*Electronic Supplementary Information*

# Zintl cluster supported low coordinate Rh(I) centers for catalytic H/D exchange between $H_2$ and $D_2$

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# 1. NMR Spectra

## 1.1. NMR spectra for [Rh(PMe$_3$){Ge$_9$(Hyp)$_3$}] (**1a**).

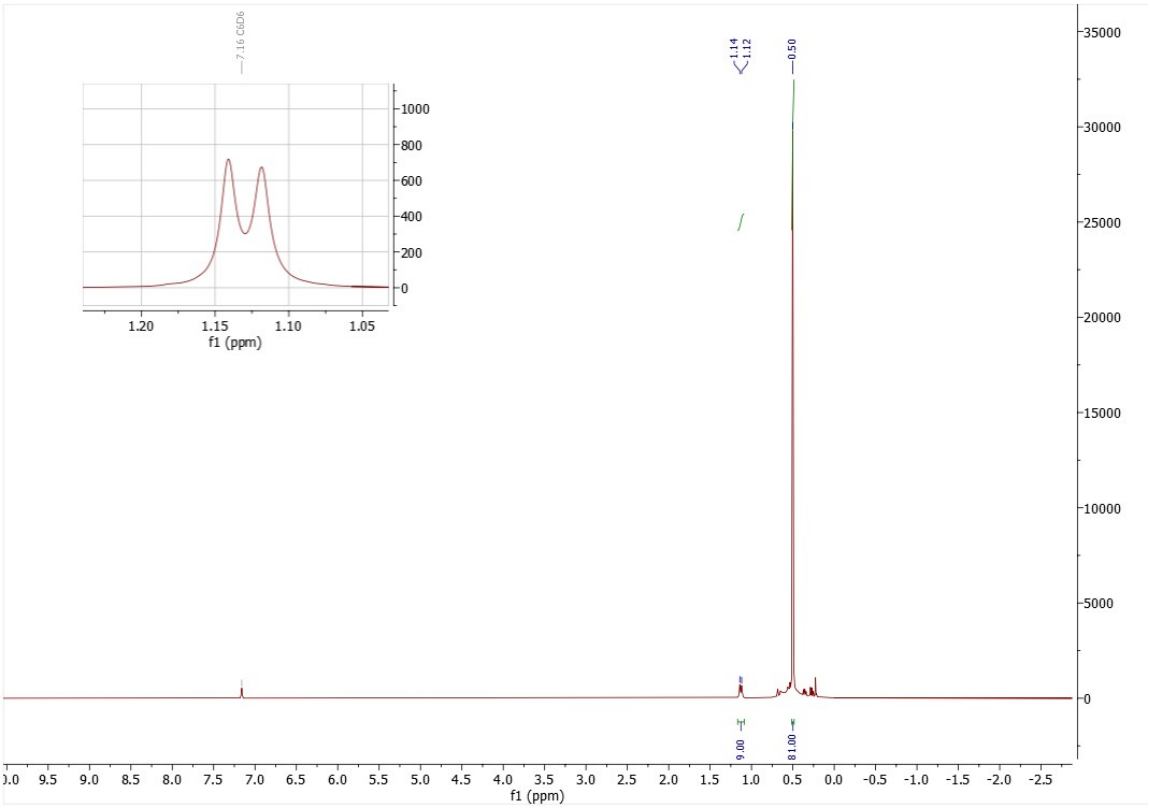



**Figure S1.** $^{1}$H NMR spectrum ($C_6D_6$, 298 K, 400 MHz) of [Rh(PMe$_3$){Ge$_9$(Hyp)$_3$}] (**1a**).

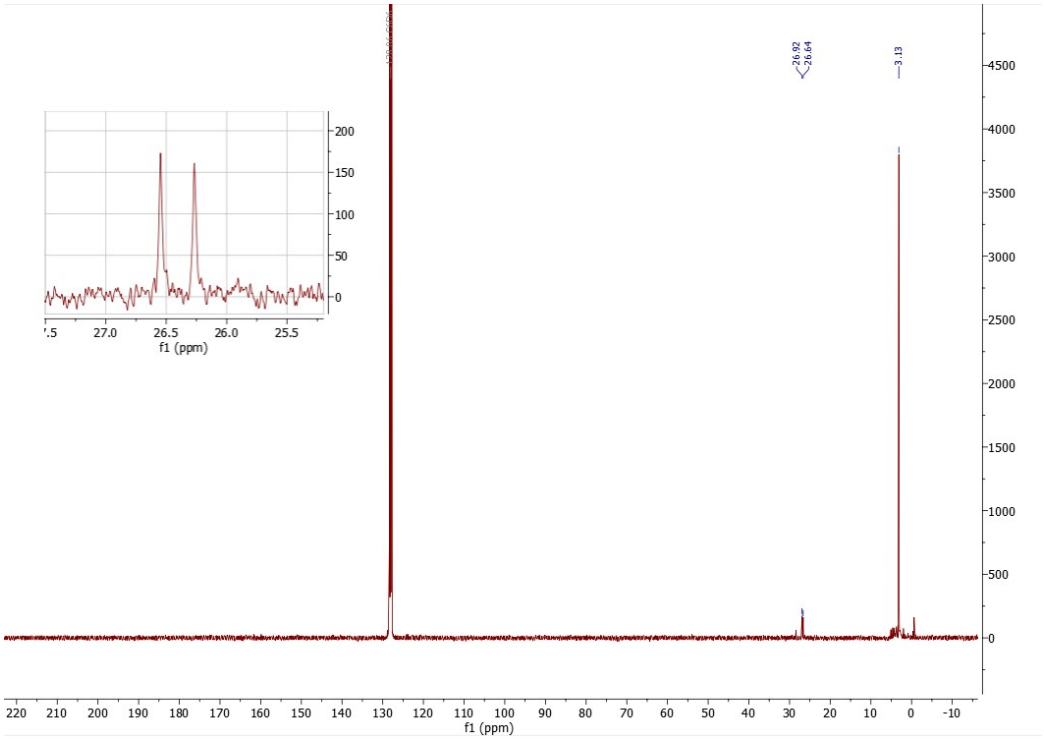



**Figure S2.** $^{13}$C{$^{1}$H} NMR spectrum ($C_6D_6$, 298 K, 100.64 MHz) of [Rh(PMe$_3$){Ge$_9$(Hyp)$_3$}] (**1a**).

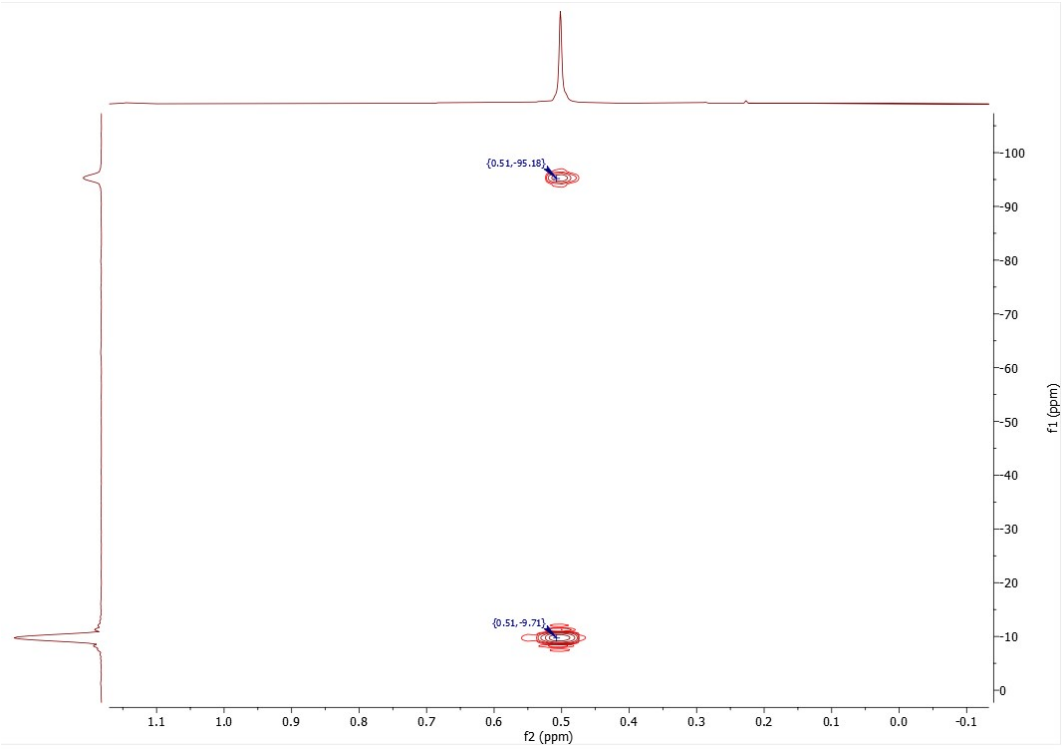



**Figure S3.** $^{1}H/^{29}Si$ HMBC NMR spectrum ($C_6D_6$, 298 K, 99.32 MHz) of [Rh(PMe$_3$){Ge$_9$(Hyp)$_3$}] (**1a**).

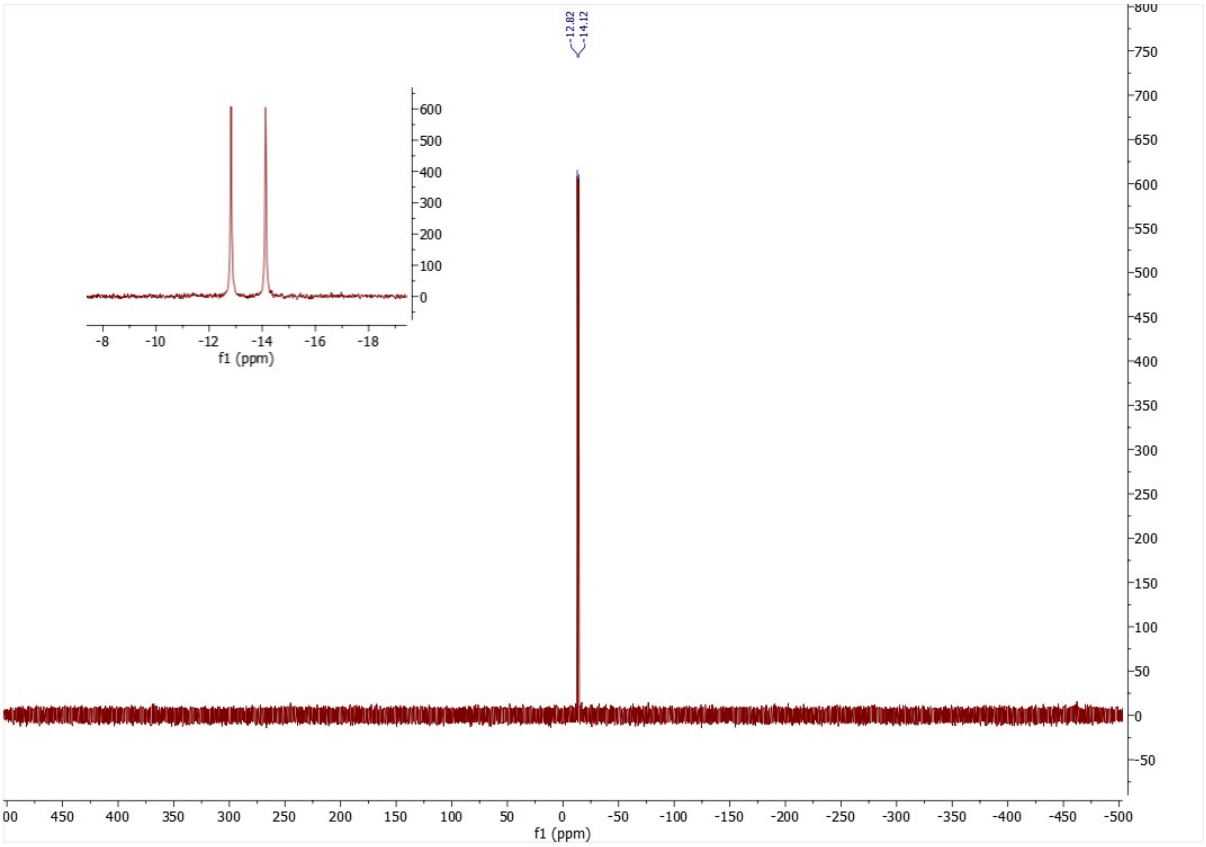



**Figure S4.** $^{31}P\{^{1}H\}$ NMR spectrum ($C_6D_6$, 298 K, 202.39 MHz) of [Rh(PMe$_3$){Ge$_9$(Hyp)$_3$}] (**1a**).

1.2. NMR spectra for [Rh(PPh$_3$){Ge$_9$(Hyp)$_3$}] (**1b**).

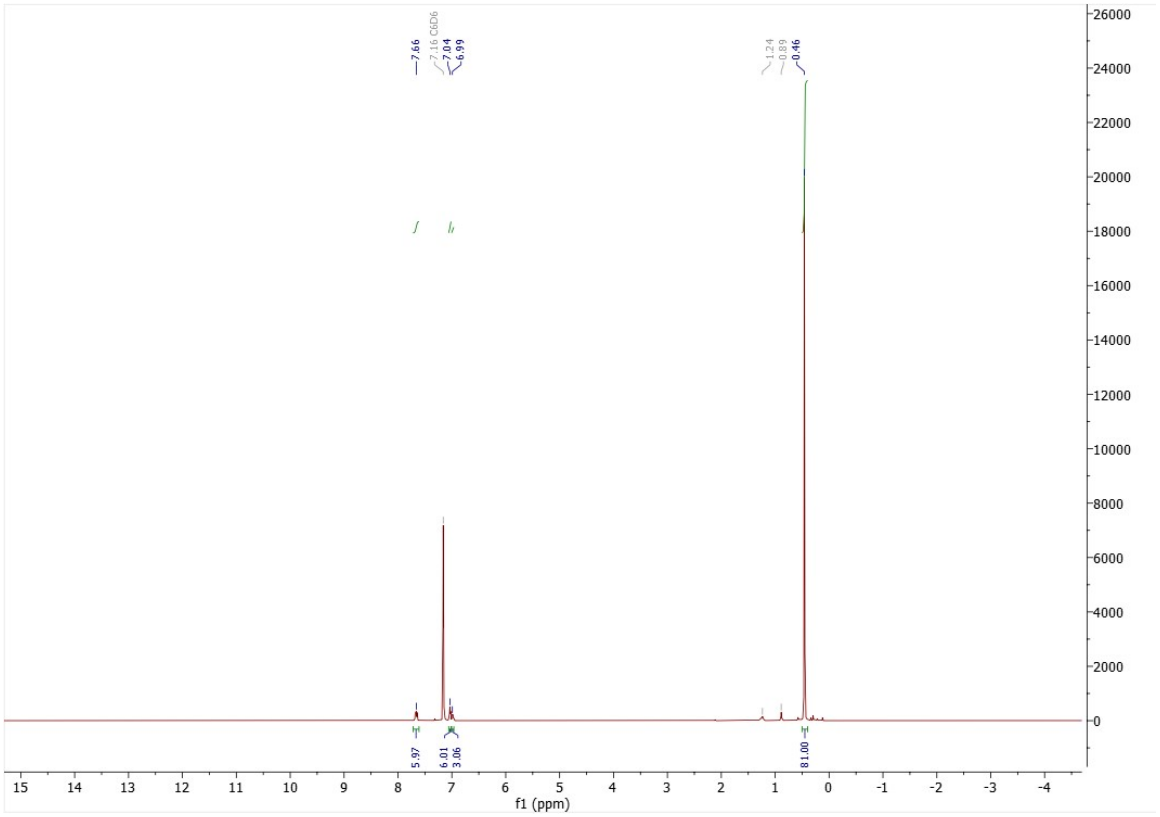



**Figure S5.** $^{1}$H NMR spectrum ($C_6D_6$, 298 K, 500 MHz) of [Rh(PPh$_3$){Ge$_9$(Hyp)$_3$}] (**1b**).

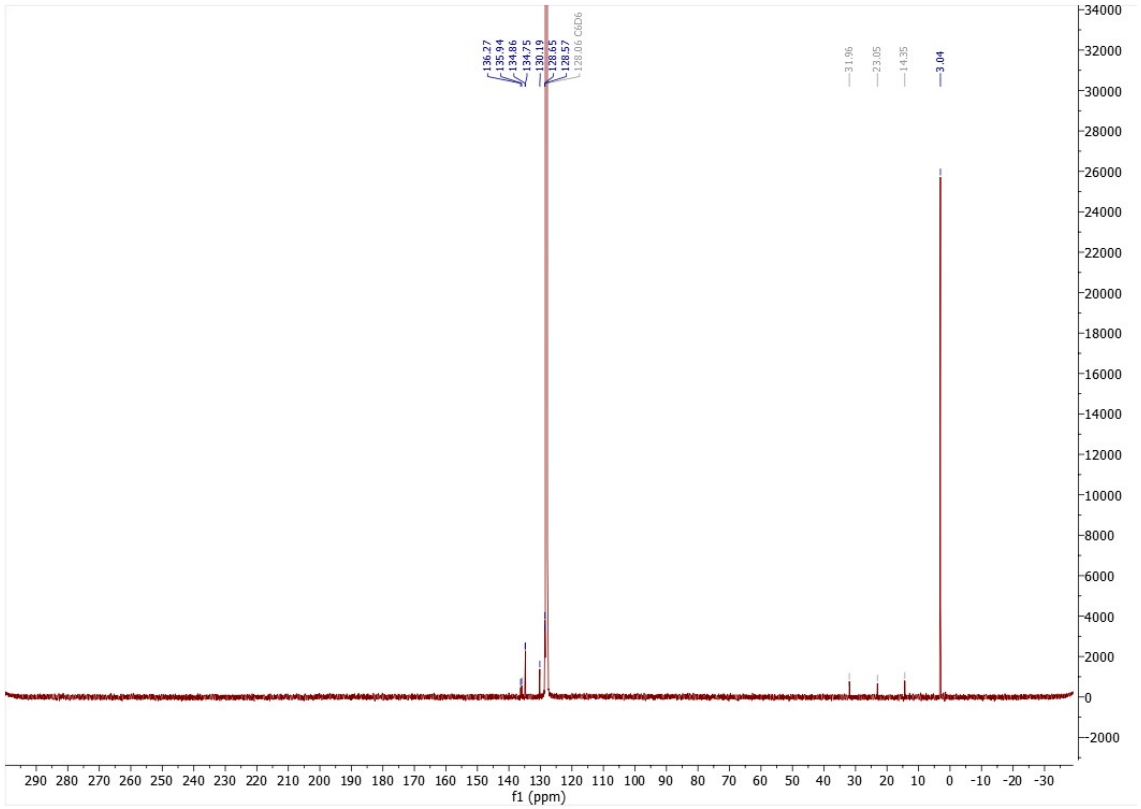



**Figure S6.** $^{13}$C{$^{1}$H} NMR spectrum ($C_6D_6$, 298 K, 125.81 MHz) of [Rh(PPh$_3$){Ge$_9$(Hyp)$_3$}] (**1b**).

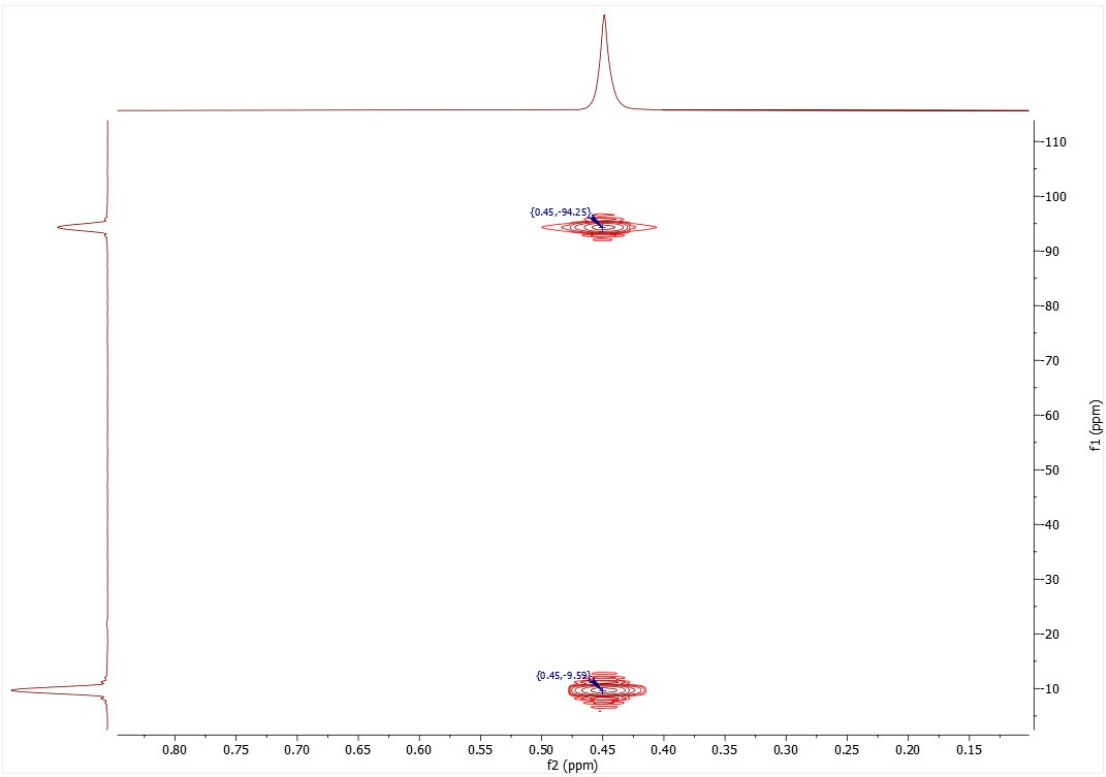



**Figure S7.** $^{1}H/^{29}Si$ HMBC NMR spectrum ($C_6D_6$, 298 K, 99.32 MHz) of [Rh(PPh$_3$){Ge$_9$(Hyp)$_3$}] (**1b**).

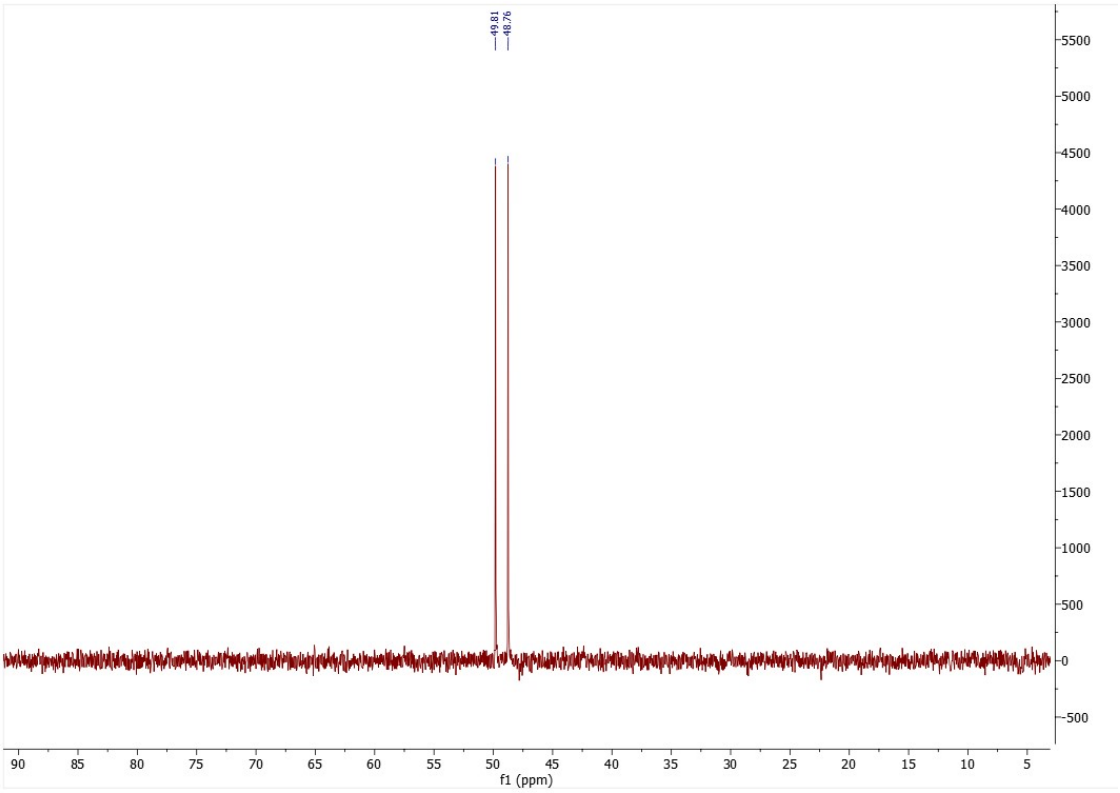



**Figure S8.** $^{31}P\{^{1}H\}$ NMR spectrum ($C_6D_6$, 298 K, 202.39 MHz) of [Rh(PPh$_3$){Ge$_9$(Hyp)$_3$}] (**1b**).

1.3. NMR spectra for [Rh(IMe$_4$){Ge$_9$(Hyp)$_3$}] (**1c**).

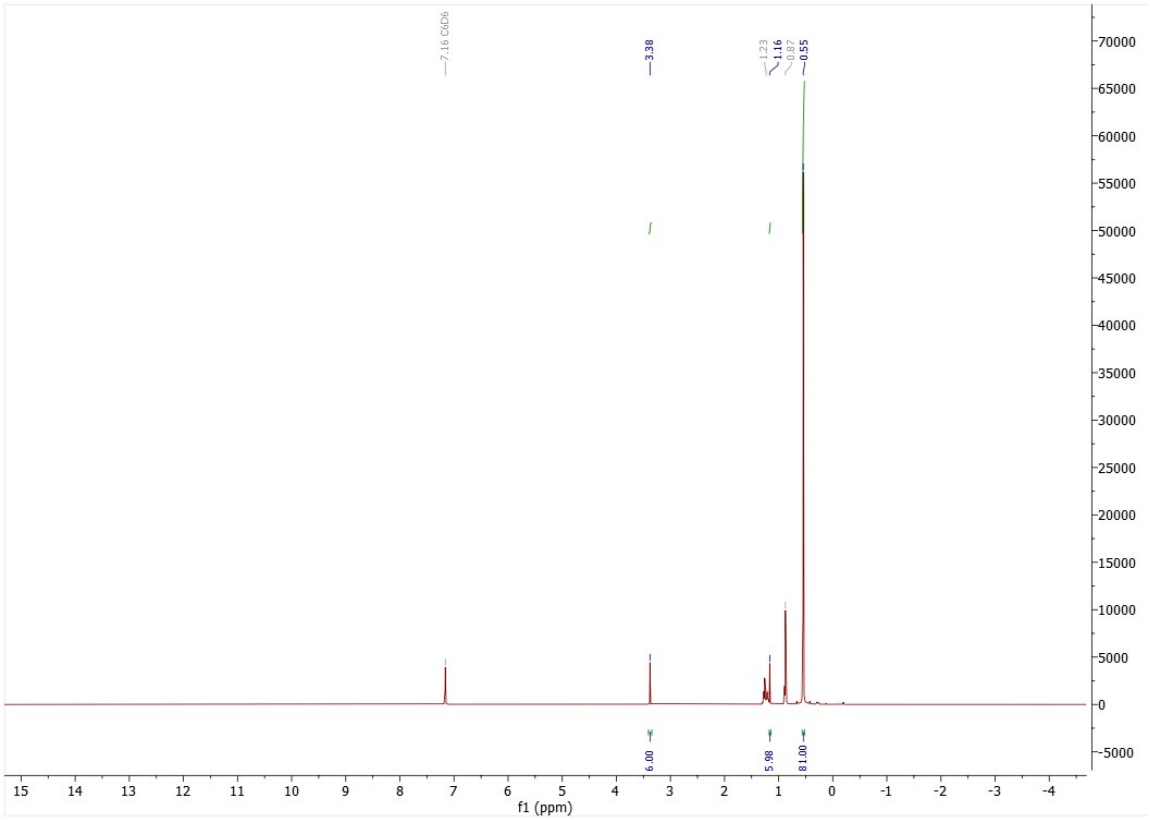



**Figure S9.** $^{1}$H NMR spectrum ($C_6D_6$, 298 K, 500 MHz) of [Rh(IMe$_4$){Ge$_9$(Hyp)$_3$}] (**1c**).

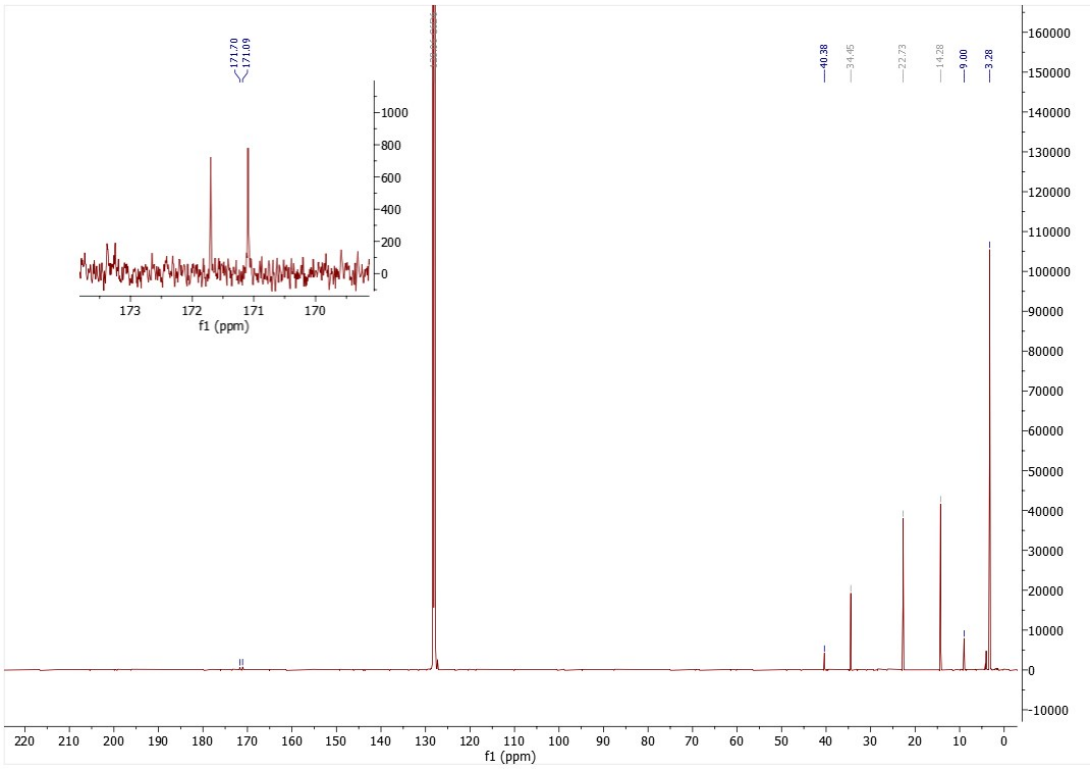



**Figure S10.** $^{13}$C{$^{1}$H} NMR spectrum ($C_6D_6$, 298 K, 125.81 MHz) of [Rh(IMe$_4$){Ge$_9$(Hyp)$_3$}] (**1c**).

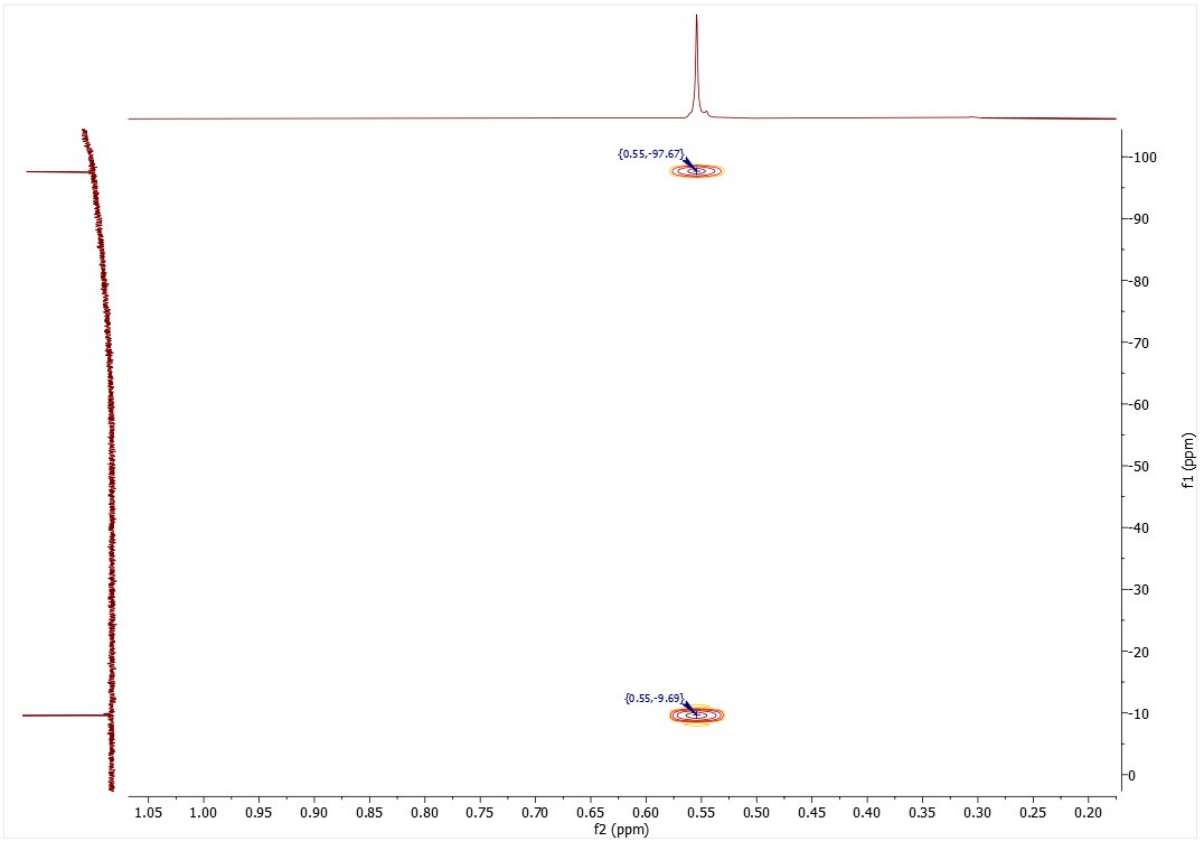



**Figure S11.** $^{1}H/^{29}Si$ HMBC NMR spectrum ($C_6D_6$, 298 K, 99.32 MHz) of [Rh(IMe$_4$){Ge$_9$(Hyp)$_3$}] (**1c**).

1.4. NMR spectra for [Rh{$Ge_9(Hyp)_3$}(μ-H)$_2$W(Cp)$_2$] (**1d**).

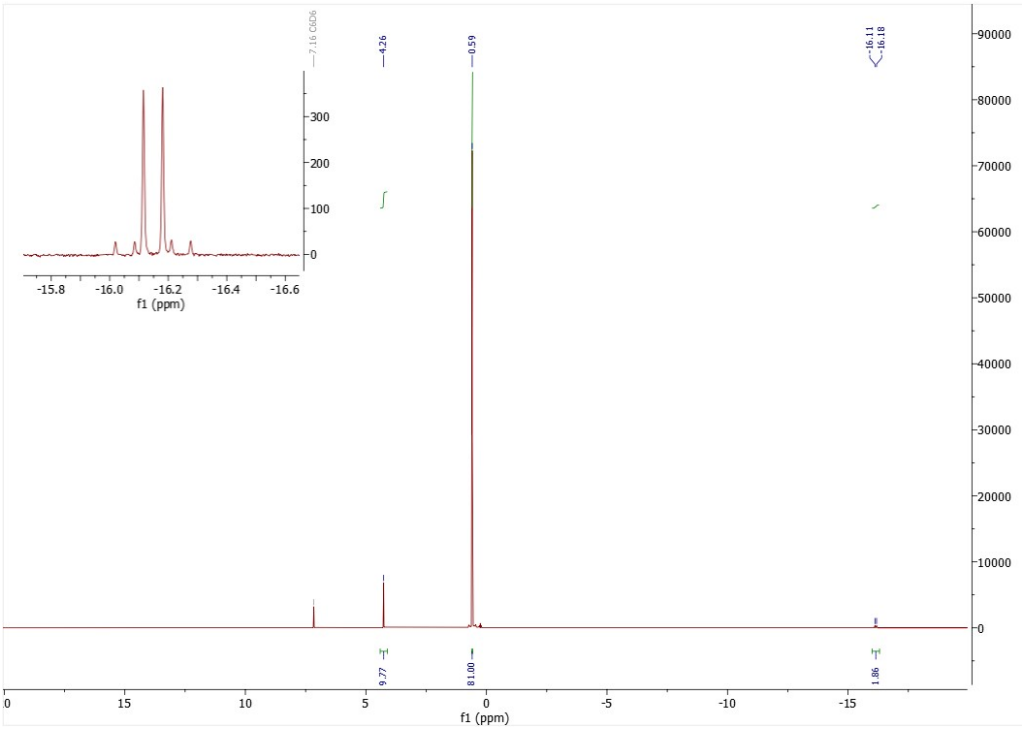



**Figure S12.** $^1$H NMR spectrum ($C_6D_6$, 298 K, 400.16 MHz) of [Rh{$Ge_9(Hyp)_3$}(μ-H)$_2$W(Cp)$_2$] (**1d**).

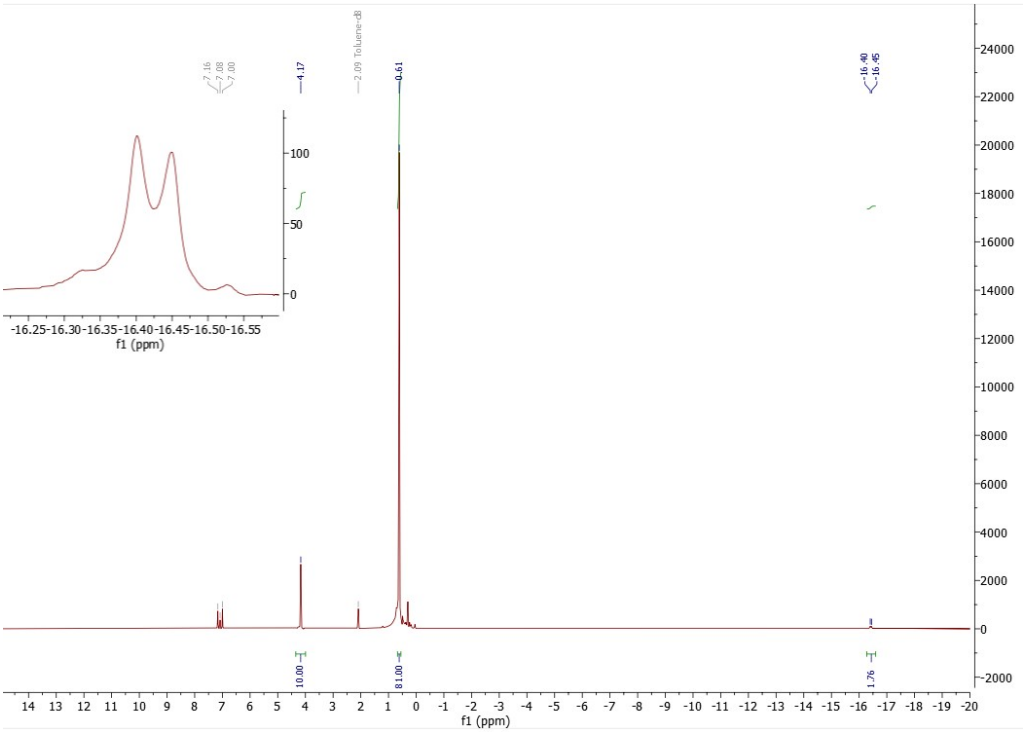



**Figure S13.** $^1$H NMR spectrum ($C_6D_6$, 193 K, 499.93 MHz) of [Rh{$Ge_9(Hyp)_3$}(μ-H)$_2$W(Cp)$_2$] (**1d**).

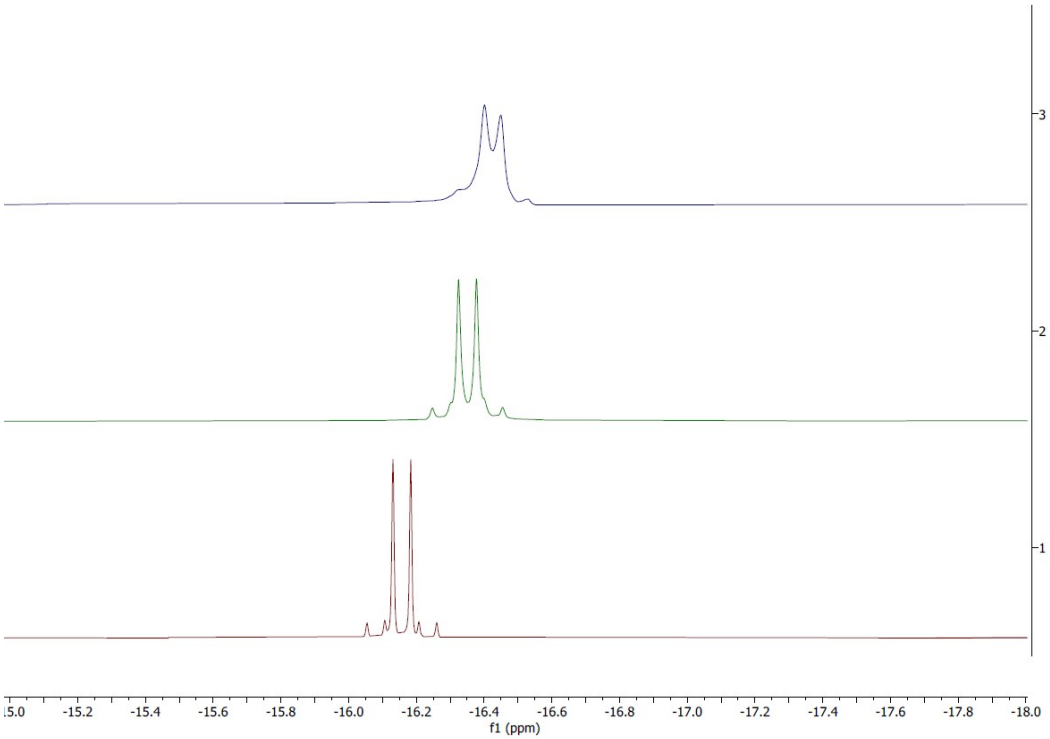



**Figure S14.** Variable temperature $^{1}$H NMR (dihydride region) spectrum ($C_7D_8$, 499.93 MHz) of [Rh{$Ge_9$(Hyp)$_3$}(μ-H)$_2$W(Cp)$_2$] (**1d**). From bottom to top: $T$ = 298, 223, and 193 K.

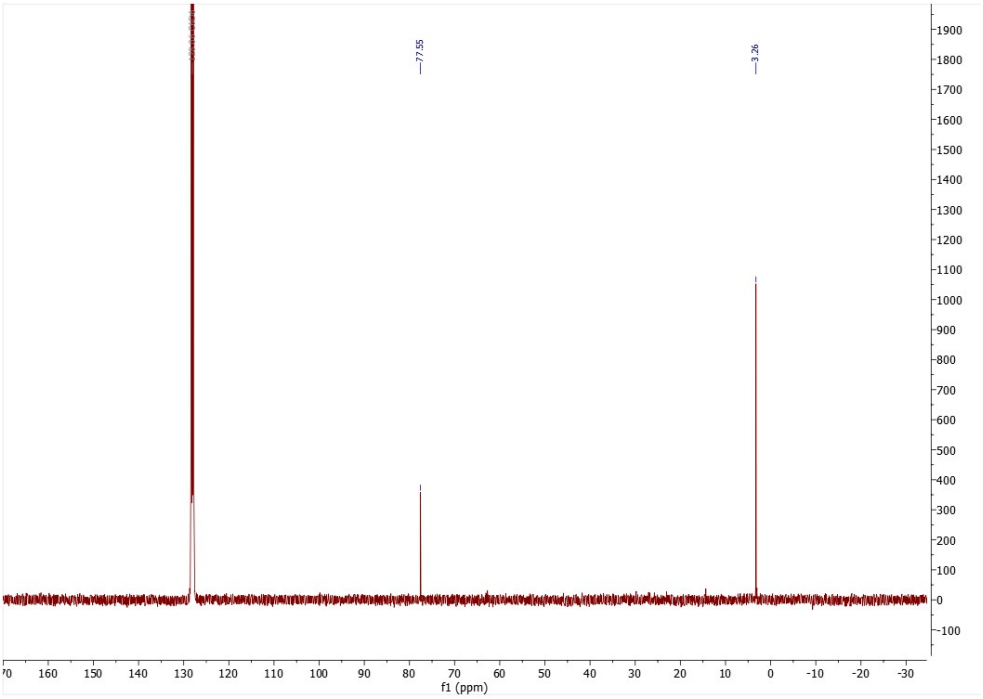



**Figure S15.** $^{13}$C{$^{1}$H} NMR spectrum ($C_6D_6$, 298 K, 100.64 MHz) of [Rh{$Ge_9$(Hyp)$_3$}(μ-H)$_2$W(Cp)$_2$] (**1d**).

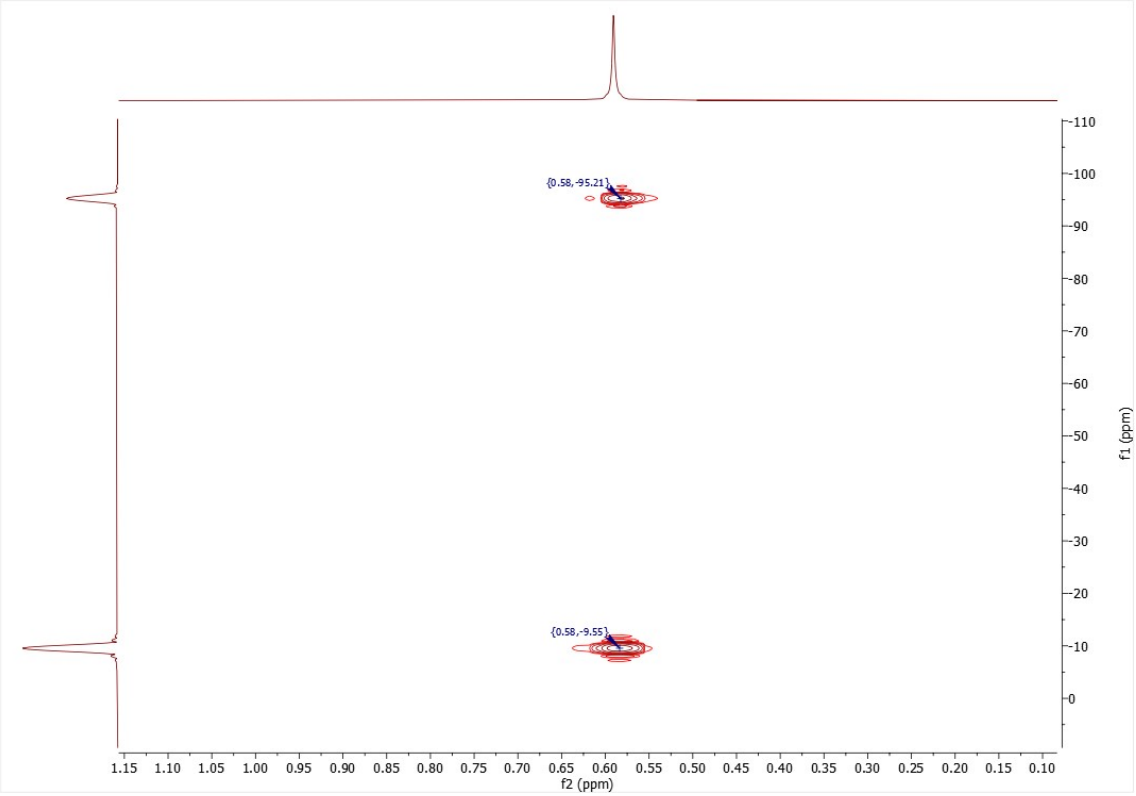



**Figure S16.** $^{29}Si/^{1}H$ HMBC NMR spectrum ($C_6D_6$, 298 K, 79.51 MHz) of [Rh{$Ge_9$(Hyp)$_3$}(μ-H)$_2$W(Cp)$_2$] (**1d**).

1.5. NMR spectra for [RhH($PPh_3$){$Ge_9$(Hyp)$_3$}][$BAr^F_4$] (**2b**[$BAr^F_4$]).

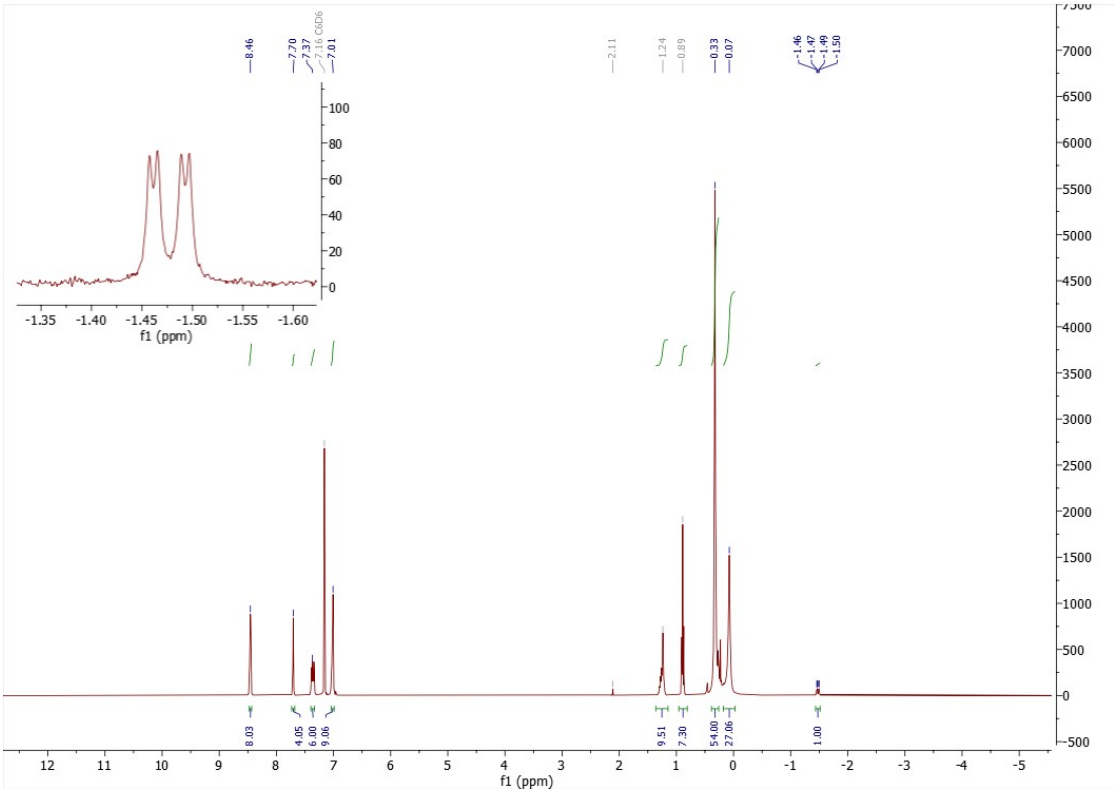



**Figure S17.** $^1$H NMR spectrum ($C_6D_6$, 298 K, 400 MHz) of [RhH($PPh_3$){$Ge_9$(Hyp)$_3$}][$BAr^F_4$] (**2b**[$BAr^F_4$]).

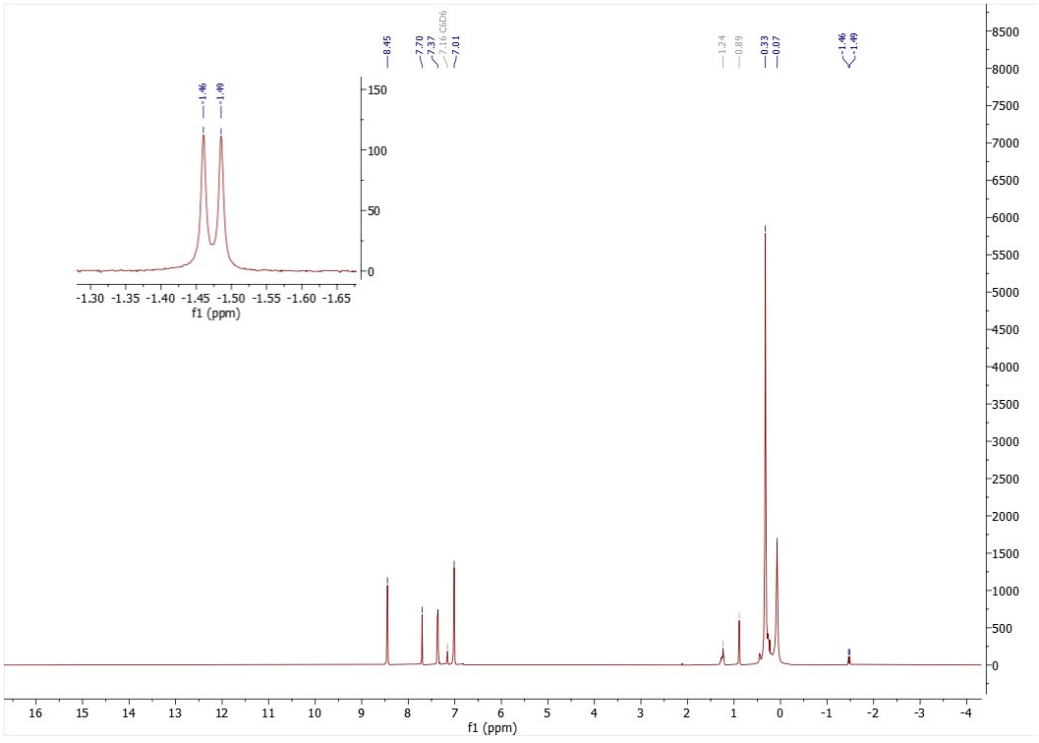



**Figure S18.** $^1$H{$^{31}$P} NMR spectrum ($C_6D_6$, 298 K, 499.94 MHz) of [RhH($PPh_3$){$Ge_9$(Hyp)$_3$}][$BAr^F_4$] (**2b**[$BAr^F_4$]).

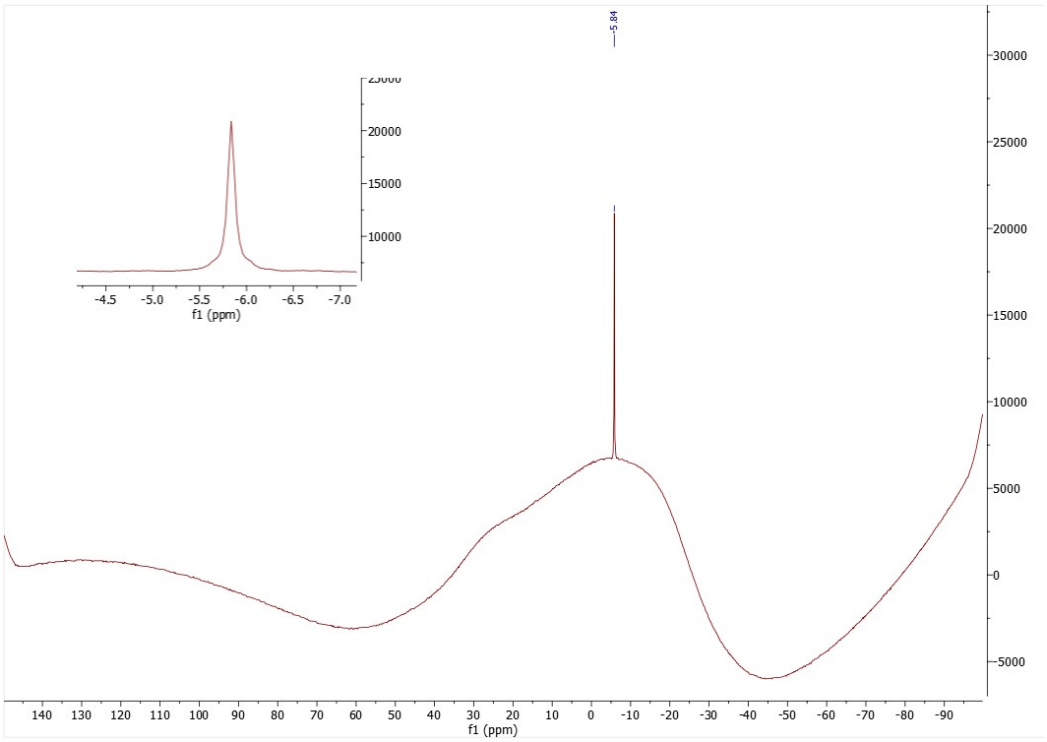



**Figure S19.** $^{11}B\{^{1}H\}$ NMR spectrum ($C_6D_6$, 298 K, 128.40 MHz) of $[RhH(PPh_3)\{Ge_9(Hyp)_3\}][BAr^F{}_4]$ (**2b**$[BAr^F{}_4]$).

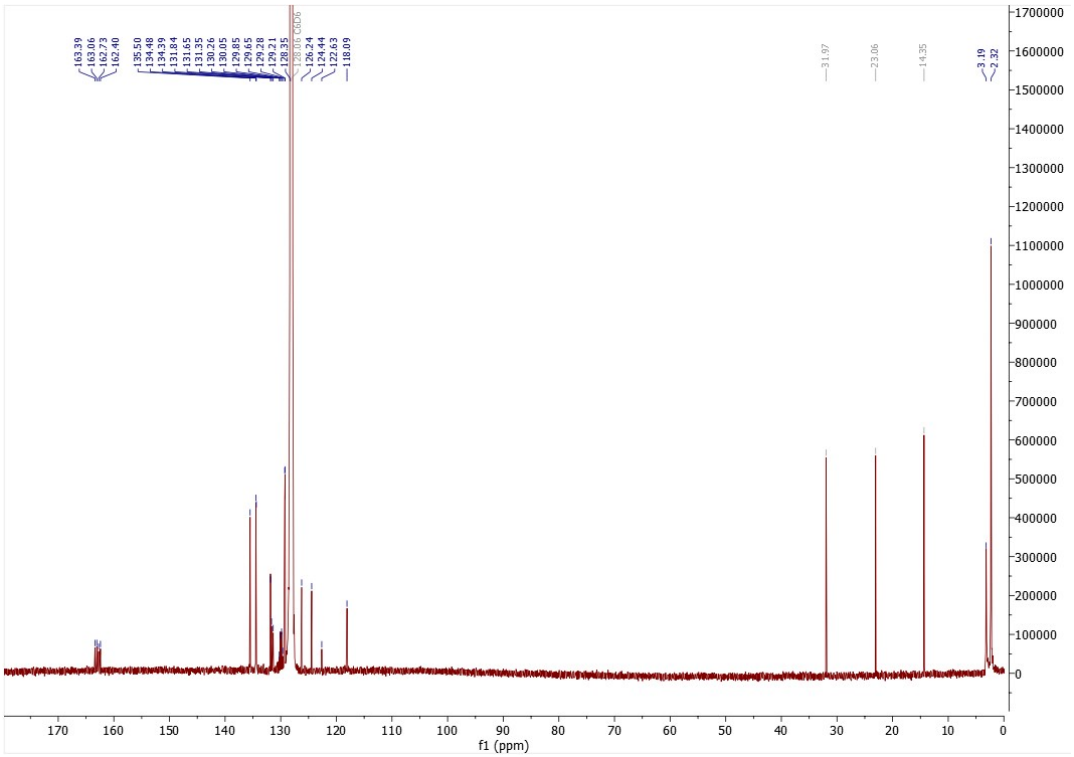



**Figure S20.** $^{13}C\{^{1}H\}$ NMR spectrum ($C_6D_6$, 298 K, 151 MHz) of $[RhH(PPh_3)\{Ge_9(Hyp)_3\}][BAr^F{}_4]$ (**2b**$[BAr^F{}_4]$).

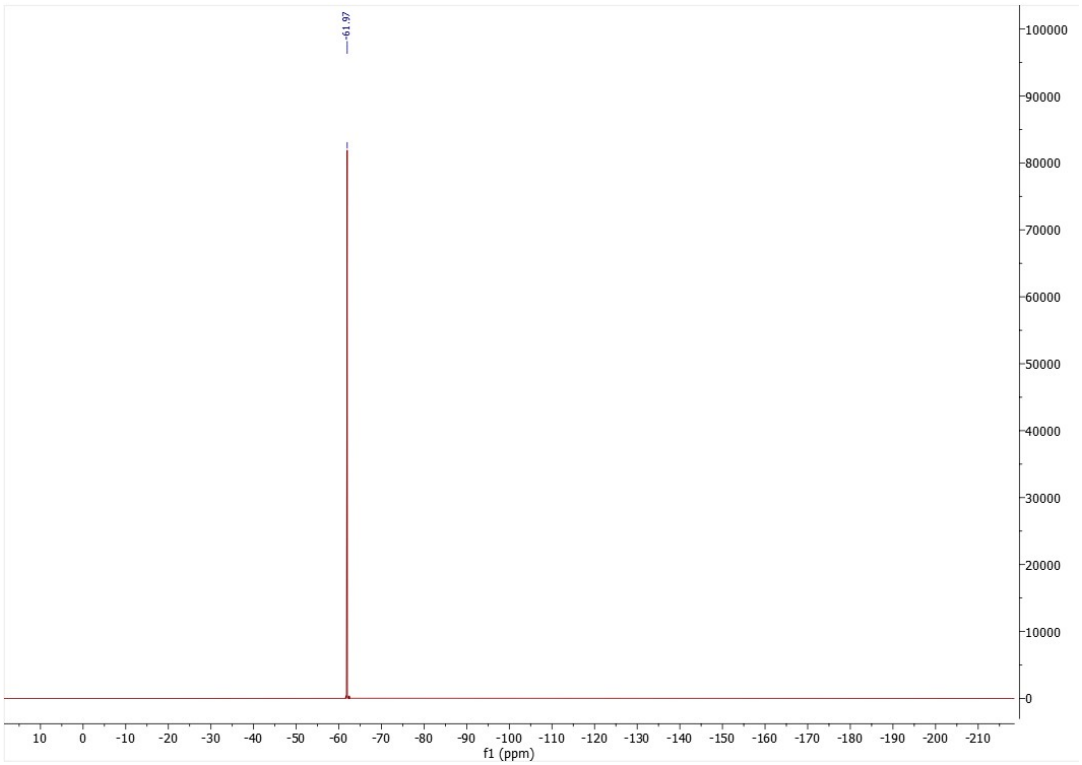



**Figure S21.** $^{19}F\{^{1}H\}$ NMR spectrum ($C_6D_6$, 298 K, 376.53 MHz) of $[RhH(PPh_3)\{Ge_9(Hyp)_3\}][BAr^F{}_4]$ (**2b**$[BAr^F{}_4]$).

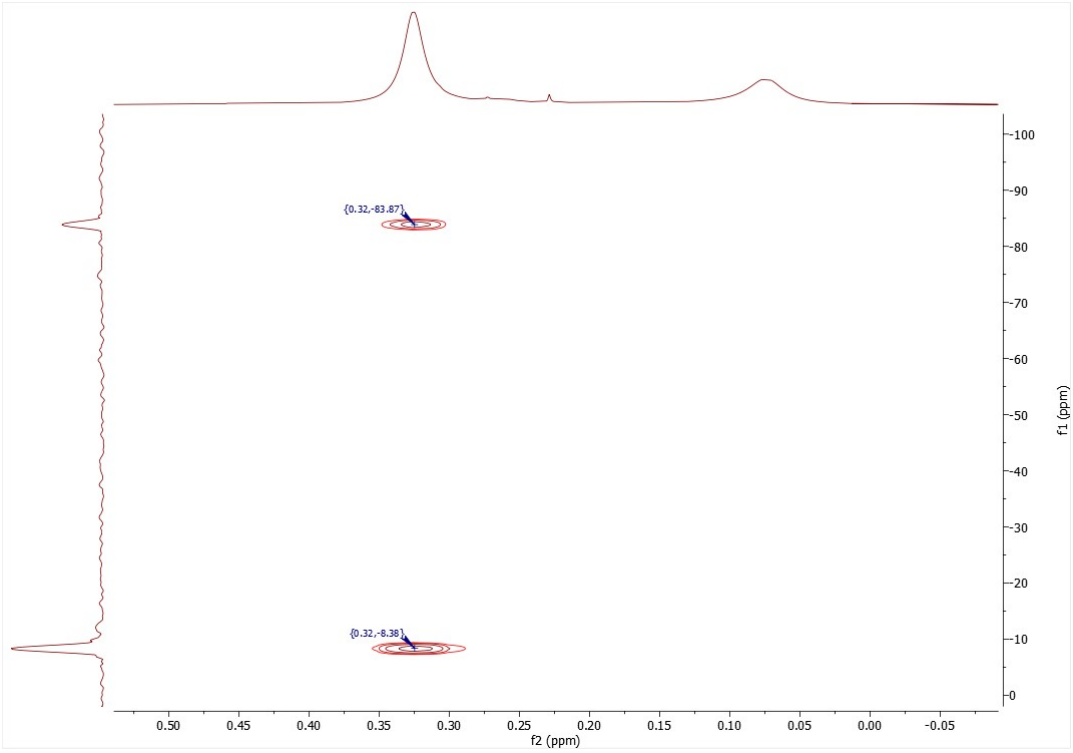



**Figure S22.** $^{1}H/^{29}Si$ HMBC NMR spectrum ($C_6D_6$, 298 K, 79.5 MHz) of $[RhH(PPh_3)\{Ge_9(Hyp)_3\}][BAr^F{}_4]$ (**2b**$[BAr^F{}_4]$).

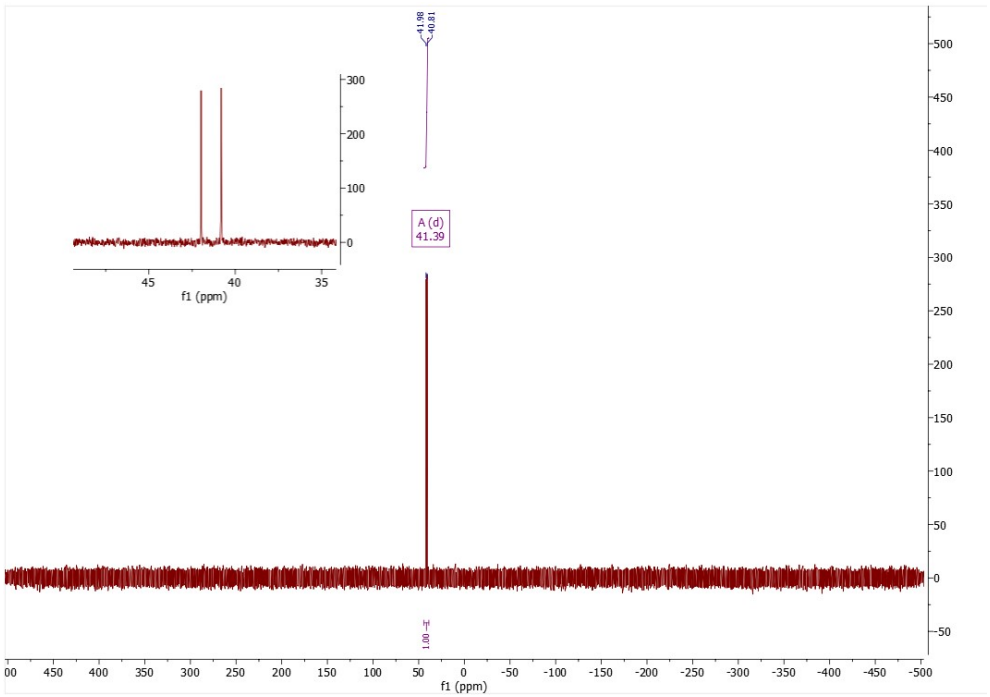



**Figure S23.** $^{31}P\{^{1}H\}$ NMR spectrum ($C_6D_6$, 298 K, 162 MHz) of $[RhH(PPh_3)\{Ge_9(Hyp)_3\}][BAr^F{}_4]$ (**2b**$[BAr^F{}_4]$).

1.6. NMR spectra for [RhH{$Ge_9$(Hyp)$_3$}(μ-H)$_2$W(Cp)$_2$][$BAr^F_4$] (**2d**[$BAr^F_4$]).

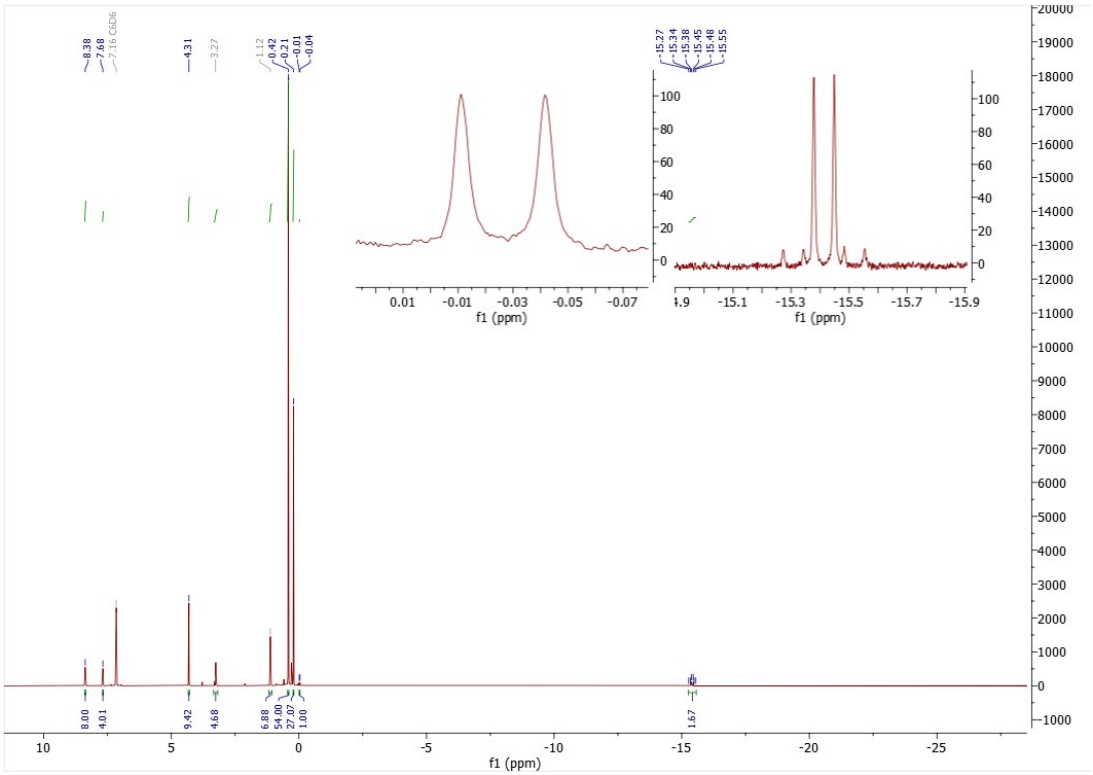



**Figure S24.** $^1$H NMR spectrum ($C_6D_6$, 298 K, 400 MHz) of [RhH{$Ge_9$(Hyp)$_3$}(μ-H)$_2$W(Cp)$_2$][$BAr^F_4$] (**2d**[$BAr^F_4$]).

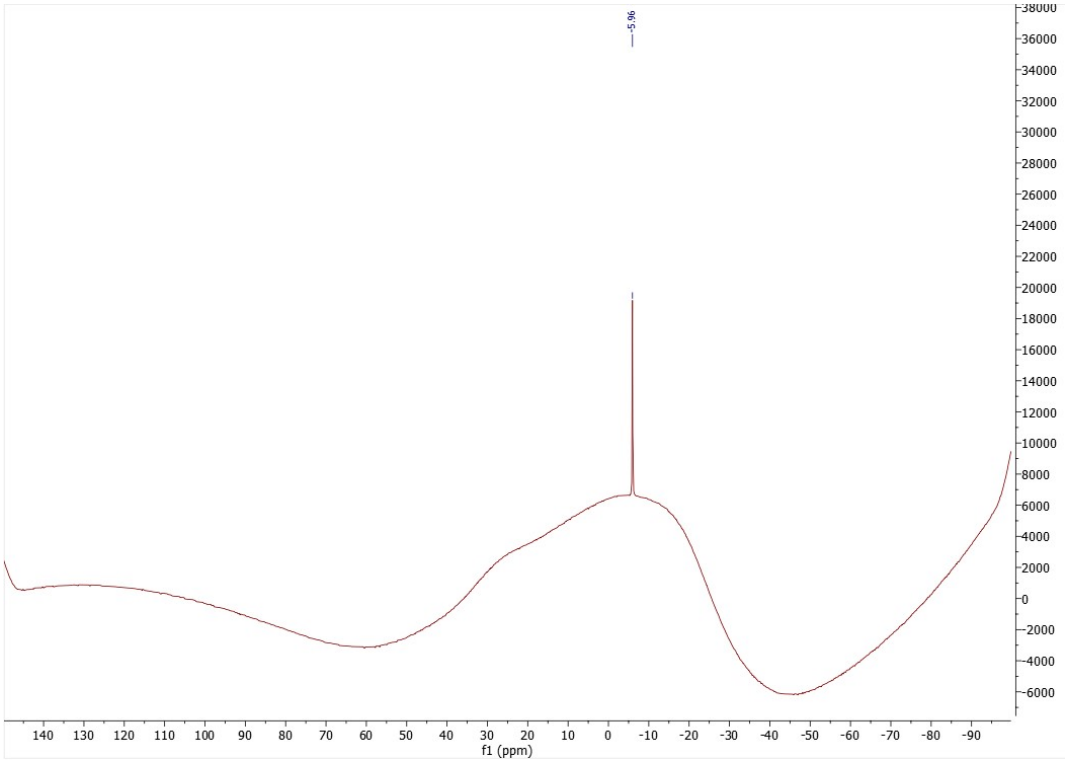



**Figure S25.** $^{11}$B{$^1$H} NMR spectrum ($C_6D_6$, 298 K, 128.40 MHz) of [RhH{$Ge_9$(Hyp)$_3$}(μ-H)$_2$W(Cp)$_2$][$BAr^F_4$] (**2d**[$BAr^F_4$]).

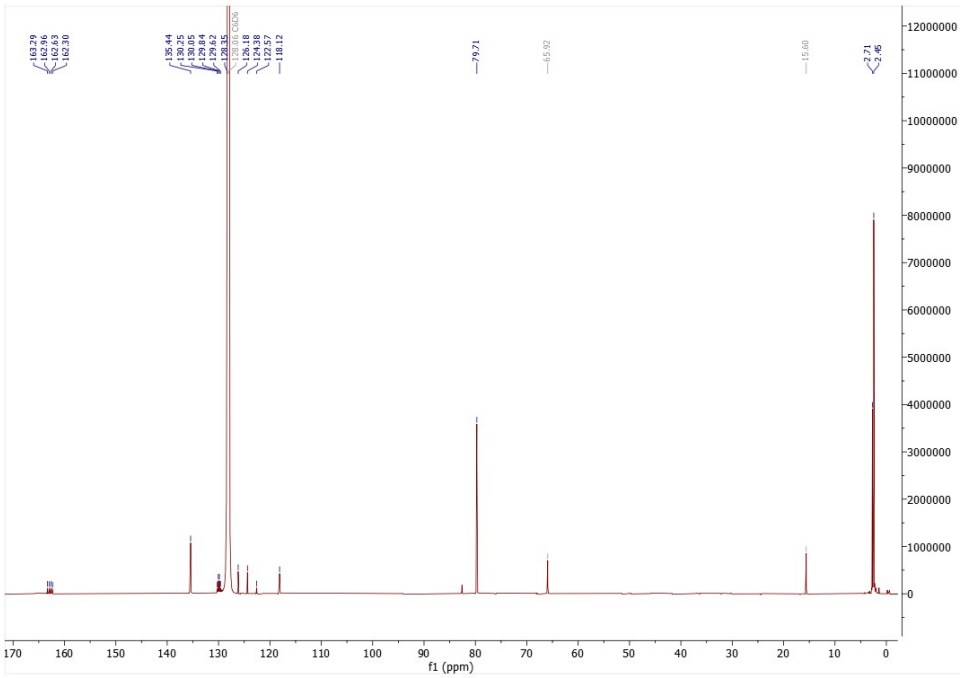



**Figure S26.** $^{13}C\{^{1}H\}$ NMR spectrum ($C_6D_6$, 298 K, 151 MHz) of [RhH{$Ge_9$(Hyp)$_3$}(μ-H)$_2$W(Cp)$_2$][$BAr^F{}_4$] (**2d**[$BAr^F{}_4$]).

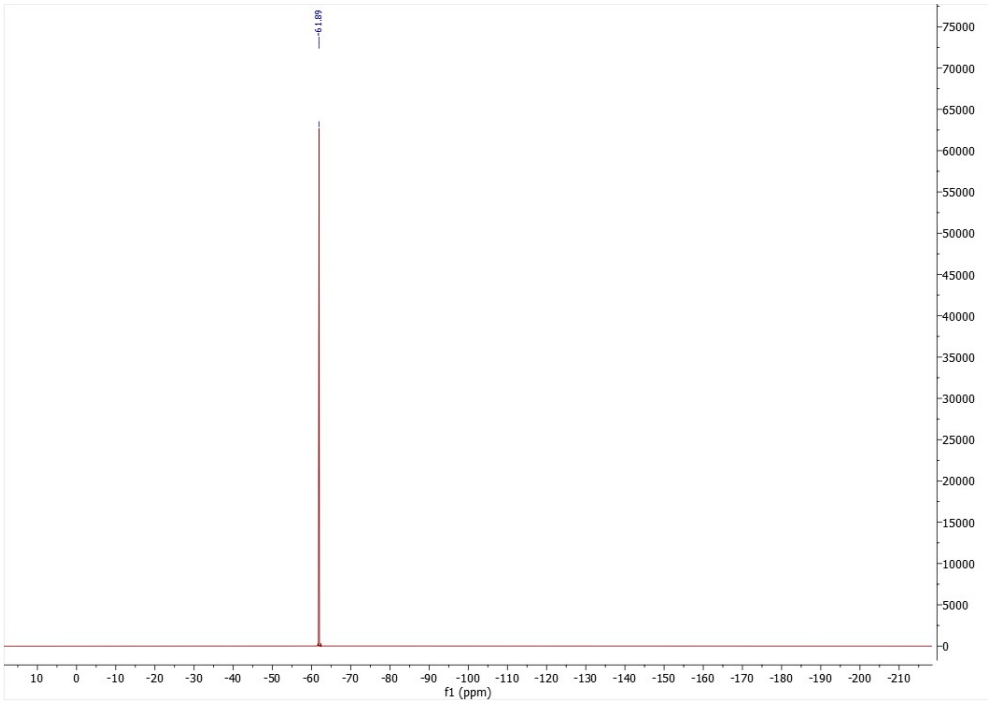



**Figure S27.** $^{19}F\{^{1}H\}$ NMR spectrum ($C_6D_6$, 298 K, 376.53 MHz) of [RhH{$Ge_9$(Hyp)$_3$}(μ-H)$_2$W(Cp)$_2$][$BAr^F{}_4$] (**2d**[$BAr^F{}_4$]).

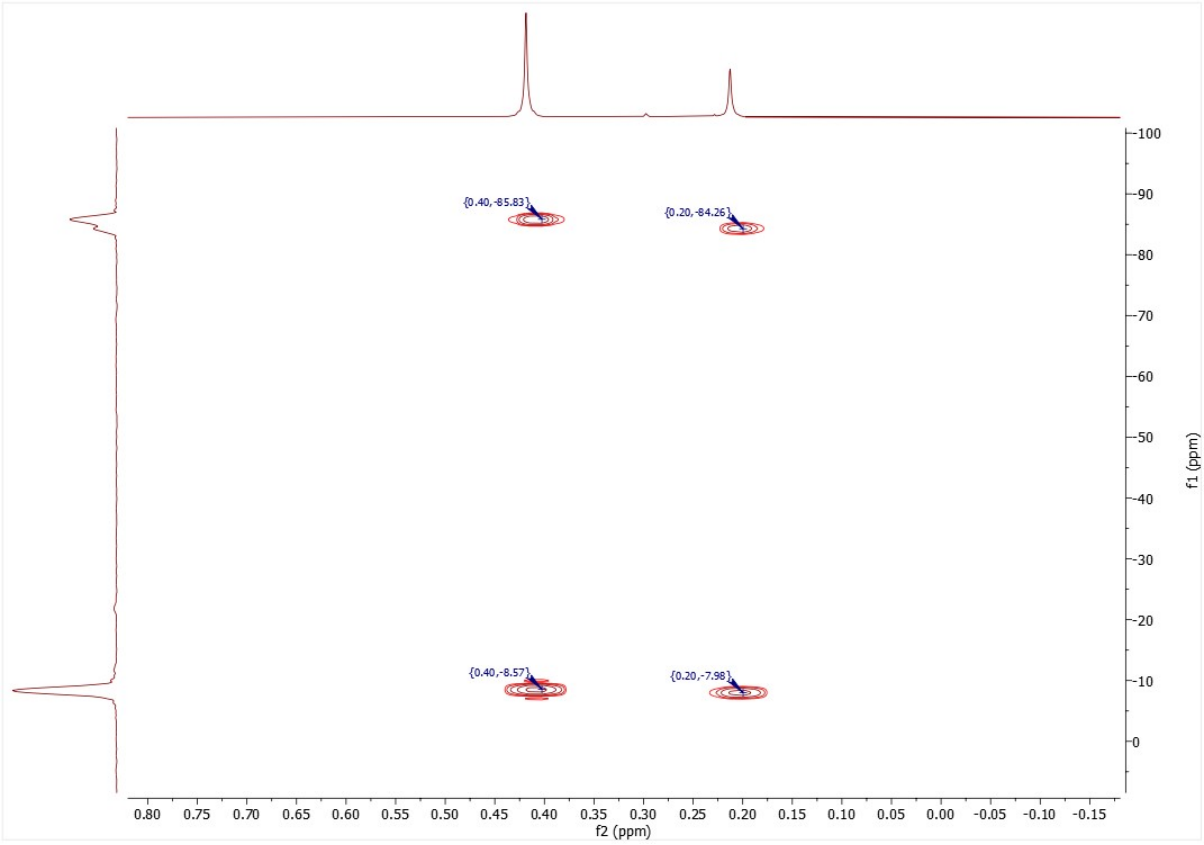



**Figure S28.** $^{1}H/^{29}Si$ HMBC NMR spectrum ($C_6D_6$, 298 K, 79.51 MHz) of $[RhH\{Ge_9(Hyp)_3\}(\mu\text{-}H)_2W(Cp)_2][BAr^F{}_4]$ (**2d**$[BAr^F{}_4]$).

1.7. NMR spectra for [Rh{$Ge_9(Hyp)_3$}(μ-D)$_2$W(Cp)$_2$] (d$_2$-**1d**).

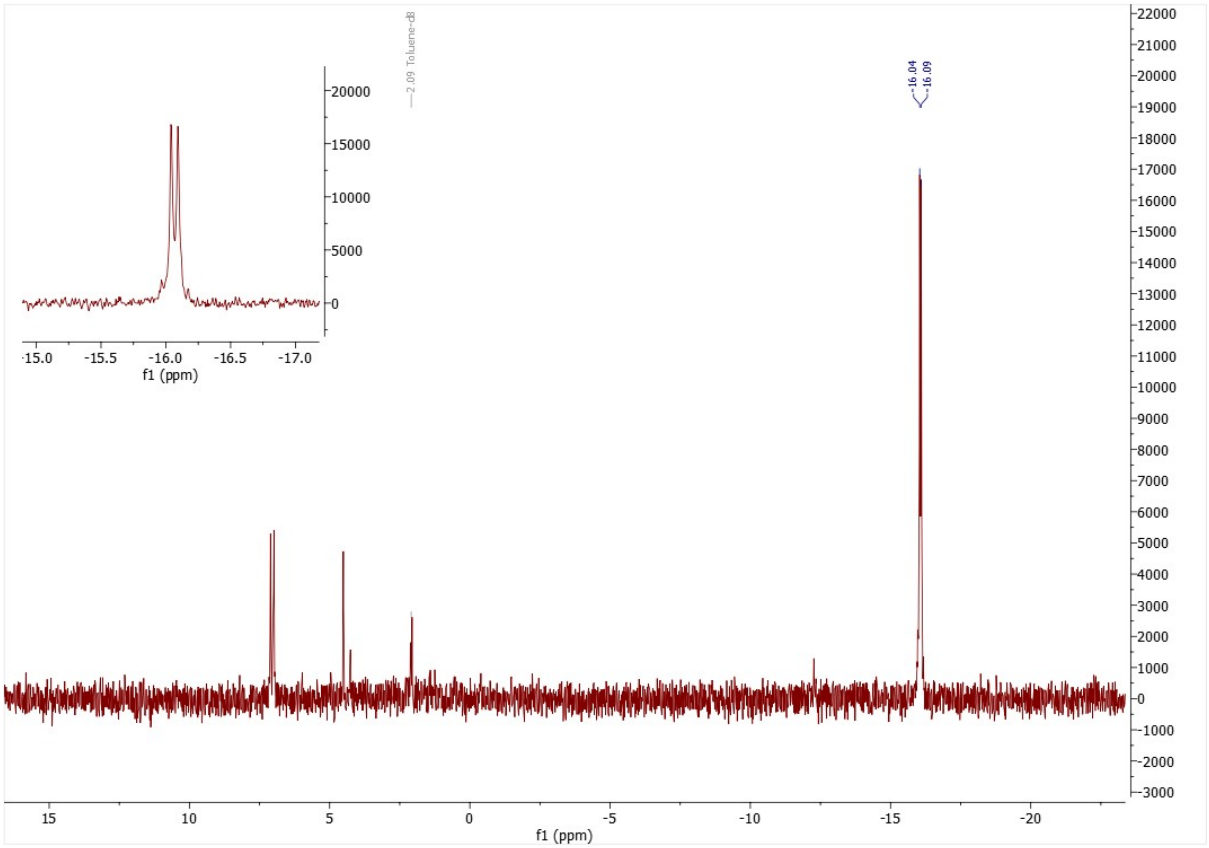
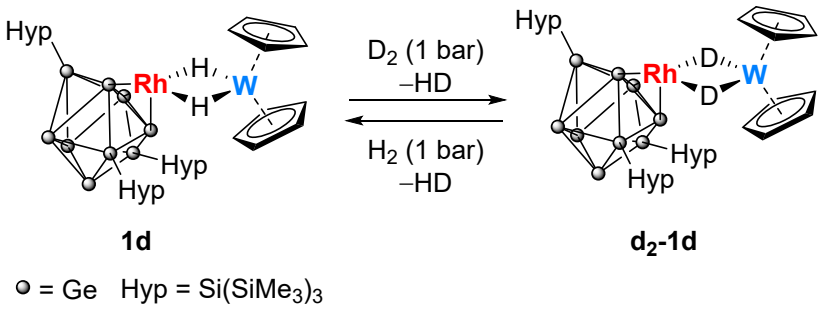



**Figure S29.** $^2$H NMR spectrum ($C_7H_8$, 298 K, 76.74 MHz) of [Rh{$Ge_9(Hyp)_3$}(μ-D)$_2$W(Cp)$_2$] (d$_2$-**1d**).




**Scheme S1:** Reversible formation of [Rh{$Ge_9(Hyp)_3$}(μ-D)$_2$W(Cp)$_2$] (d$_2$-**1d**).

To test bimetallic reactivity, a $C_6D_6$ solution of compound **1d** was placed under an atmosphere of $D_2$ (1 bar). The doublet $^1$H NMR signal for the bridging hydrides immediately started to decrease in intensity and dissolved $H_2$ and HD were observed.

The reaction was mixed by tumbling for 3 hours, resulting in a low intensity peak containing two overlapping doublet resonances. This is consistent with a mixture of compound **1d**, an isotopically shifted hydrido-deuteride complex [Rh{$Ge_9(Hyp)_3$}(μ-H)(μ-D)$W(Cp)_2$] and the unobserved dideuteride complex [Rh{$Ge_9(Hyp)_3$}(μ-$D)_2W(Cp)_2$] ($d_2$-**1d**). Replacing the atmosphere with $H_2$ resulted in complete regeneration of compound **1d** and the observation of dissolved HD over the course of a day.

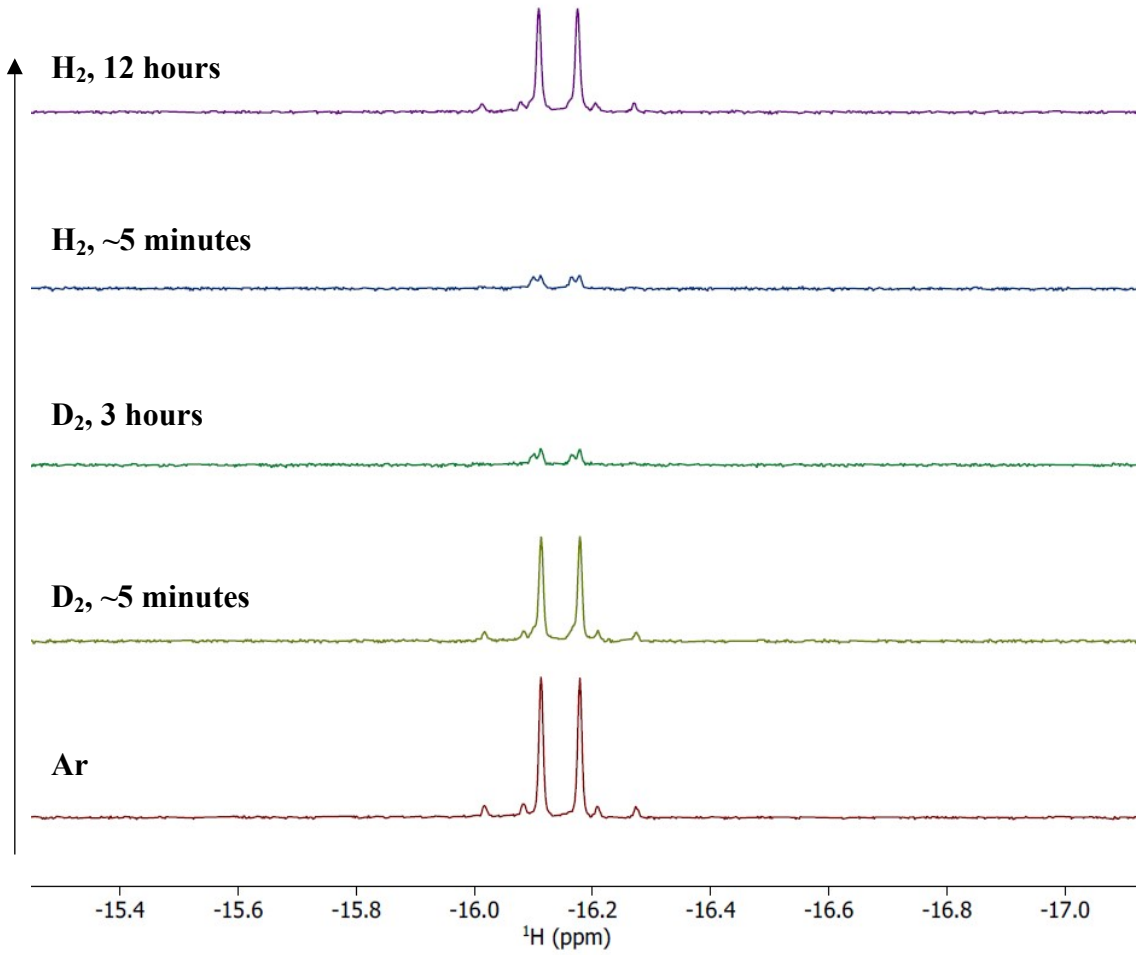



**Figure S30.** $^1H$ NMR spectra ($C_6D_6$, 298 K, 400.16 MHz) of the bridging hydride showing the reversible activation of $H_2$ and $D_2$ on changing the atmosphere. From bottom to top: Ar, $D_2$, $D_2$ (3 hours tumbled), $H_2$, $H_2$ (12 hours tumbled).

## 2. X-ray Crystallography

Single-crystal X-ray diffraction data were collected using an Oxford Diffraction Supernova dual-source diffractometer equipped with a 135 mm Atlas CCD area detector. Crystals were selected under Paratone-N oil, mounted on micromount loops and quench-cooled using an open flow $N_2$ cooling device.[1] Data were collected at 150 K using mirror monochromated Cu Kα (λ = 1.54184 Å) radiation and processed using the CrysAlisPro package, including unit cell parameter refinement and inter-frame scaling (which was carried out using SCALE3 ABSPACK within CrysAlisPro).[2] Equivalent reflections were merged and diffraction patterns processed with the CrysAlisPro suite. Structures were subsequently solved using direct methods and refined using the SHELXL package.[3] Hydrogen atoms, with the exception of metal hydrides, were typically included in calculated positions (riding model). Crystal data, details of data collections and refinements for all structures can be found in the CIF files and are summarized in Tables S1 and S2.

**Table S1.** Selected X-ray data collection and refinement parameters for **1a**, **1c**·hexane and **1d**.

| | **1a** | **1c**·hexane | **1d** |
|---|---|---|---|
| Formula | $C_{30}H_{90}Ge_9PRhSi_{12}$ | $C_{40}H_{107}Ge_9N_2RhSi_{12}$ | $C_{37}H_{93}Ge_9RhSi_{12}W$ |
| CCDC | 2155445 | 2155446 | 2155447 |
| Fw [g mol$^{-1}$] | 1575.28 | 1709.57 | 1815.26 |
| Crystal system | monoclinic | triclinic | monoclinic |
| Space group | $P2_1/c$ | $P\bar{1}$ | $P2_1/c$ |
| $a$ (Å) | 14.4411(1) | 16.3622(3) | 14.27830(10) |
| $b$ (Å) | 25.5519(2) | 19.8996(3) | 25.64300(10) |
| $c$ (Å) | 18.9046(1) | 25.9438(4) | 19.84610(10) |
| α (°) | 90 | 68.560(1) | 90 |
| β (°) | 101.771(1) | 79.856(1) | 101.575(1) |
| γ (°) | 90 | 82.113(1) | 90 |
| $V$ (Å$^3$) | 6829.06(8) | 7715.4(2) | 7118.64(7) |
| $Z$ | 4 | 4 | 4 |
| Radiation, λ (Å) | Cu Kα, 1.54184 | Cu Kα, 1.54184 | Cu Kα, 1.54184 |
| Temp (K) | 150(2) | 150(2) | 150(2) |
| $\rho_{calc}$ (g cm$^{-3}$) | 1.532 | 1.472 | 1.694 |
| μ (mm$^{-1}$) | 8.686 | 7.552 | 11.032 |
| Reflections collected | 132946 | 141405 | 196412 |
| Independent reflections | 14310 | 32320 | 14900 |
| Parameters | 569 | 1332 | 668 |
| R(int) | 0.0521 | 0.0488 | 0.0545 |
| R1/wR2,[a] $I \geq 2\sigma I$ (%) | 3.93/9.75 | 5.44/16.41 | 2.44/6.23 |
| R1/wR2,[a] all data (%) | 4.56/10.20 | 5.93/17.28 | 2.52/6.29 |
| GOF | 1.019 | 1.048 | 1.054 |

R1 = $[\Sigma||F_o| - |F_c||]/\Sigma|F_o|$; wR2 = $\{[\Sigma w[(F_o)^2 - (F_c)^2]^2]/[\Sigma w(F_o^2)^2\}^{1/2}$; w = $[\sigma^2(F_o)^2 + (AP)^2 + BP]^{-1}$, where P = $[(F_o)^2 + 2(F_c)^2]/3$ and the A and B values are 0.0442 and 15.49 for **1a**, 0.1167 and 1.9 for **1c**·hexane, and 0.0332 and 7.57 for **1d.**

**Table S2.** Selected X-ray data collection and refinement parameters for **2b**[$BAr^F_4$]·1.5hex and **2d**[$BAr^F_4$]·$Et_2O$.

| | **2b**[$BAr^F_4$]·1.5hex | **2d**[$BAr^F_4$]·$Et_2O$ |
|---|---|---|
| Formula | $C_{86}H_{130}BF_{24}Ge_9PRhSi_{12}$ | $C_{73}H_{116}BF_{24}Ge_9ORhSi_{12}W$ |
| CCDC | 2155448 | 2155449 |
| Fw [g $mol^{-1}$] | 2754.97 | 2753.61 |
| Crystal system | triclinic | monoclinic |
| Space group | *P*−1 | $P2_1/c$ |
| *a* (Å) | 15.0839(2) | 17.9023(5) |
| *b* (Å) | 19.3502(3) | 13.8042(5) |
| *c* (Å) | 21.6497(4) | 44.4206(12) |
| α (°) | 106.313(1) | 90 |
| β (°) | 96.757(1) | 96.969(3) |
| γ (°) | 92.771(1) | 90 |
| *V* ($Å^3$) | 6000.51(17) | 10896.4(6) |
| *Z* | 2 | 4 |
| Radiation, λ (Å) | Cu Kα, 1.54184 | Cu Kα, 1.54184 |
| Temp (K) | 150(2) | 150(2) |
| $\rho_{calc}$ (g $cm^{-3}$) | 1.525 | 1.679 |
| μ ($mm^{-1}$) | 5.511 | 7.778 |
| Reflections collected | 89656 | 101192 |
| Independent reflections | 24711 | 9244 |
| Parameters | 1332 | 1312 |
| R(int) | 0.0439 | 0.1242 |
| R1/wR2,[a] I ≥ 2σI (%) | 3.44/8.94 | 6.47/16.56 |
| R1/wR2,[a] all data (%) | 4.02/9.36 | 9.10/18.38 |
| GOF | 1.022 | 1.058 |

$R1 = [\Sigma||F_o| - |F_c||]/\Sigma|F_o|$; $wR2 = \{[\Sigma w[(F_o)^2 - (F_c)^2]^2]/[\Sigma w(F_o^2)^2\}^{1/2}$; $w = [\sigma^2(F_o)^2 + (AP)^2 + BP]^{-1}$, where $P = [(F_o)^2 + 2(F_c)^2]/3$ and the A and B values are 0.0518 and 2.02 for **2b**[$BAr^F_4$]·1.5hex, and 0.0908 and 0.00 for **2c**[$BAr^F_4$]·$Et_2O$**.**

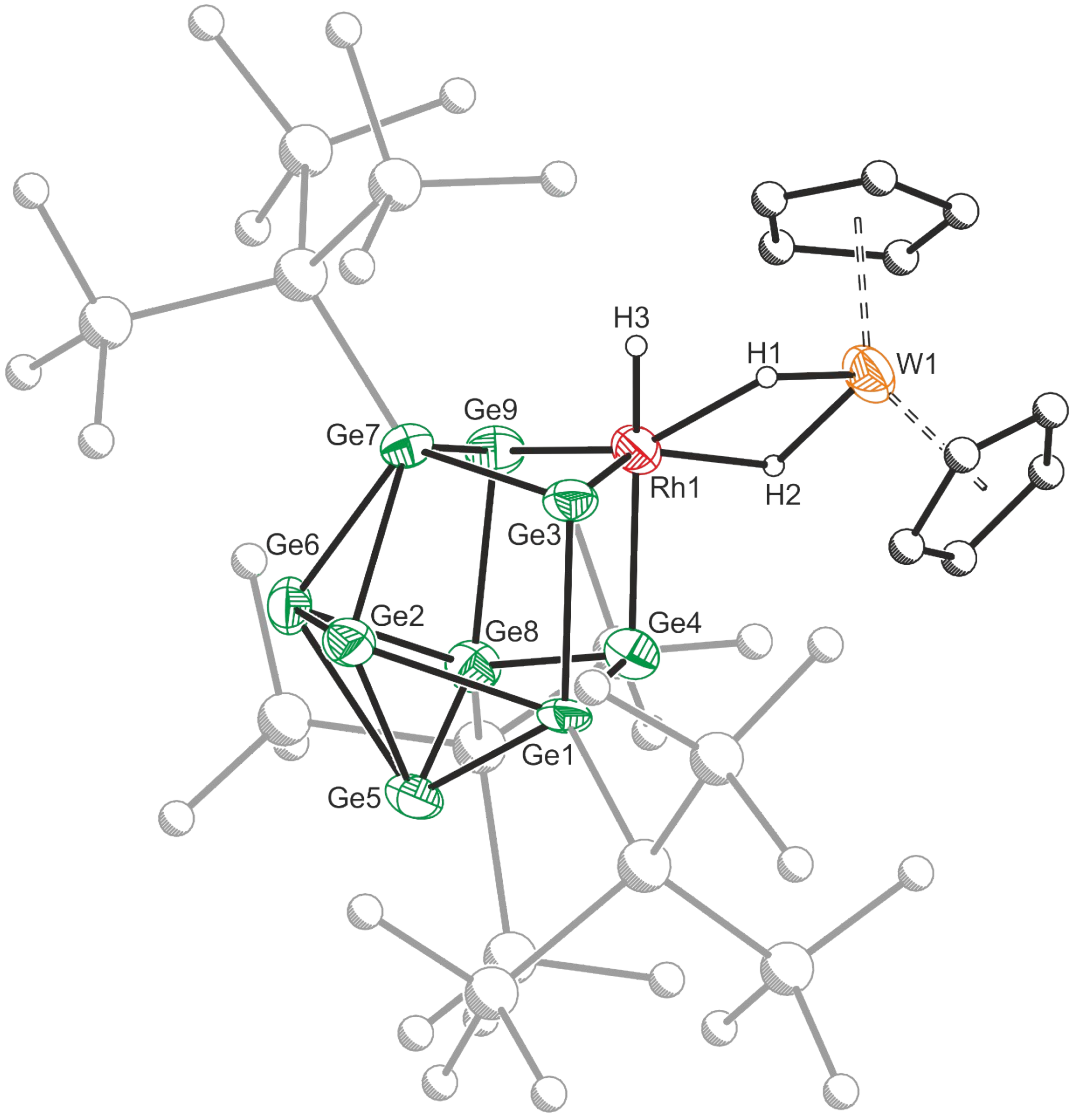
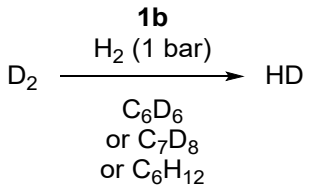



**Figure S31.** Molecular structure of the cationic portion of **2d**[$BAr^F_4$]·$Et_2O$. Anisotropic displacement ellipsoids are set at 50% probability. Only the major disordered component is shown.

# 3. Catalysis Procedures

## 3.1. H/D Scrambling




**Scheme S2.** H/D scrambling of a $H_2/D_2$ mixture in the presence of **1b**.

Compound **1b** (6 mg, 0.0034 mmol) was added to an NMR tube with a J. Young stopcock and dissolved in either $C_6D_6$, $C_7D_8$ or cyclohexane. This was freeze-pump-thaw degassed three times before charging with $D_2$ (0.5 bar) and stirring overnight to saturate the solution. The solution was then frozen, and partially degassed (~$10^2$ mbar) before charging with $H_2$ (1 bar). HD formation was observed within 5 minutes of the $H_2$ addition by $^1$H NMR spectroscopy.

A Hg drop test was used to discount the formation of a colloidal catalyst using the following method: Compound **1b** (6 mg, 0.0034 mmol) was added to an ampoule with a J. Young stopcock and dissolved in $C_6H_6$ (0.5 ml). This was freeze-pump-thaw degassed three times before charging with $H_2$ (0.5 bar) and stirred for 5 minutes before transferring via cannula onto Hg (0.5 g) and pressurizing with $D_2$ (1 bar). This was stirred for 10 minutes before transferring the headspace into an evacuated NMR tube containing degassed $C_6D_6$. The NMR tube was vigorously shaken to saturate the solution with the headspace atmosphere. Dissolved $H_2$ and HD was observed by $^1$H NMR spectroscopy.

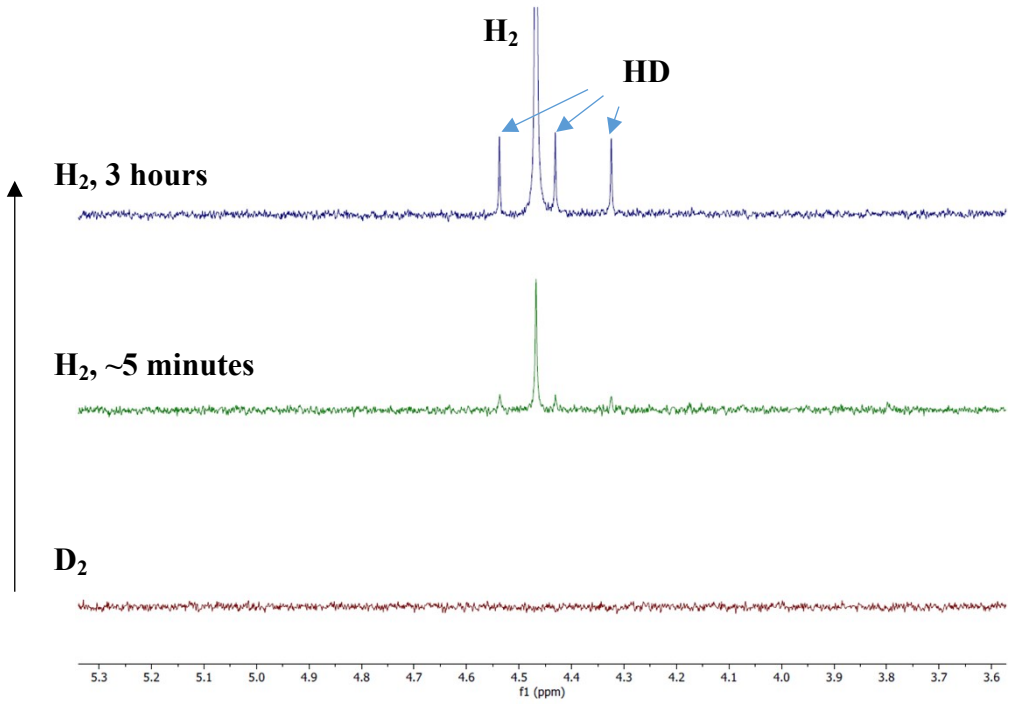



**Figure S32.** $^1$H NMR spectra ($C_6D_6$, 298 K, 400 MHz) to show HD formation from $H_2$ and $D_2$ in the presence of **1b**. Bottom to top: $D_2$ atmosphere, immediately after adding $H_2$, 3 hours standing.

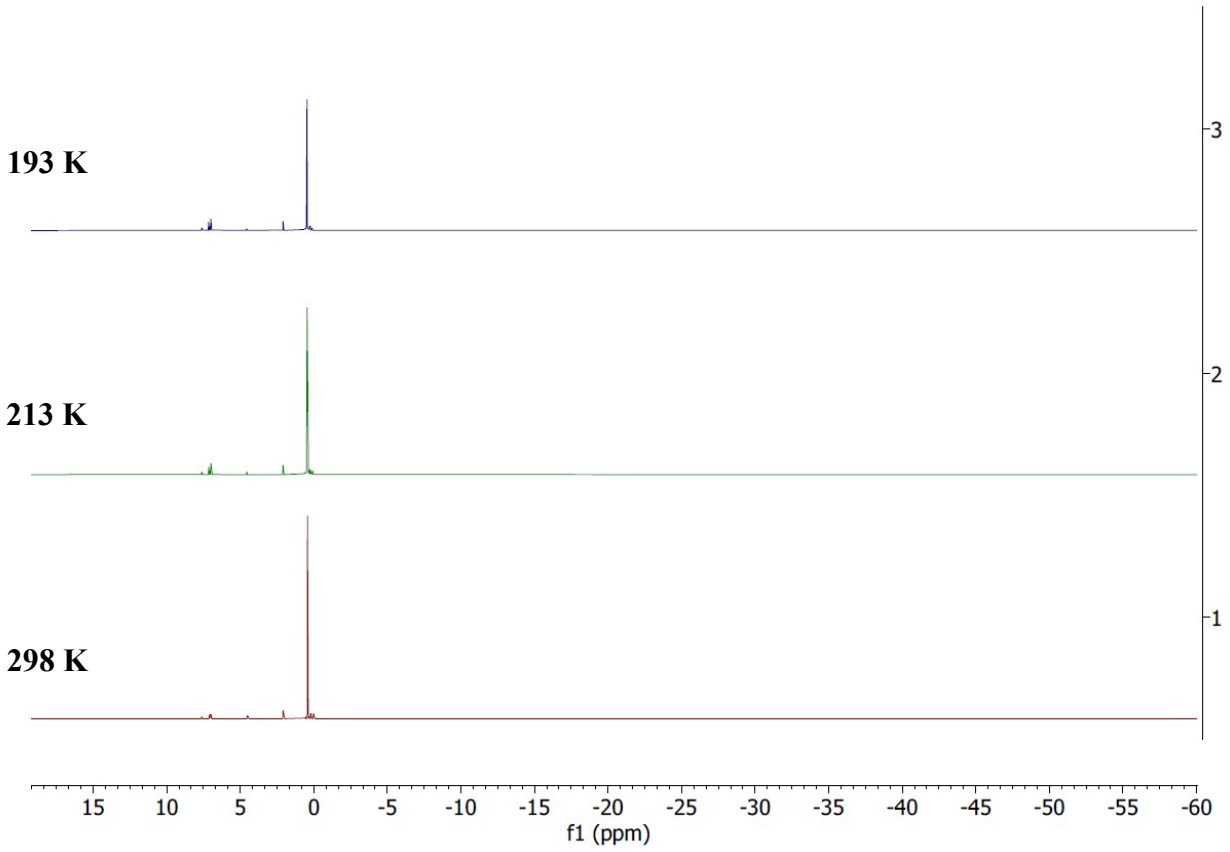
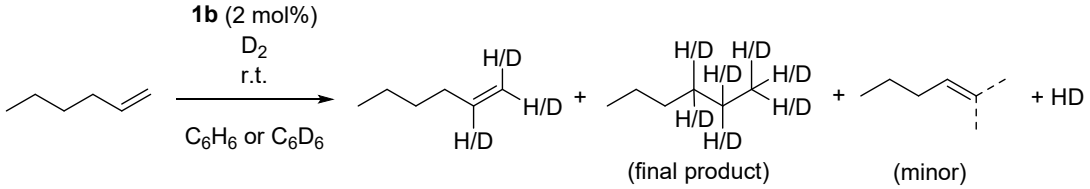



**Figure S33.** $^1$H NMR spectra ($C_7D_8$, 298 K, 500 MHz) to show no observable change or dihydride formation when **1b** is charged with $H_2$. Bottom to top: 298 K, 213 K, 193 K.

## 3.2. H/D Scrambling with Alkenes




**Scheme S3.** H/D scrambling and hydrogenation of 1-hexene in under $D_2$ the presence of **1b**.

Compound **1b** (3 mg, 0.0017 mmol) was added to was added to an NMR tube with a J. Young stopcock and dissolved in either $C_6H_6$ or $C_6D_6$. 1-hexene (10 µl, 0.08 mmol) was added using a micro-syringe. The solution was freeze-pump-thaw degassed three times before charging with $D_2$ (1 bar) and constantly mixed by tumbling. The products were identified by $^1H$ ($C_6D_6$ solution) or $^2H$ ($C_6H_6$ solution) NMR spectroscopy. After recharging the system with $D_2$, the deuterated hexenes converged to deuterated hexane.

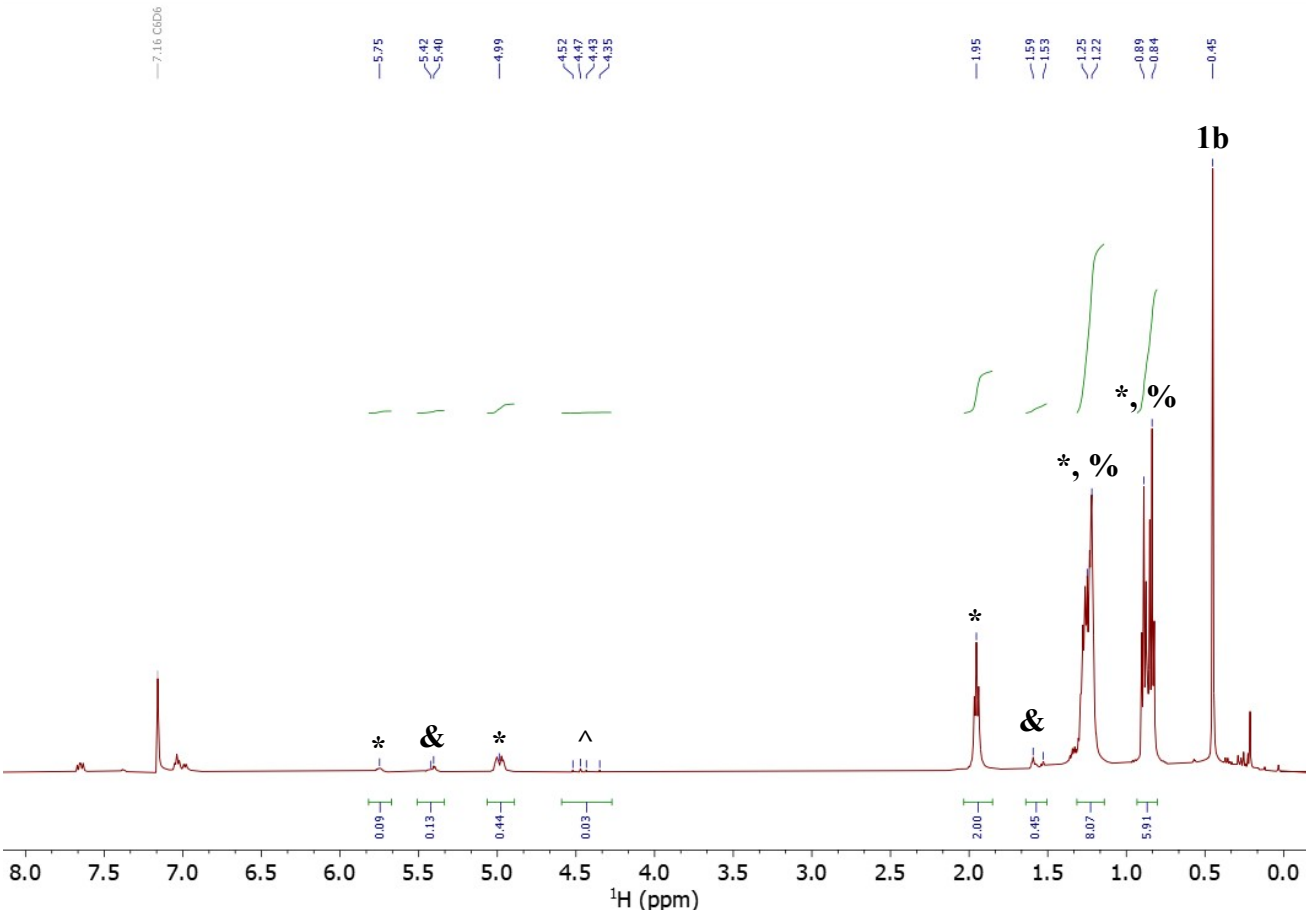



**Figure S34.** $^1$H NMR spectra ($C_6D_6$, 298 K, 500 MHz) to show the decrease in intensity at the alkenic positions when 1-hexene is charged with $D_2$ in the presence of **1b**, relative to the two vinylic protons (1.95 ppm). Of particular note is the relative integrations of the $CH_2$ (4.99 ppm) and CH (5.76 ppm) positions, showing selectivity for H/D exchange at the CH position. Assignments: ***** = 1-hexene, **&** = 2-hexenes, ^ = $H_2$, $D_2$, **%** = *n*-hexane.

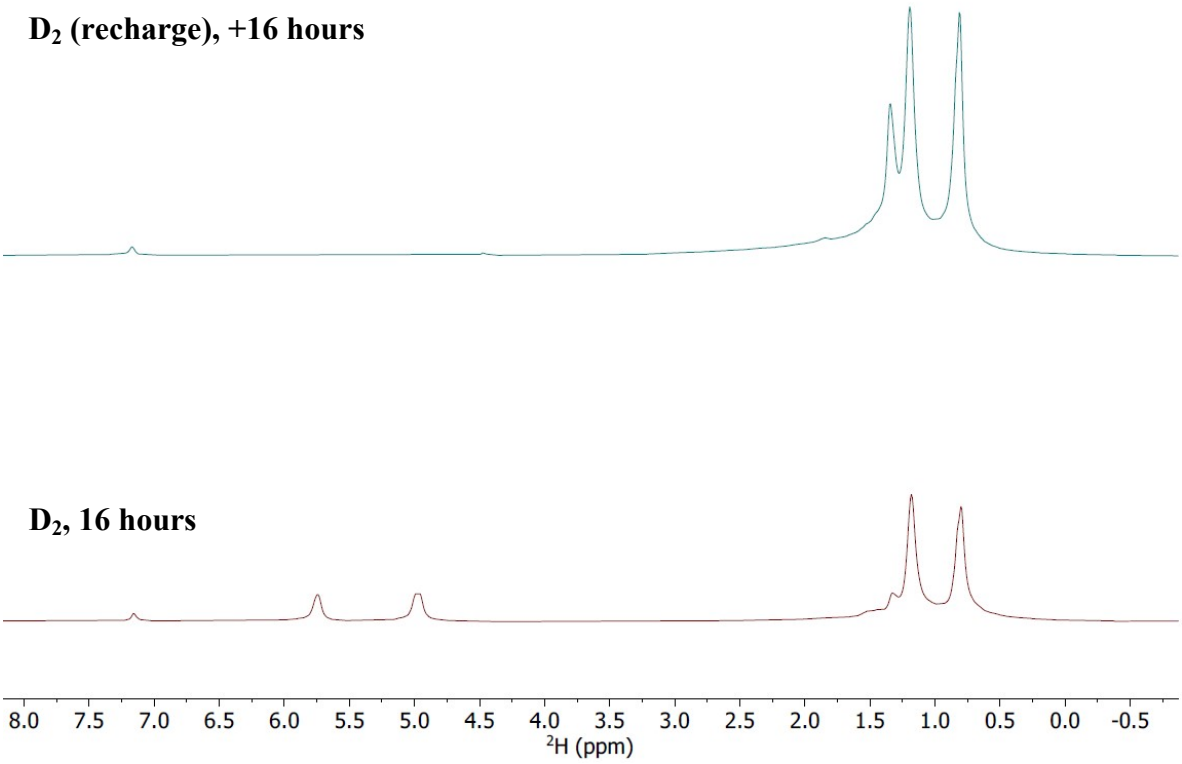
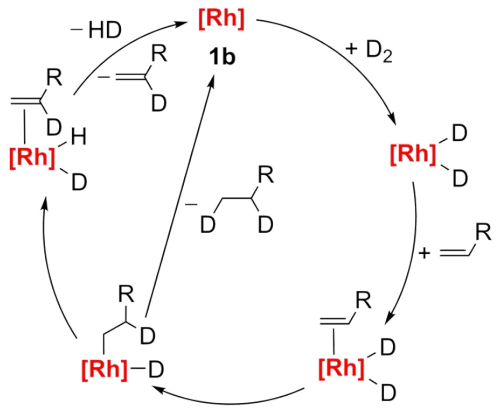



**Figure S35.** $^{2}H$ NMR spectrum ($C_6H_6$, 298 K, 76.74 MHz) of a parallel reaction in $C_6H_6$ confirming H/D exchange at the alkenic positions, in addition to hydrogenation/deuteration to *n*-hexane (bottom). On recharging the atmosphere with $D_2$, full hydrogenation/deuteration is observed.




**Scheme S4.** Proposed catalytic cycle for H/D scrambling and hydrogenation of 1-hexene in under $D_2$ the presence of **1b**.

# 4. Computational Details

## 4.1. Methodology

The geometry optimizations, PCM solvent corrections and frequency calculations were run with Gaussian 16 Revision A.03[4] and performed using the BP86[5,6] functional. Rh, Ge and Si centres were described with Stuttgart RECPs and associated basis sets,[7] with added f-orbital polarization on Rh ($\zeta$ = 1.35),[8] and d-orbital polarization on P ($\zeta$ = 0.387)  Ge ($\zeta$ = 0.230) and Si ($\zeta$ = 0.284).[9] 6-31G** basis sets were used for C and H (called BS1).[10,11] Single point energy calculations were performed on the optimised geometries, at the BP86/Def2-TZVP level of theory with added pseudopotential on Rh.[12,13] Stationary points were fully characterized via analytical frequency calculations as either minima (all positive eigenvalues) or transition states (one negative eigenvalue). IRC calculations and subsequent geometry optimizations were used to confirm the minima linked by the transition states. Energies reported in the text are based on the gas-phase free energies and incorporate a correction for dispersion effects using Grimme's D3 parameter set[14] (i.e. BP86-D3) as well as solvation (PCM approach) in benzene.

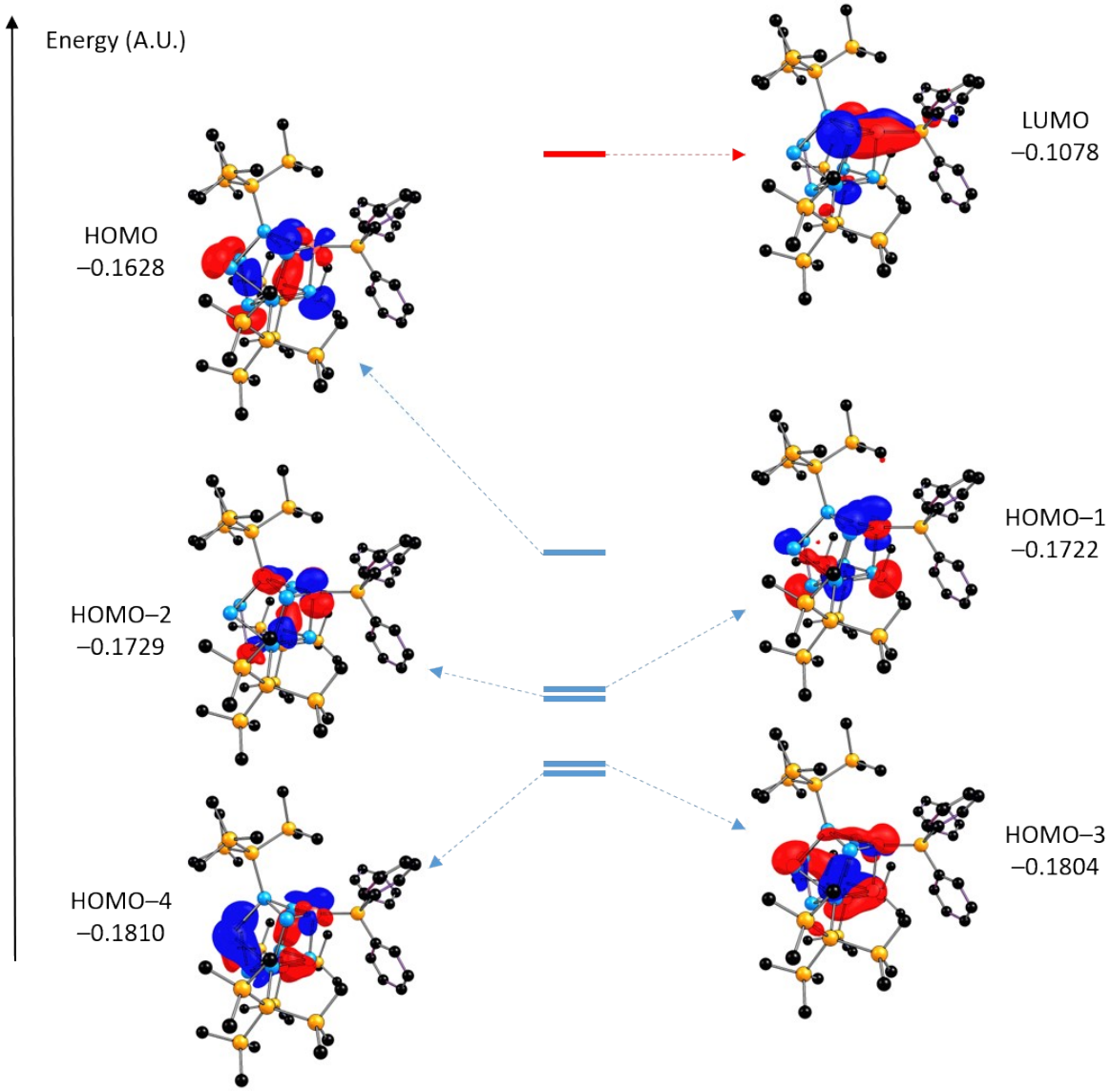
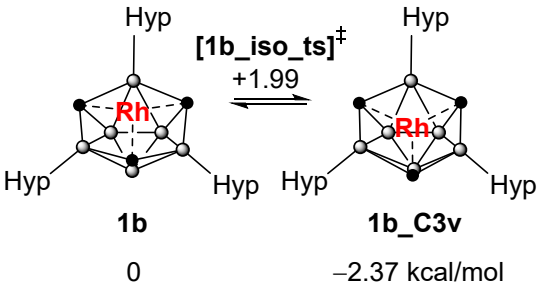



**Figure S37.** Frontier molecular orbital diagram of **1b** calculated at the BP86/Def2-TZVP level of theory.

## 4.2. Fluxional Behavior




**Scheme S6.** Isomerization of **1b**, calculated at the BP86-D3/Def2-TZVP level of theory.

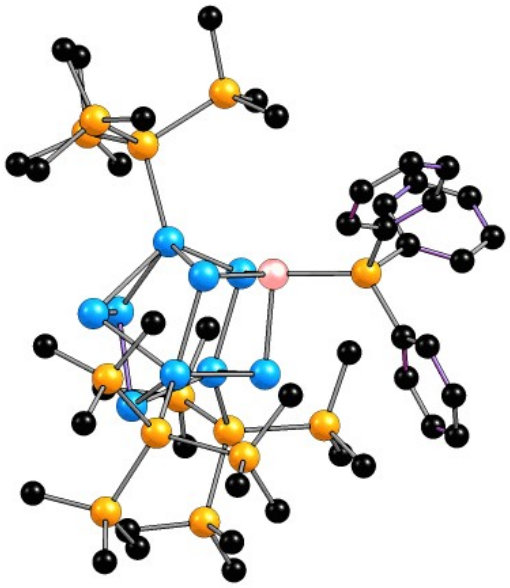


**Figure S38.** Optimized geometry of **1b** calculated at the BP86/6-31g(d,p)/SDDAll level of theory. Hydrogen atoms attached to carbon atoms omitted for clarity.

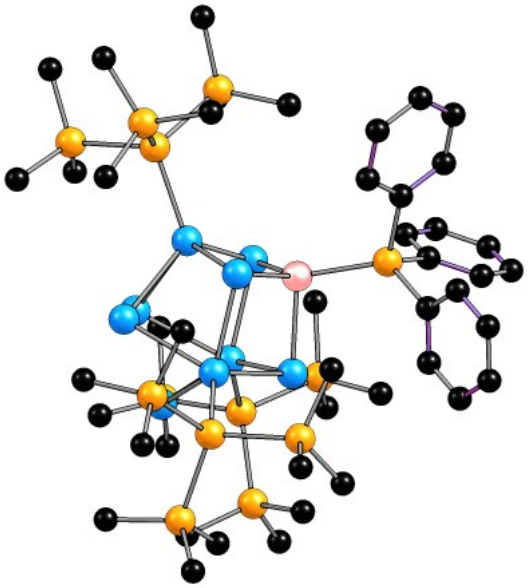


**Figure S39.** Optimized geometry of **1b_iso_ts** calculated at the BP86/6-31g(d,p)/SDDAll level of theory. Hydrogen atoms attached to carbon atoms omitted for clarity.

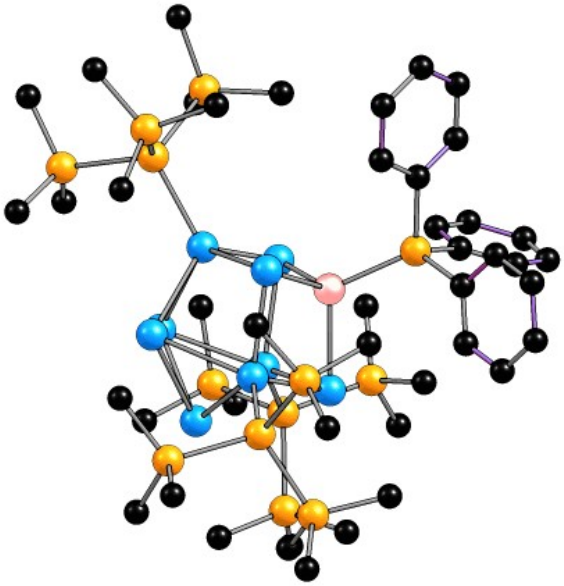
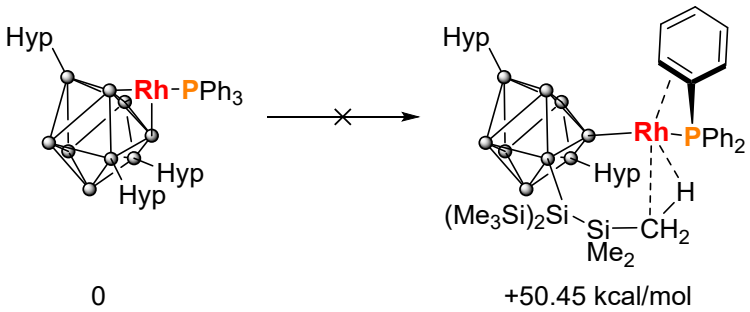


**Figure S40.** Optimized geometry of **1b_C3v** calculated at the BP86/6-31g(d,p)/SDDAll level of theory. Hydrogen atoms attached to carbon atoms omitted for clarity.

## 4.3. $\eta^3$–$\eta^1$ Isomerisation




**Scheme S7.** $\eta^3$–$\eta^1$ isomerization of **1b**, calculated at the BP86-D3/Def2-TZVP level of theory.

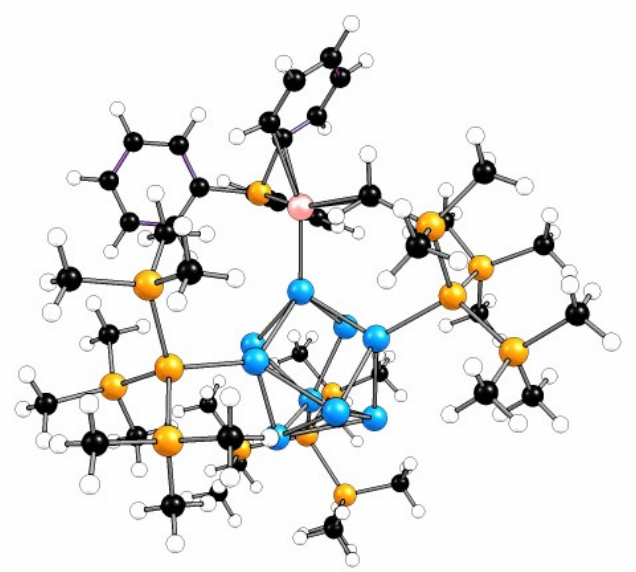
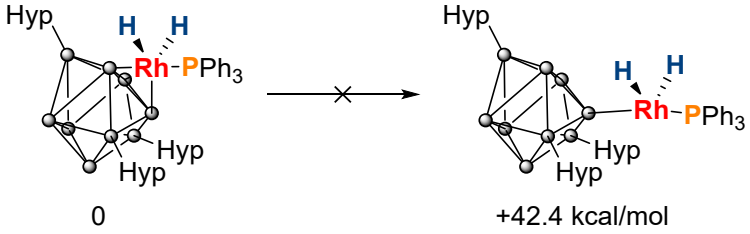


**Figure S41.** Optimized geometry of **1b_eta1** calculated at the BP86/6-31g(d,p)/SDDAll level of theory.




**Scheme S8.** $\eta^3$–$\eta^1$ isomerization of **1b_H_H**, calculated at the BP86-D3/Def2-TZVP level of theory.

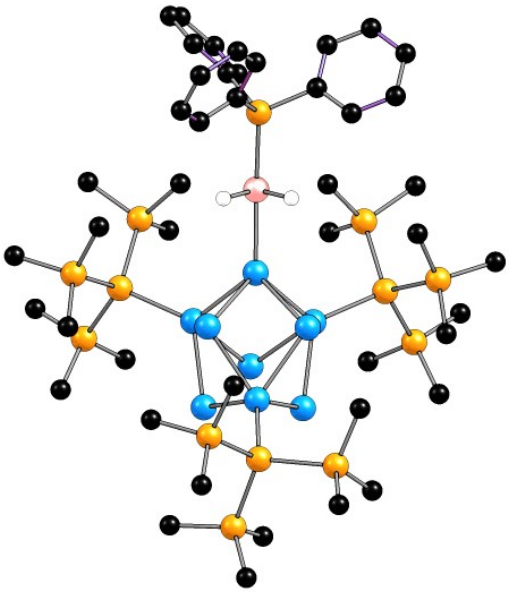
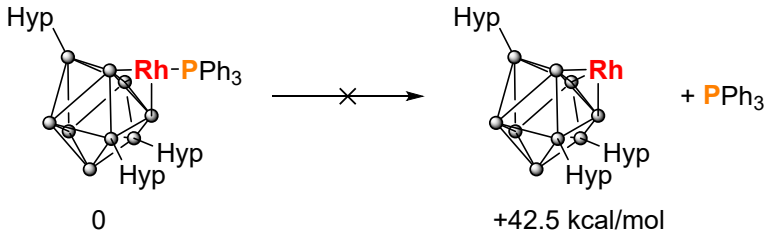


**Figure S42.** Optimized geometry of **1b_H2_eta1** calculated at the BP86/6-31g(d,p)/SDDAll level of theory. Hydrogen atoms attached to carbon atoms omitted for clarity.

4.4. Phosphine Dissociation




**Scheme S9.** Phosphine dissociation from **1b**, calculated at the BP86-D3/Def2-TZVP level of theory.

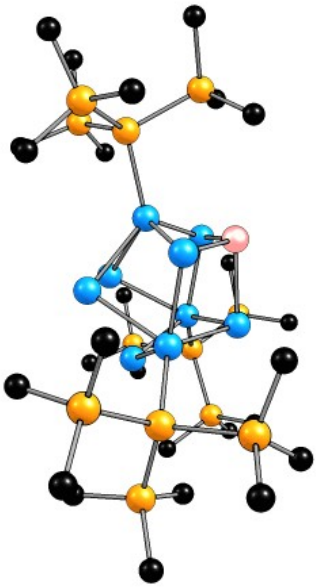
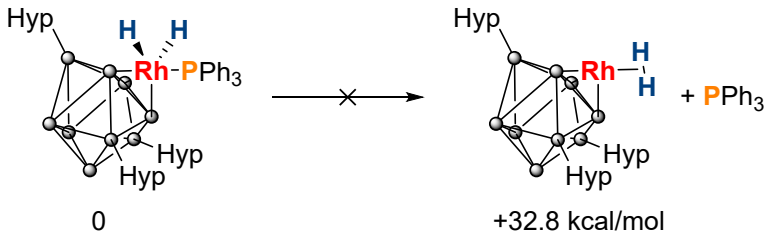


**Figure S43.** Optimized geometry of **1b_PPh3diss** calculated at the BP86/6-31g(d,p)/SDDAll level of theory. Hydrogen atoms attached to carbon atoms omitted for clarity.




**Scheme S10.** Phosphine dissociation from **1b_H_H**, calculated at the BP86-D3/Def2-TZVP level of theory.

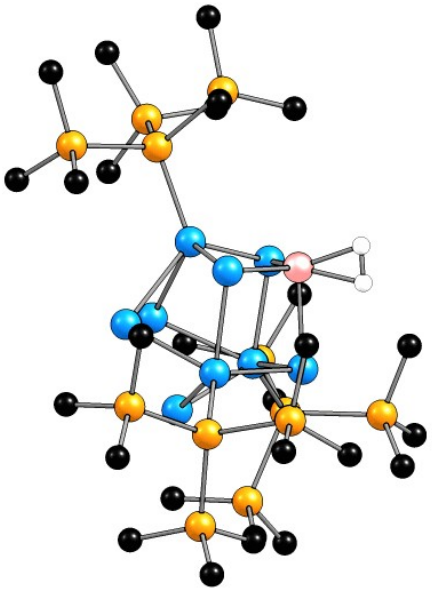
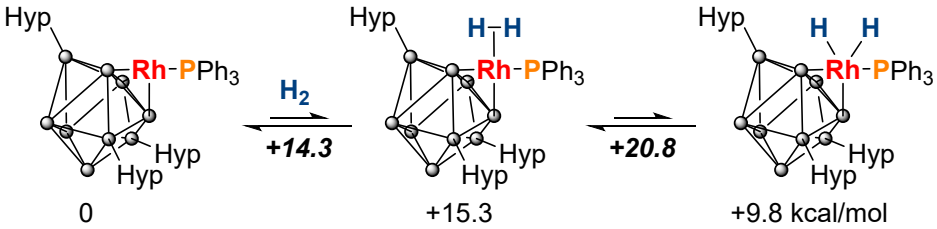


**Figure S44.** Optimized geometry of **Rh_H2** calculated at the BP86/6-31g(d,p)/SDDAll level of theory. Hydrogen atoms attached to carbon atoms omitted for clarity.

## 4.5. Oxidative Addition of $H_2$ at **1b**




**Scheme S11.** Oxidative addition of $H_2$ at **1b**, calculated at the BP86-D3/Def2-TZVP level of theory.

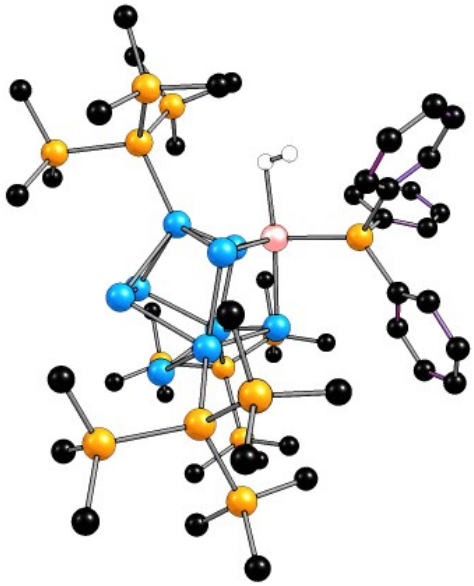


**Figure S45.** Optimized geometry of **1b_H2_diss_ts** calculated at the BP86/6-31g(d,p)/SDDAll level of theory. Hydrogen atoms attached to carbon atoms omitted for clarity.

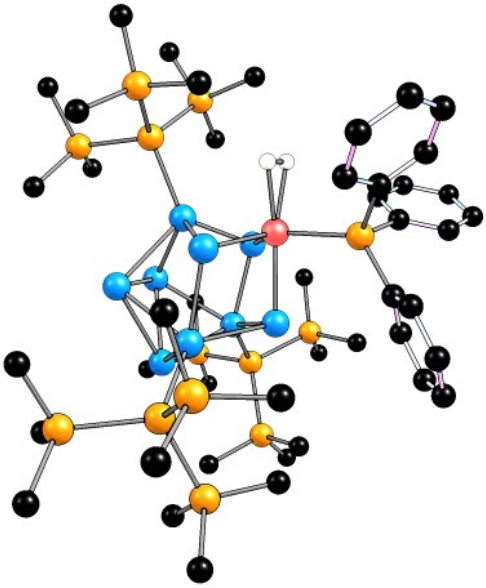


**Figure S46.** Optimized geometry of **1b_H2** calculated at the BP86/6-31g(d,p)/SDDAll level of theory. Hydrogen atoms attached to carbon atoms omitted for clarity.

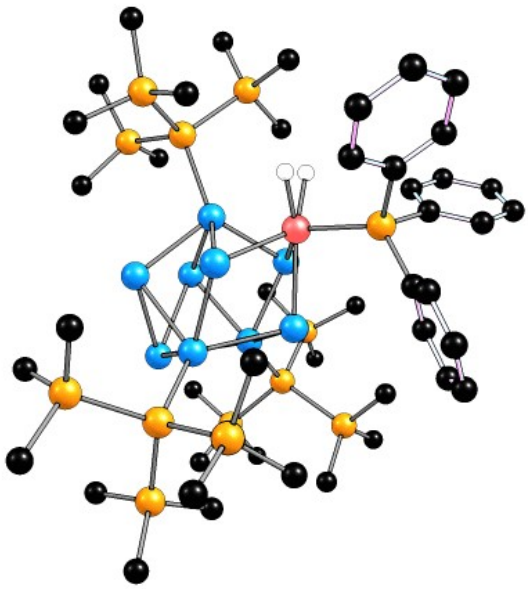


**Figure S47.** Optimized geometry of **1b_H2_oxadd_ts** calculated at the BP86/6-31g(d,p)/SDDAll level of theory. Hydrogen atoms attached to carbon atoms omitted for clarity.

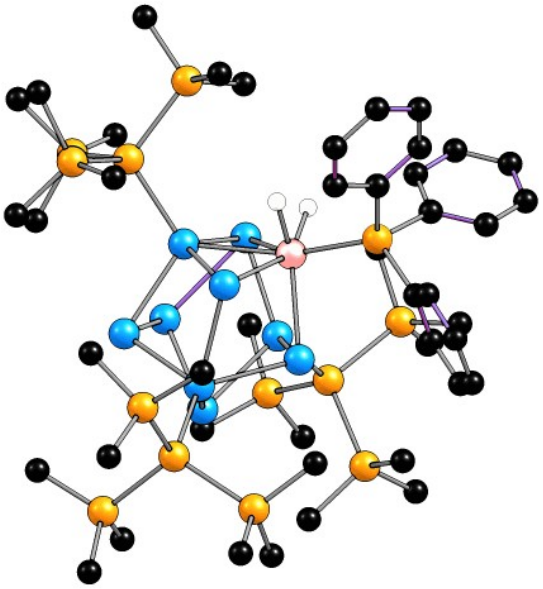
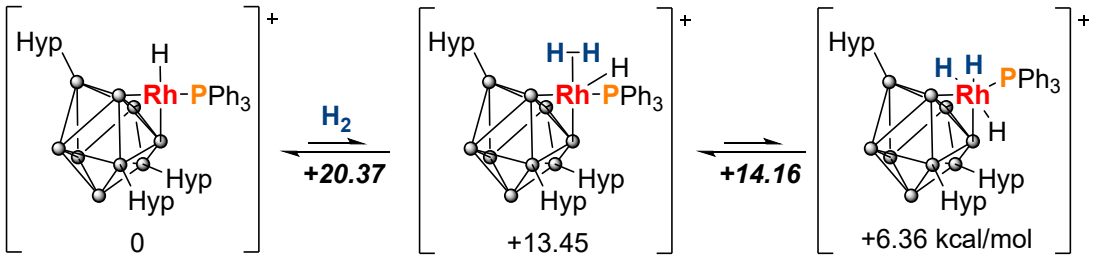


**Figure S48.** Optimized geometry of **1b_H_H** calculated at the BP86/6-31g(d,p)/SDDAll level of theory. Hydrogen atoms attached to carbon atoms omitted for clarity.

4.6. Oxidative Addition of $H_2$ at **2b**




**Scheme S12.** Oxidative addition of $H_2$ at **2b**, calculated at the BP86-D3/Def2-TZVP level of theory.

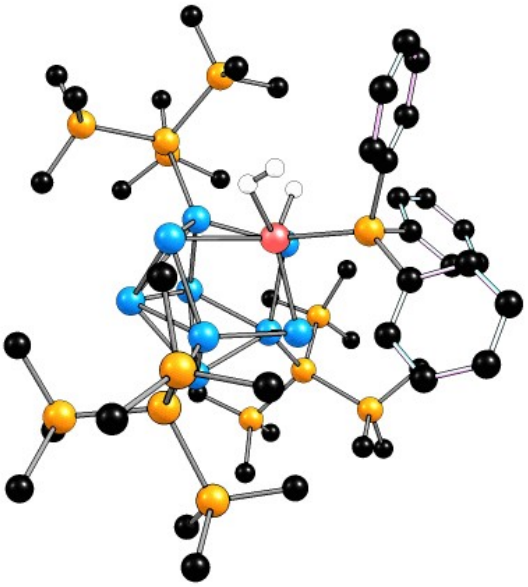


**Figure S49.** Optimized geometry of **2b_H2_diss_ts** calculated at the BP86/6-31g(d,p)/SDDAll level of theory. Hydrogen atoms attached to carbon atoms omitted for clarity.

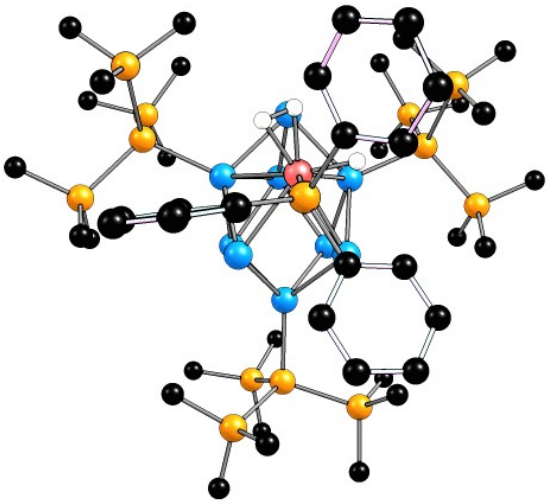


**Figure S50.** Optimized geometry of **2b_H2** calculated at the BP86/6-31g(d,p)/SDDAll level of theory. Hydrogen atoms attached to carbon atoms omitted for clarity.

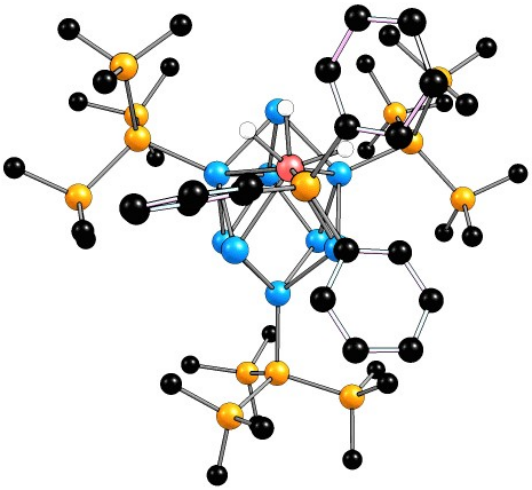


**Figure S51.** Optimized geometry of **2b_H2_oxadd_ts** calculated at the BP86/6-31g(d,p)/SDDAll level of theory. Hydrogen atoms attached to carbon atoms omitted for clarity.

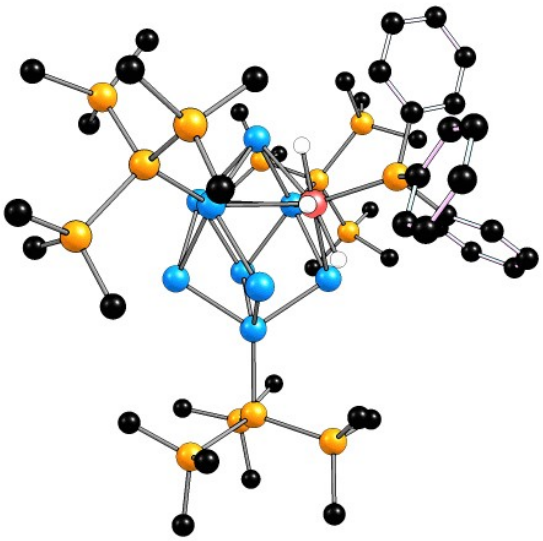


**Figure S52.** Optimized geometry of **2b_H_H** calculated at the BP86/6-31g(d,p)/SDDAll level of theory. Hydrogen atoms attached to carbon atoms omitted for clarity.

## 4.7. Computational Appendix

**Cartesian Coordinates (Å) of Optimized Geometries and Energies (hartrees) of all Species.**

**PPh3**

```
SCF  =           -701.502629721
H(0 K) =         -701.237101
H(298 K) =       -701.219663
G(298 K) =       -701.284051
SCF+D3 =         -701.538095733
PCM SCF (Benzene) =      -701.505227632
BS2 (def2-tzvp) =        -1036.57409771
Low Freq. = 22.8073cm-1, 24.7885cm-1

P         0.000147000     -0.000103000     -1.251107000
C        -1.129207000     -1.239567000     -0.416237000
C        -0.508733000      1.597479000     -0.415916000
C         1.638087000     -0.358286000     -0.415831000
C         2.472984000     -1.311150000     -1.041407000
C         3.724064000     -1.635758000     -0.495434000
C         4.167165000     -0.997805000      0.675236000
C         3.351248000     -0.039111000      1.297360000
C         2.093521000      0.278551000      0.757806000
H         2.139112000     -1.797967000     -1.965372000
H         4.357922000     -2.379396000     -0.990407000
H         5.147796000     -1.242459000      1.097046000
H         3.693549000      0.465047000      2.207814000
H         1.463094000      1.028265000      1.246792000
C        -0.099524000      2.796907000     -1.040647000
C        -0.443603000      4.042680000     -0.494538000
C        -1.218821000      4.107540000      0.675361000
C        -1.642663000      2.921683000      1.296569000
C        -1.289187000      1.673586000      0.756936000
```

| | | | |
|---|---|---|---|
| H | 0.489909000 | 2.751147000 | -1.964034000 |
| H | -0.115402000 | 4.963393000 | -0.988845000 |
| H | -1.497077000 | 5.079154000 | 1.097213000 |
| H | -2.251373000 | 2.966151000 | 2.206386000 |
| H | -1.624373000 | 0.752807000 | 1.245202000 |
| C | -2.373358000 | -1.483170000 | -1.040056000 |
| C | -3.280436000 | -2.403927000 | -0.494134000 |
| C | -2.948505000 | -3.109300000 | 0.674674000 |
| C | -1.708859000 | -2.885119000 | 1.294973000 |
| C | -0.804408000 | -1.955116000 | 0.755531000 |
| H | -2.628884000 | -0.948520000 | -1.962564000 |
| H | -4.242531000 | -2.578682000 | -0.987691000 |
| H | -3.651064000 | -3.835895000 | 1.096448000 |
| H | -1.442609000 | -3.435755000 | 2.203921000 |
| H | 0.161148000 | -1.786438000 | 1.243232000 |

**H2**

SCF = -1.17646513430
H(0 K) = -1.166541
H(298 K) = -1.163237
G(298 K) = -1.178048
SCF+D3 = -1.17646516273
PCM SCF (Benzene) = -1.17652523211
BS2 (def2-tzvp) = -1.17758514685
Low Freq. = 4356.1179cm-1

| | | | |
|---|---|---|---|
| H | 0.000000000 | 0.000000000 | 0.375260000 |
| H | 0.000000000 | 0.000000000 | -0.375260000 |

**1b**

SCF = -1972.04904032
H(0 K) = -1970.786845
H(298 K) = -1970.664346
G(298 K) = -1970.967735
SCF+D3 = -1972.35054229
PCM SCF (Benzene) = -1972.05341083
BS2 (def2-tzvp) = -24395.8954352
Low Freq. = 5.2097cm-1, 7.5107cm-1

| | | | |
|---|---|---|---|
| Rh | 1.214242000 | -0.065347000 | 1.313954000 |
| Ge | 1.865567000 | 0.072636000 | -1.371241000 |
| Ge | -1.338191000 | 2.037042000 | -0.488684000 |
| Ge | -1.366112000 | -1.940698000 | -0.650030000 |
| Ge | 1.137202000 | 2.102262000 | 0.136576000 |
| Ge | -1.270203000 | -0.030102000 | 1.235908000 |
| Ge | 1.117953000 | -2.098626000 | -0.069586000 |
| Ge | -2.248942000 | 0.119034000 | -2.089821000 |
| Ge | 0.017446000 | -1.199641000 | -2.923680000 |
| Ge | 0.030394000 | 1.493429000 | -2.812140000 |
| P | 1.362923000 | -0.252054000 | 3.639036000 |
| Si | 4.226191000 | 0.075044000 | -2.149455000 |
| Si | -2.863817000 | -3.929236000 | -0.690886000 |
| Si | -2.736662000 | 4.090633000 | -0.320173000 |
| Si | -2.141328000 | -5.422566000 | -2.428000000 |
| Si | -5.130468000 | -3.207013000 | -1.008119000 |
| Si | -2.623879000 | -4.971258000 | 1.459010000 |
| Si | -4.769170000 | 3.865893000 | -1.577928000 |
| Si | 4.835467000 | 2.311721000 | -2.783979000 |
| Si | 5.601120000 | -0.669938000 | -0.330025000 |
| Si | 4.399130000 | -1.434411000 | -4.011985000 |
| Si | -3.195360000 | 4.353121000 | 2.022006000 |

| | | | |
|---|---|---|---|
| Si | -1.410324000 | 5.924495000 | -1.126856000 |
| C | -0.153828000 | -0.080043000 | 4.720043000 |
| C | 2.067325000 | -1.886288000 | 4.222604000 |
| C | -5.948366000 | 5.313034000 | -1.139673000 |
| H | -6.242449000 | 5.281920000 | -0.076956000 |
| H | -6.870063000 | 5.244805000 | -1.745314000 |
| H | -5.486810000 | 6.294999000 | -1.334898000 |
| C | -3.531860000 | -3.949225000 | 2.800905000 |
| H | -3.194009000 | -2.898717000 | 2.792555000 |
| H | -3.333695000 | -4.371227000 | 3.802856000 |
| H | -4.623318000 | -3.953942000 | 2.642160000 |
| C | 5.403106000 | -2.552913000 | -0.049903000 |
| H | 4.342754000 | -2.822886000 | 0.095747000 |
| H | 5.968177000 | -2.865748000 | 0.846860000 |
| H | 5.785206000 | -3.131432000 | -0.907798000 |
| C | -2.352879000 | -0.932172000 | 5.361214000 |
| H | -3.142431000 | -1.682235000 | 5.248063000 |
| C | -1.188949000 | -1.032988000 | 4.585756000 |
| H | -1.077913000 | -1.865021000 | 3.881853000 |
| C | -0.310825000 | 0.978235000 | 5.635896000 |
| H | 0.483366000 | 1.720798000 | 5.755958000 |
| C | -2.003535000 | -4.529757000 | -4.110249000 |
| H | -2.963145000 | -4.077965000 | -4.411071000 |
| H | -1.700251000 | -5.244582000 | -4.896246000 |
| H | -1.249860000 | -3.724474000 | -4.070891000 |
| C | -5.430432000 | -2.685123000 | -2.822352000 |
| H | -4.745163000 | -1.872579000 | -3.117835000 |
| H | -6.465669000 | -2.320877000 | -2.949396000 |
| H | -5.281362000 | -3.529294000 | -3.516419000 |
| C | 1.736676000 | -2.440844000 | 5.477791000 |
| H | 1.013906000 | -1.936489000 | 6.126448000 |
| C | 3.556826000 | 3.079121000 | -3.977196000 |
| H | 3.471999000 | 2.496624000 | -4.909431000 |
| H | 3.854909000 | 4.109140000 | -4.243613000 |
| H | 2.554460000 | 3.119780000 | -3.517939000 |
| C | -4.411507000 | 3.916169000 | -3.455480000 |
| H | -3.977209000 | 4.882536000 | -3.761784000 |
| H | -5.346327000 | 3.769576000 | -4.025724000 |
| H | -3.708295000 | 3.117836000 | -3.746271000 |
| C | 2.538424000 | 0.996184000 | 4.396346000 |
| C | 2.325095000 | -3.645963000 | 5.896389000 |
| H | 2.056728000 | -4.068577000 | 6.870524000 |
| C | -5.664603000 | 2.227779000 | -1.176068000 |
| H | -5.044050000 | 1.363445000 | -1.467778000 |
| H | -6.616135000 | 2.168785000 | -1.734499000 |
| H | -5.891509000 | 2.137096000 | -0.101260000 |
| C | 4.242949000 | 2.942841000 | 5.525469000 |
| H | 4.908197000 | 3.695638000 | 5.961304000 |
| C | -2.505943000 | 0.130303000 | 6.268795000 |
| H | -3.418002000 | 0.212692000 | 6.869073000 |
| C | 2.992981000 | -2.558229000 | 3.397591000 |
| H | 3.238781000 | -2.143154000 | 2.414260000 |
| C | -6.331770000 | -4.640196000 | -0.583832000 |
| H | -6.133247000 | -5.535206000 | -1.196503000 |
| H | -7.374945000 | -4.327044000 | -0.769936000 |
| H | -6.253384000 | -4.931575000 | 0.477168000 |
| C | -1.485214000 | 1.083125000 | 6.402303000 |
| H | -1.595092000 | 1.912337000 | 7.109226000 |
| C | 3.299148000 | 0.697477000 | 5.546776000 |
| H | 3.234336000 | -0.293910000 | 6.005561000 |
| C | -5.531190000 | -1.729758000 | 0.134885000 |

| | | | |
|---|---|---|---|
| H | -5.408746000 | -1.995271000 | 1.197879000 |
| H | -6.573880000 | -1.398540000 | -0.018029000 |
| H | -4.868131000 | -0.874925000 | -0.079418000 |
| C | 0.048458000 | 6.271267000 | 0.061853000 |
| H | -0.305887000 | 6.594149000 | 1.055212000 |
| H | 0.691817000 | 7.071687000 | -0.345528000 |
| H | 0.671200000 | 5.369964000 | 0.196917000 |
| C | 3.248175000 | -4.306859000 | 5.070383000 |
| H | 3.701904000 | -5.248390000 | 5.397182000 |
| C | -0.704313000 | 5.562951000 | -2.864402000 |
| H | -0.068435000 | 4.661430000 | -2.857428000 |
| H | -0.091495000 | 6.413688000 | -3.212808000 |
| H | -1.507939000 | 5.397517000 | -3.600889000 |
| C | -0.786760000 | -5.120904000 | 1.966277000 |
| H | -0.210682000 | -5.707268000 | 1.231319000 |
| H | -0.699699000 | -5.621691000 | 2.947316000 |
| H | -0.312168000 | -4.128078000 | 2.045946000 |
| C | -3.406611000 | -6.851041000 | -2.613747000 |
| H | -3.552121000 | -7.398779000 | -1.668194000 |
| H | -3.052654000 | -7.571367000 | -3.373230000 |
| H | -4.389743000 | -6.474058000 | -2.942429000 |
| C | -3.836237000 | 6.124153000 | 2.380566000 |
| H | -4.098121000 | 6.223963000 | 3.449386000 |
| H | -4.735401000 | 6.361988000 | 1.788196000 |
| H | -3.068896000 | 6.882549000 | 2.150861000 |
| C | -0.436838000 | -6.170984000 | -1.988494000 |
| H | 0.312554000 | -5.379822000 | -1.817874000 |
| H | -0.074568000 | -6.810422000 | -2.813295000 |
| H | -0.490480000 | -6.791885000 | -1.078411000 |
| C | 3.607957000 | -3.126681000 | -3.611684000 |
| H | 4.076781000 | -3.597304000 | -2.731903000 |
| H | 3.722310000 | -3.812331000 | -4.470474000 |
| H | 2.529709000 | -3.015447000 | -3.405350000 |
| C | 6.532877000 | 2.288909000 | -3.675408000 |
| H | 7.320346000 | 1.831176000 | -3.054413000 |
| H | 6.845896000 | 3.321343000 | -3.914276000 |
| H | 6.478697000 | 1.728045000 | -4.623595000 |
| C | -3.378334000 | -6.732990000 | 1.437071000 |
| H | -4.434502000 | -6.721457000 | 1.120848000 |
| H | -3.329900000 | -7.181025000 | 2.445890000 |
| H | -2.825650000 | -7.394662000 | 0.749122000 |
| C | 2.644670000 | 2.276895000 | 3.816013000 |
| H | 2.076390000 | 2.505083000 | 2.906598000 |
| C | 3.487847000 | 3.246540000 | 4.381379000 |
| H | 3.560448000 | 4.236359000 | 3.918540000 |
| C | 3.581495000 | -3.759675000 | 3.820588000 |
| H | 4.294237000 | -4.271971000 | 3.166052000 |
| C | 7.448357000 | -0.315702000 | -0.700496000 |
| H | 7.775987000 | -0.787045000 | -1.641932000 |
| H | 8.079499000 | -0.712118000 | 0.115245000 |
| H | 7.641646000 | 0.767386000 | -0.777444000 |
| C | 4.976779000 | 3.431624000 | -1.239719000 |
| H | 4.033002000 | 3.430851000 | -0.667406000 |
| H | 5.195788000 | 4.472100000 | -1.539837000 |
| H | 5.783669000 | 3.095517000 | -0.567006000 |
| C | 4.148123000 | 1.666701000 | 6.104387000 |
| H | 4.738391000 | 1.420613000 | 6.993521000 |
| C | -2.486300000 | 7.507467000 | -1.240343000 |
| H | -3.290432000 | 7.390941000 | -1.986216000 |
| H | -1.863413000 | 8.365970000 | -1.549966000 |
| H | -2.953583000 | 7.758177000 | -0.273808000 |

| | | | |
|---|---|---|---|
| C | -4.520416000 | 3.100733000 | 2.598912000 |
| H | -4.205027000 | 2.065582000 | 2.385469000 |
| H | -5.488726000 | 3.274473000 | 2.100345000 |
| H | -4.680017000 | 3.189140000 | 3.688487000 |
| C | 5.124476000 | 0.242042000 | 1.277932000 |
| H | 5.311802000 | 1.325690000 | 1.197639000 |
| H | 5.701219000 | -0.146036000 | 2.136660000 |
| H | 4.046912000 | 0.111315000 | 1.494573000 |
| C | 3.539890000 | -0.708616000 | -5.557782000 |
| H | 2.476378000 | -0.495822000 | -5.356502000 |
| H | 3.590343000 | -1.427343000 | -6.395323000 |
| H | 4.019318000 | 0.228442000 | -5.887217000 |
| C | -1.611104000 | 4.069136000 | 3.053187000 |
| H | -1.824876000 | 4.206043000 | 4.128298000 |
| H | -0.811027000 | 4.772388000 | 2.768488000 |
| H | -1.232258000 | 3.043064000 | 2.909245000 |
| C | 6.249849000 | -1.723932000 | -4.420883000 |
| H | 6.776000000 | -0.780505000 | -4.641103000 |
| H | 6.341252000 | -2.378021000 | -5.306719000 |
| H | 6.773422000 | -2.217082000 | -3.584579000 |

**1b_iso_ts**

SCF = -1972.04864464
H(0 K) = -1970.786336
H(298 K) = -1970.664709
G(298 K) = -1970.963410
SCF+D3 = -1972.35143201
PCM SCF (Benzene) = -1972.05297235
BS2 (def2-tzvp) = -24395.8949558
Low Freq. = -14.9007cm-1, 10.0566cm-1

| | | | |
|---|---|---|---|
| Rh | -0.876351000 | 0.097610000 | 1.407162000 |
| Ge | -1.854793000 | 0.431844000 | -1.322834000 |
| Ge | 0.931195000 | -2.123957000 | -0.720968000 |
| Ge | 1.658697000 | 1.767966000 | -0.507556000 |
| Ge | -1.520745000 | -1.805606000 | 0.006875000 |
| Ge | 1.534109000 | -0.315788000 | 1.149826000 |
| Ge | -0.776193000 | 2.250797000 | 0.207117000 |
| Ge | 2.180871000 | -0.258851000 | -2.180915000 |
| Ge | 0.180383000 | 1.519143000 | -2.790900000 |
| Ge | -0.311261000 | -1.123917000 | -2.949987000 |
| P | -1.169882000 | -0.028897000 | 3.707506000 |
| Si | -4.205191000 | 0.914827000 | -2.001233000 |
| Si | 3.465755000 | 3.487007000 | -0.397117000 |
| Si | 1.910608000 | -4.417491000 | -0.790338000 |
| Si | 3.399272000 | 4.817382000 | -2.397615000 |
| Si | 5.573869000 | 2.353535000 | -0.185635000 |
| Si | 3.028935000 | 4.826187000 | 1.548259000 |
| Si | 4.133582000 | -4.327851000 | -1.688848000 |
| Si | -5.389325000 | -1.171928000 | -2.137077000 |
| Si | -5.222230000 | 2.374277000 | -0.386303000 |
| Si | -4.157478000 | 1.976941000 | -4.160025000 |
| Si | 1.942211000 | -5.175606000 | 1.487371000 |
| Si | 0.467179000 | -5.808512000 | -2.113474000 |
| C | -0.251747000 | -1.322025000 | 4.704157000 |
| C | -0.799731000 | 1.539242000 | 4.659070000 |
| C | 5.021367000 | -5.996503000 | -1.365603000 |
| H | 5.136361000 | -6.188209000 | -0.285423000 |
| H | 6.031221000 | -5.981156000 | -1.813789000 |
| H | 4.469983000 | -6.845257000 | -1.803132000 |
| C | 3.263531000 | 3.780763000 | 3.132541000 |

| | | | |
|---|---|---|---|
| H | 2.609829000 | 2.892634000 | 3.116315000 |
| H | 3.006790000 | 4.374433000 | 4.027867000 |
| H | 4.305821000 | 3.436639000 | 3.240207000 |
| C | -4.539265000 | 4.153275000 | -0.551413000 |
| H | -3.441983000 | 4.167613000 | -0.435125000 |
| H | -4.973385000 | 4.800010000 | 0.232342000 |
| H | -4.786200000 | 4.596315000 | -1.530635000 |
| C | 1.885654000 | -2.269166000 | 5.413713000 |
| H | 2.979310000 | -2.269426000 | 5.364504000 |
| C | 1.158780000 | -1.343804000 | 4.651023000 |
| H | 1.691571000 | -0.635736000 | 4.005489000 |
| C | -0.920833000 | -2.252825000 | 5.524870000 |
| H | -2.012879000 | -2.246932000 | 5.583050000 |
| C | 3.443373000 | 3.733275000 | -3.969698000 |
| H | 4.334482000 | 3.084921000 | -3.995918000 |
| H | 3.458550000 | 4.374037000 | -4.869716000 |
| H | 2.552409000 | 3.085146000 | -4.028428000 |
| C | 6.095370000 | 1.580040000 | -1.854429000 |
| H | 5.321306000 | 0.890973000 | -2.233088000 |
| H | 7.032885000 | 1.008184000 | -1.733908000 |
| H | 6.268201000 | 2.353804000 | -2.621139000 |
| C | -0.271245000 | 1.514198000 | 5.967084000 |
| H | -0.029017000 | 0.559124000 | 6.442463000 |
| C | -4.384422000 | -2.480390000 | -3.100713000 |
| H | -4.178645000 | -2.153831000 | -4.133430000 |
| H | -4.942139000 | -3.432988000 | -3.146947000 |
| H | -3.415355000 | -2.674255000 | -2.610571000 |
| C | 4.095149000 | -4.014149000 | -3.574438000 |
| H | 3.603322000 | -4.840116000 | -4.115041000 |
| H | 5.123610000 | -3.918375000 | -3.966407000 |
| H | 3.554486000 | -3.081668000 | -3.808626000 |
| C | -2.952625000 | -0.372098000 | 4.167215000 |
| C | -0.053970000 | 2.714155000 | 6.665067000 |
| H | 0.361287000 | 2.681721000 | 7.677969000 |
| C | 5.147754000 | -2.936195000 | -0.861729000 |
| H | 4.689535000 | -1.951861000 | -1.057766000 |
| H | 6.175801000 | -2.920658000 | -1.265948000 |
| H | 5.210186000 | -3.071246000 | 0.230407000 |
| C | -5.622561000 | -0.998374000 | 4.836696000 |
| H | -6.659782000 | -1.237159000 | 5.094320000 |
| C | 1.212433000 | -3.197220000 | 6.227144000 |
| H | 1.779940000 | -3.923937000 | 6.817884000 |
| C | -1.108422000 | 2.781180000 | 4.066035000 |
| H | -1.505343000 | 2.806477000 | 3.044349000 |
| C | 6.933666000 | 3.594036000 | 0.352429000 |
| H | 7.009650000 | 4.447559000 | -0.341443000 |
| H | 7.915920000 | 3.088519000 | 0.376662000 |
| H | 6.737229000 | 3.993014000 | 1.361771000 |
| C | -0.189644000 | -3.188670000 | 6.276925000 |
| H | -0.722992000 | -3.908263000 | 6.907117000 |
| C | -3.577606000 | 0.254074000 | 5.266022000 |
| H | -3.027240000 | 0.984197000 | 5.867147000 |
| C | 5.484039000 | 0.970238000 | 1.129471000 |
| H | 5.222404000 | 1.374053000 | 2.121704000 |
| H | 6.459732000 | 0.458860000 | 1.213450000 |
| H | 4.723774000 | 0.216711000 | 0.862785000 |
| C | -1.217684000 | -6.033397000 | -1.235636000 |
| H | -1.105832000 | -6.563979000 | -0.275118000 |
| H | -1.906153000 | -6.620605000 | -1.869348000 |
| H | -1.691167000 | -5.057663000 | -1.031687000 |
| C | -0.367432000 | 3.946136000 | 6.069866000 |

| | | | |
|---|---|---|---|
| H | -0.195540000 | 4.879710000 | 6.615820000 |
| C | 0.160179000 | -5.065247000 | -3.845745000 |
| H | -0.320716000 | -4.074568000 | -3.775617000 |
| H | -0.501658000 | -5.727449000 | -4.432431000 |
| H | 1.101761000 | -4.940903000 | -4.405763000 |
| C | 1.245633000 | 5.516251000 | 1.542031000 |
| H | 1.055555000 | 6.147818000 | 0.658657000 |
| H | 1.074215000 | 6.129218000 | 2.445226000 |
| H | 0.505484000 | 4.697857000 | 1.536275000 |
| C | 4.924083000 | 5.979382000 | -2.436431000 |
| H | 4.977809000 | 6.619079000 | -1.540231000 |
| H | 4.873919000 | 6.638166000 | -3.322100000 |
| H | 5.863380000 | 5.404497000 | -2.499203000 |
| C | 2.179239000 | -7.076816000 | 1.555473000 |
| H | 2.257434000 | -7.411634000 | 2.605592000 |
| H | 3.094509000 | -7.395263000 | 1.029483000 |
| H | 1.324355000 | -7.603181000 | 1.098645000 |
| C | 1.814040000 | 5.885764000 | -2.442824000 |
| H | 0.910778000 | 5.257708000 | -2.365051000 |
| H | 1.757974000 | 6.445131000 | -3.393817000 |
| H | 1.793892000 | 6.618025000 | -1.618433000 |
| C | -2.996002000 | 3.493042000 | -4.191193000 |
| H | -3.283964000 | 4.244740000 | -3.438100000 |
| H | -3.031891000 | 3.972718000 | -5.185942000 |
| H | -1.951357000 | 3.196827000 | -3.993381000 |
| C | -7.061703000 | -0.924825000 | -3.041333000 |
| H | -7.680996000 | -0.150208000 | -2.559753000 |
| H | -7.635084000 | -1.869380000 | -3.036497000 |
| H | -6.908265000 | -0.632198000 | -4.093579000 |
| C | 4.228511000 | 6.320207000 | 1.617410000 |
| H | 5.284142000 | 6.003905000 | 1.594313000 |
| H | 4.065019000 | 6.891074000 | 2.549286000 |
| H | 4.062032000 | 7.006994000 | 0.770480000 |
| C | -3.679909000 | -1.310740000 | 3.405149000 |
| H | -3.205347000 | -1.780632000 | 2.535501000 |
| C | -5.004699000 | -1.627481000 | 3.742991000 |
| H | -5.556462000 | -2.356414000 | 3.140476000 |
| C | -0.897939000 | 3.976658000 | 4.769361000 |
| H | -1.139712000 | 4.932781000 | 4.293918000 |
| C | -7.117819000 | 2.429224000 | -0.670159000 |
| H | -7.372120000 | 2.752895000 | -1.693016000 |
| H | -7.583204000 | 3.140383000 | 0.036032000 |
| H | -7.578081000 | 1.440981000 | -0.502368000 |
| C | -5.751624000 | -1.855445000 | -0.386448000 |
| H | -4.812766000 | -1.996188000 | 0.175868000 |
| H | -6.261469000 | -2.833255000 | -0.455326000 |
| H | -6.397651000 | -1.172303000 | 0.189966000 |
| C | -4.907641000 | -0.056761000 | 5.593929000 |
| H | -5.383980000 | 0.440179000 | 6.445805000 |
| C | 1.268635000 | -7.534911000 | -2.345115000 |
| H | 2.210535000 | -7.464680000 | -2.914745000 |
| H | 0.584565000 | -8.195018000 | -2.908367000 |
| H | 1.490896000 | -8.019799000 | -1.380461000 |
| C | 3.383999000 | -4.357999000 | 2.442980000 |
| H | 3.322431000 | -3.258269000 | 2.382658000 |
| H | 4.363772000 | -4.670057000 | 2.043930000 |
| H | 3.343756000 | -4.643446000 | 3.509250000 |
| C | -4.899316000 | 1.767283000 | 1.393315000 |
| H | -5.349039000 | 0.778022000 | 1.577241000 |
| H | -5.325877000 | 2.478719000 | 2.123424000 |
| H | -3.816242000 | 1.680472000 | 1.586364000 |

| | | | |
|---|---|---|---|
| C | -3.589918000 | 0.744056000 | -5.506616000 |
| H | -2.592645000 | 0.333449000 | -5.274640000 |
| H | -3.530382000 | 1.250033000 | -6.486906000 |
| H | -4.291822000 | -0.101027000 | -5.604894000 |
| C | 0.303720000 | -4.744659000 | 2.369695000 |
| H | 0.329183000 | -5.091495000 | 3.417969000 |
| H | -0.559561000 | -5.215457000 | 1.870236000 |
| H | 0.139061000 | -3.654135000 | 2.379600000 |
| C | -5.923143000 | 2.585944000 | -4.594785000 |
| H | -6.662933000 | 1.769328000 | -4.568615000 |
| H | -5.928631000 | 3.016746000 | -5.612347000 |
| H | -6.259102000 | 3.371625000 | -3.897232000 |

**1b_C3v**

SCF = -1972.05032790
H(0 K) = -1970.788295
H(298 K) = -1970.665623
G(298 K) = -1970.968718
SCF+D3 = -1972.35586438
PCM SCF (Benzene) = -1972.05444079
BS2 (def2-tzvp) = -24395.8957339
Low Freq. = 6.6333cm-1, 8.7855cm-1

| | | | |
|---|---|---|---|
| Rh | -0.066284005 | 0.017553001 | 1.514104107 |
| Ge | 1.187231087 | -1.864717134 | -0.877689062 |
| Ge | 1.076411079 | 1.966175140 | -0.852782059 |
| Ge | -2.182813156 | -0.018258001 | -0.937131066 |
| Ge | 2.200895159 | 0.082908006 | 0.578190043 |
| Ge | -1.187764085 | 1.941739142 | 0.483091035 |
| Ge | -1.063747079 | -1.953504139 | 0.446898032 |
| Ge | -0.733696053 | 1.377058100 | -2.774900198 |
| Ge | -0.697853053 | -1.336307097 | -2.777602198 |
| Ge | 1.640884117 | 0.061465004 | -2.715260197 |
| P | -0.120060009 | -0.055435004 | 3.809134273 |
| Si | 2.523626181 | -3.971281284 | -1.071980077 |
| Si | -4.669298334 | -0.146251010 | -1.190847088 |
| Si | 2.265146162 | 4.159664299 | -1.018052073 |
| Si | -5.329611362 | -2.437709175 | -0.900019066 |
| Si | -5.267155381 | 0.601544042 | -3.397943246 |
| Si | -5.679992425 | 1.261222090 | 0.472209034 |
| Si | 0.982850070 | 5.589329386 | -2.461416178 |
| Si | 4.822969349 | -3.402774243 | -0.673506047 |
| Si | 1.741305126 | -5.539281390 | 0.570501039 |
| Si | 2.260314165 | -4.867167349 | -3.288568236 |
| Si | 2.365796172 | 5.085956365 | 1.194726084 |
| Si | 4.480070323 | 3.791582273 | -1.872392136 |
| C | 0.233096017 | 1.559963110 | 4.689265340 |
| C | -1.749737126 | -0.563186042 | 4.583436330 |
| C | 1.608678114 | 7.393741518 | -2.289262166 |
| H | 1.455470103 | 7.777114560 | -1.266446090 |
| H | 1.056041078 | 8.053569561 | -2.982125215 |
| H | 2.682401195 | 7.478606520 | -2.525383182 |
| C | -5.477129416 | 3.106671224 | 0.011621001 |
| H | -4.412956318 | 3.368684242 | -0.113715008 |
| H | -5.892359404 | 3.745538270 | 0.811782057 |
| H | -6.003342426 | 3.354495243 | -0.925281068 |
| C | 0.059932004 | -6.289674467 | 0.051166004 |
| H | -0.693708050 | -5.500109414 | -0.108222008 |
| H | -0.315636023 | -6.962531488 | 0.843036059 |
| H | 0.143156010 | -6.876529496 | -0.878816061 |
| C | -0.268975019 | 3.937007283 | 4.939855358 |

| | | | |
|---|---|---|---|
| H | -0.811256060 | 4.826515349 | 4.603472330 |
| C | -0.450358032 | 2.719930197 | 4.266872308 |
| H | -1.122898083 | 2.666355191 | 3.402645245 |
| C | 1.115846082 | 1.644279117 | 5.785786440 |
| H | 1.649268121 | 0.753414055 | 6.129622427 |
| C | -4.221039303 | -3.616778258 | -1.915351137 |
| H | -4.266996305 | -3.390457246 | -2.993306217 |
| H | -4.543156326 | -4.663670338 | -1.770622127 |
| H | -3.166902226 | -3.536608255 | -1.599880114 |
| C | -4.700401341 | -0.666461047 | -4.712046341 |
| H | -3.611924258 | -0.837758061 | -4.657488336 |
| H | -4.936717353 | -0.296920021 | -5.725996396 |
| H | -5.204889375 | -1.638462120 | -4.580784332 |
| C | -2.250939160 | 0.058006004 | 5.747220425 |
| H | -1.703709125 | 0.887022066 | 6.205359439 |
| C | 5.337234372 | -1.852421135 | -1.664496122 |
| H | 5.210859373 | -2.003447147 | -2.749208198 |
| H | 6.397956462 | -1.610070115 | -1.472867107 |
| H | 4.728812338 | -0.979383070 | -1.373510099 |
| C | 1.161303085 | 5.060193365 | -4.290003307 |
| H | 2.202249159 | 5.155382372 | -4.641528334 |
| H | 0.527410038 | 5.696254412 | -4.933578353 |
| H | 0.846189061 | 4.012806288 | -4.432946316 |
| C | 1.087554081 | -1.227773087 | 4.632239331 |
| C | -3.451154246 | -0.386770028 | 6.326565477 |
| H | -3.831167277 | 0.107484008 | 7.227038514 |
| C | -0.869925063 | 5.547612386 | -1.997140142 |
| H | -1.279833095 | 4.530889326 | -2.121580152 |
| H | -1.443140104 | 6.228674459 | -2.651484189 |
| H | -1.035586075 | 5.855727427 | -0.951780068 |
| C | 2.992142218 | -2.895611207 | 5.884679402 |
| H | 3.729144269 | -3.545598256 | 6.367911471 |
| C | 0.614900042 | 4.015943288 | 6.029858439 |
| H | 0.763166056 | 4.968238357 | 6.549830491 |
| C | -2.469859180 | -1.633859120 | 4.014673289 |
| H | -2.095928153 | -2.109299149 | 3.099997225 |
| C | -7.173681519 | 0.778767053 | -3.505506253 |
| H | -7.692465568 | -0.160489012 | -3.253428236 |
| H | -7.465137531 | 1.062913074 | -4.532817325 |
| H | -7.541675558 | 1.564050115 | -2.823955204 |
| C | 1.309062094 | 2.869608204 | 6.446476459 |
| H | 2.001337142 | 2.922490209 | 7.293509526 |
| C | 0.718805053 | -2.033553146 | 5.729935433 |
| H | -0.307813022 | -2.009959144 | 6.106873414 |
| C | -4.500190325 | 2.299833164 | -3.815861275 |
| H | -4.813198345 | 3.076579221 | -3.098994222 |
| H | -4.817204349 | 2.617457187 | -4.825533350 |
| H | -3.397656247 | 2.252332161 | -3.803531276 |
| C | 5.528173377 | 2.823182203 | -0.598836041 |
| H | 5.660898387 | 3.394849242 | 0.335003024 |
| H | 6.530650462 | 2.609314186 | -1.010830074 |
| H | 5.052512363 | 1.861057133 | -0.342869025 |
| C | -4.157953300 | -1.457938107 | 5.758095388 |
| H | -5.093909365 | -1.801393128 | 6.211096461 |
| C | 4.459818323 | 2.817984201 | -3.515321253 |
| H | 3.989815288 | 1.827555133 | -3.389405246 |
| H | 5.492266372 | 2.664434193 | -3.877666278 |
| H | 3.900293283 | 3.356316243 | -4.298036307 |
| C | -4.891139353 | 0.985670071 | 2.188899155 |
| H | -4.990651357 | -0.058168004 | 2.528266182 |
| H | -5.374540363 | 1.637765120 | 2.938674212 |

| | | | |
|---|---|---|---|
| H | -3.814958276 | 1.227669087 | 2.167978154 |
| C | -7.142537533 | -2.679086191 | -1.474809108 |
| H | -7.833409547 | -1.997130146 | -0.952142068 |
| H | -7.468651532 | -3.715012268 | -1.271401089 |
| H | -7.245428534 | -2.502500182 | -2.558627182 |
| C | 3.629657263 | 6.526247495 | 1.256487091 |
| H | 3.613244259 | 6.999262528 | 2.255018164 |
| H | 3.402523244 | 7.304575522 | 0.509210037 |
| H | 4.656279335 | 6.167540464 | 1.073000076 |
| C | -5.214476374 | -2.944057214 | 0.942368069 |
| H | -4.186967300 | -2.800857199 | 1.317997093 |
| H | -5.479054404 | -4.009922288 | 1.063395075 |
| H | -5.896757449 | -2.348167166 | 1.571416114 |
| C | 0.422408030 | -5.058547365 | -3.770225272 |
| H | -0.117741009 | -5.712659436 | -3.066249221 |
| H | 0.341467025 | -5.500317381 | -4.779722343 |
| H | -0.089133007 | -4.080713292 | -3.783546272 |
| C | 5.965397453 | -4.850873352 | -1.195646085 |
| H | 5.693177405 | -5.791458426 | -0.689025048 |
| H | 7.014099494 | -4.616962334 | -0.938028069 |
| H | 5.918675442 | -5.024779363 | -2.283756167 |
| C | -7.553290523 | 0.873195061 | 0.601101042 |
| H | -8.065614588 | 0.996477072 | -0.367420027 |
| H | -8.030894580 | 1.556301113 | 1.326540094 |
| H | -7.727678557 | -0.159218011 | 0.948127068 |
| C | 2.418518175 | -1.270344089 | 4.167191301 |
| H | 2.707759194 | -0.661437048 | 3.302338237 |
| C | 3.366839245 | -2.092511149 | 4.794250344 |
| H | 4.395335319 | -2.113845152 | 4.419387319 |
| C | -3.662379261 | -2.083270148 | 4.601706333 |
| H | -4.209607302 | -2.913982209 | 4.144278296 |
| C | 3.009330217 | -6.965963520 | 0.752449053 |
| H | 3.197886231 | -7.472134524 | -0.208769015 |
| H | 2.629990189 | -7.720799570 | 1.464677105 |
| H | 3.975420286 | -6.597807500 | 1.136965080 |
| C | 5.113009367 | -3.052130221 | 1.185971084 |
| H | 4.442980321 | -2.249383162 | 1.538283110 |
| H | 6.155617465 | -2.728695198 | 1.356506100 |
| H | 4.928151354 | -3.948245283 | 1.801860127 |
| C | 1.667518121 | -2.865801208 | 6.347519467 |
| H | 1.366423098 | -3.490446250 | 7.195263537 |
| C | 5.329280362 | 5.478702395 | -2.204089156 |
| H | 4.800750344 | 6.044799441 | -2.989487214 |
| H | 6.365765446 | 5.314259401 | -2.550036185 |
| H | 5.369100368 | 6.108510424 | -1.300403093 |
| C | 0.657480046 | 5.782195390 | 1.703204120 |
| H | -0.122946009 | 5.004911361 | 1.640808116 |
| H | 0.355901025 | 6.622544472 | 1.055573074 |
| H | 0.692526048 | 6.150215465 | 2.744075200 |
| C | 1.521636109 | -4.710080336 | 2.275795166 |
| H | 2.462483179 | -4.273737308 | 2.648433191 |
| H | 1.170087083 | -5.450916409 | 3.016398216 |
| H | 0.775922054 | -3.898807279 | 2.223889159 |
| C | 3.117309227 | -3.741293268 | -4.574530330 |
| H | 2.714186195 | -2.715005197 | -4.537857325 |
| H | 2.955070213 | -4.134569296 | -5.594101401 |
| H | 4.205440301 | -3.685784263 | -4.403197316 |
| C | 2.902909206 | 3.762367271 | 2.461559177 |
| H | 2.915518209 | 4.185498299 | 3.481593252 |
| H | 3.911293280 | 3.378528241 | 2.233060161 |
| H | 2.205269158 | 2.908278207 | 2.457897176 |

| | | | |
|---|---|---|---|
| C | 3.070099223 | -6.604197474 | -3.364818243 |
| H | 4.131543296 | -6.580444453 | -3.068532218 |
| H | 3.013882216 | -6.997355479 | -4.396012316 |
| H | 2.548802186 | -7.318759536 | -2.705737197 |

**1b_eta1**

SCF = -1971.96969316
H(0 K) = -1970.708947
H(298 K) = -1970.586527
G(298 K) = -1970.890014
SCF+D3 = -1972.26157542
PCM SCF (Benzene) = -1971.97495005
BS2 (def2-tzvp) = -24395.8221417
Low Freq. = 4.4724cm-1, 7.3015cm-1

| | | | |
|---|---|---|---|
| C | -5.707761000 | 0.527695000 | 1.865965000 |
| C | -4.898221000 | -0.018301000 | 2.917375000 |
| C | -5.324607000 | -1.206762000 | 3.577662000 |
| C | -6.523646000 | -1.820568000 | 3.213440000 |
| C | -7.317499000 | -1.285662000 | 2.170722000 |
| C | -6.916014000 | -0.122178000 | 1.509604000 |
| P | -3.201926000 | 0.697070000 | 3.041739000 |
| C | -3.332666000 | 2.473561000 | 3.549006000 |
| C | -4.487788000 | 2.967748000 | 4.192249000 |
| C | -4.550759000 | 4.314858000 | 4.584656000 |
| C | -3.463370000 | 5.170531000 | 4.345856000 |
| C | -2.311316000 | 4.680653000 | 3.707046000 |
| C | -2.246189000 | 3.339069000 | 3.301666000 |
| C | -2.318157000 | -0.117956000 | 4.451168000 |
| C | -2.219310000 | 0.488327000 | 5.721325000 |
| C | -1.582173000 | -0.189768000 | 6.772202000 |
| C | -1.040977000 | -1.469100000 | 6.563192000 |
| C | -1.133106000 | -2.072719000 | 5.297922000 |
| C | -1.764611000 | -1.398192000 | 4.241988000 |
| Rh | -3.439625000 | -0.199633000 | 1.053848000 |
| Ge | -1.233337000 | 0.003247000 | 0.081564000 |
| Ge | 0.932261000 | 1.331144000 | 0.976918000 |
| Ge | 2.858744000 | -0.380368000 | 0.439530000 |
| Ge | 2.526379000 | 1.088190000 | -1.708680000 |
| Ge | -0.073202000 | 1.624514000 | -1.604399000 |
| Ge | 0.737733000 | -0.281252000 | -3.289677000 |
| Ge | -0.318871000 | -1.875058000 | -1.459764000 |
| Ge | 2.306687000 | -1.876634000 | -1.658928000 |
| Ge | 0.671702000 | -1.634491000 | 1.084271000 |
| Si | 5.055570000 | -0.483255000 | 1.549584000 |
| Si | 6.573488000 | -1.482345000 | -0.022574000 |
| C | 8.374634000 | -1.230363000 | 0.583865000 |
| Si | 4.808007000 | -1.837887000 | 3.515288000 |
| C | 3.910177000 | -3.476402000 | 3.116633000 |
| Si | 5.713083000 | 1.760916000 | 2.095447000 |
| C | 6.173997000 | 2.723653000 | 0.509911000 |
| C | 3.803934000 | -0.907304000 | 4.850913000 |
| C | 6.537953000 | -2.250922000 | 4.230488000 |
| Si | -1.673220000 | -3.892559000 | -1.867641000 |
| Si | -0.969199000 | -4.892757000 | -3.934407000 |
| C | 0.703731000 | -5.783211000 | -3.680395000 |
| Si | -1.540263000 | -5.456179000 | -0.053990000 |
| C | -2.344731000 | -7.127818000 | -0.538442000 |
| Si | -3.893661000 | -3.014297000 | -2.073189000 |
| C | -5.204971000 | -4.404133000 | -1.921617000 |
| C | -2.463602000 | -4.768769000 | 1.474759000 |

| | | | |
|---|---|---|---|
| C | 0.282265000 | -5.775192000 | 0.417992000 |
| Si | -0.518286000 | 3.999224000 | -2.203368000 |
| Si | 0.716008000 | 5.557731000 | -0.858974000 |
| C | 0.573786000 | 7.325908000 | -1.588942000 |
| Si | 0.124247000 | 4.231269000 | -4.512595000 |
| C | 2.028378000 | 4.267522000 | -4.684990000 |
| Si | -2.890937000 | 4.314634000 | -2.005488000 |
| C | -3.549275000 | 3.719120000 | -0.314497000 |
| C | -0.554351000 | 2.809849000 | -5.593444000 |
| C | -0.574589000 | 5.877953000 | -5.206058000 |
| C | -4.318179000 | -1.746402000 | -0.671972000 |
| C | -4.150720000 | -2.110597000 | -3.737499000 |
| C | -2.269265000 | -6.177897000 | -4.512721000 |
| C | -0.763122000 | -3.586785000 | -5.312174000 |
| C | -3.333868000 | 6.171587000 | -2.189578000 |
| C | -3.808864000 | 3.336549000 | -3.370999000 |
| C | 2.566586000 | 5.093606000 | -0.779174000 |
| C | 0.038112000 | 5.593968000 | 0.930228000 |
| C | 7.242167000 | 1.719303000 | 3.251410000 |
| C | 4.309546000 | 2.694245000 | 2.994884000 |
| C | 6.241061000 | -3.358401000 | -0.181555000 |
| C | 6.398229000 | -0.685379000 | -1.749417000 |
| H | -3.392151000 | -1.322552000 | -3.878049000 |
| H | -5.149038000 | -1.638831000 | -3.773191000 |
| H | -4.076564000 | -2.809723000 | -4.587488000 |
| H | -5.041444000 | -5.187577000 | -2.680625000 |
| H | -6.221546000 | -3.996660000 | -2.066638000 |
| H | -5.169668000 | -4.883470000 | -0.928832000 |
| H | -3.836844000 | -2.103012000 | 0.281317000 |
| H | -5.408949000 | -1.690005000 | -0.524940000 |
| H | -3.935426000 | -0.742218000 | -0.991631000 |
| H | -1.711073000 | -3.065620000 | -5.524625000 |
| H | -0.422359000 | -4.070885000 | -6.245072000 |
| H | -0.018290000 | -2.823483000 | -5.029992000 |
| H | 1.470409000 | -5.083201000 | -3.307598000 |
| H | 1.062417000 | -6.204420000 | -4.636618000 |
| H | 0.617573000 | -6.611632000 | -2.957323000 |
| H | -2.446808000 | -6.953873000 | -3.749901000 |
| H | -1.920867000 | -6.680060000 | -5.433210000 |
| H | -3.236280000 | -5.697774000 | -4.739543000 |
| H | 0.848225000 | -6.205410000 | -0.424754000 |
| H | 0.344444000 | -6.478318000 | 1.267813000 |
| H | 0.778528000 | -4.834307000 | 0.710589000 |
| H | -3.395794000 | -7.002544000 | -0.847462000 |
| H | -2.324675000 | -7.821578000 | 0.321396000 |
| H | -1.801416000 | -7.608748000 | -1.369116000 |
| H | -2.070971000 | -3.775060000 | 1.749594000 |
| H | -2.337075000 | -5.443349000 | 2.340632000 |
| H | -3.544557000 | -4.664682000 | 1.279903000 |
| H | -3.579640000 | 3.726240000 | -4.376856000 |
| H | -4.901426000 | 3.408443000 | -3.221615000 |
| H | -3.530276000 | 2.269669000 | -3.347457000 |
| H | -3.362111000 | 2.639242000 | -0.165099000 |
| H | -4.640358000 | 3.892153000 | -0.260724000 |
| H | -3.078297000 | 4.259819000 | 0.523023000 |
| H | -2.905335000 | 6.767706000 | -1.366299000 |
| H | -4.430548000 | 6.304841000 | -2.164743000 |
| H | -2.962824000 | 6.590355000 | -3.139524000 |
| H | -1.019948000 | 5.903252000 | 0.958170000 |
| H | 0.621773000 | 6.300970000 | 1.547150000 |
| H | 0.118333000 | 4.591883000 | 1.385413000 |

| | | | |
|---|---|---|---|
| H | 1.048067000 | 7.386802000 | -2.582847000 |
| H | 1.085333000 | 8.049487000 | -0.928742000 |
| H | -0.476079000 | 7.645739000 | -1.694127000 |
| H | 2.696970000 | 4.083021000 | -0.356479000 |
| H | 3.113888000 | 5.809907000 | -0.140385000 |
| H | 3.030871000 | 5.100586000 | -1.778868000 |
| H | -1.677567000 | 5.873251000 | -5.215895000 |
| H | -0.230790000 | 6.021273000 | -6.246416000 |
| H | -0.244077000 | 6.749437000 | -4.617346000 |
| H | 2.463697000 | 5.150399000 | -4.187420000 |
| H | 2.313620000 | 4.305563000 | -5.751656000 |
| H | 2.485579000 | 3.366713000 | -4.241485000 |
| H | -1.654982000 | 2.759082000 | -5.558426000 |
| H | -0.161225000 | 1.834085000 | -5.260310000 |
| H | -0.251254000 | 2.960784000 | -6.645222000 |
| H | 3.405199000 | 2.749335000 | 2.365187000 |
| H | 4.627399000 | 3.725348000 | 3.232420000 |
| H | 4.030853000 | 2.196098000 | 3.938201000 |
| H | 7.041715000 | 2.271796000 | 0.000712000 |
| H | 6.433898000 | 3.768403000 | 0.757771000 |
| H | 5.332298000 | 2.741870000 | -0.202729000 |
| H | 7.003195000 | 1.242997000 | 4.217218000 |
| H | 7.585648000 | 2.748450000 | 3.460586000 |
| H | 8.083016000 | 1.167419000 | 2.799678000 |
| H | 5.384436000 | -0.845486000 | -2.154537000 |
| H | 7.121130000 | -1.136517000 | -2.452652000 |
| H | 6.581739000 | 0.401196000 | -1.719450000 |
| H | 8.643314000 | -0.160912000 | 0.611228000 |
| H | 9.078511000 | -1.735817000 | -0.101613000 |
| H | 8.529385000 | -1.645312000 | 1.593758000 |
| H | 6.418664000 | -3.886344000 | 0.770404000 |
| H | 6.908751000 | -3.799868000 | -0.943028000 |
| H | 5.199787000 | -3.548603000 | -0.491943000 |
| H | 7.131955000 | -2.852145000 | 3.521748000 |
| H | 6.434788000 | -2.835223000 | 5.162561000 |
| H | 7.111810000 | -1.338900000 | 4.464386000 |
| H | 2.896095000 | -3.280050000 | 2.728509000 |
| H | 3.816474000 | -4.092964000 | 4.028657000 |
| H | 4.452505000 | -4.065544000 | 2.359113000 |
| H | 4.319946000 | 0.010502000 | 5.179098000 |
| H | 3.660342000 | -1.549558000 | 5.738382000 |
| H | 2.808253000 | -0.622230000 | 4.472306000 |
| H | -5.332328000 | 2.299319000 | 4.388371000 |
| H | -1.353416000 | 2.963336000 | 2.787123000 |
| H | -5.450526000 | 4.693037000 | 5.081407000 |
| H | -1.463464000 | 5.343998000 | 3.509748000 |
| H | -3.514013000 | 6.219884000 | 4.654591000 |
| H | -4.703524000 | -1.630538000 | 4.373265000 |
| H | -5.480098000 | 1.513668000 | 1.446346000 |
| H | -6.850856000 | -2.724392000 | 3.738145000 |
| H | -7.539805000 | 0.308014000 | 0.718746000 |
| H | -8.256018000 | -1.777486000 | 1.894574000 |
| H | -2.636900000 | 1.485984000 | 5.888258000 |
| H | -1.822674000 | -1.846093000 | 3.243272000 |
| H | -1.506535000 | 0.285439000 | 7.755854000 |
| H | -0.701841000 | -3.064098000 | 5.125961000 |
| H | -0.540173000 | -1.992079000 | 7.384702000 |

**1b_H2_eta1**

SCF = -1973.18143031

H(0 K) = -1971.904348

H(298 K) = -1971.781018
G(298 K) = -1972.086715
SCF+D3 = -1973.47283146
PCM SCF (Benzene) = -1973.18699251
BS2 (def2-tzvp) = -24397.0293965
Low Freq. = 7.4282cm-1, 9.7131cm-1

| | | | |
|---|---|---|---|
| Ge | 0.656817000 | -0.012226000 | -0.165290000 |
| Ge | -0.485472000 | -1.790930000 | 1.321493000 |
| Ge | -0.469308000 | 1.780236000 | 1.317410000 |
| Ge | -1.267865000 | 1.477918000 | -1.290132000 |
| Ge | -1.280272000 | -1.488680000 | -1.284984000 |
| Ge | -1.420796000 | 0.000859000 | 3.064910000 |
| Ge | -3.076191000 | 1.479682000 | 1.418486000 |
| Ge | -3.362398000 | 0.003194000 | -0.743912000 |
| Ge | -3.087583000 | -1.468172000 | 1.425136000 |
| Si | 0.609978000 | -3.949476000 | 1.799879000 |
| Si | 0.629384000 | 3.938669000 | 1.792445000 |
| Si | -5.475361000 | 0.003732000 | -2.011279000 |
| Si | 2.863621000 | -3.337790000 | 2.346412000 |
| Si | -0.487934000 | -4.921861000 | 3.701981000 |
| Si | 0.558721000 | -5.415548000 | -0.098113000 |
| Si | 2.885368000 | 3.332916000 | 2.340073000 |
| Si | 0.535599000 | 5.413438000 | -0.097450000 |
| Si | -0.453521000 | 4.900505000 | 3.710182000 |
| Si | -5.839548000 | 2.243015000 | -2.799232000 |
| Si | -7.196210000 | -0.672240000 | -0.475955000 |
| Si | -5.236948000 | -1.559484000 | -3.817802000 |
| C | 2.936501000 | -2.391818000 | 4.005899000 |
| H | 2.261274000 | -1.519891000 | 3.991994000 |
| H | 3.962167000 | -2.032010000 | 4.203413000 |
| H | 2.637511000 | -3.038048000 | 4.848269000 |
| C | 4.003648000 | -4.874518000 | 2.461307000 |
| H | 3.625591000 | -5.598929000 | 3.202056000 |
| H | 5.023046000 | -4.576500000 | 2.764882000 |
| H | 4.078509000 | -5.392240000 | 1.490271000 |
| C | 3.638811000 | -2.195205000 | 1.000473000 |
| H | 3.611799000 | -2.683623000 | 0.013330000 |
| H | 4.684531000 | -1.955117000 | 1.253459000 |
| H | 3.031370000 | -1.252491000 | 0.980289000 |
| C | -0.770330000 | -3.625854000 | 5.076202000 |
| H | 0.179284000 | -3.194660000 | 5.433420000 |
| H | -1.279843000 | -4.092818000 | 5.938274000 |
| H | -1.400035000 | -2.795066000 | 4.715522000 |
| C | -2.185036000 | -5.634778000 | 3.185705000 |
| H | -2.814716000 | -4.855623000 | 2.723880000 |
| H | -2.719380000 | -6.024800000 | 4.070488000 |
| H | -2.078410000 | -6.461638000 | 2.463785000 |
| C | 0.582855000 | -6.339949000 | 4.422240000 |
| H | 0.802778000 | -7.113114000 | 3.667514000 |
| H | 0.052704000 | -6.825722000 | 5.261158000 |
| H | 1.543818000 | -5.960218000 | 4.808731000 |
| C | -1.217545000 | -5.612253000 | -0.769799000 |
| H | -1.897198000 | -6.025033000 | -0.006319000 |
| H | -1.223756000 | -6.293205000 | -1.639711000 |
| H | -1.623674000 | -4.638884000 | -1.092661000 |
| C | 1.211930000 | -7.150979000 | 0.391459000 |
| H | 2.228936000 | -7.104436000 | 0.814996000 |
| H | 1.243805000 | -7.808157000 | -0.496299000 |
| H | 0.555728000 | -7.629026000 | 1.138114000 |
| C | 1.670678000 | -4.729373000 | -1.497980000 |

| | | | |
|---|---|---|---|
| H | 1.370653000 | -3.701974000 | -1.766343000 |
| H | 1.583404000 | -5.360634000 | -2.400519000 |
| H | 2.731703000 | -4.713966000 | -1.195233000 |
| C | 2.947168000 | 2.386817000 | 4.000249000 |
| H | 2.641412000 | 3.032457000 | 4.840560000 |
| H | 3.971868000 | 2.028365000 | 4.205588000 |
| H | 2.273386000 | 1.513856000 | 3.981625000 |
| C | 3.679489000 | 2.183402000 | 1.009154000 |
| H | 3.022070000 | 1.279363000 | 0.916768000 |
| H | 4.685920000 | 1.875897000 | 1.340956000 |
| H | 3.762992000 | 2.691699000 | 0.036211000 |
| C | 4.025740000 | 4.868679000 | 2.462385000 |
| H | 4.106628000 | 5.386131000 | 1.491789000 |
| H | 5.043355000 | 4.570917000 | 2.772663000 |
| H | 3.643569000 | 5.592942000 | 3.201082000 |
| C | 1.585361000 | 4.722004000 | -1.539942000 |
| H | 2.653075000 | 4.663219000 | -1.268924000 |
| H | 1.491407000 | 5.373958000 | -2.427187000 |
| H | 1.243389000 | 3.711011000 | -1.819831000 |
| C | 1.222672000 | 7.139906000 | 0.377035000 |
| H | 0.602481000 | 7.617463000 | 1.154122000 |
| H | 1.223266000 | 7.803895000 | -0.506223000 |
| H | 2.255942000 | 7.081440000 | 0.757627000 |
| C | -1.262736000 | 5.625585000 | -0.702933000 |
| H | -1.692870000 | 4.651740000 | -0.991372000 |
| H | -1.293055000 | 6.290071000 | -1.584947000 |
| H | -1.907019000 | 6.061787000 | 0.077849000 |
| C | 0.624179000 | 6.312753000 | 4.432125000 |
| H | 1.586190000 | 5.929746000 | 4.812637000 |
| H | 0.098667000 | 6.795458000 | 5.275727000 |
| H | 0.842018000 | 7.089355000 | 3.680244000 |
| C | -2.152879000 | 5.621870000 | 3.212881000 |
| H | -2.049231000 | 6.464240000 | 2.508719000 |
| H | -2.684374000 | 5.992568000 | 4.107642000 |
| H | -2.783773000 | 4.852363000 | 2.736816000 |
| C | -0.731437000 | 3.598329000 | 5.079494000 |
| H | 0.218079000 | 3.160006000 | 5.427982000 |
| H | -1.368296000 | 2.772830000 | 4.719206000 |
| H | -1.232425000 | 4.063877000 | 5.947329000 |
| C | -4.304471000 | 2.912486000 | -3.719006000 |
| H | -3.417977000 | 2.913345000 | -3.062177000 |
| H | -4.483749000 | 3.949325000 | -4.055798000 |
| H | -4.063672000 | 2.302178000 | -4.605168000 |
| C | -6.227659000 | 3.402504000 | -1.329058000 |
| H | -7.177631000 | 3.129096000 | -0.839922000 |
| H | -6.314574000 | 4.447790000 | -1.675909000 |
| H | -5.429591000 | 3.359636000 | -0.568707000 |
| C | -7.321511000 | 2.275318000 | -4.015049000 |
| H | -7.109449000 | 1.681541000 | -4.920166000 |
| H | -7.526060000 | 3.313027000 | -4.334639000 |
| H | -8.240121000 | 1.875352000 | -3.554970000 |
| C | -7.068163000 | 0.288356000 | 1.170308000 |
| H | -6.105335000 | 0.088445000 | 1.670651000 |
| H | -7.878481000 | -0.019690000 | 1.855291000 |
| H | -7.146451000 | 1.376887000 | 1.014773000 |
| C | -8.916340000 | -0.322099000 | -1.246809000 |
| H | -9.075125000 | 0.758472000 | -1.401013000 |
| H | -9.713135000 | -0.685751000 | -0.573208000 |
| H | -9.040398000 | -0.825566000 | -2.219986000 |
| C | -7.070600000 | -2.542181000 | -0.097523000 |
| H | -7.238864000 | -3.153278000 | -1.000106000 |

| | | | |
|---|---|---|---|
| H | -7.829432000 | -2.829750000 | 0.652214000 |
| H | -6.077333000 | -2.796061000 | 0.309822000 |
| C | -6.935128000 | -1.825091000 | -4.666695000 |
| H | -7.663481000 | -2.278388000 | -3.973342000 |
| H | -6.825856000 | -2.504774000 | -5.530907000 |
| H | -7.362202000 | -0.876979000 | -5.033366000 |
| C | -4.605617000 | -3.249860000 | -3.190383000 |
| H | -3.614691000 | -3.145982000 | -2.716560000 |
| H | -4.509608000 | -3.957330000 | -4.033516000 |
| H | -5.289641000 | -3.692138000 | -2.447821000 |
| C | -4.000851000 | -0.894897000 | -5.116972000 |
| H | -4.368168000 | 0.031797000 | -5.588892000 |
| H | -3.845205000 | -1.642558000 | -5.915299000 |
| H | -3.021610000 | -0.678619000 | -4.657886000 |
| P | 5.136040000 | -0.010634000 | -1.874302000 |
| C | 5.843915000 | 1.694271000 | -2.169170000 |
| C | 7.205770000 | 2.004844000 | -1.972828000 |
| C | 4.968347000 | 2.704541000 | -2.625806000 |
| C | 7.680373000 | 3.303329000 | -2.225886000 |
| H | 7.897861000 | 1.233234000 | -1.622371000 |
| C | 5.448214000 | 3.996748000 | -2.886757000 |
| H | 3.907120000 | 2.475928000 | -2.772039000 |
| C | 6.805075000 | 4.300454000 | -2.683564000 |
| H | 8.739601000 | 3.531810000 | -2.066616000 |
| H | 4.756683000 | 4.767988000 | -3.241245000 |
| H | 7.177564000 | 5.311256000 | -2.879816000 |
| C | 6.541909000 | -0.899804000 | -1.021292000 |
| C | 7.271819000 | -1.940592000 | -1.630337000 |
| C | 6.845135000 | -0.540640000 | 0.312105000 |
| C | 8.287124000 | -2.604750000 | -0.920572000 |
| H | 7.050287000 | -2.231505000 | -2.661452000 |
| C | 7.868516000 | -1.195423000 | 1.012919000 |
| H | 6.277603000 | 0.259954000 | 0.799836000 |
| C | 8.590146000 | -2.233539000 | 0.398257000 |
| H | 8.844822000 | -3.412687000 | -1.405954000 |
| H | 8.097615000 | -0.899535000 | 2.042169000 |
| H | 9.383523000 | -2.751021000 | 0.947385000 |
| C | 5.159297000 | -0.755226000 | -3.587773000 |
| C | 5.992938000 | -0.247515000 | -4.606549000 |
| C | 4.344661000 | -1.874179000 | -3.860689000 |
| C | 6.005740000 | -0.847617000 | -5.875993000 |
| H | 6.628588000 | 0.621561000 | -4.410697000 |
| C | 4.366448000 | -2.477067000 | -5.127991000 |
| H | 3.683181000 | -2.265784000 | -3.080638000 |
| C | 5.194388000 | -1.962927000 | -6.139115000 |
| H | 6.650822000 | -0.438840000 | -6.660912000 |
| H | 3.726052000 | -3.342673000 | -5.326486000 |
| H | 5.202935000 | -2.426798000 | -7.130989000 |
| Rh | 3.043003000 | -0.029855000 | -0.806942000 |
| H | 2.510359000 | -1.051715000 | -1.812107000 |
| H | 2.534106000 | 0.956154000 | -1.864070000 |

**1b_PPh3diss**

SCF = -1270.48818934
H(0 K) = -1269.493521
H(298 K) = -1269.389066
G(298 K) = -1269.650971
SCF+D3 = -1270.71390127
PCM SCF (Benzene) = -1270.49277358
BS2 (def2-tzvp) = -23359.2655215
Low Freq. = 8.3849cm-1, 10.1830cm-1

| | | | |
|---|---|---|---|
| Rh | 1.225343000 | -0.081074000 | -2.236266000 |
| Ge | 2.250112000 | -0.015161000 | 0.158913000 |
| Ge | -1.103918000 | -2.076755000 | -0.124201000 |
| Ge | -1.082607000 | 2.093542000 | -0.216506000 |
| Ge | 1.280032000 | -2.199240000 | -0.983129000 |
| Ge | -1.222371000 | -0.033323000 | -1.881144000 |
| Ge | 1.294383000 | 2.106469000 | -1.111594000 |
| Ge | -1.759785000 | 0.044491000 | 1.337122000 |
| Ge | 0.656295000 | 1.410383000 | 1.840442000 |
| Ge | 0.631878000 | -1.324447000 | 1.920689000 |
| Si | 4.727890000 | 0.014693000 | 0.252726000 |
| Si | -2.601087000 | 4.043659000 | 0.085999000 |
| Si | -2.617710000 | -4.036698000 | 0.111186000 |
| Si | -2.305885000 | 4.967200000 | 2.284018000 |
| Si | -4.852507000 | 3.283167000 | -0.261972000 |
| Si | -1.942809000 | 5.593520000 | -1.628844000 |
| Si | -4.705260000 | -3.394648000 | 1.105420000 |
| Si | 5.485116000 | -2.188223000 | 0.848195000 |
| Si | 5.486465000 | 0.624761000 | -1.946973000 |
| Si | 5.368098000 | 1.648119000 | 1.894784000 |
| Si | -2.922617000 | -4.770845000 | -2.159303000 |
| Si | -1.452913000 | -5.688368000 | 1.409230000 |
| C | -5.982246000 | -4.803257000 | 0.864665000 |
| H | -6.189773000 | -4.979156000 | -0.204246000 |
| H | -6.936684000 | -4.536419000 | 1.353184000 |
| H | -5.631979000 | -5.752692000 | 1.302543000 |
| C | -2.377557000 | 4.888533000 | -3.353196000 |
| H | -1.895969000 | 3.909304000 | -3.514812000 |
| H | -2.029023000 | 5.574416000 | -4.146017000 |
| H | -3.465556000 | 4.756265000 | -3.475806000 |
| C | 5.331064000 | 2.506533000 | -2.236714000 |
| H | 4.289491000 | 2.842278000 | -2.094928000 |
| H | 5.634599000 | 2.758504000 | -3.268741000 |
| H | 5.973361000 | 3.077513000 | -1.545474000 |
| C | -2.463312000 | 3.624657000 | 3.633324000 |
| H | -3.432916000 | 3.102860000 | 3.581690000 |
| H | -2.372312000 | 4.082135000 | 4.634882000 |
| H | -1.665991000 | 2.868810000 | 3.531945000 |
| C | -5.507152000 | 2.391214000 | 1.296985000 |
| H | -4.856468000 | 1.544786000 | 1.574786000 |
| H | -6.522084000 | 1.995748000 | 1.113008000 |
| H | -5.563025000 | 3.076297000 | 2.159627000 |
| C | 4.497730000 | -2.868930000 | 2.334161000 |
| H | 4.607256000 | -2.224534000 | 3.222023000 |
| H | 4.853813000 | -3.880461000 | 2.599534000 |
| H | 3.421761000 | -2.935280000 | 2.098992000 |
| C | -4.498156000 | -3.070992000 | 2.977898000 |
| H | -4.181174000 | -3.979901000 | 3.516004000 |
| H | -5.456715000 | -2.737036000 | 3.413991000 |
| H | -3.748653000 | -2.283356000 | 3.163400000 |
| C | -5.386150000 | -1.810198000 | 0.285199000 |
| H | -4.695033000 | -0.964428000 | 0.441611000 |
| H | -6.361307000 | -1.539973000 | 0.728344000 |
| H | -5.526283000 | -1.938764000 | -0.800423000 |
| C | -5.992767000 | 4.780583000 | -0.623141000 |
| H | -5.952101000 | 5.529870000 | 0.184790000 |
| H | -7.040364000 | 4.442964000 | -0.719895000 |
| H | -5.713417000 | 5.280944000 | -1.565419000 |
| C | -4.942595000 | 2.085311000 | -1.747086000 |
| H | -4.596713000 | 2.568205000 | -2.676044000 |

| | | | |
|---|---|---|---|
| H | -5.982451000 | 1.746970000 | -1.903794000 |
| H | -4.314257000 | 1.194190000 | -1.579141000 |
| C | 0.089557000 | -6.310587000 | 0.465427000 |
| H | -0.187004000 | -6.823975000 | -0.470600000 |
| H | 0.655590000 | -7.025647000 | 1.088902000 |
| H | 0.763945000 | -5.475651000 | 0.209584000 |
| C | -0.893063000 | -4.977870000 | 3.091227000 |
| H | -0.197982000 | -4.131690000 | 2.953138000 |
| H | -0.372868000 | -5.755487000 | 3.678864000 |
| H | -1.748343000 | -4.616312000 | 3.685478000 |
| C | -0.063639000 | 5.939327000 | -1.577833000 |
| H | 0.246819000 | 6.371176000 | -0.612201000 |
| H | 0.212499000 | 6.651669000 | -2.375929000 |
| H | 0.515507000 | 5.012616000 | -1.733447000 |
| C | -3.654877000 | 6.293734000 | 2.591598000 |
| H | -3.621810000 | 7.095367000 | 1.835292000 |
| H | -3.509162000 | 6.757173000 | 3.583972000 |
| H | -4.665132000 | 5.851456000 | 2.572854000 |
| C | -3.674302000 | -6.533285000 | -2.185421000 |
| H | -3.865974000 | -6.846974000 | -3.227314000 |
| H | -4.629401000 | -6.579716000 | -1.636444000 |
| H | -2.987519000 | -7.269036000 | -1.734345000 |
| C | -0.588038000 | 5.790464000 | 2.443697000 |
| H | 0.218768000 | 5.069392000 | 2.230032000 |
| H | -0.441401000 | 6.168904000 | 3.471167000 |
| H | -0.479075000 | 6.641894000 | 1.751325000 |
| C | 4.464108000 | 3.306941000 | 1.616445000 |
| H | 4.668563000 | 3.718967000 | 0.614728000 |
| H | 4.792929000 | 4.048093000 | 2.366927000 |
| H | 3.372410000 | 3.181585000 | 1.716268000 |
| C | 7.337619000 | -2.113201000 | 1.333887000 |
| H | 7.958322000 | -1.696679000 | 0.523358000 |
| H | 7.708576000 | -3.130042000 | 1.555846000 |
| H | 7.493470000 | -1.496022000 | 2.234493000 |
| C | -2.858344000 | 7.260971000 | -1.396172000 |
| H | -3.953296000 | 7.133654000 | -1.400652000 |
| H | -2.593260000 | 7.954004000 | -2.214807000 |
| H | -2.576520000 | 7.742687000 | -0.444803000 |
| C | 7.326376000 | 0.127924000 | -2.144795000 |
| H | 7.959702000 | 0.615591000 | -1.384884000 |
| H | 7.697184000 | 0.431668000 | -3.140101000 |
| H | 7.463153000 | -0.962420000 | -2.052407000 |
| C | 5.295271000 | -3.391019000 | -0.625839000 |
| H | 4.243338000 | -3.447890000 | -0.954604000 |
| H | 5.618182000 | -4.406320000 | -0.333453000 |
| H | 5.906898000 | -3.076950000 | -1.488398000 |
| C | -2.611593000 | -7.178719000 | 1.739411000 |
| H | -3.484638000 | -6.881510000 | 2.344399000 |
| H | -2.068139000 | -7.962886000 | 2.296657000 |
| H | -2.984156000 | -7.624670000 | 0.802554000 |
| C | -4.100615000 | -3.589526000 | -3.094089000 |
| H | -3.720325000 | -2.554000000 | -3.075622000 |
| H | -5.112487000 | -3.590467000 | -2.655478000 |
| H | -4.190526000 | -3.899807000 | -4.150619000 |
| C | 4.465533000 | -0.276478000 | -3.290948000 |
| H | 4.557228000 | -1.372216000 | -3.216175000 |
| H | 4.778626000 | 0.037516000 | -4.302884000 |
| H | 3.384721000 | -0.020785000 | -3.173423000 |
| C | 4.959684000 | 1.016124000 | 3.652011000 |
| H | 3.882303000 | 0.803820000 | 3.756567000 |
| H | 5.229584000 | 1.779317000 | 4.403782000 |

| | | | |
|---|---|---|---|
| H | 5.514568000 | 0.093989000 | 3.893035000 |
| C | -1.256779000 | -4.814086000 | -3.096739000 |
| H | -1.412590000 | -5.169762000 | -4.131156000 |
| H | -0.530445000 | -5.485776000 | -2.610075000 |
| H | -0.806941000 | -3.807818000 | -3.145598000 |
| C | 7.255446000 | 1.955452000 | 1.768804000 |
| H | 7.833136000 | 1.026807000 | 1.907625000 |
| H | 7.572783000 | 2.671980000 | 2.547680000 |
| H | 7.528934000 | 2.382389000 | 0.789172000 |

**Rh_H2**

SCF = -1271.69380361
H(0 K) = -1270.684551
H(298 K) = -1270.579024
G(298 K) = -1270.843958
SCF+D3 = -1271.92339197
PCM SCF (Benzene) = -1271.69606287
BS2 (def2-tzvp) = -23360.4713327
Low Freq. = 2.8816cm-1, 9.7659cm-1

| | | | |
|---|---|---|---|
| Rh | 0.796518000 | 0.030821000 | -2.335249000 |
| Ge | 1.091205000 | 2.145995000 | -1.141246000 |
| Ge | -1.201912000 | 1.940559000 | 0.006702000 |
| Si | -2.675303000 | 3.946077000 | 0.103981000 |
| Si | -3.457920000 | 4.241572000 | -2.149909000 |
| C | -4.240881000 | 5.979760000 | -2.342780000 |
| Ge | 2.194999000 | 0.113334000 | 0.109263000 |
| Si | 4.677938000 | 0.193970000 | 0.202425000 |
| Si | 5.389051000 | -1.400503000 | 1.853944000 |
| C | 7.286717000 | -1.636104000 | 1.724882000 |
| Ge | 1.302888000 | -2.033285000 | -1.117613000 |
| Ge | -1.015627000 | -2.042897000 | -0.007720000 |
| Si | -2.324542000 | -4.157541000 | 0.102954000 |
| Si | -2.587292000 | -4.849116000 | -2.185758000 |
| C | -3.202340000 | -6.662792000 | -2.248710000 |
| Ge | -1.634430000 | -0.075007000 | -1.674855000 |
| Ge | 0.635341000 | 1.390155000 | 1.957436000 |
| Ge | 0.765381000 | -1.315390000 | 1.952357000 |
| Ge | -1.681331000 | -0.084475000 | 1.691729000 |
| Si | 5.514656000 | -0.386862000 | -1.977032000 |
| C | 4.559575000 | 0.537438000 | -3.347408000 |
| Si | 5.339634000 | 2.426094000 | 0.799434000 |
| C | 5.059983000 | 3.620900000 | -0.667180000 |
| Si | -1.315132000 | 5.802369000 | 0.795215000 |
| C | -0.060568000 | 6.257764000 | -0.574459000 |
| Si | -4.493104000 | 3.569488000 | 1.626540000 |
| C | -5.328035000 | 1.882684000 | 1.306420000 |
| Si | -1.047674000 | -5.753143000 | 1.364509000 |
| C | -0.551588000 | -5.050450000 | 3.069743000 |
| Si | -4.459312000 | -3.711441000 | 1.107863000 |
| C | -5.264412000 | -2.163051000 | 0.332980000 |
| C | -0.354529000 | 5.401155000 | 2.396603000 |
| C | -2.429483000 | 7.325458000 | 1.129315000 |
| C | -3.873143000 | 3.607213000 | 3.434714000 |
| C | -5.805274000 | 4.947872000 | 1.398947000 |
| C | -4.775534000 | 2.925701000 | -2.582451000 |
| C | -2.018272000 | 4.085951000 | -3.398013000 |
| C | -2.099794000 | -7.329595000 | 1.648390000 |
| C | 0.540242000 | -6.238490000 | 0.416111000 |
| C | 5.364663000 | -2.266198000 | -2.291831000 |
| C | 7.365047000 | 0.100289000 | -2.083505000 |

| | | | |
|---|---|---|---|
| C | 4.357194000 | 3.065056000 | 2.307736000 |
| C | 7.202467000 | 2.442433000 | 1.250114000 |
| C | 4.968149000 | -0.783177000 | 3.613882000 |
| C | 4.553437000 | -3.097639000 | 1.588112000 |
| C | -5.623462000 | -5.206451000 | 0.819924000 |
| C | -4.278294000 | -3.430761000 | 2.990083000 |
| C | -3.864808000 | -3.741139000 | -3.078739000 |
| C | -0.934860000 | -4.745127000 | -3.141013000 |
| H | -2.990741000 | -7.110888000 | 2.260703000 |
| H | -1.502935000 | -8.089613000 | 2.184003000 |
| H | -2.441177000 | -7.773681000 | 0.698904000 |
| H | -4.371316000 | 1.906676000 | -2.456797000 |
| H | -5.095242000 | 3.037710000 | -3.634041000 |
| H | -5.670665000 | 3.020574000 | -1.945383000 |
| H | 3.274650000 | 3.095976000 | 2.096659000 |
| H | 4.684057000 | 4.087220000 | 2.570277000 |
| H | 4.506544000 | 2.421867000 | 3.190651000 |
| H | -1.036701000 | 5.161483000 | 3.228879000 |
| H | 0.261707000 | 6.266975000 | 2.698567000 |
| H | 0.316042000 | 4.536495000 | 2.254895000 |
| H | -3.083867000 | 2.855007000 | 3.600750000 |
| H | -4.704888000 | 3.384556000 | 4.126859000 |
| H | -3.465611000 | 4.595850000 | 3.704507000 |
| H | 5.976906000 | -2.849302000 | -1.583685000 |
| H | 5.707381000 | -2.506497000 | -3.314386000 |
| H | 4.317182000 | -2.599970000 | -2.197290000 |
| H | 0.306740000 | -6.746190000 | -0.534680000 |
| H | 1.152709000 | -6.927006000 | 1.025374000 |
| H | 1.154557000 | -5.351307000 | 0.186666000 |
| H | 0.081138000 | -4.152650000 | 2.962215000 |
| H | 0.019524000 | -5.804748000 | 3.640232000 |
| H | -1.435328000 | -4.768980000 | 3.665647000 |
| H | -5.376040000 | 5.952593000 | 1.546857000 |
| H | -6.621040000 | 4.816098000 | 2.132400000 |
| H | -6.251999000 | 4.914694000 | 0.391003000 |
| H | -5.699054000 | 1.797071000 | 0.272060000 |
| H | -6.184202000 | 1.745915000 | 1.991064000 |
| H | -4.616847000 | 1.057703000 | 1.482775000 |
| H | -4.870123000 | -3.840899000 | -2.636432000 |
| H | -3.934951000 | -4.024257000 | -4.144359000 |
| H | -3.572683000 | -2.678262000 | -3.027145000 |
| H | -0.560824000 | -3.707650000 | -3.172504000 |
| H | -1.076553000 | -5.088357000 | -4.181707000 |
| H | -0.154782000 | -5.371867000 | -2.677999000 |
| H | -1.231886000 | 4.835349000 | -3.209106000 |
| H | -2.391013000 | 4.232690000 | -4.427775000 |
| H | -1.554424000 | 3.086482000 | -3.341628000 |
| H | -3.032159000 | 7.595497000 | 0.246519000 |
| H | -1.805347000 | 8.197833000 | 1.394176000 |
| H | -3.120379000 | 7.140595000 | 1.968943000 |
| H | -6.593885000 | -5.030364000 | 1.317963000 |
| H | -5.200159000 | -6.140605000 | 1.224706000 |
| H | -5.821083000 | -5.360680000 | -0.254198000 |
| H | 0.571294000 | 5.392620000 | -0.839694000 |
| H | 0.603597000 | 7.070761000 | -0.230543000 |
| H | -0.568914000 | 6.601220000 | -1.490964000 |
| H | 5.496987000 | 0.154617000 | 3.853178000 |
| H | 5.264249000 | -1.538801000 | 4.363440000 |
| H | 3.885574000 | -0.602730000 | 3.724548000 |
| H | 7.499581000 | 1.190969000 | -1.990520000 |
| H | 7.780268000 | -0.207752000 | -3.059945000 |

| | | | |
|---|---|---|---|
| H | 7.961985000 | -0.384895000 | -1.293492000 |
| H | -5.064669000 | 6.139230000 | -1.627432000 |
| H | -4.648993000 | 6.099553000 | -3.362460000 |
| H | -3.494651000 | 6.776282000 | -2.184301000 |
| H | 7.403935000 | 1.833956000 | 2.147680000 |
| H | 7.527252000 | 3.476179000 | 1.466259000 |
| H | 7.828600000 | 2.055844000 | 0.429167000 |
| H | 3.484284000 | 0.278871000 | -3.312515000 |
| H | 4.950806000 | 0.257877000 | -4.342409000 |
| H | 4.643660000 | 1.631250000 | -3.236965000 |
| H | -2.454769000 | -7.355015000 | -1.826435000 |
| H | -3.384773000 | -6.963531000 | -3.296074000 |
| H | -4.142949000 | -6.796635000 | -1.689397000 |
| H | -3.587421000 | -2.597224000 | 3.201792000 |
| H | -3.896518000 | -4.330438000 | 3.500981000 |
| H | -5.258520000 | -3.180434000 | 3.433907000 |
| H | 5.684580000 | 3.350046000 | -1.534965000 |
| H | 5.316539000 | 4.654658000 | -0.374001000 |
| H | 4.004998000 | 3.609488000 | -0.991101000 |
| H | 3.458025000 | -3.017190000 | 1.694071000 |
| H | 4.915867000 | -3.821011000 | 2.340419000 |
| H | 4.770342000 | -3.505997000 | 0.587434000 |
| H | -6.252764000 | -1.978326000 | 0.790547000 |
| H | -5.406557000 | -2.278160000 | -0.754009000 |
| H | -4.641129000 | -1.268708000 | 0.500529000 |
| H | 7.573184000 | -2.069620000 | 0.751929000 |
| H | 7.634991000 | -2.325343000 | 2.515100000 |
| H | 7.828204000 | -0.683222000 | 1.844502000 |
| H | 0.846909000 | 0.031025000 | -4.027158000 |
| H | -0.043200000 | -0.018799000 | -3.803259000 |

**1b_H2_diss_ts**

SCF = -1973.21515743
H(0 K) = -1971.940920
H(298 K) = -1971.816691
G(298 K) = -1972.123549
SCF+D3 = -1973.51619702
PCM SCF (Benzene) = -1973.21959029
BS2 (def2-tzvp) = -24397.0625713
Low Freq. = -188.2239cm-1, 5.7910cm-1

| | | | |
|---|---|---|---|
| C | -3.866229000 | -2.351772000 | 6.188423000 |
| C | -4.044395000 | -3.548509000 | 5.476212000 |
| C | -3.345365000 | -3.754446000 | 4.275870000 |
| C | -2.476340000 | -2.765582000 | 3.788417000 |
| C | -2.282609000 | -1.564638000 | 4.505569000 |
| C | -2.987813000 | -1.365468000 | 5.710899000 |
| P | -1.083142000 | -0.296001000 | 3.816954000 |
| C | -1.529404000 | 1.260743000 | 4.755348000 |
| C | -1.111681000 | 1.472454000 | 6.088009000 |
| C | -1.505251000 | 2.630504000 | 6.777887000 |
| C | -2.318575000 | 3.586823000 | 6.147928000 |
| C | -2.734810000 | 3.383949000 | 4.822564000 |
| C | -2.340159000 | 2.228907000 | 4.128933000 |
| Rh | -1.322412000 | -0.129098000 | 1.486851000 |
| Ge | -1.153387000 | 2.078622000 | 0.339800000 |
| Ge | 1.258483000 | 2.055471000 | -0.437991000 |
| Si | 2.725314000 | 4.063829000 | -0.463519000 |
| Si | 1.995146000 | 5.467720000 | 1.343365000 |
| C | 2.908162000 | 7.152710000 | 1.298672000 |
| Ge | -2.000280000 | 0.048802000 | -1.174571000 |

| | | | |
|---|---|---|---|
| Si | -4.370495000 | 0.091105000 | -1.964927000 |
| Si | -4.367824000 | 0.341959000 | -4.366870000 |
| C | -6.139209000 | 0.026045000 | -5.032523000 |
| Ge | -1.113941000 | -2.155665000 | 0.033611000 |
| Ge | 1.318650000 | -1.920340000 | -0.647051000 |
| Si | 2.855913000 | -3.859813000 | -0.924259000 |
| Si | 2.005548000 | -5.632298000 | 0.456304000 |
| C | 2.961726000 | -7.259469000 | 0.117241000 |
| Ge | 1.173208000 | -0.038335000 | 1.276276000 |
| Ge | -0.275402000 | 1.526440000 | -2.650520000 |
| Ge | -0.214945000 | -1.192640000 | -2.808849000 |
| Ge | 2.090268000 | 0.169524000 | -2.110503000 |
| C | 0.525653000 | -0.788055000 | 4.633320000 |
| C | 1.585309000 | 0.147117000 | 4.677125000 |
| C | 2.817862000 | -0.203731000 | 5.247725000 |
| C | 3.015026000 | -1.495279000 | 5.764506000 |
| C | 1.970519000 | -2.430644000 | 5.716129000 |
| C | 0.729295000 | -2.079754000 | 5.157360000 |
| Si | -5.470382000 | -1.977499000 | -1.415090000 |
| C | -5.261547000 | -2.469954000 | 0.419356000 |
| Si | -5.555669000 | 1.975365000 | -1.040586000 |
| C | -6.014773000 | 1.706374000 | 0.798296000 |
| Si | 2.505130000 | 5.179473000 | -2.580280000 |
| C | 0.764291000 | 5.949717000 | -2.758653000 |
| Si | 4.982797000 | 3.331643000 | -0.101450000 |
| C | 5.055767000 | 2.062956000 | 1.326082000 |
| Si | 2.908123000 | -4.523677000 | -3.234182000 |
| C | 3.308188000 | -3.055541000 | -4.388244000 |
| Si | 5.026878000 | -3.180879000 | -0.158408000 |
| C | 4.899041000 | -2.277652000 | 1.520473000 |
| C | 2.789642000 | 3.979983000 | -4.038985000 |
| C | 3.809493000 | 6.580066000 | -2.697787000 |
| C | 5.691520000 | 2.521723000 | -1.681294000 |
| C | 6.099845000 | 4.818532000 | 0.364912000 |
| C | 2.362685000 | 4.621912000 | 3.021476000 |
| C | 0.117773000 | 5.816469000 | 1.253544000 |
| C | 4.263845000 | -5.857040000 | -3.483481000 |
| C | 1.222988000 | -5.260105000 | -3.757382000 |
| C | -4.775032000 | -3.399415000 | -2.488927000 |
| C | -7.351603000 | -1.817892000 | -1.751495000 |
| C | -4.539208000 | 3.588023000 | -1.169686000 |
| C | -7.191845000 | 2.235666000 | -2.006261000 |
| C | -3.843544000 | 2.112735000 | -4.863478000 |
| C | -3.215560000 | -0.895780000 | -5.253742000 |
| C | 6.157903000 | -4.711929000 | 0.072871000 |
| C | 5.853364000 | -2.011995000 | -1.425885000 |
| C | 2.209613000 | -5.193848000 | 2.308336000 |
| C | 0.152771000 | -5.968608000 | 0.123382000 |
| H | 5.267947000 | -5.452230000 | -3.272180000 |
| H | 4.257102000 | -6.207162000 | -4.531533000 |
| H | 4.107690000 | -6.732943000 | -2.832568000 |
| H | 1.890705000 | 3.625720000 | 3.067281000 |
| H | 1.964070000 | 5.227747000 | 3.854806000 |
| H | 3.446140000 | 4.493659000 | 3.182850000 |
| H | -3.610635000 | 3.514849000 | -0.576739000 |
| H | -5.127647000 | 4.440204000 | -0.784189000 |
| H | -4.255843000 | 3.810088000 | -2.211493000 |
| H | 3.626829000 | 0.533043000 | 5.280755000 |
| H | 1.440722000 | 1.158570000 | 4.283100000 |
| H | -0.082187000 | -2.813180000 | 5.138485000 |
| H | 3.784371000 | 3.507354000 | -3.992696000 |

| | | | |
|---|---|---|---|
| H | 2.712621000 | 4.525180000 | -4.996936000 |
| H | 2.034253000 | 3.175988000 | -4.043435000 |
| H | 5.050975000 | 1.691484000 | -2.024839000 |
| H | 6.700926000 | 2.117811000 | -1.485262000 |
| H | 5.773931000 | 3.250790000 | -2.504813000 |
| H | -0.470802000 | 0.737104000 | 6.584491000 |
| H | -4.977037000 | -3.237312000 | -3.560803000 |
| H | -5.239466000 | -4.358883000 | -2.198405000 |
| H | -3.683948000 | -3.496085000 | -2.358492000 |
| H | 0.981386000 | -6.173904000 | -3.189197000 |
| H | 1.239215000 | -5.522628000 | -4.830391000 |
| H | 0.409685000 | -4.531715000 | -3.598990000 |
| H | -1.171163000 | 2.785545000 | 7.809293000 |
| H | 2.534791000 | -2.272242000 | -4.318576000 |
| H | 3.350115000 | -3.401334000 | -5.436875000 |
| H | 4.277740000 | -2.593031000 | -4.141232000 |
| H | -4.730973000 | -4.314616000 | 5.851366000 |
| H | 3.979509000 | -1.769344000 | 6.204354000 |
| H | -2.641596000 | 2.083328000 | 3.085245000 |
| H | 6.071005000 | 5.609267000 | -0.403104000 |
| H | 7.148308000 | 4.485573000 | 0.468967000 |
| H | 5.793529000 | 5.266618000 | 1.325096000 |
| H | 2.113838000 | -3.438180000 | 6.120205000 |
| H | -2.858288000 | -0.438037000 | 6.276373000 |
| H | 4.708413000 | 2.505090000 | 2.274696000 |
| H | 6.091278000 | 1.707265000 | 1.472970000 |
| H | 4.419066000 | 1.188355000 | 1.111525000 |
| H | 3.273536000 | -5.120533000 | 2.589800000 |
| H | 1.746930000 | -5.974963000 | 2.938309000 |
| H | 1.729952000 | -4.230381000 | 2.549088000 |
| H | -2.620727000 | 4.490830000 | 6.687002000 |
| H | -0.456717000 | -5.070412000 | 0.325283000 |
| H | -0.209081000 | -6.783502000 | 0.776157000 |
| H | -0.026206000 | -6.264828000 | -0.923416000 |
| H | -0.156396000 | 6.332899000 | 0.318873000 |
| H | -0.192304000 | 6.453750000 | 2.101212000 |
| H | -0.461529000 | 4.878013000 | 1.300305000 |
| H | 3.712687000 | 7.303933000 | -1.871896000 |
| H | 3.686933000 | 7.130569000 | -3.647983000 |
| H | 4.835176000 | 6.174920000 | -2.674981000 |
| H | 7.174536000 | -4.391004000 | 0.363460000 |
| H | 6.241903000 | -5.302516000 | -0.854419000 |
| H | 5.777140000 | -5.377608000 | 0.865638000 |
| H | -0.019954000 | 5.180869000 | -2.657026000 |
| H | 0.654927000 | 6.417087000 | -3.753693000 |
| H | 0.582908000 | 6.727465000 | -1.998075000 |
| H | -4.547339000 | 2.871453000 | -4.482290000 |
| H | -3.812831000 | 2.202690000 | -5.964250000 |
| H | -2.838090000 | 2.350160000 | -4.475296000 |
| H | -7.816069000 | -1.077465000 | -1.078430000 |
| H | -7.846918000 | -2.789472000 | -1.573158000 |
| H | -7.564706000 | -1.514382000 | -2.789280000 |
| H | 4.003237000 | 7.028264000 | 1.316685000 |
| H | 2.620094000 | 7.762802000 | 2.173686000 |
| H | 2.647312000 | 7.723713000 | 0.391706000 |
| H | -1.955084000 | -2.914997000 | 2.835052000 |
| H | -3.483160000 | -4.680535000 | 3.708159000 |
| H | -3.360437000 | 4.129394000 | 4.320706000 |
| H | -7.000043000 | 2.529782000 | -3.051447000 |
| H | -7.776140000 | 3.045083000 | -1.532317000 |
| H | -7.817501000 | 1.328033000 | -2.016241000 |

| | | | |
|---|---|---|---|
| H | -4.196424000 | -2.602564000 | 0.673840000 |
| H | -5.782320000 | -3.426389000 | 0.607079000 |
| H | -5.685046000 | -1.711447000 | 1.097891000 |
| H | -4.413236000 | -2.180539000 | 7.121660000 |
| H | 2.792184000 | -7.615620000 | -0.912734000 |
| H | 2.616810000 | -8.050929000 | 0.806857000 |
| H | 4.048027000 | -7.135995000 | 0.258461000 |
| H | 5.211664000 | -1.141600000 | -1.644467000 |
| H | 6.057295000 | -2.530052000 | -2.377991000 |
| H | 6.815549000 | -1.638464000 | -1.031832000 |
| H | -6.615797000 | 0.792885000 | 0.941028000 |
| H | -6.608791000 | 2.563570000 | 1.163651000 |
| H | -5.115138000 | 1.623313000 | 1.429452000 |
| H | -2.158943000 | -0.727793000 | -4.986139000 |
| H | -3.315697000 | -0.774682000 | -6.347694000 |
| H | -3.463397000 | -1.939940000 | -5.001764000 |
| H | 5.898725000 | -1.946850000 | 1.854934000 |
| H | 4.476749000 | -2.932449000 | 2.300480000 |
| H | 4.249854000 | -1.388767000 | 1.447375000 |
| H | -6.439181000 | -1.025186000 | -4.885828000 |
| H | -6.162349000 | 0.230795000 | -6.118298000 |
| H | -6.894763000 | 0.667369000 | -4.551001000 |
| H | -3.443657000 | -0.031625000 | 1.463355000 |
| H | -3.564697000 | -0.399490000 | 2.130958000 |

**1b_H2**

SCF = -1973.21548071
H(0 K) = -1971.939936
H(298 K) = -1971.815753
G(298 K) = -1972.121724
SCF+D3 = -1973.51707851
PCM SCF (Benzene) = -1973.21992643
BS2 (def2-tzvp) = -24397.0624785
Low Freq. = 7.5475cm-1, 9.1755cm-1

| | | | |
|---|---|---|---|
| C | -4.091939000 | -2.489706000 | 5.998734000 |
| C | -4.259219000 | -3.666957000 | 5.252765000 |
| C | -3.515502000 | -3.856349000 | 4.076669000 |
| C | -2.613081000 | -2.870516000 | 3.647420000 |
| C | -2.429392000 | -1.689699000 | 4.400107000 |
| C | -3.179869000 | -1.506893000 | 5.579996000 |
| P | -1.189179000 | -0.425656000 | 3.781377000 |
| C | -1.591724000 | 1.099650000 | 4.789813000 |
| C | -1.217085000 | 1.208253000 | 6.147822000 |
| C | -1.572702000 | 2.344248000 | 6.892280000 |
| C | -2.303725000 | 3.382736000 | 6.291786000 |
| C | -2.674705000 | 3.283872000 | 4.941614000 |
| C | -2.318112000 | 2.150047000 | 4.193934000 |
| Rh | -1.422513000 | -0.172888000 | 1.462388000 |
| Ge | -1.120171000 | 2.071186000 | 0.374761000 |
| Ge | 1.295556000 | 2.042797000 | -0.370566000 |
| Si | 2.762263000 | 4.049371000 | -0.299078000 |
| Si | 1.992517000 | 5.383998000 | 1.543085000 |
| C | 2.937450000 | 7.050602000 | 1.615013000 |
| Ge | -1.981037000 | 0.098110000 | -1.212384000 |
| Si | -4.335447000 | 0.179049000 | -2.038581000 |
| Si | -4.308041000 | 0.624174000 | -4.410366000 |
| C | -6.061111000 | 0.316368000 | -5.125900000 |
| Ge | -1.100524000 | -2.162599000 | -0.076305000 |
| Ge | 1.337328000 | -1.874165000 | -0.693753000 |
| Si | 2.889264000 | -3.799511000 | -0.975594000 |

| | | | |
|---|---|---|---|
| Si | 2.027199000 | -5.606303000 | 0.353395000 |
| C | 3.010923000 | -7.215867000 | 0.007972000 |
| Ge | 1.091695000 | -0.084351000 | 1.315874000 |
| Ge | -0.234660000 | 1.618755000 | -2.606337000 |
| Ge | -0.187154000 | -1.106424000 | -2.850366000 |
| Ge | 2.130952000 | 0.230676000 | -2.122152000 |
| C | 0.400231000 | -0.996302000 | 4.587503000 |
| C | 1.473984000 | -0.083825000 | 4.707703000 |
| C | 2.691994000 | -0.491860000 | 5.271863000 |
| C | 2.860603000 | -1.817007000 | 5.706627000 |
| C | 1.802195000 | -2.729594000 | 5.582210000 |
| C | 0.575883000 | -2.322669000 | 5.028678000 |
| Si | -5.401534000 | -1.942252000 | -1.653224000 |
| C | -5.212615000 | -2.534125000 | 0.154600000 |
| Si | -5.564337000 | 1.956278000 | -0.972614000 |
| C | -6.038711000 | 1.519870000 | 0.830202000 |
| Si | 2.581939000 | 5.228745000 | -2.384929000 |
| C | 0.841943000 | 5.996512000 | -2.580517000 |
| Si | 5.010838000 | 3.297944000 | 0.078987000 |
| C | 5.052082000 | 1.984599000 | 1.466676000 |
| Si | 2.975130000 | -4.415552000 | -3.298243000 |
| C | 3.389771000 | -2.925354000 | -4.418143000 |
| Si | 5.044836000 | -3.125405000 | -0.163720000 |
| C | 4.884080000 | -2.268978000 | 1.536530000 |
| C | 2.902637000 | 4.073687000 | -3.871835000 |
| C | 3.881461000 | 6.638025000 | -2.432745000 |
| C | 5.741304000 | 2.534688000 | -1.514038000 |
| C | 6.128325000 | 4.762001000 | 0.611274000 |
| C | 2.278634000 | 4.451135000 | 3.190410000 |
| C | 0.127079000 | 5.777072000 | 1.401139000 |
| C | 4.335293000 | -5.742948000 | -3.554821000 |
| C | 1.298268000 | -5.143008000 | -3.859149000 |
| C | -4.649604000 | -3.277784000 | -2.796484000 |
| C | -7.278695000 | -1.802842000 | -2.017936000 |
| C | -4.575091000 | 3.590469000 | -0.949014000 |
| C | -7.194066000 | 2.269288000 | -1.933884000 |
| C | -3.828662000 | 2.444497000 | -4.748009000 |
| C | -3.108133000 | -0.505094000 | -5.375461000 |
| C | 6.186203000 | -4.652196000 | 0.042500000 |
| C | 5.877359000 | -1.915588000 | -1.387807000 |
| C | 2.181646000 | -5.200064000 | 2.217197000 |
| C | 0.187162000 | -5.961126000 | -0.027626000 |
| H | 5.336315000 | -5.341476000 | -3.323577000 |
| H | 4.341851000 | -6.073507000 | -4.609205000 |
| H | 4.171943000 | -6.630936000 | -2.922355000 |
| H | 1.783694000 | 3.465231000 | 3.170141000 |
| H | 1.862239000 | 5.025876000 | 4.036953000 |
| H | 3.352158000 | 4.289637000 | 3.384654000 |
| H | -3.649308000 | 3.480088000 | -0.357302000 |
| H | -5.180287000 | 4.396211000 | -0.495603000 |
| H | -4.287734000 | 3.907337000 | -1.964903000 |
| H | 3.511859000 | 0.227598000 | 5.364309000 |
| H | 1.351720000 | 0.954236000 | 4.381345000 |
| H | -0.246663000 | -3.039724000 | 4.951048000 |
| H | 3.899919000 | 3.607043000 | -3.821398000 |
| H | 2.838263000 | 4.645709000 | -4.814975000 |
| H | 2.153836000 | 3.264606000 | -3.913062000 |
| H | 5.099739000 | 1.723095000 | -1.897882000 |
| H | 6.743098000 | 2.114380000 | -1.313549000 |
| H | 5.845748000 | 3.290730000 | -2.310257000 |
| H | -0.638972000 | 0.408693000 | 6.621744000 |

| | | | |
|---|---|---|---|
| H | -4.826054000 | -3.047475000 | -3.860392000 |
| H | -5.100588000 | -4.263651000 | -2.583790000 |
| H | -3.560437000 | -3.360424000 | -2.642129000 |
| H | 1.053344000 | -6.071535000 | -3.316940000 |
| H | 1.327579000 | -5.378342000 | -4.938164000 |
| H | 0.480746000 | -4.421393000 | -3.691569000 |
| H | -1.273232000 | 2.418054000 | 7.943138000 |
| H | 2.615230000 | -2.143542000 | -4.344726000 |
| H | 3.446642000 | -3.251414000 | -5.472389000 |
| H | 4.355390000 | -2.467139000 | -4.148931000 |
| H | -4.971552000 | -4.430522000 | 5.582304000 |
| H | 3.813349000 | -2.134989000 | 6.142468000 |
| H | -2.582720000 | 2.085118000 | 3.132063000 |
| H | 6.114051000 | 5.579293000 | -0.128763000 |
| H | 7.173537000 | 4.419687000 | 0.717766000 |
| H | 5.811252000 | 5.177923000 | 1.582363000 |
| H | 1.922827000 | -3.763251000 | 5.922562000 |
| H | -3.060609000 | -0.594848000 | 6.171940000 |
| H | 4.695774000 | 2.400202000 | 2.423930000 |
| H | 6.082009000 | 1.614269000 | 1.616584000 |
| H | 4.410288000 | 1.123424000 | 1.216333000 |
| H | 3.237307000 | -5.116762000 | 2.525570000 |
| H | 1.715830000 | -6.000141000 | 2.820571000 |
| H | 1.682068000 | -4.248571000 | 2.464951000 |
| H | -2.576229000 | 4.269520000 | 6.873591000 |
| H | -0.439101000 | -5.074043000 | 0.172031000 |
| H | -0.178209000 | -6.789441000 | 0.606079000 |
| H | 0.035807000 | -6.245864000 | -1.081911000 |
| H | -0.100972000 | 6.348412000 | 0.486304000 |
| H | -0.202527000 | 6.374977000 | 2.269884000 |
| H | -0.471832000 | 4.850100000 | 1.375540000 |
| H | 3.760814000 | 7.339141000 | -1.590394000 |
| H | 3.778539000 | 7.213446000 | -3.370437000 |
| H | 4.908707000 | 6.237883000 | -2.396052000 |
| H | 7.195955000 | -4.329923000 | 0.354806000 |
| H | 6.287825000 | -5.217900000 | -0.898437000 |
| H | 5.801195000 | -5.341404000 | 0.812780000 |
| H | 0.059428000 | 5.221760000 | -2.517223000 |
| H | 0.752831000 | 6.489739000 | -3.565055000 |
| H | 0.639690000 | 6.752862000 | -1.803875000 |
| H | -4.559592000 | 3.147187000 | -4.313920000 |
| H | -3.786545000 | 2.629526000 | -5.836422000 |
| H | -2.835742000 | 2.676155000 | -4.325832000 |
| H | -7.772213000 | -1.112636000 | -1.312971000 |
| H | -7.756958000 | -2.792881000 | -1.907866000 |
| H | -7.476701000 | -1.442335000 | -3.040453000 |
| H | 4.027672000 | 6.904041000 | 1.685130000 |
| H | 2.614303000 | 7.630370000 | 2.498369000 |
| H | 2.735664000 | 7.663089000 | 0.720212000 |
| H | -2.057595000 | -3.006082000 | 2.711629000 |
| H | -3.644234000 | -4.766917000 | 3.482323000 |
| H | -3.234742000 | 4.093801000 | 4.462695000 |
| H | -6.996451000 | 2.650163000 | -2.949649000 |
| H | -7.798232000 | 3.027330000 | -1.403318000 |
| H | -7.802986000 | 1.354763000 | -2.025217000 |
| H | -4.149232000 | -2.689046000 | 0.406656000 |
| H | -5.738329000 | -3.496533000 | 0.291096000 |
| H | -5.636206000 | -1.810104000 | 0.870182000 |
| H | -4.673699000 | -2.330500000 | 6.912900000 |
| H | 2.867953000 | -7.556972000 | -1.031084000 |
| H | 2.660574000 | -8.022604000 | 0.676849000 |

| | | | |
|---|---|---|---|
| H | 4.092359000 | -7.082386000 | 0.174857000 |
| H | 5.229035000 | -1.047087000 | -1.594069000 |
| H | 6.101979000 | -2.406303000 | -2.349647000 |
| H | 6.828876000 | -1.541666000 | -0.969024000 |
| H | -6.639857000 | 0.596889000 | 0.884972000 |
| H | -6.635542000 | 2.339361000 | 1.269907000 |
| H | -5.142254000 | 1.379918000 | 1.456472000 |
| H | -2.060837000 | -0.329811000 | -5.078208000 |
| H | -3.196194000 | -0.299478000 | -6.457752000 |
| H | -3.329148000 | -1.572728000 | -5.211839000 |
| H | 5.874759000 | -1.933537000 | 1.892468000 |
| H | 4.460912000 | -2.949590000 | 2.293568000 |
| H | 4.223357000 | -1.387627000 | 1.478639000 |
| H | -6.330392000 | -0.752029000 | -5.074864000 |
| H | -6.080250000 | 0.614530000 | -6.189846000 |
| H | -6.840240000 | 0.890453000 | -4.599137000 |
| H | -3.320839000 | -0.655648000 | 1.442870000 |
| H | -3.339820000 | 0.031049000 | 1.848312000 |

**1b_H2_oxadd_ts**

SCF = -1973.20936262
H(0 K) = -1971.934478
H(298 K) = -1971.811374
G(298 K) = -1972.112655
SCF+D3 = -1973.51539061
PCM SCF (Benzene) = -1973.21347846
BS2 (def2-tzvp) = -24397.0525643
Low Freq. = -677.2002cm-1, 8.4514cm-1

| | | | |
|---|---|---|---|
| C | 5.772578000 | 1.825244000 | 5.105879000 |
| C | 5.864290000 | 3.047952000 | 4.422654000 |
| C | 4.897793000 | 3.381364000 | 3.459333000 |
| C | 3.849487000 | 2.491790000 | 3.175832000 |
| C | 3.745271000 | 1.264821000 | 3.867263000 |
| C | 4.715901000 | 0.939434000 | 4.836393000 |
| P | 2.296893000 | 0.145208000 | 3.464374000 |
| C | 2.794791000 | -1.488811000 | 4.234520000 |
| C | 2.693083000 | -1.716106000 | 5.625196000 |
| C | 3.103877000 | -2.940774000 | 6.175694000 |
| C | 3.619616000 | -3.950765000 | 5.346932000 |
| C | 3.721464000 | -3.732577000 | 3.963868000 |
| C | 3.308319000 | -2.510224000 | 3.410100000 |
| Rh | 1.856198000 | 0.081489000 | 1.180223000 |
| Ge | 0.729607000 | -2.056070000 | 0.193616000 |
| Ge | -1.729388000 | -1.547225000 | -0.408293000 |
| Si | -3.171292000 | -3.546909000 | 0.059984000 |
| Si | -4.028967000 | -3.386681000 | 2.299003000 |
| C | -4.729955000 | -5.087131000 | 2.840713000 |
| Ge | 1.780101000 | -0.120931000 | -1.441091000 |
| Si | 3.917669000 | -0.197142000 | -2.717088000 |
| Si | 3.529554000 | -0.999217000 | -4.955021000 |
| C | 5.099057000 | -0.687432000 | -6.012629000 |
| Ge | 0.814731000 | 2.094131000 | -0.082288000 |
| Ge | -1.660309000 | 1.606714000 | -0.618742000 |
| Si | -3.058927000 | 3.645164000 | -0.272248000 |
| Si | -2.697504000 | 4.465188000 | 1.957671000 |
| C | -3.458748000 | 6.217747000 | 2.122070000 |
| Ge | -0.750283000 | 0.153709000 | 1.544542000 |
| Ge | -0.130975000 | -1.599313000 | -2.611720000 |
| Ge | -0.033480000 | 1.297155000 | -2.803363000 |
| Ge | -2.412970000 | -0.063600000 | -2.524032000 |

| | | | |
|---|---|---|---|
| C | 0.995533000 | 0.738279000 | 4.671109000 |
| C | -0.123955000 | -0.086871000 | 4.925093000 |
| C | -1.134209000 | 0.336183000 | 5.801789000 |
| C | -1.048519000 | 1.592022000 | 6.425849000 |
| C | 0.055786000 | 2.419671000 | 6.171812000 |
| C | 1.074388000 | 1.996522000 | 5.300595000 |
| Si | 4.822450000 | 2.027597000 | -2.791936000 |
| C | 4.824237000 | 2.848462000 | -1.066104000 |
| Si | 5.452750000 | -1.699729000 | -1.631695000 |
| C | 6.308702000 | -0.890445000 | -0.123280000 |
| Si | -1.839993000 | -5.547176000 | -0.126419000 |
| C | -0.681343000 | -5.741623000 | 1.382902000 |
| Si | -4.972550000 | -3.624135000 | -1.530674000 |
| C | -5.885083000 | -1.952089000 | -1.661211000 |
| Si | -2.405944000 | 5.280898000 | -1.909787000 |
| C | -2.343387000 | 4.537537000 | -3.667333000 |
| Si | -5.354760000 | 3.009624000 | -0.557639000 |
| C | -5.735152000 | 1.440079000 | 0.463057000 |
| C | -0.783228000 | -5.563349000 | -1.716369000 |
| C | -3.001486000 | -7.073248000 | -0.183784000 |
| C | -4.313765000 | -4.094525000 | -3.262901000 |
| C | -6.250093000 | -4.944035000 | -0.980323000 |
| C | -5.437536000 | -2.099492000 | 2.415075000 |
| C | -2.651637000 | -2.890919000 | 3.527515000 |
| C | -3.685438000 | 6.709483000 | -1.914543000 |
| C | -0.688204000 | 6.003153000 | -1.483851000 |
| C | 3.804295000 | 3.126251000 | -3.980907000 |
| C | 6.633893000 | 1.968452000 | -3.417844000 |
| C | 4.554572000 | -3.286493000 | -1.056825000 |
| C | 6.835180000 | -2.211276000 | -2.857972000 |
| C | 3.170266000 | -2.878104000 | -4.942621000 |
| C | 2.076794000 | -0.115170000 | -5.825924000 |
| C | -6.506048000 | 4.415686000 | 0.051915000 |
| C | -5.744736000 | 2.660282000 | -2.395933000 |
| C | -3.527495000 | 3.316257000 | 3.240018000 |
| C | -0.838566000 | 4.592753000 | 2.379192000 |
| H | -4.678983000 | 6.357176000 | -2.238955000 |
| H | -3.362647000 | 7.497540000 | -2.618645000 |
| H | -3.795856000 | 7.169210000 | -0.918709000 |
| H | -5.104020000 | -1.104234000 | 2.078484000 |
| H | -5.785401000 | -2.007269000 | 3.459731000 |
| H | -6.302915000 | -2.393850000 | 1.797805000 |
| H | 3.755079000 | -3.047035000 | -0.334989000 |
| H | 5.265557000 | -3.978493000 | -0.570539000 |
| H | 4.091016000 | -3.813539000 | -1.907346000 |
| H | -1.991274000 | -0.318062000 | 5.991338000 |
| H | -0.197588000 | -1.073230000 | 4.455172000 |
| H | 1.936661000 | 2.645407000 | 5.121283000 |
| H | -1.409231000 | -5.484346000 | -2.620532000 |
| H | -0.207709000 | -6.504496000 | -1.778742000 |
| H | -0.069910000 | -4.722317000 | -1.725553000 |
| H | -3.559417000 | -3.369169000 | -3.611459000 |
| H | -5.139832000 | -4.103770000 | -3.996375000 |
| H | -3.849924000 | -5.095097000 | -3.263316000 |
| H | 2.284369000 | -0.938652000 | 6.278292000 |
| H | 3.863541000 | 2.761466000 | -5.020087000 |
| H | 4.183423000 | 4.163863000 | -3.964666000 |
| H | 2.740312000 | 3.146700000 | -3.689357000 |
| H | -0.708918000 | 6.562464000 | -0.533369000 |
| H | -0.356730000 | 6.696054000 | -2.277839000 |
| H | 0.064399000 | 5.201581000 | -1.392520000 |

| | | | |
|---|---|---|---|
| H | 3.016400000 | -3.105447000 | 7.254968000 |
| H | -1.578875000 | 3.744536000 | -3.735944000 |
| H | -2.086579000 | 5.323283000 | -4.400432000 |
| H | -3.311525000 | 4.099424000 | -3.960838000 |
| H | 6.689007000 | 3.736289000 | 4.635413000 |
| H | -1.838329000 | 1.921334000 | 7.109059000 |
| H | 3.366367000 | -2.343754000 | 2.329134000 |
| H | -5.794656000 | -5.940805000 | -0.862853000 |
| H | -7.052627000 | -5.024255000 | -1.735665000 |
| H | -6.720181000 | -4.669548000 | -0.020869000 |
| H | 0.134990000 | 3.397489000 | 6.658742000 |
| H | 4.655350000 | -0.009885000 | 5.376808000 |
| H | -6.281235000 | -1.625855000 | -0.685693000 |
| H | -6.732790000 | -2.038415000 | -2.364617000 |
| H | -5.211203000 | -1.163535000 | -2.037939000 |
| H | -4.623068000 | 3.290319000 | 3.115618000 |
| H | -3.309734000 | 3.668895000 | 4.263879000 |
| H | -3.143740000 | 2.285937000 | 3.149860000 |
| H | 3.934680000 | -4.906965000 | 5.777851000 |
| H | -0.370162000 | 3.593929000 | 2.396959000 |
| H | -0.710479000 | 5.043904000 | 3.379687000 |
| H | -0.294538000 | 5.213188000 | 1.648098000 |
| H | -1.805941000 | -3.597724000 | 3.493795000 |
| H | -3.047138000 | -2.873813000 | 4.559227000 |
| H | -2.267789000 | -1.884729000 | 3.283495000 |
| H | -3.676437000 | -7.115159000 | 0.686639000 |
| H | -2.397413000 | -7.998542000 | -0.189869000 |
| H | -3.620355000 | -7.072284000 | -1.096546000 |
| H | -7.561994000 | 4.140353000 | -0.121381000 |
| H | -6.312491000 | 5.363141000 | -0.477783000 |
| H | -6.380273000 | 4.598631000 | 1.132333000 |
| H | -0.002720000 | -4.876132000 | 1.473548000 |
| H | -0.061072000 | -6.648799000 | 1.268500000 |
| H | -1.248772000 | -5.835721000 | 2.323941000 |
| H | 4.013551000 | -3.454056000 | -4.526014000 |
| H | 2.989671000 | -3.238090000 | -5.971385000 |
| H | 2.271659000 | -3.102826000 | -4.343010000 |
| H | 7.282726000 | 1.412000000 | -2.720590000 |
| H | 7.036195000 | 2.993902000 | -3.504960000 |
| H | 6.710841000 | 1.489528000 | -4.407754000 |
| H | -5.512965000 | -5.445906000 | 2.152228000 |
| H | -5.176487000 | -5.005025000 | 3.848131000 |
| H | -3.939059000 | -5.854458000 | 2.885964000 |
| H | 3.111090000 | 2.737950000 | 2.404460000 |
| H | 4.963729000 | 4.330525000 | 2.917245000 |
| H | 4.114444000 | -4.518003000 | 3.309823000 |
| H | 6.431213000 | -2.773347000 | -3.716244000 |
| H | 7.567459000 | -2.860760000 | -2.345090000 |
| H | 7.378041000 | -1.334670000 | -3.248998000 |
| H | 3.796568000 | 2.964364000 | -0.681584000 |
| H | 5.284168000 | 3.851544000 | -1.126622000 |
| H | 5.393176000 | 2.252501000 | -0.333405000 |
| H | 6.526359000 | 1.554792000 | 5.853045000 |
| H | -2.944533000 | 6.940970000 | 1.467006000 |
| H | -3.356555000 | 6.575566000 | 3.162505000 |
| H | -4.530575000 | 6.228335000 | 1.864334000 |
| H | -5.085733000 | 1.873124000 | -2.800732000 |
| H | -5.616220000 | 3.564236000 | -3.014631000 |
| H | -6.789718000 | 2.319611000 | -2.507238000 |
| H | 6.906435000 | -0.013143000 | -0.422761000 |
| H | 6.990776000 | -1.616260000 | 0.355463000 |

| | | | |
|---|---|---|---|
| H | 5.577608000 | -0.560695000 | 0.632960000 |
| H | 1.116940000 | -0.333824000 | -5.328723000 |
| H | 2.003655000 | -0.461098000 | -6.872967000 |
| H | 2.209146000 | 0.979297000 | -5.835834000 |
| H | -6.790096000 | 1.139925000 | 0.332405000 |
| H | -5.555812000 | 1.606473000 | 1.538040000 |
| H | -5.098578000 | 0.601153000 | 0.136425000 |
| H | 5.289713000 | 0.391906000 | -6.136579000 |
| H | 4.957722000 | -1.119366000 | -7.019897000 |
| H | 5.999455000 | -1.144820000 | -5.571556000 |
| H | 3.300652000 | 0.718650000 | 0.901619000 |
| H | 3.348933000 | -0.491103000 | 1.006732000 |

**1b_H_H**

SCF = -1973.22553712
H(0 K) = -1971.948363
H(298 K) = -1971.825526
G(298 K) = -1972.124999
SCF+D3 = -1973.53708679
PCM SCF (Benzene) = -1973.22961216
BS2 (def2-tzvp) = -24397.0684420
Low Freq. = 6.6578cm-1, 11.2512cm-1

| | | | |
|---|---|---|---|
| C | 2.554154000 | 3.000189000 | 6.233521000 |
| C | 1.264823000 | 3.545458000 | 6.330727000 |
| C | 0.266557000 | 3.129565000 | 5.434617000 |
| C | 0.560634000 | 2.182144000 | 4.441479000 |
| C | 1.852570000 | 1.623655000 | 4.340793000 |
| C | 2.846807000 | 2.039712000 | 5.250704000 |
| P | 2.184250000 | 0.298450000 | 3.049245000 |
| C | 4.063481000 | 0.218674000 | 3.091025000 |
| C | 4.750562000 | -0.637757000 | 3.979049000 |
| C | 6.154135000 | -0.620116000 | 4.042961000 |
| C | 6.888985000 | 0.258314000 | 3.231844000 |
| C | 6.212777000 | 1.119932000 | 2.352686000 |
| C | 4.811644000 | 1.096400000 | 2.280007000 |
| Rh | 1.205389000 | 0.775471000 | 0.980506000 |
| Ge | 2.174113000 | 1.346625000 | -1.527021000 |
| Ge | 1.389844000 | -1.105140000 | -1.103613000 |
| Si | 2.983094000 | -2.825742000 | -2.001537000 |
| Si | 5.196078000 | -2.369362000 | -1.175366000 |
| C | 6.494653000 | -3.343120000 | -2.196962000 |
| Ge | -0.268410000 | 2.094790000 | -0.820571000 |
| Si | -0.434576000 | 4.569061000 | -1.135653000 |
| Si | -0.072806000 | 5.065572000 | -3.463054000 |
| C | -0.592608000 | 6.876385000 | -3.821273000 |
| Ge | -1.424676000 | 1.002725000 | 1.330142000 |
| Ge | -2.477519000 | -1.024544000 | 0.044120000 |
| Si | -4.617999000 | -2.131421000 | 0.609881000 |
| Si | -5.872414000 | -0.511702000 | 1.867411000 |
| C | -7.683310000 | -1.103538000 | 2.076235000 |
| Ge | -0.089147000 | -1.577723000 | 1.066589000 |
| Ge | -0.014844000 | 0.410023000 | -3.054600000 |
| Ge | -2.377387000 | 0.782141000 | -1.836395000 |
| Ge | -1.042618000 | -1.855210000 | -1.983137000 |
| C | 1.731186000 | -1.254472000 | 3.997356000 |
| C | 2.048522000 | -2.511628000 | 3.433131000 |
| C | 1.721926000 | -3.698896000 | 4.105675000 |
| C | 1.051161000 | -3.649240000 | 5.338873000 |
| C | 0.717844000 | -2.406463000 | 5.898131000 |
| C | 1.059586000 | -1.214511000 | 5.235864000 |

| | | | |
|---|---|---|---|
| Si | -2.623794000 | 5.308970000 | -0.470899000 |
| C | -3.081911000 | 4.687163000 | 1.276526000 |
| Si | 1.233436000 | 5.689045000 | 0.188694000 |
| C | 0.751472000 | 5.683789000 | 2.038396000 |
| Si | 3.030957000 | -2.677242000 | -4.405995000 |
| C | 3.894002000 | -1.062495000 | -4.959898000 |
| Si | 2.318761000 | -5.040985000 | -1.350471000 |
| C | 1.944420000 | -5.135759000 | 0.522760000 |
| Si | -5.743972000 | -2.701956000 | -1.435587000 |
| C | -4.617205000 | -3.706663000 | -2.605537000 |
| Si | -4.127499000 | -4.079774000 | 1.926350000 |
| C | -2.905758000 | -3.673722000 | 3.336411000 |
| C | 1.292653000 | -2.732504000 | -5.196707000 |
| C | 4.015135000 | -4.164935000 | -5.111201000 |
| C | 0.763688000 | -5.605964000 | -2.309491000 |
| C | 3.733198000 | -6.283889000 | -1.715444000 |
| C | 5.369927000 | -2.904068000 | 0.652350000 |
| C | 5.630606000 | -0.513252000 | -1.301421000 |
| C | -7.285387000 | -3.767973000 | -1.034477000 |
| C | -6.316046000 | -1.121846000 | -2.347380000 |
| C | -3.947733000 | 4.698639000 | -1.708509000 |
| C | -2.674357000 | 7.225857000 | -0.432613000 |
| C | 2.957753000 | 4.885190000 | 0.019146000 |
| C | 1.374604000 | 7.511143000 | -0.392488000 |
| C | 1.776004000 | 4.870861000 | -3.912042000 |
| C | -1.101376000 | 3.937790000 | -4.611992000 |
| C | -5.747432000 | -4.746319000 | 2.704240000 |
| C | -3.365950000 | -5.452743000 | 0.834925000 |
| C | -5.105836000 | -0.266925000 | 3.602277000 |
| C | -5.889253000 | 1.176064000 | 0.973521000 |
| H | -6.999917000 | -4.729778000 | -0.576150000 |
| H | -7.840540000 | -3.990565000 | -1.963517000 |
| H | -7.973510000 | -3.253663000 | -0.343625000 |
| H | 4.685200000 | -2.330937000 | 1.298992000 |
| H | 6.397800000 | -2.713469000 | 1.008871000 |
| H | 5.158332000 | -3.978183000 | 0.786281000 |
| H | 2.939104000 | 3.852728000 | 0.406070000 |
| H | 3.698858000 | 5.460563000 | 0.603281000 |
| H | 3.295141000 | 4.853228000 | -1.029812000 |
| H | 1.978841000 | -4.661547000 | 3.652358000 |
| H | 2.569101000 | -2.564143000 | 2.471151000 |
| H | 0.806847000 | -0.253198000 | 5.691752000 |
| H | 0.720429000 | -3.615932000 | -4.868937000 |
| H | 1.386089000 | -2.772521000 | -6.297180000 |
| H | 0.702941000 | -1.836684000 | -4.938740000 |
| H | -0.071630000 | -4.897420000 | -2.173680000 |
| H | 0.433178000 | -6.597933000 | -1.952528000 |
| H | 0.964259000 | -5.686106000 | -3.391122000 |
| H | 4.190976000 | -1.319788000 | 4.625420000 |
| H | -3.783325000 | 5.118740000 | -2.715041000 |
| H | -4.955177000 | 5.004684000 | -1.373997000 |
| H | -3.937535000 | 3.598338000 | -1.795315000 |
| H | -7.057459000 | -0.558493000 | -1.756403000 |
| H | -6.783933000 | -1.387547000 | -3.312255000 |
| H | -5.465523000 | -0.450473000 | -2.555815000 |
| H | 6.670764000 | -1.295902000 | 4.732842000 |
| H | -3.713442000 | -3.136825000 | -2.880908000 |
| H | -5.162340000 | -3.953714000 | -3.534277000 |
| H | -4.288054000 | -4.651045000 | -2.141689000 |
| H | 1.039388000 | 4.293759000 | 7.097793000 |
| H | 0.788633000 | -4.575955000 | 5.859661000 |

| | | | |
|---|---|---|---|
| H | 4.289850000 | 1.761360000 | 1.583475000 |
| H | 4.029775000 | -6.270342000 | -2.777012000 |
| H | 3.405224000 | -7.309665000 | -1.467991000 |
| H | 4.628490000 | -6.063123000 | -1.110035000 |
| H | 0.195736000 | -2.357318000 | 6.859581000 |
| H | 3.853954000 | 1.617293000 | 5.194283000 |
| H | 2.846377000 | -4.903905000 | 1.114632000 |
| H | 1.608933000 | -6.152883000 | 0.794353000 |
| H | 1.152735000 | -4.422467000 | 0.810940000 |
| H | -5.137724000 | -1.194214000 | 4.198372000 |
| H | -5.660348000 | 0.511513000 | 4.156556000 |
| H | -4.053808000 | 0.056144000 | 3.523568000 |
| H | 7.982804000 | 0.271063000 | 3.283330000 |
| H | -4.865968000 | 1.574723000 | 0.872032000 |
| H | -6.485272000 | 1.906087000 | 1.550077000 |
| H | -6.325049000 | 1.099879000 | -0.036122000 |
| H | 5.548604000 | -0.144168000 | -2.336980000 |
| H | 6.666169000 | -0.343105000 | -0.955805000 |
| H | 4.958884000 | 0.091324000 | -0.669430000 |
| H | 5.027674000 | -4.239720000 | -4.683148000 |
| H | 4.115594000 | -4.055937000 | -6.206284000 |
| H | 3.491647000 | -5.116326000 | -4.917545000 |
| H | -5.541653000 | -5.671966000 | 3.271461000 |
| H | -6.505749000 | -4.979743000 | 1.938653000 |
| H | -6.185973000 | -4.014774000 | 3.403584000 |
| H | 3.383838000 | -0.176551000 | -4.545205000 |
| H | 3.876279000 | -0.979435000 | -6.061389000 |
| H | 4.947676000 | -1.031964000 | -4.635532000 |
| H | 2.402895000 | 5.597919000 | -3.368853000 |
| H | 1.925783000 | 5.036361000 | -4.994044000 |
| H | 2.140786000 | 3.858480000 | -3.668042000 |
| H | -1.991316000 | 7.629864000 | 0.333433000 |
| H | -3.695524000 | 7.567511000 | -0.184659000 |
| H | -2.396028000 | 7.667658000 | -1.403277000 |
| H | 6.286823000 | -4.425739000 | -2.207359000 |
| H | 7.498487000 | -3.194867000 | -1.759220000 |
| H | 6.530495000 | -2.992781000 | -3.242005000 |
| H | -0.219188000 | 1.879391000 | 3.732664000 |
| H | -0.743147000 | 3.548399000 | 5.498882000 |
| H | 6.775229000 | 1.809585000 | 1.714730000 |
| H | 1.754027000 | 7.573572000 | -1.426187000 |
| H | 2.081540000 | 8.057102000 | 0.258139000 |
| H | 0.405222000 | 8.034721000 | -0.353700000 |
| H | -3.047221000 | 3.585494000 | 1.334466000 |
| H | -4.103343000 | 5.014638000 | 1.541262000 |
| H | -2.387714000 | 5.083094000 | 2.036395000 |
| H | 3.340986000 | 3.320434000 | 6.924814000 |
| H | -8.197886000 | -1.170465000 | 1.102966000 |
| H | -8.243787000 | -0.387006000 | 2.703412000 |
| H | -7.740629000 | -2.093078000 | 2.559135000 |
| H | -2.457165000 | -5.096193000 | 0.322418000 |
| H | -4.076590000 | -5.800552000 | 0.066611000 |
| H | -3.087708000 | -6.322911000 | 1.456228000 |
| H | -0.193275000 | 6.224892000 | 2.214570000 |
| H | 1.539851000 | 6.174929000 | 2.636772000 |
| H | 0.633880000 | 4.654004000 | 2.415101000 |
| H | -0.790515000 | 2.882447000 | -4.524281000 |
| H | -0.961904000 | 4.245982000 | -5.663974000 |
| H | -2.177959000 | 3.990438000 | -4.380061000 |
| H | -2.729803000 | -4.571779000 | 3.955492000 |
| H | -3.291564000 | -2.876558000 | 3.992995000 |

| | | | |
|---|---|---|---|
| H | -1.933755000 | -3.340263000 | 2.934273000 |
| H | -1.678815000 | 7.014337000 | -3.688483000 |
| H | -0.348506000 | 7.131967000 | -4.868266000 |
| H | -0.074841000 | 7.596795000 | -3.167236000 |
| H | 0.968032000 | 2.167514000 | 1.642930000 |
| H | 2.598720000 | 1.510451000 | 0.638595000 |

**2b**

SCF = -1972.45651221
H(0 K) = -1971.186498
H(298 K) = -1971.063305
G(298 K) = -1971.368302
SCF+D3 = -1972.76166889
PCM SCF (Benzene) = -1972.48205522
BS2 (def2-tzvp) = -24396.2923555
Low Freq. = 6.0160cm-1, 7.3463cm-1

| | | | |
|---|---|---|---|
| Ge | -2.300764000 | -1.373171000 | -0.089703000 |
| Ge | -2.396972000 | 0.365858000 | -2.096533000 |
| Ge | -1.755610000 | 0.897357000 | 1.096767000 |
| Ge | 0.105845000 | -1.607503000 | 0.963887000 |
| Ge | -0.796894000 | -1.950134000 | -2.185314000 |
| Ge | 0.103255000 | 0.454424000 | -3.097401000 |
| Ge | -0.675088000 | 2.102919000 | -0.963119000 |
| Ge | 1.546137000 | -1.094026000 | -1.198154000 |
| Ge | 1.849644000 | 1.449634000 | -0.928295000 |
| Rh | 0.826671000 | 0.813192000 | 1.223837000 |
| P | 1.962697000 | 0.598652000 | 3.284269000 |
| Si | -4.223203000 | -2.793522000 | 0.596922000 |
| Si | -6.167494000 | -1.372101000 | 0.524443000 |
| Si | -3.715407000 | -3.505089000 | 2.841807000 |
| Si | -4.351149000 | -4.640369000 | -0.946875000 |
| C | -7.714325000 | -2.457492000 | 0.816938000 |
| H | -7.660985000 | -3.010022000 | 1.769040000 |
| H | -7.852488000 | -3.189488000 | 0.004003000 |
| H | -8.613880000 | -1.817142000 | 0.847029000 |
| C | -6.064685000 | -0.043397000 | 1.893106000 |
| H | -6.935821000 | 0.632390000 | 1.827338000 |
| H | -5.153084000 | 0.570713000 | 1.795067000 |
| H | -6.066060000 | -0.496190000 | 2.898468000 |
| C | -6.335451000 | -0.512494000 | -1.170477000 |
| H | -7.250636000 | 0.105745000 | -1.186236000 |
| H | -6.405932000 | -1.242897000 | -1.992897000 |
| H | -5.476439000 | 0.147751000 | -1.378534000 |
| C | -5.298670000 | -4.238159000 | 3.623427000 |
| H | -5.709286000 | -5.066414000 | 3.023097000 |
| H | -6.085660000 | -3.473908000 | 3.733869000 |
| H | -5.069402000 | -4.631704000 | 4.629719000 |
| C | -2.348236000 | -4.839422000 | 2.833694000 |
| H | -2.095701000 | -5.124396000 | 3.870645000 |
| H | -1.427997000 | -4.469730000 | 2.350024000 |
| H | -2.670890000 | -5.751061000 | 2.304318000 |
| C | -3.123578000 | -2.036419000 | 3.909850000 |
| H | -3.871379000 | -1.227411000 | 3.945237000 |
| H | -2.181722000 | -1.612893000 | 3.521167000 |
| H | -2.939197000 | -2.375884000 | 4.944689000 |
| C | -5.613823000 | -5.896405000 | -0.251018000 |
| H | -5.736547000 | -6.730745000 | -0.964460000 |
| H | -6.604793000 | -5.440831000 | -0.091822000 |
| H | -5.275892000 | -6.323176000 | 0.707957000 |
| C | -2.657483000 | -5.500082000 | -1.130734000 |

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|---|---|---|---|
| H | -2.271522000 | -5.858986000 | -0.162819000 |
| H | -1.909840000 | -4.815113000 | -1.566291000 |
| H | -2.752428000 | -6.370115000 | -1.804507000 |
| C | -4.936224000 | -4.039322000 | -2.661285000 |
| H | -4.259902000 | -3.273803000 | -3.076970000 |
| H | -5.951572000 | -3.611989000 | -2.617594000 |
| H | -4.959296000 | -4.888317000 | -3.367403000 |
| Si | -1.031372000 | 4.556316000 | -1.271743000 |
| Si | -0.659102000 | 5.638575000 | 0.846942000 |
| Si | 0.485937000 | 5.341817000 | -2.971504000 |
| Si | -3.333805000 | 4.767635000 | -1.960163000 |
| Si | 3.486715000 | -2.440066000 | -2.040534000 |
| C | 1.045540000 | 5.174609000 | 1.563249000 |
| H | 1.123657000 | 4.089237000 | 1.743396000 |
| H | 1.862501000 | 5.462927000 | 0.881780000 |
| H | 1.205081000 | 5.692947000 | 2.525467000 |
| C | -0.714164000 | 7.530571000 | 0.575270000 |
| H | -1.664200000 | 7.859556000 | 0.124156000 |
| H | 0.108602000 | 7.867560000 | -0.076886000 |
| H | -0.604041000 | 8.045779000 | 1.546254000 |
| C | -2.018840000 | 5.146797000 | 2.095637000 |
| H | -1.811352000 | 5.604451000 | 3.079436000 |
| H | -2.063084000 | 4.052135000 | 2.229848000 |
| H | -3.014080000 | 5.489970000 | 1.767916000 |
| C | 2.272604000 | 5.415807000 | -2.297789000 |
| H | 2.608763000 | 4.429372000 | -1.933767000 |
| H | 2.362806000 | 6.134908000 | -1.466817000 |
| H | 2.963615000 | 5.735404000 | -3.098003000 |
| C | 0.449629000 | 4.219178000 | -4.514063000 |
| H | 1.122064000 | 4.627633000 | -5.289392000 |
| H | -0.562507000 | 4.150431000 | -4.944922000 |
| H | 0.786786000 | 3.194858000 | -4.279533000 |
| C | -0.061229000 | 7.101219000 | -3.483193000 |
| H | 0.650914000 | 7.509452000 | -4.222379000 |
| H | -0.091115000 | 7.793325000 | -2.625896000 |
| H | -1.059743000 | 7.092991000 | -3.950948000 |
| C | -4.485543000 | 3.739022000 | -0.836463000 |
| H | -5.537037000 | 3.894589000 | -1.136545000 |
| H | -4.387316000 | 4.026894000 | 0.223040000 |
| H | -4.267670000 | 2.660478000 | -0.921063000 |
| C | -3.553709000 | 4.199704000 | -3.769419000 |
| H | -4.615931000 | 4.279590000 | -4.061382000 |
| H | -3.244241000 | 3.149910000 | -3.907445000 |
| H | -2.967368000 | 4.824175000 | -4.463721000 |
| C | -3.834500000 | 6.608449000 | -1.821001000 |
| H | -3.171054000 | 7.264493000 | -2.407747000 |
| H | -3.821305000 | 6.955059000 | -0.774369000 |
| H | -4.862353000 | 6.739071000 | -2.204056000 |
| Si | 3.112605000 | -4.730932000 | -1.401686000 |
| Si | 5.539293000 | -1.587592000 | -1.113386000 |
| Si | 3.513673000 | -2.205586000 | -4.444889000 |
| C | 2.558726000 | -4.851720000 | 0.421824000 |
| H | 1.577522000 | -4.368105000 | 0.570695000 |
| H | 3.282131000 | -4.364820000 | 1.096216000 |
| H | 2.464960000 | -5.911255000 | 0.719721000 |
| C | 4.754568000 | -5.690454000 | -1.608223000 |
| H | 5.538218000 | -5.307317000 | -0.933713000 |
| H | 5.135390000 | -5.634373000 | -2.641125000 |
| H | 4.594124000 | -6.756140000 | -1.365933000 |
| C | 1.781332000 | -5.535541000 | -2.508529000 |
| H | 1.597490000 | -6.574361000 | -2.181347000 |

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|---|---|---|---|
| H | 2.097981000 | -5.567884000 | -3.564189000 |
| H | 0.823897000 | -4.989852000 | -2.456163000 |
| C | 5.603285000 | 0.320876000 | -1.181018000 |
| H | 4.796207000 | 0.769778000 | -0.576645000 |
| H | 5.501709000 | 0.696299000 | -2.212649000 |
| H | 6.568708000 | 0.679445000 | -0.781354000 |
| C | 7.004385000 | -2.270254000 | -2.135790000 |
| H | 6.998529000 | -1.882413000 | -3.167688000 |
| H | 6.998385000 | -3.371487000 | -2.182266000 |
| H | 7.954548000 | -1.958221000 | -1.666419000 |
| C | 5.739982000 | -2.154601000 | 0.695913000 |
| H | 6.671165000 | -1.739373000 | 1.120492000 |
| H | 5.800596000 | -3.253271000 | 0.767677000 |
| H | 4.899997000 | -1.819065000 | 1.325653000 |
| C | 4.079919000 | -0.449561000 | -4.938929000 |
| H | 4.087867000 | -0.354927000 | -6.039350000 |
| H | 5.097464000 | -0.229189000 | -4.575894000 |
| H | 3.398055000 | 0.321056000 | -4.540974000 |
| C | 4.763332000 | -3.487779000 | -5.119952000 |
| H | 4.425532000 | -4.519673000 | -4.927235000 |
| H | 5.767337000 | -3.368199000 | -4.682670000 |
| H | 4.853619000 | -3.365310000 | -6.214181000 |
| C | 1.820624000 | -2.558505000 | -5.251315000 |
| H | 1.075235000 | -1.788825000 | -4.989829000 |
| H | 1.416801000 | -3.539370000 | -4.951756000 |
| H | 1.932916000 | -2.557717000 | -6.350362000 |
| C | 3.018196000 | 2.119348000 | 3.501378000 |
| C | 3.885064000 | 2.501349000 | 2.454131000 |
| H | 3.908174000 | 1.921093000 | 1.524961000 |
| C | 4.713918000 | 3.623654000 | 2.595647000 |
| H | 5.384638000 | 3.908978000 | 1.778919000 |
| C | 4.677042000 | 4.381536000 | 3.778536000 |
| H | 5.320021000 | 5.260735000 | 3.886648000 |
| C | 3.813019000 | 4.009247000 | 4.820174000 |
| H | 3.781322000 | 4.594747000 | 5.744598000 |
| C | 2.986479000 | 2.880832000 | 4.687634000 |
| H | 2.323340000 | 2.594025000 | 5.508717000 |
| C | 3.149122000 | -0.800078000 | 3.629432000 |
| C | 4.459452000 | -0.552797000 | 4.091770000 |
| H | 4.825699000 | 0.473100000 | 4.185551000 |
| C | 5.294666000 | -1.624262000 | 4.451046000 |
| H | 6.308347000 | -1.419607000 | 4.809939000 |
| C | 4.831358000 | -2.945511000 | 4.359890000 |
| H | 5.482514000 | -3.777243000 | 4.646694000 |
| C | 3.527600000 | -3.197585000 | 3.899048000 |
| H | 3.157016000 | -4.224811000 | 3.825725000 |
| C | 2.693018000 | -2.132247000 | 3.530287000 |
| H | 1.677226000 | -2.338823000 | 3.173942000 |
| C | 0.875023000 | 0.581874000 | 4.802417000 |
| C | -0.333226000 | 1.309686000 | 4.822305000 |
| H | -0.666800000 | 1.839125000 | 3.924224000 |
| C | -1.116157000 | 1.356909000 | 5.985616000 |
| H | -2.050971000 | 1.926446000 | 5.984838000 |
| C | -0.706658000 | 0.670520000 | 7.140271000 |
| H | -1.321532000 | 0.701658000 | 8.045303000 |
| C | 0.493200000 | -0.057506000 | 7.128011000 |
| H | 0.821260000 | -0.594202000 | 8.023909000 |
| C | 1.284195000 | -0.102054000 | 5.968525000 |
| H | 2.220735000 | -0.666068000 | 5.977150000 |
| H | 0.077867000 | 1.936485000 | 2.030954000 |

**2b_H2_diss_ts**

SCF = -1973.61430499
H(0 K) = -1972.331332
H(298 K) = -1972.207070
G(298 K) = -1972.510484
SCF+D3 = -1973.92487574
PCM SCF (Benzene) = -1973.63994308
BS2 (def2-tzvp) = -24397.4492172
Low Freq. = -240.1228cm-1, 6.2108cm-1

| | | | |
|---|---|---|---|
| C | -3.833539000 | -1.042102000 | 6.153169000 |
| C | -4.601797000 | -1.853620000 | 5.300782000 |
| C | -4.308562000 | -1.897674000 | 3.930538000 |
| C | -3.248230000 | -1.136437000 | 3.406805000 |
| C | -2.464266000 | -0.334739000 | 4.255972000 |
| C | -2.772453000 | -0.285724000 | 5.636787000 |
| P | -0.995754000 | 0.644251000 | 3.638179000 |
| C | -1.255370000 | 2.229558000 | 4.607413000 |
| C | -0.253508000 | 2.834238000 | 5.391422000 |
| C | -0.512557000 | 4.041885000 | 6.062730000 |
| C | -1.767623000 | 4.659506000 | 5.956426000 |
| C | -2.775212000 | 4.057667000 | 5.184261000 |
| C | -2.523220000 | 2.851157000 | 4.514234000 |
| Rh | -0.549176000 | 1.145159000 | 1.313212000 |
| Ge | -1.413818000 | 2.286681000 | -0.939177000 |
| Ge | 1.142678000 | 1.909199000 | -0.863113000 |
| Si | 2.461306000 | 4.016709000 | -1.137015000 |
| Si | 2.594576000 | 5.108870000 | 1.004628000 |
| C | 3.351542000 | 6.847127000 | 0.755717000 |
| Ge | -2.052757000 | -0.197886000 | -0.999144000 |
| Si | -4.419819000 | -0.615709000 | -1.736868000 |
| Si | -4.556781000 | 0.019068000 | -4.065558000 |
| C | -6.260963000 | -0.547338000 | -4.725597000 |
| Ge | -0.713681000 | -1.422903000 | 0.927165000 |
| Ge | 1.497066000 | -2.033218000 | -0.375551000 |
| Si | 2.828174000 | -4.122676000 | -0.201708000 |
| Si | 1.763495000 | -5.514491000 | 1.449443000 |
| C | 2.430448000 | -7.294663000 | 1.243403000 |
| Ge | -0.278614000 | 0.767938000 | -3.043827000 |
| Ge | -0.331078000 | -1.826541000 | -2.258317000 |
| Ge | 1.863931000 | 0.196837000 | 1.004019000 |
| Ge | 2.071860000 | -0.231909000 | -2.205124000 |
| C | 0.449713000 | -0.192510000 | 4.480237000 |
| C | 1.738805000 | 0.384084000 | 4.403312000 |
| C | 2.830525000 | -0.217693000 | 5.048973000 |
| C | 2.657658000 | -1.419053000 | 5.755138000 |
| C | 1.388009000 | -2.013474000 | 5.811369000 |
| C | 0.288144000 | -1.405125000 | 5.182541000 |
| Si | -4.899739000 | -2.957898000 | -1.469364000 |
| C | -4.390509000 | -3.553887000 | 0.272951000 |
| Si | -5.932677000 | 0.756991000 | -0.448947000 |
| C | -6.316554000 | -0.027534000 | 1.249135000 |
| Si | 1.364101000 | 5.405124000 | -2.772964000 |
| C | -0.217601000 | 6.185179000 | -2.039744000 |
| Si | 4.654998000 | 3.340186000 | -1.874395000 |
| C | 5.320210000 | 1.890524000 | -0.822248000 |
| Si | 2.772637000 | -5.154613000 | -2.381606000 |
| C | 3.150794000 | -3.900490000 | -3.769249000 |
| Si | 5.057693000 | -3.477151000 | 0.436824000 |
| C | 5.025074000 | -2.244227000 | 1.894372000 |
| C | 0.904509000 | 4.411317000 | -4.336055000 |

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|---|---|---|---|
| C | 2.576991000 | 6.797497000 | -3.270698000 |
| C | 4.625706000 | 2.814183000 | -3.709479000 |
| C | 5.842234000 | 4.826832000 | -1.675780000 |
| C | 3.709893000 | 4.106827000 | 2.191523000 |
| C | 0.873411000 | 5.300503000 | 1.804180000 |
| C | 4.112196000 | -6.519198000 | -2.404521000 |
| C | 1.062868000 | -5.942965000 | -2.697724000 |
| C | -3.981294000 | -4.002829000 | -2.776719000 |
| C | -6.783328000 | -3.225954000 | -1.668260000 |
| C | -5.227069000 | 2.508964000 | -0.165335000 |
| C | -7.580111000 | 0.915974000 | -1.407035000 |
| C | -4.405414000 | 1.914688000 | -4.244063000 |
| C | -3.221520000 | -0.816655000 | -5.143452000 |
| C | 5.997334000 | -5.052822000 | 0.976144000 |
| C | 5.968676000 | -2.676788000 | -1.037632000 |
| C | 2.168507000 | -4.908178000 | 3.214276000 |
| C | -0.130674000 | -5.527485000 | 1.210861000 |
| H | 5.124273000 | -6.095276000 | -2.295562000 |
| H | 4.075731000 | -7.054799000 | -3.369948000 |
| H | 3.962583000 | -7.260054000 | -1.602215000 |
| H | 3.346458000 | 3.069723000 | 2.296842000 |
| H | 3.714189000 | 4.573553000 | 3.192793000 |
| H | 4.752462000 | 4.066233000 | 1.834915000 |
| H | -4.307661000 | 2.477211000 | 0.443292000 |
| H | -5.968611000 | 3.129192000 | 0.369499000 |
| H | -4.987665000 | 3.011846000 | -1.116869000 |
| H | 3.817192000 | 0.252526000 | 4.991725000 |
| H | 1.896052000 | 1.311163000 | 3.842344000 |
| H | -0.695398000 | -1.876990000 | 5.248539000 |
| H | 1.789548000 | 3.942653000 | -4.796565000 |
| H | 0.447384000 | 5.082773000 | -5.084609000 |
| H | 0.177072000 | 3.612501000 | -4.110923000 |
| H | 3.934138000 | 1.971625000 | -3.879452000 |
| H | 5.634355000 | 2.491876000 | -4.023742000 |
| H | 4.320171000 | 3.646253000 | -4.365325000 |
| H | 0.724157000 | 2.359302000 | 5.505358000 |
| H | -4.331073000 | -3.772199000 | -3.796615000 |
| H | -4.161816000 | -5.077236000 | -2.594890000 |
| H | -2.891829000 | -3.830454000 | -2.743650000 |
| H | 0.835378000 | -6.733153000 | -1.962977000 |
| H | 1.040847000 | -6.401395000 | -3.702356000 |
| H | 0.258968000 | -5.188790000 | -2.653224000 |
| H | 0.272628000 | 4.493539000 | 6.677501000 |
| H | 2.364520000 | -3.130217000 | -3.842054000 |
| H | 3.199072000 | -4.423946000 | -4.740711000 |
| H | 4.114714000 | -3.390140000 | -3.609864000 |
| H | -5.429289000 | -2.445338000 | 5.704755000 |
| H | 3.509386000 | -1.890195000 | 6.255502000 |
| H | -3.328303000 | 2.376283000 | 3.942994000 |
| H | 5.483688000 | 5.717180000 | -2.217652000 |
| H | 6.834979000 | 4.562306000 | -2.081607000 |
| H | 5.976146000 | 5.101463000 | -0.616337000 |
| H | 1.244133000 | -2.954196000 | 6.351958000 |
| H | -2.180164000 | 0.342513000 | 6.309165000 |
| H | 5.344797000 | 2.142044000 | 0.250744000 |
| H | 6.348171000 | 1.638474000 | -1.137983000 |
| H | 4.698267000 | 0.987398000 | -0.949653000 |
| H | 3.251509000 | -4.954640000 | 3.416878000 |
| H | 1.661291000 | -5.552530000 | 3.954623000 |
| H | 1.833687000 | -3.870998000 | 3.380611000 |
| H | -1.964883000 | 5.599406000 | 6.481230000 |

| | | | |
|---|---|---|---|
| H | -0.558303000 | -4.524033000 | 1.381174000 |
| H | -0.597930000 | -6.222205000 | 1.931289000 |
| H | -0.411022000 | -5.850248000 | 0.194899000 |
| H | 0.172162000 | 5.837454000 | 1.144534000 |
| H | 0.958522000 | 5.868175000 | 2.747906000 |
| H | 0.437384000 | 4.315302000 | 2.037337000 |
| H | 2.910694000 | 7.387878000 | -2.401855000 |
| H | 2.079010000 | 7.486388000 | -3.976136000 |
| H | 3.471167000 | 6.393425000 | -3.773832000 |
| H | 7.040121000 | -4.794393000 | 1.232912000 |
| H | 6.025414000 | -5.808159000 | 0.173768000 |
| H | 5.538007000 | -5.516025000 | 1.865128000 |
| H | -0.925641000 | 5.412772000 | -1.692796000 |
| H | -0.728686000 | 6.792553000 | -2.807779000 |
| H | 0.013296000 | 6.845440000 | -1.187347000 |
| H | -5.208381000 | 2.442315000 | -3.703179000 |
| H | -4.472419000 | 2.199654000 | -5.309010000 |
| H | -3.437252000 | 2.278453000 | -3.859412000 |
| H | -7.355308000 | -2.694145000 | -0.889732000 |
| H | -7.017006000 | -4.301996000 | -1.580741000 |
| H | -7.145610000 | -2.882200000 | -2.650841000 |
| H | 4.331811000 | 6.806776000 | 0.253948000 |
| H | 3.493591000 | 7.332325000 | 1.737979000 |
| H | 2.687544000 | 7.493089000 | 0.157598000 |
| H | -3.033193000 | -1.169998000 | 2.333242000 |
| H | -4.904723000 | -2.524268000 | 3.260732000 |
| H | -3.763657000 | 4.521799000 | 5.108258000 |
| H | -7.453125000 | 1.467631000 | -2.352804000 |
| H | -8.307684000 | 1.472750000 | -0.789635000 |
| H | -8.020047000 | -0.067885000 | -1.638818000 |
| H | -3.308039000 | -3.428518000 | 0.447599000 |
| H | -4.633579000 | -4.623561000 | 0.399962000 |
| H | -4.932920000 | -2.987069000 | 1.047740000 |
| H | -4.059504000 | -0.996433000 | 7.223246000 |
| H | 2.165801000 | -7.717812000 | 0.260334000 |
| H | 1.991356000 | -7.947417000 | 2.018832000 |
| H | 3.526945000 | -7.336253000 | 1.349818000 |
| H | 5.435515000 | -1.785883000 | -1.409873000 |
| H | 6.080617000 | -3.383147000 | -1.876878000 |
| H | 6.980820000 | -2.361081000 | -0.727940000 |
| H | -6.766214000 | -1.028586000 | 1.139777000 |
| H | -7.039984000 | 0.604888000 | 1.794352000 |
| H | -5.414480000 | -0.123025000 | 1.874812000 |
| H | -2.208715000 | -0.455894000 | -4.896758000 |
| H | -3.411721000 | -0.581961000 | -6.206147000 |
| H | -3.228114000 | -1.913148000 | -5.031277000 |
| H | 6.056736000 | -2.015553000 | 2.216232000 |
| H | 4.477176000 | -2.649610000 | 2.760670000 |
| H | 4.542620000 | -1.295362000 | 1.602872000 |
| H | -6.347086000 | -1.646714000 | -4.720962000 |
| H | -6.372767000 | -0.209277000 | -5.771468000 |
| H | -7.100877000 | -0.134276000 | -4.145333000 |
| H | -1.841936000 | 3.100474000 | 2.229527000 |
| H | 0.645514000 | 1.872327000 | 2.031953000 |
| H | -1.769435000 | 2.956488000 | 1.475540000 |

**2b_H2**

SCF = -1973.62379228
H(0 K) = -1972.339141
H(298 K) = -1972.215185
G(298 K) = -1972.519446

SCF+D3 = -1973.93754732
PCM SCF (Benzene) = -1973.64952477
BS2 (def2-tzvp) = -24397.4575056
Low Freq. = 7.0700cm-1, 8.2862cm-1

| | | | |
|---|---|---|---|
| C | 1.808412000 | 2.605061000 | 6.541015000 |
| C | 1.621132000 | 3.843803000 | 5.903140000 |
| C | 1.353204000 | 3.886352000 | 4.527667000 |
| C | 1.268269000 | 2.694525000 | 3.786242000 |
| C | 1.439842000 | 1.451028000 | 4.420797000 |
| C | 1.720710000 | 1.414345000 | 5.806876000 |
| P | 1.299341000 | -0.166115000 | 3.496159000 |
| C | 2.779296000 | -1.068908000 | 4.210310000 |
| C | 2.664037000 | -2.172690000 | 5.078954000 |
| C | 3.816079000 | -2.780054000 | 5.609327000 |
| C | 5.089665000 | -2.291072000 | 5.285760000 |
| C | 5.211165000 | -1.179424000 | 4.434586000 |
| C | 4.065639000 | -0.573028000 | 3.900673000 |
| Rh | 1.404888000 | -0.248443000 | 1.099689000 |
| Ge | 2.668640000 | -0.264685000 | -1.467174000 |
| Ge | 0.729149000 | -1.916033000 | -1.015417000 |
| Si | 1.453439000 | -4.274357000 | -1.462474000 |
| Si | 3.315672000 | -4.780106000 | -0.018772000 |
| C | 4.111618000 | -6.412881000 | -0.616948000 |
| Ge | 1.100945000 | 1.756435000 | -0.880799000 |
| Si | 2.264652000 | 3.932652000 | -1.369681000 |
| Si | 2.688463000 | 4.024013000 | -3.747846000 |
| C | 3.223067000 | 5.810425000 | -4.175338000 |
| Ge | -0.690959000 | 1.494887000 | 1.049462000 |
| Ge | -2.589992000 | 0.269728000 | -0.322931000 |
| Si | -5.031804000 | 0.512638000 | 0.013148000 |
| Si | -5.361863000 | 2.023857000 | 1.859376000 |
| C | -7.191896000 | 2.576974000 | 1.851538000 |
| Ge | 0.511987000 | 0.050611000 | -3.144794000 |
| Ge | -1.305223000 | 1.694204000 | -2.079008000 |
| Ge | -0.972724000 | -1.438548000 | 0.979931000 |
| Ge | -1.602980000 | -1.275892000 | -2.168262000 |
| C | -0.176569000 | -0.983514000 | 4.283025000 |
| C | -0.424079000 | -2.356835000 | 4.044955000 |
| C | -1.535293000 | -2.989012000 | 4.625974000 |
| C | -2.429946000 | -2.253302000 | 5.419637000 |
| C | -2.208026000 | -0.883747000 | 5.632722000 |
| C | -1.086084000 | -0.249567000 | 5.072449000 |
| Si | 0.827918000 | 5.748652000 | -0.712576000 |
| C | 0.195937000 | 5.506754000 | 1.073908000 |
| Si | 4.367635000 | 4.013559000 | -0.189964000 |
| C | 4.107545000 | 4.364792000 | 1.670057000 |
| Si | 2.132222000 | -4.371740000 | -3.776397000 |
| C | 3.815010000 | -3.501495000 | -4.019705000 |
| Si | -0.404285000 | -5.751372000 | -1.052939000 |
| C | -1.190641000 | -5.440068000 | 0.660275000 |
| Si | -5.873940000 | 1.425054000 | -2.055680000 |
| C | -5.177397000 | 0.492052000 | -3.568046000 |
| Si | -5.895813000 | -1.693850000 | 0.445884000 |
| C | -4.892384000 | -2.566015000 | 1.815295000 |
| C | 0.844990000 | -3.564470000 | -4.932143000 |
| C | 2.309143000 | -6.212147000 | -4.265861000 |
| C | -1.742480000 | -5.533727000 | -2.398346000 |
| C | 0.230149000 | -7.555657000 | -1.091910000 |
| C | 2.724828000 | -4.999012000 | 1.785568000 |
| C | 4.644184000 | -3.409764000 | -0.056853000 |

| | | | |
|---|---|---|---|
| C | -7.776913000 | 1.240727000 | -2.039302000 |
| C | -5.422413000 | 3.274405000 | -2.199262000 |
| C | -0.668349000 | 5.884432000 | -1.891214000 |
| C | 1.819294000 | 7.383668000 | -0.768581000 |
| C | 5.361170000 | 2.391152000 | -0.372489000 |
| C | 5.420909000 | 5.431227000 | -0.924402000 |
| C | 4.091255000 | 2.819742000 | -4.228919000 |
| C | 1.143010000 | 3.618691000 | -4.792852000 |
| C | -7.709940000 | -1.518525000 | 1.022756000 |
| C | -5.837386000 | -2.751040000 | -1.142441000 |
| C | -4.983730000 | 1.150637000 | 3.515315000 |
| C | -4.245063000 | 3.562241000 | 1.694801000 |
| H | -8.082032000 | 0.181157000 | -2.043766000 |
| H | -8.201055000 | 1.714952000 | -2.942293000 |
| H | -8.231593000 | 1.724616000 | -1.159476000 |
| H | 2.264590000 | -4.069647000 | 2.162725000 |
| H | 3.584019000 | -5.236042000 | 2.437705000 |
| H | 1.990374000 | -5.815792000 | 1.881185000 |
| H | 4.837302000 | 1.532694000 | 0.080680000 |
| H | 6.338221000 | 2.496372000 | 0.132580000 |
| H | 5.550785000 | 2.146997000 | -1.430433000 |
| H | -1.703175000 | -4.055614000 | 4.448054000 |
| H | 0.263600000 | -2.941569000 | 3.424929000 |
| H | -0.915805000 | 0.813639000 | 5.262394000 |
| H | -0.161323000 | -3.991813000 | -4.791526000 |
| H | 1.139379000 | -3.725157000 | -5.984657000 |
| H | 0.776530000 | -2.475242000 | -4.766955000 |
| H | -2.105684000 | -4.492562000 | -2.448096000 |
| H | -2.607657000 | -6.184571000 | -2.179583000 |
| H | -1.361159000 | -5.807222000 | -3.396159000 |
| H | 1.680000000 | -2.556289000 | 5.360336000 |
| H | -0.351516000 | 6.124812000 | -2.919636000 |
| H | -1.346819000 | 6.687072000 | -1.551662000 |
| H | -1.245486000 | 4.944180000 | -1.925582000 |
| H | -5.871583000 | 3.868068000 | -1.385843000 |
| H | -5.797724000 | 3.677721000 | -3.156567000 |
| H | -4.330144000 | 3.426711000 | -2.174508000 |
| H | 3.709450000 | -3.635006000 | 6.284732000 |
| H | -4.085707000 | 0.623830000 | -3.657159000 |
| H | -5.638695000 | 0.884213000 | -4.491841000 |
| H | -5.387447000 | -0.588750000 | -3.516013000 |
| H | 1.689842000 | 4.772513000 | 6.478390000 |
| H | -3.297213000 | -2.746411000 | 5.869636000 |
| H | 4.180006000 | 0.306620000 | 3.258698000 |
| H | 0.739028000 | -7.797019000 | -2.038998000 |
| H | -0.622497000 | -8.248972000 | -0.980088000 |
| H | 0.932960000 | -7.754288000 | -0.265737000 |
| H | -2.903114000 | -0.302564000 | 6.246643000 |
| H | 1.874133000 | 0.455196000 | 6.311391000 |
| H | -0.458816000 | -5.596155000 | 1.470321000 |
| H | -2.030279000 | -6.139794000 | 0.820099000 |
| H | -1.581536000 | -4.411653000 | 0.748376000 |
| H | -5.674048000 | 0.309367000 | 3.693400000 |
| H | -5.102627000 | 1.865310000 | 4.349357000 |
| H | -3.953049000 | 0.759629000 | 3.545077000 |
| H | 5.984083000 | -2.765587000 | 5.701329000 |
| H | -3.177644000 | 3.285072000 | 1.738362000 |
| H | -4.448689000 | 4.264091000 | 2.523079000 |
| H | -4.421372000 | 4.094974000 | 0.746148000 |
| H | 5.012605000 | -3.223122000 | -1.078653000 |
| H | 5.504674000 | -3.709658000 | 0.567742000 |

| | | | |
|---|---|---|---|
| H | 4.247565000 | -2.462294000 | 0.344854000 |
| H | 3.009079000 | -6.753705000 | -3.608961000 |
| H | 2.693476000 | -6.281064000 | -5.299215000 |
| H | 1.337688000 | -6.732845000 | -4.235877000 |
| H | -8.146161000 | -2.520515000 | 1.183805000 |
| H | -8.331429000 | -0.996734000 | 0.276845000 |
| H | -7.781029000 | -0.965396000 | 1.974058000 |
| H | 3.781884000 | -2.448285000 | -3.691846000 |
| H | 4.091704000 | -3.512902000 | -5.088926000 |
| H | 4.618452000 | -4.007742000 | -3.459419000 |
| H | 5.042789000 | 3.084713000 | -3.738949000 |
| H | 4.254986000 | 2.852843000 | -5.320730000 |
| H | 3.845189000 | 1.779062000 | -3.957299000 |
| H | 2.644273000 | 7.381759000 | -0.036775000 |
| H | 1.152924000 | 8.228903000 | -0.520204000 |
| H | 2.248257000 | 7.574337000 | -1.765484000 |
| H | 3.386605000 | -7.242280000 | -0.648754000 |
| H | 4.925541000 | -6.701081000 | 0.072142000 |
| H | 4.549022000 | -6.302765000 | -1.623156000 |
| H | 1.066994000 | 2.735828000 | 2.710743000 |
| H | 1.207910000 | 4.846362000 | 4.023316000 |
| H | 6.199704000 | -0.778681000 | 4.188575000 |
| H | 5.705402000 | 5.226180000 | -1.969546000 |
| H | 6.351758000 | 5.536711000 | -0.338847000 |
| H | 4.893980000 | 6.398875000 | -0.896144000 |
| H | -0.394721000 | 4.579593000 | 1.176025000 |
| H | -0.446529000 | 6.354286000 | 1.371345000 |
| H | 1.042821000 | 5.455936000 | 1.778535000 |
| H | 2.026356000 | 2.564540000 | 7.612964000 |
| H | -7.438397000 | 3.152932000 | 0.944191000 |
| H | -7.386504000 | 3.226594000 | 2.723518000 |
| H | -7.881829000 | 1.719246000 | 1.909838000 |
| H | -4.810422000 | -2.835908000 | -1.536070000 |
| H | -6.473006000 | -2.325625000 | -1.936535000 |
| H | -6.204510000 | -3.770781000 | -0.929366000 |
| H | 3.621404000 | 5.341675000 | 1.830338000 |
| H | 5.084256000 | 4.390174000 | 2.185716000 |
| H | 3.487573000 | 3.593900000 | 2.156841000 |
| H | 0.852211000 | 2.558294000 | -4.701277000 |
| H | 1.360721000 | 3.815207000 | -5.858030000 |
| H | 0.274965000 | 4.234005000 | -4.504433000 |
| H | -5.328226000 | -3.559442000 | 2.023738000 |
| H | -4.894921000 | -1.988201000 | 2.753852000 |
| H | -3.841271000 | -2.711679000 | 1.513183000 |
| H | 2.397720000 | 6.524457000 | -4.017461000 |
| H | 3.505930000 | 5.858475000 | -5.242217000 |
| H | 4.087373000 | 6.147495000 | -3.581223000 |
| H | 2.883358000 | 0.589232000 | 1.359225000 |
| H | 1.684397000 | -1.757433000 | 1.465446000 |
| H | 3.127582000 | -0.245040000 | 1.125724000 |

**2b_H2_oxadd_ts**

SCF = -1973.62182862
H(0 K) = -1972.339038
H(298 K) = -1972.215461
G(298 K) = -1972.517500
SCF+D3 = -1973.93751249
PCM SCF (Benzene) = -1973.64747567
BS2 (def2-tzvp) = -24397.4545063
Low Freq. = -640.0738cm-1, 5.0703cm-1

| | | | |
|---|---|---|---|
| C | 1.796771000 | 2.680513000 | 6.520775000 |
| C | 1.257228000 | 3.860635000 | 5.980877000 |
| C | 0.823182000 | 3.881787000 | 4.647643000 |
| C | 0.926675000 | 2.727332000 | 3.852066000 |
| C | 1.453047000 | 1.538452000 | 4.390251000 |
| C | 1.894851000 | 1.524639000 | 5.733437000 |
| P | 1.537409000 | -0.041603000 | 3.397174000 |
| C | 3.174840000 | -0.734267000 | 3.981096000 |
| C | 3.262863000 | -1.726316000 | 4.980023000 |
| C | 4.519203000 | -2.161199000 | 5.436980000 |
| C | 5.695483000 | -1.606112000 | 4.912313000 |
| C | 5.614073000 | -0.607626000 | 3.927032000 |
| C | 4.363531000 | -0.176162000 | 3.462385000 |
| Rh | 1.476192000 | 0.079680000 | 1.011210000 |
| Ge | 2.613580000 | 0.328239000 | -1.602845000 |
| Ge | 1.041474000 | -1.685506000 | -1.072946000 |
| Si | 2.187760000 | -3.857342000 | -1.589651000 |
| Si | 4.210385000 | -3.982949000 | -0.285508000 |
| C | 5.265696000 | -5.429946000 | -0.956978000 |
| Ge | 0.676913000 | 1.963046000 | -0.871051000 |
| Si | 1.385484000 | 4.339773000 | -1.291832000 |
| Si | 1.670196000 | 4.581807000 | -3.679479000 |
| C | 1.833450000 | 6.448026000 | -4.067252000 |
| Ge | -0.971012000 | 1.321104000 | 1.116749000 |
| Ge | -2.640654000 | -0.222708000 | -0.253428000 |
| Si | -5.066026000 | -0.469958000 | 0.173212000 |
| Si | -5.621742000 | 0.978167000 | 2.016514000 |
| C | -7.525479000 | 1.138361000 | 2.083876000 |
| Ge | 0.349164000 | 0.217783000 | -3.158980000 |
| Ge | -1.706260000 | 1.457786000 | -1.991177000 |
| Ge | -0.671813000 | -1.577153000 | 0.976403000 |
| Ge | -1.411446000 | -1.527079000 | -2.129687000 |
| C | 0.264252000 | -1.123066000 | 4.217798000 |
| C | 0.264630000 | -2.515735000 | 3.966558000 |
| C | -0.697160000 | -3.343744000 | 4.567038000 |
| C | -1.686886000 | -2.789472000 | 5.395210000 |
| C | -1.709262000 | -1.404767000 | 5.624910000 |
| C | -0.737092000 | -0.572572000 | 5.044081000 |
| Si | -0.341067000 | 5.813127000 | -0.488175000 |
| C | -0.784435000 | 5.417677000 | 1.327443000 |
| Si | 3.488976000 | 4.784408000 | -0.194763000 |
| C | 3.247376000 | 5.060815000 | 1.679362000 |
| Si | 2.708534000 | -3.814105000 | -3.946275000 |
| C | 4.167553000 | -2.630349000 | -4.290749000 |
| Si | 0.693010000 | -5.675278000 | -1.078195000 |
| C | -0.000911000 | -5.537551000 | 0.696480000 |
| Si | -6.138637000 | 0.217749000 | -1.876037000 |
| C | -5.312382000 | -0.583431000 | -3.398633000 |
| Si | -5.446314000 | -2.797510000 | 0.665387000 |
| C | -4.245850000 | -3.417615000 | 2.013094000 |
| C | 1.212099000 | -3.273474000 | -5.001574000 |
| C | 3.206680000 | -5.582124000 | -4.479761000 |
| C | -0.762604000 | -5.711918000 | -2.314226000 |
| C | 1.661139000 | -7.320004000 | -1.208717000 |
| C | 3.803406000 | -4.312157000 | 1.552098000 |
| C | 5.241114000 | -2.380416000 | -0.401957000 |
| C | -7.964790000 | -0.342349000 | -1.797110000 |
| C | -6.070067000 | 2.116991000 | -2.054898000 |
| C | -1.913474000 | 5.661743000 | -1.561096000 |
| C | 0.296009000 | 7.615278000 | -0.561953000 |
| C | 4.753780000 | 3.375007000 | -0.448630000 |

| | | | |
|---|---|---|---|
| C | 4.227946000 | 6.381132000 | -0.945256000 |
| C | 3.254788000 | 3.684126000 | -4.256586000 |
| C | 0.185543000 | 3.912515000 | -4.675925000 |
| C | -7.240601000 | -2.982164000 | 1.298339000 |
| C | -5.219594000 | -3.852006000 | -0.909458000 |
| C | -5.000776000 | 0.233436000 | 3.662188000 |
| C | -4.857619000 | 2.711110000 | 1.784691000 |
| H | -8.052134000 | -1.441221000 | -1.772516000 |
| H | -8.499040000 | 0.015935000 | -2.695090000 |
| H | -8.483319000 | 0.062698000 | -0.912765000 |
| H | 3.196635000 | -3.493688000 | 1.975527000 |
| H | 4.736394000 | -4.374179000 | 2.139647000 |
| H | 3.254505000 | -5.258860000 | 1.686442000 |
| H | 4.418276000 | 2.434217000 | 0.019391000 |
| H | 5.717415000 | 3.657330000 | 0.012429000 |
| H | 4.934373000 | 3.175418000 | -1.517453000 |
| H | -0.674580000 | -4.421454000 | 4.378553000 |
| H | 1.033206000 | -2.959512000 | 3.324794000 |
| H | -0.752564000 | 0.501907000 | 5.247250000 |
| H | 0.320647000 | -3.889874000 | -4.800142000 |
| H | 1.460081000 | -3.373363000 | -6.073413000 |
| H | 0.943196000 | -2.218770000 | -4.818177000 |
| H | -1.323820000 | -4.761339000 | -2.312302000 |
| H | -1.465318000 | -6.521166000 | -2.047332000 |
| H | -0.413629000 | -5.896601000 | -3.343746000 |
| H | 2.356193000 | -2.160846000 | 5.409724000 |
| H | -1.724734000 | 5.973284000 | -2.601788000 |
| H | -2.711860000 | 6.308273000 | -1.155576000 |
| H | -2.294083000 | 4.625808000 | -1.580779000 |
| H | -6.607636000 | 2.622741000 | -1.235774000 |
| H | -6.543026000 | 2.420877000 | -3.005615000 |
| H | -5.030064000 | 2.484724000 | -2.063105000 |
| H | 4.571827000 | -2.933901000 | 6.210691000 |
| H | -4.273039000 | -0.235711000 | -3.524765000 |
| H | -5.870262000 | -0.309556000 | -4.311725000 |
| H | -5.297735000 | -1.683252000 | -3.326806000 |
| H | 1.180747000 | 4.761340000 | 6.598145000 |
| H | -2.437084000 | -3.436005000 | 5.861067000 |
| H | 4.316700000 | 0.605292000 | 2.697740000 |
| H | 2.127679000 | -7.450764000 | -2.198373000 |
| H | 0.971450000 | -8.167306000 | -1.045521000 |
| H | 2.454537000 | -7.383241000 | -0.445571000 |
| H | -2.477582000 | -0.966018000 | 6.269206000 |
| H | 2.320529000 | 0.613038000 | 6.163787000 |
| H | 0.809154000 | -5.563186000 | 1.444375000 |
| H | -0.680179000 | -6.384349000 | 0.900657000 |
| H | -0.568020000 | -4.601405000 | 0.839766000 |
| H | -5.493187000 | -0.729201000 | 3.878781000 |
| H | -5.230441000 | 0.923265000 | 4.493944000 |
| H | -3.910906000 | 0.065350000 | 3.649493000 |
| H | 6.672080000 | -1.945437000 | 5.271619000 |
| H | -3.755056000 | 2.664873000 | 1.794672000 |
| H | -5.177852000 | 3.374280000 | 2.607983000 |
| H | -5.172088000 | 3.172419000 | 0.834336000 |
| H | 5.501721000 | -2.135064000 | -1.444319000 |
| H | 6.181258000 | -2.504346000 | 0.164855000 |
| H | 4.696357000 | -1.523633000 | 0.028603000 |
| H | 4.036505000 | -5.983460000 | -3.875770000 |
| H | 3.533677000 | -5.566460000 | -5.534838000 |
| H | 2.357619000 | -6.281612000 | -4.404457000 |
| H | -7.458648000 | -4.048146000 | 1.488958000 |

| | | | |
|---|---|---|---|
| H | -7.976745000 | -2.613674000 | 0.565395000 |
| H | -7.395219000 | -2.434525000 | 2.242863000 |
| H | 3.953380000 | -1.604916000 | -3.943884000 |
| H | 4.363632000 | -2.584397000 | -5.376751000 |
| H | 5.092537000 | -2.971190000 | -3.796809000 |
| H | 4.159118000 | 4.114972000 | -3.795770000 |
| H | 3.359529000 | 3.776156000 | -5.352257000 |
| H | 3.225416000 | 2.608835000 | -4.010803000 |
| H | 1.157533000 | 7.768338000 | 0.109164000 |
| H | -0.505780000 | 8.303509000 | -0.239999000 |
| H | 0.600978000 | 7.905849000 | -1.580132000 |
| H | 4.716517000 | -6.385450000 | -0.949942000 |
| H | 6.165315000 | -5.552414000 | -0.327595000 |
| H | 5.603783000 | -5.237635000 | -1.988750000 |
| H | 0.593226000 | 2.755151000 | 2.809594000 |
| H | 0.401937000 | 4.795611000 | 4.217756000 |
| H | 6.526153000 | -0.161812000 | 3.517575000 |
| H | 4.495706000 | 6.246092000 | -2.006122000 |
| H | 5.149927000 | 6.648620000 | -0.398561000 |
| H | 3.534166000 | 7.234502000 | -0.872320000 |
| H | -1.173455000 | 4.389982000 | 1.435107000 |
| H | -1.558996000 | 6.115538000 | 1.691736000 |
| H | 0.102416000 | 5.521708000 | 1.974713000 |
| H | 2.145111000 | 2.658216000 | 7.558262000 |
| H | -7.923372000 | 1.627597000 | 1.179405000 |
| H | -7.815290000 | 1.755233000 | 2.953178000 |
| H | -8.018746000 | 0.157951000 | 2.186964000 |
| H | -4.207483000 | -3.736582000 | -1.332521000 |
| H | -5.948882000 | -3.578404000 | -1.689707000 |
| H | -5.367989000 | -4.920369000 | -0.671528000 |
| H | 2.602412000 | 5.933469000 | 1.876022000 |
| H | 4.224787000 | 5.253928000 | 2.156698000 |
| H | 2.796260000 | 4.185592000 | 2.175231000 |
| H | 0.112652000 | 2.813196000 | -4.616248000 |
| H | 0.308620000 | 4.182121000 | -5.740219000 |
| H | -0.771269000 | 4.334644000 | -4.327096000 |
| H | -4.471539000 | -4.470684000 | 2.258950000 |
| H | -4.330114000 | -2.824999000 | 2.938579000 |
| H | -3.197277000 | -3.363751000 | 1.673859000 |
| H | 0.892515000 | 6.985089000 | -3.862191000 |
| H | 2.062676000 | 6.575497000 | -5.140453000 |
| H | 2.637956000 | 6.931404000 | -3.490484000 |
| H | 3.050782000 | 0.398883000 | 0.863736000 |
| H | 2.198221000 | -1.310768000 | 1.227067000 |
| H | 2.398815000 | 1.367143000 | 1.277821000 |

**2b_H_H**

SCF = -1973.62913735
H(0 K) = -1972.344607
H(298 K) = -1972.220967
G(298 K) = -1972.523816
SCF+D3 = -1973.94716296
PCM SCF (Benzene) = -1973.65936784
BS2 (def2-tzvp) = -24397.4609980
Low Freq. = 3.8840cm-1, 5.8495cm-1

| | | | |
|---|---|---|---|
| C | 3.459667000 | 3.360815000 | 5.680269000 |
| C | 2.178853000 | 3.704457000 | 6.138105000 |
| C | 1.049359000 | 3.070242000 | 5.592681000 |
| C | 1.200847000 | 2.105009000 | 4.586526000 |
| C | 2.487816000 | 1.754370000 | 4.121951000 |

| | | | |
|---|---|---|---|
| C | 3.618104000 | 2.385147000 | 4.680827000 |
| P | 2.654601000 | 0.405646000 | 2.841035000 |
| C | 4.462937000 | 0.469849000 | 2.396205000 |
| C | 5.382969000 | -0.456576000 | 2.929781000 |
| C | 6.753057000 | -0.335312000 | 2.641106000 |
| C | 7.216304000 | 0.711631000 | 1.829876000 |
| C | 6.304108000 | 1.639474000 | 1.298609000 |
| C | 4.934263000 | 1.516277000 | 1.573344000 |
| Rh | 1.100790000 | 0.713400000 | 1.080277000 |
| Ge | 2.203066000 | 1.031273000 | -1.484373000 |
| Ge | 1.201733000 | -1.339247000 | -0.977330000 |
| Si | 2.604474000 | -3.232639000 | -1.902853000 |
| Si | 4.896246000 | -2.987598000 | -1.187398000 |
| C | 6.025391000 | -4.007955000 | -2.347014000 |
| Ge | -0.206781000 | 2.068638000 | -0.921686000 |
| Si | -0.240227000 | 4.546318000 | -1.313493000 |
| Si | 0.896219000 | 4.991059000 | -3.393344000 |
| C | 0.498126000 | 6.789545000 | -3.909097000 |
| Ge | -1.568440000 | 1.296633000 | 1.192133000 |
| Ge | -2.664968000 | -0.860752000 | 0.162401000 |
| Si | -4.836666000 | -1.750491000 | 0.954278000 |
| Si | -6.397628000 | 0.084911000 | 0.904055000 |
| C | -8.145019000 | -0.611422000 | 1.244244000 |
| Ge | -0.040572000 | 0.231230000 | -3.000585000 |
| Ge | -2.412187000 | 0.815126000 | -1.861692000 |
| Ge | -0.370099000 | -1.731054000 | 1.116777000 |
| Ge | -1.297018000 | -1.869310000 | -1.869248000 |
| C | 2.494419000 | -1.144110000 | 3.864146000 |
| C | 2.386330000 | -2.396341000 | 3.221804000 |
| C | 2.286922000 | -3.574688000 | 3.977973000 |
| C | 2.288419000 | -3.515229000 | 5.381301000 |
| C | 2.398011000 | -2.273846000 | 6.025929000 |
| C | 2.503349000 | -1.091690000 | 5.274235000 |
| Si | -2.550351000 | 5.227194000 | -1.447082000 |
| C | -3.587227000 | 4.458293000 | -0.038373000 |
| Si | 0.849565000 | 5.659348000 | 0.522932000 |
| C | -0.218218000 | 5.551836000 | 2.102622000 |
| Si | 2.547993000 | -3.093825000 | -4.318259000 |
| C | 3.528120000 | -1.569006000 | -4.922135000 |
| Si | 1.732494000 | -5.361422000 | -1.191523000 |
| C | 1.440456000 | -5.384965000 | 0.697068000 |
| Si | -5.484969000 | -3.554333000 | -0.505914000 |
| C | -4.052945000 | -4.793086000 | -0.742583000 |
| Si | -4.412492000 | -2.493485000 | 3.208541000 |
| C | -3.387601000 | -1.203383000 | 4.177095000 |
| C | 0.782451000 | -3.016584000 | -5.042409000 |
| C | 3.361712000 | -4.680535000 | -5.013015000 |
| C | 0.099048000 | -5.787186000 | -2.083083000 |
| C | 3.024385000 | -6.712195000 | -1.599560000 |
| C | 5.148278000 | -3.644902000 | 0.589240000 |
| C | 5.450911000 | -1.164550000 | -1.269743000 |
| C | -6.962024000 | -4.458080000 | 0.303609000 |
| C | -6.013448000 | -2.877068000 | -2.210503000 |
| C | -3.314408000 | 4.725499000 | -3.123492000 |
| C | -2.629462000 | 7.130834000 | -1.277079000 |
| C | 2.566214000 | 4.908529000 | 0.893239000 |
| C | 1.091929000 | 7.496581000 | 0.050443000 |
| C | 2.787071000 | 4.811608000 | -3.188062000 |
| C | 0.306608000 | 3.820868000 | -4.781436000 |
| C | -6.092347000 | -2.735010000 | 4.088560000 |
| C | -3.462088000 | -4.150140000 | 3.208840000 |

| | | | |
|---|---|---|---|
| C | -5.959525000 | 1.365104000 | 2.252493000 |
| C | -6.402689000 | 0.942825000 | -0.800615000 |
| H | -6.678655000 | -4.917446000 | 1.265140000 |
| H | -7.312308000 | -5.265880000 | -0.363404000 |
| H | -7.811542000 | -3.780058000 | 0.486532000 |
| H | 4.545382000 | -3.090495000 | 1.326399000 |
| H | 6.209524000 | -3.536214000 | 0.875522000 |
| H | 4.889823000 | -4.714260000 | 0.666066000 |
| H | 2.461741000 | 3.886000000 | 1.291200000 |
| H | 3.083602000 | 5.519994000 | 1.653786000 |
| H | 3.199898000 | 4.872457000 | -0.008367000 |
| H | 2.197082000 | -4.537537000 | 3.466182000 |
| H | 2.379966000 | -2.452169000 | 2.127933000 |
| H | 2.592187000 | -0.131241000 | 5.788824000 |
| H | 0.137515000 | -3.819119000 | -4.648313000 |
| H | 0.837853000 | -3.132966000 | -6.139809000 |
| H | 0.290856000 | -2.051567000 | -4.834025000 |
| H | -0.676331000 | -5.021915000 | -1.908071000 |
| H | -0.289212000 | -6.753937000 | -1.716167000 |
| H | 0.246633000 | -5.876299000 | -3.172180000 |
| H | 5.035560000 | -1.266061000 | 3.577871000 |
| H | -2.790856000 | 5.203922000 | -3.967776000 |
| H | -4.372619000 | 5.039520000 | -3.163257000 |
| H | -3.280946000 | 3.633001000 | -3.274512000 |
| H | -6.892607000 | -2.216515000 | -2.130922000 |
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| H | 7.457851000 | -1.060130000 | 3.060859000 |
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| H | -4.392987000 | -5.642645000 | -1.361083000 |
| H | -3.693449000 | -5.194031000 | 0.219055000 |
| H | 2.059230000 | 4.463336000 | 6.917771000 |
| H | 2.203955000 | -4.434581000 | 5.969326000 |
| H | 4.233718000 | 2.248725000 | 1.158044000 |
| H | 3.264301000 | -6.743120000 | -2.674588000 |
| H | 2.625339000 | -7.701940000 | -1.314244000 |
| H | 3.964455000 | -6.557385000 | -1.044545000 |
| H | 2.402389000 | -2.218728000 | 7.119195000 |
| H | 4.622559000 | 2.118343000 | 4.340805000 |
| H | 2.387416000 | -5.205304000 | 1.233366000 |
| H | 1.049945000 | -6.368873000 | 1.011931000 |
| H | 0.714248000 | -4.614250000 | 1.009835000 |
| H | -6.020101000 | 0.927103000 | 3.262673000 |
| H | -6.668207000 | 2.211287000 | 2.210957000 |
| H | -4.942485000 | 1.770152000 | 2.115388000 |
| H | 8.284759000 | 0.806518000 | 1.611878000 |
| H | -5.423110000 | 1.393823000 | -1.033549000 |
| H | -7.157927000 | 1.748782000 | -0.811164000 |
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| H | 6.525348000 | -1.086254000 | -1.026958000 |
| H | 4.901108000 | -0.541821000 | -0.544579000 |
| H | 4.376953000 | -4.848784000 | -4.621505000 |
| H | 3.432163000 | -4.594158000 | -6.112260000 |
| H | 2.753158000 | -5.572427000 | -4.788978000 |
| H | -5.925715000 | -3.134125000 | 5.104934000 |
| H | -6.739761000 | -3.446020000 | 3.549448000 |
| H | -6.639101000 | -1.782670000 | 4.187904000 |
| H | 3.097895000 | -0.630669000 | -4.532283000 |
| H | 3.500064000 | -1.517808000 | -6.025088000 |
| H | 4.585959000 | -1.613683000 | -4.614418000 |

| | | | |
|---|---|---|---|
| H | 3.187544000 | 5.538932000 | -2.462364000 |
| H | 3.287907000 | 4.991206000 | -4.156039000 |
| H | 3.063939000 | 3.798593000 | -2.848189000 |
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| H | 6.657615000 | 2.459581000 | 0.665764000 |
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| H | 4.344445000 | 3.848763000 | 6.101450000 |
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| H | 0.299652000 | 6.048793000 | 2.942064000 |
| H | -0.399529000 | 4.502520000 | 2.391369000 |
| H | 0.573032000 | 2.770752000 | -4.570980000 |
| H | 0.786143000 | 4.103969000 | -5.735434000 |
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| H | -3.868402000 | -0.211420000 | 4.175400000 |
| H | -2.377011000 | -1.095982000 | 3.746844000 |
| H | -0.575637000 | 6.923262000 | -4.121111000 |
| H | 1.053771000 | 7.037464000 | -4.831137000 |
| H | 0.787679000 | 7.518949000 | -3.135222000 |
| H | 0.791132000 | 2.032638000 | 1.845043000 |
| H | 2.290448000 | 1.648529000 | 0.523482000 |
| H | 0.061615000 | 0.008173000 | 2.165531000 |

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