871	0.543105480023
C	0.554422015564	0.867974012384	3.023038726576
C	1.377411063271	0.952553600539	1.702203287249
H	2.285571956753	-1.630645731850	1.894614284071
H	-0.133329135341	-1.716705069792	0.020654076327
H	1.483065785879	-0.846916312672	4.006784517543
H	0.926073620791	1.648216473145	3.708041113806
H	1.927273946558	-3.048321473020	0.920633485360
H	1.460931104953	-1.402389315786	-0.625868591680
H	0.023471260518	-0.218325626389	4.760886888060
H	-0.478130288062	1.169488723937	2.772615078163
C	0.447942639540	-2.656230276571	2.426310582230
H	0.984296643768	-3.234234660779	3.201728440239
H	-0.248389283206	-3.362960093012	1.937263522345
C	-0.368283640724	-1.554934282365	3.102577085541
H	-1.051635844529	-1.090303965101	2.366359082876
H	-1.023010819669	-2.032234462360	3.852180849915
C	1.034631903881	5.826844554574	-0.627758104005
C	1.371938277723	4.732057913730	0.401405886751
C	3.746076180072	4.408886477399	-2.428266582080
C	3.780421409032	3.724919764517	-1.046042329541
C	2.586662780238	2.849547720736	-0.815679597179
H	0.746336913315	6.718126081315	-0.043606649315
H	0.591475359977	4.757025995082	1.183026750594
H	4.629068471011	5.070154235205	-2.465075393125
H	3.849476648440	4.494638672053	-0.263980969671

H	0.138165645304	5.528841591049	-1.197899775584
H	2.305020280337	4.993276995094	0.928908457043
H	3.885368151260	3.652401804557	-3.219102583542
H	4.684208028986	3.096959667403	-0.988956373216
C	2.116510507277	6.252504775999	-1.626962951314
H	3.025962843036	6.574553646470	-1.085298139513
H	1.731502901896	7.159485748766	-2.123690450446
C	2.483668543198	5.222505307795	-2.709686350090
H	1.627225493689	4.540735703037	-2.872702977155
H	2.640924281733	5.740361735685	-3.671095060230
B	0.975700915637	2.289754643146	1.033480280623
C	-0.095822442928	2.429136598375	0.059508801503
C	1.488717874206	3.301169397600	-0.121058273294

Thermochemistry (use all positive eigenvalues) at 298.15 K, 1.00 Atm
E(el) = -1421.475476591073
ZPVE = 0.725464515193
Enthalpie(0K) = -1420.750012075880
E(tr) = 0.001416276854
E(rot) = 0.001416276854
E(vib) = 0.753062044990
H-E(el) = 0.756838783266
Enthalpie = -1420.718637807807
S(el) = 0.000000000000
S(tr) = 0.000070817727
S(rot) = 0.000058314465 (Symmetry number = 1)
S(vib) = 0.000169556828
G-E(el) = 0.667784652014
Free Energy = -1420.807691939059

Table S20. Cartesian coordinates and energies of Int_9a.

C	3.252029389972	2.235951706027	-2.693798687944
C	3.221553197611	1.339624799811	-3.747961269068
C	3.225098921891	1.776418204060	-1.357028165981
C	3.206533493726	-0.035157879269	-3.482705558208
C	3.292861290746	0.376952067490	-1.089187350822
C	3.274545343774	-0.505895829331	-2.174709976826
C	3.020395189351	0.197356086033	1.458165550407
C	3.702153377091	-0.111914097916	0.260694095277
H	3.232163073190	3.311200455361	-2.888257584638
H	3.194081013460	1.703870901567	-4.777720308369
H	3.169483412344	-0.748309282829	-4.310918696821
H	3.330526964024	-1.581253623771	-1.986293332359
C	3.605498057838	-0.197502794326	2.666798631299
C	4.896668999386	-0.843652841893	0.309415368935
C	5.450948476852	-1.248441500352	1.521512865537
C	4.807620314680	-0.905638191737	2.705122608671
H	3.122928784512	0.035757166379	3.615832841208
H	5.418191236384	-1.073156113058	-0.623982252820
H	6.386960159974	-1.813411429655	1.534689427922
H	5.231223798839	-1.195324954410	3.671012384871
C	-1.342730044707	0.336338810447	-2.877485022236
C	-0.608477502191	-0.126840342086	-1.608279907961
C	-1.225140554300	3.376239920371	-2.562491031595
C	0.048489352711	0.799995854373	-0.580590653322
C	-1.437245608340	2.787604101584	-1.150371601155
C	-0.157683825991	2.261506319258	-0.537610473206
H	-2.318124389447	0.785277227482	-2.634520368300
H	0.207774237602	-0.790920254342	-1.949705486825
H	-2.197412107287	3.420862685061	-3.086102566751
H	-2.182509975621	1.983899653974	-1.161302601074
H	-1.594903712159	-0.599157791960	-3.407889789173
H	-1.312244775788	-0.792876108382	-1.082116897254
H	-0.879323810371	4.419195597652	-2.452120407519
H	-1.863460281000	3.564844728053	-0.497709251368
C	-0.603772534217	1.227578688513	-3.878503120327
H	-1.267184670750	1.338653575415	-4.756059379661
H	0.298058454724	0.698656591729	-4.240764353400

C	-0.191671467774	2.622850740809	-3.401241502169
H	0.739288799425	2.553259758212	-2.813467861926
H	0.063166470469	3.230491270402	-4.287848342427
C	-0.865979070325	-1.642049196575	1.318508172272
C	0.543479725560	-1.261763772986	0.774837755164
C	-0.470222032758	1.436031250677	2.867382586693
C	0.743922424505	0.194896488886	0.430809161458
C	1.002291464495	0.999441064147	2.796237391444
C	1.680449067533	0.934474901925	1.397084598753
H	-0.718506873900	-2.312718930187	2.183259708836
H	0.758507260789	-1.875800706934	-0.116485185671
H	-0.581960021927	2.062508906075	3.768941172652
H	1.076774722743	-0.001554945807	3.255053097886
H	-1.387258182829	-2.251093717805	0.560704890025
H	1.301955173028	-1.553422649232	1.515671793826
H	-0.737019857019	2.087179892771	2.018993524629
H	1.613198349593	1.662651464381	3.431160582081
C	-1.832394986457	-0.526480686868	1.738351629268
H	-2.797829261777	-1.026984223964	1.934007797836
H	-2.020373310895	0.157939636248	0.891597129823
C	-1.499185296406	0.302229630286	2.986468348296
H	-2.444548856224	0.767156812102	3.319621690096
H	-1.193267615581	-0.377635080139	3.805246482097
C	0.688742607433	5.193790695553	1.626069127484
C	0.508003105715	4.599674457307	0.218217723667
C	4.219678702102	4.317945944786	1.174390344901
C	3.732710084024	4.036664394654	-0.257491523413
H	0.241831959306	4.506476766245	2.368343636283
H	1.157113938064	5.143081022890	-0.495361046664
H	4.946670481925	3.538087089218	1.459661574294
H	4.569868866137	4.053014054364	-0.972302950390
H	0.094465044057	6.122567482229	1.671666412992
H	-0.513426358295	4.834231835742	-0.111109350735
H	4.761866534838	5.278602144650	1.175561739075
H	3.032309738239	4.833641088737	-0.573906434571
C	2.116785242675	5.547925133282	2.048640686681
H	2.054629852040	6.088440655182	3.007918391100
H	2.530952188317	6.272695959513	1.323105101999
C	3.095804852770	4.369843232287	2.204838558523
H	3.546823037362	4.375734043198	3.209531093231
H	2.529065562199	3.402521237556	2.202246171281
B	1.929747215632	2.324081088127	0.696580149941
C	3.045739168465	2.721787025831	-0.286317308041
C	0.719074687552	3.107626265815	0.106135352766

Thermochemistry (use all positive eigenvalues) at 298.15 K, 1.00 Atm
E(el) = -1421.491134221601
ZPVE = 0.725496507632
Enthalpie(0K) = -1420.765637713969
E(tr) = 0.001416276854
E(rot) = 0.001416276854
E(vib) = 0.753681473074
H-E(el) = 0.757458211350
Enthalpie = -1420.733676010251
S(el) = 0.000000000000
S(tr) = 0.000070817727
S(rot) = 0.000058101047 (Symmetry number = 1)
S(vib) = 0.000173552189
G-E(el) = 0.667276493346
Free Energy = -1420.823857728255

Table S21. Cartesian coordinates and energies of Int_9b.

C	4.320241005166	4.476946862593	0.256260295437
C	5.582432433713	4.449591932541	0.812814560758
C	3.503548787419	3.310416137225	0.216242062989
C	6.059015143802	3.248788680479	1.349707457245
C	4.013505956141	2.081927502783	0.748060916335
C	5.286419476882	2.087205668899	1.317118903682

C	3.287016779045	0.779063057904	0.678712240031
H	3.933566400213	5.422088711819	-0.126910399878
H	6.192245545388	5.354863757420	0.848153450775
H	7.051072434819	3.215450462947	1.808831582239
H	5.686391964810	1.171378345578	1.756801290086
C	1.463196859173	-0.764485130520	1.019146631727
C	4.054119584889	-0.302333382697	0.209212319383
C	3.544048813601	-1.591627512570	0.139216503910
C	2.239313195180	-1.823324958312	0.565669726158
H	0.442957554810	-0.974694002680	1.340147961514
H	5.078579182918	-0.117458027132	-0.123324585241
H	4.166237566973	-2.407805797247	-0.237081851588
H	1.816395434164	-2.831377168063	0.544012137973
C	-3.743315269453	1.737836401529	1.388248301699
C	-2.765178569248	0.563903524774	1.214212372448
C	-3.197216419711	1.619272719608	-2.085441776370
C	-1.360590129855	0.995109562511	0.840128496203
C	-2.054209621210	0.690202437800	-1.629570838471
C	-1.069401773980	1.216674994010	-0.597530229685
H	-3.415661295138	2.362362103902	2.236244145423
H	-3.177249735014	-0.128508688284	0.465977103065
H	-2.768155797725	2.585939608094	-2.394635638213
H	-1.480501507062	0.438214248226	-2.533891484513
H	-4.724134149663	1.313409300751	1.673038179986
H	-2.757711155967	-0.004059943268	2.154951979662
H	-3.623876996751	1.166485928284	-2.998315857464
H	-2.486566446544	-0.262612339522	-1.284558468127
C	-3.935802514221	2.640053637173	0.170160785210
H	-3.013516637723	3.222839997940	-0.018043682118
H	-4.709486473557	3.383348803399	0.430517124482
C	-4.342077568978	1.897354777224	-1.111512113418
H	-4.855738644031	0.952274112452	-0.851087172729
H	-5.086215083498	2.500079549361	-1.661222592994
C	-1.430819369887	1.523356176148	4.218501239085
C	-0.631432267745	0.650293243012	3.235408579976
C	0.839495393196	3.885152310010	2.909937950745
C	-0.411960060062	1.152350657438	1.814139653354
C	1.535805576266	2.543979993198	2.678469450125
H	-1.527478773006	0.947564944927	5.156413402299
H	-1.147726539786	-0.322631804400	3.179959252318
H	1.414335791107	4.418077883486	3.689647069389
H	1.528032662793	1.953289322046	3.606790437789
H	-2.455806331821	1.642749578768	3.831794117466
H	0.350773675535	0.422692095774	3.679609141404
H	0.915608256297	4.503584589661	1.995404578793
H	2.599324248474	2.751297528033	2.502382112558
C	-0.878994786805	2.910900511237	4.559205410053
H	0.051735530563	2.810631207153	5.148886505108
H	-1.608468560743	3.386736769897	5.237694534059
C	-0.626523670229	3.831943248855	3.352947102720
H	-1.270772452443	3.527041519872	2.508642642787
H	-0.931605224515	4.862970709996	3.603254880628
C	-0.304047478537	3.122331689213	-3.246419364252
C	0.460033401788	2.008075613619	-2.485499066253
C	2.298154537219	4.810707324488	-2.314683637668
C	0.096467172927	1.811667944180	-1.023473920115
C	1.630929161574	4.593568624843	-0.912672670372
H	-0.862840383569	3.757097010092	-2.535825579700
H	1.541192753146	2.209140889678	-2.543882584875
H	3.035580048850	5.621947481289	-2.207998955046
H	0.541145116429	4.504524721231	-1.018602133225
H	-1.068853700971	2.652547527224	-3.886757087131
H	0.339136943365	1.057339459590	-3.034563565606
H	2.876493767139	3.920640116582	-2.615028309203
H	1.809851328100	5.485760663822	-0.289632142237
C	0.583529453780	4.014515430076	-4.123537874398
H	-0.042527237204	4.460105885343	-4.916929894232
H	1.329595926052	3.383794409708	-4.643765139011
C	1.303672193921	5.174090847633	-3.422667310604
H	1.861663811132	5.730214428565	-4.196920674620

H	0.556270494105	5.882486649339	-3.018968028851
B	1.080284050323	2.276560237388	0.045813733366
C	1.942036964392	0.557662140921	1.074883062225
C	0.965387110441	1.704466404918	1.515806839088
C	2.167326993538	3.377458409587	-0.237099651633

Thermochemistry (use all positive eigenvalues) at 298.15 K, 1.00 Atm
E(el) = -1421.516828554179
ZPVE = 0.727506903355
Enthalpie(0K) = -1420.789321650824
E(tr) = 0.001416276854
E(rot) = 0.001416276854
E(vib) = 0.755485020390
H-E(el) = 0.759261758667
Enthalpie = -1420.757566795513
S(el) = 0.000000000000
S(tr) = 0.000070817727
S(rot) = 0.000058686725 (Symmetry number = 1)
S(vib) = 0.000173207305
G-E(el) = 0.669008248345
Free Energy = -1420.847820305834

Table S22. Cartesian coordinates and energies of Int_9c.

C	4.364723425145	4.342613043252	0.513873480355
C	5.176655755546	4.680314370110	1.586403456776
C	3.928742240828	3.007596275239	0.334208224420
C	5.640955719582	3.678524283318	2.441894753427
C	4.435898761755	1.981777707674	1.188611086873
C	5.302258979253	2.343992673109	2.219216190003
B	1.592310131353	1.995126177377	-0.340718776799
C	4.237242958271	0.564134686142	0.802135916702
H	3.993272865281	5.125307684933	-0.152390017235
H	5.456365586943	5.723733608942	1.751056224832
H	6.292409525661	3.936453512838	3.281315213369
H	5.715618633164	1.564930565575	2.864922483619
C	2.957035443861	-1.142467613647	-0.305022725929
C	5.392783359315	-0.208855625046	0.600372359513
C	5.335164464285	-1.441073789768	-0.040133782321
C	4.110647079284	-1.883302963686	-0.540026733348
H	2.010861813711	-1.509600352221	-0.705758372781
H	6.361687457413	0.198648921779	0.902398293976
H	6.247349512491	-2.023420007700	-0.195357749421
H	4.048884673680	-2.812814479959	-1.112997917083
C	-2.771733255844	-0.361094928558	1.744890309511
C	-1.984761227109	-0.487448875730	0.427804245160
C	-2.711484627834	3.019956260243	0.727828998727
C	-0.743560187018	0.390079778964	0.302775312977
C	-2.269794714396	2.237161813033	-0.524105209907
C	-0.868954998830	1.693613617345	-0.349533157409
H	-2.073469926286	-0.486928193023	2.593127202267
H	-2.665594146976	-0.313649237969	-0.417547998988
H	-2.051641194414	3.896863861914	0.857475508707
H	-2.337494112882	2.908132285498	-1.387767212074
H	-3.472240310760	-1.213842010373	1.794462946090
H	-1.682174816035	-1.538149598564	0.314363190702
H	-3.723651472373	3.413925537807	0.523579856191
H	-2.997515739083	1.440462345488	-0.717200328017
C	-3.572300801255	0.925233867010	1.974211965720
H	-4.109758088496	0.797846453537	2.930005043142
H	-4.358075201557	1.019118891030	1.200407649114
C	-2.746813757253	2.222002656629	2.033856228597
H	-3.163603966406	2.888057737862	2.809042618267
H	-1.717184339597	1.987063694149	2.363763042907
C	1.564270042636	-1.775354415115	2.521152907690
C	0.511124401574	-1.448700915706	1.452558771968
C	1.978105926044	1.108943693990	3.381839696387
C	0.457791575427	-0.072787930498	0.792025978352
C	1.609058178864	1.723306469832	2.025116638031

H	2.558283764814	-1.392733938732	2.251491961447
H	-0.462094187208	-1.650294019475	1.920083148070
H	2.949916592943	0.587307406777	3.325188651590
H	2.217276791617	2.625277499916	1.905910439475
H	1.670682753935	-2.873339210572	2.549580047393
H	0.584751842435	-2.195633267342	0.641249657090
H	2.148062895455	1.974055878040	4.045703955610
H	0.569017747011	2.080080401431	2.083528608314
C	1.193574450705	-1.290668231108	3.920588689909
H	2.024137503855	-1.539911351796	4.606796156849
H	0.310334091861	-1.848275066062	4.284025416522
C	0.902052670773	0.205731397634	4.006176313819
H	-0.071564774035	0.420988627934	3.527023048968
H	0.773396573334	0.472055505933	5.069581965564
C	-0.371397155472	3.451669735117	-3.067076613497
C	-0.039892886632	3.726039020054	-1.582847372581
C	3.091990500053	2.298862526551	-3.171265149995
C	0.218495495271	2.468423629377	-0.766355176875
C	3.214835405576	3.336161771755	-2.021686798375
H	-0.898043388218	4.335738119954	-3.468719161001
H	-0.872985859635	4.296075949370	-1.142975642158
H	3.632710995806	2.755792272536	-4.017648935185
H	2.500903853205	4.155983912833	-2.224487451399
H	-1.091395317753	2.615426104501	-3.121741346803
H	0.814537077422	4.416088195806	-1.523656161715
H	3.652561043475	1.387903359671	-2.899520447618
H	4.224843509647	3.769162297285	-2.048697310125
C	0.798479964059	3.141058325887	-4.009219262321
H	1.428791572452	4.043792288263	-4.120673071237
H	0.363131448850	2.974651706600	-5.009603385731
C	1.681650196012	1.932149150570	-3.636485631082
H	1.174422542797	1.302842700661	-2.885113426847
H	1.809985107381	1.280725041407	-4.517700159502
C	1.683249553718	0.795138306482	0.709052074517
C	2.932306278265	2.776667216337	-0.682479111864
C	2.977470923506	0.048545093865	0.437285384731

Thermochemistry (use all positive eigenvalues) at 298.15 K, 1.00 Atm
E(el) = -1421.494677525551
ZPVE = 0.726931912441
Enthalpie(0K) = -1420.767745613110
E(tr) = 0.001416276854
E(rot) = 0.001416276854
E(vib) = 0.754686723167
H-E(el) = 0.758463461443
Enthalpie = -1420.736214064108
S(el) = 0.000000000000
S(tr) = 0.000070817727
S(rot) = 0.000058565389 (Symmetry number = 1)
S(vib) = 0.000169991543
G-E(el) = 0.669204906443
Free Energy = -1420.825472619108

Table S23. Cartesian coordinates and energies of TS_9a.

C	4.189286210284	4.541602543335	0.339472722511
C	5.459280757614	4.591861159736	0.876198866026
C	3.466092740628	3.319784119719	0.260151617802
C	6.039120509651	3.411596755562	1.355807831703
C	4.080527270018	2.113026443539	0.726453965414
C	5.361873826961	2.198168276595	1.282637230428
C	3.408767570559	0.796088610860	0.629356053713
H	3.723034590450	5.469178976160	0.005634605687
H	5.994799793264	5.541303856202	0.945077442319
H	7.035479020101	3.438339382663	1.805750169716
H	5.842572430032	1.310068098846	1.695248204913
C	1.462523832845	-0.650575167805	0.531239877216
C	4.211324552814	-0.353572390761	0.500316376790
C	3.656747085653	-1.621078298059	0.401086399928

C	2.268607647423	-1.771865374190	0.422190619061
H	0.378518402044	-0.778592828899	0.545756185547
H	5.297007575639	-0.253685373254	0.446507061018
H	4.308967159559	-2.492872877433	0.303081561653
H	1.814723879853	-2.763206748040	0.344968126103
C	-3.747425332077	1.836350687944	1.394877849237
C	-2.818473987586	0.624086555624	1.192755796173
C	-3.263695567993	1.745956782604	-2.087431432668
C	-1.411789007702	1.024335866580	0.808832881514
C	-2.154062161290	0.768841030276	-1.658039257271
C	-1.134425738588	1.228814002564	-0.621423627560
H	-3.382404444809	2.433800865001	2.246781179068
H	-3.260718879070	-0.034694142691	0.432568254575
H	-2.802286604041	2.699205921188	-2.393062557931
H	-1.597457003503	0.509261599287	-2.571207684925
H	-4.736907268483	1.441059971749	1.689769234528
H	-2.824807306881	0.044944716694	2.125516961350
H	-3.724229306612	1.322852154614	-2.998567991399
H	-2.621325259527	-0.176167657652	-1.335077142524
C	-3.927175079324	2.763297422674	0.193655122175
H	-2.988888921713	3.317211515242	-0.000897274646
H	-4.670503221003	3.527131887290	0.481504107049
C	-4.382011063033	2.057335374913	-1.092338146215
H	-4.930052349796	1.130253659305	-0.836765289684
H	-5.109855512316	2.698217889177	-1.620286874313
C	-1.449793224838	1.507912532182	4.242475388579
C	-0.696749169217	0.647187481450	3.215845618597
C	0.957483111664	3.804216432384	3.071020955764
C	-0.461670075283	1.188101352590	1.807337979726
C	1.551295639897	2.435691474034	2.701963979963
H	-1.597764447633	0.884044345815	5.142306859647
H	-1.244623658336	-0.304226222778	3.124671889944
H	1.589169745571	4.214520875144	3.879744456282
H	1.538348132507	1.774683543496	3.579927450747
H	-2.459793789724	1.723311224595	3.856632158314
H	0.277752612973	0.359807903242	3.641692259888
H	1.069670051527	4.487899561011	2.208899203425
H	2.611612346694	2.595656761163	2.480463190679
C	-0.804917134656	2.827812351715	4.676760599090
H	0.121629109540	2.622143918446	5.245827472047
H	-1.495497169676	3.300046062351	5.397126699540
C	-0.500009652269	3.818826031773	3.540121603175
H	-1.177994976862	3.629246442606	2.687927283293
H	-0.722310163472	4.846766237724	3.875366838257
C	-0.272016456821	2.961437894760	-3.290739606584
C	0.474241825700	1.867616085499	-2.481331254833
C	2.263933748433	4.703577438313	-2.298933103607
C	0.078246814086	1.722310488314	-1.024879999264
C	1.550445702953	4.463530189065	-0.927833725963
H	-0.857347794462	3.605580437314	-2.612095342699
H	1.558234582333	2.058527108997	-2.528163882042
H	2.977072414864	5.533185684494	-2.168913848082
H	0.473968397966	4.306677371479	-1.075348588108
H	-1.013886555673	2.473165103544	-3.944004028219
H	0.346173163657	0.897723173250	-2.996009972687
H	2.875544071488	3.827807707151	-2.576683996545
H	1.647361357095	5.371954452516	-0.308708440099
C	0.634474752238	3.848959174769	-4.153214570215
H	0.030526708998	4.266349077733	-4.978452194600
H	1.411236942886	3.222149711993	-4.631473472900
C	1.304731086997	5.034716812539	-3.446763327856
H	1.877790697526	5.591687466419	-4.209303589454
H	0.527751597451	5.731443201338	-3.079862841637
B	1.157576062448	2.086642922595	0.041622683051
C	2.001774953393	0.643687862964	0.610412085552
C	0.826522171337	1.813758065675	1.527538363860
C	2.130058077188	3.289227229460	-0.217487103923

Thermochemistry (use all positive eigenvalues) at 298.15 K, 1.00 Atm
E(el) = -1421.505274303684

ZPVE = 0.726866484071
Enthalpie(0K) = -1420.778407819613
E(tr) = 0.001416276854
E(rot) = 0.001416276854
E(vib) = 0.754264067001
H-E(el) = 0.758040805278
Enthalpie = -1420.747233498406
S(el) = 0.000000000000
S(tr) = 0.000070817727
S(rot) = 0.000058703664 (Symmetry number = 1)
S(vib) = 0.000167655531
G-E(el) = 0.669437506065
Free Energy = -1420.835836797619

Table S24. Cartesian coordinates and energies of TS_9b.

C	3.879861015803	4.328350911339	0.613313661556
C	4.698028688909	4.816071152323	1.634371636391
C	3.830863253218	2.951687247335	0.408054104188
C	5.433376702817	3.943274430744	2.444662379623
C	4.548705482366	2.076652081086	1.227124622714
C	5.368234527807	2.564980119040	2.244330123118
B	1.465466473045	2.115427708280	-0.272148058759
C	4.293217063369	0.690715011621	0.813085558527
H	3.301707056980	5.010845486780	-0.015307034871
H	4.764994067218	5.894753471206	1.800489338770
H	6.061509919171	4.346182906371	3.243598451006
H	5.931204269503	1.878201675123	2.881895625742
C	2.872557536174	-0.654292179724	-0.643771484901
C	5.321984761296	-0.232242985672	0.634226840943
C	5.130949398233	-1.344546985470	-0.179061117549
C	3.919586126048	-1.523690289439	-0.866122665125
H	1.909392409504	-0.836196987577	-1.127140578886
H	6.306121066449	-0.024303649539	1.063105145613
H	5.952014396564	-2.050419654736	-0.331608124470
H	3.798867012827	-2.362614682427	-1.555367246651
C	-2.755996641311	-0.377733131781	1.702964127392
C	-1.952916336648	-0.450232057643	0.391892865223
C	-2.871293108866	3.029231847390	0.728464118191
C	-0.745024593192	0.474921113068	0.316235248256
C	-2.348810485961	2.302350755985	-0.523542125409
C	-0.931160055511	1.821186337594	-0.314549345386
H	-2.055239778286	-0.482252681187	2.552851863161
H	-2.630755893832	-0.281473221187	-0.457795653811
H	-2.274385639830	3.946459579007	0.883022498882
H	-2.400029512506	2.995650808905	-1.374157774221
H	-3.418376396226	-1.261462744775	1.738778167769
H	-1.610647741921	-1.487315229198	0.263554042112
H	-3.906035408857	3.356523973490	0.517883919795
H	-3.032056496395	1.479811649953	-0.770531369935
C	-3.619341004528	0.867151735779	1.937081923746
H	-4.162600078001	0.702768293359	2.884058077394
H	-4.398832235370	0.928950697403	1.153566465253
C	-2.865929950092	2.207073460723	2.020969117522
H	-3.321957605433	2.834033756095	2.806702965322
H	-1.824873501698	2.025664497173	2.350072975657
C	1.779849763342	-1.702191047229	2.294633249668
C	0.614899195292	-1.377015658037	1.350646492117
C	2.093504526552	1.114545735751	3.449762091944
C	0.451306260605	0.039610354928	0.812099923133
C	1.629934825371	1.803330019597	2.162122508531
H	2.710605705759	-1.207862843873	1.976162335659
H	-0.307355113348	-1.689320955973	1.864236445810
H	3.097386029964	0.671658245089	3.314443461784
H	2.207553012383	2.730737323639	2.061356588062
H	1.981928490328	-2.784045266601	2.213847199497
H	0.687441431368	-2.043756467985	0.469885019738
H	2.229201654064	1.927813714499	4.183380987790
H	0.586237800955	2.134550428570	2.301020250942

C	1.505746783401	-1.377206694790	3.760987499217
H	2.409000061836	-1.625498609477	4.348967149739
H	0.700018925764	-2.036213608469	4.134763081439
C	1.119281584984	0.075860676319	4.029251281996
H	0.103392089492	0.269988918793	3.635954929884
H	1.046031218716	0.213248903580	5.122101749348
C	-0.152427661417	3.630225447414	-3.054316481120
C	-0.047657409973	3.884099363675	-1.536791948276
C	3.038613942040	1.479775292685	-3.157375468663
C	0.115643725046	2.627391930739	-0.704739843737
C	3.644233415225	2.267565351879	-1.998140132179
H	-0.458557107241	4.577953527872	-3.532332599880
H	-0.929141274102	4.461144721794	-1.211173723326
H	3.621781061864	1.751388801577	-4.055666102094
H	3.632015405045	3.355427213436	-2.235328833824
H	-0.962571669302	2.903469582617	-3.252414229441
H	0.819123582445	4.547176959391	-1.363109041303
H	3.224820612424	0.404774905283	-2.990274281823
H	4.716103487873	2.024013382592	-1.888891023597
C	1.144927657883	3.155382581887	-3.718633026252
H	1.951591112507	3.846171685512	-3.413400824890
H	1.050441300440	3.287661938204	-4.810597538887
C	1.548884267609	1.694119041964	-3.428978554488
H	0.968813104157	1.296669685710	-2.580424760390
H	1.267029861365	1.058081545991	-4.285639489893
C	1.616242423651	1.002878095411	0.808411140841
C	2.999452760543	2.281433818726	-0.648209617635
C	2.983921187764	0.444357978474	0.263959227078

Thermochemistry (use all positive eigenvalues) at 298.15 K, 1.00 Atm
E(el) = -1421.480149512106
ZPVE = 0.724310795728
Enthalpie(0K) = -1420.755838716378
E(tr) = 0.001416276854
E(rot) = 0.001416276854
E(vib) = 0.751979557231
H-E(el) = 0.755756295508
Enthalpie = -1420.724393216598
S(el) = 0.000000000000
S(tr) = 0.000070817727
S(rot) = 0.000058410596 (Symmetry number = 1)
S(vib) = 0.000169808862
G-E(el) = 0.666598358926
Free Energy = -1420.813551153180

Table S25. Cartesian coordinates and energies of Int_10.

C	4.509002025124	3.918452850440	0.854033342860
C	5.865045122258	4.141353299752	0.895966652344
C	3.958414779125	2.679962708825	0.404286776962
C	6.728575118423	3.114785457715	0.485743072452
C	4.853115937158	1.631623550724	-0.020388233188
C	6.232955042837	1.898027739229	0.044829448916
C	4.370689671518	0.320953869445	-0.506065421896
H	3.843339176089	4.709752866418	1.199048329189
H	6.261943012621	5.093807268413	1.254318822594
H	7.810980380281	3.267869714209	0.519687876388
H	6.955879610610	1.136635297273	-0.245518553204
C	2.578556263940	-1.276031428757	-0.835860120256
C	5.268398365539	-0.636297595395	-1.031234317438
C	4.826609931062	-1.884087789251	-1.442647245905
C	3.470429971274	-2.213464506978	-1.338546682537
H	1.517410245982	-1.536426927823	-0.757999971544
H	6.331571936711	-0.415678480505	-1.132169911998
H	5.541564934086	-2.605772771513	-1.847441333459
H	3.116519018065	-3.198634286096	-1.656558897200
C	-2.584491548210	2.379939349892	2.013787262894
C	-2.163769778820	0.911255167232	1.783507167604
C	-2.608943862664	1.986747464649	-1.499663280314

C	-0.770157650585	0.830773480874	1.229105026453
C	-1.852724956221	0.709805642601	-1.099018819408
C	-0.634031538051	0.883029407221	-0.199453461647
H	-1.928234035568	2.837453789995	2.775095251172
H	-2.885371970303	0.448340066049	1.100491258443
H	-1.894047301041	2.700899907717	-1.945994787932
H	-1.514844357895	0.218633011134	-2.023773615499
H	-3.599762881620	2.350189864831	2.447248113338
H	-2.251808909700	0.368914887777	2.732417590110
H	-3.305977050116	1.710729933651	-2.310808786198
H	-2.559230421288	-0.005976095191	-0.652118046912
C	-2.599702025979	3.266898040826	0.767037763865
H	-1.564687432572	3.474207751316	0.438091460585
H	-3.014425262482	4.242438112467	1.073641646749
C	-3.413017633481	2.713209076919	-0.415408135256
H	-4.214012010206	2.049298258086	-0.037650777132
H	-3.931857449704	3.550129938863	-0.914012008628
C	-0.220814881094	-0.834872579164	4.145532576405
C	0.013218698220	0.601471893188	3.650268161606
C	3.008708994358	-1.152658145669	2.729152219422
C	0.321959780766	0.745894831774	2.165075912876
C	2.758590655293	0.370767158656	2.633472847930
H	-0.934044332726	-1.343512437669	3.470224653421
H	0.829742972832	1.047093594667	4.238025265634
H	3.478947765425	-1.493510363960	1.791955530614
H	3.698318118136	0.826455541001	2.285572100434
H	-0.719441418294	-0.770917273053	5.129099960178
H	-0.868166233781	1.206914210493	3.901854155202
H	3.758595129557	-1.299529992761	3.527224534503
H	2.578089954712	0.764607789007	3.645965750312
C	1.022505190768	-1.716163141627	4.304832457350
H	0.685055792122	-2.662058118006	4.763442732142
H	1.707735273264	-1.253845655866	5.041185381288
C	1.797035026917	-2.040561207837	3.015908545270
H	2.175016251041	-3.076182558434	3.075178025112
H	1.104956713149	-2.026073404232	2.153043867624
C	1.858967511978	2.325317072649	-2.673484999515
C	0.813226618846	1.293023455035	-2.227225088291
C	1.507798888079	4.723272920696	-0.394862617940
C	1.630405659201	3.633720670691	0.701367019029
H	2.243876288594	2.018292339503	-3.660375251104
H	1.140222284625	0.295592459356	-2.584503372151
H	1.062622143231	5.592645935643	0.116188450193
H	0.620829850782	3.245853794262	0.904529132474
H	2.736726092906	2.308767272816	-2.006254431656
H	-0.127985667455	1.508813417743	-2.754466571621
H	2.509312757467	5.041493303492	-0.734040777538
H	1.970848912220	4.124774008454	1.628275107025
C	1.308075074561	3.745764669134	-2.817485872763
H	0.571791778279	3.738012472160	-3.642524967137
H	2.129854314769	4.407638675723	-3.148547613846
C	0.626463194116	4.380303720517	-1.602636959261
H	0.170774567858	5.322767308677	-1.953255489247
H	-0.220885084356	3.751760830723	-1.271478968201
B	1.935453906491	1.043878073365	0.156205803429
C	1.628342286638	0.715876989406	1.709674832879
C	0.616541885973	1.107947644680	-0.746498399816
C	3.001774444516	-0.000552580263	-0.426550023456
C	2.546618848652	2.498262724045	0.386805112350

Thermochemistry (use all positive eigenvalues) at 298.15 K, 1.00 Atm
E(el) = -1421.533937750642
ZPVE = 0.731770027840
Enthalpie(0K) = -1420.802167722802
E(tr) = 0.001416276854
E(rot) = 0.001416276854
E(vib) = 0.759148176504
H-E(el) = 0.762924914780
Enthalpie = -1420.771012835862
S(el) = 0.000000000000

S(tr) = 0.000070817727
S(rot) = 0.000058561984 (Symmetry number = 1)
S(vib) = 0.000166940781
G-E(el) = 0.674576959749
Free Energy = -1420.859360790893

Table S26. Cartesian coordinates and energies of TS_10.

C	5.533421894152	3.154194851127	-0.158507431072
C	6.673373522308	2.967041260527	-0.899147848732
C	4.448366458545	2.217375724434	-0.182757081394
C	6.759935508245	1.831834707965	-1.723208709133
C	4.629486116148	0.975725865670	-0.891107662323
C	5.770316912511	0.863357729388	-1.708913401765
C	3.716266541973	-0.169853007973	-0.717180131267
H	5.465899776863	4.038999705579	0.473903145467
H	7.488822778293	3.692843989745	-0.862438536108
H	7.634275567694	1.689994453154	-2.364862556635
H	5.910595296197	-0.011093910368	-2.343155684986
C	1.777206112082	-1.206136429679	0.263021514675
C	4.109682837129	-1.442594538919	-1.191025863481
C	3.345214858008	-2.572305739141	-0.950841657153
C	2.170356906631	-2.453334968508	-0.207051566637
H	0.867749154599	-1.151442797203	0.859961953138
H	5.046656761900	-1.573296772735	-1.732588230151
H	3.676449899746	-3.545554409233	-1.323213909117
H	1.565558105775	-3.336418135854	0.018884220720
C	-3.386825825472	0.275489091555	1.092046238277
C	-2.032021152176	-0.445367222323	0.986934828613
C	-2.209032135278	1.258673180256	-2.147743481329
C	-0.845200617302	0.474054858330	0.908000184415
C	-0.905268672529	0.606272882359	-1.660009302636
C	-0.407510994643	0.954856037508	-0.270657096951
H	-3.482502181908	0.747831097558	2.086071411319
H	-2.042101076265	-1.082257074744	0.086052075508
H	-2.106881165939	2.358208005372	-2.118459347074
H	-0.109995432820	0.857360514775	-2.383538684817
H	-4.176248735246	-0.496371842521	1.038803836641
H	-1.928860751484	-1.131515266020	1.843047823934
H	-2.309380958020	0.992692142946	-3.215272268545
H	-1.012493617931	-0.492231471591	-1.707331706825
C	-3.652652204984	1.337767869303	0.021940352256
H	-2.993319329771	2.209108196272	0.190883880287
H	-4.680457042744	1.707169150756	0.182714643972
C	-3.506700104966	0.862016423207	-1.435967844045
H	-3.636204847814	-0.235834762050	-1.490084580791
H	-4.332859636703	1.286794520975	-2.032338454509
C	-0.221313398777	-0.733262162034	4.138584070194
C	-0.660823075227	0.588317651361	3.480951649891
C	3.020606057721	0.557475987361	3.503904892710
C	-0.062454730277	0.878961370670	2.118496783456
C	2.057138229100	1.700103764713	3.157594102628
H	-0.324786990188	-1.554811172286	3.405242877525
H	-0.444397395455	1.418572972617	4.173971659022
H	3.766404639003	0.442101997654	2.695273544545
H	2.652517970207	2.610719871188	3.013167508566
H	-0.948079126713	-0.947981330785	4.942641865842
H	-1.756771978228	0.567286806557	3.383201087082
H	3.584903081712	0.871706218346	4.401421363485
H	1.420710602966	1.906574343955	4.033457126589
C	1.183624985956	-0.798577949502	4.754839102160
H	1.219502903172	-1.733876200600	5.340704924190
H	1.302739717847	0.018303713663	5.492712043711
C	2.367924289362	-0.801262183625	3.772453017446
H	3.157884809565	-1.468067191994	4.160816121202
H	2.041481858451	-1.250956866941	2.819998125683
C	1.232770761124	3.812857904926	-1.770931644466
C	0.347097011945	3.297548518072	-0.621176983479
C	3.240455835526	5.176401213920	0.041755845060

C	3.017402750987	3.928056660790	0.956839978859
H	0.794904349471	3.485221602897	-2.728501986203
H	-0.716828100941	3.380510592801	-0.887346481961
H	3.827513923415	5.896566531549	0.633264714724
H	2.042386219863	4.014994779164	1.454514093677
H	2.229992205712	3.341860293157	-1.724613633619
H	0.480358238213	3.930881254955	0.270974966558
H	3.864983893048	4.912655364654	-0.827791789695
H	3.756506760204	3.990413019137	1.779296278934
C	1.388828421940	5.330830671674	-1.757008859513
H	0.411927427838	5.810555567328	-1.947801535917
H	2.045964907792	5.610019069434	-2.600211083986
C	1.977550983639	5.890219570939	-0.457394817767
H	2.230054566956	6.950030952284	-0.633246986597
H	1.217139542456	5.902918365810	0.345565412836
B	2.026628721488	1.441594665180	0.455071222764
C	1.174625114706	1.403852213308	1.964549698577
C	0.685783767522	1.918672878251	-0.185846955202
C	2.512735431810	-0.036420076554	0.014142552976
C	3.198887489539	2.542031950698	0.401716766632

Thermochemistry (use all positive eigenvalues) at 298.15 K, 1.00 Atm
E(el) = -1421.476668736221
ZPVE = 0.725755831848
Enthalpie(0K) = -1420.750912904373
E(tr) = 0.001416276854
E(rot) = 0.001416276854
E(vib) = 0.753300130319
H-E(el) = 0.757076868595
Enthalpie = -1420.719591867626
S(el) = 0.000000000000
S(tr) = 0.000070817727
S(rot) = 0.000058773206 (Symmetry number = 1)
S(vib) = 0.000170551224
G-E(el) = 0.667589484537
Free Energy = -1420.809079251684

Table S27. Cartesian coordinates and energies of Int_11.

C	3.687338769158	4.251954446865	0.496421324317
C	4.531267457465	4.874191439821	1.419337735246
C	3.816548289717	2.879493882226	0.287396126330
C	5.493117685224	4.135328340005	2.118417865625
C	4.785950545924	2.137278148465	0.990319378229
C	5.630084900657	2.762411388946	1.908283861672
B	1.552766510607	2.049951489420	-0.041996613137
C	4.658699681814	0.729458020336	0.608922137337
H	2.936626421070	4.834710361474	-0.045490351896
H	4.439249719130	5.949348989522	1.597263541427
H	6.144621182832	4.640377036147	2.837319905191
H	6.380897174058	2.187716959875	2.457685102172
C	3.248573485418	-0.640227239333	-0.816214902168
C	5.352309635133	-0.399792686622	1.050798245552
C	4.999806059375	-1.646118624328	0.535999929797
C	3.954289527666	-1.765431733527	-0.388167324018
H	2.416170460193	-0.750317986263	-1.515956715809
H	6.156349473963	-0.307818205052	1.786485694371
H	5.535260053328	-2.540917953990	0.865950672725
H	3.677507043841	-2.753078368456	-0.767891944028
C	-2.837570966698	-0.461037058454	1.297355093154
C	-1.866961508356	-0.363216376778	0.096060761548
C	-2.889560663920	3.041522082810	0.762955194953
C	-0.715593391754	0.593381244589	0.259583753548
C	-2.274640533549	2.494899093790	-0.537610718967
C	-0.878021060216	1.967753100832	-0.311421895114
H	-2.258851899499	-0.678568911741	2.212222377045
H	-2.442485955116	-0.103549718474	-0.804047721023
H	-2.295730254403	3.912094573916	1.095294972427
H	-2.256621358520	3.316606722738	-1.263663166126

H	-3.471100204354	-1.345142786599	1.112810327522
H	-1.456391386960	-1.368233667632	-0.079503181559
H	-3.897163019909	3.422768619638	0.516132494173
H	-2.940552151263	1.733221956357	-0.969651355865
C	-3.742274015891	0.741463467786	1.570374287665
H	-4.397447920217	0.454747561038	2.410859284666
H	-4.415561514527	0.907190091291	0.708721043950
C	-3.009981905448	2.047926159281	1.921171017159
H	-3.542325000190	2.561751199980	2.739749078820
H	-2.007265136204	1.811158961628	2.327097680805
C	1.690289971271	-1.698197906641	2.314440861867
C	0.497233630797	-1.290846384630	1.449791624504
C	2.148652473384	0.847316726802	3.821798729908
C	0.399388399971	0.155075692776	0.990907528686
C	1.885831939690	1.652997752328	2.552183401802
H	2.588131735330	-1.120762104506	2.030731849484
H	-0.427262409047	-1.614556255242	1.954153932892
H	3.123626508365	0.338697278930	3.716049344718
H	2.740446362792	2.319363614088	2.370024927675
H	1.929759836831	-2.750205950895	2.086493283090
H	0.539357307132	-1.870162449184	0.509469343787
H	2.295198519421	1.605154985002	4.608772360759
H	1.058466715723	2.384451463324	2.759478809094
C	1.420563454001	-1.579249529521	3.811591974453
H	2.315595807528	-1.920169262807	4.363784148300
H	0.598610980646	-2.264626255406	4.088874830683
C	1.079654240896	-0.159523279108	4.256277087262
H	0.090312412622	0.142503739088	3.862586127125
H	0.983733494714	-0.144432847743	5.354971351089
C	-0.219306681646	3.815384210969	-2.891763102051
C	0.209082397585	3.966392319992	-1.415157284660
C	2.769067187938	1.645690549846	-3.287650767292
C	0.236714427533	2.691313433283	-0.602173564812
C	3.324356729119	2.443455080922	-2.108388219998
H	-0.485880348422	4.821923135395	-3.259749619618
H	-0.489949348407	4.667142766527	-0.924327425566
H	3.299264937430	2.005585948456	-4.188839185322
H	3.020779366716	3.499340403627	-2.201812669628
H	-1.141229094696	3.211741007369	-2.949933905136
H	1.195863546240	4.455372056241	-1.382296141607
H	3.045979588696	0.582870903782	-3.187838418401
H	4.425808814815	2.442835096019	-2.193444537780
C	0.817474340377	3.220341954157	-3.845012612830
H	1.697335578557	3.889047682109	-3.872675851857
H	0.388561920409	3.264597852711	-4.861268975775
C	1.266732222325	1.773840486079	-3.542301892399
H	0.703903043972	1.365351764038	-2.685270684612
H	1.010862206857	1.120297638201	-4.394106932331
C	1.333260133204	1.187122977970	1.263354189398
C	3.022825045954	1.980656042681	-0.658758407477
C	3.617782612590	0.615833306155	-0.332040593950

Thermochemistry (use all positive eigenvalues) at 298.15 K, 1.00 Atm
E(el) = -1421.519377685645
ZPVE = 0.727138622847
Enthalpie(0K) = -1420.792239062798
E(tr) = 0.001416276854
E(rot) = 0.001416276854
E(vib) = 0.755014397289
H-E(el) = 0.758791135566
Enthalpie = -1420.760586550079
S(el) = 0.000000000000
S(tr) = 0.000070817727
S(rot) = 0.000058569874 (Symmetry number = 1)
S(vib) = 0.000171864387
G-E(el) = 0.668972855049
Free Energy = -1420.850404830596

Table S28. Cartesian coordinates and energies of TS_11.

C	3.958973425916	4.086579429005	0.410238894791
C	4.760974482771	4.606706266633	1.428406101816
C	3.967483256999	2.710966161647	0.185516129455
C	5.558664924705	3.761998167148	2.210146893318
C	4.782748757684	1.865003240612	0.957980025809
C	5.579165006705	2.386178580384	1.979313441453
B	1.723637299410	1.968591847275	-0.201523530549
C	3.644002169424	0.492668466250	-0.546493193207
C	4.591312978973	0.488155009639	0.496514897676
H	3.332030265649	4.749805935751	-0.192228680363
H	4.764339175994	5.683789635319	1.618059452869
H	6.177169960081	4.186691614501	3.006033745373
H	6.210278230037	1.730540759475	2.585730188730
C	3.218062828717	-0.710858381044	-1.107879868922
C	5.150197936952	-0.707437244202	0.951242172800
C	4.744321218175	-1.903848158074	0.361629212636
C	3.780673675674	-1.906005460120	-0.653788732692
H	2.445634336034	-0.730472293782	-1.880501994296
H	5.883802784551	-0.707907605649	1.762256298208
H	5.171750022526	-2.850538029205	0.704218017396
H	3.458463067157	-2.854486451402	-1.092855805414
C	-2.691542790283	-0.680760535801	1.441580953450
C	-1.801411135881	-0.445666101822	0.207949320146
C	-3.016715115218	2.779147062095	0.796694319418
C	-0.707753104076	0.571107655580	0.418908466917
C	-2.197441407479	2.486928762655	-0.480896421327
C	-0.819953526024	1.932527595061	-0.227942383577
H	-2.172755138547	-1.356059012865	2.144239310482
H	-2.428968935799	-0.127650366852	-0.637626090958
H	-2.350574461092	3.209871389856	1.568131223291
H	-2.110037096924	3.430438362861	-1.032589174052
H	-3.595873967430	-1.221371218133	1.109127909414
H	-1.353658894142	-1.407183210459	-0.095792263967
H	-3.718565313940	3.585890857264	0.524202179864
H	-2.773115765428	1.809584317036	-1.135454740110
C	-3.104883871335	0.571877042736	2.214194156045
H	-2.213387499998	1.023016403180	2.689811764764
H	-3.749281285783	0.237462115165	3.045887624486
C	-3.852025876814	1.650829675436	1.415796679579
H	-4.468001486981	1.176836140597	0.627591251252
H	-4.566785432579	2.140656843645	2.099727271230
C	1.899823521019	-1.159118360259	2.678500107548
C	0.833740658269	-1.079316118031	1.587955372036
C	1.773761147835	1.686712187621	3.773742927678
C	0.410140338356	0.297875073465	1.120500512017
C	1.478304103440	2.306903863403	2.394632081082
C	1.324698828542	1.460681495359	1.192733190861
H	2.760846167276	-0.518250546779	2.411951472868
H	-0.059237375583	-1.636878802228	1.909877477540
H	2.819026842648	1.334248374200	3.782667117729
H	2.184902118422	3.125969691471	2.196318065939
H	2.294570216962	-2.188986258674	2.681253360252
H	1.217877396131	-1.595438193587	0.688910739089
H	1.736667248479	2.541007725765	4.467671489141
H	0.464785762825	2.764651387852	2.456704530296
C	1.395215006049	-0.829566393506	4.080929889436
H	2.232175105068	-0.956931643415	4.791521453174
H	0.624142577964	-1.567148015370	4.369263358986
C	0.822737867845	0.579718142621	4.244766515475
H	-0.143305280964	0.665018192745	3.713301032395
H	0.589736435053	0.735213042382	5.311427940805
C	-0.144651992842	3.864219148677	-2.792238419097
C	0.320995329616	3.929197469045	-1.321397035404
C	2.847809180422	1.730823338567	-3.464538789261
C	0.317694197240	2.595515212245	-0.589697838529
C	3.466879302783	2.436164881182	-2.258143599208
C	3.164435880632	1.911082406097	-0.838025887070
H	-0.428598496095	4.889317379847	-3.090521495739

H	-0.330151850513	4.632278563956	-0.773901344931
H	3.331734166326	2.155969117086	-4.363357582482
H	3.200738634089	3.506545184552	-2.285264219325
H	-1.063982981676	3.257227541052	-2.861757843870
H	1.330541822481	4.372269865660	-1.291181413814
H	3.123491086163	0.662924686707	-3.458522662397
H	4.565517713120	2.397031699792	-2.367400340995
C	0.873883436899	3.342356341460	-3.806066994130
H	1.750521897767	4.015657682442	-3.798930424895
H	0.427992310239	3.460549830394	-4.809020595046
C	1.333479262483	1.878470634683	-3.623217489403
H	0.820938740890	1.415080156520	-2.762136730205
H	1.024092693076	1.281716286056	-4.498508247454

Thermochemistry (use all positive eigenvalues) at 298.15 K, 1.00 Atm
E(el) = -1421.504257984435
ZPVE = 0.724418125281
Enthalpie(0K) = -1420.779839859154
E(tr) = 0.001416276854
E(rot) = 0.001416276854
E(vib) = 0.752566588247
H-E(el) = 0.756343326524
Enthalpie = -1420.747914657911
S(el) = 0.000000000000
S(tr) = 0.000070817727
S(rot) = 0.000058533132 (Symmetry number = 1)
S(vib) = 0.000176995003
G-E(el) = 0.665006307528
Free Energy = -1420.839251676907