Electronic Supplementary Material (ESI) for ChemComm.

Stoichiometric and catalytic isomerization of alkenylboranes using bulky Lewis bases

Fu An Tsao[a,b], Anson Sathaseevan[a], Hui Zhu[c], Stefan Grimme[c], Gerhard Erker[b] and Douglas W. Stephan[a*]

[a]University of Toronto, Department of Chemistry, 80 St. George St., Toronto, Ontario, Canada
[b]Organisch Chemisches Institut, Westfälische Wilhelms-Universität, 48149 Münster, Corrensstr. 40, Germany
[c]Mulliken Center for Theoretical Chemistry, Institut fuer Physikalische und Theoretische Chemie,Universitaet Bonn, Beringstrasse 4, D-53115 Bonn, Germany
grimme grimme@thch.uni-bonn.de

Supporting Information

General experimental procedure

All experimental manipulations were conducted in an O_2-free, N_2-filled MBraun LABmaster SP dry box equipped with a -35 ^oC freezer. All proteo solvents (purchased from Caledon Laboratories) were purified using a Grubbs-type column system (Innovative Technologies) and stored over 4 Å sieves in Straus flasks. $CDCl_3$ (purchased from Cambridge Isotopes) was dried over CaH_2 and distilled under reduced pressure. All solvents were degassed by repeated freeze-pump-thaw cycles prior to use.

All chemicals were used as received unless otherwise noted. $B(C_6F_5)_3$ was purchased from Boulder Scientific. Triethylamine, diphenylphosphine oxide, pyridine, 1-pentyne, 1-hexyne and N-propargylphthalimide were purchased from Sigma Aldrich. 2,5-diisopropylaniline, 4-phenyl-1-butyne, 1-methyl-1-pentyne and 3-methyl-1-butyne were purchased from Alfa Aesar, Tricyclohexylphosphine was purchased from Strem Chemicals. 3-methoxy-1-propyne and 3,3-dimethyl-1-butyne were purchased from TCI Chemicals. All liquid reagents were degassed by repeated freeze-pump-thaw cycles and stored over 4 Å sieves before use; all solid reagents were placed under dynamic vacuum for 1 hour prior to use.

NMR spectroscopy was performed on either a Bruker Advance III 400 MHz, an Agilent DD2 500 MHz, or an Agilent DD2 600 MHz. Unless otherwise stated, all spectra were obtained at room temperature. All NMR spectra were referenced to residual proteo solvent peaks of CD_2Cl_2 (^1H = 5.32 ppm; ^{13}C = 53.84 ppm) or an external standard (^{19}F: $CFCl_3$ (δ 0.00), ^{11}B: $(Et_2O)BF_3$ (δ 0.00)).

Single-crystal X-ray crystallographic analyses were performed on crystals coated in Paratone-N oil and mounted on a Bruker Kappa Apex II diffractometer. Combustion elemental analyses were performed on a on a PerkinElmer CHN Analyzer.

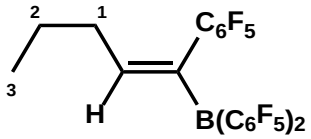
General procedure for NMR-scale reactions of substrates in Table 1

$B(C_6F_5)_3$ (15.0 mg, 0.03 mmol) was dissolved in 1 ml of toluene-d^8 and mixed with 1 eq of alkyne at room temperature in a 1-dram screwcap vial in an N_2-filled glovebox. This solution was mixed several times using a glass pipette and then transferred to a 5-mm NMR tube. NMR spectra were recorded to ensure the completion of 1,1-carboboration reaction. Once this has been confirmed, 1 or 0.1 eq of H*t*Bu_2P was added to the sample and NMR spectra were recorded at multiple time intervals afterwards. Reaction progress and E/Z ratios were monitored and determined by *in situ* $^{19}F\{^1H\}$ NMR spectra.

General procedure for the isolation of 1a-1e

$B(C_6F_5)_3$ was dissolved in 3 ml of dichloromethane (DCM) and added to 1 eq of alkyne at room temperature. This mixture was stirred for 1 h (**1a, 1b, 1e, 1f**) or 24 h (**1c, 1d**) to ensure the completion of the 1,1-carboboration reaction. 1 eq of H*t*Bu_2P was then added as a solution in 1 ml of dichloromethane and the mixture was allowed to stir for another 3 h before all volatiles were removed under reduced pressure. The isomerized products were then isolated by either repeated trituration in pentane or by recrystallization from a saturated solution in pentane at -35 ^oC.

Synthesis of 1a



161.6 mg (0.32 mmol) of $B(C_6F_5)_3$ was reacted with 24.0 mg (0.35 mmol) of 1-pentyne. After isomerization, it was purified by recrystallization from a 4:1 solvent mixture of pentane:DCM to give 97.8 mg (0.17 mmol, 54%) of ***Z*-1a**.

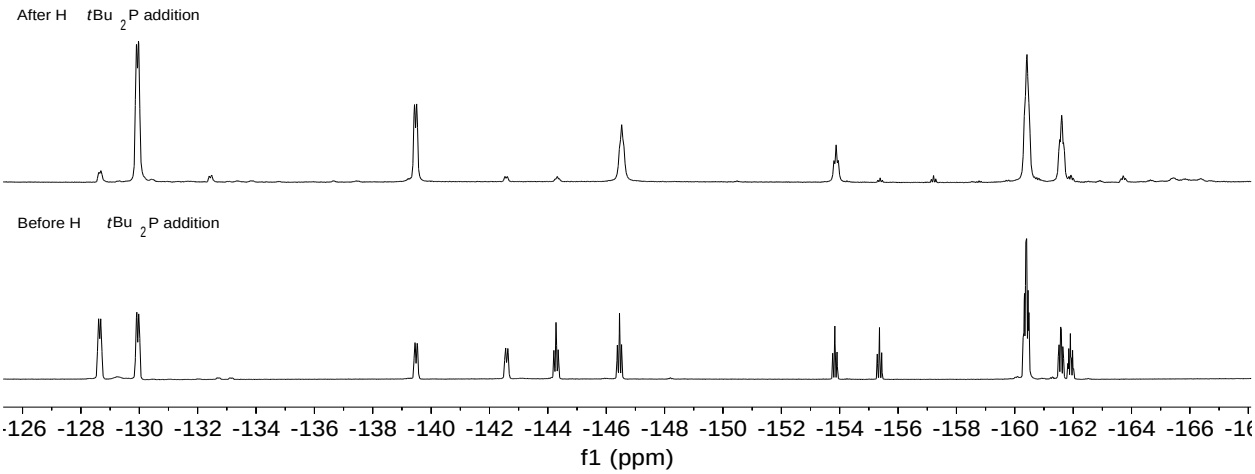
^{1}H (400.0 MHz, $CDCl_3$): δ 7.21 (t, 1H, $^3J_{H-H}$ = 7.3 Hz, *H*C=CB), 2.28 (m, 2H, H^1), 1.55 (m, 2H, H^2), 0.91 (t, 3H, $^3J_{H-H}$ = 7.3 Hz, H^3)

^{11}B{^{1}H} (128 MHz, $CDCl_3$): δ 62.9 (br s, $v_{1/2}$ ≈ 940 Hz)

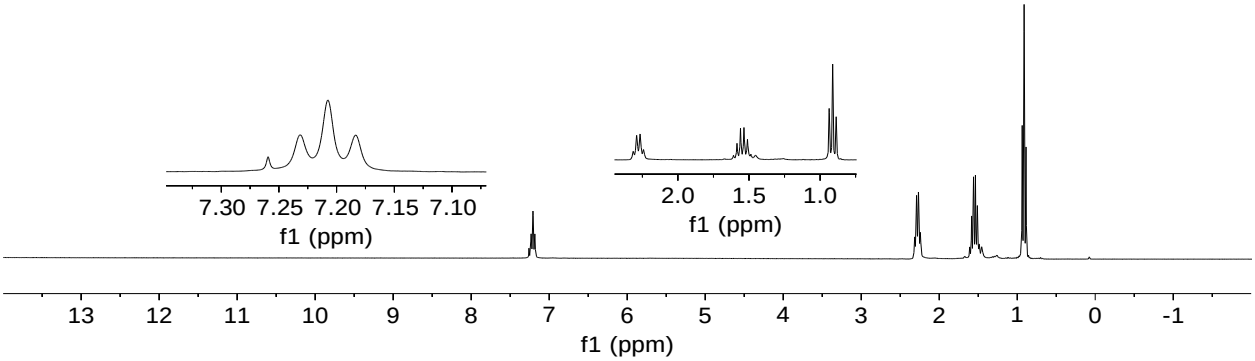
^{13}C{^{1}H} (100 MHz, $CDCl_3$): δ (C_6F_5 signals not listed) n.o. (HC=*C*B), 172.0 (s, H*C*=CB), 35.4 (s, C^1), 21.4 (s, C^2), 13.9 (s, C^3)

^{19}F{^{1}H} NMR (377 MHz, $CDCl_3$): δ -129.5 (d, 4F, $^3J_{F-F}$ = 17.7 Hz, *o*-$B(C_6F_5)_2$), -139.2 (d, 2F, $^3J_{F-F}$ = 19.6 Hz, *o*-C_6F_5), -147.4 (t, 2F, $^3J_{F-F}$ = 20.0 Hz, *p*-$B(C_6F_5)_2$), -154.3 (t, 1F, $^3J_{F-F}$ = 22.2 Hz, *p*-C_6F_5), -160.3 (m, 4F, *m*-$B(C_6F_5)_2$), -161.5 (m, 2F, *m*-C_6F_5)

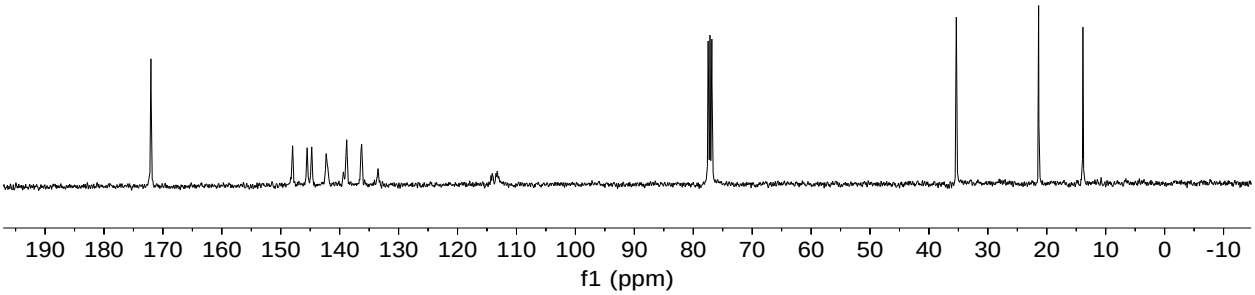
Anal. Calc. for $C_{23}H_8BF_{15}$: C 47.62% H 1.39%. Found: C 47.54% H 1.65%



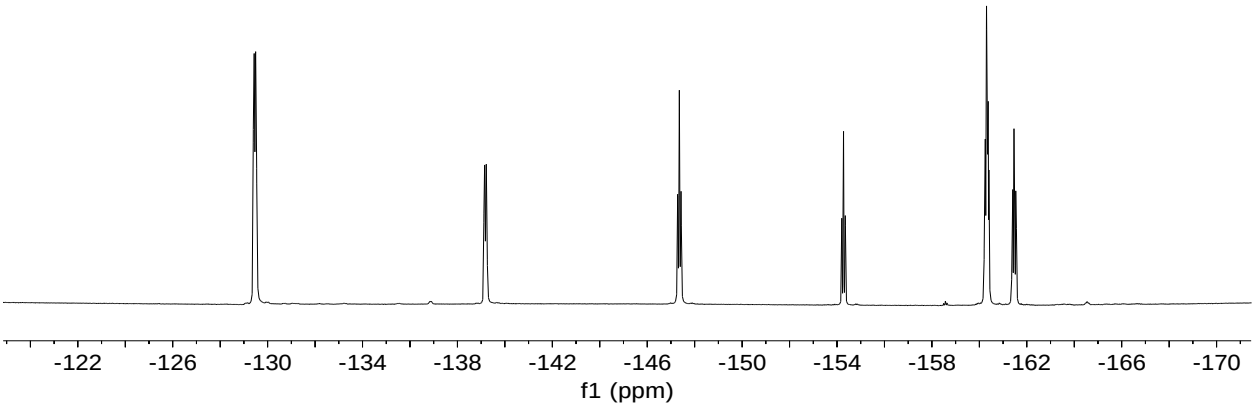
***in situ* ^{19}F{^{1}H} (377 MHz, $CDCl_3$) NMR spectrum of the isomerization of E/Z-1a**



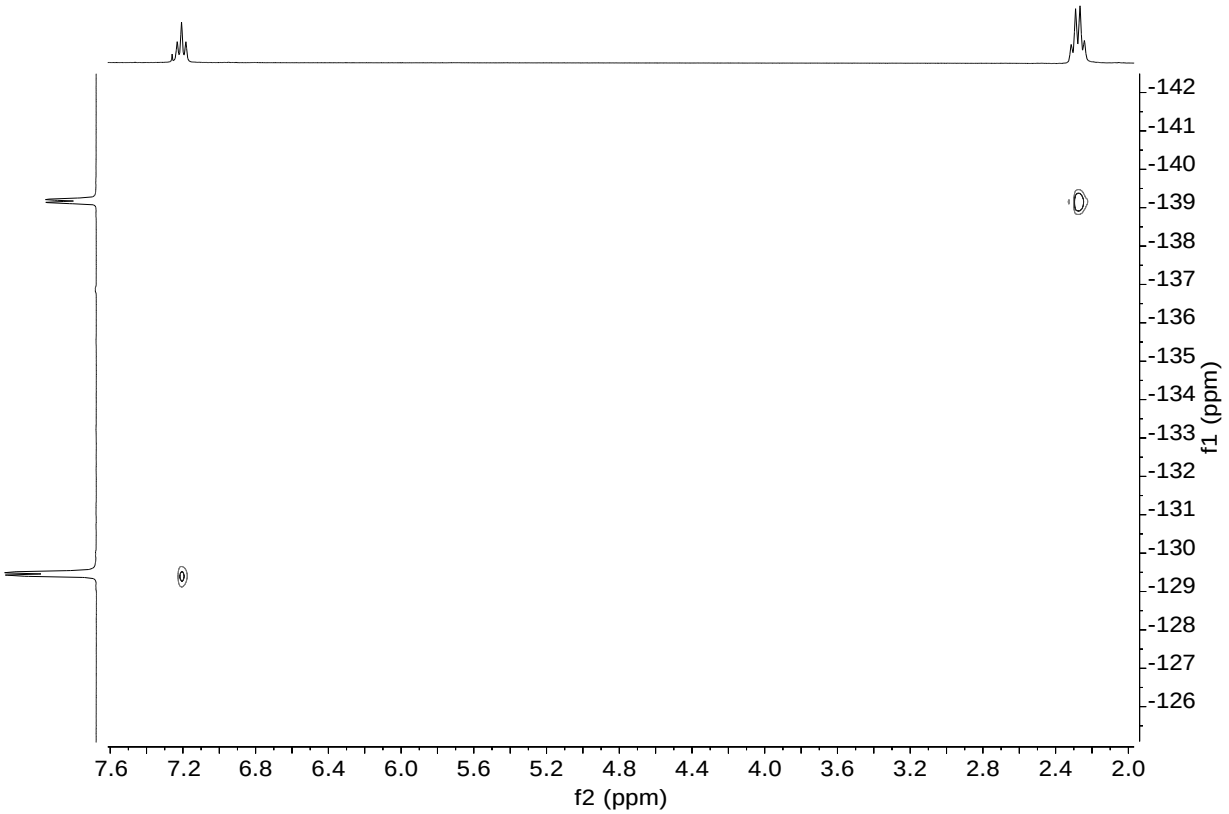
^{1}H (400.0 MHz, $CDCl_3$) NMR spectrum of *Z*-1a



^{13}C{^{1}H} (100 MHz, $CDCl_3$) NMR spectrum of *Z*-1a

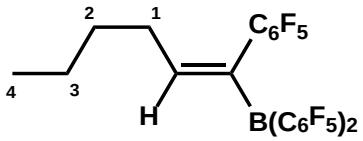


^{19}F{^{1}H} (377 MHz, $CDCl_3$) NMR spectrum of *Z*-1a



^{1}H{^{19}F}HOESY spectrum of *Z*-1a

Synthesis of 1b



157.7 mg (0.31 mmol) of $B(C_6F_5)_3$ was reacted with 26.3 mg (0.32 mmol) of 1-hexyne. After isomerization, it was purified by recrystallization from pentane to give 141.9 mg (0.24 mmol, 77%) of ***Z*-1b**

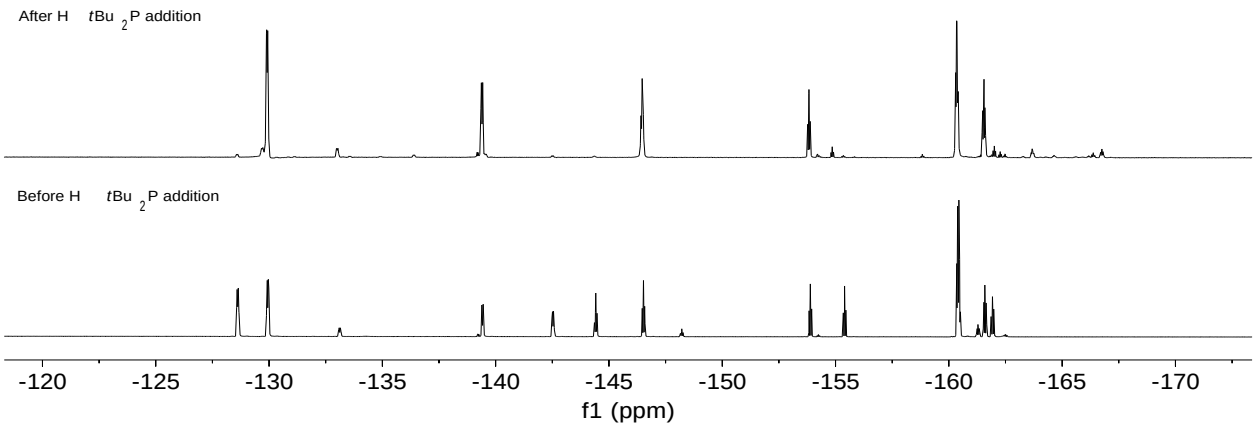
^{1}H (400.0 MHz, $CDCl_3$): δ 7.20 (t, 1H, $^{3}J_{H\text{-}H}$ = 7.3 Hz, *H*C=CB), 2.29 (m, 2H, H^1), 1.49 (m, 2H, H^2), 1.30 (m, 2H, H^3), 0.87 (t, 3H, $^{3}J_{H\text{-}H}$ = 7.3 Hz, H^4)

^{11}B{^{1}H} (128 MHz, $CDCl_3$): δ 61.3(br s, $v_{1/2}$ ≈ 960 Hz)

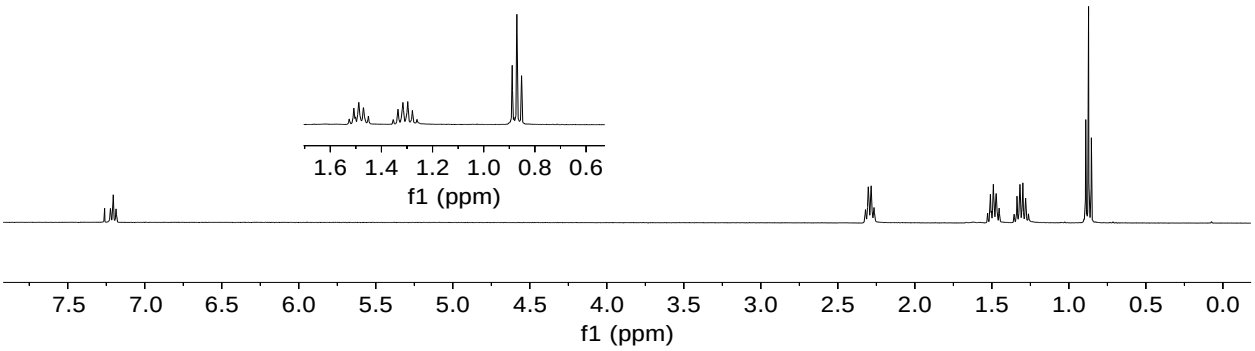
^{13}C{^{1}H} (100 MHz, $CDCl_3$): δ (C_6F_5 signals not listed) n.o. (HC=*C*B), 172.3 (s, H*C*=CB), 33.2 (s, C^1), 30.0 (s, C^2), 22.6 (s, C^3), 13.8 (s, C^4)

^{19}F{^{1}H} NMR (377 MHz, $CDCl_3$): δ -129.5 (d, 4F, $^{3}J_{F\text{-}F}$ = 17.1 Hz*, o*-$B(C_6F_5)_2$), -139.1 (d, 2F, $^{3}J_{F\text{-}F}$ = 19.6 Hz*, o*-C_6F_5), -147.3 (t, 2F, $^{3}J_{F\text{-}F}$ = 21.0 Hz*, p*-$B(C_6F_5)_2$), -154.2 (t, 1F, $^{3}J_{F\text{-}F}$ = 22.1 Hz*, p*-C_6F_5), -160.2 (m, 4F, *m*-$B(C_6F_5)_2$), -161.3 (m, 2F, *m*-C_6F_5)

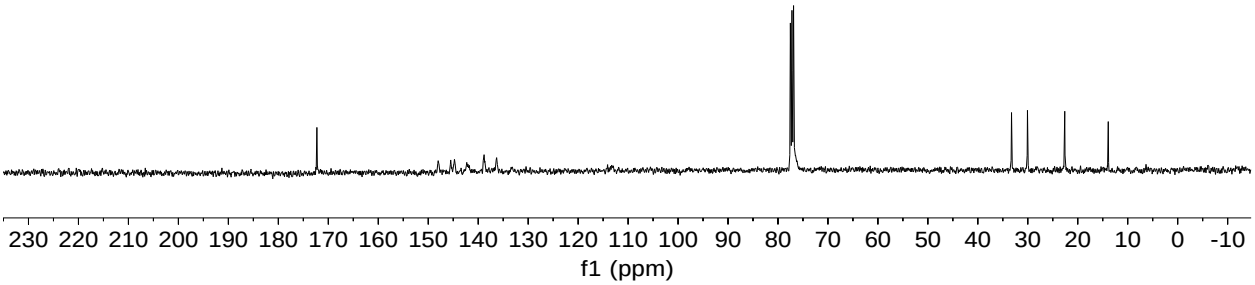
Anal. Calc. for $C_{24}H_{10}BF_{15}$: C 48.52% H 1.70%. Found: C 48.69% H 1.63%



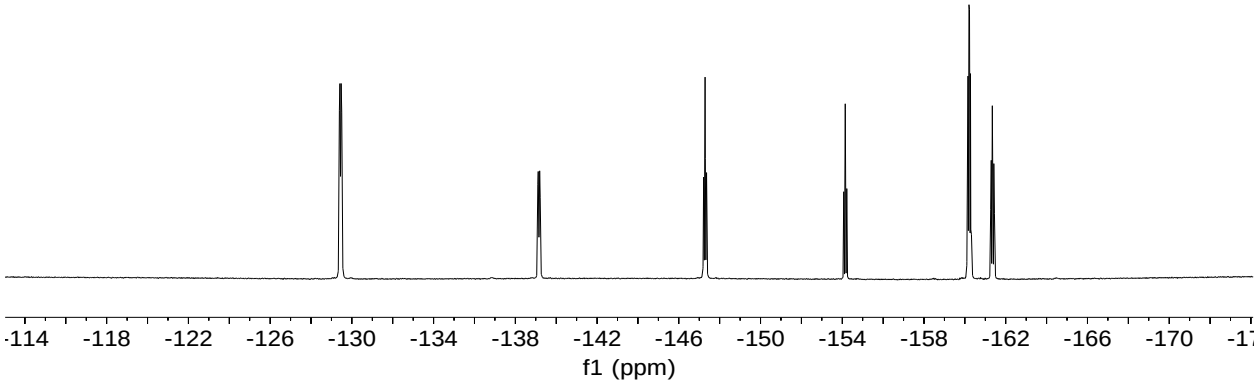
***in situ* $^{19}F\{^{1}H\}$ (377 MHz, $CDCl_3$) NMR spectrum of the isomerization of E/*Z*-1b**



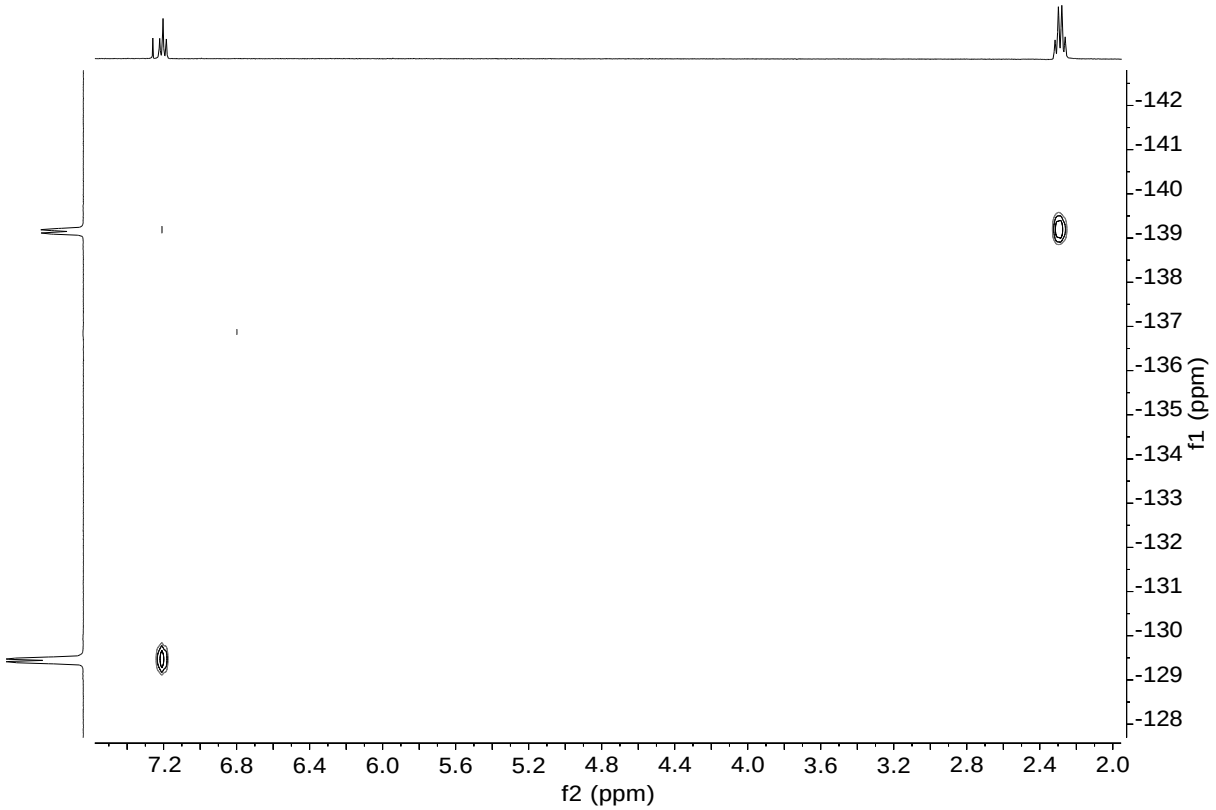
^{1}H (400.0 MHz, $CDCl_3$) NMR spectrum of *Z*-1b



$^{13}C\{^{1}H\}$ (100 MHz, $CDCl_3$) NMR spectrum of *Z*-1b

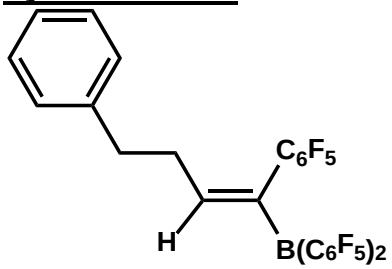


$^{19}F\{^{1}H\}$ (377 MHz, $CDCl_3$) NMR spectrum of *Z*-1b



$^{1}H\{^{19}F\}$HOESY spectrum of *Z*-1b

Synthesis of 1c



153.4 mg (0.30 mmol) of $B(C_6F_5)_3$ was reacted with 42.4 mg (0.33 mmol) of 4-phenyl-1-butyne. After isomerization, it was purified by repeated washing with pentane to give 188.2 mg (0.30 mmol, 96%) of ***Z*-1c**

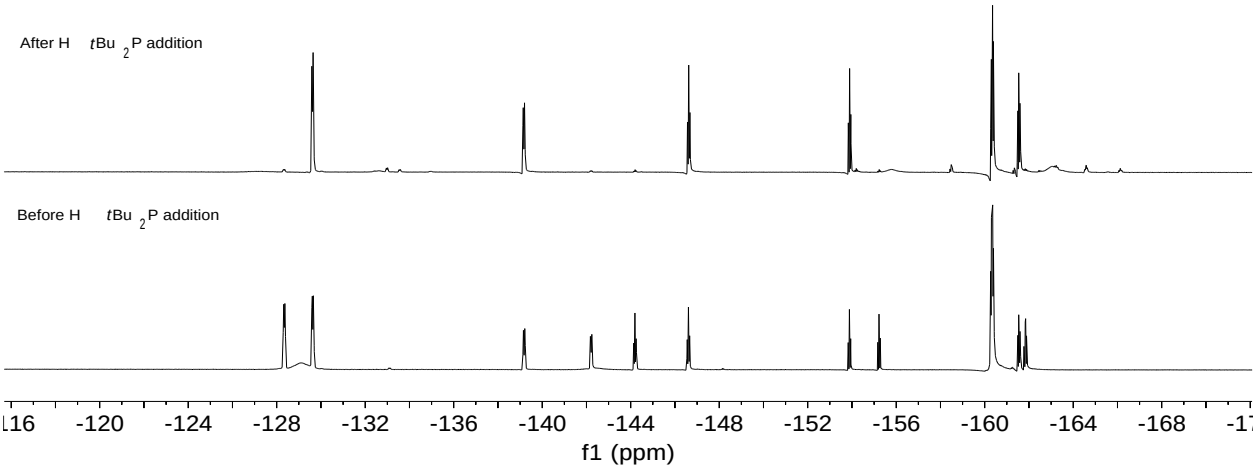
^{1}H (400.0 MHz, $CDCl_3$): δ 7.26 (m, 2H, Ph), 7.20 (m, 1H, Ph), 7.13 (t, $^3J_{H-H}$ = 7.2 Hz, *H*C=CB), 7.09 (m, 2H, Ph), 2.8 (t, 2H, $^3J_{H-H}$ = 7.5 Hz, PhC*H*$_2$CH$_2$), 2.62 (m, 2H, PhCH$_2$C*H*$_2$)

^{11}B{^{1}H} (128 MHz, $CDCl_3$): δ 61.8 (br s, $v_{1/2}$ ≈ 1030 Hz)

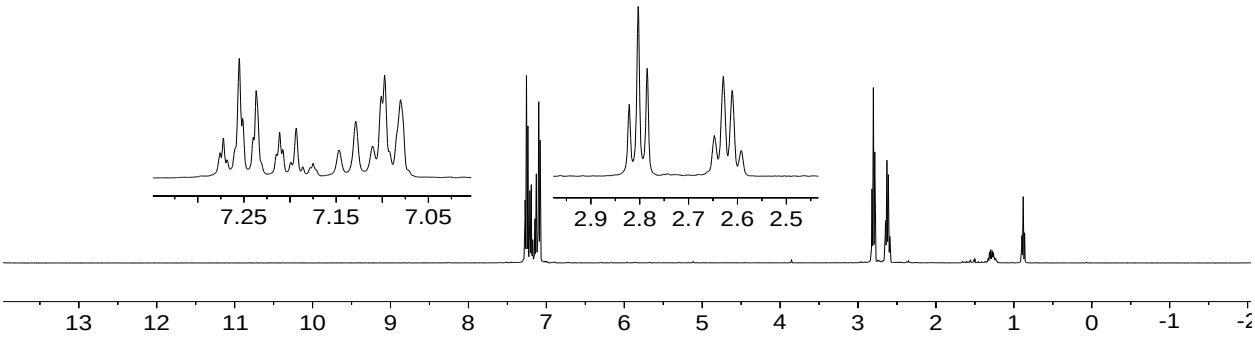
^{13}C{^{1}H} (100 MHz, $CDCl_3$): δ (C_6F_5 signals not listed) n.o. (HC=*C*B), 169.8 (s, H*C*=CB), 139.7 (s, *i*-Ph), 128.7 (s, Ph), 128.4 (s, Ph), 126.7 (s, *p*-Ph), 34.8 (s, Ph*C*H$_2$CH$_2$), 33.9 (s, PhCH$_2$*C*H$_2$)

^{19}F{^{1}H} NMR (377 MHz, $CDCl_3$): δ -129.1 (d, 4F, $^3J_{F-F}$ = 18 Hz, *o*-B(C_6F_5)$_2$), -138.9 (d, 2F, $^3J_{F-F}$ = 19 Hz, *o*-C_6F_5), -147.1 (t, 2F, $^3J_{F-F}$ = 20 Hz, *p*-B(C_6F_5)$_2$), -154.0 (t, 1F, $^3J_{F-F}$ = 20 Hz, *p*-C_6F_5), -160.1 (m, 4F, *m*-B(C_6F_5)$_2$), -161.2 (m, 2F, *m*-C_6F_5)

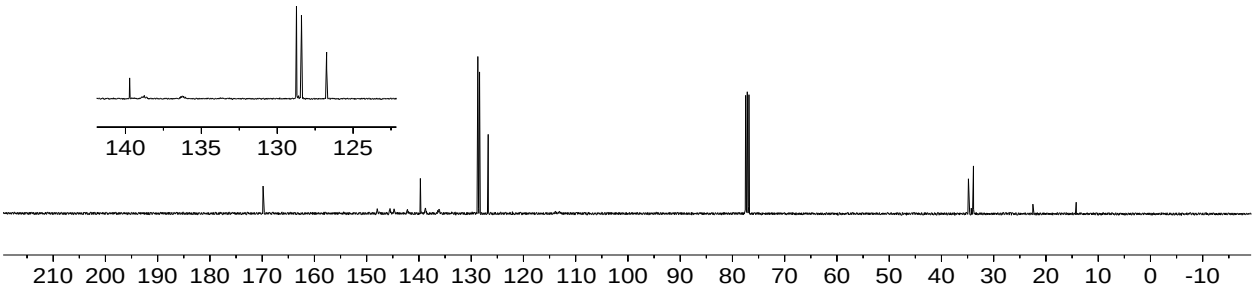
Anal. Calc. for $C_{28}H_{10}BF_{15}$: C 52.37% H 1.57%. Found: C 52.86% H 1.71%



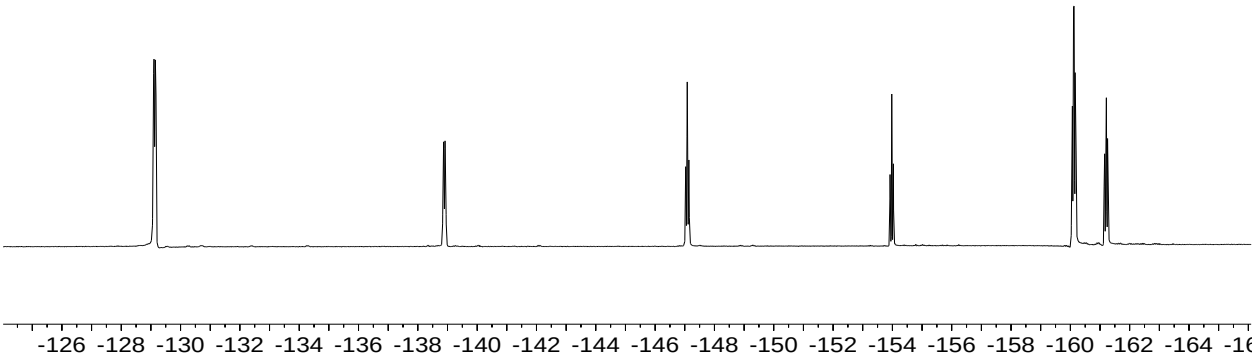
***in situ* ^{19}F{^{1}H} (377 MHz, $CDCl_3$) NMR spectrum of the isomerization of E/Z-1c**



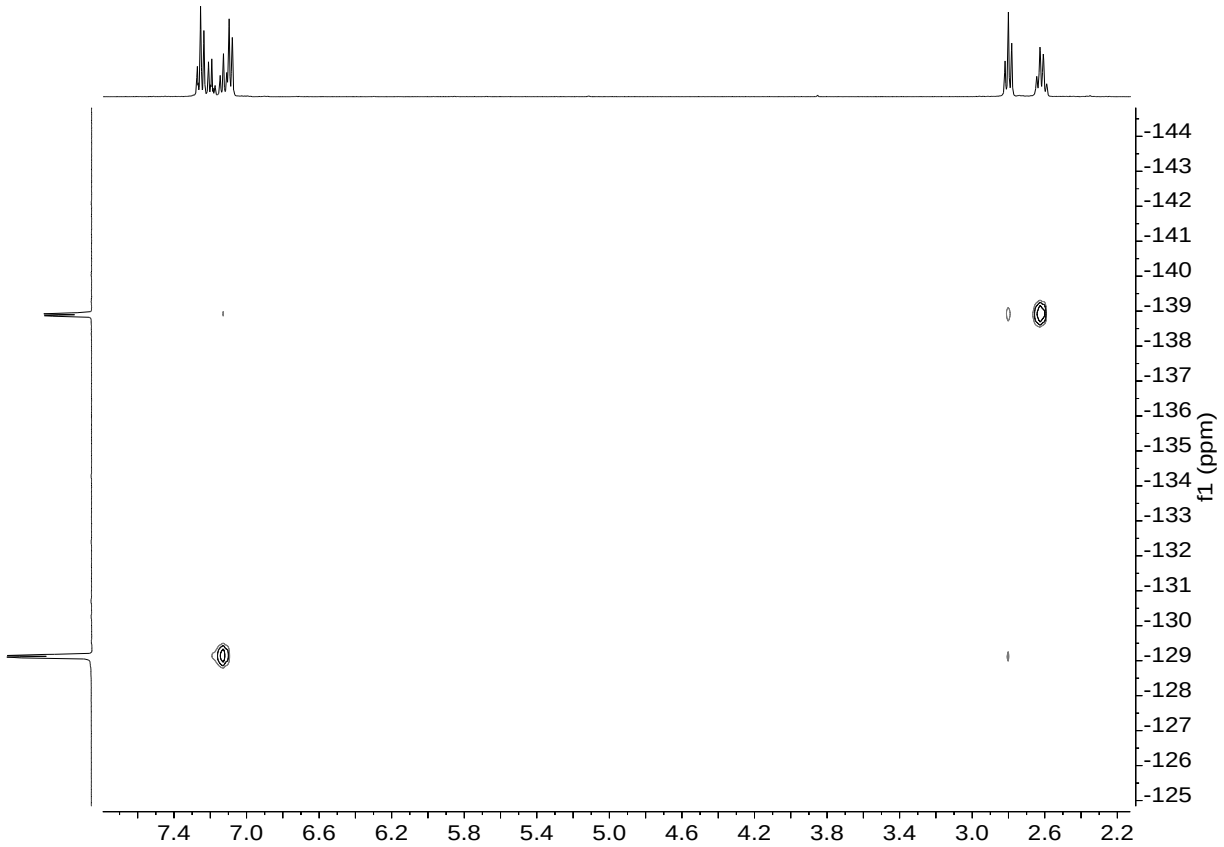
^{1}H (400.0 MHz, $CDCl_3$) NMR spectrum of *Z*-1c



^{13}C{^{1}H} (100 MHz, $CDCl_3$) NMR spectrum of *Z*-1c

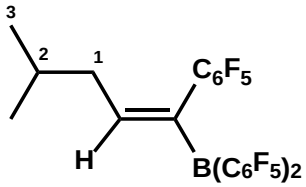


^{19}F{^{1}H} (377 MHz, $CDCl_3$) NMR spectrum of *Z*-1c



^{1}H{^{19}F}HOESY spectrum of *Z*-1c

Synthesis of 1d



94.4 mg (0.18 mmol) of $B(C_6F_5)_3$ was reacted with 16.1 mg (0.20 mmol) of 3-methyl-1-butyne. After isomerization, it was purified by recrystallization from a 4:1 solvent mixture of pentane:DCM to give 71.4 mg (0.12 mmol, 67%) of ***Z*-1d**

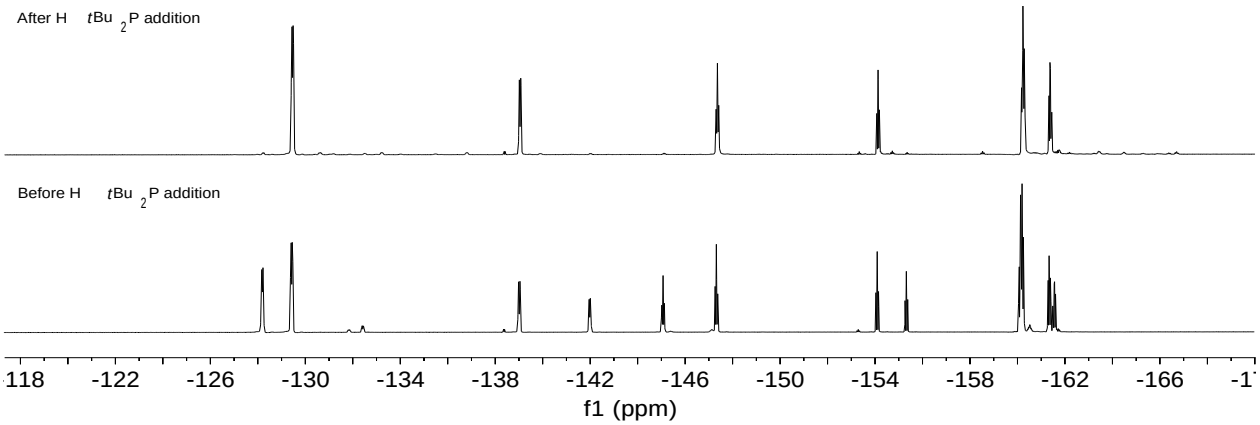
^{1}H (400.0 MHz, $CDCl_3$): δ 7.25 (t, $^{3}J_{H\text{-}H}$ = 6.9 Hz, *H*C=CB), 2.2 (app t, 2H, $^{3}J_{H\text{-}H}$ = 6.8 Hz, H^1), 1.86 (m, 1H, H^2), 0.90 (d, 6H, $^{3}J_{H\text{-}H}$ = 6.8 Hz, H^3)

^{11}B{^{1}H} (128 MHz, $CDCl_3$): δ 61.9 (br s, $v_{1/2}$ ≈ 960 Hz)

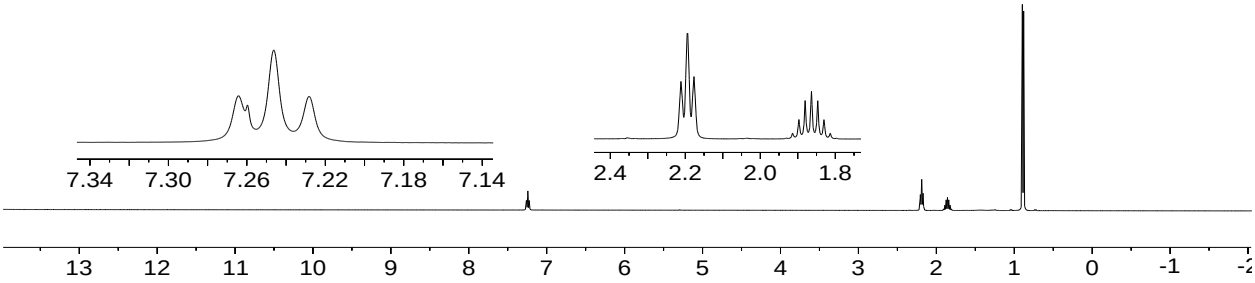
^{13}C{^{1}H} (100 MHz, $CDCl_3$): δ (C_6F_5 signals not listed) n.o. (HC=*C*B), 171.6 (s, H*C*=CB), 42.2 (s, C^1), 28.4 (s, C^2), 22.5 (s, C^3)

^{19}F{^{1}H} NMR (377 MHz, $CDCl_3$): δ -129.4 (d, 4F, $^{3}J_{F\text{-}F}$ = 18 Hz*, o*-$B(C_6F_5)_2$), -139.0 (d, 2F, $^{3}J_{F\text{-}F}$ = 21 Hz*, o*-C_6F_5), -147.3 (t, 2F, $^{3}J_{F\text{-}F}$ = 18 Hz*, p*-$B(C_6F_5)_2$), -154.1 (t, 1F, $^{3}J_{F\text{-}F}$ = 20 Hz*, p*-C_6F_5), -160.2 (m, 4F, *m*-$B(C_6F_5)_2$), -161.3 (m, 2F, *m*-C_6F_5)

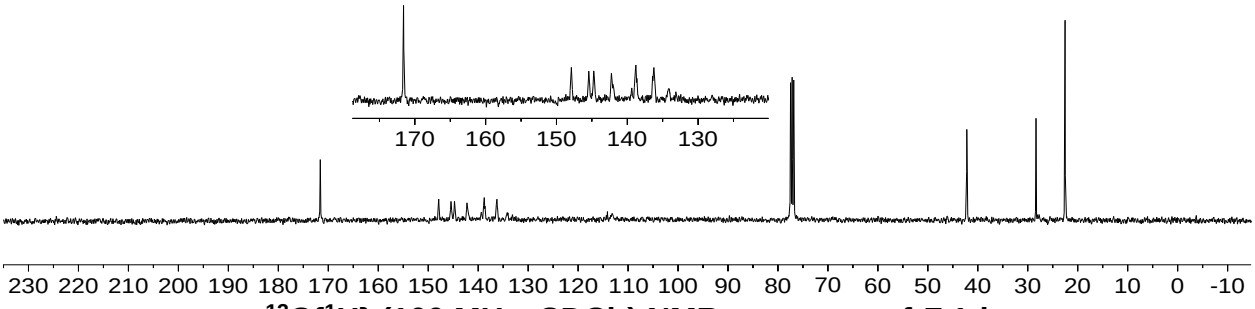
Anal. Calc. for $C_{24}H_{10}BF_{15}$: C 48.52% H 1.70%. Found: C 48.52% H 1.73%



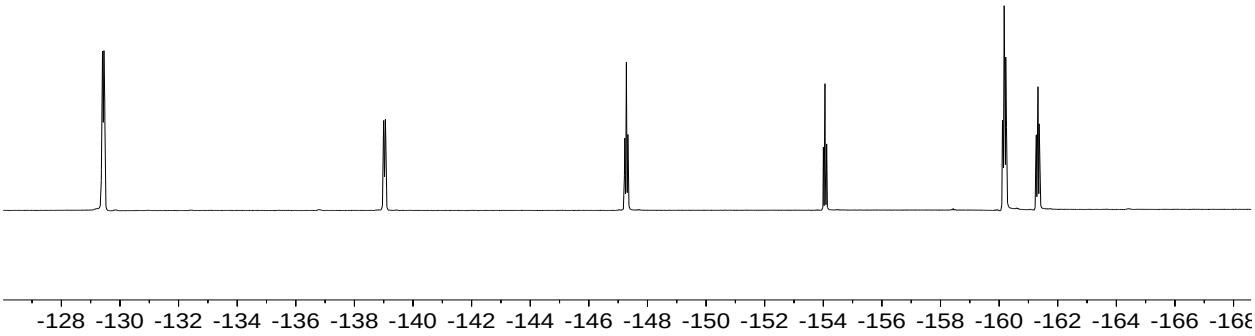
***in situ* $^{19}F\{^{1}H\}$ (377 MHz, $CDCl_3$) NMR spectrum of the isomerization of E/*Z*-1d**



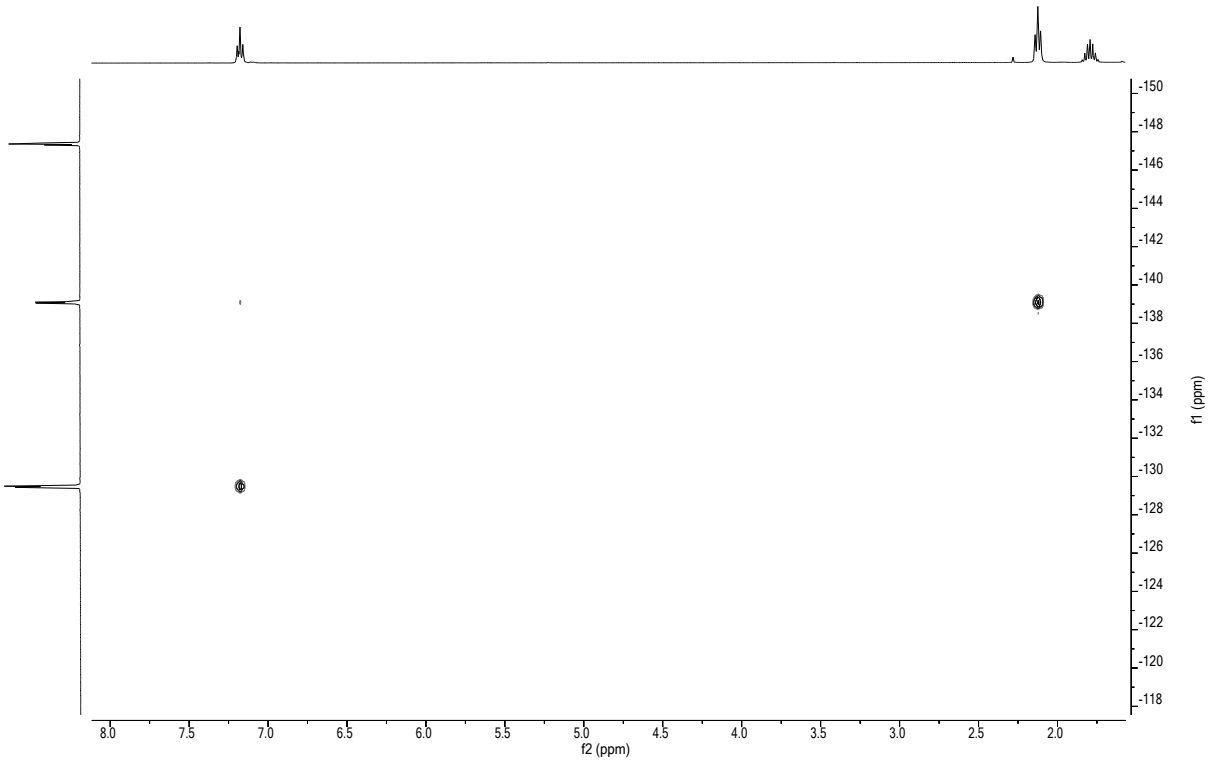
^{1}H (400.0 MHz, $CDCl_3$) NMR spectrum of *Z*-1d



$^{13}C\{^{1}H\}$ (100 MHz, $CDCl_3$) NMR spectrum of *Z*-1d

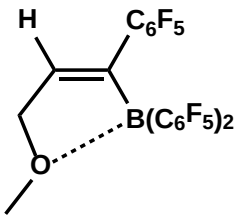


$^{19}F\{^{1}H\}$ (377 MHz, $CDCl_3$) NMR spectrum of *Z*-1d



$^{1}H\{^{19}F\}$HOESY spectrum of *Z*-1d

Synthesis of 1g



187.9 mg (0.37 mmol) of $B(C_6F_5)_3$ was reacted with 26.2 mg (0.37 mmol) of 3-methoxy-1-propyne. After isomerization, it was purified by recrystallization from pentane to give 116.8 mg (0.20 mmol, 54%) of ***E*-1g**

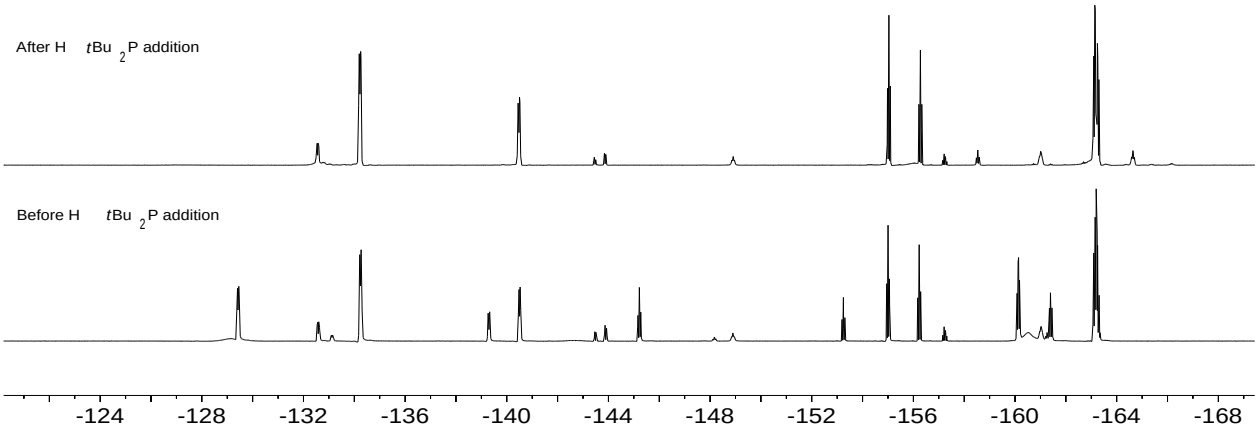
^{1}H (500.0 MHz, $CDCl_3$): δ 6.30 (s, 1H, *H*C=CB), 5.13 (s, 2H, C*H*$_2$OCH$_3$), 3.86 (m, 3H, CH$_2$OC*H*$_3$)

^{11}B{^{1}H} (128 MHz, $CDCl_3$): δ 7.3 (br s, $v_{1/2}$ ≈ 1 Hz)

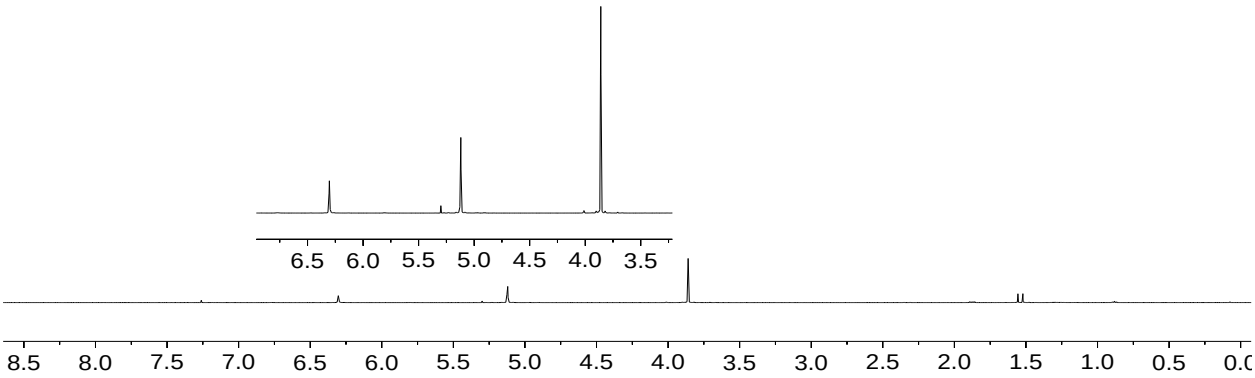
^{13}C{^{1}H} (100 MHz, $CDCl_3$): δ (C_6F_5 signals not listed) n.o. (HC=*C*B), 128.2 (s, H*C*=CB), 84.2 (s, *C*H$_2$OCH$_3$), 61.7 (s, CH$_2$O*C*H$_3$)

^{19}F{^{1}H} NMR (377 MHz, $CDCl_3$): δ -134.3 (d, 4F, $^{3}J_{F-F}$ = 22.0 Hz*, o*-B(C_6F_5)$_2$), -140.0 (m, 2F, *o*-C_6F_5), -155.1 (t, 2F, $^{3}J_{F-F}$ = 19.3 Hz*, p*-B(C_6F_5)$_2$), -156.4 (t, 1F, $^{3}J_{F-F}$ = 21.8 Hz*, p*-C_6F_5), -162.9 - -163.2 (m, 6F, *m*-B(C_6F_5)$_2$ + *m*-C_6F_5)

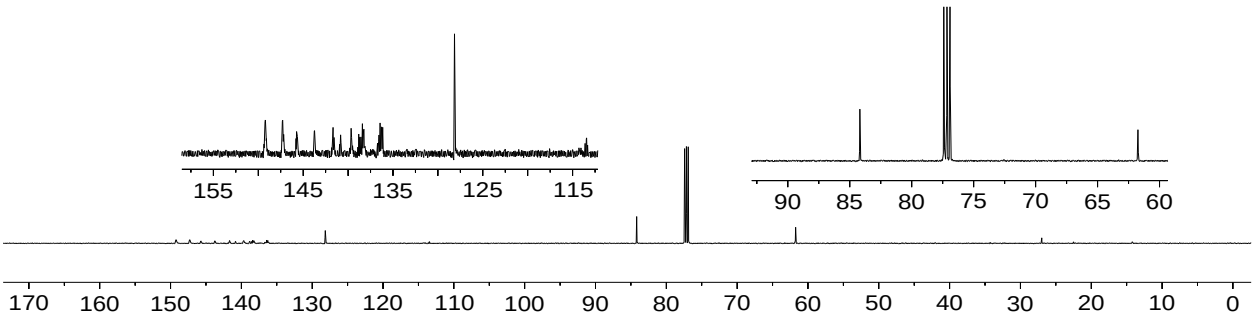
Anal. Calc. for $C_{22}H_6BF_{15}O$: C 45.40% H 1.04%. Found: C 45.40% H 1.16%



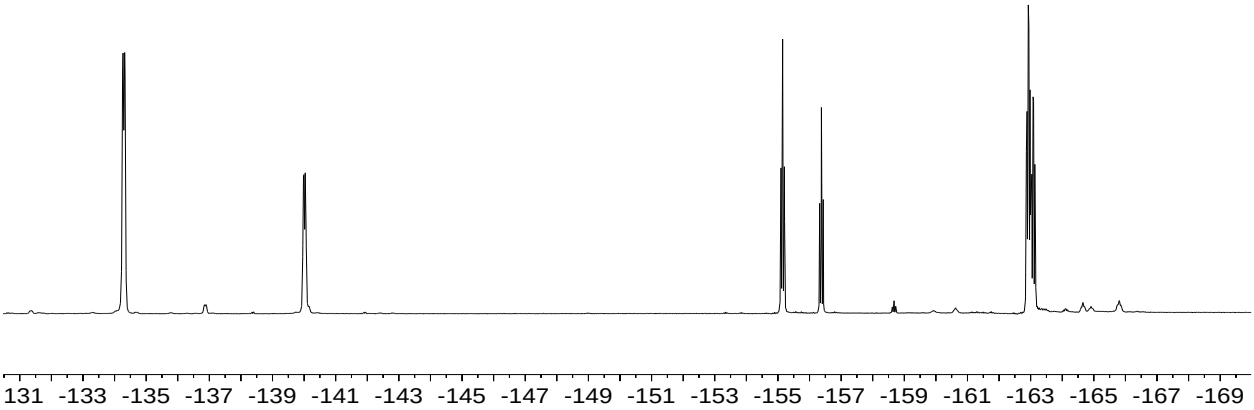
***in situ* ^{19}F{^{1}H} (377 MHz, $CDCl_3$) NMR spectrum of the isomerization of E/Z-1g**



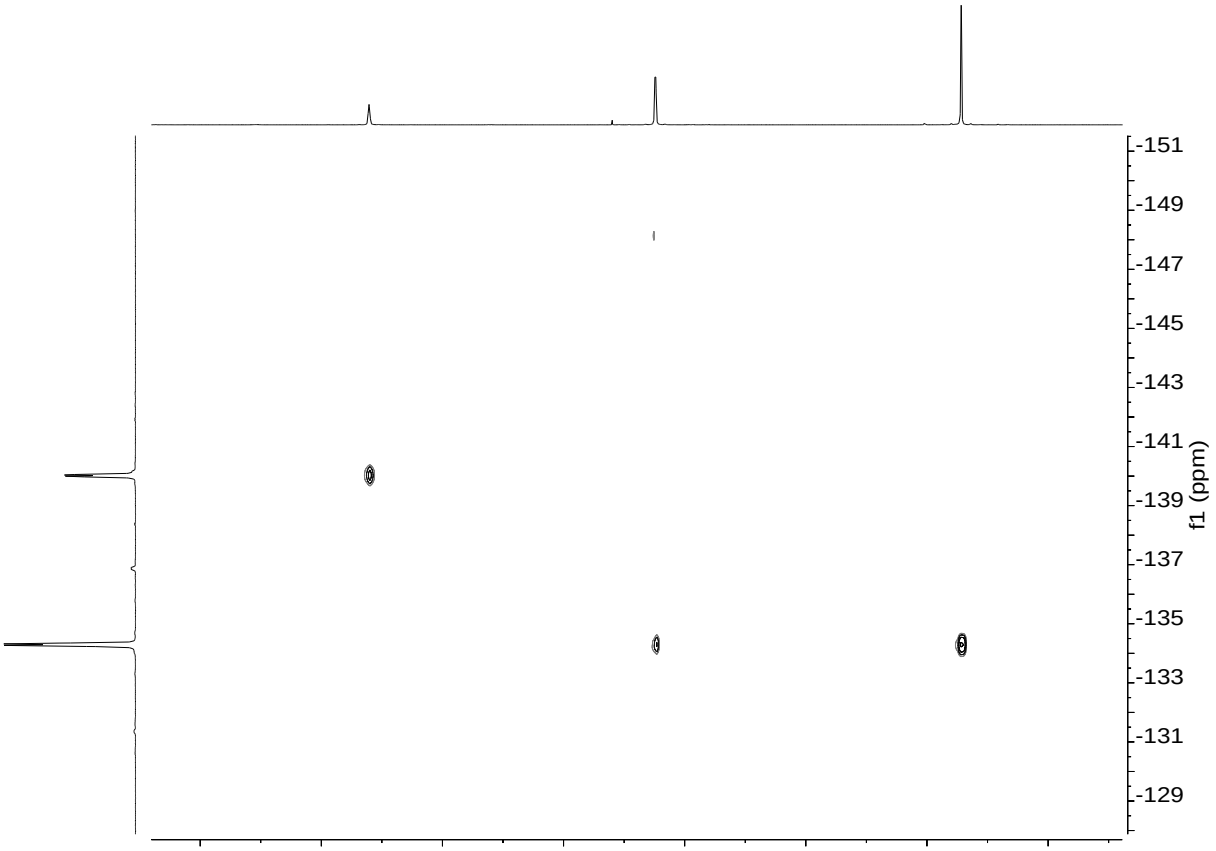
^{1}H (400.0 MHz, $CDCl_3$) NMR spectrum of *E*-1g



^{13}C{^{1}H} (100 MHz, $CDCl_3$) NMR spectrum of *E*-1g

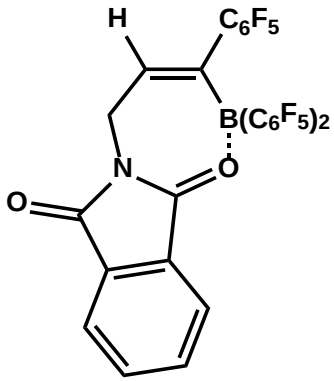


^{19}F{^{1}H} (377 MHz, $CDCl_3$) NMR spectrum of *E*-1g



^{1}H{^{19}F}HOESY spectrum of *E*-1g

Synthesis of 1h



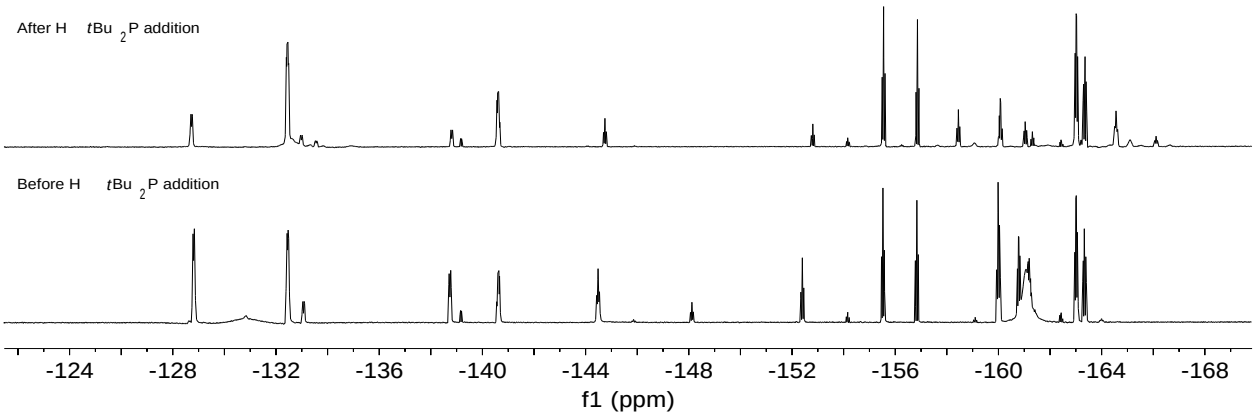
164.6 mg (0.32 mmol) of $B(C_6F_5)_3$ was reacted with 60.0 mg (0.32 mmol) of N-propargylphthalimide. After isomerization completes after 24 h, it was purified by first triturating with pentane, then recrystallized from a 4:1 solvent mixture of pentane:DCM to give 182.7 mg (0.26 mmol, 82%) of ***E*-1c**

^{1}H (400.0 MHz, $CDCl_3$): δ 7.95 (m, 2H, Ar), 7.85 (m, 2H, Ar), 6.37 (t, 1H, $^{3}J_{H\text{-}H}$ = 6.8 Hz, *H*C=CB), 4.48 (d, 2H, $^{3}J_{H\text{-}H}$ = 7.0 Hz, C*H*$_2$N)

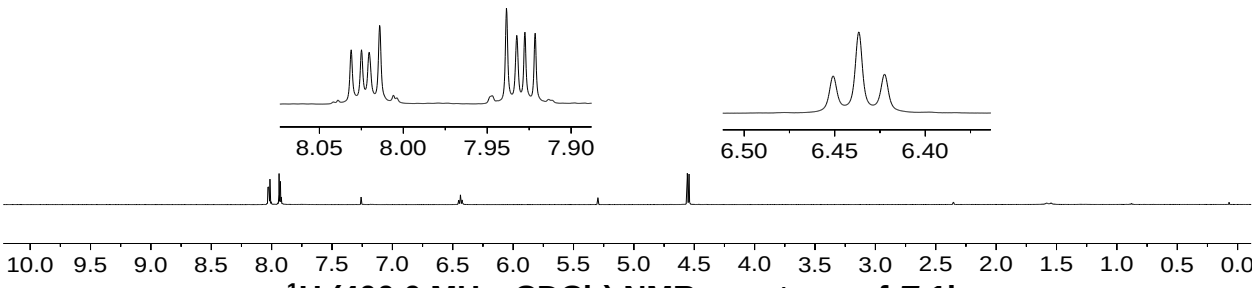
^{11}B{^{1}H} (128 MHz, $CDCl_3$): δ 3.5 (br s, $v_{1/2}$ ≈ 600 Hz)

$^{13}C\{^{1}H\}$ (100 MHz, $CDCl_3$): δ (C_6F_5 signals not listed) n.o. (HC=*C*B), 136.6 (s, Ar), 132.8 (s, H*C*=CB), 125.7 (s, Ar), 38.3 (s, *C*H_2N)
$^{19}F\{^{1}H\}$ NMR (377 MHz, $CDCl_3$): δ -132.6 (m, 4F, *o*-B(C_6F_5)$_2$), -140.6 (m, 2F, *o*-C_6F_5), -155.8 (t, 2F, $^{3}J_{F-F}$ = 20.0 Hz, *p*-B(C_6F_5)$_2$), -156.8 (t, 1F, $^{3}J_{F-F}$ = 20.2 Hz, *p*-C_6F_5), -162.9 - -163.1 (m, 6F, *m*-B(C_6F_5)$_2$ + *m*-C_6F_5)

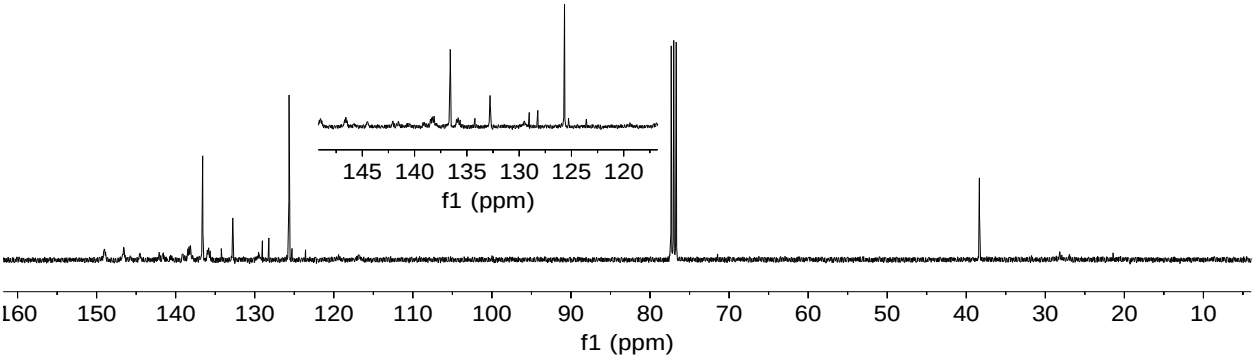
Anal. Calc. for $C_{29}H_7BF_{15}NO_2$: C 49.96% H 1.01%. N: 2.01. Found: C 49.82% H 1.30% N: 1.84



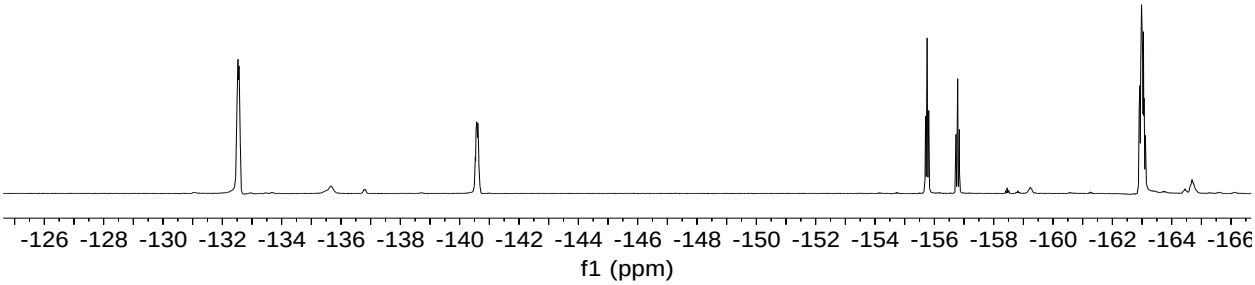
***in situ* $^{19}F\{^{1}H\}$ (377 MHz, $CDCl_3$) NMR spectrum of the isomerization of E/Z-1h**



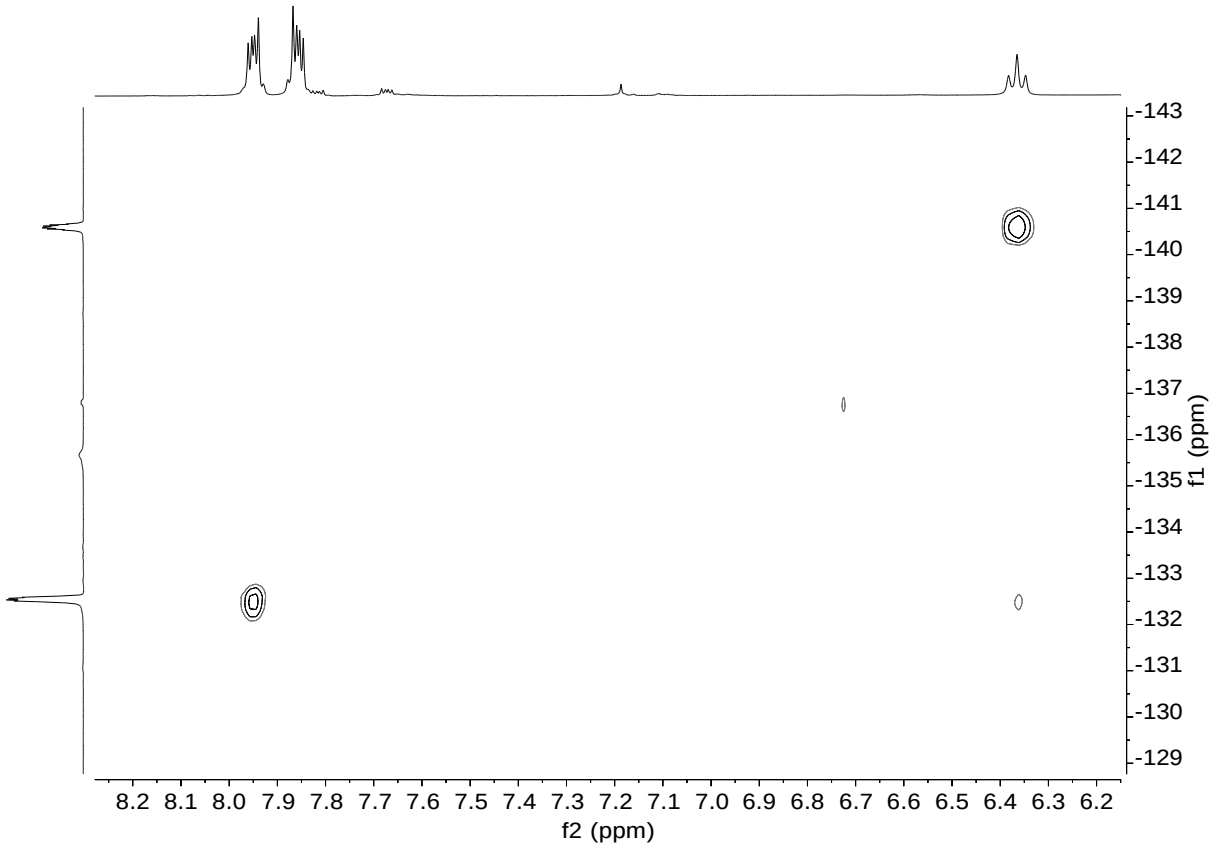
^{1}H (400.0 MHz, $CDCl_3$) NMR spectrum of *E*-1h



$^{13}C\{^{1}H\}$ (100 MHz, $CDCl_3$) NMR spectrum of *E*-1h

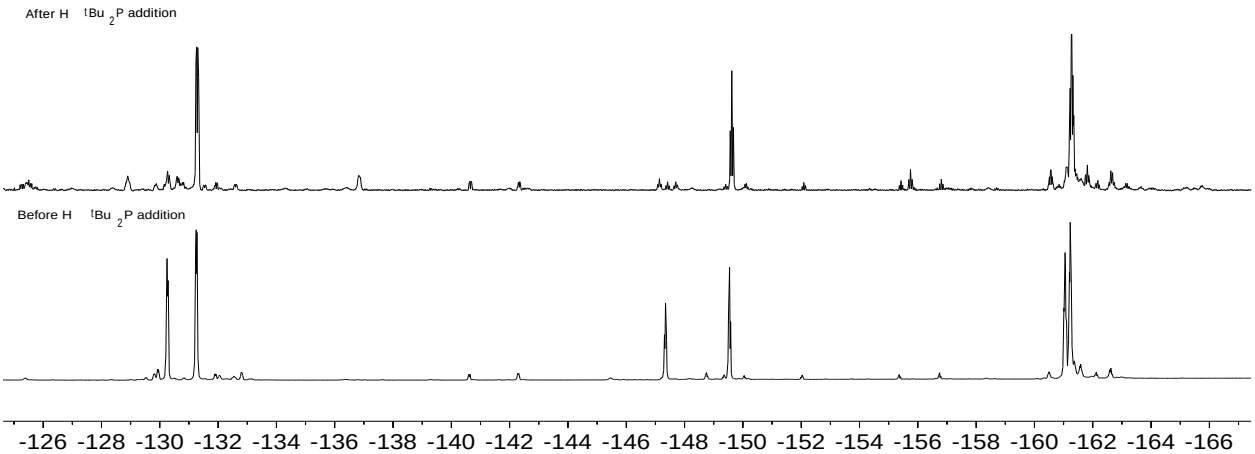


$^{19}F\{^{1}H\}$ (377 MHz, $CDCl_3$) NMR spectrum of *E*-1h

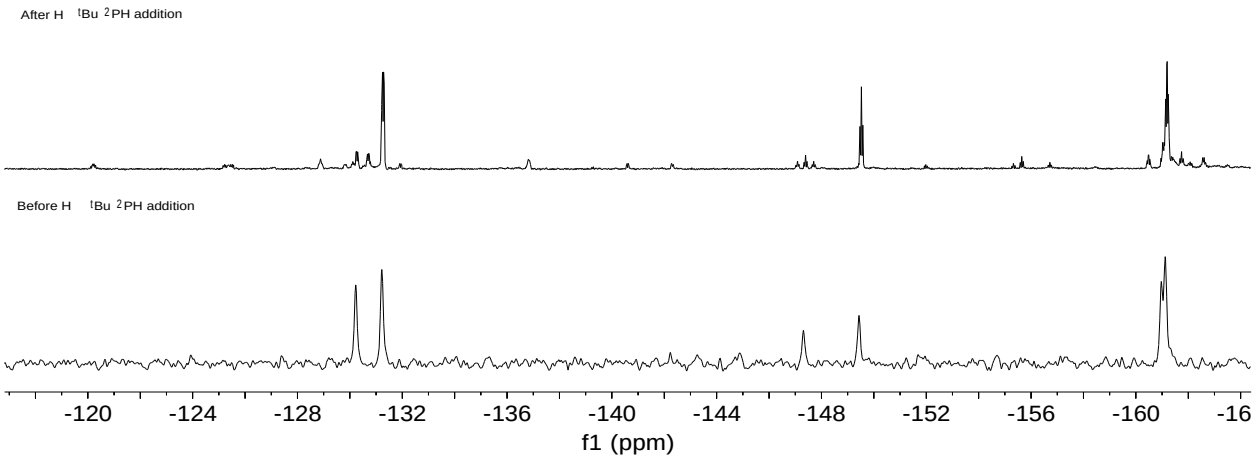


^{1}H{^{19}F}HOESY spectrum of *E*-1h

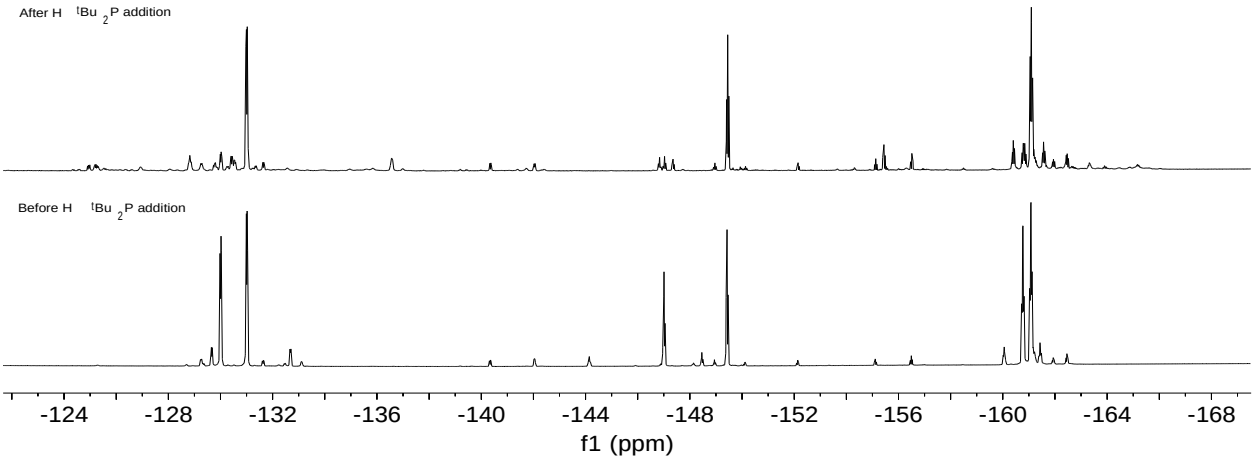
***In situ* ^{19}F{^{1}H} NMR spectra of entries 9-12 in Table 1.**



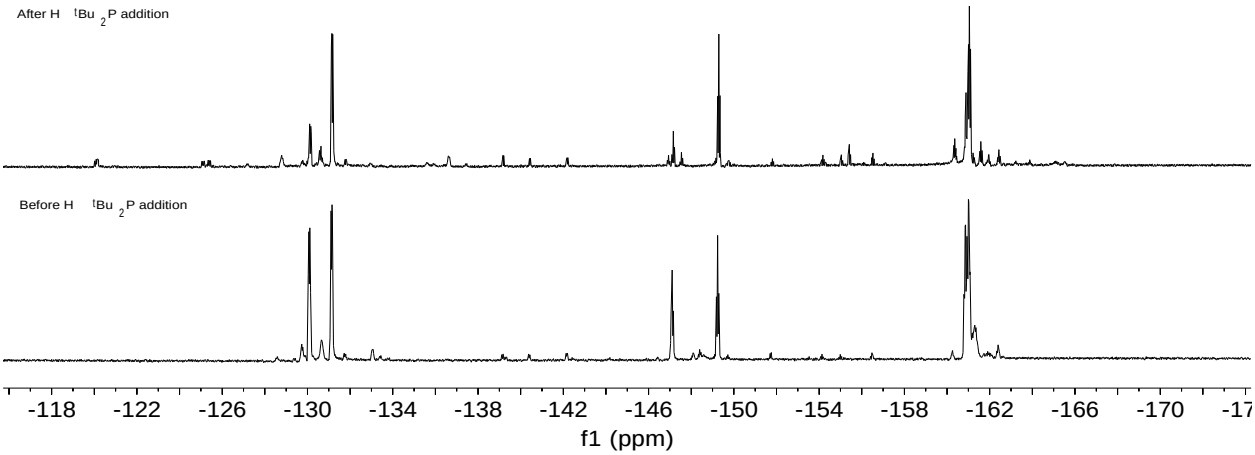
***in situ* ^{19}F{^{1}H} (377 MHz, $CDCl_3$) NMR spectrum of the isomerization of E/Z-2a**



***in situ* $^{19}F\{^{1}H\}$ (377 MHz, $CDCl_3$) NMR spectrum of the isomerization of E/Z-2b**



***in situ* $^{19}F\{^{1}H\}$ (377 MHz, $CDCl_3$) NMR spectrum of the isomerization of E/Z-2c**



***in situ* $^{19}F\{^{1}H\}$ (377 MHz, $CDCl_3$) NMR spectrum of the isomerization of E/Z-2d**

Computational Studies

Computational details: The TURBOMOLE V7.0 suite of programs[1] was used for all DFT calculations. All structures are fully optimized at the TPSS-D3/def2-TZVP + COSMO (toluene) level of theory, which combines the TPSS meta-GGA density functional[2] with the BJ-damped DFT-D3 dispersion correction[3, 4] and the large def2-TZVP AO basis set[5-7], together with the COSMO (for toluene solvent: dielectric constant ε_r=2.38 , R_{sol}= 3.48 Å) solvation model[8]. The density-fitting RI-J approach[9, 10] is used to accelerate the geometry optimization and harmonic frequency calculations. Vibrational frequency analysis is used to identify the nature of located stationary points and to provide thermal and free-energy corrections according to the modified ideal gas–rigid rotor–harmonic oscillator model.[11] The structures are characterized as true minima (with no imaginary frequency) or transition states (with only one imaginary frequency). Better free energies in toluene solution are obtained from the sum of more reliable PW6B95-D3/def2-QZVP single-point energies,[7, 12] COSMO-RS[13] solvation free energies (default Gsolv using the BP_TZVP_C30_1301.ctd parameter file), and TPSS-D3/def2-TZVP thermal corrections at 298.15 K related to ideal gas under 1 atm (*i.e.*, 0.04 mol/L concentration). In our discussion, the final PW6B95-D3/def2-QZVP + COSMO-RS(toluene) free energies (in kcal/mol) are used unless specified otherwise.

References:

[1] TURBOMOLE V7.0 **2015**, a development of University of Karlsruhe and Forschungszentrum Karlsruhe GmbH, 1989-2007, TURBOMOLE GmbH, since 2007; available from http://www.turbomole.com .

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Scheme S1. The PW6B95-D3/def2-QZVP + COSMO-RS(toluene) // TPSS-D3/def2-TZVP + COSMO(toluene) computed reaction free energy path (in kcal/mol) for the *t*Bu$_2$PH (**P**) catalyzed Z to E isomerization of **1g** in toluene solution. For each structure, the crucial P, O, C, B and H atoms are shown as violet, red, grey, yellow and white balls, respectively, the C and F backbone atoms are indicated by sticks, and other H-atoms are omitted for clarity.

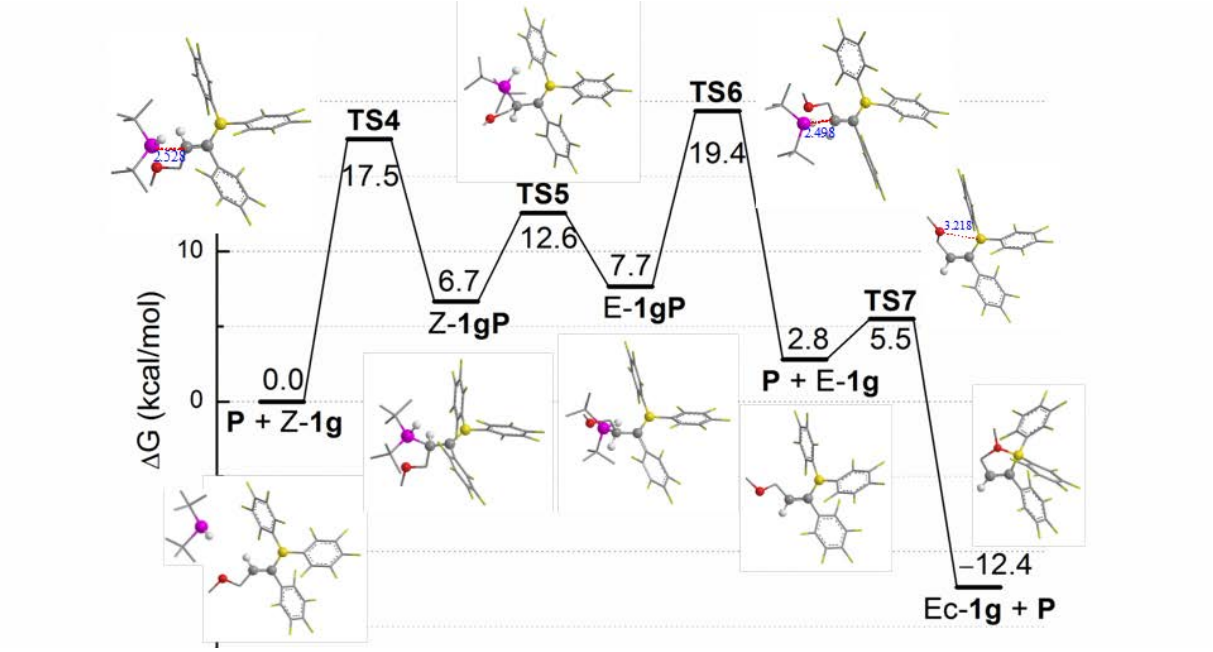

Table S1. The TPSS-D3/def2-TZVP + COSMO(toluene) computed zero-point energies (ZPE), enthalpy and free energy corrections (Hc and Gc) at 298.15 K, the COSMO-RS (toluene) solvation enthalpy and free energy corrections (Hsol and Gsol), the PW6B95-D3/def2-QZVP single-point and relative energies (TE and RE), and the final relative free energies (ΔG). For each transition structure, the TPSS-D3/def2-TZVP + COSMO(toluene) computed imaginary frequency (IF) is also shown.

Name	IF	ZPE	Hc	Gc	Hs	Gs	TE	RE	ΔG
	cm^{-1}	kcal/mol	kcal/mol	kcal/mol	kcal/mol	kcal/mol	Eh	kal/mol	kal/mol
E-**1a** + **P**	0	324.06	355.81	262.34	-26.75	-19.01	-3066.072444	0.0	0.0
TS1	-132.8	325.30	356.93	279.40	-24.47	-19.08	-3066.068593	2.4	19.4
E-**1aP**	0	326.40	358.04	280.73	-28.44	-22.68	-3066.081933	-6.0	8.8
TS2	0	326.61	358.20	280.93	-26.61	-21.06	-3066.072932	-0.3	16.2

Z-**1aP**	0	326.17	358.03	279.95	-27.57	-21.91	-3066.078910	-4.1	10.6
TS3	-128.1	325.28	356.93	279.30	-24.65	-19.18	-3066.071473	0.6	17.4
Z-**1a** + **P**	0	323.93	355.76	262.01	-27.52	-19.58	-3066.076737	-2.7	-3.6
Z-**1g** + **P**	0	309.18	340.70	247.67	-27.97	-19.87	-3102.012089	0.0	0.0
TS4	-58.3	310.22	341.81	264.23	-23.70	-18.34	-3102.013069	-0.6	17.5
Z-**1gP**	0	311.42	343.16	265.15	-27.02	-21.43	-3102.026820	-9.2	6.7
TS5	0	311.75	343.22	266.10	-26.12	-20.59	-3102.020273	-5.1	12.6
E-**1gP**	0	311.78	343.24	266.22	-25.90	-20.47	-3102.028469	-10.3	7.7
TS6	-88.8	310.02	341.70	263.88	-23.41	-18.11	-3102.009885	1.4	19.3
E-**1g** + **P**	0	309.08	340.65	247.44	-27.52	-19.56	-3102.007768	2.7	2.8
TS7	0	309.04	340.70	247.15	-27.25	-19.43	-3102.003177	5.6	5.5
Ec-**1g** + **P**	0	309.69	340.90	248.62	-30.78	-22.74	-3102.028753	-10.5	-12.4

Table S2: The TPSS-D3/def2-TZVP + COSMO(toluene) optimized Cartesian coordinates (in angstrom, xyz file format). For each structure, the structure labelling, number of atoms and total energy are followed by atom name and atomic coordinates.

P (*t*Bu$_2$PH)
28
Energy = -657.8858321078
P -0.0001320 -0.9549098 -0.3191643
H 0.0708490 -1.6308880 0.9290401
C -1.5672170 0.0340367 0.0802511
C -2.7131960 -0.9236403 -0.3121491
C -1.7331049 0.4089996 1.5614349
C -1.6440994 1.2909173 -0.8012499
H -2.6711852 -1.1795512 -1.3757147
H -2.6700492 -1.8549169 0.2649424
H -3.6794704 -0.4440144 -0.1066009
H -0.9656761 1.1076911 1.8998797
H -2.7118282 0.8859515 1.7118109
H -1.6907952 -0.4812886 2.1978578
H -2.6367106 1.7489544 -0.7015803
H -0.9013255 2.0382270 -0.5053006
H -1.4883845 1.0494478 -1.8587362
C 1.5583885 0.0917055 -0.0827766
C 1.8275851 0.8727376 -1.3831053
C 1.5698017 1.0501351 1.1149554
C 2.6764381 -0.9560859 0.1004384
H 1.8445991 0.2014848 -2.2483547
H 1.0691507 1.6405485 -1.5618584
H 2.8028738 1.3723609 -1.3165194
H 1.3601484 0.5242372 2.0518158
H 2.5616843 1.5154604 1.2011471
H 0.8386743 1.8553815 0.9974357
H 3.6511432 -0.4512800 0.1175871
H 2.5582363 -1.5033741 1.0419596
H 2.6836355 -1.6814127 -0.7211495

E-**1a**

47
Energy = -2404.975863163

C	2.0784550	0.1014846	0.4705067
C	-0.2649081	1.0578051	-0.4810408
C	-1.4887296	-1.6131862	0.4330180
C	2.9350495	0.9586489	-0.2340023
C	2.6275692	-0.4977846	1.6135067
C	-1.1506352	0.9512326	-1.5621030
C	-0.2272044	2.3112845	0.1454302
C	-1.9537086	-0.8508071	1.5111585
C	-2.4599093	-2.3458172	-0.2618346
C	4.2508856	1.1978407	0.1424587
C	3.9310478	-0.2627942	2.0363344
C	-1.9447263	2.0042893	-2.0008819
C	-1.0201196	3.3821311	-0.2498308
C	-3.2888781	-0.8090003	1.8931654
C	-3.8057148	-2.3229257	0.0937050
C	4.7489397	0.5851918	1.2913457
C	-1.8808324	3.2269801	-1.3352096
C	-4.2235237	-1.5535932	1.1769778
F	2.5019804	1.5638610	-1.3616552
F	1.8798133	-1.3171360	2.3778677
F	-1.2329398	-0.2031500	-2.2569117
F	0.5784157	2.5105079	1.2096096
F	-1.0689732	-0.1208827	2.2302628
F	-2.1194791	-3.0804095	-1.3400851
F	5.0420990	2.0073182	-0.5790518
F	4.4113885	-0.8412959	3.1486078
F	-2.7633778	1.8607833	-3.0554413
F	-0.9668768	4.5580635	0.3950284
F	-3.6816422	-0.0692130	2.9431869
F	-4.7074059	-3.0314186	-0.6063933
F	6.0084494	0.8115605	1.6790712
F	-2.6405115	4.2502611	-1.7398122
F	-5.5164404	-1.5318785	1.5302446
B	0.6009874	-0.1577254	0.0140681
C	-0.0491095	-1.5699268	0.0591961
C	0.5750950	-2.7316591	-0.2614539
H	-0.0009737	-3.6558023	-0.2011793
C	1.9537405	-2.9113022	-0.8006839
C	1.9164987	-3.4491066	-2.2509036
H	2.4877914	-3.6413181	-0.1756402
H	2.5203224	-1.9771922	-0.7800018
C	3.3235589	-3.6810625	-2.8072966
H	1.3428376	-4.3837283	-2.2750926
H	1.3758761	-2.7305559	-2.8783816
H	3.2803952	-4.0529224	-3.8360619
H	3.9027519	-2.7504570	-2.8093697
H	3.8685200	-4.4152092	-2.2031347

TS1
75
Energy = -3062.864006015

C	-1.1842772	1.7757977	0.1121368
C	1.4819019	1.6185123	-0.1177989
C	1.3981670	-1.3220881	0.4056070

C	-1.4708144	2.7393377	1.0778443
C	-2.0641505	1.7225145	-0.9653869
C	2.5482451	1.6527151	0.7856817
C	1.6924563	2.3030188	-1.3169806
C	2.0288059	-1.4074485	-0.8429440
C	2.0661409	-1.9592365	1.4609563
C	-2.5723388	3.5863783	1.0070550
C	-3.1714245	2.5573942	-1.0862795
C	3.7509924	2.3000919	0.5197408
C	2.8818371	2.9535390	-1.6283589
C	3.2380032	-2.0657325	-1.0389172
C	3.2740455	-2.6297679	1.2983359
C	-3.4293959	3.4930521	-0.0880261
C	3.9198185	2.9511942	-0.6996042
C	3.8671391	-2.6828468	0.0392400
F	-0.6579981	2.8557375	2.1554119
F	-1.8571076	0.8225210	-1.9600440
F	2.4327497	1.0571382	1.9951655
F	0.7177747	2.3194951	-2.2565206
F	1.4352635	-0.8723888	-1.9336931
F	1.5518797	-1.9073782	2.7109227
F	-2.8208641	4.4880571	1.9739067
F	-3.9982489	2.4615272	-2.1450925
F	4.7470398	2.3102109	1.4253010
F	3.0436225	3.5778598	-2.8096995
F	3.7916633	-2.1341090	-2.2639951
F	3.8841686	-3.2094775	2.3484820
F	-4.4983909	4.3001734	-0.1797836
F	5.0743097	3.5776120	-0.9758387
F	5.0334072	-3.3257894	-0.1342190
B	0.1184978	0.8656416	0.2054208
C	0.1284954	-0.5735518	0.5953342
C	-0.9273881	-1.2934523	1.2318794
H	-0.6281388	-2.2585270	1.6439088
C	-1.9781624	-0.6273136	2.0977040
C	-2.8683833	-1.6205693	2.8467037
H	-2.5810866	0.0787045	1.5218824
H	-1.4285948	-0.0233581	2.8330133
C	-3.9193973	-0.9262318	3.7160806
H	-2.2360638	-2.2651681	3.4706002
H	-3.3648473	-2.2857811	2.1261890
H	-4.5363425	-1.6551434	4.2511072
H	-3.4434321	-0.2757729	4.4581994
H	-4.5850566	-0.3030226	3.1073134
P	-2.2073189	-2.3986868	-0.4209285
H	-1.6087290	-1.7924095	-1.5413478
C	-4.0424076	-2.1957440	-0.8727950
C	-4.5036977	-0.8416538	-0.3007022
C	-4.2006486	-2.1599484	-2.4041518
C	-4.9165926	-3.2986971	-0.2563119
H	-5.5224721	-0.6412645	-0.6529785
H	-4.5193700	-0.8513515	0.7913581
H	-3.8681646	-0.0198037	-0.6349315
H	-3.8873751	-3.0915417	-2.8787222
H	-5.2599232	-1.9972752	-2.6420584
H	-3.6265690	-1.3359305	-2.8382061

H	-5.9674094	-3.0585107	-0.4582441
H	-4.7132463	-4.2835510	-0.6821579
H	-4.7930341	-3.3556372	0.8298875
C	-1.6280787	-4.1771575	-0.6212227
C	-2.0291505	-4.9780103	0.6320426
C	-2.1555562	-4.8566968	-1.8957389
C	-0.0910883	-4.1283251	-0.7101620
H	-1.6569899	-4.5011730	1.5449955
H	-3.1119274	-5.0924603	0.7208539
H	-1.5871894	-5.9793984	0.5712778
H	-1.8684825	-4.2994174	-2.7925836
H	-1.7095923	-5.8570933	-1.9639124
H	-3.2406948	-4.9778429	-1.8899397
H	0.3607917	-3.7226866	0.1976347
H	0.2447705	-3.5317000	-1.5634180
H	0.2808771	-5.1512229	-0.8423068

E-**1aP**
75
Energy = -3062.873451523

C	-1.0065468	1.6380713	-0.2952719
C	1.6709452	1.4145839	-0.2729040
C	1.4237014	-1.5185524	0.4292083
C	-1.4172377	2.4936328	0.7300770
C	-1.7151136	1.7699229	-1.4895859
C	2.6182325	1.4596712	0.7559263
C	2.0389638	2.0872949	-1.4400210
C	2.3235121	-1.6309191	-0.6490287
C	1.8104812	-2.2289477	1.5793820
C	-2.4728252	3.3927347	0.6075207
C	-2.7726217	2.6601386	-1.6629872
C	3.8498710	2.0978690	0.6341362
C	3.2582362	2.7350926	-1.6066872
C	3.5070507	-2.3578801	-0.5848718
C	2.9795222	-2.9754523	1.6705744
C	-3.1584614	3.4745621	-0.6028443
C	4.1740692	2.7383165	-0.5581993
C	3.8440258	-3.0383684	0.5819778
F	-0.7682208	2.4654589	1.9175789
F	-1.3944160	0.9999902	-2.5629524
F	2.3584361	0.8841843	1.9536794
F	1.1907999	2.1044565	-2.4972003
F	2.0285273	-1.0678070	-1.8427930
F	1.0421339	-2.1646164	2.6975140
F	-2.8405095	4.1791496	1.6355793
F	-3.4342149	2.7287516	-2.8350816
F	4.7264758	2.1127335	1.6582511
F	3.5655048	3.3514455	-2.7653743
F	4.3153294	-2.4416227	-1.6602085
F	3.2977274	-3.6102963	2.8161378
F	-4.1858310	4.3278588	-0.7432346
F	5.3581138	3.3600782	-0.6938673
F	4.9836417	-3.7494987	0.6539419
B	0.2653264	0.6787957	-0.0944124
C	0.1894054	-0.7171260	0.3424807

C	-1.0561167	-1.3985095	0.9061699
H	-0.8014313	-2.4301814	1.1803159
C	-1.6479987	-0.7495291	2.1721172
C	-2.5475507	-1.6899020	2.9758310
H	-2.1654701	0.1796680	1.9261688
H	-0.7864028	-0.4621304	2.7812662
C	-3.1650689	-1.0067059	4.1985852
H	-1.9535492	-2.5568367	3.2931456
H	-3.3478955	-2.0896545	2.3375288
H	-3.7849409	-1.7018544	4.7738358
H	-2.3827304	-0.6206877	4.8610003
H	-3.7938896	-0.1595081	3.8999909
P	-2.2486066	-1.7052226	-0.5097865
H	-1.7726242	-0.8990874	-1.5449408
C	-4.0789381	-1.2390408	-0.4672579
C	-4.2904271	-0.0047869	0.4309500
C	-4.4436334	-0.8411674	-1.9160858
C	-5.0025729	-2.3709425	0.0099040
H	-5.2956764	0.3827575	0.2308191
H	-4.2320785	-0.2573599	1.4900519
H	-3.5739761	0.7910579	0.2147780
H	-4.3295447	-1.6645911	-2.6226981
H	-5.4953778	-0.5335194	-1.9225733
H	-3.8428675	0.0021530	-2.2656366
H	-6.0255664	-1.9787635	0.0374456
H	-4.9948589	-3.2279398	-0.6670839
H	-4.7523845	-2.7153123	1.0166304
C	-1.9369729	-3.4356231	-1.1273760
C	-2.3045879	-4.4732301	-0.0502566
C	-2.7104783	-3.7091936	-2.4298646
C	-0.4277253	-3.5355637	-1.4315737
H	-1.7736871	-4.2909140	0.8892530
H	-3.3761449	-4.5009748	0.1550176
H	-2.0030165	-5.4619102	-0.4129611
H	-2.4712010	-2.9735067	-3.2038099
H	-2.4064782	-4.6947807	-2.8000063
H	-3.7921514	-3.7305932	-2.2809431
H	0.1779381	-3.4629374	-0.5261943
H	-0.0970859	-2.7637591	-2.1320632
H	-0.2431740	-4.5171674	-1.8826977

TS2

75

Energy = -3062.867015690

C	-1.2413935	1.2251963	0.7805026
C	1.1853214	1.4668448	-0.2910682
C	1.5611875	-1.4747762	-0.3459640
C	-1.6553265	1.0659141	2.1043600
C	-1.9789707	2.1516942	0.0379119
C	1.7270946	2.4156164	0.5794495
C	1.7206581	1.4771818	-1.5816890
C	1.8629203	-2.3196657	-1.4263537
C	2.6769433	-1.1399428	0.4479509
C	-2.7375355	1.7470342	2.6563568
C	-3.0707672	2.8509953	0.5439409
C	2.7406741	3.2990459	0.2232253

C	2.7331933	2.3436573	-1.9834993
C	3.1435520	-2.7662825	-1.7302541
C	3.9743005	-1.5544853	0.1620513
C	-3.4535925	2.6447245	1.8680453
C	3.2497016	3.2605285	-1.0723096
C	4.2163175	-2.3729460	-0.9367027
F	-0.9914516	0.2147582	2.9233443
F	-1.6613973	2.3645221	-1.2628219
F	1.2783415	2.4828895	1.8577799
F	1.2467694	0.6280756	-2.5272561
F	0.8747996	-2.7220460	-2.2699606
F	2.5203239	-0.4109793	1.5727743
F	-3.1011207	1.5486903	3.9383474
F	-3.7650648	3.7109210	-0.2244566
F	3.2404198	4.1815242	1.1111186
F	3.2120769	2.3141151	-3.2440897
F	3.3552376	-3.5548355	-2.8024707
F	4.9974648	-1.1943156	0.9608872
F	-4.5059137	3.3045052	2.3791055
F	4.2277827	4.1060210	-1.4418635
F	5.4637064	-2.7839342	-1.2226812
B	0.0271425	0.4660446	0.1688108
C	0.2023075	-0.9763238	-0.0018764
C	-0.7446667	-2.1595545	0.2523870
H	-0.5491800	-2.9170207	-0.5200999
C	-0.4588832	-2.8675777	1.5993063
C	-0.8422596	-4.3491682	1.6222352
H	-0.8952847	-2.3169165	2.4342545
H	0.6266546	-2.7896085	1.7319465
C	-0.5594061	-5.0047364	2.9762469
H	-0.2830633	-4.8674847	0.8321340
H	-1.9031268	-4.4758774	1.3701999
H	-0.8100625	-6.0702515	2.9632140
H	0.4996796	-4.9083791	3.2397261
H	-1.1433870	-4.5287929	3.7727865
P	-2.4977719	-1.7075528	-0.1649840
H	-2.5760791	-0.3205072	-0.0471054
C	-3.9293927	-2.2302024	0.9380458
C	-3.5073449	-2.2318269	2.4208826
C	-5.0087656	-1.1329461	0.7759932
C	-4.5125417	-3.6047738	0.5709459
H	-4.4219054	-2.3079589	3.0195715
H	-2.8735933	-3.0825612	2.6685945
H	-2.9960681	-1.3110781	2.7110823
H	-5.4055267	-1.0677742	-0.2369329
H	-5.8376719	-1.3807594	1.4479072
H	-4.6213894	-0.1515896	1.0668898
H	-5.3473029	-3.8110215	1.2499451
H	-4.8988930	-3.6350005	-0.4496451
H	-3.7802383	-4.4074244	0.6895867
C	-2.7725300	-2.0123820	-1.9832483
C	-2.4765084	-3.4807187	-2.3417615
C	-4.2070197	-1.6478496	-2.4098631
C	-1.8128729	-1.0626462	-2.7351558
H	-1.4367013	-3.7501670	-2.1441585
H	-3.1294127	-4.1768178	-1.8085754

H	-2.6519517	-3.6088182	-3.4153798
H	-4.4541659	-0.6126206	-2.1571497
H	-4.2541510	-1.7412702	-3.5006114
H	-4.9635831	-2.3123626	-1.9874480
H	-0.7762672	-1.1778755	-2.4270863
H	-2.0972978	-0.0179157	-2.5802290
H	-1.8941902	-1.2885776	-3.8048443

Z-**1aP**
75
Energy = -3062.871931564

C	0.6677844	2.2152292	0.1174727
C	-1.8743206	1.3772766	-0.2078925
C	-1.0038967	-1.4538542	0.2727751
C	0.8434325	3.0783795	-0.9659974
C	1.4194323	2.5292745	1.2510420
C	-2.6325170	0.9376059	-1.2934747
C	-2.5533432	2.1939533	0.6984894
C	-1.8623361	-1.5457915	1.3811453
C	-1.2932075	-2.3488629	-0.7638612
C	1.7150913	4.1620784	-0.9544014
C	2.3048089	3.6032926	1.3102372
C	-3.9746166	1.2628366	-1.4704410
C	-3.8930918	2.5439751	0.5641380
C	-2.9210077	-2.4468818	1.4560615
C	-2.3374172	-3.2674196	-0.7230363
C	2.4554381	4.4245981	0.1962863
C	-4.6101874	2.0712732	-0.5321040
C	-3.1604015	-3.3183981	0.3974177
F	0.1700299	2.8417632	-2.1189093
F	1.3048393	1.7772835	2.3750433
F	-2.0616052	0.1698684	-2.2539134
F	-1.8992430	2.6679365	1.7881186
F	-1.6837740	-0.7294375	2.4395533
F	-0.5481993	-2.3351487	-1.8994624
F	1.8673289	4.9472320	-2.0387531
F	3.0092228	3.8616416	2.4300134
F	-4.6629684	0.8148193	-2.5402941
F	-4.5053042	3.3242694	1.4770927
F	-3.7109464	-2.4913658	2.5454337
F	-2.5602575	-4.0994616	-1.7592678
F	3.3070635	5.4641355	0.2311724
F	-5.9060257	2.3971096	-0.6854092
F	-4.1725373	-4.1995632	0.4572144
B	-0.3464034	0.9860008	0.0320725
C	0.0552282	-0.4047787	0.2156841
C	1.4510260	-0.8022486	0.6266721
H	2.0452182	0.1157625	0.7052495
C	1.5274356	-1.5214920	1.9839844
C	2.9390032	-1.7640257	2.5149346
H	0.9616536	-2.4570826	1.9444368
H	0.9874717	-0.8696445	2.6786496
C	2.9430464	-2.5559199	3.8249020
H	3.4364253	-0.7976209	2.6645881
H	3.5362335	-2.3016411	1.7654301

H	3.9614422	-2.7033999	4.1982897
H	2.3716560	-2.0289441	4.5966632
H	2.4856640	-3.5426864	3.6870256
P	2.3954240	-1.6396650	-0.8047252
H	1.5355696	-1.4380350	-1.8860333
C	3.8654932	-0.6109050	-1.3211782
C	3.3287384	0.8119258	-1.5851121
C	4.9402725	-0.5516441	-0.2243244
C	4.4490991	-1.1499657	-2.6408812
H	4.1488242	1.4076791	-2.0013178
H	2.5041890	0.8140951	-2.3043690
H	2.9902431	1.3001884	-0.6700396
H	5.3715323	-1.5314308	-0.0076785
H	5.7472453	0.1048759	-0.5682063
H	4.5419721	-0.1319629	0.7037328
H	5.2368061	-0.4607783	-2.9659195
H	4.8968610	-2.1398351	-2.5349952
H	3.6908032	-1.1856771	-3.4290578
C	2.6856281	-3.5049940	-0.8710253
C	1.6693044	-4.2161454	0.0439651
C	2.4260772	-3.9362765	-2.3318678
C	4.1032079	-3.9294402	-0.4502822
H	1.9284601	-4.0979245	1.0975748
H	0.6458386	-3.8655096	-0.1089731
H	1.6971526	-5.2857594	-0.1921713
H	3.1038777	-3.4503516	-3.0370678
H	2.5897435	-5.0180882	-2.3976446
H	1.3964676	-3.7267502	-2.6312982
H	4.3359610	-3.6416925	0.5778319
H	4.8756925	-3.5305927	-1.1102689
H	4.1509428	-5.0230126	-0.5058239

TS3

75

Energy = -3062.866110589

C	1.1732559	1.9488746	0.0626517
C	-1.4751129	1.6366664	-0.3079459
C	-1.2581390	-1.2491418	0.5503491
C	1.5608754	2.6117803	-1.1029290
C	1.9328960	2.2386740	1.1975082
C	-2.2822476	1.2147001	-1.3651502
C	-1.9800030	2.6978880	0.4463389
C	-2.1521376	-1.0319893	1.6061516
C	-1.6674554	-2.1876034	-0.3994523
C	2.6431004	3.4821615	-1.1667805
C	3.0201185	3.1092213	1.1821566
C	-3.5156655	1.7887874	-1.6574775
C	-3.2103257	3.2966437	0.1954356
C	-3.3699073	-1.6971602	1.7170561
C	-2.8733527	-2.8773392	-0.3177189
C	3.3800315	3.7308963	-0.0108733
C	-3.9835032	2.8362350	-0.8677664
C	-3.7328927	-2.6297092	0.7485890
F	0.8871876	2.3733851	-2.2548446
F	1.6149593	1.6813054	2.3908878
F	-1.8595249	0.2201873	-2.1809703

F	-1.2657367	3.1676891	1.4970046
F	-1.8411066	-0.1413613	2.5713956
F	-0.8854504	-2.4435873	-1.4751805
F	2.9959146	4.0711455	-2.3242826
F	3.7210660	3.3611718	2.3033379
F	-4.2552973	1.3530971	-2.6949048
F	-3.6619590	4.3061132	0.9623391
F	-4.1939481	-1.4555321	2.7527077
F	-3.2162102	-3.7718396	-1.2632625
F	4.4305783	4.5660529	-0.0470896
F	-5.1715191	3.4025648	-1.1331071
F	-4.9013404	-3.2842883	0.8426242
B	-0.0788778	0.9701195	0.0536356
C	0.0068865	-0.4608432	0.4436170
C	1.2008095	-1.0332923	0.9661649
H	2.0443384	-0.3461022	0.9999238
C	1.1579398	-1.9793381	2.1462824
C	2.5126432	-2.5121278	2.6081473
H	0.4582478	-2.7996151	1.9545639
H	0.7143001	-1.3945365	2.9664727
C	2.3968626	-3.4462775	3.8151835
H	3.1679485	-1.6661463	2.8518474
H	2.9964083	-3.0454120	1.7780075
H	3.3803924	-3.8089236	4.1302932
H	1.9374928	-2.9313886	4.6660602
H	1.7753910	-4.3176405	3.5775686
P	2.2889385	-2.2953806	-0.7185454
H	1.4739615	-1.8893785	-1.7889992
C	3.9182345	-1.5335178	-1.2727707
C	3.6336388	-0.0283863	-1.4434428
C	4.9951817	-1.7144666	-0.1891494
C	4.3995260	-2.0868894	-2.6245767
H	4.5496176	0.4622660	-1.7934089
H	2.8465432	0.1550934	-2.1810347
H	3.3423527	0.4413438	-0.5011838
H	5.2567533	-2.7635794	-0.0338177
H	5.9026983	-1.1831861	-0.4993108
H	4.6695707	-1.2945590	0.7675746
H	5.2947814	-1.5300167	-2.9295269
H	4.6680119	-3.1443148	-2.5737582
H	3.6400560	-1.9544753	-3.4012385
C	2.2508821	-4.1796951	-0.9471378
C	1.1181540	-4.7266256	-0.0547157
C	1.9370762	-4.5171968	-2.4163207
C	3.5658716	-4.8444114	-0.5094477
H	1.3408805	-4.5829057	1.0054984
H	0.1563113	-4.2616930	-0.2803211
H	1.0217380	-5.8039392	-0.2356198
H	2.7104751	-4.1562312	-3.0976548
H	1.8742146	-5.6080839	-2.5212049
H	0.9769367	-4.0913147	-2.7214418
H	3.8183062	-4.6055321	0.5284819
H	4.4087418	-4.5667138	-1.1458950
H	3.4404731	-5.9317784	-0.5773121

Z-**1a**
47
Energy = -2404.979502596
C -2.2356633 0.0620783 -0.0516137
C 0.0212685 -1.4236461 -0.1812152
C 1.6142724 1.2380899 -0.0373971
C -3.0803426 -0.7579725 -0.8095655
C -2.8749125 0.9213147 0.8518653
C 1.0172493 -1.7849233 -1.0961428
C -0.3038803 -2.3938462 0.7744950
C 2.0477930 0.7724071 1.2083838
C 2.6149401 1.5856796 -0.9503028
C -4.4658970 -0.7235292 -0.7082224
C -4.2574649 0.9701587 0.9969510
C 1.6610908 -3.0163740 -1.0702549
C 0.3290262 -3.6297753 0.8459362
C 3.3923453 0.6625371 1.5447453
C 3.9694225 1.4835458 -0.6457765
C -5.0565639 0.1467962 0.2063762
C 1.3163270 -3.9422673 -0.0870127
C 4.3602529 1.0219211 0.6089443
F -2.5489995 -1.6085820 -1.7154040
F -2.1489119 1.7122174 1.6700548
F 1.3562719 -0.9362490 -2.0907345
F -1.2429355 -2.1289839 1.7081337
F 1.1321507 0.4214023 2.1378632
F 2.2817477 2.0021329 -2.1878413
F -5.2375128 -1.5092803 -1.4761349
F -4.8292173 1.7958080 1.8887499
F 2.5983895 -3.3268345 -1.9802543
F 0.0031656 -4.5210089 1.7953695
F 3.7637337 0.2229332 2.7583784
F 4.9009807 1.8180113 -1.5538991
F -6.3885989 0.1918056 0.3244253
F 1.9281116 -5.1311366 -0.0432476
F 5.6614275 0.9253886 0.9160332
B -0.6729927 -0.0138104 -0.2020933
C 0.1628374 1.2760007 -0.3572069
C -0.4338891 2.4185557 -0.7872672
H -1.4961096 2.3564520 -1.0279170
C 0.1617446 3.7744626 -0.9302636
C -0.6661011 4.8250041 -0.1556180
H 0.1697467 4.0525975 -1.9944439
H 1.2002871 3.7874501 -0.5840243
C -0.0887927 6.2339168 -0.3130977
H -1.7021363 4.8012997 -0.5157025
H -0.6936319 4.5460174 0.9042533
H -0.6835925 6.9633800 0.2459757
H 0.9403822 6.2802540 0.0603653
H -0.0788287 6.5378323 -1.3659589

Z-**1g**
45
Energy = -2440.883848384
C -2.2273623 -0.0463611 0.0513237

C	0.0864050	-1.4213884	-0.2131621
C	1.5519545	1.3183934	0.0643742
C	-3.0591164	-0.8690390	-0.7183706
C	-2.8732911	0.7477883	1.0085785
C	1.0937618	-1.6799800	-1.1509720
C	-0.1923461	-2.4644990	0.6795546
C	1.9940651	0.8002475	1.2878111
C	2.5456614	1.7845092	-0.8019505
C	-4.4409767	-0.8965730	-0.5773757
C	-4.2516978	0.7304138	1.1951028
C	1.7887980	-2.8822871	-1.2065393
C	0.4931749	-3.6737327	0.6695442
C	3.3362207	0.7554079	1.6459485
C	3.8984502	1.7509001	-0.4747385
C	-5.0388831	-0.0915998	0.3910956
C	1.4879292	-3.8832982	-0.2842360
C	4.2957865	1.2363182	0.7566253
F	-2.5198878	-1.6577523	-1.6744292
F	-2.1542589	1.5305182	1.8381226
F	1.3927205	-0.7549876	-2.0885290
F	-1.1355821	-2.3020921	1.6312211
F	1.0873327	0.3339742	2.1735194
F	2.2118333	2.2481332	-2.0233795
F	-5.2026808	-1.6801526	-1.3572421
F	-4.8305620	1.4894324	2.1390336
F	2.7337708	-3.0937898	-2.1364368
F	0.2109496	-4.6366707	1.5605456
F	3.7132927	0.2644696	2.8371717
F	4.8208913	2.2020810	-1.3399904
F	-6.3671993	-0.1092880	0.5485996
F	2.1490092	-5.0451429	-0.3182846
F	5.5938278	1.2044158	1.0862312
B	-0.6702079	-0.0476470	-0.1436734
C	0.1040462	1.2900865	-0.2669745
C	-0.5565939	2.3984418	-0.6817346
H	-1.6180984	2.3115307	-0.9095284
C	-0.0086537	3.7715401	-0.8716819
H	0.3230871	3.8979974	-1.9177111
H	0.8685270	3.9463857	-0.2264422
C	-0.6395453	6.0426858	-0.8164789
H	-1.4915358	6.6783033	-0.5698970
H	0.2172368	6.3135187	-0.1824499
H	-0.3638487	6.1846955	-1.8718437
O	-1.0503489	4.6959591	-0.5741194

TS4

73

Energy = -3098.777167526

C	1.0643460	1.9932350	0.1082020
C	-1.5931200	1.6932770	-0.2211680
C	-1.3572950	-1.2143090	0.6156320
C	1.4273190	2.6525240	-1.0678430
C	1.8648700	2.2612590	1.2204270
C	-2.4171160	1.2555590	-1.2592760
C	-2.0808980	2.7703650	0.5220960
C	-2.2736460	-0.9984290	1.6506330

C	-1.7267170	-2.1687320	-0.3344920
C	2.5252750	3.4999290	-1.1620880
C	2.9685710	3.1091510	1.1734030
C	-3.6512680	1.8311730	-1.5443100
C	-3.3124240	3.3695080	0.2788440
C	-3.4802480	-1.6862530	1.7453960
C	-2.9201320	-2.8807270	-0.2666200
C	3.3032770	3.7273580	-0.0289540
C	-4.1024590	2.8943130	-0.7655280
C	-3.8045130	-2.6371800	0.7808850
F	0.7125280	2.4330150	-2.1974840
F	1.5697850	1.7070180	2.4202220
F	-2.0078730	0.2474260	-2.0640700
F	-1.3488440	3.2533120	1.5536230
F	-1.9928500	-0.0928400	2.6117020
F	-0.9185170	-2.4095760	-1.3906640
F	2.8541130	4.0857430	-2.3274480
F	3.7099560	3.3415640	2.2716740
F	-4.4065740	1.3827940	-2.5638890
F	-3.7485990	4.3932630	1.0344140
F	-4.3284030	-1.4497920	2.7621300
F	-3.2296720	-3.7907210	-1.2080750
F	4.3699320	4.5386900	-0.0959950
F	-5.2906050	3.4617000	-1.0237800
F	-4.9608640	-3.3141960	0.8605730
B	-0.1957390	1.0302550	0.1269170
C	-0.1010500	-0.4122640	0.5136480
C	1.1015180	-0.9811210	0.9634480
H	1.9671610	-0.3257730	0.9858480
C	1.1267640	-2.0343040	2.0311740
H	0.3628630	-2.8060790	1.8593940
H	0.8784340	-1.5272200	2.9806820
C	2.5319360	-3.4713700	3.2734460
H	3.5469940	-3.8720220	3.2672210
H	2.3616030	-2.9126730	4.2037250
H	1.8091970	-4.2977960	3.2126800
P	2.3129250	-2.3026560	-0.8192590
H	1.5972750	-1.9632820	-1.9880470
C	3.9491110	-1.4663680	-1.2265850
C	3.5912310	0.0131900	-1.4708430
C	4.9006270	-1.5513130	-0.0191160
C	4.6271360	-2.0160900	-2.4916450
H	4.5049890	0.5573780	-1.7383200
H	2.8726570	0.1304230	-2.2883850
H	3.1759150	0.4800040	-0.5749990
H	5.2560620	-2.5703390	0.1502370
H	5.7734940	-0.9150870	-0.2091410
H	4.4125720	-1.2077500	0.8976080
H	5.5219180	-1.4147440	-2.6993560
H	4.9460370	-3.0544720	-2.3740740
H	3.9663500	-1.9482210	-3.3614630
C	2.3969180	-4.1831710	-1.0161700
C	1.1666690	-4.7623310	-0.2888580
C	2.3276770	-4.5845150	-2.5003260
C	3.6615980	-4.7532860	-0.3549470
H	1.2039520	-4.5400890	0.7800420

H	0.2314580	-4.3761500	-0.7006240
H	1.1652550	-5.8524690	-0.4113910
H	3.1781230	-4.2078000	-3.0721400
H	2.3291830	-5.6803020	-2.5722390
H	1.4071390	-4.2173310	-2.9649740
H	3.7441710	-4.4281460	0.6854660
H	4.5721040	-4.4653910	-0.8862690
H	3.5999680	-5.8484330	-0.3681750
O	2.4230650	-2.6112390	2.1362750

Z-**1gP**
73
Energy = -3098.788121948

C	0.6078898	2.2306694	0.1272056
C	-1.9439611	1.3890652	-0.1633562
C	-1.0390819	-1.4520854	0.2304262
C	0.7948332	3.0697853	-0.9730404
C	1.3609882	2.5579443	1.2557010
C	-2.7076291	0.9771503	-1.2556010
C	-2.6227193	2.1652232	0.7778355
C	-1.8934993	-1.6162607	1.3319700
C	-1.3154350	-2.2895502	-0.8568549
C	1.6775977	4.1447059	-0.9801994
C	2.2563830	3.6244828	1.2966895
C	-4.0561634	1.2893999	-1.4061465
C	-3.9687374	2.5004109	0.6709660
C	-2.9438371	-2.5299279	1.3546382
C	-2.3517053	-3.2176253	-0.8694086
C	2.4176760	4.4221213	0.1671096
C	-4.6918106	2.0555535	-0.4330361
C	-3.1750274	-3.3394141	0.2459102
F	0.1192922	2.8189037	-2.1212455
F	1.2393589	1.8247406	2.3913530
F	-2.1370359	0.2500931	-2.2469528
F	-1.9608341	2.6106246	1.8747996
F	-1.7123889	-0.8640544	2.4372062
F	-0.5597852	-2.2103679	-1.9810662
F	1.8396014	4.9075585	-2.0788343
F	2.9619097	3.8967177	2.4122545
F	-4.7508620	0.8683197	-2.4825891
F	-4.5811608	3.2394899	1.6173106
F	-3.7324321	-2.6462025	2.4396240
F	-2.5648375	-3.9943843	-1.9492229
F	3.2802005	5.4529933	0.1834704
F	-5.9937609	2.3676932	-0.5601603
F	-4.1785620	-4.2321235	0.2539368
B	-0.4115296	1.0039781	0.0554871
C	0.0022222	-0.3854047	0.2202551
C	1.4087361	-0.7624919	0.5973178
H	1.9913814	0.1621690	0.6700211
C	1.5347487	-1.4736673	1.9391667
H	0.8309477	-2.3140381	2.0133447
H	1.2950010	-0.7549561	2.7325319
C	3.1305920	-2.5368126	3.3428586
H	4.1754369	-2.8526495	3.3466535

H	2.9603365	-1.8128762	4.1502138
H	2.4798119	-3.4092791	3.4976399
P	2.3995019	-1.6275960	-0.7678485
H	1.6051720	-1.4042435	-1.8964833
C	3.9118240	-0.6205212	-1.1883968
C	3.4066708	0.8035556	-1.5090264
C	4.9057752	-0.5594457	-0.0174700
C	4.5809863	-1.1828862	-2.4569993
H	4.2624896	1.3892240	-1.8626714
H	2.6446138	0.8033648	-2.2944671
H	2.9983910	1.3066434	-0.6307778
H	5.3307504	-1.5383235	0.2127155
H	5.7237173	0.1135381	-0.2985510
H	4.4340601	-0.1724154	0.8891805
H	5.3956571	-0.5053262	-2.7367155
H	5.0112132	-2.1743552	-2.3027063
H	3.8798102	-1.2265857	-3.2962553
C	2.6421875	-3.4918900	-0.7964833
C	1.5431398	-4.1667387	0.0462493
C	2.4886970	-3.9390397	-2.2667624
C	4.0121676	-3.9210740	-0.2457115
H	1.7004810	-3.9910120	1.1109591
H	0.5386020	-3.8362008	-0.2268654
H	1.6009987	-5.2462929	-0.1327578
H	3.2454669	-3.4960660	-2.9180733
H	2.6083888	-5.0278930	-2.3030704
H	1.4982269	-3.6911512	-2.6578372
H	4.1485821	-3.5775225	0.7806132
H	4.8409581	-3.5598867	-0.8581727
H	4.0467073	-5.0165965	-0.2536636
O	2.8813442	-1.9350850	2.0696527

TS5

73

Energy = -3098.782327598

C	0.9360592	1.6118384	-0.4798712
C	-1.6272045	1.3059926	0.1778237
C	-1.4091235	-1.6481093	0.0650633
C	1.5662050	1.6591704	-1.7242729
C	1.3604670	2.5789337	0.4354161
C	-2.2131582	2.1896949	-0.7312196
C	-2.3348658	1.1282856	1.3692875
C	-1.6918441	-2.5797290	1.0758157
C	-2.4407977	-1.4947136	-0.8820804
C	2.5723741	2.5692384	-2.0394087
C	2.3648034	3.5045589	0.1682875
C	-3.4219860	2.8393278	-0.5043375
C	-3.5461455	1.7580602	1.6404742
C	-2.8899622	-3.2773880	1.1754341
C	-3.6582870	-2.1640026	-0.8033815
C	2.9781904	3.4968481	-1.0830564
C	-4.0955413	2.6187278	0.6942841
C	-3.8907122	-3.0630464	0.2328980
F	1.2053134	0.7902558	-2.6998924
F	0.8088037	2.6098252	1.6732988

F	-1.6035288	2.4262716	-1.9194856
F	-1.8435773	0.3242446	2.3447013
F	-0.7765298	-2.8141013	2.0523640
F	-2.2677445	-0.6937568	-1.9544817
F	3.1573077	2.5638276	-3.2528990
F	2.7554563	4.3968086	1.0971852
F	-3.9513083	3.6690064	-1.4251885
F	-4.1876878	1.5545311	2.8090273
F	-3.0979108	-4.1374741	2.1915993
F	-4.6054594	-1.9710795	-1.7416849
F	3.9512940	4.3782007	-1.3653771
F	-5.2643454	3.2366798	0.9385970
F	-5.0602603	-3.7198251	0.3182484
B	-0.2366306	0.5817829	-0.1307657
C	-0.1428521	-0.8752883	-0.0505965
C	1.0566212	-1.8201360	-0.2024528
H	0.9145541	-2.6830805	0.4617201
O	1.9649521	-3.5634190	-1.5989519
C	1.1013132	-2.4243006	-1.6080659
H	1.4054667	-1.6943508	-2.3665969
H	0.0746135	-2.7414648	-1.8423780
C	1.9336194	-4.2608746	-2.8470642
H	2.6139314	-5.1091259	-2.7537328
H	0.9186352	-4.6218005	-3.0626897
H	2.2636667	-3.6114773	-3.6711658
P	2.6292100	-1.1108899	0.4793600
H	2.4936500	0.2774320	0.4359040
C	4.2413660	-1.3574725	-0.4411475
C	4.0115170	-1.1849294	-1.9565103
C	5.1946915	-0.2228931	0.0008764
C	4.8590781	-2.7378666	-0.1653246
H	4.9975923	-1.1192009	-2.4295838
H	3.4870741	-2.0400634	-2.3781822
H	3.4690948	-0.2666703	-2.1949325
H	5.4843635	-0.2842431	1.0487567
H	6.1040586	-0.3049369	-0.6045526
H	4.7564830	0.7628461	-0.1881631
H	5.7647823	-2.8355812	-0.7744635
H	5.1492175	-2.8552795	0.8821140
H	4.1687142	-3.5376343	-0.4427816
C	2.6854122	-1.4995587	2.3015375
C	2.5449748	-3.0138559	2.5474848
C	3.9900940	-0.9980167	2.9473293
C	1.5118471	-0.7282561	2.9461233
H	1.5874812	-3.4039095	2.1985669
H	3.3507347	-3.5836258	2.0777518
H	2.5961086	-3.1832381	3.6286109
H	4.1507605	0.0699651	2.7733699
H	3.8939617	-1.1466595	4.0285729
H	4.8675329	-1.5557503	2.6119867
H	0.5480516	-0.9936954	2.5163446
H	1.6455732	0.3521804	2.8394393
H	1.5041854	-0.9695627	4.0155112

E-**1gP**

73
Energy = -3098.788156309

C	-0.9913673	1.6662157	-0.3033219
C	-1.4135237	2.5466048	0.6952490
C	-1.6777549	1.7759038	-1.5129982
B	0.2750991	0.7085754	-0.0687857
C	-2.4585662	3.4515988	0.5346873
F	-0.7895128	2.5331847	1.8977891
C	-2.7242444	2.6707399	-1.7243878
F	-1.3450009	0.9796510	-2.5622944
C	1.6824733	1.4464228	-0.2263026
C	0.2009261	-0.6908214	0.3565433
C	-3.1209271	3.5126409	-0.6897451
F	-2.8393115	4.2613733	1.5396444
F	-3.3653492	2.7180455	-2.9084407
C	2.6185930	1.4853114	0.8128822
C	2.0613853	2.1288335	-1.3844319
C	1.4373913	-1.4932178	0.4267278
C	-1.0430159	-1.3968351	0.8807887
F	-4.1385010	4.3705211	-0.8671383
C	3.8493582	2.1283798	0.7098489
F	2.3478324	0.8984639	2.0026588
C	3.2806118	2.7813212	-1.5325348
F	1.2250766	2.1519118	-2.4507922
C	2.3244865	-1.5939348	-0.6628330
C	1.8348996	-2.2169482	1.5642145
H	-0.7895251	-2.4245340	1.1647437
C	-1.6445465	-0.7754260	2.1355281
P	-2.2643934	-1.7048096	-0.5031679
C	4.1846076	2.7792798	-0.4737721
F	4.7146580	2.1375592	1.7435193
F	3.5988375	3.4073735	-2.6828669
C	3.5097839	-2.3198764	-0.6185163
F	2.0166847	-1.0176187	-1.8464088
C	3.0058964	-2.9626647	1.6357957
F	1.0739500	-2.1704862	2.6877997
H	-2.0303006	0.2339880	1.9516822
H	-0.8464575	-0.7041069	2.8838175
O	-2.6848940	-1.6433832	2.5955152
H	-1.7905575	-0.9280452	-1.5631687
C	-4.0754161	-1.2098769	-0.4073997
C	-1.9728989	-3.4501868	-1.0832203
F	5.3680102	3.4056970	-0.5911964
C	3.8593225	-3.0118598	0.5377595
F	4.3071868	-2.3912710	-1.7026108
F	3.3356655	-3.6113031	2.7700075
C	-3.2180081	-1.2155045	3.8512815
C	-4.2296678	0.0747374	0.4295173
C	-4.5135380	-0.8918531	-1.8551279
C	-4.9579658	-2.3104965	0.2011409
C	-2.2979073	-4.4630059	0.0307495
C	-2.7923742	-3.7622849	-2.3480009
C	-0.4728842	-3.5435897	-1.4367284
F	5.0006657	-3.7214247	0.5906400
H	-3.9976830	-1.9283870	4.1254485
H	-2.4345686	-1.2083718	4.6207232

H	-3.6510999	-0.2072086	3.7738777
H	-5.2415074	0.4598898	0.2603443
H	-4.1145893	-0.1341580	1.4921263
H	-3.5217114	0.8511437	0.1324676
H	-4.4458464	-1.7539303	-2.5201247
H	-5.5613314	-0.5726938	-1.8226551
H	-3.9254282	-0.0749330	-2.2827116
H	-5.9779555	-1.9178060	0.2836833
H	-4.9979445	-3.2041112	-0.4265771
H	-4.6119660	-2.5829068	1.2006690
H	-1.7531187	-4.2480469	0.9545787
H	-3.3639899	-4.4974180	0.2607477
H	-1.9908938	-5.4560958	-0.3151043
H	-2.5909963	-3.0455025	-3.1500798
H	-2.4955263	-4.7551649	-2.7041917
H	-3.8668312	-3.7873023	-2.1526583
H	0.1637921	-3.4369238	-0.5559719
H	-0.1752403	-2.7903923	-2.1718918
H	-0.2920202	-4.5362032	-1.8642787

TS6

73

Energy = -3098.774690892

C	-1.0128453	1.8924597	0.7329998
C	-1.1515845	2.6453030	1.8979526
C	-1.9845904	2.0991060	-0.2427608
B	0.2250107	0.9196576	0.5134329
C	-2.2039040	3.5302757	2.1111171
F	-0.2413746	2.4987053	2.8911004
C	-3.0466996	2.9833078	-0.0796308
F	-1.9085887	1.4247793	-1.4160547
C	1.6151133	1.6439414	0.2616433
C	0.1495054	-0.5764301	0.5537502
C	-3.1594245	3.6986333	1.1104117
F	-2.3116342	4.2200055	3.2607636
F	-3.9642620	3.1515359	-1.0503119
C	2.7490568	1.3849279	1.0374252
C	1.7835504	2.5970128	-0.7463461
C	1.3349633	-1.3371644	0.0727375
C	-0.9019947	-1.3655091	1.0670763
F	-4.1823298	4.5487400	1.2909243
C	3.9746759	2.0086725	0.8254028
F	2.6793260	0.5120533	2.0684386
C	2.9929756	3.2350808	-1.0002738
F	0.7427423	2.9070838	-1.5539027
C	1.8387570	-1.1716390	-1.2233326
C	2.0255886	-2.2509569	0.8798631
H	-0.6828242	-2.4207168	1.2204645
C	-1.9081941	-0.8790306	2.0695256
P	-2.4448403	-2.1187721	-0.7467224
C	4.0974014	2.9374066	-0.2052837
F	5.0362807	1.7324311	1.6048131
F	3.1102597	4.1279279	-1.9996808
C	2.9534030	-1.8577878	-1.6940688
F	1.2098221	-0.3451422	-2.0874004

C	3.1417810	-2.9545162	0.4390180
F	1.6260577	-2.4575434	2.1543181
H	-2.3812445	0.0652520	1.7756391
H	-1.3652282	-0.7011894	3.0136991
O	-2.8876303	-1.8947958	2.2775370
H	-1.9338824	-1.4264854	-1.8667311
C	-4.2931032	-1.7810514	-0.9591018
C	-1.9836485	-3.8842575	-1.2062832
F	5.2719107	3.5462227	-0.4278963
C	3.6101410	-2.7570293	-0.8577919
F	3.3876517	-1.6785866	-2.9549178
F	3.7803484	-3.8108961	1.2564712
C	-3.7557408	-1.5719310	3.3659113
C	-4.5655477	-0.4248857	-0.2804209
C	-4.6787763	-1.6649954	-2.4445775
C	-5.1276730	-2.8618729	-0.2544385
C	-2.2538054	-4.8046041	-0.0004269
C	-2.6994231	-4.4186190	-2.4571385
C	-0.4686047	-3.8608703	-1.4882656
F	4.6846704	-3.4301480	-1.2988560
H	-4.4784483	-2.3859746	3.4439871
H	-3.1910176	-1.4876375	4.3046825
H	-4.2869939	-0.6264059	3.1816901
H	-5.6298995	-0.1833929	-0.3892508
H	-4.3290768	-0.4612347	0.7846818
H	-3.9929541	0.3773233	-0.7495421
H	-4.5444902	-2.6023120	-2.9867301
H	-5.7384327	-1.3846700	-2.5107226
H	-4.0932950	-0.8864431	-2.9437846
H	-6.1813575	-2.5576679	-0.2707361
H	-5.0543402	-3.8310155	-0.7549073
H	-4.8204308	-2.9792509	0.7883466
H	-1.7637826	-4.4345734	0.9055366
H	-3.3215767	-4.9004645	0.2094785
H	-1.8592625	-5.8040557	-0.2196896
H	-2.5229112	-3.7773859	-3.3261624
H	-2.3025168	-5.4160330	-2.6868210
H	-3.7770100	-4.5182779	-2.3064864
H	0.1051940	-3.5436024	-0.6140768
H	-0.2231002	-3.1973001	-2.3234908
H	-0.1446916	-4.8749924	-1.7510091

E-**1g**
45
Energy = -2440.880287531

C	2.0327327	0.1022111	0.3617173
C	-0.3132069	1.1877102	-0.4545058
C	-1.5548952	-1.5548703	0.2934952
C	2.9023877	0.9767268	-0.3063560
C	2.5956707	-0.6123411	1.4297368
C	-1.2515311	1.1667781	-1.4966374
C	-0.2102988	2.4025575	0.2390291
C	-1.9803194	-0.8631328	1.4334961
C	-2.5487245	-2.2475120	-0.4101742
C	4.2415903	1.1234315	0.0329177
C	3.9244484	-0.4742467	1.8142555

C	-2.0349496	2.2636929	-1.8359205
C	-0.9892388	3.5144190	-0.0568375
C	-3.3000629	-0.8509202	1.8672445
C	-3.8801461	-2.2522275	-0.0033636
C	4.7530717	0.3945987	1.1059245
C	-1.9041755	3.4441000	-1.1065323
C	-4.2586905	-1.5540294	1.1410908
F	2.4564467	1.6940072	-1.3594526
F	1.8359029	-1.4500616	2.1627957
F	-1.3979753	0.0586430	-2.2514802
F	0.6487978	2.5188639	1.2729554
F	-1.0691825	-0.1782729	2.1650182
F	-2.2453753	-2.9123163	-1.5414472
F	5.0425833	1.9548108	-0.6507820
F	4.4170112	-1.1631130	2.8553276
F	-2.9062702	2.2023695	-2.8550676
F	-0.8715535	4.6493614	0.6494466
F	-3.6540574	-0.1797616	2.9753678
F	-4.8057377	-2.9196678	-0.7114414
F	6.0349072	0.5321653	1.4576897
F	-2.6512336	4.5082842	-1.4163282
F	-5.5370589	-1.5611508	1.5432217
B	0.5364586	-0.0726967	-0.0662195
C	-0.1283310	-1.4825405	-0.1192509
C	0.4899347	-2.6084391	-0.5455832
H	-0.0619329	-3.5464491	-0.5802466
C	1.9021978	-2.7516901	-1.0180588
H	2.5397284	-3.0872674	-0.1784790
H	2.3207552	-1.8086756	-1.3960877
C	3.2322566	-3.9838830	-2.5238720
H	3.1521605	-4.7540016	-3.2926457
H	3.6653581	-3.0718417	-2.9605751
H	3.8848217	-4.3374377	-1.7117206
O	1.9086234	-3.7426394	-2.0443174

TS7

45

Energy = -2440.876447595

C	1.9012370	-0.6618540	0.1656540
C	-0.6108560	-0.6720450	-0.7688820
C	-1.4005690	1.3803940	1.3141620
C	2.2651880	-2.0070130	0.2159980
C	2.9220410	0.2461420	-0.1131900
C	-1.8389670	-1.2697530	-0.4610170
C	-0.3397110	-0.5014410	-2.1315000
C	-1.5634930	2.2093910	0.1993290
C	-2.5091450	1.2523920	2.1586210
C	3.5755970	-2.4367650	0.0351570
C	4.2404380	-0.1447850	-0.3234070
C	-2.7517190	-1.6674540	-1.4306200
C	-1.2375020	-0.8623170	-3.1301310
C	-2.7529950	2.8704750	-0.0821720
C	-3.7153130	1.8987850	1.9015450
C	4.5675490	-1.4971210	-0.2408010
C	-2.4482360	-1.4546090	-2.7747210
C	-3.8381950	2.7116370	0.7772060

F	1.3237080	-2.9435540	0.4602200
F	2.6347280	1.5649790	-0.1910410
F	-2.1600010	-1.5102130	0.8276940
F	0.8136890	0.0809620	-2.5200260
F	-0.5234710	2.3884470	-0.6450330
F	-2.4492990	0.4548510	3.2426370
F	3.8936770	-3.7397760	0.1203440
F	5.1951560	0.7593220	-0.5986380
F	-3.9113150	-2.2527600	-1.0925910
F	-0.9531250	-0.6516640	-4.4245330
F	-2.8608750	3.6627700	-1.1608310
F	-4.7633320	1.7397900	2.7259890
F	5.8338160	-1.8941960	-0.4272170
F	-3.3166890	-1.8225230	-3.7228590
F	-4.9925530	3.3443770	0.5271560
B	0.4003650	-0.2178420	0.3472290
C	-0.1163680	0.6540430	1.5283880
C	0.4520560	0.7260130	2.7564410
H	-0.0283360	1.3420560	3.5144350
C	1.6884810	-0.0018780	3.2057070
H	1.9375190	0.2966950	4.2335120
H	2.5507690	0.2409090	2.5664910
C	2.5489340	-2.1639170	3.6161110
H	2.7080980	-2.0150140	4.6932760
H	2.3211460	-3.2126010	3.4181790
H	3.4631790	-1.8749030	3.0769540
O	1.4257740	-1.4090010	3.1556550

Ec-**1g**
45
Energy = -2440.902146844

C	1.9477655	-0.4335240	0.0902978
C	-0.6053724	-1.5151930	0.1309629
C	-0.9305765	1.6154034	0.9720690
C	2.2846624	-1.0121834	-1.1378940
C	2.9382156	0.3999981	0.6230954
C	-1.2582636	-2.6594202	0.5882483
C	-1.1468397	-0.9696309	-1.0365789
C	-0.3400512	2.6524647	0.2457362
C	-2.3281390	1.5663256	0.9615652
C	3.4711215	-0.7429311	-1.8177109
C	4.1369105	0.6952548	-0.0157096
C	-2.3598513	-3.2247123	-0.0525559
C	-2.2474477	-1.4905006	-1.7051698
C	-1.0871600	3.5961202	-0.4506738
C	-3.1022634	2.4903818	0.2649957
C	4.4026690	0.1234536	-1.2565039
C	-2.8640407	-2.6345224	-1.2055229
C	-2.4775966	3.5126787	-0.4436626
F	1.4624736	-1.9058402	-1.7357119
F	2.7677371	0.9525327	1.8504395
F	-0.8425947	-3.3065176	1.7112752
F	-0.5708443	0.1328802	-1.5835170
F	1.0037775	2.7594804	0.2067314
F	-2.9721479	0.5832132	1.6259182
F	3.7315809	-1.3262607	-3.0015757

F	5.0419365	1.5123768	0.5536332
F	-2.9404754	-4.3365092	0.4379263
F	-2.7174933	-0.9086246	-2.8236976
F	-0.4795461	4.5854724	-1.1275630
F	-4.4438131	2.4033392	0.2733920
F	5.5534112	0.3876503	-1.8917135
F	-3.9270424	-3.1633145	-1.8321442
F	-3.2103708	4.4168228	-1.1109487
B	0.5630079	-0.6851810	0.9040283
C	-0.1350608	0.5698540	1.6512119
C	-0.0751990	0.4662208	2.9837580
H	-0.5375155	1.1422281	3.6974552
C	0.7004303	-0.7031778	3.4819626
H	0.1403023	-1.3619084	4.1547224
H	1.6611128	-0.4352298	3.9391887
C	2.0246508	-2.4616940	2.3219105
H	1.7818235	-3.1391013	3.1412572
H	2.0095143	-2.9905986	1.3713248
H	2.9874735	-1.9703983	2.4818658
O	0.9759988	-1.4602258	2.2537691