Electronic Supplementary Material (ESI) for RSC Advances.

DFT Calculations Bring Insight to Internal Alkyne-to-Vinylidene Transformations at Rhodium PNP- and PONOP-Pincer Complexes

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Breakdown of Energy Contributions

The following tables detail the evolution of the relative energies as the successive corrections to the initial SCF energy are included. Terms used are:

ΔE_{BS1}	SCF energy computed with the BP86 functional with BS1
ΔH_{BS1}	Enthalpy at 0 K with BS1
ΔG_{BS1}	Free energy at 298.15 K and 1 atm with BS1
$\Delta G_{BS1/DFB}$	Free energy corrected for 1,2-difluorobenzene (DFB) solvent with BS1
$\Delta G_{BS1/DFB+D3}$	Free energy corrected for DFB and dispersion effects with BS1
ΔE_{BS2}	SCF energy computed with the BP86 functional with BS2
ΔG_{DFB}	Free energy corrected for basis set (BS2), dispersion effects and DFB solvent
ΔG_{FB}	Free energy corrected for basis set (BS2), dispersion effects and fluorobenzene solvent (FB, in blue)

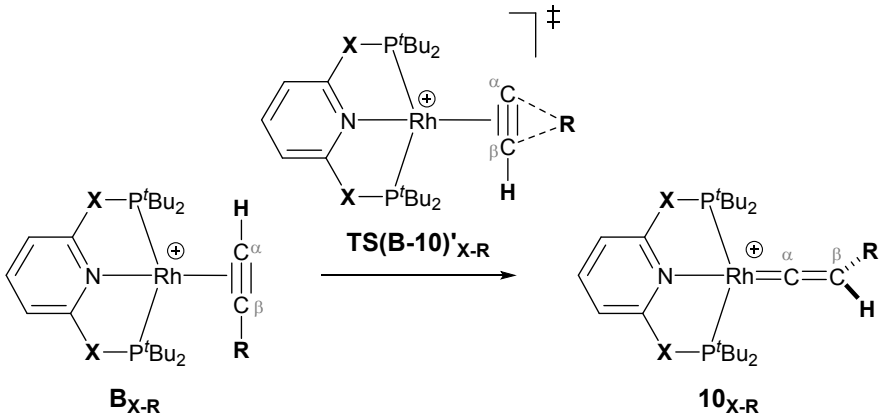
In each case the final data used in the main article is highlighted in bold.

Table S1 – Relative energies (kcal/mol) for computed structures in Pathways **I**, **II** and **III**. Data in bold are those used in the main text. All energies are quoted relative to **9_X and HC≡CR** at 0.0 kcal mol^{-1} (X = CH_2 and O; R = ^{t}Bu and Ar′ (3,5-^{t}Bu$_2$C$_6$H$_3$)).

	ΔE_{BS1}	ΔH_{BS1}	ΔG_{BS1}	$\Delta G_{BS1/DFB}$	$\Delta G_{BS1/DFB+D3}$	ΔE_{BS2}	ΔG_{DFB}	ΔG_{FB}
9_X + HC≡CR	0.0	0.0	0.0	0.0	0.0	0.0	**0.0**	0.0
A_C	-9.1	-10.9	-26.3	-2.8	+23.5	-12.5	**+20.0**	+18.1
$B_{C\text{-}tBu}$	-38.0	-37.7	-38.2	-7.5	-1.9	-36.3	**-0.2**	-3.7
$TS(B\text{-}10)_{C\text{-}tBu}$	+3.7	1.7	+1.5	+31.5	+37.8	+6.0	**+40.1**	+36.8
$TS(B\text{-}C)_{C\text{-}tBu}$	-30.7	-32.2	-34.3	-2.8	+7.2	-29.1	**+8.8**	+5.2
$C_{C\text{-}tBu}$	-40.5	-42.0	-45.1	-14.2	-2.9	-40.6	**-3.0**	-6.4
$TS(C\text{-}D)_{C\text{-}tBu}$	+2.6	0.8	0.0	+28.5	35.9	+4.4	**+37.7**	+34.8
$D_{C\text{-}tBu}$	+2.0	0.5	-0.3	+27.8	+35.0	+3.4	**+36.4**	+33.6
$TS(C\text{-}10)_{C\text{-}tBu}$	-29.7	-32.6	-35.1	-3.9	+7.8	-28.7	**+8.7**	+5.3
$TS(C\text{-}E)_{C\text{-}tBu}$	-38.2	-40.7	-42.7	-13.5	-2.8	-38.2	**-2.8**	-5.8
$E_{C\text{-}tBu}$	-42.9	-44.4	-46.3	-23.6	-13.7	-42.3	**-8.1**	-10.6
$10_{C\text{-}tBu}$	-52.3	-52.4	-53.9	-27.0	-17.1	-50.6	**-12.1**	-15.5
A_O	-5.3	-7.2	-22.5	+1.8	+26.0	-8.3	**23.0**	+20.9
$B_{O\text{-}tBu}$	-41.1	-41.6	-42.7	-9.8	-5.5	-39.2	**-3.7**	-7.7
$TS(B\text{-}10)_{\text{-}tBu}$	+2.5	-0.1	-1.6	+30.9	+36.9	4.9	**+39.4**	+35.5
$TS(B\text{-}C)_{O\text{-}tBu}$	-32.7	-34.7	-37.7	-4.4	+4.6	-30.8	**+6.5**	+2.4
$C_{O\text{-}tBu}$	-38.4	-40.0	-43.6	-9.9	+0.9	-38.0	**+1.3**	-2.8
$TS(C\text{-}D)_{O\text{-}tBu}$	+1.6	-1.1	-2.3	29.7	+36.5	+3.7	**+38.5**	+34.7
$D_{O\text{-}tBu}$	+1.5	-0.7	-2.6	28.7	+35.2	+3.3	**+37.0**	+33.4
$TS(C\text{-}10)_{O\text{-}tBu}$	-28.5	-31.6	-35.4	-2.2	+8.9	-27.3	**+10.2**	+6.2
$TS(C\text{-}E)_{O\text{-}tBu}$	-35.2	-38.0	-41.7	-9.5	+0.3	-34.7	**+0.8**	-2.9
$E_{O\text{-}tBu}$	-39.1	-40.8	-42.2	-11.2	-1.8	-37.9	**-0.6**	-4.0
$10_{O\text{-}tBu}$	-49.7	-50.2	-53.4	-20.1	-10.9	-47.6	**-8.9**	-12.9
$B_{C\text{-}Ar}$	-47.6	-48.0	-48.9	-16.7	-13.7	-46.5	**-12.6**	-16.1
$TS(B\text{-}10)_{C\text{-}Ar}$	-3.4	-5.8	-7.0	+24.8	+28.5	-1.6	**+30.3**	+26.9
$TS(B\text{-}C)_{\text{-}Ar}$	-41.7	-43.1	-43.9	-10.0	-1.3	-40.2	**+0.2**	-3.7
$C_{C\text{-}Ar}$	-44.5	-45.8	-47.5	-15.2	-4.2	-44.8	**-4.5**	-8.1
$TS(C\text{-}D)_{\text{-}Ar}$	-4.3	-6.4	-8.0	+23.0	28.2	-2.7	**+29.8**	+26.5
$TS(C\text{-}10)_{\text{-}Ar}$	-32.8	-35.9	-37.9	-4.7	+7.0	-32.2	**+7.6**	3.9
$TS(C\text{-}E)_{\text{-}Ar}$	-40.8	-43.5	-45.4	-15.6	-5.0	-41.3	**-5.5**	-8.5
$D_{C\text{-}Ar}$	-45.4	-47.1	-49.5	-21.8	-11.5	-45.3	**-11.4**	-13.7
$10_{C\text{-}Ar}$	-53.9	-54.2	-56.3	-25.7	-16.6	-52.9	**-15.7**	-18.9
$B_{O\text{-}Ar}$	-47.8	-48.2	-49.4	-14.4	-12.6	-46.2	**-11.0**	-15.3
$TS(B\text{-}10)_{O\text{-}Ar}$	-4.6	-7.3	-8.5	26.2	+28.9	-2.5	**+31.0**	+26.8
$TS(B\text{-}C)_{O\text{-}Ar}$	-40.2	-41.7	-44.1	-7.9	+1.1	-38.6	**+2.8**	-1.6

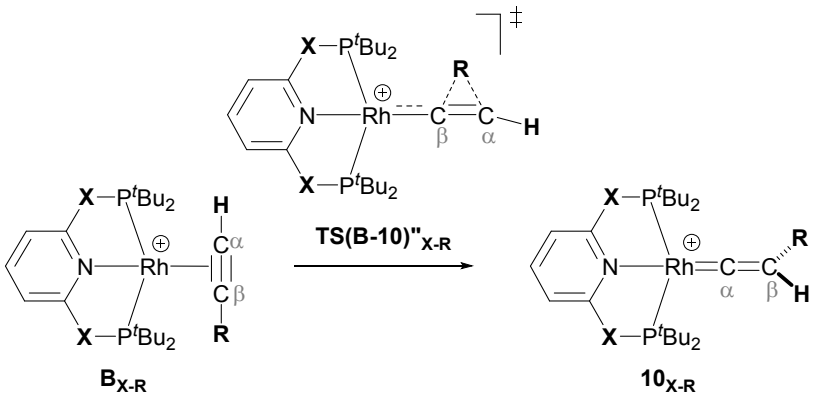
$\mathbf{C_{O\text{-}Ar}}$	-42.1	-43.7	-47.0	-11.6	-1.1	-41.9	**-1.0**	-5.2
$\mathbf{TS(C\text{-}D)_{O\text{-}Ar}}$	-4.5	-6.8	-7.8	+26.5	+29.8	-2.7	**+31.6**	+27.6
$\mathbf{TS(C\text{-}10)_{O\text{-}Ar}}$	-31.7	-34.9	-38.6	-3.0	+8.2	-30.8	**+9.1**	+4.9
$\mathbf{TS(C\text{-}E)_{O\text{-}Ar}}$	-37.8	-40.7	-43.9	-10.9	-1.3	-37.7	**-1.2**	-5.0
$\mathbf{E_{O\text{-}Ar}}$	-41.4	-43.2	-45.8	-14.3	-5.1	-40.7	**-4.4**	-7.7
$\mathbf{10_{O\text{-}Ar}}$	-51.1	-51.5	-54.5	-20.5	-12.6	-49.4	**-10.9**	-15.0
$\mathbf{TS(C\text{-}10)_{C\text{-}NMe2}}$	-37.4	-39.7	-41.8	-10.0	+3.0	-35.7	**+4.7**	+1.2
$\mathbf{A_{NH}}$	-6.8	-8.9	-25.1	-1.8	23.7	-10.1	**+20.3**	18.4
$\mathbf{B_{NH}}$	-48.2	-48.8	-50.4	-17.4	-14.5	-46.9	**-13.2**	-17.0
$\mathbf{10_{NH}}$	-52.9	-53.5	-57.0	-25.2	-16.7	-51.5	**-15.3**	-18.9
$\mathbf{A_S}$	-19.5	-22.1	-39.0	-10.2	16.2	-23.1	**+12.6**	9.5
$\mathbf{B_S}$	-56.4	-56.9	-60.9	-26.4	-23.3	-54.7	**-21.5**	-25.6
$\mathbf{10_S}$	-64.7	-65.0	-69.4	-35.6	-26.2	-63.2	**-24.7**	-28.7

Table S2 – DFT calculated free energies in kcal mol^{-1} for the direct 1,2-R transfer in the Rh-alkyne species $\mathbf{B_{X\text{-}R}}$ to form the Rh-vinylidene species $\mathbf{10_{X\text{-}R}}$ *via* Pathway **I**. All free energies are quoted with respect to $\mathbf{9_X}$ and **HC≡CR** (X = CH_2 and O, R = ^{t}Bu and Ar′ (3,5-^{t}Bu$_2$C$_6$H$_3$)).



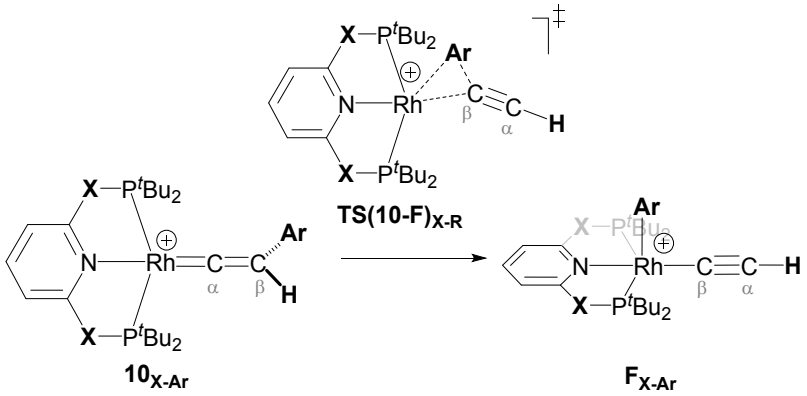
	ΔE_{BS1}	ΔH_{BS1}	ΔG_{BS1}	$\Delta G_{BS1/DFB}$	$\Delta G_{BS1/DFB+D3}$	ΔE_{BS2}	ΔG_{DFB}	ΔG_{FB}
$\mathbf{9_X}$ + **HC≡CR**	0.0	0.0	0.0	0.0	0.0	0.0	**0.0**	0.0
$\mathbf{B_{C\text{-}tBu}}$	-38.0	-37.7	-38.2	-7.5	-1.9	-36.3	**-0.2**	-3.7
TS(B-10)'$_{C\text{-}tBu}$	21.9	20.3	20.3	50.3	56.5	22.8	**57.4**	54.2
$\mathbf{B_{C\text{-}Ar}}$	-47.6	-48.0	-48.9	-16.7	-13.7	-46.5	**-12.6**	-16.1
TS(B-10)'$_{C\text{-}Ar}$	6.0	4.7	5.6	38.6	41.3	8.2	**43.5**	39.8
$\mathbf{B_{O\text{-}tBu}}$	-41.1	-41.6	-42.7	-9.8	-5.5	-39.2	**-3.7**	-7.7
TS(B-10)'$_{O\text{-}tBu}$	15.8	13.2	11.3	43.4	48.5	16.3	**49.0**	45.3
$\mathbf{B_{O\text{-}Ar}}$	-47.8	-48.2	-49.4	-14.4	-12.6	-46.2	**-11.0**	-15.3
TS(B-10)'$_{O\text{-}Ar}$	0.8	-0.6	-0.3	35.3	36.7	3.3	**39.2**	34.9

Table S3 – DFT calculated free energies in kcal mol^{-1} for the indirect 1,2-R transfer in the Rh-alkyne species $\mathbf{B_{X\text{-}R}}$ to form the Rh-vinylidene species $\mathbf{10_{X\text{-}R}}$ *via* Pathway **III**. All free energies are quoted with respect to $\mathbf{9_X}$ and **HC≡CR** (X = CH_2 and O, R = ^{t}Bu and Ar′ (3,5-^{t}Bu$_2$C$_6$H$_3$)).



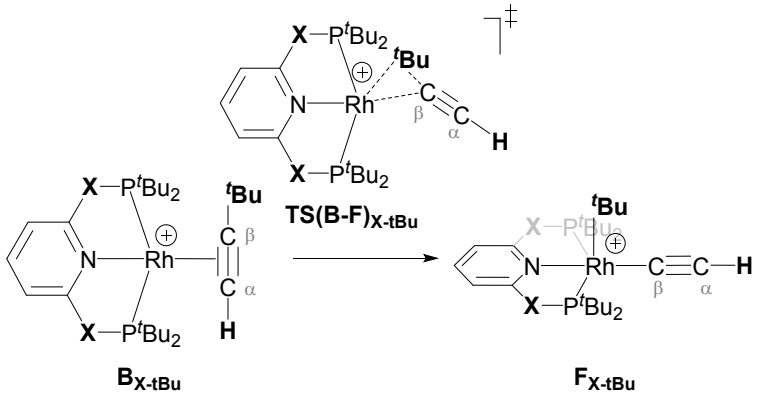
	ΔE_{BS1}	ΔH_{BS1}	ΔG_{BS1}	$\Delta G_{BS1/DFB}$	$\Delta G_{BS1/DFB+D3}$	ΔE_{BS2}	ΔG_{DFB}	ΔG_{FB}
$\mathbf{9_X}$ **+ HC≡CR**	0.0	0.0	0.0	0.0	0.0	0.0	**0.0**	0.0
$\mathbf{B_{C\text{-}tBu}}$	-38.0	-37.7	-38.2	-7.5	-1.9	-36.3	**-0.2**	-3.7
TS(B-10)"$_{C\text{-}tBu}$	5.3	3.8	3.6	34.4	39.6	6.3	**40.6**	37.2
$\mathbf{B_{C\text{-}Ar}}$	-47.6	-48.0	-48.9	-16.7	-13.7	-46.5	**-12.6**	-16.1
TS(B-10)"$_{C\text{-}Ar}$	-5.8	-7.6	-7.9	25.0	28.1	-4.2	**29.8**	26.1
$\mathbf{B_{O\text{-}tBu}}$	-41.1	-41.6	-42.7	-9.8	-5.5	-39.2	**-3.7**	-7.7
TS(B-10)"$_{O\text{-}tBu}$	2.4	0.9	0.4	32.7	37.3	4.0	**38.9**	35.0
$\mathbf{B_{O\text{-}Ar}}$	-47.8	-48.2	-49.4	-14.4	-12.6	-46.2	**-11.0**	-15.3
TS(B-10)"$_{O\text{-}Ar}$	-8.9	-11.1	-12.4	22.5	24.7	-7.2	**26.4**	22.2

Table S4 – DFT calculated free energies in kcal mol^{-1} for transfer of the R group onto the Rh in $\mathbf{10_{X\text{-}Ar}}$ *via* $\mathbf{TS(10\text{-}F)_{X\text{-}R}}$ to give the Rh—R species $\mathbf{F_{X\text{-}Ar}}$. Free energies are reported with respect to $\mathbf{9_X}$ and HC≡CAr′ (X = CH_2 and O).



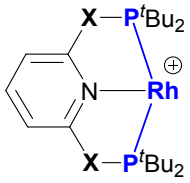
	ΔE_{BS1}	ΔH_{BS1}	ΔG_{BS1}	$\Delta G_{BS1/DFB}$	$\Delta G_{BS1/DFB+D3}$	ΔE_{BS2}	ΔG_{DFB}	ΔG_{FB}
$\mathbf{9_X}$ **+ HC≡CAr′**	0.0	0.0	0.0	0.0	0.0	0.0	**0.0**	0.0
$\mathbf{B_{C\text{-}Ar}}$	-47.6	-48.0	-48.9	-16.7	-13.7	-46.5	**-12.6**	-16.1
$\mathbf{10_{C\text{-}tBu}}$	-52.3	-52.4	-53.9	-27.0	-17.1	-50.6	**-12.1**	-15.5
$\mathbf{TS(10\text{-}F)_{C\text{-}Ar}}$	+6.8	+5.1	+6.1	+37.6	+32.6	+6.9	**32.7**	+29.3
$\mathbf{F_{C\text{-}Ar}}$	-19.9	-20.9	-20.3	+9.1	+1.2	-19.9	**+1.1**	-1.8
$\mathbf{B_{O\text{-}Ar}}$	-47.8	-48.2	-49.4	-14.4	-12.6	-46.2	**-11.0**	-15.3
$\mathbf{10_{O\text{-}Ar}}$	-51.1	-51.5	-54.5	-20.5	-12.6	-49.4	**-10.9**	-15.0
$\mathbf{TS(10\text{-}F)_{O\text{-}Ar}}$	+10.5	+9.0	+9.7	+44.3	+38.3	+11.2	**+39.0**	+34.9
$\mathbf{F_{O\text{-}Ar}}$	-15.9	-16.9	-16.7	+16.8	+7.4	-15.2	**+8.1**	+4.2

Table S5 – DFT calculated free energies in kcal mol^{-1} for transfer of the R group onto the Rh in $\mathbf{B_{X\text{-}tBu}}$ *via* **TS(B-F)** $_{\mathbf{X\text{-}tBu}}$ to give the Rh-^{t}Bu species $\mathbf{F_{X\text{-}tBu}}$. Free energies are reported with respect to $\mathbf{9_X}$ and HC≡C^{t}Bu (X = CH_2 and O).

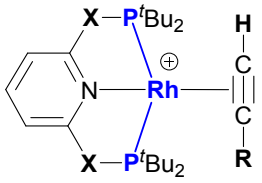


	ΔE_{BS1}	ΔH_{BS1}	ΔG_{BS1}	$\Delta G_{BS1/DFB}$	$\Delta G_{BS1/DFB+D3}$	ΔE_{BS2}	ΔG_{DFB}	ΔG_{FB}
9_X + HC≡CtBu	0.0	0.0	0.0	0.0	0.0	0.0	**0.0**	0.0
$B_{C\text{-}tBu}$	-38.0	-37.7	-38.2	-7.5	-1.9	-36.3	**-0.2**	-3.7
TS(B-F)$_{C\text{-}tBu}$	16.7	15.1	15.4	46.1	46.1	17.1	**46.6**	43.1
$F_{C\text{-}tBu}$	4.6	4.1	4.4	33.8	32.0	5.4	**32.8**	29.7
$B_{O\text{-}tBu}$	-41.1	-41.6	-42.7	-9.8	-5.5	-39.2	**-3.7**	-7.7
TS(B-F)$_{O\text{-}tBu}$	16.4	15.0	14.9	47.9	47.2	17.0	**47.8**	43.8
$F_{O\text{-}tBu}$	5.7	5.0	5.0	37.4	34.3	7.3	**35.9**	32.0

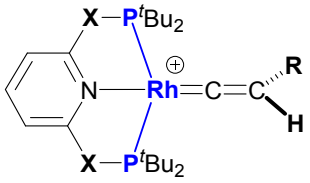
Table S6 – The P—Rh—P bite angles (θ, in degrees) in species $\mathbf{A_X}$, $\mathbf{B_{X\text{-}R}}$ and $\mathbf{10_{X\text{-}R}}$ (X = CH_2 and O, R = ^{t}Bu and Ar′).



$\mathbf{A_X}$



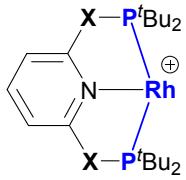
$\mathbf{B_{X\text{-}R}}$



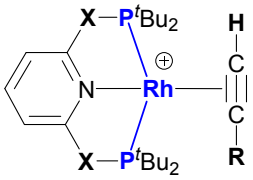
$\mathbf{10_{X\text{-}R}}$

Species	P—Rh—P	**Species**	P—Rh—P	**Species**	P—Rh—P	**Species**	P—Rh—P
$\mathbf{A_C}$	171.1	$\mathbf{A_O}$	166.0	$\mathbf{A_C}$	171.1	$\mathbf{A_O}$	166.0
$\mathbf{B_{C\text{-}tBu}}$	161.1	$\mathbf{B_{O\text{-}tBu}}$	162.5	$\mathbf{B_{C\text{-}Ar}}$	163.4	$\mathbf{B_{O\text{-}Ar}}$	162.5
$\mathbf{10_{C\text{-}tBu}}$	166.3	$\mathbf{10_{O\text{-}tBu}}$	162.9	$\mathbf{10_{C\text{-}Ar}}$	166.7	$\mathbf{10_{O\text{-}Ar}}$	163.0

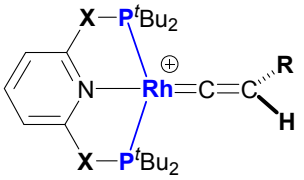
Table S7 – The HOMOs (in eV) of $\mathbf{A_X}$, $\mathbf{B_{X\text{-}R}}$ and $\mathbf{10_{X\text{-}R}}$ (X = CH_2 and O, R = ^{t}Bu and Ar).



$\mathbf{A_X}$



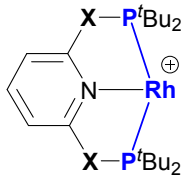
$\mathbf{B_{X\text{-}R}}$



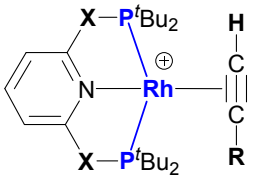
$\mathbf{10_{X\text{-}R}}$

Species	HOMO	**Species**	HOMO	**Species**	HOMO	**Species**	HOMO
$\mathbf{A_C}$	-7.03	$\mathbf{A_O}$	-7.38	$\mathbf{A_C}$	-7.03	$\mathbf{A_O}$	-7.38
$\mathbf{B_{C\text{-}tBu}}$	-7.05	$\mathbf{B_{O\text{-}tBu}}$	-7.54	$\mathbf{B_{C\text{-}Ar}}$	-6.87	$\mathbf{B_{O\text{-}Ar}}$	-7.30
$\mathbf{10_{C\text{-}tBu}}$	-7.31	$\mathbf{10_{O\text{-}tBu}}$	-7.65	$\mathbf{10_{C\text{-}Ar}}$	-6.97	$\mathbf{10_{O\text{-}Ar}}$	-7.23

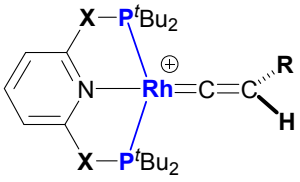
Table S8 – The P—Rh—P bite angles (θ, in degrees) in species $\mathbf{A_X}$, $\mathbf{B_{X\text{-}R}}$ and $\mathbf{10_{X\text{-}R}}$ (X = NH, CH_2, O and S).



$\mathbf{A_X}$



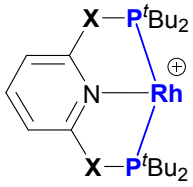
$\mathbf{B_{X\text{-}R}}$



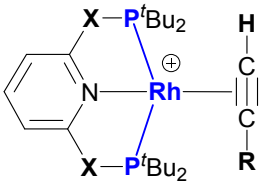
$\mathbf{10_{X\text{-}R}}$

Species	P—Rh—P	**Species**	P—Rh—P	**Species**	P—Rh—P	**Species**	P—Rh—P
$\mathbf{A_C}$	171.1	$\mathbf{A_O}$	166.0	$\mathbf{A_{NH}}$	169.0	$\mathbf{A_S}$	178.8
$\mathbf{B_{C\text{-}Ar}}$	163.4	$\mathbf{B_{O\text{-}Ar}}$	162.5	$\mathbf{B_{NH\text{-}Ar}}$	169.9	$\mathbf{B_{S\text{-}Ar}}$	167.5
$\mathbf{10_{C\text{-}Ar}}$	166.7	$\mathbf{10_{O\text{-}Ar}}$	163.0	$\mathbf{10_{NH\text{-}Ar}}$	165.8	$\mathbf{10_{S\text{-}Ar}}$	176.4

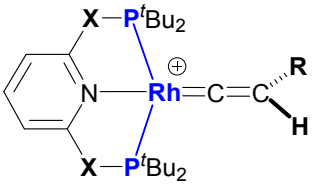
Table S9 – The HOMOs (in eV) of $\mathbf{A_X}$, $\mathbf{B_{X\text{-}Ar}}$ and $\mathbf{10_{X\text{-}Ar}}$ (X = CH_2 and NH, O and S).



$\mathbf{A_X}$



$\mathbf{B_{X\text{-}R}}$



$\mathbf{10_{X\text{-}R}}$

Species	HOMO	**Species**	HOMO	**Species**	HOMO	**Species**	HOMO
$\mathbf{A_C}$	-7.03	$\mathbf{A_O}$	-7.38	$\mathbf{A_S}$	-7.25	$\mathbf{A_{NH}}$	-7.00
$\mathbf{B_{C\text{-}Ar}}$	-6.87	$\mathbf{B_{O\text{-}Ar}}$	-7.30	$\mathbf{B_{S\text{-}Ar}}$	-7.25	$\mathbf{B_{NH\text{-}Ar}}$	-7.01
$\mathbf{10_{C\text{-}Ar}}$	-6.97	$\mathbf{10_{O\text{-}Ar}}$	-7.24	$\mathbf{10_{S\text{-}Ar}}$	-7.31	$\mathbf{10_{NH\text{-}Ar}}$	-7.04

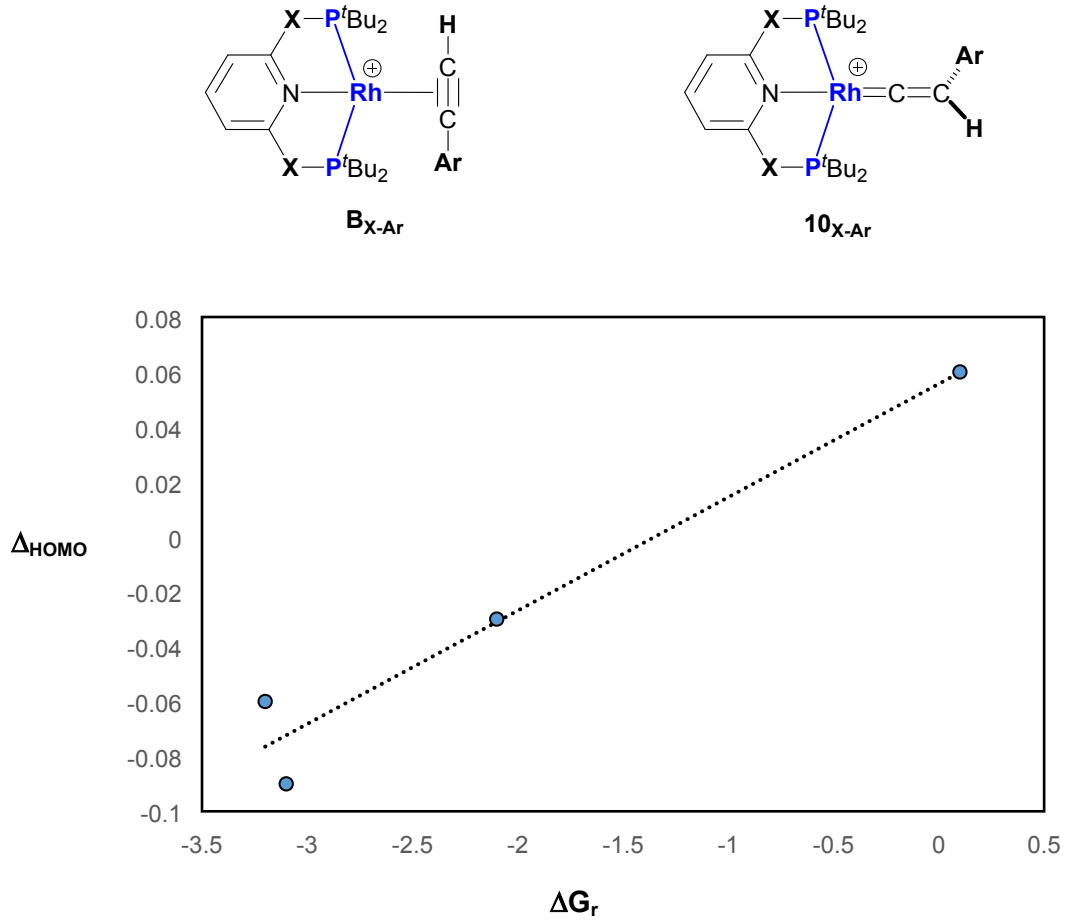
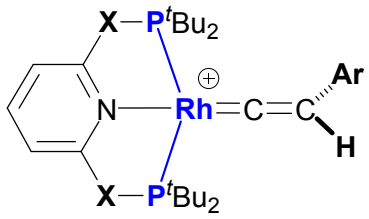


Figure S1 – Plot of the difference between the free energies of $\mathbf{B}_{\mathbf{X\text{-}Ar}}$ and $\mathbf{10}_{\mathbf{X\text{-}Ar}}$ ($\Delta\mathbf{G}_\mathbf{r}$, in kcal mol^{-1}) and difference between the HOMOs of $\mathbf{B}_{\mathbf{X\text{-}Ar}}$ and $\mathbf{10}_{\mathbf{X\text{-}Ar}}$ ($\Delta_{\mathbf{HOMO}}$ (in eV); X = NH, CH_2, O and S).



$10_{X\text{-}R}$

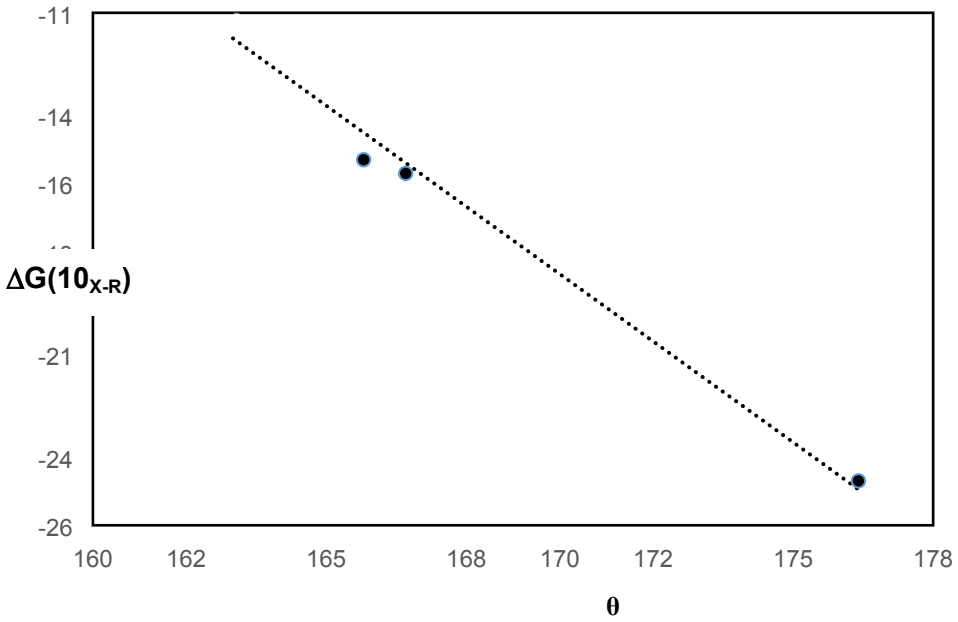


Figure S2 – Plot of the relative free energy of **$10_{X\text{-}R}$** with respect to **$B_{X\text{-}R}$** (ΔG, in kcal mol^{-1},) *vs* the P–Rh–P bite angle of **$10_{X\text{-}R}$** (θ (in degrees); X = NH, CH_2, O and S).

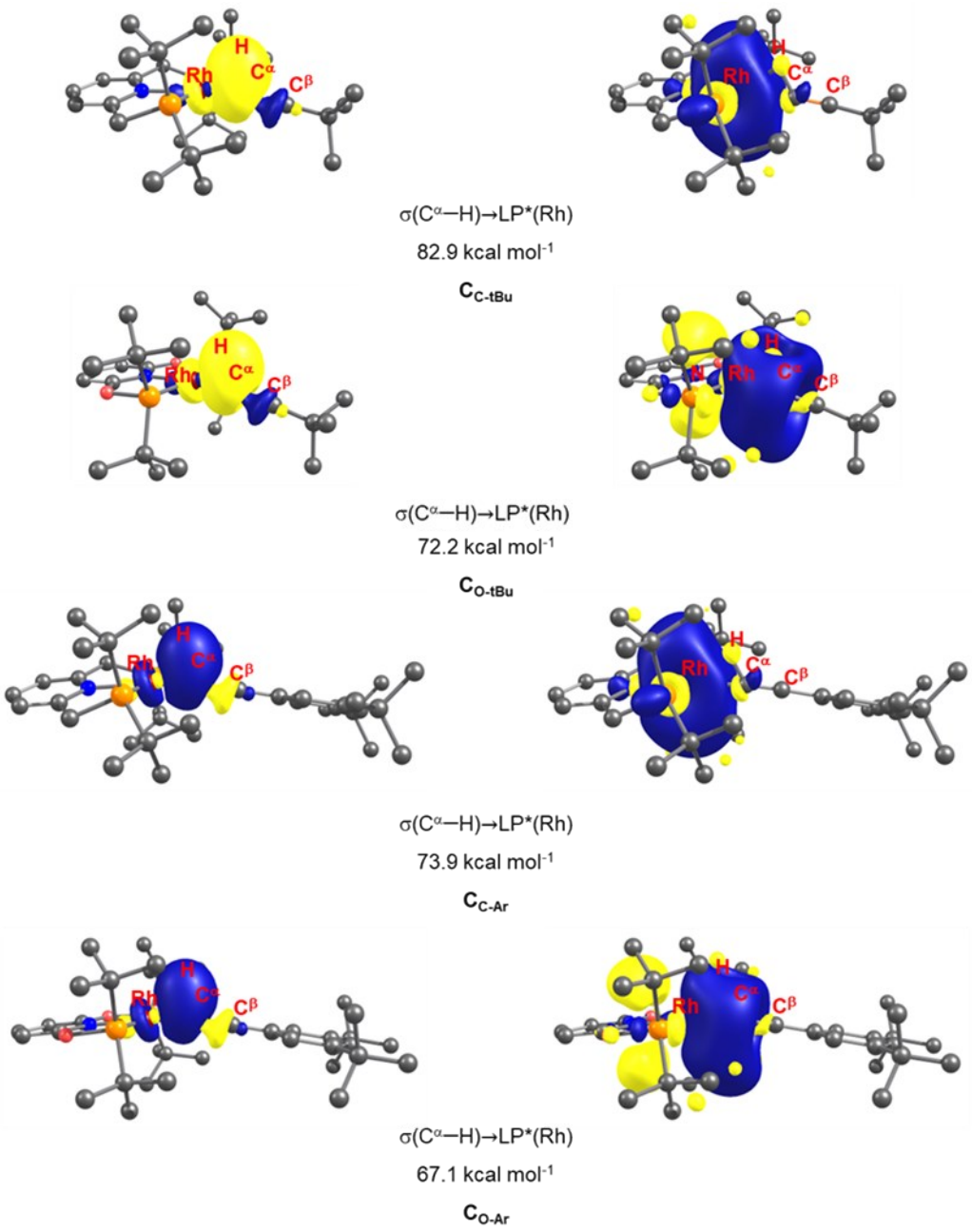


Figure **S3**. NBO donor-acceptor interactions derived from second-order perturbation theory, showing the interactions between the C$^{\alpha}$–H bonding orbital (left) and an empty Rh orbital (LP*, right) in $\mathbf{C_{X\text{-}R}}$ with the stabilisation energies (in kcal mol^{-1}).

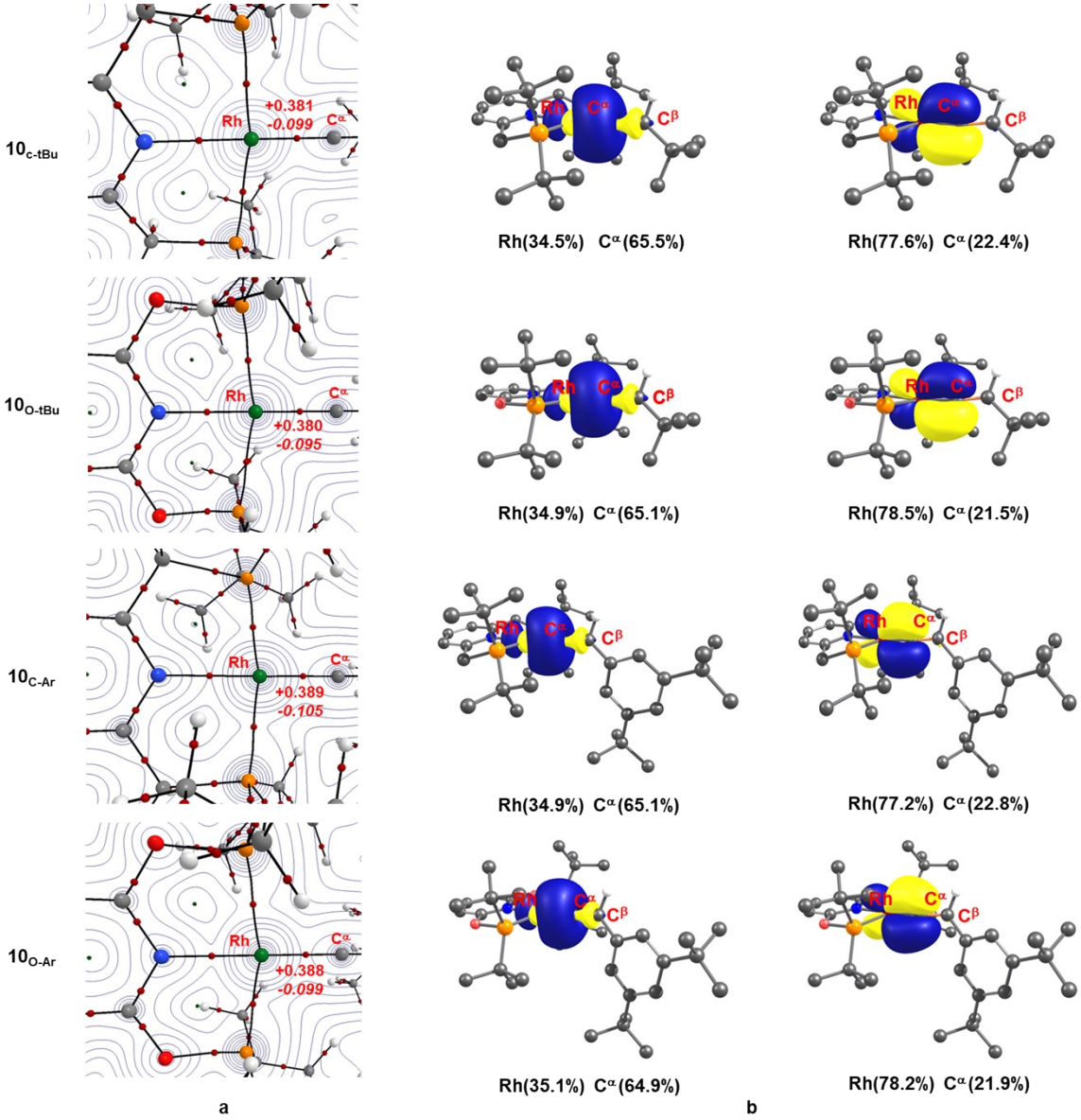


Figure **S4**. (**a**) QTAIM molecular graph of $\mathbf{10_{X\text{-}R}}$; the electron density contours are computed in the {Rh/P/C$^{\alpha}$} plane with bond critical points (BCPs) shown as small red spheres; for the Rh—C$^{\alpha}$ BCP, the Laplacian of the electron density ($\nabla^2\rho(r)$ in eÅ^{-5}) is shown in plain and total energy densities (H(r) in a.u.) is shown in italic; (**b**) NBO σ- and π- bonding orbitals of the Rh—C$^{\alpha}$ interaction and the contribution of the Rh and C$^{\alpha}$ centres in the corresponding interactions in $\mathbf{10_{X\text{-}R}}$.

Cartesian Coordinates and Computed Energies (in Hartrees)

9_c

SCF (BP86) Energy = -2473.63991160
Enthalpy 0K = -2472.254901
Enthalpy 298K = -2472.173582
Free Energy 298K = -2472.365403
Lowest Frequency = 7.6621 cm^{-1}
Second Frequency = 14.0646 cm^{-1}
SCF (BP86-D3BJ) Energy = -2474.111384
SCF (FB) Energy = -2473.763495
SCF (DFB) Energy = -2473.78008
SCF (BS2) Energy = -3812.790739

Rh	2.70768	-2.09034	1.15331
P	4.14307	-2.74359	-0.61842
P	1.82376	-1.84213	3.41662
N	4.02373	-3.47044	2.23615
C	1.11905	-1.47635	-0.23631
H	1.43377	-1.92392	-1.18720
C	1.84738	-0.32656	0.16302
H	2.64532	-0.01583	-0.52382
C	1.26907	0.86581	0.90858
H	2.09724	1.49017	1.28802
H	0.68662	0.54923	1.78817
C	-0.35043	-1.73662	0.03443
H	-0.60610	-1.52407	1.08418
H	-0.56427	-2.80826	-0.12871
C	5.23812	-3.84529	1.72348
C	6.10940	-4.69678	2.42265
H	7.06908	-4.96522	1.97274
C	5.74636	-5.17927	3.68355
H	6.41464	-5.83950	4.24421
C	4.50590	-4.80210	4.20831
H	4.17240	-5.16657	5.18352
C	3.66495	-3.95766	3.46616
C	5.63597	-3.29315	0.38766
H	6.26484	-4.01267	-0.16262
H	6.24845	-2.38598	0.53903
C	2.31108	-3.58168	3.97282
H	2.24554	-3.71677	5.06339
H	1.56306	-4.24712	3.50734
C	3.61789	-4.37599	-1.55684
C	3.39912	-5.44983	-0.46497
H	4.33686	-5.75121	0.03020
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C	4.67170	-4.87977	-2.56405
H	4.73144	-4.24288	-3.46044
H	4.37651	-5.88894	-2.90473
H	5.68131	-4.97054	-2.13024
C	2.27406	-4.16052	-2.28844
H	1.45552	-3.96366	-1.57803
H	2.01849	-5.08554	-2.83652
H	2.31036	-3.34416	-3.02805
C	5.01237	-1.45755	-1.80206
C	5.37781	-0.22422	-0.93825
H	4.52449	0.18496	-0.37731
H	5.76526	0.56942	-1.60248
H	6.17793	-0.44566	-0.21174
C	4.03155	-1.04928	-2.92057
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H	4.47943	-0.23343	-3.51694
H	3.07028	-0.68280	-2.52511
C	6.32083	-1.98400	-2.43743
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H	-0.90038	-0.46580	2.68932
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H	0.39682	-1.05917	6.20865
C	2.98876	-0.66573	4.47583
C	4.27304	-0.43326	3.64272
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H	4.89064	0.33387	4.14575
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H	-1.43377	1.92392	1.18720
C	-1.84738	0.32656	-0.16302
H	-2.64532	0.01583	0.52382
C	-1.26907	-0.86581	-0.90858
H	-2.09724	-1.49017	-1.28802
H	-0.68662	-0.54923	-1.78817
C	0.35043	1.73662	-0.03443
H	0.60610	1.52407	-1.08418
H	0.56427	2.80826	0.12871
Rh	-2.70768	2.09034	-1.15331
P	-4.14307	2.74359	0.61842
P	-1.82376	1.84213	-3.41662
N	-4.02373	3.47044	-2.23615
C	-5.23812	3.84529	-1.72348
C	-6.10940	4.69678	-2.42265
H	-7.06908	4.96522	-1.97274
C	-5.74636	5.17927	-3.68355
H	-6.41464	5.83950	-4.24421
C	-4.50590	4.80210	-4.20831
H	-4.17240	5.16657	-5.18352
C	-3.66495	3.95766	-3.46616
C	-5.63597	3.29315	-0.38766
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H	-6.24845	2.38598	-0.53903
C	-2.31108	3.58168	-3.97282
H	-2.24554	3.71677	-5.06339
H	-1.56306	4.24712	-3.50734
C	-3.61789	4.37599	1.55684
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H	-2.97785	6.35432	0.93995

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H	-4.73144	4.24288	3.46044
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H	-5.68131	4.97054	2.13024
C	-2.27406	4.16052	2.28844
H	-1.45552	3.96366	1.57803
H	-2.01849	5.08554	2.83652
H	-2.31036	3.34416	3.02805
C	-5.01237	1.45755	1.80206
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H	-5.76526	-0.56942	1.60248
H	-6.17793	0.44566	0.21174
C	-4.03155	1.04928	2.92057
H	-3.82644	1.88217	3.61276
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C	0.75716	0.55186	-3.77795
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H	0.90038	0.46580	-2.68932
C	0.00126	1.95593	-5.70917
H	-0.55020	2.83574	-6.07786
H	1.04820	2.07444	-6.04465
H	-0.39682	1.05917	-6.20865
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H	-4.89064	-0.33387	-4.14575
H	-4.04333	0.08283	-2.62064
C	-3.38773	1.27383	-5.83729
H	-2.52877	1.47047	-6.49581
H	-4.04441	0.55744	-6.36409
H	-3.96352	2.20702	-5.72267
C	-2.30529	-0.70208	-4.69531
H	-3.03562	-1.39079	-5.15747
H	-1.44403	-0.64297	-5.37887
H	-1.97651	-1.16243	-3.74883

8

SCF (BP86) Energy = -1392.85822202
Enthalpy 0K = -1392.077791
Enthalpy 298K = -1392.033095
Free Energy 298K = -1392.148433
Lowest Frequency = 23.4026 cm^{-1}
Second Frequency = 38.6423 cm^{-1}
SCF (BP86-D3BJ) Energy = -1393.106437
SCF (FB) Energy = -1392.899301
SCF (DFB) Energy = -1392.90509
SCF (BS2) Energy = -2062.471272

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C	2.57506	4.50396	-0.82070
H	3.37973	4.89938	-1.45446
C	1.29403	4.13313	-1.54417
H	1.33329	4.53883	-2.56899
H	0.42448	4.61783	-1.05717
C	1.90801	3.85388	1.57618
H	0.93032	4.37375	1.53194
H	2.33511	4.09486	2.56415
C	0.05142	2.14729	-0.55439
H	-0.97196	2.46056	-0.80546
C	0.32868	2.00572	0.82838
H	-0.50864	2.20235	1.51185
C	1.66116	2.30542	1.48961
H	1.65797	1.87404	2.50686
H	2.49678	1.84019	0.94540
C	1.03405	2.58561	-1.61851
H	1.99254	2.05609	-1.52102
H	0.62382	2.32516	-2.61128
Rh	-0.16282	0.04177	0.01916
P	-2.50575	0.26510	0.11932
P	2.04905	-0.97459	-0.08797
N	-0.72296	-2.05381	-0.06666
C	-1.96264	-2.45921	0.35692
C	-2.35929	-3.80430	0.29425
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C	-1.46750	-4.76614	-0.19473
H	-1.75673	-5.82017	-0.24454
C	-0.20051	-4.35325	-0.62008
H	0.52180	-5.07074	-1.01849
C	0.14461	-2.99258	-0.55577
C	-2.86519	-1.40496	0.92612
H	-3.92321	-1.70536	0.86661
H	-2.61856	-1.26473	1.99321
C	1.46342	-2.49553	-1.05872
H	2.20802	-3.30625	-1.08468
H	1.33071	-2.13157	-2.09275
C	-3.37873	0.14936	-1.62909
C	-2.36809	-0.52641	-2.58724
H	-2.17952	-1.57818	-2.31801
H	-2.78697	-0.51602	-3.61061
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H	-5.43662	-0.29025	-0.91545
H	-5.11407	-0.69632	-2.61364
H	-4.47933	-1.74273	-1.33184
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H	-4.02771	1.48001	-3.21265
H	-4.48685	2.06858	-1.60338
C	-3.47086	1.47023	1.31471
C	-2.92915	1.21911	2.74504
H	-1.82708	1.19247	2.78631
H	-3.26997	2.03896	3.40234
H	-3.31308	0.28238	3.18177
C	-3.20652	2.94740	0.93629
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H	-3.74994	3.59334	1.64974
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H	-5.46158	1.83389	2.09076
H	-5.46351	1.48990	0.35026
C	3.64386	-0.55641	-1.16758
C	3.16178	-0.35307	-2.62664

H	2.27594	0.29862	-2.69870
H	3.97302	0.12437	-3.20513
H	2.93398	-1.30712	-3.12991
C	4.33956	0.73695	-0.68593
H	4.69640	0.66990	0.35211
H	5.22546	0.91227	-1.32358
H	3.70369	1.63140	-0.77146
C	4.68067	-1.70261	-1.14987
H	4.26020	-2.67365	-1.45890
H	5.48157	-1.45760	-1.87177
H	5.16189	-1.82565	-0.16714
C	2.59242	-1.72774	1.64579
C	1.35254	-1.67019	2.57083
H	0.55592	-2.35536	2.24010
H	1.65298	-1.97620	3.59040
H	0.92454	-0.65419	2.62111
C	3.06412	-3.19416	1.54399
H	3.93713	-3.32426	0.88685
H	3.35945	-3.54063	2.55150
H	2.26112	-3.86655	1.19880
C	3.70814	-0.86928	2.28166
H	3.88464	-1.22860	3.31198
H	4.66563	-0.95078	1.74432
H	3.43200	0.19522	2.34989

HCCtBu

SCF (BP86) Energy = -234.586240585
Enthalpy 0K = -234.449584
Enthalpy 298K = -234.440795
Free Energy 298K = -234.480158
Lowest Frequency = 169.3417 cm^{-1}
Second Frequency = 169.4574 cm^{-1}
SCF (BP86-D3BJ) Energy = -234.6063448
SCF (FB) Energy = -234.5884013
SCF (DFB) Energy = -234.5888902
SCF (BS2) Energy = -234.647662

C	2.39701	0.00001	0.00004
H	3.47016	-0.00003	0.00003
C	1.17635	0.00003	0.00005
C	-0.29938	0.00002	0.00004
C	-0.81204	1.24798	0.76779
C	-0.81201	-1.28898	0.69686
H	-0.45850	-2.18995	0.16902
H	-0.45806	-1.34117	1.73961
H	-1.91621	-1.29967	0.70297
H	-0.45855	1.24157	1.81198
H	-1.91624	1.25862	0.77405
H	-0.45817	2.17711	0.29151
C	-0.81192	0.04094	-1.46473
H	-0.45806	-0.83615	-2.03114
H	-1.91612	0.04120	-1.47711
H	-0.45825	0.94842	-1.98121

A_C

SCF (BP86) Energy = -1080.79612092
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Enthalpy 298K = -1080.158071
Free Energy 298K = -1080.258904
Lowest Frequency = 24.9345 cm^{-1}
Second Frequency = 28.1670 cm^{-1}
SCF (BP86-D3BJ) Energy = -1080.977565
SCF (FB) Energy = -1080.844237
SCF (DFB) Energy = -1080.851914
SCF (BS2) Energy = -1750.339368

Rh	-0.00020	-0.43189	0.00068
P	-2.31385	-0.25110	-0.13326
P	2.31373	-0.25129	0.13349
N	-0.00013	1.55263	0.00051
C	-1.12436	2.25687	-0.39461
C	-1.13732	3.65867	-0.38500
H	-2.04758	4.17598	-0.70027
C	0.00035	4.37570	-0.00005
H	0.00052	5.46918	-0.00025
C	1.13778	3.65846	0.38520
H	2.04821	4.17559	0.70027
C	1.12434	2.25666	0.39536
C	-2.32245	1.48182	-0.88088
H	-3.25133	2.04940	-0.70831
H	-2.22842	1.33103	-1.97068
C	2.32205	1.48131	0.88195
H	3.25110	2.04899	0.71062
H	2.22702	1.32963	1.97155
C	-3.34269	-0.09742	1.49588
C	-2.48842	0.77891	2.44301
H	-2.36653	1.80802	2.06347
H	-2.99607	0.84822	3.42228
H	-1.48460	0.34859	2.59964
C	-4.72341	0.56358	1.30128
H	-5.39354	-0.02048	0.65419
H	-5.21453	0.65376	2.28742
H	-4.64764	1.58470	0.89125
C	-3.50271	-1.50189	2.11851
H	-2.53101	-2.01150	2.24027
H	-3.95204	-1.40207	3.12307
H	-4.16934	-2.15157	1.52828
C	-3.10274	-1.44681	-1.43138
C	-2.50228	-1.08849	-2.81094
H	-1.40455	-0.96504	-2.76181
H	-2.71744	-1.90958	-3.51814
H	-2.94464	-0.17326	-3.23914
C	-2.60900	-2.86214	-1.04083
H	-2.96968	-3.18473	-0.05162
H	-2.97223	-3.59514	-1.78368
H	-1.50365	-2.91710	-1.04205
C	-4.64069	-1.41435	-1.51106
H	-5.02709	-0.40506	-1.73124
H	-4.97279	-2.07796	-2.33055
H	-5.11821	-1.77848	-0.58743
C	3.10428	-1.44695	1.43060
C	2.50430	-1.08963	2.81063
H	1.40647	-0.96686	2.76220
H	2.72033	-1.91092	3.51735
H	2.94631	-0.17431	3.23900
C	2.61142	-2.86254	1.03978
H	2.97173	-3.18445	0.05021
H	2.97575	-3.59553	1.78210
H	1.50613	-2.91840	1.04168
C	4.64224	-1.41335	1.50956
H	5.02802	-0.40380	1.72964
H	4.97517	-2.07679	2.32885
H	5.11961	-1.77705	0.58570
C	3.34130	-0.09665	-1.49639
C	2.48589	0.77919	-2.44294
H	2.36379	1.80825	-2.06335

H	2.99281	0.84865	-3.42257
H	1.48216	0.34836	-2.59876
C	4.72166	0.56534	-1.30255
H	5.39261	-0.01830	-0.65592
H	5.21214	0.65598	-2.28896
H	4.64536	1.58635	-0.89236
C	3.50193	-1.50092	-2.11932
H	3.95051	-1.40062	-3.12417
H	4.16942	-2.15020	-1.52965
H	2.53052	-2.01123	-2.24052

$B_{C\text{-}tBu}$

SCF (BP86) Energy = -1315.42848687
Enthalpy 0K = -1314.686830
Enthalpy 298K = -1314.641976
Free Energy 298K = -1314.758068
Lowest Frequency = 21.0087 cm^{-1}
Second Frequency = 32.1843 cm^{-1}
SCF (BP86-D3BJ) Energy = -1315.662926
SCF (FB) Energy = -1315.469708
SCF (DFB) Energy = -1315.475431
SCF (BS2) Energy = -1985.025037

Rh	0.02956	0.15491	0.10794
P	2.39016	-0.17053	0.01237
P	-2.31358	-0.30501	0.21738
N	0.08858	-1.93374	-0.41823
C	1.19585	-2.48121	-1.01430
C	1.23904	-3.83680	-1.37821
H	2.13744	-4.23410	-1.85807
C	0.13058	-4.65520	-1.13343
H	0.14331	-5.71092	-1.42057
C	-0.98706	-4.10297	-0.49731
H	-1.85931	-4.71681	-0.25738
C	-0.97880	-2.74694	-0.13312
C	2.35607	-1.56518	-1.26895
H	3.30249	-2.12626	-1.33390
H	2.20764	-1.05693	-2.23741
C	-2.09796	-2.13634	0.65203
H	-3.02575	-2.72175	0.56054
H	-1.80699	-2.13697	1.71721
C	3.10029	-1.00239	1.63004
C	1.92596	-1.72209	2.33634
H	1.56459	-2.59100	1.76286
H	2.27679	-2.09541	3.31624
H	1.07142	-1.04373	2.50274
C	4.21034	-2.03762	1.34977
H	5.08618	-1.61118	0.83987
H	4.56111	-2.45010	2.31366
H	3.83981	-2.88981	0.75557
C	3.62393	0.10562	2.57119
H	2.86793	0.88873	2.75181
H	3.87332	-0.34480	3.54909
H	4.53960	0.58646	2.19319
C	3.69583	1.03667	-0.77554
C	3.26869	1.25231	-2.24846
H	2.18266	1.41147	-2.35523
H	3.77781	2.15072	-2.64122
H	3.56680	0.41036	-2.89516
C	3.62324	2.38402	-0.02321
H	3.97195	2.30683	1.01766
H	4.27133	3.11898	-0.53451
H	2.59739	2.78095	-0.00613
C	5.14334	0.50269	-0.75836
H	5.23954	-0.48202	-1.24622
H	5.78307	1.20667	-1.32222
H	5.56014	0.43382	0.25849
C	-3.45897	0.27272	1.67937
C	-2.72597	-0.07557	2.99821
H	-1.67207	0.24893	2.98431
H	-3.22846	0.44949	3.83039
H	-2.76119	-1.15190	3.23510
C	-3.62199	1.80649	1.61381
H	-4.12121	2.14546	0.69414
H	-4.24223	2.13670	2.46715
H	-2.64625	2.31130	1.68688
C	-4.83990	-0.41613	1.67117
H	-4.76621	-1.51639	1.70361
H	-5.39758	-0.10364	2.57329
H	-5.45156	-0.13319	0.80011
C	-3.28275	-0.38671	-1.48466
C	-2.20027	-0.43551	-2.58974
H	-1.59997	-1.35883	-2.54398
H	-2.69269	-0.40818	-3.57949
H	-1.50938	0.42249	-2.52160
C	-4.17921	-1.63854	-1.60209
H	-4.94057	-1.69985	-0.80862
H	-4.71623	-1.59833	-2.56745
H	-3.59421	-2.57300	-1.60290
C	-4.14447	0.87569	-1.69482
H	-4.57206	0.84606	-2.71362
H	-4.98843	0.93989	-0.99037
H	-3.55465	1.80256	-1.61760
C	0.11034	1.77560	1.42902
H	0.28547	1.74738	2.49986
C	-0.05511	2.38386	0.32594
C	-0.26218	3.62740	-0.49992
C	0.28075	3.48099	-1.93918
C	0.46749	4.79630	0.22156
H	0.08102	4.93259	1.24486
H	1.55408	4.62606	0.28214
H	0.29992	5.73361	-0.33695
H	1.37429	3.35913	-1.94766
H	0.04059	4.38749	-2.52026
H	-0.17115	2.61393	-2.44995
C	-1.77013	3.97737	-0.57226
H	-2.19312	4.15347	0.42898
H	-1.90300	4.89680	-1.16781
H	-2.34371	3.17378	-1.05875

TS(B-10)$_{C\text{-}tBu}$

SCF (BP86) Energy = -1315.36208646
Enthalpy 0K = -1314.624048
Enthalpy 298K = -1314.579593
Free Energy 298K = -1314.694761
Lowest Frequency = -595.8778 cm^{-1}
Second Frequency = 24.5848 cm^{-1}
SCF (BP86-D3BJ) Energy = -1315.595362
SCF (FB) Energy = -1315.404228
SCF (DFB) Energy = -1315.410234
SCF (BS2) Energy = -1984.957568

Rh	0.05131	0.14752	0.10433
P	2.40033	-0.16280	0.02204
P	-2.29902	-0.32117	0.23109
N	0.11314	-1.88862	-0.52659

C	1.22822	-2.41130	-1.13462
C	1.27725	-3.74825	-1.55776
H	2.17984	-4.12000	-2.05013
C	0.17130	-4.58238	-1.35509
H	0.18794	-5.62321	-1.69143
C	-0.94461	-4.06449	-0.68811
H	-1.81118	-4.69351	-0.46739
C	-0.94246	-2.72658	-0.26323
C	2.39190	-1.48495	-1.33038
H	3.33892	-2.04318	-1.41092
H	2.25363	-0.92328	-2.27072
C	-2.04735	-2.16545	0.57651
H	-2.97062	-2.75706	0.48544
H	-1.72876	-2.20778	1.63307
C	3.03977	-1.06166	1.63325
C	1.83162	-1.79622	2.26374
H	1.48577	-2.63869	1.64360
H	2.14455	-2.21096	3.23985
H	0.98293	-1.11066	2.43093
C	4.15294	-2.09441	1.35772
H	5.06257	-1.65400	0.92502
H	4.44154	-2.56467	2.31564
H	3.80823	-2.90679	0.69583
C	3.52073	0.00702	2.64046
H	2.74683	0.77173	2.82721
H	3.73222	-0.48640	3.60639
H	4.45017	0.50629	2.32423
C	3.74707	1.07065	-0.65867
C	3.39183	1.36415	-2.13624
H	2.31669	1.56228	-2.27879
H	3.94491	2.26200	-2.46627
H	3.69085	0.54221	-2.80724
C	3.68547	2.39210	0.14161
H	3.85221	2.25472	1.22006
H	4.47089	3.07504	-0.23052
H	2.72095	2.90644	0.00192
C	5.18158	0.50296	-0.60096
H	5.27317	-0.47039	-1.11126
H	5.85782	1.20613	-1.12142
H	5.55689	0.39672	0.42863
C	-3.35066	0.18963	1.78775
C	-2.51242	-0.14531	3.04551
H	-1.49906	0.28574	2.99038
H	-3.01760	0.29377	3.92492
H	-2.43753	-1.22922	3.23539
C	-3.58536	1.71630	1.77329
H	-4.16517	2.05485	0.90187
H	-4.15614	1.99628	2.67732
H	-2.62944	2.26481	1.80681
C	-4.69768	-0.56174	1.85490
H	-4.57010	-1.65733	1.87042
H	-5.21176	-0.28471	2.79345
H	-5.37521	-0.30190	1.02646
C	-3.38028	-0.34569	-1.40955
C	-2.37168	-0.27168	-2.58000
H	-1.69952	-1.14519	-2.60281
H	-2.92711	-0.25044	-3.53595
H	-1.74017	0.63045	-2.52296
C	-4.21008	-1.64176	-1.54404
H	-4.90065	-1.80003	-0.70020
H	-4.82535	-1.57102	-2.45958
H	-3.57551	-2.53622	-1.65538
C	-4.33685	0.86379	-1.48574
H	-4.80815	0.87578	-2.48555
H	-5.15082	0.80606	-0.74605
H	-3.82057	1.82637	-1.35762
C	-0.05823	1.76829	1.42654
H	0.97998	2.50113	0.98025
C	-0.03635	2.40421	0.25681
C	-0.32158	3.64545	-0.57697
C	0.51305	3.68295	-1.87569
C	-0.00021	4.88511	0.30144
H	-0.60456	4.89050	1.22269
H	1.06601	4.91527	0.58548
H	-0.22138	5.80430	-0.26666
H	1.59265	3.75746	-1.67092
H	0.22560	4.56743	-2.46874
H	0.33205	2.78393	-2.48778
C	-1.82003	3.65577	-0.95424
H	-2.46685	3.62432	-0.06428
H	-2.04108	4.58280	-1.50958
H	-2.06339	2.80414	-1.60821

TS(B-C)$_{C\text{-}tBu}$

SCF (BP86) Energy = -1315.41692298
Enthalpy 0K = -1314.678080
Enthalpy 298K = -1314.633086
Free Energy 298K = -1314.751863
Lowest Frequency = -143.3884 cm^{-1}
Second Frequency = 13.1341 cm^{-1}
SCF (BP86-D3BJ) Energy = -1315.644376
SCF (FB) Energy = -1315.457148
SCF (DFB) Energy = -1315.462639
SCF (BS2) Energy = -1985.01344

Rh	0.05616	-0.05106	0.18849
P	2.40589	-0.00807	0.02443
P	-2.19184	-0.72892	0.22979
N	0.35070	-2.05620	-0.42557
C	1.52693	-2.44864	-1.02108
C	1.74124	-3.77264	-1.43314
H	2.69388	-4.03657	-1.90067
C	0.73287	-4.72850	-1.26508
H	0.87977	-5.76172	-1.59247
C	-0.46642	-4.33033	-0.66356
H	-1.27666	-5.04559	-0.49725
C	-0.62939	-3.00312	-0.23843
C	2.56086	-1.38504	-1.25962
H	3.57208	-1.81625	-1.33130
H	2.34330	-0.89501	-2.22522
C	-1.86346	-2.57017	0.49991
H	-2.72404	-3.21483	0.26149
H	-1.67169	-2.66667	1.58337
C	3.34864	-0.70011	1.58423
C	2.36656	-1.65972	2.29843
H	2.12288	-2.54059	1.68223
H	2.83883	-2.02456	3.22935
H	1.41962	-1.15678	2.55959
C	4.63180	-1.48098	1.22820
H	5.37157	-0.87560	0.68343
H	5.11144	-1.81958	2.16492
H	4.41700	-2.38617	0.63640
C	3.68905	0.45992	2.54497
H	2.81296	1.09502	2.76326
H	4.03723	0.03860	3.50556
H	4.49847	1.10052	2.16016
C	3.36611	1.45166	-0.81886

C	2.67080	1.69378	-2.18119
H	1.57196	1.73293	-2.07996
H	3.01304	2.66203	-2.58951
H	2.92526	0.92689	-2.93167
C	3.20715	2.72845	0.03787
H	3.71196	2.65461	1.01210
H	3.66463	3.57741	-0.50291
H	2.14648	2.96565	0.21488
C	4.86242	1.15668	-1.05028
H	5.03147	0.22163	-1.61065
H	5.30111	1.97735	-1.64751
H	5.42927	1.10662	-0.10687
C	-3.34668	-0.30088	1.73245
C	-2.55082	-0.65086	3.01419
H	-1.53102	-0.22822	2.99587
H	-3.07797	-0.22585	3.88718
H	-2.47317	-1.73694	3.18790
C	-3.63743	1.21661	1.75255
H	-4.24269	1.54508	0.89505
H	-4.20917	1.45576	2.66781
H	-2.70973	1.80947	1.76659
C	-4.67196	-1.09051	1.71743
H	-4.51741	-2.18115	1.65903
H	-5.22065	-0.88973	2.65604
H	-5.32997	-0.78569	0.88792
C	-3.13519	-0.67440	-1.47545
C	-2.03898	-0.74013	-2.56612
H	-1.49479	-1.69877	-2.55102
H	-2.51540	-0.64363	-3.55947
H	-1.29905	0.07045	-2.44932
C	-4.11218	-1.85233	-1.67711
H	-4.89373	-1.90472	-0.90396
H	-4.62173	-1.72704	-2.65017
H	-3.59152	-2.82340	-1.71459
C	-3.89366	0.66184	-1.61655
H	-4.25469	0.76201	-2.65646
H	-4.77658	0.71579	-0.95965
H	-3.24464	1.52893	-1.40608
C	-0.20547	1.86723	0.90879
H	0.06844	1.62847	1.95203
C	-0.55449	2.93071	0.32296
C	-0.95549	4.16750	-0.35454
C	-0.66609	4.03191	-1.87973
C	-0.09786	5.33400	0.22841
H	-0.26825	5.45416	1.31041
H	0.97705	5.16676	0.05695
H	-0.39065	6.27269	-0.27171
H	0.40426	3.85860	-2.07032
H	-0.96283	4.97026	-2.37803
H	-1.24289	3.20473	-2.32383
C	-2.46218	4.46748	-0.12877
H	-2.69092	4.57346	0.94389
H	-2.72912	5.41195	-0.63225
H	-3.09607	3.66686	-0.54215

TS(C-D)$_{C\text{-}tBu}$

SCF (BP86) Energy = -1315.36375662
Enthalpy 0K = -1314.625498
Enthalpy 298K = -1314.580950
Free Energy 298K = -1314.697117
Lowest Frequency = -280.8519 cm^{-1}
Second Frequency = 12.2741 cm^{-1}
SCF (BP86-D3BJ) Energy = -1315.595234
SCF (FB) Energy = -1315.407748
SCF (DFB) Energy = -1315.414368
SCF (BS2) Energy = -1984.960123

Rh	-0.00824	0.03417	-0.01530
P	2.35048	-0.30849	-0.07934
P	-2.38664	-0.26789	0.07017
N	-0.04254	-2.08401	-0.04720
C	1.07810	-2.78528	-0.42741
C	1.10904	-4.18841	-0.40030
H	2.01977	-4.70656	-0.71166
C	-0.02496	-4.90184	0.00040
H	-0.01882	-5.99565	0.02053
C	-1.16860	-4.18735	0.37076
H	-2.07558	-4.70518	0.69386
C	-1.15647	-2.78370	0.34693
C	2.24886	-1.99676	-0.92338
H	3.18223	-2.57737	-0.85627
H	2.08305	-1.75863	-1.98900
C	-2.35718	-2.00553	0.79948
H	-3.28569	-2.56756	0.60629
H	-2.29227	-1.86036	1.89377
C	3.13606	-0.68325	1.66413
C	1.97229	-1.13484	2.57959
H	1.53862	-2.09648	2.25912
H	2.35845	-1.27208	3.60651
H	1.16159	-0.38536	2.60940
C	4.20175	-1.79879	1.62552
H	5.05286	-1.56302	0.96944
H	4.60344	-1.93847	2.64581
H	3.77794	-2.76848	1.31499
C	3.74277	0.61311	2.24350
H	3.02503	1.45083	2.23097
H	4.02336	0.43449	3.29738
H	4.65668	0.92333	1.71280
C	3.57370	0.61658	-1.27661
C	2.95889	0.55760	-2.69657
H	1.90070	0.87487	-2.70345
H	3.52491	1.25063	-3.34485
H	3.04383	-0.44075	-3.15792
C	3.68045	2.09798	-0.86527
H	4.11491	2.24060	0.13526
H	4.33531	2.62032	-1.58602
H	2.69367	2.58160	-0.89746
C	4.97535	-0.03068	-1.28472
H	4.95146	-1.10606	-1.52853
H	5.58212	0.46329	-2.06537
H	5.50781	0.10234	-0.32938
C	-3.48890	0.65685	1.37780
C	-2.57141	0.96841	2.58389
H	-1.75208	1.65753	2.32190
H	-3.17270	1.45030	3.37628
H	-2.12075	0.06120	3.02294
C	-4.02356	1.97624	0.78137
H	-4.80375	1.80050	0.02380
H	-4.48312	2.57477	1.58889
H	-3.22785	2.58611	0.32548
C	-4.67561	-0.20331	1.87223
H	-4.35169	-1.11042	2.40831
H	-5.26382	0.39726	2.58998
H	-5.35665	-0.50285	1.06247
C	-3.27853	-0.46610	-1.64127
C	-2.44423	-1.49699	-2.43812
H	-2.47659	-2.50722	-1.99553

H	-2.86518	-1.57439	-3.45683
H	-1.39278	-1.17775	-2.53154
C	-4.73301	-0.96253	-1.51563
H	-5.39512	-0.21036	-1.05829
H	-5.12454	-1.16221	-2.52988
H	-4.82311	-1.90357	-0.94582
C	-3.23368	0.88018	-2.39884
H	-3.63349	0.72043	-3.41693
H	-3.85175	1.65608	-1.92247
H	-2.20082	1.25700	-2.49110
C	-0.08892	1.63649	-1.40745
H	-0.60626	1.78107	0.55776
C	-0.16397	2.41432	-0.32716
C	0.14461	3.86137	0.10176
C	0.71169	4.64229	-1.10689
C	1.13222	3.88284	1.29065
H	0.72932	3.32733	2.15621
H	2.10626	3.44589	1.02232
H	1.30593	4.92390	1.61336
H	1.67193	4.23059	-1.45435
H	0.87601	5.69600	-0.82330
H	0.00686	4.61990	-1.95400
C	-1.17769	4.53780	0.54729
H	-1.61863	4.03246	1.42382
H	-0.98405	5.58727	0.83062
H	-1.92009	4.53863	-0.26803

$C_{C\text{-}tBu}$

SCF (BP86) Energy = -1315.43251607
Enthalpy 0K = -1314.693645
Enthalpy 298K = -1314.648370
Free Energy 298K = -1314.768392
Lowest Frequency = 8.3428 cm^{-1}
Second Frequency = 15.9817 cm^{-1}
SCF (BP86-D3BJ) Energy = -1315.657877
SCF (FB) Energy = -1315.473546
SCF (DFB) Energy = -1315.479325
SCF (BS2) Energy = -1985.031789

Rh	0.01978	-0.18737	0.08799
P	2.35959	-0.31827	-0.01394
P	-2.29113	-0.56620	0.13965
N	0.12773	-2.27812	-0.16500
C	1.29753	-2.87914	-0.56944
C	1.37804	-4.26627	-0.76730
H	2.32816	-4.70447	-1.08482
C	0.24702	-5.06624	-0.57565
H	0.29367	-6.14766	-0.73394
C	-0.94520	-4.45292	-0.17618
H	-1.85017	-5.04255	-0.00643
C	-0.98353	-3.06608	0.03306
C	2.49523	-2.00645	-0.84641
H	3.43131	-2.53307	-0.59400
H	2.53588	-1.79719	-1.93157
C	-2.24023	-2.40995	0.54122
H	-3.13598	-2.95312	0.19603
H	-2.24139	-2.46307	1.64611
C	3.23933	-0.53512	1.69483
C	2.60461	-1.78334	2.35190
H	2.85962	-2.71712	1.82292
H	2.99029	-1.87678	3.38324
H	1.50585	-1.69734	2.40582
C	4.76520	-0.72816	1.58750
H	5.28047	0.18157	1.24062
H	5.16644	-0.96627	2.58960
H	5.04327	-1.56302	0.92160
C	2.91506	0.69674	2.57051
H	1.82689	0.81809	2.70357
H	3.36197	0.55365	3.57102
H	3.31973	1.63358	2.15775
C	3.33428	0.82195	-1.23343
C	2.39233	1.04263	-2.44129
H	1.44423	1.51205	-2.13534
H	2.89579	1.70540	-3.16883
H	2.15663	0.10313	-2.97222
C	3.60813	2.18061	-0.55292
H	4.34751	2.09966	0.26034
H	4.02557	2.87794	-1.30207
H	2.68346	2.62850	-0.15256
C	4.65892	0.19857	-1.72741
H	4.50760	-0.75452	-2.26123
H	5.12656	0.89540	-2.44679
H	5.38361	0.03003	-0.91764
C	-3.38994	0.13739	1.56870
C	-2.49214	0.18917	2.82784
H	-1.64799	0.88567	2.70360
H	-3.09918	0.53940	3.68249
H	-2.08041	-0.79758	3.10246
C	-3.84174	1.57090	1.21576
H	-4.58706	1.58486	0.40417
H	-4.31935	2.02419	2.10336
H	-2.99187	2.21100	0.92610
C	-4.62015	-0.74994	1.86584
H	-4.34171	-1.76424	2.19691
H	-5.19310	-0.29053	2.69180
H	-5.30081	-0.84096	1.00691
C	-3.14067	-0.45142	-1.59497
C	-2.33299	-1.38672	-2.52642
H	-2.43056	-2.45065	-2.25197
H	-2.71721	-1.27797	-3.55680
H	-1.26111	-1.12334	-2.53670
C	-4.62175	-0.87832	-1.59564
H	-5.26123	-0.17443	-1.03969
H	-4.98842	-0.89468	-2.63840
H	-4.77473	-1.89063	-1.18362
C	-2.99512	0.99693	-2.11444
H	-3.35185	1.03889	-3.15975
H	-3.59227	1.71561	-1.53276
H	-1.94384	1.32729	-2.09310
C	-0.10227	1.82555	0.14820
H	0.00265	1.16002	1.16690
C	-0.20064	3.06742	0.05724
C	-0.29420	4.52639	-0.12955
C	0.17328	4.87753	-1.57187
C	0.63204	5.23312	0.90101
H	0.32998	4.99848	1.93490
H	1.68316	4.92931	0.76744
H	0.56825	6.32610	0.76346
H	1.21574	4.56271	-1.74074
H	0.11254	5.96944	-1.71928
H	-0.46544	4.39126	-2.32719
C	-1.75684	5.00563	0.07284
H	-2.11178	4.77908	1.09178
H	-1.81628	6.09752	-0.07486
H	-2.43582	4.52403	-0.64985

TS(C-10)$_{C\text{-}tBu}$

SCF (BP86) Energy = -1315.41521036
Enthalpy 0K = -1314.678637
Enthalpy 298K = -1314.633195
Free Energy 298K = -1314.752998
Lowest Frequency = -789.3127 cm^{-1}
Second Frequency = 12.4710 cm^{-1}
SCF (BP86-D3BJ) Energy = -1315.639942
SCF (FB) Energy = -1315.455734
SCF (DFB) Energy = -1315.46151764
SCF (BS2) Energy = -1985.012905

Rh	-0.00084	-0.16828	0.03687
P	2.31618	-0.43715	-0.05461
P	-2.31802	-0.44190	0.09179
N	-0.00115	-2.29063	-0.04013
C	1.13887	-2.98365	-0.37358
C	1.16060	-4.38589	-0.42756
H	2.09137	-4.89459	-0.69342
C	-0.00524	-5.11264	-0.16497
H	-0.00638	-6.20558	-0.21155
C	-1.17036	-4.40828	0.15577
H	-2.10346	-4.93574	0.37229
C	-1.14559	-3.00663	0.22265
C	2.36805	-2.19424	-0.74223
H	3.28633	-2.73992	-0.46610
H	2.38949	-2.07379	-1.84126
C	-2.37887	-2.24776	0.63852
H	-3.29293	-2.76871	0.30626
H	-2.41602	-2.21522	1.74327
C	3.20027	-0.56261	1.66412
C	2.49736	-1.71187	2.42457
H	2.69560	-2.70003	1.97651
H	2.87964	-1.74014	3.46122
H	1.40518	-1.55819	2.46699
C	4.71182	-0.85126	1.57705
H	5.27820	-0.00592	1.15471
H	5.10327	-1.02726	2.59591
H	4.93812	-1.75377	0.98394
C	2.94959	0.75221	2.43681
H	1.86823	0.93768	2.55461
H	3.38955	0.66856	3.44730
H	3.40490	1.62829	1.94897
C	3.36621	0.53126	-1.36240
C	2.44095	0.71405	-2.58923
H	1.51297	1.24550	-2.32506
H	2.97757	1.29825	-3.35943
H	2.15824	-0.24786	-3.05161
C	3.73369	1.92055	-0.79873
H	4.46915	1.85973	0.01983
H	4.19078	2.52685	-1.60214
H	2.84312	2.45937	-0.43478
C	4.64678	-0.21280	-1.80276
H	4.43162	-1.19551	-2.25415
H	5.15572	0.38924	-2.57777
H	5.36271	-0.35981	-0.98105
C	-3.40621	0.41368	1.44758
C	-2.52280	0.50085	2.71467
H	-1.60241	1.07924	2.53559
H	-3.09560	0.99707	3.51945
H	-2.22234	-0.49173	3.09265
C	-3.77167	1.84150	0.98872
H	-4.49463	1.83928	0.15692
H	-4.24393	2.38241	1.82905
H	-2.88133	2.41274	0.67743
C	-4.69151	-0.37314	1.79044
H	-4.47943	-1.38306	2.17878
H	-5.23475	0.16748	2.58713
H	-5.37622	-0.46912	0.93549
C	-3.15909	-0.42404	-1.65250
C	-2.41587	-1.49050	-2.49145
H	-2.59982	-2.51704	-2.13221
H	-2.77759	-1.43855	-3.53451
H	-1.32688	-1.31075	-2.49802
C	-4.66655	-0.74370	-1.63466
H	-5.25971	0.05029	-1.15345
H	-5.02728	-0.83115	-2.67606
H	-4.89200	-1.70080	-1.13364
C	-2.90722	0.95923	-2.29463
H	-3.28030	0.94724	-3.33508
H	-3.42779	1.77306	-1.76620
H	-1.82993	1.19331	-2.31757
C	-0.00574	1.78792	0.03446
H	0.11054	2.06216	1.18098
C	-0.01246	3.06484	0.01283
C	0.00011	4.54002	-0.01826
C	0.06209	4.92769	-1.52930
C	1.25429	5.09037	0.71359
H	1.24488	4.81698	1.78191
H	2.18320	4.70794	0.26127
H	1.26343	6.19109	0.64503
H	0.97594	4.54048	-2.00706
H	0.06872	6.02820	-1.60464
H	-0.81442	4.54915	-2.07908
C	-1.28791	5.12519	0.61916
H	-1.36843	4.84732	1.68309
H	-1.26332	6.22614	0.55618
H	-2.18955	4.77003	0.09489

$D_{C\text{-}tBu}$
SCF (BP86) Energy = -1315.36477713
Enthalpy 0K = -1314.625878
Enthalpy 298K = -1314.581042
Free Energy 298K = -1314.697676
Lowest Frequency = 10.4549 cm^{-1}
Second Frequency = 31.3418 cm^{-1}
SCF (BP86-D3BJ) Energy = -1315.596551
SCF (FB) Energy = -1315.409167
SCF (DFB) Energy = -1315.415953
SCF (BS2) Energy = -1984.961713

Rh	-0.00042	0.04022	0.02809
P	2.37557	-0.24572	-0.04501
P	-2.36095	-0.31604	0.10572
N	0.03537	-2.06646	-0.18151
C	1.17001	-2.70638	-0.62130
C	1.23116	-4.10533	-0.71176
H	2.15050	-4.57605	-1.06963
C	0.11500	-4.87413	-0.36442
H	0.14472	-5.96535	-0.43710
C	-1.03898	-4.22022	0.07802
H	-1.92989	-4.78408	0.36671
C	-1.05664	-2.81902	0.17143
C	2.32131	-1.84864	-1.04227
H	3.26846	-2.41064	-1.02908
H	2.14663	-1.51243	-2.07985
C	-2.25899	-2.10365	0.71248

H	-3.18078	-2.67551	0.51717
H	-2.15763	-2.02755	1.81104
C	3.09956	-0.75316	1.69053
C	1.91777	-1.31419	2.51920
H	1.53653	-2.26537	2.11292
H	2.26582	-1.51092	3.55007
H	1.07735	-0.59758	2.56952
C	4.20035	-1.83114	1.60472
H	5.07671	-1.51058	1.02265
H	4.55180	-2.06036	2.62749
H	3.82335	-2.77587	1.17815
C	3.63685	0.50876	2.40128
H	2.88544	1.31597	2.43923
H	3.89424	0.24816	3.44394
H	4.55096	0.90225	1.92974
C	3.63054	0.80615	-1.09404
C	3.13189	0.79870	-2.56032
H	2.05728	1.04359	-2.63465
H	3.69482	1.56956	-3.11708
H	3.32774	-0.16044	-3.06877
C	3.61823	2.26386	-0.58831
H	3.93856	2.36169	0.45994
H	4.31889	2.85715	-1.20348
H	2.61533	2.70132	-0.69847
C	5.06366	0.23563	-1.03326
H	5.11812	-0.82204	-1.34193
H	5.69399	0.80941	-1.73707
H	5.52023	0.33580	-0.03567
C	-3.48188	0.46231	1.49248
C	-2.52924	0.81597	2.65807
H	-1.78568	1.57509	2.36638
H	-3.12052	1.22255	3.49878
H	-1.98182	-0.06443	3.03917
C	-4.17325	1.74277	0.98054
H	-4.97471	1.51979	0.25840
H	-4.64217	2.26117	1.83662
H	-3.46851	2.44532	0.51227
C	-4.56080	-0.52160	2.00373
H	-4.13451	-1.40152	2.51204
H	-5.18255	0.00544	2.75017
H	-5.23475	-0.87143	1.20721
C	-3.26802	-0.42986	-1.60355
C	-2.39657	-1.34682	-2.49362
H	-2.36142	-2.38739	-2.12828
H	-2.83877	-1.37231	-3.50597
H	-1.36875	-0.95761	-2.58382
C	-4.69057	-1.01406	-1.48579
H	-5.37564	-0.34944	-0.93605
H	-5.10507	-1.13523	-2.50322
H	-4.71124	-2.01017	-1.01083
C	-3.31048	0.97232	-2.25207
H	-3.72396	0.87033	-3.27208
H	-3.95723	1.67486	-1.70549
H	-2.29849	1.40328	-2.33624
C	-0.01802	1.58178	-1.46678
H	-0.08100	1.69252	0.62340
C	-0.04184	2.38517	-0.41890
C	-0.06044	3.86220	-0.00433
C	0.43187	4.68454	-1.22232
C	0.85057	4.11342	1.22003
H	0.51699	3.52583	2.09464
H	1.90093	3.85696	1.01211
H	0.81256	5.17926	1.50229
H	1.46800	4.42793	-1.49407
H	0.39558	5.76031	-0.97859
H	-0.20696	4.50635	-2.10246
C	-1.49957	4.30780	0.35184
H	-1.87851	3.77527	1.24039
H	-1.51047	5.38703	0.58524
H	-2.18943	4.13270	-0.48998

TS(C-E)$_{C\text{-}tBu}$

SCF (BP86) Energy = -1315.42880900
Enthalpy 0K = -1314.691619
Enthalpy 298K = -1314.646611
Free Energy 298K = -1314.765219
Lowest Frequency = -642.3505 cm^{-1}
Second Frequency = 15.5195 cm^{-1}
SCF (BP86-D3BJ) Energy = -1315.655218
SCF (FB) Energy = -1315.471692
SCF (DFB) Energy = -1315.47812
SCF (BS2) Energy = -1985.027935

Rh	0.00849	-0.17359	-0.00867
P	-2.32329	-0.47347	0.05735
P	2.34308	-0.39595	-0.09672
N	0.03912	-2.30854	-0.00318
C	-1.09168	-3.02164	0.31300
C	-1.08620	-4.42498	0.33603
H	-2.00594	-4.96034	0.58709
C	0.09606	-5.12015	0.05824
H	0.11772	-6.21371	0.08004
C	1.25051	-4.39039	-0.24785
H	2.19089	-4.89884	-0.47739
C	1.19994	-2.98846	-0.28374
C	-2.33546	-2.25576	0.69330
H	-3.24317	-2.80575	0.39249
H	-2.37269	-2.17232	1.79567
C	2.40991	-2.18847	-0.69559
H	3.34110	-2.70357	-0.40553
H	2.41844	-2.11551	-1.79957
C	-3.20613	-0.55456	-1.65829
C	-2.48644	-1.66258	-2.46297
H	-2.65401	-2.66871	-2.04296
H	-2.88616	-1.66835	-3.49302
H	-1.39970	-1.48222	-2.52173
C	-4.70878	-0.88472	-1.55233
H	-5.28499	-0.06849	-1.08881
H	-5.11387	-1.03162	-2.57012
H	-4.90361	-1.81401	-0.99008
C	-3.00570	0.79404	-2.38557
H	-1.93727	1.04144	-2.49691
H	-3.44273	0.72062	-3.39781
H	-3.49827	1.63286	-1.87126
C	-3.33698	0.46313	1.40866
C	-2.37417	0.62428	2.60991
H	-1.48222	1.20996	2.33505
H	-2.90374	1.15508	3.42204
H	-2.04405	-0.34576	3.02384
C	-3.71703	1.86309	0.87993
H	-4.48073	1.81677	0.08660
H	-4.14699	2.45238	1.71019
H	-2.83496	2.40513	0.50030
C	-4.60186	-0.29986	1.86093
H	-4.37196	-1.28688	2.29601
H	-5.10006	0.28883	2.65263
H	-5.33207	-0.44051	1.05039

C	3.41263	0.52735	-1.41402
C	2.52892	0.68475	-2.67404
H	1.66487	1.34087	-2.48474
H	3.13597	1.14370	-3.47539
H	2.15426	-0.27918	-3.06093
C	3.78246	1.92999	-0.88562
H	4.52188	1.88731	-0.06977
H	4.23975	2.50990	-1.70768
H	2.89468	2.48224	-0.53617
C	4.69096	-0.25819	-1.78714
H	4.46972	-1.23128	-2.25633
H	5.25907	0.33193	-2.52884
H	5.35592	-0.43061	-0.92807
C	3.14323	-0.40871	1.66370
C	2.37115	-1.47696	2.47490
H	2.52052	-2.49905	2.08820
H	2.73738	-1.46318	3.51729
H	1.28705	-1.26845	2.50205
C	4.64571	-0.75309	1.66235
H	5.25490	0.03355	1.18995
H	4.99184	-0.84656	2.70806
H	4.86356	-1.71272	1.16273
C	2.90288	0.97115	2.31868
H	3.21223	0.92129	3.37854
H	3.48743	1.77179	1.84143
H	1.83916	1.25857	2.28077
C	-0.01916	1.79220	0.03300
H	-0.05794	0.79880	-1.22722
C	-0.04392	3.03568	-0.03208
C	-0.09709	4.51293	-0.00023
C	-0.51194	4.97529	1.42516
C	-1.14652	5.01499	-1.03074
H	-0.88137	4.69995	-2.05355
H	-2.15126	4.62540	-0.79749
H	-1.19206	6.11763	-1.01113
H	-1.50515	4.58199	1.69709
H	-0.55512	6.07766	1.46032
H	0.21501	4.63360	2.18017
C	1.29162	5.11191	-0.34979
H	1.61501	4.80311	-1.35774
H	1.24305	6.21441	-0.32895
H	2.05622	4.78978	0.37660

$E_{C\text{-}tBu}$

SCF (BP86) Energy = -1315.43634721
Enthalpy 0K = -1314.697420
Enthalpy 298K = -1314.652265
Free Energy 298K = -1314.770842
Lowest Frequency = 16.5130 cm^{-1}
Second Frequency = 19.8705 cm^{-1}
SCF (BP86-D3BJ) Energy = -1315.66336
SCF (FB) Energy = -1315.481579
SCF (DFB) Energy = -1315.488927
SCF (BS2) Energy = -1985.034525

Rh	0.00869	-0.18129	-0.00992
P	-2.32851	-0.45237	0.05546
P	2.34078	-0.42189	-0.09678
N	0.02045	-2.32493	0.02694
C	-1.12671	-3.02204	0.31015
C	-1.14448	-4.42560	0.31033
H	-2.07624	-4.95055	0.53831
C	0.03159	-5.13462	0.04022
H	0.03631	-6.22857	0.04612
C	1.20119	-4.41861	-0.23965
H	2.13647	-4.93853	-0.46477
C	1.17181	-3.01521	-0.25621
C	-2.36130	-2.23776	0.68728
H	-3.27621	-2.77488	0.38533
H	-2.39895	-2.15519	1.78988
C	2.39999	-2.22894	-0.65154
H	3.31913	-2.74307	-0.32354
H	2.44288	-2.18622	-1.75642
C	-3.24119	-0.49523	-1.64331
C	-2.59796	-1.63694	-2.46493
H	-2.78748	-2.63314	-2.03109
H	-3.03791	-1.63261	-3.47827
H	-1.50838	-1.50469	-2.57474
C	-4.75492	-0.75771	-1.50404
H	-5.28059	0.07649	-1.01360
H	-5.19095	-0.86854	-2.51345
H	-4.97811	-1.68662	-0.95154
C	-2.99006	0.84732	-2.36627
H	-1.91406	1.06771	-2.45611
H	-3.41701	0.78927	-3.38379
H	-3.46596	1.69724	-1.85429
C	-3.28493	0.50391	1.43342
C	-2.28428	0.63816	2.60744
H	-1.39703	1.22323	2.31278
H	-2.78023	1.16710	3.44168
H	-1.95417	-0.34020	3.00210
C	-3.64212	1.91425	0.91687
H	-4.42544	1.88853	0.14201
H	-4.03767	2.51113	1.75874
H	-2.75490	2.43349	0.51753
C	-4.55424	-0.23103	1.91728
H	-4.33629	-1.22297	2.34740
H	-5.01993	0.36910	2.72008
H	-5.30647	-0.35539	1.12446
C	3.39462	0.48259	-1.43535
C	2.49384	0.61714	-2.68567
H	1.61300	1.24551	-2.48071
H	3.07999	1.09346	-3.49235
H	2.14848	-0.35890	-3.07145
C	3.75684	1.89523	-0.92867
H	4.50073	1.86945	-0.11600
H	4.20678	2.46507	-1.76166
H	2.86497	2.44475	-0.58556
C	4.67457	-0.30092	-1.80547
H	4.45708	-1.28656	-2.24983
H	5.22867	0.27710	-2.56690
H	5.35113	-0.44760	-0.95044
C	3.13912	-0.39901	1.66392
C	2.37086	-1.45515	2.49458
H	2.52181	-2.48328	2.12533
H	2.73776	-1.42260	3.53620
H	1.28534	-1.25226	2.52082
C	4.64201	-0.74209	1.66283
H	5.24769	0.03605	1.17239
H	4.99259	-0.81509	2.70868
H	4.85883	-1.71086	1.18072
C	2.90114	0.99232	2.29482
H	3.20812	0.95979	3.35593
H	3.48809	1.78288	1.80433
H	1.83947	1.28780	2.25076
C	0.00121	1.77722	-0.02733
H	-0.02948	-0.15793	-1.52447
C	-0.00743	3.02067	-0.04218

C	-0.04509	4.50031	-0.01237
C	-0.45498	4.97496	1.40953
C	-1.08688	5.01210	-1.04544
H	-0.82555	4.68675	-2.06598
H	-2.09660	4.63604	-0.81094
H	-1.11932	6.11555	-1.03264
H	-1.45261	4.59370	1.68332
H	-0.48657	6.07795	1.44213
H	0.26769	4.62820	2.16669
C	1.34932	5.08534	-0.36277
H	1.66983	4.76948	-1.36950
H	1.31340	6.18860	-0.34547
H	2.11056	4.75728	0.36476

$10_{C\text{-}tBu}$

SCF (BP86) Energy = -1315.45119958
Enthalpy 0K = -1314.710171
Enthalpy 298K = -1314.665198
Free Energy 298K = -1314.783080
Lowest Frequency = 18.7166 cm^{-1}
Second Frequency = 31.6497 cm^{-1}
SCF (BP86-D3BJ) Energy = -1315.678862
SCF (FB) Energy = -1315.492862
SCF (DFB) Energy = -1315.498767
SCF (BS2) Energy = -1985.047832

Rh	0.00502	-0.11476	0.04181
P	2.34241	-0.37102	-0.03130
P	-2.32635	-0.42062	0.10508
N	0.02572	-2.27589	-0.13237
C	1.18154	-2.93408	-0.46670
C	1.21614	-4.33334	-0.57963
H	2.15400	-4.82821	-0.84608
C	0.04770	-5.07386	-0.36970
H	0.05601	-6.16405	-0.46318
C	-1.13119	-4.39783	-0.03611
H	-2.06017	-4.94534	0.14462
C	-1.11801	-2.99944	0.09011
C	2.41182	-2.11481	-0.76677
H	3.32470	-2.66013	-0.47243
H	2.47465	-1.96800	-1.86091
C	-2.35529	-2.26301	0.53830
H	-3.26555	-2.76769	0.17247
H	-2.39860	-2.30071	1.64271
C	3.17536	-0.54323	1.70585
C	2.43884	-1.69993	2.42183
H	2.62477	-2.68007	1.95092
H	2.80502	-1.76308	3.46253
H	1.34933	-1.52606	2.45616
C	4.68502	-0.84831	1.64809
H	5.26898	0.00137	1.26019
H	5.04817	-1.04999	2.67250
H	4.91909	-1.73968	1.04114
C	2.91992	0.76076	2.49541
H	1.84257	0.98595	2.55401
H	3.30312	0.63720	3.52467
H	3.42952	1.63112	2.05448
C	3.40650	0.63196	-1.29428
C	2.50704	0.81276	-2.54040
H	1.54994	1.29745	-2.28874
H	3.03686	1.44342	-3.27744
H	2.28108	-0.14543	-3.04076
C	3.72718	2.01533	-0.68859
H	4.46357	1.94982	0.12884
H	4.16625	2.66032	-1.47120
H	2.82229	2.51504	-0.30465
C	4.71227	-0.07932	-1.71277
H	4.52992	-1.05884	-2.18546
H	5.22740	0.54634	-2.46437
H	5.40983	-0.22425	-0.87519
C	-3.39664	0.33430	1.52874
C	-2.48461	0.34916	2.77865
H	-1.56951	0.93850	2.61041
H	-3.04051	0.79892	3.62145
H	-2.18130	-0.66425	3.09529
C	-3.78223	1.78471	1.16627
H	-4.51138	1.82817	0.34098
H	-4.25777	2.25870	2.04419
H	-2.90049	2.38745	0.89428
C	-4.66741	-0.48778	1.83998
H	-4.44115	-1.51909	2.15798
H	-5.19959	-0.00499	2.67981
H	-5.36733	-0.53289	0.99301
C	-3.18024	-0.31840	-1.62747
C	-2.42871	-1.32110	-2.53470
H	-2.58685	-2.37040	-2.23308
H	-2.80676	-1.21771	-3.56791
H	-1.34348	-1.11904	-2.55048
C	-4.68229	-0.66270	-1.61026
H	-5.27925	0.09170	-1.07366
H	-5.05484	-0.69096	-2.65067
H	-4.88824	-1.65201	-1.16671
C	-2.95808	1.10521	-2.18624
H	-3.34454	1.15169	-3.22065
H	-3.48238	1.87684	-1.60171
H	-1.88475	1.35728	-2.20832
C	-0.02789	1.70408	0.34089
H	-0.19945	3.10991	1.79857
C	-0.08578	2.97366	0.70702
C	-0.04845	4.28652	-0.10137
C	0.17023	4.02365	-1.60440
C	1.09677	5.16976	0.45200
H	0.96035	5.37790	1.52725
H	2.07915	4.68616	0.32027
H	1.12020	6.13776	-0.07856
H	1.14207	3.53802	-1.79159
H	0.15936	4.97681	-2.16004
H	-0.62487	3.38151	-2.01993
C	-1.39789	5.01904	0.10617
H	-1.59721	5.20361	1.17586
H	-1.38102	5.99699	-0.40653
H	-2.23777	4.43454	-0.30561

TS(B-10)'$_{C\text{-}tBu}$

SCF (BP86) Energy = -1315.33306337
Enthalpy 0K = -1314.594363
Enthalpy 298K = -1314.549666
Free Energy 298K = -1314.664721
Lowest Frequency = -464.8404 cm^{-1}
Second Frequency = 23.6300 cm^{-1}
SCF (BP86-D3BJ) Energy = -1315.56652
SCF (FB) Energy = -1315.37512
SCF (DFB) Energy = -1315.38131
SCF (BS2) Energy = -1984.930783

Rh	0.05269	0.06265	-0.01206
P	2.42484	-0.09675	-0.04898

P	-2.26940	-0.46700	0.09051
N	0.23647	-2.07309	-0.05566
C	1.40674	-2.67891	-0.44760
C	1.53144	-4.07499	-0.52461
H	2.48427	-4.50518	-0.84492
C	0.44362	-4.89298	-0.20624
H	0.52341	-5.98234	-0.26611
C	-0.74766	-4.28110	0.19477
H	-1.62320	-4.87710	0.46603
C	-0.82591	-2.88148	0.26850
C	2.56639	-1.80364	-0.82434
H	3.52436	-2.30120	-0.59787
H	2.54642	-1.62466	-1.91535
C	-2.07767	-2.22134	0.75786
H	-2.96033	-2.85090	0.55852
H	-2.00599	-2.10284	1.85488
C	3.23707	-0.29258	1.70862
C	2.56487	-1.51160	2.38174
H	2.83031	-2.46481	1.89508
H	2.91139	-1.57262	3.42956
H	1.46609	-1.41335	2.39142
C	4.76283	-0.51149	1.67527
H	5.31011	0.38287	1.33852
H	5.11059	-0.73798	2.70003
H	5.05718	-1.36305	1.03891
C	2.90178	0.96135	2.54778
H	1.81255	1.05490	2.69269
H	3.36228	0.86023	3.54736
H	3.28811	1.89217	2.10176
C	3.54247	0.94216	-1.26133
C	2.72656	1.13395	-2.56146
H	1.76904	1.64915	-2.37939
H	3.32823	1.73934	-3.26415
H	2.50963	0.17663	-3.06788
C	3.85139	2.32332	-0.64326
H	4.49015	2.25077	0.25225
H	4.40196	2.93029	-1.38488
H	2.93238	2.87158	-0.38390
C	4.86610	0.22413	-1.61512
H	4.70413	-0.75315	-2.09871
H	5.40995	0.85148	-2.34484
H	5.53036	0.07969	-0.75184
C	-3.52126	0.22275	1.42066
C	-2.65802	0.58974	2.65049
H	-1.85669	1.30160	2.39868
H	-3.30245	1.04271	3.42612
H	-2.18020	-0.29648	3.10338
C	-4.25121	1.47393	0.89354
H	-4.96237	1.23098	0.08768
H	-4.83437	1.92656	1.71610
H	-3.55913	2.24282	0.51922
C	-4.58205	-0.81761	1.85287
H	-4.14255	-1.70164	2.34136
H	-5.24750	-0.34301	2.59717
H	-5.21540	-1.15786	1.02045
C	-3.11047	-0.72295	-1.64281
C	-2.17538	-1.65743	-2.44631
H	-2.13949	-2.67992	-2.03499
H	-2.55728	-1.73360	-3.48069
H	-1.14720	-1.25879	-2.49273
C	-4.51902	-1.34503	-1.57169
H	-5.25633	-0.67029	-1.10825
H	-4.87003	-1.54899	-2.60002
H	-4.53601	-2.30642	-1.03045
C	-3.16203	0.63863	-2.36788
H	-3.51707	0.48108	-3.40277
H	-3.86068	1.34366	-1.88980
H	-2.16350	1.10350	-2.41662
C	0.35643	2.15067	0.48063
H	0.85784	2.52798	1.36645
C	0.15826	2.07370	-0.81272
C	-0.75715	3.83118	-0.06963
C	0.38162	4.79012	-0.38482
C	-1.34668	4.05873	1.32533
H	-2.05773	3.27381	1.61881
H	-0.57716	4.15073	2.10840
H	-1.90697	5.01409	1.30016
H	1.17753	4.76648	0.37765
H	-0.02828	5.81859	-0.40031
H	0.82551	4.58213	-1.36999
C	-1.83718	3.82948	-1.14336
H	-1.41043	3.78565	-2.15471
H	-2.53805	2.99189	-1.02762
H	-2.42094	4.76729	-1.03957

TS(B-10)"$_{\text{C-tBu}}$

SCF (BP86) Energy = -1315.35950815
Enthalpy 0K = -1314.620639
Enthalpy 298K = -1314.575751
Free Energy 298K = -1314.691455
Lowest Frequency = -435.6637 cm^{-1}
Second Frequency = 21.0132 cm^{-1}
SCF (BP86-D3BJ) Energy = -1315.594527
SCF (FB) Energy = -1315.400572
SCF (DFB) Energy = -1315.406347
SCF (BS2) Energy = -1984.957103

Rh	-0.05205	-0.10420	0.04730
P	2.29373	0.29797	0.14765
P	-2.37745	0.22589	-0.03225
N	-0.07970	2.03094	-0.12124
C	1.01586	2.77538	0.24864
C	1.05676	4.16927	0.09541
H	1.95629	4.71189	0.39870
C	-0.05747	4.84657	-0.41267
H	-0.04527	5.93317	-0.53781
C	-1.19485	4.09944	-0.73529
H	-2.09765	4.58498	-1.11611
C	-1.18406	2.70383	-0.58173
C	2.14345	2.02923	0.88988
H	3.08047	2.60631	0.86383
H	1.88509	1.85612	1.94945
C	-2.39454	1.88770	-0.92797
H	-3.32004	2.46176	-0.75242
H	-2.37126	1.63509	-2.00385
C	3.21139	0.64305	-1.55361
C	2.09794	0.89429	-2.59810
H	1.51407	1.80093	-2.37184
H	2.56163	1.03398	-3.59246
H	1.39277	0.04803	-2.65679
C	4.12732	1.88505	-1.48974
H	4.91151	1.80389	-0.72057
H	4.63644	1.99928	-2.46437
H	3.55884	2.81341	-1.31691
C	4.04752	-0.57308	-2.00642
H	3.45032	-1.49615	-2.07074
H	4.44130	-0.37187	-3.01959

H	4.91598	-0.75977	-1.35507
C	3.48608	-0.52534	1.44578
C	2.77393	-0.43962	2.81869
H	1.72256	-0.76928	2.75597
H	3.29781	-1.10025	3.53324
H	2.79949	0.57532	3.24840
C	3.66995	-2.01811	1.10215
H	4.16017	-2.18118	0.13067
H	4.30523	-2.49042	1.87392
H	2.69893	-2.53602	1.10424
C	4.86059	0.17011	1.53489
H	4.77772	1.24589	1.76312
H	5.44147	-0.28997	2.35555
H	5.45462	0.05438	0.61437
C	-3.56116	-0.78465	-1.19086
C	-2.71633	-1.11658	-2.44531
H	-1.72565	-1.52376	-2.18564
H	-3.25456	-1.85395	-3.06856
H	-2.54789	-0.22592	-3.07516
C	-3.99808	-2.07688	-0.46744
H	-4.74360	-1.86888	0.31727
H	-4.47281	-2.76386	-1.19173
H	-3.15184	-2.60576	-0.00319
C	-4.81730	-0.00932	-1.65059
H	-4.57037	0.91360	-2.20029
H	-5.38711	-0.65176	-2.34719
H	-5.49176	0.25011	-0.82233
C	-3.20093	0.58568	1.69049
C	-2.40352	1.74791	2.32735
H	-2.53578	2.69976	1.78618
H	-2.76752	1.90380	3.35931
H	-1.32553	1.51784	2.37528
C	-4.68981	0.97689	1.60790
H	-5.32921	0.13720	1.29266
H	-5.03359	1.28517	2.61244
H	-4.87057	1.82837	0.92991
C	-3.02808	-0.66280	2.58415
H	-3.41194	-0.43753	3.59606
H	-3.58085	-1.53699	2.20679
H	-1.96379	-0.93637	2.67555
C	-0.05138	-2.04991	0.53368
C	-0.17811	-2.75591	1.57972
H	-0.27565	-3.40418	2.43617
C	0.26438	-3.66405	-0.42853
C	-1.08783	-4.15989	-0.92288
H	-0.90597	-5.01276	-1.60508
H	-1.72255	-4.52219	-0.09929
H	-1.63491	-3.39532	-1.48816
C	1.00287	-4.78318	0.33193
H	0.36698	-5.28716	1.07736
H	1.29901	-5.54845	-0.40972
H	1.92176	-4.43100	0.82374
C	1.14449	-3.13190	-1.55880
H	2.10667	-2.76348	-1.17835
H	1.35284	-3.97656	-2.24574
H	0.64936	-2.32403	-2.11658

TS(B-F)$_{C\text{-}tBu}$

SCF (BP86) Energy = -1315.34138384
Enthalpy 0K = -1314.602636
Enthalpy 298K = -1314.557787
Free Energy 298K = -1314.672611
Lowest Frequency = -228.9709 cm^{-1}
Second Frequency = 33.9755 cm^{-1}
SCF (BP86-D3BJ) Energy = -1315.584824
SCF (FB) Energy = -1315.38253
SCF (DFB) Energy = -1315.388362
SCF (BS2) Energy = -1984.939804

Rh	-0.04265	-0.32745	-0.05144
P	2.32360	0.13856	0.25066
P	-2.37106	0.12657	0.02308
N	-0.05720	1.75409	-0.63434
C	0.99676	2.57660	-0.33288
C	1.00269	3.93210	-0.70194
H	1.87080	4.54919	-0.45444
C	-0.10832	4.48103	-1.35092
H	-0.11896	5.53393	-1.64762
C	-1.22069	3.66170	-1.57964
H	-2.12546	4.05780	-2.04854
C	-1.17679	2.31078	-1.20440
C	2.10345	2.00082	0.50092
H	3.04221	2.55798	0.35247
H	1.82570	2.11981	1.56464
C	-2.36462	1.40971	-1.37184
H	-3.29835	1.99061	-1.44728
H	-2.26083	0.81848	-2.29879
C	3.64701	0.16554	-1.21270
C	2.98162	0.96167	-2.36170
H	2.90144	2.03745	-2.13659
H	3.60491	0.86526	-3.26926
H	1.97236	0.58943	-2.60594
C	4.97686	0.85407	-0.83451
H	5.60586	0.21564	-0.19559
H	5.54668	1.04157	-1.76334
H	4.85009	1.82781	-0.33433
C	3.97804	-1.25273	-1.72254
H	3.10510	-1.76080	-2.15602
H	4.73499	-1.16949	-2.52395
H	4.40623	-1.89911	-0.93997
C	3.12284	-0.36173	1.95954
C	2.00852	-0.23026	3.02504
H	1.12654	-0.84029	2.77873
H	2.41404	-0.57973	3.99254
H	1.68827	0.81544	3.17695
C	3.57375	-1.83662	1.89765
H	4.39004	-1.99904	1.17464
H	3.95836	-2.13494	2.89006
H	2.73335	-2.50600	1.65421
C	4.30740	0.53534	2.38259
H	4.05237	1.60827	2.39198
H	4.59015	0.26591	3.41661
H	5.19963	0.39637	1.75717
C	-3.87493	-1.00494	-0.48332
C	-3.67677	-1.38090	-1.97275
H	-2.65421	-1.71874	-2.20170
H	-4.36375	-2.20757	-2.22765
H	-3.91999	-0.54310	-2.64706
C	-3.86285	-2.27807	0.39797
H	-4.24416	-2.07709	1.40971
H	-4.52530	-3.03817	-0.05477
H	-2.85702	-2.70981	0.50794
C	-5.24832	-0.30846	-0.36283
H	-5.30479	0.62917	-0.94130
H	-6.01818	-0.98777	-0.77346
H	-5.53052	-0.09816	0.67980
C	-2.81574	1.11770	1.65156

C	-1.52260	1.75883	2.20978
H	-1.15271	2.57898	1.57485
H	-1.74909	2.18816	3.20325
H	-0.71825	1.01306	2.32869
C	-3.84558	2.24118	1.40535
H	-4.81052	1.87826	1.02429
H	-4.04450	2.75140	2.36578
H	-3.46064	3.00705	0.71087
C	-3.33254	0.11663	2.70951
H	-3.41729	0.64012	3.67902
H	-4.33078	-0.28009	2.47002
H	-2.63778	-0.72947	2.84713
C	-0.15481	-2.04112	0.87869
C	-0.30603	-2.88605	1.78533
H	-0.41590	-3.62190	2.56210
C	0.18616	-2.88561	-1.14029
C	0.26976	-2.09562	-2.44341
H	1.09727	-1.37545	-2.46736
H	0.44963	-2.83780	-3.25496
H	-0.66402	-1.57080	-2.69114
C	-0.98609	-3.84711	-1.14831
H	-0.83869	-4.50941	-2.02763
H	-1.02259	-4.46845	-0.24410
H	-1.95570	-3.35419	-1.28493
C	1.48440	-3.57719	-0.76772
H	1.34496	-4.27442	0.06929
H	1.81845	-4.15249	-1.65667
H	2.28659	-2.87661	-0.51256

$F_{C\text{-}tBu}$

SCF (BP86) Energy = -1315.36066149
Enthalpy 0K = -1314.620224
Enthalpy 298K = -1314.575252
Free Energy 298K = -1314.690048
Lowest Frequency = 18.8888 cm^{-1}
Second Frequency = 38.0231 cm^{-1}
SCF (BP86-D3BJ) Energy = -1315.655218
SCF (FB) Energy = -1315.471692
SCF (DFB) Energy = -1315.47812
SCF (BS2) Energy = -1985.027935

Rh	-0.07153	-0.50051	-0.06287
P	2.38526	-0.05216	0.25489
P	-2.41384	0.04537	0.02593
N	0.00089	1.69202	-0.49304
C	1.05315	2.44506	-0.04521
C	1.07778	3.84128	-0.20660
H	1.94499	4.40678	0.14551
C	-0.01899	4.49186	-0.78139
H	-0.01373	5.57681	-0.92221
C	-1.14549	3.73263	-1.12261
H	-2.04782	4.20924	-1.51505
C	-1.11723	2.33992	-0.95047
C	2.12173	1.74984	0.75520
H	3.06271	2.32284	0.74085
H	1.78629	1.71906	1.80885
C	-2.33699	1.49908	-1.19385
H	-3.24958	2.11766	-1.17542
H	-2.28489	1.01986	-2.18807
C	3.76772	0.25367	-1.15386
C	3.23615	1.36898	-2.08680
H	3.26298	2.36266	-1.61233
H	3.89217	1.41966	-2.97461
H	2.21086	1.19068	-2.44612
C	5.10555	0.74092	-0.55419
H	5.67124	-0.07673	-0.08351
H	5.72651	1.12691	-1.38364
H	4.99756	1.56006	0.17461
C	4.06900	-1.00215	-1.99981
H	3.22893	-1.29511	-2.64479
H	4.92202	-0.77026	-2.66361
H	4.36242	-1.87138	-1.38936
C	3.16500	-0.81782	1.87439
C	2.05739	-0.81543	2.95373
H	1.15224	-1.35072	2.63030
H	2.45321	-1.33323	3.84682
H	1.78845	0.20546	3.27843
C	3.55608	-2.27682	1.55220
H	4.35806	-2.33809	0.79736
H	3.93708	-2.75856	2.47088
H	2.68821	-2.86059	1.20486
C	4.37448	-0.04680	2.45047
H	4.17368	1.02989	2.58427
H	4.58739	-0.45704	3.45429
H	5.29027	-0.16066	1.85713
C	-4.10228	-0.80917	-0.53563
C	-4.23169	-0.75316	-2.07990
H	-3.34849	-1.10701	-2.63109
H	-5.07375	-1.40437	-2.37456
H	-4.47254	0.26245	-2.43445
C	-4.12356	-2.27045	-0.03481
H	-4.07914	-2.33412	1.06250
H	-5.07039	-2.74015	-0.35796
H	-3.29401	-2.86624	-0.43650
C	-5.34103	-0.06330	0.01437
H	-5.36785	0.99768	-0.28448
H	-6.23741	-0.54151	-0.42146
H	-5.44366	-0.12984	1.10659
C	-2.64395	0.78668	1.82461
C	-1.25404	1.22236	2.34978
H	-0.88480	2.13603	1.86060
H	-1.34289	1.43857	3.43053
H	-0.50251	0.41596	2.24284
C	-3.57485	2.01608	1.88390
H	-4.61956	1.79259	1.63244
H	-3.56584	2.40831	2.91768
H	-3.22258	2.83189	1.22955
C	-3.13739	-0.35471	2.74519
H	-3.13140	0.01050	3.78831
H	-4.16508	-0.67769	2.52372
H	-2.46936	-1.23168	2.69100
C	-0.30091	-2.14549	0.94838
C	-0.51226	-3.14043	1.65306
H	-0.65190	-3.99705	2.28751
C	0.09368	-1.90176	-1.75201
C	0.29052	-0.96047	-2.93749
H	1.20694	-0.35980	-2.86362
H	0.37023	-1.56450	-3.86641
H	-0.56558	-0.27843	-3.07644
C	-1.15825	-2.75163	-1.94566
H	-0.99899	-3.39859	-2.83288
H	-1.34050	-3.40306	-1.07985
H	-2.05269	-2.15272	-2.14620
C	1.26388	-2.86711	-1.52901
H	1.00879	-3.61325	-0.76328
H	1.46265	-3.40159	-2.48112
H	2.19310	-2.37668	-1.22629

9$_o$

SCF (BP86) Energy = -2617.37083069
Enthalpy 0K = -2616.080830
Enthalpy 298K = -2615.999755
Free Energy 298K = -2616.193459
Lowest Frequency = 10.7412 cm^{-1}
Second Frequency = 15.1242 cm^{-1}
SCF (BP86-D3BJ) Energy = -2617.80779
SCF (FB) Energy = -2617.495255
SCF (DFB) Energy = -2617.512123
SCF (BS2) Energy = -3956.582084

Rh	2.75469	-2.03675	1.15829
P	4.02833	-2.84698	-0.62848
P	2.03521	-1.69508	3.40281
N	4.07000	-3.33930	2.18531
C	1.20827	-1.38514	-0.27483
H	1.57293	-1.74683	-1.24618
C	1.87025	-0.24072	0.23584
H	2.71598	0.14022	-0.35437
C	1.17746	0.86858	1.01191
H	1.93826	1.51883	1.47564
H	0.56438	0.46110	1.83381
C	-0.25426	-1.73510	-0.07389
H	-0.56186	-1.59581	0.97481
H	-0.40269	-2.80580	-0.29933
C	5.13093	-3.92665	1.54600
C	6.02688	-4.79113	2.18866
H	6.85114	-5.22387	1.61994
C	5.81471	-5.07288	3.54332
H	6.49423	-5.74755	4.07198
C	4.73739	-4.49480	4.22333
H	4.53808	-4.68450	5.27898
C	3.89232	-3.63044	3.51195
O	5.31810	-3.66238	0.23748
O	2.85950	-3.06338	4.15618
C	3.34877	-4.37571	-1.61640
C	2.36767	-5.07739	-0.64650
H	2.88203	-5.47062	0.24627
H	1.90734	-5.93742	-1.16591
H	1.56425	-4.40361	-0.30410
C	4.46692	-5.36724	-2.00650
H	5.17173	-4.95178	-2.74071
H	3.99238	-6.25176	-2.46842
H	5.03939	-5.71291	-1.13322
C	2.59659	-3.91605	-2.88466
H	1.79902	-3.18288	-2.67564
H	2.11096	-4.79793	-3.34002
H	3.27466	-3.49344	-3.64296
C	5.16053	-1.68441	-1.66126
C	5.84130	-0.76199	-0.62112
H	5.10695	-0.23049	0.00831
H	6.44451	-0.00782	-1.15752
H	6.51972	-1.32478	0.03944
C	4.29654	-0.83946	-2.62447
H	3.82255	-1.44629	-3.41102
H	4.95247	-0.10628	-3.12694
H	3.51039	-0.26713	-2.10445
C	6.23554	-2.45407	-2.45689
H	6.81069	-3.14499	-1.82152
H	6.94570	-1.72145	-2.88109
H	5.80800	-3.01654	-3.30188
C	0.31764	-2.18071	4.15249
C	-0.05136	-3.51914	3.46825
H	-0.06310	-3.43661	2.36855
H	-1.06100	-3.82217	3.79938
H	0.64733	-4.32328	3.74708
C	-0.75115	-1.11545	3.82766
H	-0.54895	-0.14902	4.31381
H	-1.72485	-1.47659	4.20481
H	-0.86618	-0.94370	2.74514
C	0.38736	-2.38428	5.68163
H	1.17944	-3.08999	5.97276
H	-0.57665	-2.80648	6.01917
H	0.53356	-1.43760	6.22578
C	2.91679	-0.27113	4.41077
C	4.09703	0.20144	3.52861
H	4.83012	-0.60404	3.35561
H	4.62431	1.02339	4.04648
H	3.76468	0.56988	2.54439
C	3.47620	-0.77693	5.75924
H	2.69626	-1.15146	6.43743
H	3.97208	0.07396	6.26054
H	4.22886	-1.56868	5.62899
C	1.94880	0.90465	4.66693
H	2.52567	1.74348	5.09647
H	1.16498	0.64570	5.39658
H	1.46889	1.27836	3.74857
C	-1.20827	1.38514	0.27483
H	-1.57293	1.74683	1.24618
C	-1.87025	0.24072	-0.23584
H	-2.71598	-0.14022	0.35437
C	-1.17746	-0.86858	-1.01191
H	-1.93826	-1.51883	-1.47564
H	-0.56438	-0.46110	-1.83381
C	0.25426	1.73510	0.07389
H	0.56186	1.59581	-0.97481
H	0.40269	2.80580	0.29933
Rh	-2.75469	2.03675	-1.15829
P	-4.02833	2.84698	0.62848
P	-2.03521	1.69508	-3.40281
N	-4.07000	3.33930	-2.18531
C	-5.13093	3.92665	-1.54600
C	-6.02688	4.79113	-2.18866
H	-6.85114	5.22387	-1.61994
C	-5.81471	5.07288	-3.54332
H	-6.49423	5.74755	-4.07198
C	-4.73739	4.49480	-4.22333
H	-4.53808	4.68450	-5.27898
C	-3.89232	3.63044	-3.51195
O	-5.31810	3.66238	-0.23748
O	-2.85950	3.06338	-4.15618
C	-3.34877	4.37571	1.61640
C	-2.36767	5.07739	0.64650
H	-2.88203	5.47062	-0.24627
H	-1.90734	5.93742	1.16591
H	-1.56425	4.40361	0.30410
C	-4.46692	5.36724	2.00650
H	-5.17173	4.95178	2.74071
H	-3.99238	6.25176	2.46842
H	-5.03939	5.71291	1.13322
C	-2.59659	3.91605	2.88466
H	-1.79902	3.18288	2.67564
H	-2.11096	4.79793	3.34002
H	-3.27466	3.49344	3.64296
C	-5.16053	1.68441	1.66126
C	-5.84130	0.76199	0.62112

H	-5.10695	0.23049	-0.00831
H	-6.44451	0.00782	1.15752
H	-6.51972	1.32478	-0.03944
C	-4.29654	0.83946	2.62447
H	-3.82255	1.44629	3.41102
H	-4.95247	0.10628	3.12694
H	-3.51039	0.26713	2.10445
C	-6.23554	2.45407	2.45689
H	-6.81069	3.14499	1.82152
H	-6.94570	1.72145	2.88109
H	-5.80800	3.01654	3.30188
C	-0.31764	2.18071	-4.15249
C	0.05136	3.51914	-3.46825
H	0.06310	3.43661	-2.36855
H	1.06100	3.82217	-3.79938
H	-0.64733	4.32328	-3.74708
C	0.75115	1.11545	-3.82766
H	0.54895	0.14902	-4.31381
H	1.72485	1.47659	-4.20481
H	0.86618	0.94370	-2.74514
C	-0.38736	2.38428	-5.68163
H	-1.17944	3.08999	-5.97276
H	0.57665	2.80648	-6.01917
H	-0.53356	1.43760	-6.22578
C	-2.91679	0.27113	-4.41077
C	-4.09703	-0.20144	-3.52861
H	-4.83012	0.60404	-3.35561
H	-4.62431	-1.02339	-4.04648
H	-3.76468	-0.56988	-2.54439
C	-3.47620	0.77693	-5.75924
H	-2.69626	1.15146	-6.43743
H	-3.97208	-0.07396	-6.26054
H	-4.22886	1.56868	-5.62899
C	-1.94880	-0.90465	-4.66693
H	-2.52567	-1.74348	-5.09647
H	-1.16498	-0.64570	-5.39658
H	-1.46889	-1.27836	-3.74857

8_o

SCF (BP86) Energy = -1464.72451816
Enthalpy 0K = -1463.992143
Enthalpy 298K = -1463.947274
Free Energy 298K = -1464.064842
Lowest Frequency = 18.1088 cm^{-1}
Second Frequency = 26.4435 cm^{-1}
SCF (BP86-D3BJ) Energy = -1464.956261
SCF (FB) Energy = -1464.764617
SCF (DFB) Energy = -1464.770104
SCF (BS2) Energy = -2134.367708

C	2.88639	4.41089	0.38931
H	3.91954	4.70427	0.61640
C	2.45792	4.58215	-0.87857
H	3.17113	5.00425	-1.59832
C	1.08808	4.24106	-1.43343
H	0.98931	4.68412	-2.43839
H	0.29698	4.70964	-0.81449
C	2.09755	3.82691	1.54604
H	1.11198	4.32595	1.62989
H	2.62828	4.04105	2.48867
C	-0.01118	2.21116	-0.35481
H	-1.05488	2.54921	-0.41945
C	0.46227	1.96922	0.95543
H	-0.27317	2.07677	1.76619
C	1.87299	2.27690	1.42565
H	2.03641	1.80296	2.40879
H	2.62833	1.86678	0.73591
C	0.80480	2.69908	-1.53324
H	1.76003	2.15842	-1.61450
H	0.24389	2.48882	-2.46191
Rh	-0.14766	0.04047	0.06270
P	-2.46198	0.24957	0.09594
P	2.00287	-0.96863	-0.02790
N	-0.70209	-1.98116	-0.18091
C	-2.00834	-2.37612	-0.05518
C	-2.41885	-3.70850	-0.20104
H	-3.47518	-3.95595	-0.08742
C	-1.44580	-4.66935	-0.50035
H	-1.73568	-5.71683	-0.62438
C	-0.10534	-4.29629	-0.64163
H	0.68436	-5.01293	-0.87142
C	0.22834	-2.94352	-0.46926
O	-2.94041	-1.44128	0.21650
O	1.51212	-2.57596	-0.59463
C	-3.37750	0.66691	-1.56585
C	-2.41000	0.20126	-2.68079
H	-2.25570	-0.89075	-2.66155
H	-2.84895	0.45574	-3.66274
H	-1.42133	0.68352	-2.60317
C	-4.71427	-0.09316	-1.71155
H	-5.47669	0.23950	-0.99256
H	-5.10921	0.10279	-2.72493
H	-4.58764	-1.18077	-1.60512
C	-3.62850	2.18593	-1.68944
H	-2.71209	2.78915	-1.57985
H	-4.02860	2.39142	-2.69880
H	-4.37663	2.54719	-0.96607
C	-3.38551	0.86117	1.66811
C	-2.68940	0.13810	2.84654
H	-1.60119	0.31998	2.86055
H	-3.11370	0.51570	3.79417
H	-2.85758	-0.95018	2.81223
C	-3.20118	2.38941	1.81054
H	-3.71482	2.95516	1.01825
H	-3.63904	2.70538	2.77428
H	-2.14180	2.69359	1.82258
C	-4.88739	0.50926	1.65710
H	-5.06482	-0.55822	1.45331
H	-5.30586	0.73393	2.65498
H	-5.45137	1.11144	0.92738
C	3.31855	-0.74703	-1.43117
C	2.49270	-0.66174	-2.73763
H	1.74480	0.14770	-2.70541
H	3.17941	-0.45810	-3.57894
H	1.97059	-1.60799	-2.95062
C	4.13236	0.55151	-1.23833
H	4.75935	0.52993	-0.33422
H	4.81112	0.66340	-2.10304
H	3.50797	1.45815	-1.20260
C	4.28568	-1.94824	-1.51120
H	3.75471	-2.90877	-1.59066
H	4.90611	-1.83153	-2.41844
H	4.97487	-1.98907	-0.65279
C	2.80612	-1.53803	1.66208
C	1.70177	-1.36227	2.73151
H	0.81978	-1.98983	2.51939
H	2.10278	-1.67153	3.71427

H 1.35908 -0.31838 2.81214
C 3.23078 -3.02336 1.62987
H 3.99624 -3.23627 0.87003
H 3.66220 -3.27306 2.61635
H 2.37872 -3.69823 1.45884
C 4.02903 -0.66520 2.01945
H 4.34738 -0.91644 3.04748
H 4.88777 -0.86300 1.35849
H 3.81260 0.41384 2.00162

A_O

SCF (BP86) Energy = -1152.65482641
Enthalpy 0K = -1152.100117
Enthalpy 298K = -1152.063943
Free Energy 298K = -1152.164526
Lowest Frequency = 20.3372 cm^{-1}
Second Frequency = 31.2022 cm^{-1}
SCF (BP86-D3BJ) Energy = -1152.821592
SCF (FB) Energy = -1152.703619
SCF (DFB) Energy = -1152.711718
SCF (BS2) Energy = -1822.227633

Rh 0.00000 -0.57528 0.10578
P 2.28202 -0.30044 0.05120
P -2.28202 -0.30044 0.05120
N 0.00000 1.40174 -0.13732
C 1.18250 2.10813 -0.22983
C 1.21181 3.49636 -0.41054
H 2.18071 3.99385 -0.47595
C 0.00000 4.18928 -0.50024
H 0.00000 5.27348 -0.64204
C -1.21181 3.49636 -0.41054
H -2.18070 3.99386 -0.47595
C -1.18250 2.10813 -0.22983
O 2.35554 1.44590 -0.13995
O -2.35554 1.44590 -0.13995
C 3.17744 -0.89649 -1.53424
C 2.48271 -0.16531 -2.70695
H 2.70280 0.91407 -2.70594
H 2.85585 -0.58686 -3.65734
H 1.38712 -0.30228 -2.68050
C 4.69260 -0.62389 -1.56772
H 5.24288 -1.21371 -0.81742
H 5.08232 -0.91628 -2.55963
H 4.92613 0.44315 -1.42265
C 2.88591 -2.41426 -1.63367
H 1.80002 -2.62038 -1.64221
H 3.30039 -2.79611 -2.58386
H 3.34694 -2.99452 -0.81803
C 3.30022 -0.47383 1.66478
C 2.35315 0.00896 2.79008
H 1.41181 -0.56697 2.81393
H 2.86167 -0.11792 3.76275
H 2.09951 1.07681 2.68311
C 3.62729 -1.97084 1.86476
H 4.35449 -2.34536 1.12608
H 4.07754 -2.10634 2.86421
H 2.72567 -2.60832 1.82651
C 4.58258 0.38407 1.67322
H 4.36707 1.44339 1.46291
H 5.03153 0.32788 2.68139
H 5.33823 0.03102 0.95727
C -3.17744 -0.89649 -1.53424
C -2.48270 -0.16533 -2.70695
H -1.38711 -0.30230 -2.68049
H -2.85584 -0.58687 -3.65734
H -2.70278 0.91407 -2.70595
C -2.88593 -2.41426 -1.63366
H -3.34696 -2.99452 -0.81801
H -3.30041 -2.79611 -2.58384
H -1.80004 -2.62039 -1.64220
C -4.69260 -0.62387 -1.56772
H -4.92612 0.44317 -1.42267
H -5.08232 -0.91627 -2.55963
H -5.24288 -1.21368 -0.81741
C -3.30022 -0.47383 1.66478
C -2.35315 0.00897 2.79008
H -2.09952 1.07682 2.68311
H -2.86167 -0.11792 3.76275
H -1.41181 -0.56697 2.81393
C -4.58259 0.38407 1.67322
H -5.33823 0.03101 0.95727
H -5.03153 0.32788 2.68139
H -4.36707 1.44339 1.46291
C -3.62729 -1.97084 1.86476
H -4.07754 -2.10634 2.86421
H -4.35448 -2.34536 1.12607
H -2.72566 -2.60832 1.82652

$B_{O\text{-}tBu}$

SCF (BP86) Energy = -1387.29807486
Enthalpy 0K = -1386.604571
Enthalpy 298K = -1386.559577
Free Energy 298K = -1386.676898
Lowest Frequency = 23.1101 cm^{-1}
Second Frequency = 27.6162 cm^{-1}
SCF (BP86-D3BJ) Energy = -1387.516554
SCF (FB) Energy = -1387.33849
SCF (DFB) Energy = -1387.34399
SCF (BS2) Energy = -2056.924554

Rh -0.00009 0.11249 0.16550
P 2.31227 -0.24084 0.06419
P -2.31223 -0.24083 0.06424
N -0.00004 -1.96299 -0.13477
C 1.17566 -2.66846 -0.19393
C 1.21442 -4.06231 -0.34477
H 2.18109 -4.56593 -0.38812
C -0.00006 -4.75291 -0.42207
H -0.00007 -5.84075 -0.53701
C -1.21454 -4.06233 -0.34438
H -2.18121 -4.56598 -0.38741
C -1.17576 -2.66850 -0.19342
O 2.34072 -2.00217 -0.09444
O -2.34079 -2.00227 -0.09308
C 3.42012 -0.10083 1.62579
C 2.65270 -0.86331 2.73277
H 2.61629 -1.94612 2.53249
H 3.17837 -0.71541 3.69310
H 1.61890 -0.49671 2.84892
C 4.82175 -0.71794 1.45040
H 5.45783 -0.12295 0.77615
H 5.32212 -0.73552 2.43570
H 4.77912 -1.75440 1.07985
C 3.52882 1.39548 2.00029
H 2.54108 1.87201 2.10772

H	4.05204	1.47779	2.97003
H	4.11288	1.97146	1.26514
C	3.21837	0.15409	-1.59349
C	2.12374	0.01428	-2.67907
H	1.26205	0.67533	-2.48339
H	2.55331	0.28765	-3.66000
H	1.75445	-1.02227	-2.75806
C	3.73747	1.60620	-1.55175
H	4.58689	1.72517	-0.85993
H	4.09444	1.88715	-2.55892
H	2.95127	2.32616	-1.26943
C	4.37087	-0.82068	-1.91438
H	4.04066	-1.87029	-1.89841
H	4.73541	-0.59694	-2.93352
H	5.22452	-0.71285	-1.23040
C	-3.42081	-0.09994	1.62524
C	-2.65398	-0.86188	2.73301
H	-1.62026	-0.49523	2.84962
H	-3.18021	-0.71356	3.69297
H	-2.61742	-1.94477	2.53321
C	-3.52984	1.39655	1.99894
H	-4.11360	1.97209	1.26319
H	-4.05355	1.47930	2.96836
H	-2.54221	1.87325	2.10660
C	-4.82235	-0.71718	1.44949
H	-4.77954	-1.75373	1.07923
H	-5.32306	-0.73450	2.43462
H	-5.45821	-0.12240	0.77485
C	-3.21746	0.15336	-1.59410
C	-2.12240	0.01254	-2.67913
H	-1.75348	-1.02419	-2.75748
H	-2.55143	0.28562	-3.66037
H	-1.26053	0.67334	-2.48336
C	-4.37016	-0.82121	-1.91484
H	-5.22415	-0.71243	-1.23144
H	-4.73404	-0.59820	-2.93438
H	-4.04041	-1.87095	-1.89779
C	-3.73600	1.60570	-1.55356
H	-4.09264	1.88601	-2.56102
H	-4.58551	1.72557	-0.86201
H	-2.94954	2.32554	-1.27164
C	-0.00043	1.64620	1.59599
H	-0.00094	1.51156	2.67265
C	-0.00010	2.32205	0.51974
C	0.00008	3.64548	-0.19993
C	0.00067	3.49674	-1.73695
C	1.26031	4.43723	0.24791
H	1.26279	4.59359	1.33888
H	2.19013	3.91306	-0.02646
H	1.27009	5.42589	-0.24270
H	0.89281	2.95519	-2.09094
H	0.00052	4.49394	-2.20847
H	-0.89085	2.95458	-2.09156
C	-1.26065	4.43698	0.24694
H	-1.26407	4.59320	1.33793
H	-1.27013	5.42570	-0.24355
H	-2.19017	3.91272	-0.02830

TS(B-10)$_{o\text{-}tBu}$

SCF (BP86) Energy = -1387.22856413
Enthalpy 0K = -1386.538460
Enthalpy 298K = -1386.493833
Free Energy 298K = -1386.611358
Lowest Frequency = -590.3387 cm^{-1}
Second Frequency = 12.6015 cm^{-1}
SCF (BP86-D3BJ) Energy = -1387.44418
SCF (FB) Energy = -1387.26948
SCF (DFB) Energy = -1387.275165
SCF (BS2) Energy = -2056.854194

Rh	0.02479	0.11215	0.11548
P	2.32986	-0.24047	0.06198
P	-2.29041	-0.28628	0.08266
N	0.05166	-1.88661	-0.49136
C	1.23168	-2.55248	-0.71215
C	1.28804	-3.90042	-1.09027
H	2.26133	-4.36435	-1.25577
C	0.08401	-4.60018	-1.22908
H	0.09649	-5.65455	-1.51971
C	-1.13395	-3.95801	-0.98618
H	-2.09510	-4.46702	-1.07010
C	-1.11078	-2.60554	-0.61333
O	2.39186	-1.88189	-0.56448
O	-2.28129	-1.99282	-0.37085
C	3.21411	-0.53576	1.74833
C	2.32305	-1.55540	2.49723
H	2.32367	-2.54307	2.00823
H	2.72313	-1.68802	3.51850
H	1.28233	-1.19935	2.58372
C	4.64053	-1.09971	1.59596
H	5.34966	-0.34519	1.22034
H	5.00011	-1.41336	2.59271
H	4.67450	-1.98173	0.93701
C	3.23630	0.79014	2.54160
H	2.21829	1.16451	2.74114
H	3.71238	0.60200	3.52082
H	3.82399	1.57902	2.04397
C	3.44506	0.55717	-1.28725
C	2.52883	0.67283	-2.52941
H	1.59596	1.21734	-2.31264
H	3.07278	1.21038	-3.32723
H	2.25991	-0.32187	-2.92213
C	3.88489	1.95462	-0.79958
H	4.62932	1.89570	0.01105
H	4.35640	2.49804	-1.63806
H	3.03738	2.56905	-0.44843
C	4.67845	-0.29361	-1.65948
H	4.40052	-1.32392	-1.92875
H	5.15691	0.16637	-2.54319
H	5.43228	-0.32987	-0.86068
C	-3.15083	-0.47661	1.79227
C	-2.18591	-1.33529	2.64459
H	-1.18926	-0.86909	2.71998
H	-2.60089	-1.42010	3.66515
H	-2.07627	-2.35594	2.24316
C	-3.27743	0.92328	2.43361
H	-3.98139	1.57783	1.89669
H	-3.66095	0.80245	3.46278
H	-2.29759	1.42753	2.50803
C	-4.52286	-1.17445	1.70114
H	-4.45634	-2.15147	1.19619
H	-4.89350	-1.35386	2.72660
H	-5.27910	-0.55944	1.18805
C	-3.50349	0.30145	-1.31134
C	-2.59531	0.71293	-2.49336
H	-1.98639	-0.13285	-2.85514
H	-3.22678	1.05499	-3.33331
H	-1.90651	1.53008	-2.22374

C	-4.45203	-0.82657	-1.77540
H	-5.10450	-1.19459	-0.97016
H	-5.10227	-0.41642	-2.56948
H	-3.90463	-1.68268	-2.19570
C	-4.33790	1.50678	-0.82675
H	-4.86072	1.94656	-1.69516
H	-5.10941	1.20945	-0.09917
H	-3.72859	2.30378	-0.37368
C	-0.05061	1.66566	1.53192
H	1.04852	2.34620	1.20049
C	0.04980	2.41680	0.44161
C	-0.11334	3.76695	-0.24321
C	0.43499	3.77180	-1.68627
C	0.64765	4.81393	0.61788
H	0.25564	4.84893	1.64739
H	1.72916	4.59584	0.65982
H	0.52607	5.81286	0.16711
H	1.52091	3.59102	-1.71375
H	0.24727	4.75749	-2.14414
H	-0.05961	3.00622	-2.30599
C	-1.61877	4.12854	-0.26314
H	-2.05911	4.09085	0.74622
H	-1.73405	5.15335	-0.65435
H	-2.18067	3.45605	-0.92843

TS(B-C)$_{O\text{-}tBu}$

SCF (BP86) Energy = -1387.28468888
Enthalpy 0K = -1386.593586
Enthalpy 298K = -1386.548514
Free Energy 298K = -1386.668911
Lowest Frequency = -136.0195 cm^{-1}
Second Frequency = 12.9844 cm^{-1}
SCF (BP86-D3BJ) Energy = -1387.495595
SCF (FB) Energy = -1387.324574
SCF (DFB) Energy = -1387.329988
SCF (BS2) Energy = -2056.911156

Rh	0.00002	-0.04585	0.20532
P	2.28076	-0.38253	0.09431
P	-2.28069	-0.38276	0.09430
N	0.00012	-2.04369	-0.38977
C	1.17306	-2.72738	-0.57959
C	1.21328	-4.07716	-0.95569
H	2.18133	-4.56205	-1.08988
C	0.00026	-4.74976	-1.14274
H	0.00031	-5.80363	-1.43499
C	-1.21284	-4.07727	-0.95576
H	-2.18084	-4.56224	-1.08999
C	-1.17276	-2.72748	-0.57965
O	2.34170	-2.07214	-0.40084
O	-2.34145	-2.07234	-0.40096
C	3.28246	-0.52890	1.72828
C	2.46416	-1.50056	2.61290
H	2.45228	-2.52162	2.19905
H	2.93006	-1.54742	3.61360
H	1.42017	-1.16281	2.73649
C	4.70836	-1.08073	1.53251
H	5.37233	-0.35395	1.03834
H	5.14390	-1.29485	2.52543
H	4.71538	-2.01940	0.95607
C	3.32679	0.86088	2.40210
H	2.31938	1.28236	2.55377
H	3.79608	0.75627	3.39675
H	3.92352	1.59087	1.83294
C	3.26707	0.36088	-1.37904
C	2.25143	0.39800	-2.54684
H	1.34807	0.97680	-2.28864
H	2.73154	0.86867	-3.42420
H	1.93354	-0.61512	-2.84477
C	3.69140	1.79830	-1.00915
H	4.49977	1.81460	-0.26026
H	4.07439	2.30390	-1.91398
H	2.84555	2.39472	-0.62470
C	4.48853	-0.48230	-1.79975
H	4.21346	-1.52913	-2.00072
H	4.89985	-0.05674	-2.73317
H	5.29380	-0.47041	-1.05137
C	-3.28235	-0.52935	1.72828
C	-2.46395	-1.50101	2.61280
H	-1.41998	-1.16319	2.73637
H	-2.92981	-1.54796	3.61352
H	-2.45201	-2.52204	2.19889
C	-3.32678	0.86037	2.40221
H	-3.92356	1.59037	1.83311
H	-3.79608	0.75565	3.39684
H	-2.31940	1.28191	2.55393
C	-4.70821	-1.08129	1.53249
H	-4.71516	-2.01991	0.95596
H	-5.14371	-1.29553	2.52540
H	-5.37225	-0.35452	1.03840
C	-3.26709	0.36065	-1.37898
C	-2.25148	0.39794	-2.54680
H	-1.93350	-0.61513	-2.84480
H	-2.73164	0.86863	-3.42412
H	-1.34817	0.97680	-2.28857
C	-4.48848	-0.48262	-1.79973
H	-5.29374	-0.47086	-1.05134
H	-4.89985	-0.05703	-2.73311
H	-4.21332	-1.52941	-2.00077
C	-3.69156	1.79800	-1.00900
H	-4.07462	2.30362	-1.91378
H	-4.49991	1.81417	-0.26008
H	-2.84575	2.39448	-0.62453
C	-0.00009	1.86496	1.02429
H	-0.00005	1.51912	2.07305
C	-0.00018	3.01029	0.49365
C	-0.00032	4.33446	-0.13206
C	-0.00055	4.14409	-1.68134
C	1.27296	5.11995	0.29608
H	1.30549	5.26061	1.38844
H	2.19107	4.59793	-0.01705
H	1.26102	6.11582	-0.17789
H	0.89517	3.59956	-2.01921
H	-0.00066	5.14192	-2.15143
H	-0.89632	3.59949	-2.01894
C	-1.27354	5.11983	0.29646
H	-1.30577	5.26048	1.38883
H	-1.26182	6.11571	-0.17750
H	-2.19170	4.59774	-0.01641

C$_{O\text{-}tBu}$

SCF (BP86) Energy = -1387.29375677
Enthalpy 0K = -1386.601980
Enthalpy 298K = -1386.556743
Free Energy 298K = -1386.678182
Lowest Frequency = 9.7432 cm^{-1}
Second Frequency = 19.2155 cm^{-1}

SCF (BP86-D3BJ) Energy = -1387.501871
SCF (FB) Energy = -1387.333129
SCF (DFB) Energy = -1387.338486
SCF (BS2) Energy = -2056.922584

Rh	-0.00011	-0.10366	0.10463
P	2.28958	-0.43326	0.06845
P	-2.29003	-0.43159	0.06841
N	-0.00085	-2.14190	-0.25206
C	1.17756	-2.83356	-0.38757
C	1.21393	-4.20990	-0.65014
H	2.17975	-4.70815	-0.74463
C	-0.00184	-4.89147	-0.78000
H	-0.00223	-5.96589	-0.98492
C	-1.21712	-4.20899	-0.65027
H	-2.18330	-4.70652	-0.74487
C	-1.17976	-2.83267	-0.38770
O	2.34411	-2.16650	-0.26170
O	-2.34582	-2.16475	-0.26196
C	3.24545	-0.39615	1.73028
C	2.47180	-1.35054	2.67093
H	2.55443	-2.40113	2.34972
H	2.90326	-1.27227	3.68481
H	1.40227	-1.08406	2.73358
C	4.71232	-0.85312	1.60950
H	5.33040	-0.12890	1.05557
H	5.14010	-0.93609	2.62499
H	4.80294	-1.84058	1.12924
C	3.16491	1.04496	2.28496
H	2.12282	1.38469	2.40582
H	3.63835	1.06282	3.28289
H	3.69642	1.77568	1.65541
C	3.28045	0.18231	-1.45392
C	2.27797	0.10823	-2.63139
H	1.37727	0.71565	-2.44103
H	2.77120	0.49335	-3.54224
H	1.96400	-0.92880	-2.83893
C	3.67907	1.65309	-1.20082
H	4.46503	1.74568	-0.43350
H	4.08599	2.07530	-2.13724
H	2.81439	2.27161	-0.90373
C	4.51521	-0.68397	-1.77807
H	4.25171	-1.74656	-1.89584
H	4.93987	-0.33483	-2.73663
H	5.30675	-0.60179	-1.01952
C	-3.24576	-0.39399	1.73032
C	-2.47282	-1.34916	2.67077
H	-1.40305	-1.08361	2.73332
H	-2.90410	-1.27065	3.68471
H	-2.55640	-2.39963	2.34943
C	-3.16402	1.04696	2.28522
H	-3.69487	1.77824	1.65577
H	-3.63749	1.06507	3.28314
H	-2.12164	1.38579	2.40620
C	-4.71301	-0.84973	1.60958
H	-4.80446	-1.83706	1.12920
H	-5.14079	-0.93248	2.62508
H	-5.33052	-0.12495	1.05576
C	-3.28059	0.18486	-1.45380
C	-2.27827	0.11021	-2.63135
H	-1.96505	-0.92701	-2.83905
H	-2.77128	0.49580	-3.54212
H	-1.37711	0.71697	-2.44099
C	-4.51599	-0.68051	-1.77794
H	-5.30741	-0.59786	-1.01933
H	-4.94048	-0.33096	-2.73643
H	-4.25324	-1.74327	-1.89586
C	-3.67815	1.65590	-1.20048
H	-4.08487	2.07850	-2.13680
H	-4.46395	1.74896	-0.43306
H	-2.81300	2.27378	-0.90343
C	0.00066	1.92279	0.21355
H	0.00034	1.25213	1.21864
C	0.00129	3.16668	0.11172
C	0.00212	4.62577	-0.08430
C	0.00422	4.91551	-1.61454
C	1.27220	5.24338	0.56350
H	1.29971	5.05052	1.64844
H	2.18983	4.83173	0.11230
H	1.27217	6.33575	0.40891
H	0.89923	4.49367	-2.09986
H	0.00488	6.00711	-1.77505
H	-0.88988	4.49442	-2.10216
C	-1.26908	5.24450	0.56021
H	-1.29955	5.05168	1.64508
H	-1.26771	6.33687	0.40562
H	-2.18590	4.83364	0.10665

TS(C-D)$_{o\text{-}tBu}$
SCF (BP86) Energy = -1387.22994128
Enthalpy 0K = -1386.540024
Enthalpy 298K = -1386.495682
Free Energy 298K = -1386.612452
Lowest Frequency = -48.4631 cm^{-1}
Second Frequency = 16.1993 cm^{-1}
SCF (BP86-D3BJ) Energy = -1387.444468
SCF (FB) Energy = -1387.271412
SCF (DFB) Energy = -1387.277305
SCF (BS2) Energy = -2056.856196

Rh	0.00004	0.05567	0.02913
P	-2.31985	-0.28585	-0.00464
P	2.31990	-0.28566	-0.00481
N	0.00011	-2.01684	-0.09852
C	-1.17973	-2.72321	-0.10544
C	-1.21493	-4.12464	-0.12799
H	-2.18123	-4.63070	-0.13362
C	0.00025	-4.81813	-0.13959
H	0.00031	-5.91193	-0.15458
C	1.21536	-4.12449	-0.12896
H	2.18173	-4.63044	-0.13535
C	1.18002	-2.72307	-0.10637
O	-2.34251	-2.05156	-0.10090
O	2.34272	-2.05127	-0.10274
C	-3.32338	0.06976	-1.61398
C	-2.28534	0.04275	-2.76128
H	-1.79425	-0.94091	-2.85111
H	-2.80472	0.24360	-3.71584
H	-1.50079	0.80648	-2.62985
C	-4.40515	-0.99831	-1.88473
H	-5.19082	-1.01527	-1.11597
H	-4.88915	-0.75510	-2.84795
H	-3.97774	-2.00867	-1.96796
C	-3.96401	1.47042	-1.51710
H	-3.23597	2.25308	-1.24906
H	-4.38170	1.73565	-2.50493

H	-4.79406	1.49868	-0.79347
C	-3.32192	-0.09004	1.62240
C	-2.46789	-0.78731	2.70863
H	-1.46048	-0.34387	2.77676
H	-2.96655	-0.64545	3.68424
H	-2.38176	-1.87258	2.53558
C	-3.43538	1.41485	1.95551
H	-4.05430	1.96645	1.23065
H	-3.92171	1.51156	2.94293
H	-2.44310	1.89010	2.02155
C	-4.71638	-0.74345	1.54130
H	-4.66831	-1.79785	1.22561
H	-5.16901	-0.71717	2.54898
H	-5.39685	-0.19797	0.86796
C	3.32361	0.07158	-1.61363
C	2.28570	0.04615	-2.76108
H	1.50145	0.81008	-2.62898
H	2.80528	0.24775	-3.71538
H	1.79420	-0.93722	-2.85196
C	3.96450	1.47200	-1.51500
H	4.79469	1.49911	-0.79149
H	4.38206	1.73849	-2.50255
H	3.23667	2.25444	-1.24575
C	4.40518	-0.99640	-1.88553
H	3.97748	-2.00648	-1.97058
H	4.88973	-0.75180	-2.84812
H	5.19046	-1.01483	-1.11641
C	3.32171	-0.09131	1.62260
C	2.46742	-0.78954	2.70802
H	2.38121	-1.87464	2.53396
H	2.96592	-0.64866	3.68385
H	1.46005	-0.34605	2.77640
C	4.71612	-0.74478	1.54114
H	5.39676	-0.19878	0.86839
H	5.16861	-0.71940	2.54891
H	4.66800	-1.79890	1.22453
C	3.43523	1.41323	1.95722
H	3.92140	1.50891	2.94482
H	4.05431	1.96550	1.23302
H	2.44296	1.88848	2.02358
C	0.00047	1.67308	1.43215
H	-0.00027	1.68640	-0.58794
C	0.00004	2.50752	0.42473
C	-0.00031	3.94521	-0.06708
C	-0.00090	4.83362	1.20542
C	-1.26297	4.24045	-0.90975
H	-1.30092	3.60974	-1.81536
H	-2.18026	4.07320	-0.32159
H	-1.25768	5.29382	-1.23830
H	-0.89451	4.64587	1.82185
H	-0.00096	5.89571	0.90652
H	0.89233	4.64616	1.82249
C	1.26253	4.24130	-0.90921
H	1.30141	3.61044	-1.81467
H	1.25654	5.29459	-1.23797
H	2.17967	4.07490	-0.32057

$D_{O\text{-}tBu}$

SCF (BP86) Energy = -1387.23016835
Enthalpy 0K = -1386.539397
Enthalpy 298K = -1386.494342
Free Energy 298K = -1386.612997
Lowest Frequency = 20.1225 cm^{-1}
Second Frequency = 21.2946 cm^{-1}

SCF (BP86-D3BJ) Energy = -1387.445262
SCF (FB) Energy = -1387.272307
SCF (DFB) Energy = -1387.278507
SCF (BS2) Energy = -2056.856702

Rh	-0.00001	0.06477	-0.02880
P	-2.32579	-0.27632	-0.03406
P	2.32571	-0.27651	-0.03399
N	-0.00009	-1.99756	0.11217
C	-1.18032	-2.70298	0.16875
C	-1.21478	-4.09872	0.29607
H	-2.18151	-4.60203	0.34045
C	-0.00023	-4.78965	0.36197
H	-0.00028	-5.87879	0.46369
C	1.21440	-4.09881	0.29651
H	2.18107	-4.60219	0.34123
C	1.18009	-2.70306	0.16919
O	-2.34457	-2.03848	0.09343
O	2.34439	-2.03863	0.09442
C	-3.25397	-0.12195	-1.71741
C	-2.17354	-0.36117	-2.79957
H	-1.74117	-1.37411	-2.73489
H	-2.63946	-0.26347	-3.79693
H	-1.35074	0.37103	-2.73200
C	-4.37739	-1.16724	-1.88396
H	-5.20770	-1.01766	-1.17941
H	-4.78810	-1.06769	-2.90507
H	-4.00469	-2.19648	-1.77032
C	-3.81877	1.30854	-1.84907
H	-3.05790	2.08481	-1.66325
H	-4.18605	1.44930	-2.88148
H	-4.67065	1.48313	-1.17279
C	-3.38963	0.11420	1.51732
C	-2.58589	-0.44978	2.71349
H	-1.57863	-0.00406	2.76963
H	-3.12551	-0.18927	3.64175
H	-2.50479	-1.54841	2.67527
C	-3.51223	1.64819	1.66104
H	-4.09066	2.10783	0.84410
H	-4.04934	1.86160	2.60273
H	-2.52272	2.12831	1.72228
C	-4.78326	-0.54303	1.45373
H	-4.72974	-1.62556	1.25671
H	-5.27163	-0.40678	2.43547
H	-5.43508	-0.07209	0.70069
C	3.25352	-0.12306	-1.71763
C	2.17281	-0.36290	-2.79939
H	1.34983	0.36912	-2.73182
H	2.63840	-0.26544	-3.79692
H	1.74071	-1.37594	-2.73423
C	3.81820	1.30739	-1.85016
H	4.67026	1.48236	-1.17420
H	4.18518	1.44767	-2.88273
H	3.05733	2.08369	-1.66449
C	4.37694	-1.16838	-1.88391
H	4.00439	-2.19757	-1.76935
H	4.78721	-1.06955	-2.90526
H	5.20754	-1.01820	-1.17983
C	3.38991	0.11462	1.51698
C	2.58654	-0.44897	2.71358
H	2.50559	-1.54762	2.67581
H	3.12635	-0.18799	3.64160
H	1.57923	-0.00337	2.76979

C	4.78356	-0.54255	1.45323
H	5.43513	-0.07183	0.69984
H	5.27219	-0.40592	2.43479
H	4.73007	-1.62515	1.25661
C	3.51248	1.64867	1.66004
H	4.05001	1.86251	2.60140
H	4.09050	2.10803	0.84264
H	2.52296	2.12874	1.72154
C	0.00008	1.62175	1.46138
H	-0.00116	1.71522	-0.62866
C	-0.00013	2.42344	0.41612
C	0.00038	3.88810	-0.01737
C	0.00113	4.73477	1.28065
C	-1.26149	4.20841	-0.85225
H	-1.28375	3.62182	-1.78818
H	-2.18158	3.99991	-0.28187
H	-1.26836	5.27603	-1.13148
H	-0.89141	4.52722	1.89248
H	0.00146	5.80659	1.01879
H	0.89393	4.52653	1.89188
C	1.26193	4.20739	-0.85308
H	1.28313	3.62073	-1.78899
H	1.26940	5.27499	-1.13238
H	2.18224	3.99825	-0.28329

TS(C-10)$_{O\text{-}tBu}$

SCF (BP86) Energy = -1387.27797551
Enthalpy 0K = -1386.588668
Enthalpy 298K = -1386.543222
Free Energy 298K = -1386.665148
Lowest Frequency = -743.9309 cm^{-1}
Second Frequency = 13.7542 cm^{-1}
SCF (BP86-D3BJ) Energy = -1387.48558
SCF (FB) Energy = -1387.317865
SCF (DFB) Energy = -1387.323448
SCF (BS2) Energy = -2056.905489

Rh	0.00204	-0.08086	0.04590
P	2.28143	-0.40518	0.01550
P	-2.27223	-0.44132	0.02910
N	0.01829	-2.16194	-0.05271
C	1.19825	-2.85383	-0.14084
C	1.24830	-4.25278	-0.21867
H	2.21776	-4.74871	-0.28394
C	0.03944	-4.95880	-0.20994
H	0.04775	-6.05090	-0.27048
C	-1.18000	-4.27638	-0.12588
H	-2.14187	-4.79097	-0.11887
C	-1.15123	-2.87672	-0.04956
O	2.35863	-2.16107	-0.15617
O	-2.32188	-2.20693	0.03571
C	3.26413	-0.22664	1.65732
C	2.49289	-1.08720	2.68654
H	2.56974	-2.16295	2.46174
H	2.93010	-0.91987	3.68733
H	1.42422	-0.81200	2.72845
C	4.72672	-0.70296	1.56709
H	5.34841	-0.02885	0.95658
H	5.15977	-0.71235	2.58389
H	4.80656	-1.72450	1.16239
C	3.19991	1.25566	2.08930
H	2.15806	1.59886	2.20519
H	3.69595	1.36073	3.07092
H	3.71413	1.92994	1.38606
C	3.26910	0.06835	-1.56129
C	2.26862	-0.13128	-2.72581
H	1.35196	0.46667	-2.58633
H	2.75255	0.18128	-3.66907
H	1.97695	-1.18926	-2.83584
C	3.65469	1.56036	-1.45687
H	4.43837	1.73712	-0.70194
H	4.05806	1.89332	-2.43015
H	2.78469	2.19813	-1.22192
C	4.51363	-0.80999	-1.80670
H	4.26285	-1.88209	-1.80984
H	4.92618	-0.55846	-2.80059
H	5.31024	-0.63938	-1.06849
C	-3.30355	-0.14127	1.62167
C	-2.33331	-0.44987	2.78761
H	-1.42041	0.16790	2.73970
H	-2.84721	-0.24364	3.74403
H	-2.02757	-1.50936	2.79413
C	-3.71127	1.34780	1.66129
H	-4.48196	1.58884	0.91110
H	-4.13886	1.57546	2.65425
H	-2.85081	2.02290	1.50890
C	-4.54091	-1.05530	1.74049
H	-4.27392	-2.11888	1.64240
H	-4.98585	-0.91105	2.74173
H	-5.31792	-0.82015	0.99934
C	-3.21874	-0.11749	-1.61110
C	-2.38784	-0.83888	-2.69958
H	-2.42661	-1.93444	-2.58831
H	-2.80705	-0.58632	-3.69016
H	-1.33082	-0.51964	-2.68312
C	-4.66535	-0.64681	-1.62041
H	-5.32856	-0.06122	-0.96401
H	-5.06699	-0.56117	-2.64650
H	-4.72178	-1.70772	-1.32872
C	-3.18793	1.40466	-1.87775
H	-3.62440	1.59721	-2.87445
H	-3.77961	1.97589	-1.14442
H	-2.15696	1.79507	-1.87684
C	-0.01533	1.88808	0.06768
H	0.02882	2.17273	1.21459
C	-0.02879	3.16262	0.02786
C	-0.04652	4.63499	-0.00994
C	-0.13340	5.00922	-1.52411
C	1.25641	5.21745	0.60029
H	1.34951	4.95439	1.66700
H	2.14719	4.84683	0.06837
H	1.23799	6.31732	0.52217
H	0.73694	4.63204	-2.08434
H	-0.14831	6.10907	-1.60553
H	-1.05272	4.61498	-1.98554
C	-1.28929	5.18762	0.73846
H	-1.25866	4.92579	1.80923
H	-1.30613	6.28742	0.65885
H	-2.22322	4.79416	0.30640

TS(C-E)$_{O\text{-}tBu}$

SCF (BP86) Energy = -1387.28865618
Enthalpy 0K = -1386.598844
Enthalpy 298K = -1386.553762
Free Energy 298K = -1386.675244
Lowest Frequency = -628.8056 cm^{-1}
Second Frequency = 5.9072 cm^{-1}

SCF (BP86-D3BJ) Energy = -1387.498408
SCF (FB) Energy = -1387.329755
SCF (DFB) Energy = -1387.335665
SCF (BS2) Energy = -2056.91727

Rh	0.00016	-0.09021	-0.00391
P	-2.29534	-0.42468	-0.02704
P	2.29569	-0.42427	-0.02716
N	0.00029	-2.18115	0.04911
C	-1.17999	-2.87807	0.07563
C	-1.21760	-4.27818	0.12923
H	-2.18176	-4.78816	0.14693
C	0.00055	-4.96925	0.15576
H	0.00065	-6.06235	0.19701
C	1.21857	-4.27797	0.12865
H	2.18282	-4.78780	0.14592
C	1.18072	-2.87786	0.07509
O	-2.34344	-2.19102	0.04706
O	2.34404	-2.19064	0.04603
C	-3.26802	-0.14048	-1.65078
C	-2.48912	-0.91415	-2.74132
H	-2.52381	-2.00343	-2.57923
H	-2.95709	-0.70401	-3.71945
H	-1.43339	-0.59847	-2.79669
C	-4.72157	-0.64980	-1.58504
H	-5.34698	-0.03768	-0.91648
H	-5.16300	-0.58140	-2.59555
H	-4.78156	-1.70278	-1.26621
C	-3.22634	1.37388	-1.96038
H	-2.19872	1.77360	-1.96296
H	-3.65559	1.53600	-2.96521
H	-3.82256	1.96579	-1.24862
C	-3.23750	-0.02782	1.59258
C	-2.20926	-0.30251	2.71768
H	-1.30799	0.32568	2.60980
H	-2.67442	-0.06179	3.69060
H	-1.90572	-1.36281	2.75186
C	-3.59535	1.47495	1.57255
H	-4.40625	1.69890	0.86060
H	-3.95271	1.76562	2.57672
H	-2.72221	2.10617	1.33169
C	-4.48681	-0.90468	1.81303
H	-4.24888	-1.97896	1.76737
H	-4.88570	-0.69103	2.82111
H	-5.28909	-0.69287	1.09168
C	3.26839	-0.13890	-1.65072
C	2.49087	-0.91366	-2.74146
H	1.43469	-0.59949	-2.79702
H	2.95871	-0.70268	-3.71948
H	2.52714	-2.00290	-2.57950
C	3.22470	1.37540	-1.96036
H	3.81759	1.96892	-1.24725
H	3.65594	1.53808	-2.96426
H	2.19615	1.77276	-1.96522
C	4.72265	-0.64611	-1.58451
H	4.78410	-1.69900	-1.26562
H	5.16423	-0.57714	-2.59492
H	5.34698	-0.03302	-0.91584
C	3.23762	-0.02818	1.59282
C	2.20938	-0.30401	2.71765
H	1.90624	-1.36443	2.75116
H	2.67437	-0.06373	3.69076
H	1.30786	0.32390	2.61005
C	4.48714	-0.90489	1.81266
H	5.28938	-0.69232	1.09150
H	4.88594	-0.69185	2.82091
H	4.24949	-1.97920	1.76622
C	3.59502	1.47470	1.57395
H	3.95258	1.76466	2.57826
H	4.40562	1.69945	0.86192
H	2.72166	2.10588	1.33377
C	0.00092	1.88187	0.03925
H	0.00038	0.85786	-1.24304
C	0.00336	3.12441	-0.02113
C	0.00137	4.60136	0.01776
C	-0.27698	5.06756	1.47495
C	-1.11126	5.14585	-0.91984
H	-0.94099	4.83167	-1.96299
H	-2.10549	4.78746	-0.60608
H	-1.11765	6.24904	-0.89070
H	-1.25694	4.70624	1.82762
H	-0.27970	6.17042	1.51662
H	0.49829	4.69721	2.16555
C	1.37978	5.14644	-0.44442
H	1.60490	4.83301	-1.47729
H	1.37696	6.24963	-0.41397
H	2.18890	4.78709	0.21274

$E_{O\text{-}tBu}$
SCF (BP86) Energy = -1387.29489217
Enthalpy 0K = -1386.603342
Enthalpy 298K = -1386.559120
Free Energy 298K = -1386.676023
Lowest Frequency = -4.2366 cm^{-1}
Second Frequency = 21.3155 cm^{-1}
SCF (BP86-D3BJ) Energy = -1387.505307
SCF (FB) Energy = -1387.337383
SCF (DFB) Energy = -1387.343817
SCF (BS2) Energy = -2056.922463

Rh	-0.00045	-0.09834	0.02127
P	2.29497	-0.43061	0.03626
P	-2.29612	-0.42767	0.03653
N	-0.00174	-2.19526	-0.08376
C	1.17757	-2.88729	-0.10822
C	1.21585	-4.28732	-0.16798
H	2.17929	-4.79867	-0.18817
C	-0.00353	-4.97709	-0.19733
H	-0.00424	-6.06998	-0.24312
C	-1.22202	-4.28580	-0.16680
H	-2.18612	-4.79595	-0.18607
C	-1.18195	-2.88582	-0.10713
O	2.34107	-2.19427	-0.07987
O	-2.34456	-2.19135	-0.07785
C	3.29632	-0.16493	1.64423
C	2.60726	-1.02078	2.73253
H	2.67317	-2.09919	2.51753
H	3.11795	-0.83555	3.69401
H	1.54602	-0.74946	2.86567
C	4.77289	-0.58990	1.51024
H	5.33505	0.06584	0.82690
H	5.25117	-0.51008	2.50285
H	4.87878	-1.63369	1.17314
C	3.17809	1.33384	2.00829
H	2.12957	1.67306	2.04170
H	3.62197	1.48520	3.00845

H	3.72410	1.98098	1.30430
C	3.19919	0.01963	-1.58990
C	2.13163	-0.18502	-2.69326
H	1.25609	0.47133	-2.53962
H	2.57294	0.07862	-3.67138
H	1.79310	-1.23329	-2.75747
C	3.58673	1.51331	-1.51690
H	4.41560	1.69311	-0.81338
H	3.92982	1.83703	-2.51595
H	2.73028	2.14984	-1.23303
C	4.42123	-0.87373	-1.88335
H	4.15811	-1.94308	-1.88517
H	4.80267	-0.61863	-2.88856
H	5.24393	-0.71749	-1.17100
C	-3.29716	-0.15859	1.64415
C	-2.61124	-1.01649	2.73281
H	-1.54893	-0.74920	2.86564
H	-3.12104	-0.82871	3.69426
H	-2.68135	-2.09475	2.51838
C	-3.17392	1.33987	2.00780
H	-3.71450	1.98938	1.30185
H	-3.62022	1.49331	3.00658
H	-2.12392	1.67424	2.04413
C	-4.77512	-0.57851	1.50987
H	-4.88456	-1.62196	1.17287
H	-5.25327	-0.49698	2.50241
H	-5.33490	0.07915	0.82641
C	-3.19914	0.02192	-1.59054
C	-2.13243	-0.18870	-2.69360
H	-1.79764	-1.23827	-2.75589
H	-2.57292	0.07469	-3.67216
H	-1.25446	0.46476	-2.54140
C	-4.42406	-0.86818	-1.88184
H	-5.24647	-0.70711	-1.17024
H	-4.80432	-0.61466	-2.88790
H	-4.16452	-1.93842	-1.88058
C	-3.58169	1.51699	-1.52067
H	-3.92446	1.83963	-2.52018
H	-4.40938	1.70110	-0.81687
H	-2.72292	2.15126	-1.23871
C	0.00004	1.86675	0.03877
H	-0.00030	-0.05416	1.53655
C	-0.00121	3.10905	0.04208
C	0.00221	4.58752	-0.00033
C	0.25356	5.05659	-1.46052
C	1.13119	5.13253	0.91687
H	0.98070	4.81504	1.96201
H	2.11951	4.77433	0.58422
H	1.13800	6.23602	0.89026
H	1.22622	4.69401	-1.83230
H	0.25735	6.15954	-1.50343
H	-0.53480	4.68765	-2.13731
C	-1.36604	5.13578	0.48759
H	-1.57306	4.81928	1.52330
H	-1.36295	6.23926	0.45978
H	-2.18783	4.77919	-0.15557

$10_{o\text{-}tBu}$

SCF (BP86) Energy = -1387.31173059
Enthalpy 0K = -1386.618202
Enthalpy 298K = -1386.573141
Free Energy 298K = -1386.693896
Lowest Frequency = 12.5499 cm^{-1}
Second Frequency = 21.5117 cm^{-1}
SCF (BP86-D3BJ) Energy = -1387.522322
SCF (FB) Energy = -1387.35165
SCF (DFB) Energy = -1387.357062
SCF (BS2) Energy = -2056.937959

Rh	-0.01781	-0.02705	0.05775
P	2.27166	-0.45351	0.03231
P	-2.32391	-0.29120	0.04299
N	-0.09254	-2.12213	-0.15412
C	1.06183	-2.85268	-0.25620
C	1.05044	-4.24836	-0.39365
H	1.99509	-4.78813	-0.47205
C	-0.19143	-4.89532	-0.42229
H	-0.23024	-5.98351	-0.52850
C	-1.38442	-4.16928	-0.31410
H	-2.36520	-4.64642	-0.33008
C	-1.29600	-2.77653	-0.17772
O	2.24601	-2.20810	-0.22905
O	-2.43132	-2.05755	-0.05789
C	3.20004	-0.41005	1.71023
C	2.31346	-1.22426	2.68283
H	2.28536	-2.29398	2.41943
H	2.73757	-1.14044	3.69943
H	1.27914	-0.83871	2.71190
C	4.61420	-1.01848	1.65221
H	5.31249	-0.39604	1.07044
H	5.01404	-1.07943	2.68062
H	4.61252	-2.03816	1.23480
C	3.24963	1.06303	2.17760
H	2.24876	1.52466	2.19377
H	3.65380	1.09031	3.20550
H	3.90781	1.68438	1.55040
C	3.33351	0.02467	-1.49289
C	2.34449	0.01163	-2.68365
H	1.50037	0.70420	-2.52581
H	2.88255	0.32213	-3.59752
H	1.93744	-0.99743	-2.86617
C	3.87483	1.45470	-1.27516
H	4.67159	1.48670	-0.51465
H	4.31164	1.81710	-2.22288
H	3.08201	2.16533	-0.98408
C	4.48582	-0.96226	-1.77399
H	4.12185	-1.99381	-1.89621
H	4.97431	-0.66259	-2.71874
H	5.25551	-0.95446	-0.98884
C	-3.32838	-0.04344	1.65726
C	-2.35467	-0.43017	2.79672
H	-1.43426	0.17733	2.77669
H	-2.85957	-0.26480	3.76558
H	-2.06938	-1.49464	2.74879
C	-3.69411	1.45409	1.76631
H	-4.47885	1.74293	1.04849
H	-4.09063	1.64831	2.77899
H	-2.82070	2.11247	1.61864
C	-4.58795	-0.93029	1.74019
H	-4.34885	-1.99678	1.60790
H	-5.03240	-0.80689	2.74424
H	-5.35576	-0.65006	1.00497
C	-3.24937	0.15695	-1.57575
C	-2.41766	-0.49777	-2.70516
H	-2.46139	-1.59822	-2.66607
H	-2.83327	-0.18029	-3.67821
H	-1.35967	-0.18261	-2.66807

C	-4.70182	-0.35406	-1.62702
H	-5.35952	0.18955	-0.93056
H	-5.09833	-0.18673	-2.64486
H	-4.77212	-1.43304	-1.41562
C	-3.19778	1.69374	-1.73165
H	-3.59922	1.96033	-2.72578
H	-3.80756	2.21769	-0.97916
H	-2.16495	2.07445	-1.67000
C	0.02140	1.79668	0.39736
H	-0.15272	3.22548	1.84304
C	0.02085	3.06401	0.76341
C	0.23233	4.34936	-0.06318
C	0.42427	4.03357	-1.56043
C	1.48449	5.07555	0.48669
H	1.37566	5.31112	1.55922
H	2.39154	4.46042	0.36205
H	1.63892	6.02605	-0.05344
H	1.30215	3.38721	-1.72917
H	0.58057	4.96762	-2.12610
H	-0.46028	3.52817	-1.98350
C	-1.01236	5.25071	0.12624
H	-1.17500	5.49481	1.19013
H	-0.87849	6.20053	-0.42050
H	-1.92311	4.76143	-0.25782

TS(B-10)'$_{o\text{-}tBu}$

SCF (BP86) Energy = -1387.20741801
Enthalpy 0K = -1386.517314
Enthalpy 298K = -1386.472305
Free Energy 298K = -1386.590702
Lowest Frequency = -164.5946 cm^{-1}
Second Frequency = 19.6956 cm^{-1}
SCF (BP86-D3BJ) Energy = -1387.424559
SCF (FB) Energy = -1387.248829
SCF (DFB) Energy = -1387.254707
SCF (BS2) Energy = -2056.836092

Rh	0.10962	0.06024	-0.12832
P	2.44696	0.11162	-0.07447
P	-2.12808	-0.44319	-0.11213
N	0.46497	-1.92281	0.31494
C	1.73192	-2.41617	0.48009
C	1.98784	-3.75694	0.78023
H	3.01780	-4.09474	0.90144
C	0.88620	-4.61738	0.91136
H	1.05164	-5.67373	1.14392
C	-0.41526	-4.14306	0.74384
H	-1.28793	-4.79125	0.83531
C	-0.61621	-2.77863	0.43390
O	2.78067	-1.56446	0.34872
O	-1.84182	-2.32070	0.25778
C	3.31856	0.93769	1.42624
C	2.34286	0.72441	2.60889
H	2.24069	-0.34336	2.86427
H	2.73786	1.24567	3.49983
H	1.33533	1.11876	2.38763
C	4.68256	0.30896	1.77968
H	5.45732	0.52146	1.02928
H	5.02628	0.73716	2.73878
H	4.60758	-0.78194	1.90700
C	3.46898	2.44587	1.13519
H	2.51129	2.90717	0.83511
H	3.80975	2.95834	2.05275
H	4.21661	2.64832	0.35095
C	3.43290	0.19412	-1.72074
C	2.80566	-0.90185	-2.61560
H	1.71069	-0.78474	-2.69844
H	3.23541	-0.82031	-3.63015
H	3.02291	-1.91336	-2.23743
C	3.17700	1.57700	-2.36077
H	3.57030	2.40976	-1.75534
H	3.68632	1.61455	-3.34040
H	2.10253	1.74540	-2.54110
C	4.94430	-0.06036	-1.56238
H	5.15311	-0.99019	-1.00986
H	5.39396	-0.16102	-2.56688
H	5.45786	0.77517	-1.06034
C	-3.25697	-0.25988	1.45184
C	-2.31108	-0.38904	2.66860
H	-1.51198	0.37140	2.65092
H	-2.89890	-0.25014	3.59404
H	-1.84024	-1.38334	2.71517
C	-3.97080	1.10296	1.49339
H	-4.63686	1.26015	0.63149
H	-4.58870	1.14764	2.40851
H	-3.25214	1.93177	1.52918
C	-4.32190	-1.37921	1.50029
H	-3.87948	-2.38210	1.42402
H	-4.84508	-1.30790	2.47087
H	-5.08467	-1.26075	0.71384
C	-3.09097	-0.76601	-1.78441
C	-2.06645	-0.62353	-2.93216
H	-1.21928	-1.31934	-2.81383
H	-2.57344	-0.86673	-3.88347
H	-1.66830	0.39939	-3.01425
C	-3.68581	-2.19235	-1.83430
H	-4.39585	-2.39309	-1.01936
H	-4.23786	-2.28630	-2.78694
H	-2.90865	-2.96852	-1.81082
C	-4.22733	0.26542	-1.95941
H	-4.68138	0.11744	-2.95597
H	-5.03089	0.12929	-1.21706
H	-3.86251	1.30217	-1.90115
C	-0.36973	1.79012	-1.02947
H	0.11070	2.52880	-1.66310
C	-1.55557	1.46019	-0.54948
C	-1.28821	3.89944	0.29027
C	-0.20394	4.66340	-0.42363
C	-1.01714	3.60109	1.73187
H	-1.81970	3.03214	2.22057
H	-0.06029	3.06999	1.86494
H	-0.92143	4.56843	2.27254
H	0.80839	4.29103	-0.20130
H	-0.24521	5.71036	-0.05147
H	-0.35814	4.71739	-1.51325
C	-2.68260	4.20413	-0.16432
H	-2.78997	4.10613	-1.25685
H	-3.44871	3.59749	0.33516
H	-2.89106	5.27113	0.07418

TS(B-10)"$_{o\text{-}tBu}$

SCF (BP86) Energy = -1387.22870948
Enthalpy 0K = -1386.536772
Enthalpy 298K = -1386.492190
Free Energy 298K = -1386.608164
Lowest Frequency = -384.4696 cm^{-1}
Second Frequency = 17.4560 cm^{-1}

SCF (BP86-D3BJ) Energy = -1387.446754
SCF (FB) Energy = -1387.269765
SCF (DFB) Energy = -1387.27551
SCF (BS2) Energy = -2056.855701

Rh	0.00002	0.13682	-0.08958
P	2.29605	-0.24113	0.01122
P	-2.29599	-0.24121	0.01120
N	0.00006	-1.96109	-0.11197
C	1.16989	-2.67117	-0.17955
C	1.21204	-4.06944	-0.27971
H	2.18101	-4.56851	-0.32514
C	0.00011	-4.76663	-0.32809
H	0.00013	-5.85729	-0.40983
C	-1.21183	-4.06949	-0.27972
H	-2.18079	-4.56859	-0.32515
C	-1.16974	-2.67121	-0.17958
O	2.33497	-1.99649	-0.15532
O	-2.33484	-1.99657	-0.15537
C	3.23174	-0.14740	1.71370
C	2.12386	-0.19556	2.79181
H	1.54784	-1.13488	2.74392
H	2.59063	-0.13867	3.79224
H	1.40965	0.63915	2.69416
C	4.18288	-1.34755	1.92016
H	4.99471	-1.38258	1.17907
H	4.64796	-1.24504	2.91762
H	3.65000	-2.30914	1.89326
C	4.03247	1.16665	1.83503
H	3.42108	2.06308	1.65141
H	4.42431	1.24458	2.86534
H	4.90027	1.18904	1.15654
C	3.43615	0.14243	-1.48880
C	2.65517	-0.37024	-2.72271
H	1.64356	0.06797	-2.77759
H	3.20667	-0.08540	-3.63700
H	2.55712	-1.46761	-2.71728
C	3.61767	1.67273	-1.59998
H	4.19132	2.09477	-0.75989
H	4.18201	1.89408	-2.52410
H	2.64887	2.19373	-1.66712
C	4.80499	-0.56301	-1.41115
H	4.70160	-1.64974	-1.26471
H	5.33924	-0.40352	-2.36551
H	5.44343	-0.15531	-0.61102
C	-3.23175	-0.14753	1.71367
C	-2.12390	-0.19535	2.79183
H	-1.40994	0.63958	2.69422
H	-2.59072	-0.13860	3.79224
H	-1.54758	-1.13449	2.74397
C	-4.03278	1.16635	1.83488
H	-4.90052	1.18854	1.15630
H	-4.42476	1.24421	2.86515
H	-3.42156	2.06290	1.65132
C	-4.18262	-1.34788	1.92019
H	-3.64955	-2.30936	1.89328
H	-4.64768	-1.24545	2.91767
H	-4.99448	-1.38309	1.17914
C	-3.43612	0.14229	-1.48881
C	-2.65517	-0.37045	-2.72272
H	-2.55727	-1.46783	-2.71733
H	-3.20660	-0.08551	-3.63702
H	-1.64349	0.06762	-2.77757
C	-4.80496	-0.56313	-1.41110
H	-5.44336	-0.15544	-0.61094
H	-5.33925	-0.40363	-2.36543
H	-4.70156	-1.64987	-1.26469
C	-3.61761	1.67258	-1.60006
H	-4.18220	1.89389	-2.52404
H	-4.19104	2.09470	-0.75985
H	-2.64882	2.19355	-1.66749
C	0.00000	2.05306	-0.67237
C	0.00008	2.71659	-1.75455
H	0.00025	3.30282	-2.65947
C	-0.00017	3.65631	0.19616
C	-1.27335	3.57398	1.03435
H	-1.32303	4.47304	1.67794
H	-2.17507	3.56536	0.40257
H	-1.26719	2.68010	1.67446
C	-0.00026	4.98469	-0.60661
H	-0.90022	5.10759	-1.23043
H	-0.00040	5.80764	0.13098
H	0.89975	5.10780	-1.23030
C	1.27293	3.57419	1.03449
H	2.17473	3.56561	0.40280
H	1.32246	4.47330	1.67802
H	1.26681	2.68035	1.67466

TS(B-F)$_{o\text{-}tBu}$
SCF (BP86) Energy = -1387.20634180
Enthalpy 0K = -1386.514360
Enthalpy 298K = -1386.469775
Free Energy 298K = -1386.585035
Lowest Frequency = -263.8705 cm^{-1}
Second Frequency = 14.1794 cm^{-1}
SCF (BP86-D3BJ) Energy = -1387.432793
SCF (FB) Energy = -1387.246558
SCF (DFB) Energy = -1387.252043
SCF (BS2) Energy = -2056.834875

Rh	0.02204	-0.32970	-0.06580
P	2.35051	0.10112	0.04303
P	-2.34739	0.08788	0.00562
N	0.01544	1.77148	-0.29150
C	1.17022	2.50459	-0.18529
C	1.20115	3.90321	-0.28742
H	2.15997	4.41750	-0.20930
C	-0.00742	4.58142	-0.47277
H	-0.01528	5.67209	-0.55450
C	-1.20860	3.86728	-0.53009
H	-2.17900	4.35307	-0.64052
C	-1.15716	2.47044	-0.41773
O	2.32787	1.86134	0.03634
O	-2.31603	1.79217	-0.43697
C	3.49729	-0.04312	-1.52731
C	2.61235	0.41339	-2.71426
H	2.38474	1.49042	-2.65348
H	3.16977	0.24840	-3.65381
H	1.66012	-0.13389	-2.78491
C	4.72461	0.89468	-1.46501
H	5.50320	0.53139	-0.78020
H	5.17101	0.93032	-2.47550
H	4.45453	1.92345	-1.18400
C	3.98110	-1.49535	-1.72013
H	3.16122	-2.22627	-1.79069
H	4.55121	-1.55410	-2.66483

H	4.65922	-1.81543	-0.91249
C	3.28264	-0.11597	1.71773
C	2.31373	0.42392	2.79635
H	1.35070	-0.10910	2.78654
H	2.78108	0.27051	3.78598
H	2.13386	1.50515	2.67829
C	3.54666	-1.62028	1.94843
H	4.24932	-2.04269	1.21131
H	4.01288	-1.74138	2.94312
H	2.61418	-2.20558	1.94338
C	4.60542	0.67575	1.78690
H	4.48792	1.72704	1.48164
H	4.94778	0.67026	2.83739
H	5.40310	0.21437	1.18616
C	-3.73797	-0.36141	-1.30509
C	-3.02116	-0.75619	-2.61481
H	-2.51135	-1.72784	-2.53740
H	-3.77514	-0.84557	-3.41745
H	-2.28938	0.00526	-2.93589
C	-4.62091	-1.53071	-0.81610
H	-5.28296	-1.23439	0.01226
H	-5.26899	-1.84656	-1.65334
H	-4.04817	-2.41698	-0.49992
C	-4.63930	0.86180	-1.60350
H	-4.08176	1.68164	-2.07802
H	-5.42008	0.52827	-2.31104
H	-5.14715	1.25734	-0.71344
C	-3.09659	0.25086	1.77948
C	-2.02230	0.97876	2.62114
H	-1.85645	2.01340	2.27694
H	-2.37799	1.03342	3.66603
H	-1.06208	0.43885	2.61216
C	-4.40396	1.06827	1.80959
H	-5.24335	0.54629	1.32438
H	-4.68833	1.22300	2.86622
H	-4.28573	2.06193	1.34869
C	-3.32462	-1.16665	2.35274
H	-3.62390	-1.06511	3.41187
H	-4.13234	-1.70777	1.83767
H	-2.40516	-1.77236	2.32143
C	0.02772	-1.84069	1.18714
C	0.01987	-2.44581	2.27390
H	0.02097	-2.95252	3.22223
C	0.03503	-2.87583	-0.62366
C	0.21967	-2.38632	-2.06678
H	1.24728	-2.06230	-2.27114
H	0.02446	-3.25953	-2.72714
H	-0.47298	-1.58966	-2.37381
C	-1.31426	-3.56703	-0.45144
H	-1.34827	-4.41612	-1.16296
H	-1.45369	-3.95666	0.56537
H	-2.15258	-2.90236	-0.69944
C	1.19475	-3.79791	-0.24518
H	1.00419	-4.33114	0.69595
H	1.30995	-4.54002	-1.06082
H	2.15001	-3.26156	-0.15304

$F_{O\text{-}tBu}$

SCF (BP86) Energy = -1387.22340978
Enthalpy 0K = -1386.530277
Enthalpy 298K = -1386.485284
Free Energy 298K = -1386.600743
Lowest Frequency = 28.4797 cm^{-1}
Second Frequency = 33.1132 cm^{-1}

Rh	-0.06452	-0.55796	0.01497
P	-2.36827	0.01344	0.09712
P	2.36065	-0.04429	0.20167
N	-0.02653	1.52208	-0.57331
C	-1.17898	2.15985	-0.94057
C	-1.21958	3.52266	-1.26270
H	-2.15997	3.97318	-1.58377
C	-0.04254	4.26691	-1.09928
H	-0.03979	5.33601	-1.33085
C	1.11454	3.66307	-0.59209
H	2.02825	4.22451	-0.39124
C	1.07466	2.28706	-0.31270
O	-2.32427	1.43630	-0.95355
O	2.14700	1.71167	0.27257
C	-2.67802	0.79409	1.85455
C	-1.29968	1.22713	2.40337
H	-0.89230	2.10682	1.88050
H	-1.41483	1.50111	3.46814
H	-0.56461	0.40565	2.35796
C	-3.59594	2.03451	1.84838
H	-4.64880	1.80397	1.64539
H	-3.54865	2.49286	2.85305
H	-3.25912	2.79449	1.12497
C	-3.23049	-0.33280	2.75820
H	-2.59411	-1.23504	2.73068
H	-3.24253	0.03226	3.80110
H	-4.26365	-0.61302	2.50156
C	-4.02939	-0.70455	-0.62853
C	-3.92970	-0.71333	-2.17360
H	-3.10126	-1.31808	-2.56572
H	-4.86465	-1.15018	-2.56732
H	-3.83713	0.30637	-2.57748
C	-4.24824	-2.12841	-0.06215
H	-4.50317	-2.11121	1.00813
H	-5.10141	-2.58485	-0.59487
H	-3.38077	-2.79172	-0.18732
C	-5.24150	0.18115	-0.26134
H	-5.10979	1.22901	-0.57296
H	-6.11820	-0.21711	-0.80355
H	-5.48627	0.14576	0.81026
C	3.08966	-0.41068	1.94997
C	2.01667	-0.01270	2.98610
H	1.10498	-0.61882	2.86938
H	2.42013	-0.21662	3.99452
H	1.76786	1.06036	2.93904
C	3.29021	-1.94646	2.00209
H	4.07767	-2.29930	1.31893
H	3.60382	-2.21475	3.02725
H	2.35227	-2.48711	1.79119
C	4.40154	0.32536	2.28667
H	4.30552	1.41929	2.19588
H	4.65252	0.10228	3.33941
H	5.25263	-0.01556	1.67804
C	3.83721	0.06188	-1.12645
C	3.22303	0.25600	-2.53125
H	2.52498	1.10992	-2.56714
H	4.04378	0.48485	-3.23471
H	2.71184	-0.63722	-2.91462
C	4.72046	1.30571	-0.85588
H	5.20420	1.30317	0.12768
H	5.52210	1.30441	-1.61673
H	4.15859	2.24420	-0.96491
C	4.71635	-1.20713	-1.09391
H	5.42583	-1.15692	-1.93968

H	5.31655	-1.27242	-0.17316
H	4.14802	-2.14417	-1.20389
C	-0.30971	-3.11589	1.90056
C	-0.18716	-2.16841	1.11474
C	0.00161	-1.94617	-1.69062
H	-0.38690	-3.93637	2.59138
C	-0.14506	-1.00304	-2.88304
H	0.62319	-0.21851	-2.91159
H	-0.04742	-1.59362	-3.81892
H	-1.13295	-0.51824	-2.91096
C	1.33391	-2.69578	-1.64953
H	1.38073	-3.36860	-2.53064
H	2.20596	-2.03632	-1.70316
H	1.41029	-3.31908	-0.74615
C	-1.11075	-2.99267	-1.65851
H	-1.04095	-3.58925	-2.59122
H	-1.00697	-3.67408	-0.80313
H	-2.11235	-2.55394	-1.63824

B_{C-Ar}

SCF (BP86) Energy = -1703.74570599
Enthalpy 0K = -1702.817243
Enthalpy 298K = -1702.761544
Free Energy 298K = -1702.902945
Lowest Frequency = 10.5454 cm^{-1}
Second Frequency = 12.8652 cm^{-1}
SCF (BP86-D3BJ) Energy = -1704.034476
SCF (FB) Energy = -1703.785879
SCF (DFB) Energy = -1703.791802
SCF (BS2) Energy = -2373.429615

Rh	1.19341	-0.01302	-0.42300
P	1.40872	-2.36315	-0.21731
P	1.62443	2.32108	-0.40556
N	2.69102	-0.04002	1.10041
C	2.89011	-1.17375	1.85200
C	3.87056	-1.22270	2.85503
H	3.99707	-2.13984	3.43650
C	4.66078	-0.09532	3.10798
H	5.42267	-0.11393	3.89304
C	4.46498	1.05239	2.33265
H	5.07601	1.94575	2.48779
C	3.48622	1.05514	1.32506
C	1.99605	-2.35280	1.58337
H	2.47197	-3.29370	1.90490
H	1.06907	-2.23495	2.17233
C	3.32935	2.24493	0.41577
H	3.58497	3.17871	0.94396
H	4.05332	2.14507	-0.41386
C	2.94499	-3.00647	-1.23415
C	3.90273	-1.80486	-1.42482
H	4.35895	-1.47914	-0.47604
H	4.72424	-2.10943	-2.09966
H	3.38477	-0.93872	-1.87456
C	3.72049	-4.14133	-0.53221
H	3.11611	-5.04420	-0.36373
H	4.57451	-4.43324	-1.17090
H	4.14265	-3.81795	0.43416
C	2.46613	-3.46351	-2.63023
H	1.87372	-2.68355	-3.13855
H	3.35024	-3.67109	-3.26020
H	1.86957	-4.38837	-2.59456
C	-0.02040	-3.68232	-0.20291
C	-0.96618	-3.33518	0.96970
H	-1.27489	-2.27705	0.96585
H	-1.88373	-3.94242	0.86757
H	-0.52926	-3.58254	1.95188
C	-0.81479	-3.56024	-1.52513
H	-0.20380	-3.78294	-2.41257
H	-1.64433	-4.29050	-1.50555
H	-1.24993	-2.55687	-1.64695
C	0.48429	-5.12886	-0.01829
H	1.09275	-5.25315	0.89359
H	-0.39196	-5.79545	0.08326
H	1.06538	-5.49118	-0.88057
C	2.04836	3.18675	-2.09125
C	2.79610	2.13198	-2.94178
H	2.20741	1.21109	-3.07024
H	2.99827	2.55851	-3.94127
H	3.77301	1.85354	-2.50911
C	0.73292	3.57271	-2.80313
H	0.22872	4.41853	-2.30896
H	0.96015	3.88941	-3.83736
H	0.02642	2.72741	-2.85596
C	2.95629	4.42833	-1.94628
H	3.91518	4.19952	-1.45145
H	3.20049	4.80337	-2.95720
H	2.47500	5.25230	-1.40118
C	0.61291	3.46775	0.78812
C	0.69405	2.78660	2.17470
H	1.71050	2.81540	2.60279
H	0.02995	3.32437	2.87547
H	0.36436	1.73449	2.13171
C	1.15336	4.90812	0.89384
H	0.96734	5.48978	-0.02254
H	0.62423	5.42425	1.71605
H	2.23115	4.95478	1.12532
C	-0.86196	3.49914	0.33164
H	-1.45117	4.06792	1.07423
H	-0.99211	3.99965	-0.64007
H	-1.29587	2.49005	0.26270
C	-0.00521	0.01295	-2.14548
H	0.22938	-0.00155	-3.20404
C	-0.83120	0.03822	-1.17314
C	-2.12892	0.04379	-0.54099
C	-3.27873	0.00704	-1.37186
C	-2.28125	0.08563	0.86503
H	-3.13783	-0.02440	-2.45487
H	-1.37494	0.11960	1.47606
C	-4.56809	0.01486	-0.81576
C	-3.55998	0.08750	1.45368
C	-4.67684	0.05363	0.59279
H	-5.67790	0.05925	1.03674
C	-5.84534	-0.01620	-1.68348
C	-6.67700	-1.27712	-1.32626
C	-5.52658	-0.05718	-3.19418
H	-4.95947	0.83191	-3.52068
H	-4.95210	-0.95839	-3.47096
H	-6.46718	-0.07710	-3.76960
H	-6.10616	-2.19979	-1.52760
H	-7.59955	-1.30739	-1.93153
H	-6.97480	-1.28873	-0.26452
C	-3.77533	0.13017	2.98250
C	-2.44239	0.13534	3.76250
C	-4.58995	-1.11489	3.42436
H	-5.57702	-1.15709	2.93520
H	-4.05358	-2.04808	3.18080

H	-4.75936	-1.09216	4.51497
H	-1.84445	-0.77084	3.55969
H	-2.64677	0.16057	4.84609
H	-1.82707	1.01965	3.52151
C	-4.56130	1.41637	3.35304
H	-4.00296	2.32170	3.05915
H	-5.54545	1.45311	2.85738
H	-4.73381	1.45851	4.44265
C	-6.68753	1.25593	-1.39743
H	-6.12368	2.17046	-1.64903
H	-7.60963	1.24511	-2.00408
H	-6.98641	1.32382	-0.33812

TS(B-10)$_{C-Ar}$

SCF (BP86) Energy = -1703.67519659
Enthalpy 0K = -1702.749993
Enthalpy 298K = -1702.694684
Free Energy 298K = -1702.836213
Lowest Frequency = -650.9261 cm^{-1}
Second Frequency = 7.7380 cm^{-1}
SCF (BP86-D3BJ) Energy = -1703.962758
SCF (FB) Energy = -1703.71588
SCF (DFB) Energy = -1703.721913
SCF (BS2) Energy = -2373.358009

Rh	1.24522	0.08455	-0.36527
P	2.26615	-2.03615	-0.19680
P	0.74762	2.40331	-0.23348
N	3.04278	0.70711	0.58736
C	3.87229	-0.20184	1.19719
C	5.08348	0.19143	1.78704
H	5.71570	-0.56199	2.26447
C	5.45673	1.54039	1.77385
H	6.39229	1.86447	2.23930
C	4.61517	2.46447	1.14534
H	4.88103	3.52374	1.09481
C	3.42426	2.02617	0.54438
C	3.41331	-1.63259	1.25120
H	4.26818	-2.32242	1.33998
H	2.79215	-1.76481	2.15444
C	2.55284	2.97195	-0.23163
H	2.68810	4.01185	0.10572
H	2.85819	2.92979	-1.29226
C	3.45681	-2.43417	-1.68194
C	3.94573	-1.06718	-2.21992
H	4.56852	-0.52885	-1.48585
H	4.57040	-1.24430	-3.11496
H	3.10008	-0.41950	-2.50584
C	4.68502	-3.28249	-1.29054
H	4.42389	-4.27530	-0.89653
H	5.30291	-3.44107	-2.19326
H	5.32768	-2.77193	-0.55365
C	2.64838	-3.13457	-2.79615
H	1.74671	-2.55966	-3.07017
H	3.27827	-3.20552	-3.70145
H	2.35524	-4.16165	-2.52482
C	1.33642	-3.62281	0.43959
C	0.76865	-3.29228	1.84064
H	0.26379	-2.31053	1.85858
H	0.02070	-4.05948	2.11014
H	1.54026	-3.31000	2.62812
C	0.14228	-3.93298	-0.49462
H	0.43203	-4.05173	-1.54967
H	-0.32121	-4.88373	-0.17353
H	-0.63865	-3.15835	-0.42178
C	2.25363	-4.85957	0.54132
H	3.15667	-4.67048	1.14586
H	1.69542	-5.67583	1.03591
H	2.56483	-5.23384	-0.44670
C	0.00992	3.38090	-1.74353
C	0.87945	3.04530	-2.97936
H	1.01521	1.95769	-3.10692
H	0.36349	3.42480	-3.87981
H	1.86779	3.53452	-2.95287
C	-1.42488	2.87663	-2.02065
H	-2.11131	3.03575	-1.17641
H	-1.82973	3.43113	-2.88685
H	-1.43353	1.80679	-2.28076
C	-0.00000	4.90777	-1.52069
H	0.99688	5.30849	-1.26990
H	-0.32083	5.40005	-2.45703
H	-0.70945	5.21457	-0.73564
C	0.06163	3.05424	1.47109
C	0.50723	2.02868	2.54043
H	1.60342	1.99485	2.65488
H	0.08200	2.32516	3.51729
H	0.15890	1.01037	2.29912
C	0.61166	4.44301	1.86262
H	0.37778	5.22768	1.12796
H	0.15161	4.74467	2.82149
H	1.70220	4.42928	2.02538
C	-1.48131	3.09160	1.42949
H	-1.85818	3.29524	2.44870
H	-1.86365	3.89381	0.77836
H	-1.91380	2.13157	1.10098
C	0.11142	-0.25678	-2.06767
H	-0.43313	-1.52268	-1.67533
C	-0.74911	-0.52060	-1.06771
C	-2.10997	-0.54674	-0.51042
C	-2.31739	-0.67694	0.87846
C	-3.21190	-0.48155	-1.39546
H	-1.43936	-0.72573	1.52738
H	-3.01977	-0.38897	-2.46714
C	-3.62224	-0.73480	1.40650
C	-4.52684	-0.53690	-0.90222
C	-4.69630	-0.66302	0.49480
H	-5.71668	-0.71039	0.88985
C	-3.90789	-0.88608	2.91641
C	-4.75795	0.31703	3.40499
C	-2.61174	-0.93578	3.75445
H	-1.97744	-1.79728	3.48135
H	-2.01395	-0.01403	3.64461
H	-2.86516	-1.03975	4.82275
H	-4.22180	1.26999	3.25586
H	-4.97933	0.21415	4.48143
H	-5.72100	0.38564	2.87258
C	-5.76340	-0.46879	-1.82422
C	-5.37575	-0.33296	-3.31311
C	-6.62849	0.75834	-1.43029
H	-6.97560	0.70168	-0.38505
H	-6.06288	1.69843	-1.54880
H	-7.52230	0.81432	-2.07530
H	-4.80153	0.58941	-3.50868
H	-6.28907	-0.28819	-3.92939
H	-4.78281	-1.19438	-3.66661
C	-4.69412	-2.20291	3.15707
H	-4.11252	-3.08002	2.82531

H	-4.91326	-2.32405	4.23209
H	-5.65564	-2.21297	2.61769
C	-6.59881	-1.76603	-1.65348
H	-6.01160	-2.65717	-1.93355
H	-6.94511	-1.90153	-0.61528
H	-7.49231	-1.72873	-2.30030

TS(B-C)$_{C-Ar}$

SCF (BP86) Energy = -1703.73631205
Enthalpy 0K = -1702.809367
Enthalpy 298K = -1702.754165
Free Energy 298K = -1702.895027
Lowest Frequency = -36.3608 cm^{-1}
Second Frequency = 8.8987 cm^{-1}
SCF (BP86-D3BJ) Energy = -1704.01612
SCF (FB) Energy = -1703.774232
SCF (DFB) Energy = -1703.77957
SCF (BS2) Energy = -2373.419562

Rh	1.59996	-0.05507	0.24332
P	2.11989	2.21942	0.17555
P	1.58849	-2.38025	0.07123
N	3.49657	-0.25025	-0.69608
C	4.14124	0.84339	-1.22749
C	5.39472	0.73483	-1.84855
H	5.86719	1.63439	-2.25314
C	6.01408	-0.51443	-1.96197
H	6.98697	-0.61653	-2.45131
C	5.35604	-1.62950	-1.43226
H	5.80462	-2.62533	-1.48895
C	4.11386	-1.47602	-0.79794
C	3.43685	2.17449	-1.17420
H	4.16130	3.00335	-1.09909
H	2.88534	2.32031	-2.12177
C	3.44096	-2.66070	-0.15535
H	3.67536	-3.59185	-0.69857
H	3.84181	-2.78020	0.86850
C	3.04792	2.89859	1.73565
C	4.30169	2.00915	1.91087
H	5.04020	2.15437	1.10473
H	4.79790	2.27517	2.86202
H	4.03514	0.93902	1.95204
C	3.47837	4.37407	1.61745
H	2.61967	5.06437	1.62071
H	4.10792	4.63539	2.48798
H	4.07982	4.56964	0.71325
C	2.14133	2.70514	2.97218
H	1.87939	1.64262	3.11014
H	2.68644	3.03491	3.87540
H	1.20935	3.28892	2.91684
C	0.85785	3.49985	-0.54308
C	0.07275	2.73713	-1.63699
H	-0.43646	1.84870	-1.23118
H	-0.68685	3.41343	-2.07132
H	0.72059	2.40518	-2.46714
C	-0.11969	3.93534	0.56995
H	0.36413	4.57570	1.32537
H	-0.93738	4.52894	0.12062
H	-0.57108	3.06874	1.08170
C	1.52196	4.74257	-1.17677
H	2.19842	4.48307	-2.00811
H	0.73092	5.38954	-1.59903
H	2.08481	5.34651	-0.45042
C	1.20970	-3.49306	1.61322
C	1.75226	-2.72342	2.84099
H	1.26877	-1.74082	2.95603
H	1.55186	-3.31554	3.75274
H	2.84276	-2.55926	2.79307
C	-0.31737	-3.66093	1.76563
H	-0.74749	-4.29427	0.97264
H	-0.53338	-4.15492	2.73059
H	-0.83565	-2.68719	1.76241
C	1.89084	-4.87877	1.55424
H	2.98951	-4.80765	1.49369
H	1.65708	-5.42749	2.48511
H	1.53881	-5.49490	0.71435
C	0.79198	-3.07121	-1.55507
C	1.52567	-2.36373	-2.71907
H	2.58169	-2.67035	-2.80388
H	1.02857	-2.63226	-3.66910
H	1.48816	-1.26594	-2.61161
C	0.91294	-4.59811	-1.72403
H	0.30151	-5.15092	-0.99283
H	0.54811	-4.87819	-2.72959
H	1.95471	-4.95360	-1.64776
C	-0.69215	-2.64445	-1.58808
H	-1.12866	-2.92752	-2.56362
H	-1.28913	-3.13609	-0.80407
H	-0.79726	-1.55358	-1.46863
C	-0.18430	0.13825	1.20744
H	0.17587	0.24385	2.25172
C	-1.42010	0.17045	0.88175
C	-2.77274	0.19714	0.50583
C	-3.54064	-1.00710	0.50604
C	-3.39824	1.43285	0.15698
H	-3.03943	-1.93623	0.78496
H	-2.78996	2.33938	0.17247
C	-4.89944	-0.99225	0.16809
C	-4.75425	1.47776	-0.18979
C	-5.47004	0.25679	-0.17515
H	-6.53203	0.28052	-0.44218
C	-5.77717	-2.26154	0.16278
C	-6.94095	-2.08059	1.17414
C	-4.97805	-3.52152	0.56074
H	-4.14856	-3.72161	-0.14009
H	-4.56415	-3.44301	1.58110
H	-5.64293	-4.40093	0.54249
H	-6.55938	-1.93017	2.19830
H	-7.58239	-2.97855	1.17650
H	-7.57953	-1.21785	0.92086
C	-5.47996	2.78483	-0.57259
C	-4.53773	4.00732	-0.52430
C	-6.64939	3.02915	0.41864
H	-7.38543	2.20807	0.40166
H	-6.28037	3.13162	1.45328
H	-7.18271	3.95772	0.15202
H	-4.12740	4.17207	0.48727
H	-5.09684	4.91538	-0.80460
H	-3.69650	3.90662	-1.23248
C	-6.04045	2.65413	-2.01421
H	-5.22983	2.48614	-2.74370
H	-6.75641	1.82035	-2.10635
H	-6.57062	3.57918	-2.29881
C	-6.35622	-2.47730	-1.26110
H	-5.55088	-2.61584	-2.00252
H	-6.99429	-3.37752	-1.27686
H	-6.97609	-1.62655	-1.59013

$C_{C\text{-}Ar}$

SCF (BP86) Energy = -1703.74066861
Enthalpy 0K = -1702.813665
Enthalpy 298K = -1702.757994
Free Energy 298K = -1702.900785
Lowest Frequency = 7.1847 cm^{-1}
Second Frequency = 13.4312 cm^{-1}
SCF (BP86-D3BJ) Energy = -1704.01675
SCF (FB) Energy = -1703.780561
SCF (DFB) Energy = -1703.786443
SCF (BS2) Energy = -2373.426879

Rh	1.69118	0.00607	0.10953
P	2.03275	2.31229	-0.12944
P	1.85518	-2.32410	0.25398
N	3.77072	-0.09845	-0.22526
C	4.46181	0.98727	-0.71253
C	5.84131	0.92710	-0.96293
H	6.35195	1.81551	-1.34456
C	6.54066	-0.26395	-0.74285
H	7.61454	-0.32732	-0.94130
C	5.83463	-1.37299	-0.26430
H	6.34320	-2.32168	-0.07202
C	4.46012	-1.26959	-0.00338
C	3.69138	2.24380	-1.02752
H	4.31074	3.13989	-0.85230
H	3.44010	2.24107	-2.10452
C	3.70997	-2.43472	0.58671
H	4.15279	-3.39251	0.26557
H	3.80535	-2.39194	1.68793
C	2.39973	3.26191	1.51509
C	3.60716	2.54574	2.16467
H	4.53904	2.67943	1.58976
H	3.77788	2.97545	3.16839
H	3.41898	1.46494	2.28373
C	2.73238	4.75320	1.31059
H	1.86295	5.33316	0.96237
H	3.04546	5.18621	2.27832
H	3.56377	4.91035	0.60214
C	1.17916	3.10783	2.45081
H	0.95593	2.04555	2.64611
H	1.40654	3.58726	3.42024
H	0.27082	3.58383	2.05067
C	0.94044	3.32367	-1.36352
C	0.57604	2.34113	-2.50227
H	0.03041	1.46342	-2.12183
H	-0.06638	2.86577	-3.23309
H	1.46424	1.98305	-3.05267
C	-0.35431	3.76869	-0.65022
H	-0.16804	4.54308	0.11167
H	-1.04225	4.20499	-1.39714
H	-0.86830	2.91593	-0.17678
C	1.66678	4.54962	-1.96053
H	2.57522	4.27370	-2.52167
H	0.98715	5.04427	-2.67832
H	1.94260	5.29734	-1.20273
C	1.11166	-3.28831	1.75959
C	1.20964	-2.34365	2.98126
H	0.59560	-1.43829	2.85365
H	0.84117	-2.87997	3.87469
H	2.24431	-2.02448	3.19579
C	-0.37586	-3.60184	1.48917
H	-0.50460	-4.36712	0.70672
H	-0.83180	-4.00065	2.41355
H	-0.93874	-2.69884	1.19917
C	1.88148	-4.59150	2.07362
H	2.93461	-4.40681	2.34353
H	1.40865	-5.07698	2.94679
H	1.85864	-5.31459	1.24550
C	1.58765	-3.23599	-1.43195
C	2.56332	-2.57222	-2.43272
H	3.62142	-2.76659	-2.18899
H	2.37663	-2.98901	-3.43902
H	2.40976	-1.48054	-2.48539
C	1.86022	-4.75180	-1.37604
H	1.11633	-5.28868	-0.76620
H	1.79821	-5.16422	-2.39990
H	2.86666	-4.99123	-0.99184
C	0.14241	-2.96440	-1.90760
H	0.02173	-3.36394	-2.93111
H	-0.60972	-3.45537	-1.27116
H	-0.07793	-1.88478	-1.92912
C	-0.30960	0.07924	0.27938
H	0.35146	0.13557	1.27726
C	-1.56517	0.08383	0.22944
C	-2.97876	0.07415	0.12344
C	-3.67124	-1.15292	-0.07007
C	-3.71428	1.28724	0.21905
H	-3.08450	-2.07125	-0.14359
H	-3.16209	2.21699	0.37210
C	-5.06980	-1.18182	-0.17478
C	-5.11432	1.28941	0.13115
C	-5.75866	0.04742	-0.06719
H	-6.85134	0.03689	-0.14134
C	-5.86400	-2.48731	-0.39582
C	-6.84060	-2.70025	0.79160
C	-4.94138	-3.72202	-0.49288
H	-4.23833	-3.64477	-1.34070
H	-4.35897	-3.87470	0.43256
H	-5.55106	-4.62724	-0.65153
H	-6.29350	-2.78916	1.74569
H	-7.42302	-3.62608	0.64301
H	-7.55790	-1.86857	0.89048
C	-5.95556	2.57948	0.24047
C	-5.07774	3.83208	0.45426
C	-6.92850	2.45528	1.44344
H	-7.61507	1.59953	1.33238
H	-6.37631	2.32463	2.38972
H	-7.54438	3.36725	1.52940
H	-4.49242	3.77084	1.38836
H	-5.72031	4.72551	0.52613
H	-4.38000	3.99441	-0.38586
C	-6.77060	2.77194	-1.06631
H	-6.10399	2.87062	-1.94008
H	-7.45252	1.92638	-1.25618
H	-7.38520	3.68637	-0.99934
C	-6.67169	-2.37784	-1.71673
H	-6.00205	-2.23210	-2.58152
H	-7.25206	-3.30163	-1.88473
H	-7.38445	-1.53666	-1.69647

$TS(C\text{-}D)_{C\text{-}Ar}$

SCF (BP86) Energy = -1703.67671836
Enthalpy 0K = -1702.750836
Enthalpy 298K = -1702.695386
Free Energy 298K = -1702.837846
Lowest Frequency = -289.2775 cm^{-1}
Second Frequency = 4.9307 cm^{-1}

SCF (BP86-D3BJ) Energy = -1703.962095
SCF (FB) Energy = -1703.718223
SCF (DFB) Energy = -1703.724606
SCF (BS2) Energy = -2373.359839

Rh	1.31222	0.07110	-0.22090
P	0.57222	2.28205	-0.45817
P	2.69396	-1.87229	0.04827
N	2.99750	1.01139	0.68404
C	3.18105	2.37106	0.57196
C	4.23034	3.03125	1.22793
H	4.32772	4.11518	1.12231
C	5.15285	2.29561	1.98053
H	5.97885	2.79347	2.49656
C	5.00683	0.90575	2.03629
H	5.71862	0.28845	2.59130
C	3.92942	0.28465	1.38444
C	2.26149	3.11550	-0.35529
H	2.20504	4.18405	-0.09807
H	2.68027	3.05115	-1.37575
C	3.76558	-1.21028	1.45287
H	4.74961	-1.70519	1.51194
H	3.21988	-1.47519	2.37826
C	-0.44541	3.12852	0.96447
C	-0.05568	2.38200	2.26195
H	1.02190	2.46157	2.48409
H	-0.60430	2.82958	3.11081
H	-0.31398	1.31196	2.20835
C	-0.10808	4.62806	1.12437
H	-0.26595	5.20928	0.20255
H	-0.77385	5.05332	1.89721
H	0.92533	4.79506	1.47079
C	-1.95863	2.96496	0.71237
H	-2.24872	1.91690	0.53516
H	-2.50339	3.31005	1.60981
H	-2.30612	3.57884	-0.13400
C	-0.04666	2.74496	-2.23394
C	1.01896	2.23035	-3.23303
H	1.25026	1.16343	-3.06845
H	0.61448	2.33157	-4.25620
H	1.95676	2.81024	-3.20588
C	-1.36414	1.99670	-2.52999
H	-2.19252	2.29603	-1.87210
H	-1.66691	2.21856	-3.56917
H	-1.22898	0.90652	-2.44561
C	-0.23730	4.26714	-2.40231
H	0.67557	4.83953	-2.16450
H	-0.48887	4.47940	-3.45752
H	-1.06520	4.65577	-1.78779
C	2.11293	-3.57684	0.77500
C	1.02200	-3.28089	1.83222
H	0.09135	-2.92158	1.36966
H	0.78556	-4.22002	2.36435
H	1.34333	-2.54949	2.59446
C	1.49901	-4.44575	-0.34538
H	2.26263	-4.82493	-1.04296
H	1.01347	-5.32583	0.11429
H	0.73477	-3.89856	-0.92205
C	3.26950	-4.33427	1.46671
H	3.65852	-3.79702	2.34747
H	2.88094	-5.30353	1.82910
H	4.10927	-4.54996	0.79191
C	3.88582	-2.09066	-1.46613
C	4.56883	-0.71968	-1.68695
H	5.25371	-0.44811	-0.86592
H	5.16967	-0.77212	-2.61284
H	3.82954	0.09091	-1.80838
C	4.97630	-3.16323	-1.26186
H	4.56289	-4.18361	-1.23310
H	5.67401	-3.12282	-2.11845
H	5.57639	-2.99925	-0.34997
C	3.03935	-2.42240	-2.71654
H	3.70236	-2.41877	-3.60093
H	2.57250	-3.41663	-2.65707
H	2.23521	-1.68699	-2.87441
C	0.01461	-1.25283	-1.30476
H	-0.14395	-0.96789	0.69157
C	-0.80295	-1.03312	-0.25486
C	-2.24632	-0.85015	-0.04323
C	-3.14075	-0.95912	-1.13354
C	-2.75958	-0.67118	1.26099
H	-2.72950	-1.13407	-2.13282
H	-2.05669	-0.61893	2.10033
C	-4.53117	-0.88924	-0.93828
C	-4.14541	-0.59186	1.49526
C	-5.00403	-0.69782	0.37969
H	-6.08119	-0.64723	0.54440
C	-5.48216	-1.04817	-2.14612
C	-5.25692	-2.44462	-2.78599
C	-5.17428	0.05385	-3.19448
H	-5.33895	1.06023	-2.77231
H	-4.13306	0.00038	-3.55480
H	-5.83590	-0.05990	-4.07066
H	-4.21860	-2.57630	-3.13375
H	-5.92148	-2.57387	-3.65784
H	-5.47728	-3.25094	-2.06596
C	-4.67646	-0.43278	2.93791
C	-4.11309	0.87346	3.55729
C	-4.21087	-1.64638	3.78714
H	-4.60009	-2.59208	3.37346
H	-3.11103	-1.72333	3.82936
H	-4.57877	-1.54951	4.82338
H	-3.01003	0.87356	3.58557
H	-4.47310	0.99059	4.59424
H	-4.44042	1.75690	2.98233
C	-6.96910	-0.93234	-1.74500
H	-7.26563	-1.71618	-1.02699
H	-7.20414	0.05155	-1.30323
H	-7.60207	-1.05141	-2.64036
C	-6.21876	-0.36705	2.99382
H	-6.61718	0.49258	2.42773
H	-6.68568	-1.28726	2.60298
H	-6.54479	-0.25255	4.04120

TS(C-10)$_{C\text{-}Ar}$
SCF (BP86) Energy = -1703.72209941
Enthalpy 0K = -1702.797832
Enthalpy 298K = -1702.741976
Free Energy 298K = -1702.885532
Lowest Frequency = -659.6256 cm^{-1}
Second Frequency = 6.9136 cm^{-1}
SCF (BP86-D3BJ) Energy = -1703.997127
SCF (FB) Energy = -1703.760689
SCF (DFB) Energy = -1703.766389
SCF (BS2) Energy = -2373.40685

Rh	-1.65729	0.02392	0.05280
P	-1.99746	-2.26094	0.37411
P	-1.84415	2.31413	-0.32378
N	-3.77385	0.06898	-0.10320
C	-4.49509	-1.09323	-0.24355
C	-5.89504	-1.08367	-0.34259
H	-6.42896	-2.03203	-0.44918
C	-6.58701	0.13199	-0.32666
H	-7.67737	0.15637	-0.41202
C	-5.85247	1.31586	-0.20081
H	-6.35356	2.28755	-0.17860
C	-4.45516	1.26315	-0.07974
C	-3.73749	-2.39266	-0.34801
H	-4.32139	-3.22578	0.07912
H	-3.58955	-2.62610	-1.41880
C	-3.66459	2.52870	0.13382
H	-4.14173	3.38237	-0.37710
H	-3.66551	2.76517	1.21411
C	-2.19287	-2.81428	2.22047
C	-3.33895	-1.95499	2.80423
H	-4.32068	-2.20575	2.36858
H	-3.40637	-2.14040	3.89177
H	-3.15170	-0.87788	2.65215
C	-2.52387	-4.30859	2.40192
H	-1.68502	-4.96284	2.11520
H	-2.73744	-4.50344	3.46905
H	-3.41699	-4.61703	1.83199
C	-0.89106	-2.45769	2.97402
H	-0.67614	-1.37781	2.89720
H	-1.01327	-2.70031	4.04546
H	-0.01684	-3.01857	2.60723
C	-1.02186	-3.55299	-0.68880
C	-0.77954	-2.87055	-2.05638
H	-0.22891	-1.92252	-1.94772
H	-0.19109	-3.55210	-2.69820
H	-1.72047	-2.65405	-2.59180
C	0.34128	-3.84189	-0.02392
H	0.23897	-4.40494	0.91795
H	0.95036	-4.46163	-0.70743
H	0.90471	-2.91542	0.17808
C	-1.78705	-4.87653	-0.91181
H	-2.75128	-4.72658	-1.42518
H	-1.17855	-5.53181	-1.56185
H	-1.97557	-5.42625	0.02182
C	-0.98340	3.58837	0.85330
C	-0.96143	2.92386	2.25028
H	-0.42558	1.96147	2.23549
H	-0.45372	3.60002	2.96268
H	-1.97504	2.73666	2.64571
C	0.46899	3.82417	0.38532
H	0.51727	4.39685	-0.55501
H	1.00210	4.41484	1.15294
H	1.01468	2.87616	0.24609
C	-1.72948	4.93813	0.94889
H	-2.75688	4.82773	1.33366
H	-1.19080	5.59079	1.66027
H	-1.77679	5.47077	-0.01218
C	-1.73578	2.83400	-2.18470
C	-2.80681	1.99606	-2.92221
H	-3.83539	2.27892	-2.64116
H	-2.70567	2.16610	-4.00960
H	-2.67435	0.91700	-2.73127
C	-1.98885	4.33275	-2.43955
H	-1.18573	4.96912	-2.03475
H	-2.02485	4.51095	-3.53010
H	-2.95107	4.67835	-2.02391
C	-0.34511	2.42172	-2.71940
H	-0.30711	2.60970	-3.80804
H	0.47486	2.99259	-2.25681
H	-0.15837	1.34824	-2.54987
C	0.28024	0.00242	0.10968
H	0.74275	-0.36501	1.17993
C	1.56330	0.01579	0.09986
C	2.99392	-0.02172	0.06899
C	3.75001	1.02520	0.65352
C	3.65549	-1.10340	-0.56557
H	3.21615	1.84900	1.13670
H	3.04845	-1.89606	-1.01268
C	5.15423	1.00317	0.61753
C	5.05835	-1.14663	-0.63276
C	5.77548	-0.08796	-0.03141
H	6.86557	-0.11343	-0.07124
C	5.95728	2.15052	1.26921
C	5.60882	2.22190	2.78021
C	5.57500	3.49138	0.58690
H	5.81489	3.47249	-0.48982
H	4.49969	3.71513	0.69044
H	6.13464	4.32397	1.04707
H	4.53448	2.40845	2.94818
H	6.16850	3.04334	3.25991
H	5.87389	1.28261	3.29470
C	5.75648	-2.32658	-1.34438
C	5.29888	-2.36869	-2.82709
C	5.35887	-3.65289	-0.64279
H	5.67511	-3.65443	0.41423
H	4.26929	-3.82390	-0.67077
H	5.84331	-4.50781	-1.14539
H	4.20732	-2.49966	-2.91892
H	5.78153	-3.21297	-3.34905
H	5.57333	-1.43946	-3.35463
C	7.48295	1.95298	1.13133
H	7.82689	1.02685	1.62342
H	7.80387	1.92728	0.07564
H	8.00727	2.79497	1.61318
C	7.29591	-2.20419	-1.31413
H	7.64906	-1.29309	-1.82720
H	7.69147	-2.20020	-0.28374
H	7.74311	-3.06779	-1.83401

TS(C-E)$_{C\text{-}Ar}$

SCF (BP86) Energy = -1703.73482687
Enthalpy 0K = -1702.809971
Enthalpy 298K = -1702.754397
Free Energy 298K = -1702.897367
Lowest Frequency = -647.5198 cm^{-1}
Second Frequency = 6.7275 cm^{-1}
SCF (BP86-D3BJ) Energy = -1704.011606
SCF (FB) Energy = -1703.777826
SCF (DFB) Energy = -1703.784687
SCF (BS2) Energy = -2373.421257

Rh	-1.65788	-0.00230	-0.00240
P	-1.89144	-2.30913	0.35446
P	-1.93085	2.30512	-0.34502
N	-3.78879	-0.00705	0.07171
C	-4.46795	-1.12121	0.50434
C	-5.87045	-1.15424	0.53363

H	-6.37787	-2.05726	0.88392
C	-6.60147	-0.02797	0.13824
H	-7.69505	-0.03525	0.16642
C	-5.90685	1.10721	-0.29463
H	-6.44332	2.00274	-0.61998
C	-4.50411	1.09379	-0.33422
C	-3.66452	-2.29324	1.01152
C	-3.74424	2.27575	-0.88657
C	-0.92871	-3.22737	1.75633
C	-0.73847	-2.21184	2.90791
H	-1.69115	-1.79107	3.27463
H	-0.26183	-2.73052	3.75938
H	-0.08336	-1.37819	2.61003
C	-1.70104	-4.45678	2.28746
H	-1.88784	-5.21488	1.51286
H	-1.09391	-4.93625	3.07652
H	-2.66559	-4.18588	2.74820
C	0.46102	-3.65292	1.23480
H	1.00636	-2.80490	0.78840
H	1.05903	-4.02770	2.08506
H	0.39813	-4.46922	0.49724
C	-1.96375	-3.30394	-1.30251
C	-3.05849	-2.62324	-2.15891
H	-2.85138	-1.54954	-2.31289
H	-3.07944	-3.10305	-3.15401
H	-4.06704	-2.72513	-1.72421
C	-0.60649	-3.14547	-2.02607
H	0.20920	-3.67494	-1.51125
H	-0.69114	-3.57432	-3.04114
H	-0.31710	-2.08587	-2.12074
C	-2.30787	-4.79546	-1.12136
H	-3.25042	-4.95312	-0.56939
H	-2.43558	-5.25618	-2.11813
H	-1.50565	-5.35024	-0.60968
C	-1.90692	3.40681	1.24067
C	-2.97984	2.81973	2.18814
H	-2.80955	1.74697	2.38123
H	-2.92710	3.35134	3.15533
H	-4.00463	2.94903	1.80101
C	-0.52408	3.27680	1.91745
H	0.28944	3.69006	1.30227
H	-0.53973	3.83707	2.86976
H	-0.27936	2.22697	2.14740
C	-2.22225	4.88874	0.95363
H	-3.17408	5.02641	0.41254
H	-2.31554	5.42629	1.91484
H	-1.42091	5.38308	0.38197
C	-1.04512	3.10347	-1.86478
C	-0.98016	1.98962	-2.93783
H	-1.98086	1.64539	-3.25626
H	-0.47790	2.39067	-3.83701
H	-0.40652	1.11940	-2.57988
C	-1.79797	4.32545	-2.43563
H	-1.86641	5.15975	-1.72208
H	-1.24589	4.69401	-3.31929
H	-2.81681	4.07762	-2.77786
C	0.39408	3.49711	-1.46709
H	0.94379	3.79936	-2.37683
H	0.41490	4.35527	-0.77573
H	0.93659	2.65169	-1.01222
C	0.29734	0.00163	-0.08003
H	-0.67443	0.18491	1.19834
C	1.54451	0.00761	-0.00378
C	2.97106	0.01043	-0.00306
C	3.68578	1.18303	0.35155
C	3.69521	-1.15873	-0.34970
H	3.11454	2.07671	0.62141
H	3.13122	-2.05434	-0.62815
C	5.09067	1.20150	0.37231
C	5.10031	-1.17035	-0.35466
C	5.77110	0.01711	0.01291
H	6.86200	0.01966	0.01915
C	5.83322	2.49440	0.77879
C	5.42256	2.88652	2.22329
C	5.44336	3.63764	-0.19579
H	5.72821	3.38942	-1.23245
H	4.35841	3.83708	-0.18229
H	5.95908	4.57225	0.08629
H	4.33662	3.06104	2.30902
H	5.93652	3.81507	2.52777
H	5.69428	2.09422	2.94147
C	5.85383	-2.45917	-0.75390
C	5.46282	-2.85079	-2.20398
C	5.45737	-3.60580	0.21400
H	5.72825	-3.35792	1.25452
H	4.37364	-3.81035	0.18657
H	5.98093	-4.53752	-0.06310
H	4.37887	-3.03022	-2.30347
H	5.98499	-3.77632	-2.50364
H	5.73953	-2.05592	-2.91736
C	7.36864	2.32990	0.74051
H	7.71803	1.54947	1.43829
H	7.73267	2.07993	-0.27097
H	7.84864	3.27726	1.03864
C	7.38788	-2.28767	-0.69624
H	7.74237	-1.50496	-1.38884
H	7.73809	-2.03705	0.31997
H	7.87593	-3.23250	-0.98930
H	-4.26731	3.22012	-0.65956
H	-3.71968	2.19127	-1.98922
H	-4.19661	-3.24263	0.83198
H	-3.55874	-2.19355	2.10840

E_{C-Ar}

SCF (BP86) Energy = -1703.74219930
Enthalpy 0K = -1702.815783
Enthalpy 298K = -1702.759968
Free Energy 298K = -1702.903927
Lowest Frequency = 5.4161 cm^{-1}
Second Frequency = 10.9140 cm^{-1}
SCF (BP86-D3BJ) Energy = -1704.019347
SCF (FB) Energy = -1703.787548
SCF (DFB) Energy = -1703.795464
SCF (BS2) Energy = -2373.427734

Rh	1.66394	-0.00229	-0.00788
P	1.88623	-2.29887	-0.43372
P	1.93704	2.29449	0.40683
N	3.80386	-0.02383	-0.00976
C	4.48304	-1.12460	-0.46828
C	5.88623	-1.15793	-0.48412
H	6.39763	-2.05251	-0.85016
C	6.61283	-0.04055	-0.05650
H	7.70662	-0.04767	-0.07373
C	5.91444	1.08689	0.39108
H	6.44813	1.97633	0.73726
C	4.51124	1.07142	0.41814

C	3.68380	-2.28171	-1.02240
C	3.74054	2.24134	0.98471
C	0.94717	-3.13127	-1.89979
C	0.81998	-2.05897	-3.00754
H	1.79886	-1.67974	-3.35200
H	0.32478	-2.51603	-3.88332
H	0.20978	-1.20560	-2.67307
C	1.70156	-4.35909	-2.45841
H	1.83266	-5.15872	-1.71448
H	1.11204	-4.78038	-3.29262
H	2.69232	-4.09942	-2.86755
C	-0.46997	-3.53314	-1.43540
H	-1.00228	-2.68536	-0.97298
H	-1.05179	-3.85589	-2.31755
H	-0.45421	-4.38026	-0.73065
C	1.88636	-3.35298	1.18703
C	2.97280	-2.73423	2.09924
H	2.79156	-1.66150	2.29011
H	2.95291	-3.25136	3.07539
H	3.99057	-2.84592	1.68952
C	0.51255	-3.19243	1.87766
H	-0.29951	-3.67716	1.31559
H	0.55677	-3.66707	2.87466
H	0.24070	-2.13214	2.01214
C	2.20051	-4.84385	0.95321
H	3.15301	-5.00158	0.41877
H	2.29151	-5.34759	1.93305
H	1.39904	-5.35715	0.39895
C	1.92480	3.46387	-1.12664
C	3.04547	2.96862	-2.07079
H	2.91965	1.90660	-2.34097
H	3.00471	3.55710	-3.00485
H	4.05337	3.10409	-1.64382
C	0.56295	3.31525	-1.84165
H	-0.27279	3.69763	-1.23621
H	0.58801	3.89657	-2.78104
H	0.34584	2.26426	-2.09211
C	2.18265	4.93982	-0.75919
H	3.12204	5.08205	-0.19769
H	2.26939	5.52836	-1.69054
H	1.35647	5.37579	-0.17591
C	1.01021	3.00347	1.94522
C	0.93663	1.83327	2.95676
H	1.93379	1.47608	3.27251
H	0.41909	2.18243	3.86881
H	0.36441	0.98380	2.54724
C	1.73644	4.20150	2.59514
H	1.81064	5.07139	1.92621
H	1.16014	4.51883	3.48320
H	2.75034	3.94749	2.94764
C	-0.42506	3.39874	1.53510
H	-0.99808	3.64806	2.44649
H	-0.44163	4.29063	0.88786
H	-0.94515	2.57042	1.02570
C	-0.28464	0.00692	0.00153
H	1.62873	0.26254	-1.50193
C	-1.53129	0.00169	-0.02669
C	-2.96025	0.00728	-0.01518
C	-3.67655	1.14575	-0.46378
C	-3.68481	-1.12331	0.43956
H	-3.10550	2.01009	-0.81698
H	-3.12049	-1.99384	0.78849
C	-5.08180	1.16722	-0.47280
C	-5.09015	-1.12998	0.45921
C	-5.76272	0.02218	-0.00416
H	-6.85362	0.02794	0.00021
C	-5.82419	2.42258	-0.98420
C	-5.42786	2.68434	-2.46181
C	-5.42058	3.64586	-0.11851
H	-5.69634	3.49126	0.93866
H	-4.33500	3.83780	-0.15975
H	-5.93538	4.55455	-0.47699
H	-4.34220	2.84491	-2.57394
H	-5.94161	3.58483	-2.84185
H	-5.71043	1.83291	-3.10412
C	-5.84212	-2.37727	0.97634
C	-5.43734	-2.64355	2.45084
C	-5.45856	-3.60471	0.10746
H	-5.74068	-3.44683	-0.94753
H	-4.37481	-3.80836	0.14027
H	-5.98042	-4.50784	0.46974
H	-4.35266	-2.81602	2.55459
H	-5.95794	-3.53840	2.83485
H	-5.70564	-1.78913	3.09534
C	-7.35973	2.26934	-0.91578
H	-7.71921	1.43207	-1.53849
H	-7.71355	2.11043	0.11751
H	-7.83962	3.18905	-1.29097
C	-7.37641	-2.20745	0.91992
H	-7.72198	-1.36646	1.54548
H	-7.73651	-2.04449	-0.11056
H	-7.86329	-3.12200	1.29870
H	4.27109	3.18978	0.79566
H	3.69163	2.12705	2.08396
H	4.20023	-3.23937	-0.84060
H	3.62150	-2.16365	-2.12090

$10_{C\text{-}Ar}$

SCF (BP86) Energy = -1703.75576952
Enthalpy 0K = -1702.826981
Enthalpy 298K = -1702.771327
Free Energy 298K = -1702.914878
Lowest Frequency = 6.7929 cm^{-1}
Second Frequency = 10.8392 cm^{-1}
SCF (BP86-D3BJ) Energy = -1704.034853
SCF (FB) Energy = -1703.797932
SCF (DFB) Energy = -1703.804302
SCF (BS2) Energy = -2373.439885

Rh	-1.50254	0.04525	-0.20774
P	-1.48273	2.38226	0.04315
P	-2.05428	-2.23378	-0.36000
N	-3.58825	0.25777	0.32708
C	-4.05395	1.44386	0.83505
C	-5.40491	1.60363	1.18297
H	-5.74758	2.56126	1.58421
C	-6.29067	0.53105	1.02988
H	-7.34440	0.63730	1.30497
C	-5.80883	-0.67882	0.51723
H	-6.47597	-1.53340	0.37547
C	-4.45572	-0.79159	0.16000
C	-3.06818	2.56402	1.06440
H	-3.55285	3.54469	0.92011
H	-2.73984	2.52979	2.11987
C	-3.93645	-2.05708	-0.47838
H	-4.46871	-2.93999	-0.08542
H	-4.15726	-2.01466	-1.56123

C	-1.83747	3.34720	-1.59462
C	-3.17668	2.79791	-2.13967
H	-4.03628	3.05475	-1.49774
H	-3.36541	3.24539	-3.13229
H	-3.14385	1.70172	-2.26394
C	-1.94224	4.87350	-1.40720
H	-0.97590	5.32926	-1.13915
H	-2.26179	5.32921	-2.36230
H	-2.68804	5.16103	-0.64634
C	-0.72056	3.00392	-2.60655
H	-0.64612	1.91520	-2.76155
H	-0.95946	3.47566	-3.57707
H	0.26710	3.37367	-2.29146
C	-0.16652	3.23763	1.16752
C	0.11399	2.23739	2.31332
H	0.47745	1.27117	1.92800
H	0.89119	2.66074	2.97471
H	-0.77537	2.04544	2.93945
C	1.13060	3.45512	0.35803
H	1.01244	4.23096	-0.41581
H	1.92550	3.79891	1.04403
H	1.48384	2.52673	-0.12024
C	-0.65138	4.57534	1.76963
H	-1.55610	4.45986	2.38988
H	0.14122	4.96921	2.43150
H	-0.85057	5.34204	1.00693
C	-1.63123	-3.23946	-1.95507
C	-1.73136	-2.23398	-3.12690
H	-1.04941	-1.37917	-2.99283
H	-1.46273	-2.75155	-4.06576
H	-2.75263	-1.83494	-3.25810
C	-0.18035	-3.76086	-1.85640
H	-0.07671	-4.56297	-1.10784
H	0.11250	-4.18882	-2.83234
H	0.53287	-2.95623	-1.61303
C	-2.60141	-4.41400	-2.21305
H	-3.64618	-4.08360	-2.33814
H	-2.30867	-4.91038	-3.15616
H	-2.57224	-5.17586	-1.42050
C	-1.75722	-3.22646	1.27201
C	-2.52857	-2.47162	2.38019
H	-3.62254	-2.51717	2.24548
H	-2.29964	-2.94082	3.35412
H	-2.22433	-1.41196	2.43637
C	-2.23856	-4.68913	1.21033
H	-1.63674	-5.29845	0.51763
H	-2.13613	-5.14192	2.21355
H	-3.30025	-4.77767	0.92249
C	-0.24796	-3.16674	1.59906
H	-0.07500	-3.63538	2.58485
H	0.36935	-3.70385	0.86322
H	0.10540	-2.12342	1.64623
C	0.23592	-0.12436	-0.75602
H	1.44905	-0.33754	-2.37325
C	1.45667	-0.24117	-1.27238
C	2.79108	-0.22793	-0.63383
C	3.92773	-0.06020	-1.45306
C	2.96626	-0.39356	0.75864
H	3.78323	0.06202	-2.53252
H	2.08194	-0.55187	1.38570
C	5.22703	-0.04668	-0.91249
C	4.25009	-0.39164	1.33513
C	5.36090	-0.21246	0.48170
H	6.36147	-0.21212	0.91561
C	6.44181	0.13938	-1.84874
C	6.31620	1.49871	-2.58754
C	6.46771	-1.01157	-2.88990
H	6.56236	-1.99253	-2.39373
H	5.55256	-1.03138	-3.50551
H	7.32678	-0.88921	-3.57248
H	5.39625	1.55491	-3.19372
H	7.17368	1.64407	-3.26763
H	6.30160	2.33866	-1.87201
C	4.40958	-0.60619	2.85821
C	3.82388	-1.99101	3.24306
C	3.64264	0.50480	3.62250
H	4.04054	1.50332	3.37240
H	2.56583	0.49785	3.38261
H	3.74379	0.36002	4.71251
H	2.75281	-2.06738	2.98916
H	3.92487	-2.16161	4.32940
H	4.35389	-2.80390	2.71824
C	7.78290	0.12808	-1.08245
H	7.84230	0.94407	-0.34160
H	7.95157	-0.82899	-0.55936
H	8.61513	0.26642	-1.79309
C	5.88657	-0.56641	3.30966
H	6.48555	-1.36099	2.83285
H	6.36022	0.40533	3.08769
H	5.94334	-0.72042	4.40058

TS(B-10)'$_{C\text{-}Ar}$

SCF (BP86) Energy = -1703.66028863
Enthalpy 0K = -1702.733191
Enthalpy 298K = -1702.678258
Free Energy 298K = -1702.816169
Lowest Frequency = -290.2984 cm^{-1}
Second Frequency = 17.3842 cm^{-1}
SCF (BP86-D3BJ) Energy = -1703.949513
SCF (FB) Energy = -1703.699365
SCF (DFB) Energy = -1703.70501
SCF (BS2) Energy = -2373.342504

Rh	1.13582	-0.04828	-0.32868
P	1.79062	-2.26059	0.13328
P	1.07590	2.32745	-0.55239
N	3.11657	0.37210	0.25826
C	3.86790	-0.54930	0.95008
C	5.19131	-0.28332	1.33678
H	5.74345	-1.04657	1.89186
C	5.78112	0.94525	1.02441
H	6.80797	1.16877	1.32761
C	5.02639	1.87576	0.30148
H	5.45117	2.83957	0.00808
C	3.71305	1.56633	-0.08029
C	3.21925	-1.85349	1.30700
H	3.96778	-2.65932	1.38646
H	2.74218	-1.75804	2.30028
C	2.91556	2.50714	-0.93243
H	3.28828	3.53994	-0.84872
H	3.01848	2.19801	-1.98792
C	2.61843	-3.13721	-1.38528
C	3.71358	-2.18115	-1.91288
H	4.54808	-2.05761	-1.20222
H	4.13461	-2.60535	-2.84259
H	3.29921	-1.18542	-2.14577
C	3.26160	-4.49415	-1.03295

H	2.51830	-5.25410	-0.74628
H	3.78971	-4.87713	-1.92556
H	4.01061	-4.41326	-0.22669
C	1.55734	-3.32003	-2.49380
H	1.11673	-2.35410	-2.78901
H	2.04642	-3.75941	-3.38276
H	0.73827	-3.99029	-2.19437
C	0.78462	-3.51637	1.23051
C	-0.06523	-2.66242	2.19659
H	-0.80944	-2.06547	1.64999
H	-0.60093	-3.33645	2.89010
H	0.54879	-1.98081	2.81224
C	-0.15096	-4.39800	0.37472
H	0.40607	-5.11213	-0.25330
H	-0.78728	-4.99423	1.05431
H	-0.80152	-3.78495	-0.26607
C	1.72183	-4.42688	2.06129
H	2.32142	-3.86952	2.79907
H	1.09184	-5.13218	2.63312
H	2.40256	-5.02950	1.44211
C	0.29113	3.29142	-2.05544
C	0.77257	2.56864	-3.34049
H	0.68567	1.47060	-3.28077
H	0.16410	2.91269	-4.19586
H	1.82193	2.80569	-3.58194
C	-1.25523	3.25254	-1.98970
H	-1.65246	3.88140	-1.18041
H	-1.65925	3.64933	-2.93868
H	-1.66380	2.24108	-1.84870
C	0.74459	4.76665	-2.12299
H	1.84161	4.87702	-2.13874
H	0.36159	5.21376	-3.05884
H	0.34302	5.36764	-1.29183
C	0.86330	3.31983	1.11757
C	1.21431	2.33931	2.26196
H	2.27887	2.05524	2.25051
H	1.01212	2.83384	3.23015
H	0.61997	1.41165	2.20872
C	1.79787	4.54480	1.21887
H	1.64736	5.27552	0.40984
H	1.59285	5.06573	2.17217
H	2.86151	4.25519	1.23717
C	-0.60450	3.77137	1.27437
H	-0.75885	4.13292	2.30745
H	-0.85815	4.60549	0.60092
H	-1.31836	2.94925	1.09734
C	-0.67047	-0.15053	-1.43528
H	-0.87088	0.42860	-2.33279
C	-0.61349	-1.37917	-0.90541
C	-2.02931	-0.50830	-0.51316
C	-3.17600	-0.83929	-1.28989
C	-2.19051	0.03418	0.78862
H	-3.01945	-1.26791	-2.28320
H	-1.28431	0.27953	1.34943
C	-4.46644	-0.63565	-0.78990
C	-3.47556	0.18790	1.34576
C	-4.58150	-0.13419	0.53080
H	-5.58619	0.00120	0.94446
C	-5.73795	-0.95642	-1.60316
C	-6.56866	-2.03061	-0.85072
C	-5.40716	-1.49477	-3.01219
H	-4.83349	-0.76453	-3.60941
H	-4.83568	-2.43829	-2.97099
H	-6.34308	-1.70160	-3.55715
H	-5.99431	-2.96467	-0.72901
H	-7.48550	-2.26454	-1.41859
H	-6.87734	-1.68953	0.15160
C	-3.71740	0.68003	2.79016
C	-2.39906	0.88685	3.56601
C	-4.56163	-0.37525	3.55504
H	-5.54722	-0.53878	3.08902
H	-4.04155	-1.34737	3.59613
H	-4.73767	-0.03743	4.59084
H	-1.81091	-0.04517	3.63053
H	-2.62383	1.20936	4.59647
H	-1.76621	1.66626	3.10941
C	-6.58223	0.33699	-1.75715
H	-6.02073	1.11741	-2.29885
H	-7.50271	0.12203	-2.32659
H	-6.88483	0.75287	-0.78151
C	-4.48867	2.02624	2.75263
H	-3.90833	2.80496	2.22842
H	-5.46051	1.92895	2.24051
H	-4.68625	2.38076	3.77904

TS(B-10)"$_{C\text{-}Ar}$

SCF (BP86) Energy = -1703.67908546
Enthalpy 0K = -1702.752845
Enthalpy 298K = -1702.697291
Free Energy 298K = -1702.837622
Lowest Frequency = -346.8243 cm^{-1}
Second Frequency = 8.5270 cm^{-1}
SCF (BP86-D3BJ) Energy = -1703.967604
SCF (FB) Energy = -1703.718401
SCF (DFB) Energy = -1703.724061
SCF (BS2) Energy = -2373.362192

Rh	1.23136	-0.04824	0.12715
P	1.26997	-2.40092	0.07784
P	1.88361	2.21093	0.12536
N	3.21420	-0.28825	-0.68741
C	3.82636	-1.51785	-0.72493
C	5.08382	-1.70888	-1.31839
H	5.52172	-2.71094	-1.32450
C	5.76850	-0.62154	-1.87016
H	6.75137	-0.75134	-2.33235
C	5.16456	0.63786	-1.80583
H	5.66040	1.52127	-2.21776
C	3.89641	0.77870	-1.22076
C	3.13386	-2.66136	-0.04325
H	3.39565	-3.62340	-0.51462
H	3.49224	-2.71048	1.00141
C	3.22791	2.12355	-1.19239
H	3.97256	2.93256	-1.10166
H	2.70025	2.28222	-2.15106
C	0.60836	-3.20991	-1.55822
C	1.37771	-2.51817	-2.70866
H	2.44898	-2.77905	-2.72158
H	0.94792	-2.84797	-3.67210
H	1.28623	-1.41933	-2.65295
C	0.80786	-4.73510	-1.64684
H	0.17889	-5.28170	-0.92578
H	0.51459	-5.07686	-2.65675
H	1.85739	-5.04026	-1.49608
C	-0.88720	-2.86294	-1.70241
H	-1.06087	-1.77687	-1.62584
H	-1.24542	-3.19829	-2.69310

H	-1.50599	-3.36661	-0.94318
C	0.89984	-3.47304	1.66241
C	1.38038	-2.62637	2.86541
H	0.87403	-1.64864	2.90213
H	1.15736	-3.17312	3.80023
H	2.46859	-2.44272	2.85011
C	-0.61368	-3.72035	1.80893
H	-1.02932	-4.31809	0.98148
H	-0.79988	-4.28264	2.74230
H	-1.16998	-2.77278	1.88152
C	1.64384	-4.82813	1.67212
H	2.73884	-4.71707	1.61751
H	1.42344	-5.33969	2.62710
H	1.32404	-5.49896	0.86182
C	0.79801	3.64881	-0.58646
C	-0.04188	3.00296	-1.71427
H	-0.63031	2.14154	-1.36130
H	-0.73660	3.75751	-2.12721
H	0.58791	2.65559	-2.55200
C	-0.12334	4.19602	0.52493
H	0.43376	4.80381	1.25637
H	-0.89170	4.85138	0.07683
H	-0.64054	3.39377	1.07620
C	1.61369	4.81553	-1.18942
H	2.24285	4.49981	-2.03741
H	0.90703	5.57008	-1.58161
H	2.25404	5.32114	-0.45222
C	2.82013	2.75640	1.73796
C	3.97029	1.74291	1.94460
H	4.74629	1.81823	1.16452
H	4.45812	1.95260	2.91408
H	3.59477	0.70583	1.96575
C	3.40716	4.18047	1.67059
H	2.62839	4.95912	1.64846
H	4.01693	4.35834	2.57558
H	4.07125	4.32545	0.80142
C	1.85031	2.63528	2.93499
H	2.40079	2.84949	3.86944
H	1.00930	3.34342	2.87635
H	1.44254	1.61289	3.00693
C	-0.64007	0.18912	0.87038
C	-0.93863	0.35495	2.11111
H	-1.24538	0.52464	3.13321
C	-2.15992	0.23062	0.45981
C	-2.78695	1.46862	0.16960
C	-2.92855	-0.96029	0.44087
H	-2.20270	2.38526	0.24544
H	-2.44603	-1.89980	0.70805
C	-4.13978	1.52178	-0.21204
C	-4.28703	-0.93964	0.07943
C	-4.85701	0.30761	-0.25466
H	-5.91393	0.33753	-0.53823
C	-5.17151	-2.20568	0.06010
C	-4.40787	-3.46586	0.51978
C	-5.68952	-2.44337	-1.38362
H	-6.28219	-1.59022	-1.75366
H	-4.85322	-2.60274	-2.08560
H	-6.33659	-3.33706	-1.41313
H	-3.56274	-3.70230	-0.14977
H	-5.08685	-4.33473	0.50729
H	-4.02210	-3.36266	1.54892
C	-4.86538	2.84186	-0.55226
C	-5.38744	2.77340	-2.01257
C	-3.94056	4.07064	-0.42419
H	-3.55600	4.19249	0.60349
H	-3.08167	4.00997	-1.11496
H	-4.50319	4.98500	-0.67610
H	-4.55633	2.64518	-2.72702
H	-5.91920	3.70586	-2.26944
H	-6.09126	1.93753	-2.16041
C	-6.06300	3.03436	0.41686
H	-6.79345	2.21191	0.34219
H	-5.72230	3.08984	1.46487
H	-6.59414	3.97241	0.18006
C	-6.37883	-2.00190	1.01524
H	-7.00444	-1.14426	0.71794
H	-7.02158	-2.89905	1.00760
H	-6.04212	-1.83173	2.05212

TS(10-F)$_{C\text{-}Ar}$

SCF (BP86) Energy = -1703.65895427
Enthalpy 0K = -1702.732549
Enthalpy 298K = -1702.677166
Free Energy 298K = -1702.815332
Lowest Frequency = -296.5141 cm^{-1}
Second Frequency = 18.3772 cm^{-1}
SCF (BP86-D3BJ) Energy = -1703.960357
SCF (FB) Energy = -1703.700005
SCF (DFB) Energy = -1703.706172
SCF (BS2) Energy = -2373.344556

Rh	0.73740	0.24221	-0.26323
P	2.45130	-1.42146	-0.51146
P	-0.18807	2.43137	0.04324
N	2.12313	0.93237	1.21356
C	2.97391	0.04245	1.82094
C	3.81288	0.44092	2.87363
H	4.46174	-0.29935	3.34935
C	3.81594	1.77639	3.29316
H	4.45928	2.10017	4.11672
C	3.00734	2.69552	2.61560
H	3.01921	3.75675	2.87796
C	2.18078	2.25443	1.57008
C	3.01785	-1.36806	1.29444
C	1.38766	3.21726	0.73789
C	3.94323	-0.71779	-1.56261
C	4.31907	0.68116	-1.02231
H	4.72299	0.65385	0.00311
H	5.10792	1.09892	-1.67383
H	3.45932	1.37040	-1.04924
C	5.19622	-1.61658	-1.49546
H	5.04912	-2.59216	-1.98257
H	6.01910	-1.10962	-2.03196
H	5.54333	-1.78738	-0.46190
C	3.48175	-0.54042	-3.02735
H	2.57904	0.08705	-3.09135
H	4.29331	-0.04360	-3.58995
H	3.26803	-1.49397	-3.52994
C	2.26975	-3.34115	-0.83332
C	0.89918	-3.77673	-0.27850
H	0.06481	-3.26616	-0.78146
H	0.78625	-4.86422	-0.44167
H	0.81471	-3.60710	0.80809
C	2.29723	-3.65131	-2.34582
H	3.28853	-3.49214	-2.79695
H	2.04733	-4.71911	-2.48345
H	1.55161	-3.05627	-2.89651

C	3.37007	-4.14823	-0.10463
H	3.30027	-4.05920	0.99204
H	3.22528	-5.21709	-0.34631
H	4.39085	-3.88078	-0.41258
C	-0.49637	3.55007	-1.51891
C	0.43707	3.00461	-2.62405
H	0.21246	1.95642	-2.87420
H	0.30884	3.62218	-3.53224
H	1.50267	3.06340	-2.33934
C	-1.96225	3.41960	-1.98018
H	-2.66679	3.89393	-1.27818
H	-2.07836	3.92777	-2.95457
H	-2.26053	2.36840	-2.11519
C	-0.16590	5.04050	-1.27322
H	0.89511	5.20739	-1.02553
H	-0.36345	5.59505	-2.20881
H	-0.78301	5.49834	-0.48678
C	-1.46011	2.78797	1.47629
C	-0.85463	2.16090	2.75410
H	0.04815	2.68843	3.10367
H	-1.60256	2.22477	3.56532
H	-0.60860	1.09544	2.60728
C	-1.70294	4.29437	1.70658
H	-2.26489	4.75770	0.88025
H	-2.31451	4.41436	2.61978
H	-0.77516	4.86968	1.86502
C	-2.80549	2.09104	1.19069
H	-3.49849	2.32047	2.02126
H	-3.27913	2.44090	0.26151
H	-2.69937	0.99840	1.13355
C	0.00135	-0.53272	-1.91539
H	-0.24083	-1.24227	-4.10812
C	-0.08289	-0.92275	-3.09382
C	-1.25007	-0.69096	-0.49890
C	-2.45750	-0.35556	-1.14495
C	-1.29112	-1.50705	0.65646
H	-2.42268	0.23301	-2.06382
H	-0.36523	-1.77886	1.16398
C	-3.69523	-0.86214	-0.69119
C	-2.52235	-1.94238	1.19372
C	-3.70334	-1.63179	0.48646
H	-4.65389	-2.01739	0.86254
C	-4.97536	-0.60746	-1.52314
C	-4.79935	-1.26376	-2.91924
C	-5.21321	0.91378	-1.70031
H	-5.36419	1.40998	-0.72632
H	-4.37058	1.40832	-2.21204
H	-6.11563	1.08792	-2.31167
H	-3.94020	-0.83991	-3.46632
H	-5.70220	-1.10201	-3.53372
H	-4.63843	-2.35135	-2.82740
C	-2.61279	-2.76519	2.49953
C	-1.24239	-2.94409	3.18897
C	-3.18500	-4.17209	2.17794
H	-4.18919	-4.11168	1.72701
H	-2.53195	-4.71512	1.47351
H	-3.26764	-4.77186	3.10117
H	-0.53860	-3.52316	2.56563
H	-1.37257	-3.50130	4.13191
H	-0.77700	-1.97385	3.43846
C	-6.23248	-1.21338	-0.85926
H	-6.15776	-2.30929	-0.75512
H	-6.42299	-0.78037	0.13805
H	-7.11593	-1.00299	-1.48506
C	-3.55643	-2.04244	3.49802
H	-3.17027	-1.04116	3.75579
H	-4.57269	-1.91726	3.09026
H	-3.64172	-2.62634	4.43098
H	2.29132	-2.00371	1.83522
H	4.01667	-1.80543	1.45937
H	1.18740	4.15234	1.28522
H	1.99440	3.48522	-0.14758

F_{C-Ar}

SCF (BP86) Energy = -1703.70149825
Enthalpy 0K = -1702.773932
Enthalpy 298K = -1702.718073
Free Energy 298K = -1702.857447
Lowest Frequency = 18.5143 cm^{-1}
Second Frequency = 25.5712 cm^{-1}
SCF (BP86-D3BJ) Energy = -1704.007772
SCF (FB) Energy = -1703.744948
SCF (DFB) Energy = -1703.751885
SCF (BS2) Energy = -2373.387231

Rh	0.93141	0.06133	-0.40716
P	1.20903	-2.30275	-0.42398
P	1.25162	2.40161	0.04118
N	1.38449	-0.16731	1.68931
C	1.31744	-1.41015	2.27046
C	1.60508	-1.59291	3.63174
H	1.53943	-2.59458	4.06522
C	1.95349	-0.48984	4.42117
H	2.16113	-0.61238	5.48831
C	2.04903	0.76768	3.81671
H	2.35046	1.64616	4.39401
C	1.78514	0.90333	2.44282
C	0.88185	-2.57663	1.41613
C	2.05156	2.21948	1.75111
C	3.09269	-2.71270	-0.68930
C	3.89554	-1.84981	0.31280
H	3.69446	-2.11442	1.36382
H	4.97312	-2.01460	0.13180
H	3.70164	-0.77148	0.18201
C	3.43031	-4.19728	-0.44223
H	2.98334	-4.86211	-1.19700
H	4.52666	-4.32364	-0.50909
H	3.12553	-4.54541	0.55943
C	3.50352	-2.30547	-2.12375
H	3.19914	-1.27516	-2.36905
H	4.60350	-2.37240	-2.20740
H	3.07432	-2.96762	-2.88916
C	0.07194	-3.61884	-1.27990
C	-1.36605	-3.05921	-1.28856
H	-1.44514	-2.15021	-1.90063
H	-2.03004	-3.82927	-1.72208
H	-1.74716	-2.82228	-0.28137
C	0.52527	-3.82111	-2.74259
H	1.48117	-4.36285	-2.81989
H	-0.23570	-4.43241	-3.26048
H	0.60968	-2.86241	-3.28085
C	0.08028	-4.96357	-0.51665
H	-0.33729	-4.87140	0.49973
H	-0.56860	-5.67083	-1.06451
H	1.07642	-5.42343	-0.44505
C	2.72037	3.11541	-1.01292
C	3.68390	1.92613	-1.24102

H	3.19366	1.10905	-1.79693
H	4.54188	2.27084	-1.84722
H	4.10079	1.53024	-0.29715
C	2.17600	3.59188	-2.37714
H	1.57124	4.50836	-2.28422
H	3.03055	3.83297	-3.03544
H	1.57844	2.80946	-2.87364
C	3.50340	4.25585	-0.32451
H	3.93361	3.96213	0.64805
H	4.35396	4.52759	-0.97610
H	2.90509	5.16484	-0.17563
C	-0.15490	3.70604	0.31690
C	-0.99550	3.22548	1.52192
H	-0.42965	3.24253	2.46896
H	-1.84739	3.91864	1.64527
H	-1.40477	2.21545	1.37044
C	0.39241	5.11711	0.61676
H	0.87124	5.57757	-0.26120
H	-0.45848	5.76411	0.89826
H	1.10487	5.13681	1.45928
C	-1.04603	3.74293	-0.94307
H	-1.87233	4.45614	-0.76944
H	-0.50123	4.08050	-1.83777
H	-1.48835	2.75777	-1.15275
C	0.82062	0.18538	-2.36174
H	0.89603	0.27019	-4.67208
C	0.85604	0.21627	-3.59877
C	-1.10875	0.03579	-0.13567
C	-1.96803	0.30113	-1.21428
C	-1.64993	-0.27583	1.12986
H	-1.54898	0.53394	-2.19368
H	-1.00126	-0.43606	1.98996
C	-3.37605	0.22586	-1.05557
C	-3.04907	-0.35027	1.31815
C	-3.88777	-0.10304	0.21018
H	-4.96998	-0.16626	0.34760
C	-4.28265	0.48492	-2.28232
C	-3.95765	-0.55339	-3.38908
C	-4.02309	1.91230	-2.83108
H	-4.25225	2.67828	-2.07049
H	-2.97552	2.04669	-3.14926
H	-4.66396	2.10369	-3.70934
H	-2.90593	-0.49000	-3.71602
H	-4.59405	-0.37776	-4.27394
H	-4.14517	-1.58163	-3.03501
C	-3.67713	-0.68433	2.69142
C	-2.61857	-0.92185	3.79016
C	-4.53587	-1.97107	2.56102
H	-5.34164	-1.85459	1.81807
H	-3.91767	-2.83277	2.25443
H	-5.00618	-2.21611	3.52930
H	-1.95768	-1.77418	3.55075
H	-3.12076	-1.15603	4.74383
H	-1.98984	-0.03003	3.95920
C	-5.78324	0.36668	-1.93283
H	-6.04522	-0.64289	-1.57208
H	-6.08789	1.10039	-1.16668
H	-6.38757	0.56106	-2.83475
C	-4.58260	0.49368	3.14130
H	-3.99800	1.42280	3.25483
H	-5.39027	0.69020	2.41754
H	-5.05247	0.26449	4.11368
H	-0.22000	-2.66964	1.47745
H	1.30971	-3.51923	1.79530
H	1.79203	3.06607	2.40802
H	3.14274	2.28921	1.58588

B_{O-Ar}

SCF (BP86) Energy = -1775.61055155
Enthalpy 0K = -1774.729112
Enthalpy 298K = -1774.673594
Free Energy 298K = -1774.815429
Lowest Frequency = 12.5151 cm^{-1}
Second Frequency = 16.2450 cm^{-1}
SCF (BP86-D3BJ) Energy = -1775.883185
SCF (FB) Energy = -1775.649205
SCF (DFB) Energy = -1775.6546
SCF (BS2) Energy = -2445.323999

Rh	-1.18940	0.14644	-0.34431
P	-0.81360	2.40023	0.16598
P	-2.18416	-1.94705	-0.54915
N	-2.90677	0.49964	0.79166
C	-3.15805	1.74026	1.32220
C	-4.30460	2.01513	2.08277
H	-4.44963	3.01974	2.48235
C	-5.22193	0.98009	2.29384
H	-6.12409	1.16658	2.88379
C	-4.99897	-0.29017	1.74954
H	-5.69663	-1.11794	1.88370
C	-3.83351	-0.49190	0.99675
O	-2.27568	2.73354	1.10976
O	-3.62391	-1.70490	0.44861
C	-1.09170	3.65691	-1.26093
C	-2.40693	3.21283	-1.94490
H	-3.27965	3.35085	-1.28598
H	-2.56431	3.83407	-2.84503
H	-2.36750	2.15543	-2.25851
C	-1.22038	5.11907	-0.79154
H	-0.26132	5.52948	-0.43870
H	-1.54015	5.73600	-1.65104
H	-1.97399	5.23861	0.00308
C	0.08284	3.50466	-2.25465
H	0.21018	2.46098	-2.58719
H	-0.12909	4.12107	-3.14687
H	1.03908	3.85355	-1.83408
C	0.44982	2.97853	1.49806
C	0.48952	1.81805	2.52007
H	0.80594	0.87175	2.05312
H	1.21778	2.06760	3.31257
H	-0.48908	1.66470	3.00601
C	1.83378	3.14778	0.83501
H	1.87070	4.03005	0.17546
H	2.58684	3.30333	1.62842
H	2.14388	2.25894	0.26044
C	0.03017	4.27404	2.22453
H	-0.98189	4.20007	2.65095
H	0.73538	4.44144	3.05885
H	0.07390	5.16106	1.57696
C	-3.07661	-2.43872	-2.18303
C	-3.59207	-1.10504	-2.77618
H	-2.77923	-0.38117	-2.94896
H	-4.08313	-1.31231	-3.74414
H	-4.34021	-0.62840	-2.12059
C	-2.04148	-3.07873	-3.13524
H	-1.74944	-4.09006	-2.80945
H	-2.49331	-3.17683	-4.13869

H	-1.12638	-2.47149	-3.24217
C	-4.27820	-3.38348	-1.96875
H	-4.99934	-2.97337	-1.24507
H	-4.80132	-3.50149	-2.93505
H	-3.97881	-4.38642	-1.63365
C	-1.42438	-3.42569	0.40943
C	-1.17717	-2.88777	1.83950
H	-2.12175	-2.70340	2.37633
H	-0.60730	-3.64330	2.40956
H	-0.59344	-1.95040	1.83126
C	-2.33599	-4.66654	0.47631
H	-2.41831	-5.17613	-0.49661
H	-1.89073	-5.38992	1.18352
H	-3.34715	-4.42436	0.84034
C	-0.07568	-3.77697	-0.25940
H	0.42818	-4.54779	0.35116
H	-0.20247	-4.19436	-1.27067
H	0.60003	-2.90909	-0.32485
C	-0.01590	-0.06820	-2.06875
H	-0.32720	-0.13315	-3.10586
C	0.83372	-0.25139	-1.13643
C	2.15891	-0.39831	-0.58191
C	3.26054	0.00501	-1.37959
C	2.39523	-0.96003	0.69424
H	3.05950	0.43786	-2.36432
H	1.53435	-1.27082	1.29387
C	4.58098	-0.15337	-0.92487
C	3.70595	-1.13905	1.17747
C	4.77376	-0.72485	0.35287
H	5.79414	-0.85463	0.71577
C	3.93632	-1.79292	2.55891
C	3.36447	-3.23595	2.53620
C	3.20857	-0.97061	3.65469
H	3.59665	0.06135	3.69961
H	2.12071	-0.91845	3.47831
H	3.36244	-1.43513	4.64412
H	2.28254	-3.24312	2.31954
H	3.51410	-3.72153	3.51626
H	3.86766	-3.84991	1.77003
C	5.75738	0.28516	-1.82570
C	5.62333	1.79749	-2.14782
C	5.71551	-0.52874	-3.14701
H	5.81359	-1.60993	-2.95053
H	4.77428	-0.36933	-3.69975
H	6.54634	-0.22482	-3.80707
H	4.68051	2.02594	-2.67310
H	6.45341	2.12199	-2.79886
H	5.65608	2.40436	-1.22673
C	5.43341	-1.87247	2.93173
H	6.00616	-2.48759	2.21678
H	5.90031	-0.87379	2.98347
H	5.54097	-2.33882	3.92536
C	7.12955	0.05288	-1.15533
H	7.23465	0.62530	-0.21745
H	7.30716	-1.01368	-0.93431
H	7.93177	0.38494	-1.83533

TS(B-10)$_{o\text{-}Ar}$

SCF (BP86) Energy = -1775.54175745
Enthalpy 0K = -1774.663837
Enthalpy 298K = -1774.608648
Free Energy 298K = -1774.750311
Lowest Frequency = -691.6370 cm^{-1}
Second Frequency = 12.7050 cm^{-1}
SCF (BP86-D3BJ) Energy = -1775.813016
SCF (FB) Energy = -1775.58062
SCF (DFB) Energy = -1775.586143
SCF (BS2) Energy = -2445.254441

Rh	1.22629	0.15325	-0.31561
P	2.43428	-1.82378	-0.52638
P	0.61078	2.33554	0.22987
N	2.90990	0.68203	0.79354
C	3.93510	-0.20779	0.99595
C	5.08963	0.12024	1.71956
H	5.86769	-0.63318	1.84967
C	5.19861	1.41528	2.23965
H	6.09058	1.70064	2.80484
C	4.17666	2.34838	2.03547
H	4.22643	3.36836	2.41906
C	3.04731	1.94748	1.30620
O	3.83243	-1.44999	0.47892
O	2.06014	2.84095	1.10924
C	3.35590	-2.14685	-2.18522
C	3.72950	-0.73923	-2.71039
H	4.43307	-0.22199	-2.03620
H	4.23238	-0.85240	-3.68798
H	2.83790	-0.10670	-2.84997
C	4.63905	-2.98686	-2.01540
H	4.43349	-4.03569	-1.75802
H	5.18058	-2.98507	-2.97855
H	5.31138	-2.56335	-1.25318
C	2.38014	-2.82175	-3.17388
H	1.44909	-2.24228	-3.30047
H	2.86454	-2.87206	-4.16565
H	2.13117	-3.85497	-2.88169
C	1.84644	-3.40339	0.39264
C	1.54554	-2.93724	1.83722
H	0.85528	-2.07537	1.85412
H	1.07241	-3.76997	2.38795
H	2.46486	-2.65650	2.37561
C	0.53922	-3.89022	-0.27403
H	0.68622	-4.21821	-1.31546
H	0.15936	-4.76089	0.29043
H	-0.25015	-3.12005	-0.25349
C	2.89204	-4.53573	0.41756
H	3.87388	-4.18970	0.77764
H	2.54093	-5.32238	1.11001
H	3.01994	-5.00675	-0.56960
C	0.66449	3.62523	-1.19354
C	2.01987	3.39841	-1.90483
H	2.13560	2.35228	-2.23549
H	2.05821	4.04403	-2.80062
H	2.87275	3.66670	-1.26069
C	-0.48410	3.29335	-2.17257
H	-1.48087	3.42331	-1.72158
H	-0.41878	3.98186	-3.03427
H	-0.40125	2.26550	-2.56861
C	0.56588	5.08486	-0.70858
H	1.31835	5.32027	0.06096
H	0.74947	5.75281	-1.56959
H	-0.43451	5.32971	-0.31747
C	-0.66204	2.74537	1.61814
C	-0.58645	1.54637	2.59276
H	0.41282	1.45197	3.05057
H	-1.31188	1.70861	3.41072
H	-0.83399	0.59556	2.09440

C	-0.32178	4.03962	2.38838
H	-0.42825	4.94466	1.77405
H	-1.02928	4.12939	3.23267
H	0.69674	4.01715	2.80439
C	-2.07372	2.83919	1.00037
H	-2.81124	2.91510	1.81962
H	-2.19171	3.73800	0.37323
H	-2.33889	1.95086	0.40330
C	0.11422	-0.04088	-2.07678
H	-0.36273	-1.37014	-1.85348
C	-0.75236	-0.46240	-1.14434
C	-2.12509	-0.58816	-0.63703
C	-2.38721	-1.21961	0.59761
C	-3.18750	-0.10129	-1.43491
H	-1.54273	-1.58581	1.18678
H	-2.95067	0.37284	-2.39001
C	-3.70893	-1.37084	1.05725
C	-4.51957	-0.23483	-1.00371
C	-4.74342	-0.86910	0.23847
H	-5.77700	-0.98144	0.58255
C	-4.05493	-2.06146	2.39387
C	-4.81989	-1.06531	3.30569
C	-2.79468	-2.53970	3.14760
H	-2.22131	-3.28045	2.56333
H	-2.12342	-1.70134	3.40443
H	-3.09093	-3.02467	4.09257
H	-4.20249	-0.17948	3.53358
H	-5.08471	-1.55139	4.26044
H	-5.75597	-0.71420	2.84072
C	-5.71680	0.27059	-1.83738
C	-5.26996	0.93494	-3.15813
C	-6.51486	1.31338	-1.00991
H	-6.89949	0.88847	-0.06776
H	-5.88810	2.18581	-0.75732
H	-7.38164	1.67332	-1.59039
H	-4.62991	1.81714	-2.98185
H	-6.15660	1.27909	-3.71597
H	-4.72374	0.23228	-3.81105
C	-4.95250	-3.29649	2.11205
H	-4.43391	-4.02735	1.46836
H	-5.21379	-3.79925	3.05915
H	-5.89496	-3.01667	1.61294
C	-6.63824	-0.93057	-2.18181
H	-6.09968	-1.68777	-2.77658
H	-7.02834	-1.42549	-1.27686
H	-7.50439	-0.58521	-2.77204

TS(B-C)$_{o\text{-}Ar}$

SCF (BP86) Energy = -1775.54175745
Enthalpy 0K = -1774.663837
Enthalpy 298K = -1774.608648
Free Energy 298K = -1774.750311
Lowest Frequency = -691.6370 cm^{-1}
Second Frequency = 12.7050 cm^{-1}
SCF (BP86-D3BJ) Energy = -1775.859728
SCF (FB) Energy = -1775.635557
SCF (DFB) Energy = -1775.64073
SCF (BS2) Energy = -2445.311889

Rh	1.22629	0.15325	-0.31561
P	2.43428	-1.82378	-0.52638
P	0.61078	2.33554	0.22987
N	2.90990	0.68203	0.79354
C	3.93510	-0.20779	0.99595
C	5.08963	0.12024	1.71956
H	5.86769	-0.63318	1.84967
C	5.19861	1.41528	2.23965
H	6.09058	1.70064	2.80484
C	4.17666	2.34838	2.03547
H	4.22643	3.36836	2.41906
C	3.04731	1.94748	1.30620
O	3.83243	-1.44999	0.47892
O	2.06014	2.84095	1.10924
C	3.35590	-2.14685	-2.18522
C	3.72950	-0.73923	-2.71039
H	4.43307	-0.22199	-2.03620
H	4.23238	-0.85240	-3.68798
H	2.83790	-0.10670	-2.84997
C	4.63905	-2.98686	-2.01540
H	4.43349	-4.03569	-1.75802
H	5.18058	-2.98507	-2.97855
H	5.31138	-2.56335	-1.25318
C	2.38014	-2.82175	-3.17388
H	1.44909	-2.24228	-3.30047
H	2.86454	-2.87206	-4.16565
H	2.13117	-3.85497	-2.88169
C	1.84644	-3.40339	0.39264
C	1.54554	-2.93724	1.83722
H	0.85528	-2.07537	1.85412
H	1.07241	-3.76997	2.38795
H	2.46486	-2.65650	2.37561
C	0.53922	-3.89022	-0.27403
H	0.68622	-4.21821	-1.31546
H	0.15936	-4.76089	0.29043
H	-0.25015	-3.12005	-0.25349
C	2.89204	-4.53573	0.41756
H	3.87388	-4.18970	0.77764
H	2.54093	-5.32238	1.11001
H	3.01994	-5.00675	-0.56960
C	0.66449	3.62523	-1.19354
C	2.01987	3.39841	-1.90483
H	2.13560	2.35228	-2.23549
H	2.05821	4.04403	-2.80062
H	2.87275	3.66670	-1.26069
C	-0.48410	3.29335	-2.17257
H	-1.48087	3.42331	-1.72158
H	-0.41878	3.98186	-3.03427
H	-0.40125	2.26550	-2.56861
C	0.56588	5.08486	-0.70858
H	1.31835	5.32027	0.06096
H	0.74947	5.75281	-1.56959
H	-0.43451	5.32971	-0.31747
C	-0.66204	2.74537	1.61814
C	-0.58645	1.54637	2.59276
H	0.41282	1.45197	3.05057
H	-1.31188	1.70861	3.41072
H	-0.83399	0.59556	2.09440
C	-0.32178	4.03962	2.38838
H	-0.42825	4.94466	1.77405
H	-1.02928	4.12939	3.23267
H	0.69674	4.01715	2.80439
C	-2.07372	2.83919	1.00037
H	-2.81124	2.91510	1.81962
H	-2.19171	3.73800	0.37323
H	-2.33889	1.95086	0.40330
C	0.11422	-0.04088	-2.07678
H	-0.36273	-1.37014	-1.85348

C	-0.75236	-0.46240	-1.14434
C	-2.12509	-0.58816	-0.63703
C	-2.38721	-1.21961	0.59761
C	-3.18750	-0.10129	-1.43491
H	-1.54273	-1.58581	1.18678
H	-2.95067	0.37284	-2.39001
C	-3.70893	-1.37084	1.05725
C	-4.51957	-0.23483	-1.00371
C	-4.74342	-0.86910	0.23847
H	-5.77700	-0.98144	0.58255
C	-4.05493	-2.06146	2.39387
C	-4.81989	-1.06531	3.30569
C	-2.79468	-2.53970	3.14760
H	-2.22131	-3.28045	2.56333
H	-2.12342	-1.70134	3.40443
H	-3.09093	-3.02467	4.09257
H	-4.20249	-0.17948	3.53358
H	-5.08471	-1.55139	4.26044
H	-5.75597	-0.71420	2.84072
C	-5.71680	0.27059	-1.83738
C	-5.26996	0.93494	-3.15813
C	-6.51486	1.31338	-1.00991
H	-6.89949	0.88847	-0.06776
H	-5.88810	2.18581	-0.75732
H	-7.38164	1.67332	-1.59039
H	-4.62991	1.81714	-2.98185
H	-6.15660	1.27909	-3.71597
H	-4.72374	0.23228	-3.81105
C	-4.95250	-3.29649	2.11205
H	-4.43391	-4.02735	1.46836
H	-5.21379	-3.79925	3.05915
H	-5.89496	-3.01667	1.61294
C	-6.63824	-0.93057	-2.18181
H	-6.09968	-1.68777	-2.77658
H	-7.02834	-1.42549	-1.27686
H	-7.50439	-0.58521	-2.77204

$C_{O\text{-}Ar}$

SCF (BP86) Energy = -1775.60148460
Enthalpy 0K = -1774.721821
Enthalpy 298K = -1774.666087
Free Energy 298K = -1774.811699
Lowest Frequency = 7.1135 cm^{-1}
Second Frequency = 12.7580 cm^{-1}
SCF (BP86-D3BJ) Energy = -1775.860315
SCF (FB) Energy = -1775.639365
SCF (DFB) Energy = -1775.644736
SCF (BS2) Energy = -2445.317225

Rh	-1.60177	-0.00223	0.13226
P	-1.92050	-2.28748	0.03517
P	-1.93614	2.28367	0.08770
N	-3.64453	-0.00355	-0.21871
C	-4.32615	-1.18036	-0.40293
C	-5.70242	-1.21878	-0.66584
H	-6.19192	-2.18455	-0.79901
C	-6.39554	-0.00507	-0.74522
H	-7.46998	-0.00577	-0.94992
C	-5.72294	1.20963	-0.56605
H	-6.22849	2.17474	-0.62113
C	-4.34637	1.17286	-0.30485
O	-3.64735	-2.34559	-0.32612
O	-3.68839	2.33831	-0.12152
C	-1.90770	-3.28849	1.67153
C	-2.87578	-2.53731	2.61675
H	-3.92148	-2.61288	2.27811
H	-2.81241	-2.99295	3.62112
H	-2.61224	-1.46921	2.70850
C	-2.36555	-4.75087	1.50741
H	-1.63297	-5.35750	0.95165
H	-2.46818	-5.20324	2.51043
H	-3.34420	-4.82662	1.00695
C	-0.47565	-3.22544	2.25102
H	-0.13153	-2.18802	2.39670
H	-0.47536	-3.71791	3.23993
H	0.26172	-3.74909	1.62248
C	-1.27413	-3.23655	-1.50163
C	-1.33180	-2.20521	-2.65475
H	-0.72728	-1.30984	-2.43183
H	-0.93221	-2.67504	-3.57177
H	-2.36606	-1.88685	-2.86919
C	0.19463	-3.63421	-1.23582
H	0.27968	-4.43601	-0.48403
H	0.63228	-4.01839	-2.17475
H	0.80441	-2.77245	-0.91316
C	-2.12845	-4.46646	-1.87178
H	-3.18986	-4.20411	-2.00208
H	-1.76038	-4.86679	-2.83378
H	-2.05681	-5.27550	-1.13078
C	-1.81549	3.29424	1.71249
C	-2.38390	2.36064	2.80892
H	-1.83478	1.40577	2.86595
H	-2.29535	2.86926	3.78579
H	-3.45068	2.13618	2.64389
C	-0.32204	3.57596	1.99078
H	0.09638	4.32306	1.29725
H	-0.22222	3.98499	3.01209
H	0.29641	2.66291	1.93834
C	-2.63284	4.60236	1.68727
H	-3.68159	4.42688	1.40041
H	-2.63128	5.03381	2.70453
H	-2.20510	5.35695	1.01156
C	-1.40800	3.20850	-1.50939
C	-1.91487	2.31101	-2.66493
H	-3.01571	2.27346	-2.70741
H	-1.55739	2.73322	-3.62126
H	-1.52755	1.28046	-2.58160
C	-2.00845	4.62111	-1.64459
H	-1.55241	5.33666	-0.94304
H	-1.80573	4.99340	-2.66519
H	-3.10045	4.62665	-1.49855
C	0.13637	3.25536	-1.54237
H	0.45481	3.63703	-2.52918
H	0.55107	3.93436	-0.78015
H	0.58245	2.25629	-1.40472
C	0.40917	-0.00565	0.34093
H	-0.23213	-0.00437	1.33708
C	1.66376	-0.00728	0.27346
C	3.07473	-0.00065	0.15859
C	3.78010	1.23066	0.08150
C	3.79807	-1.22341	0.12848
H	3.20466	2.16069	0.10836
H	3.23699	-2.16041	0.19383
C	5.17934	1.25572	-0.02587
C	5.19761	-1.23223	0.02271
C	5.85776	0.01567	-0.05281
H	6.94570	0.02200	-0.13517

C	5.91938	2.60947	-0.10806
C	5.61366	3.43609	1.16967
C	5.42358	3.38628	-1.35701
H	5.63262	2.82477	-2.28344
H	4.33839	3.58090	-1.31715
H	5.93568	4.36167	-1.42577
H	4.53437	3.63361	1.28498
H	6.12852	4.41134	1.12324
H	5.95956	2.91015	2.07570
C	5.95754	-2.57709	-0.00620
C	5.47255	-3.41055	-1.22246
C	5.66492	-3.35627	1.30401
H	6.00379	-2.78944	2.18776
H	4.58873	-3.56473	1.42870
H	6.19397	-4.32497	1.29599
H	4.39040	-3.61947	-1.17352
H	5.99892	-4.38028	-1.25269
H	5.67275	-2.88357	-2.17089
C	7.45039	2.43806	-0.21987
H	7.87410	1.91830	0.65674
H	7.73973	1.88230	-1.12847
H	7.92818	3.43042	-0.27576
C	7.48576	-2.38768	-0.12681
H	7.76615	-1.86394	-1.05699
H	7.90250	-1.82763	0.72805
H	7.97811	-3.37434	-0.14425

TS(C-D)$_{O\text{-}Ar}$

SCF (BP86) Energy = -1775.54168760
Enthalpy 0K = -1774.663114
Enthalpy 298K = -1774.608083
Free Energy 298K = -1774.749224
Lowest Frequency = -235.7898 cm^{-1}
Second Frequency = 9.5233 cm^{-1}
SCF (BP86-D3BJ) Energy = -1775.81188
SCF (FB) Energy = -1775.580964
SCF (DFB) Energy = -1775.586755
SCF (BS2) Energy = -2445.254759

Rh	1.24909	0.08209	-0.14872
P	0.47197	2.24323	0.10265
P	2.70742	-1.77984	-0.26832
N	2.97779	0.94551	0.65200
C	3.00550	2.27804	0.98077
C	4.14524	2.90888	1.49665
H	4.09969	3.97091	1.74175
C	5.30126	2.14106	1.67884
H	6.20564	2.60550	2.08208
C	5.30672	0.78393	1.34000
H	6.18811	0.15185	1.45725
C	4.13121	0.22183	0.82137
O	1.88323	3.01134	0.81764
O	4.14410	-1.08024	0.47399
C	-0.80984	2.77567	1.43060
C	-0.63783	1.76331	2.58698
H	0.38368	1.78123	3.00272
H	-1.33492	2.03323	3.40031
H	-0.86954	0.73429	2.27028
C	-0.53630	4.20057	1.96185
H	-0.66483	4.97570	1.19335
H	-1.26655	4.40688	2.76501
H	0.47242	4.29601	2.39075
C	-2.23383	2.68182	0.84039
H	-2.46028	1.69021	0.41531
H	-2.95843	2.86107	1.65471
H	-2.41388	3.44996	0.07096
C	0.36422	3.20092	-1.55657
C	1.73549	3.00357	-2.24707
H	1.98191	1.93538	-2.37403
H	1.68955	3.46008	-3.25205
H	2.55244	3.49510	-1.69415
C	-0.73984	2.53844	-2.41207
H	-1.74043	2.62351	-1.95939
H	-0.77463	3.04925	-3.39111
H	-0.52696	1.47206	-2.59645
C	0.08973	4.70688	-1.36980
H	0.82093	5.18347	-0.69723
H	0.17429	5.19984	-2.35534
H	-0.92643	4.90879	-0.99495
C	2.46575	-3.25712	0.93560
C	2.25646	-2.62100	2.33082
H	1.41473	-1.90749	2.34112
H	2.02902	-3.42505	3.05328
H	3.15890	-2.09684	2.68404
C	1.19736	-4.04257	0.52694
H	1.30420	-4.54332	-0.44746
H	1.01920	-4.82690	1.28445
H	0.29883	-3.40704	0.48470
C	3.69036	-4.19413	0.97359
H	4.62693	-3.64947	1.17284
H	3.54707	-4.92309	1.79197
H	3.80244	-4.77190	0.04281
C	3.45109	-2.24344	-1.97975
C	3.39788	-0.93392	-2.80358
H	4.01783	-0.13708	-2.35671
H	3.80135	-1.13747	-3.81206
H	2.36253	-0.57202	-2.91087
C	4.91295	-2.72959	-1.87957
H	5.00785	-3.69610	-1.36399
H	5.29603	-2.86518	-2.90701
H	5.56095	-1.99807	-1.37297
C	2.55874	-3.31201	-2.64993
H	2.90157	-3.44544	-3.69198
H	2.64116	-4.29247	-2.15308
H	1.50072	-3.00300	-2.68030
C	0.07222	-1.11543	-1.48747
H	-0.11645	-1.04886	0.55637
C	-0.77264	-1.03871	-0.44639
C	-2.22170	-0.89439	-0.23895
C	-3.06808	-0.62218	-1.33865
C	-2.78453	-1.11524	1.03714
H	-2.61506	-0.47331	-2.32366
H	-2.11788	-1.35578	1.87333
C	-4.46406	-0.56629	-1.17816
C	-4.17758	-1.06713	1.23650
C	-4.98850	-0.78576	0.11611
H	-6.07011	-0.74791	0.25312
C	-5.36579	-0.29378	-2.40311
C	-5.16016	-1.42839	-3.44288
C	-4.97491	1.06570	-3.04166
H	-5.11923	1.89615	-2.32903
H	-3.92287	1.07794	-3.37370
H	-5.60402	1.26503	-3.92637
H	-4.11362	-1.48835	-3.78621
H	-5.79407	-1.25128	-4.32896
H	-5.43322	-2.40923	-3.01832
C	-4.76600	-1.35228	2.63681
C	-4.18437	-0.34286	3.66146

C	-4.38079	-2.79510	3.06182
H	-4.78139	-3.53797	2.35156
H	-3.28711	-2.93174	3.11254
H	-4.79285	-3.01950	4.06090
H	-3.08369	-0.39702	3.71586
H	-4.57725	-0.55598	4.67058
H	-4.46373	0.69254	3.40039
C	-6.86350	-0.23958	-2.03030
H	-7.22021	-1.19589	-1.61083
H	-7.08010	0.56209	-1.30307
H	-7.46117	-0.03499	-2.93420
C	-6.30581	-1.23364	2.66370
H	-6.64790	-0.22156	2.38648
H	-6.78845	-1.96144	1.98925
H	-6.67258	-1.43839	3.68348

TS(C-10)$_{o\text{-}Ar}$

SCF (BP86) Energy = -1775.58495610
Enthalpy 0K = -1774.707946
Enthalpy 298K = -1774.652095
Free Energy 298K = -1774.798294
Lowest Frequency = -603.8489 cm^{-1}
Second Frequency = 4.3197 cm^{-1}
SCF (BP86-D3BJ) Energy = -1775.842685
SCF (FB) Energy = -1775.622451
SCF (DFB) Energy = -1775.62787
SCF (BS2) Energy = -2445.299445

Rh	-1.58239	0.00048	0.04733
P	-1.92320	-2.27475	0.02094
P	-1.91935	2.27663	0.01562
N	-3.66452	0.00207	-0.06910
C	-4.36477	-1.17293	-0.15254
C	-5.76386	-1.21094	-0.23803
H	-6.26880	-2.17596	-0.29972
C	-6.45832	0.00473	-0.24193
H	-7.55013	0.00574	-0.30874
C	-5.76621	1.21915	-0.16276
H	-6.27291	2.18520	-0.16595
C	-4.36713	1.17855	-0.07822
O	-3.68137	-2.33874	-0.15622
O	-3.68646	2.34316	0.00137
C	-1.75888	-3.25144	1.66753
C	-2.61351	-2.46465	2.68990
H	-3.68960	-2.53163	2.46342
H	-2.45248	-2.89668	3.69399
H	-2.32643	-1.39881	2.72486
C	-2.24911	-4.70975	1.58589
H	-1.57879	-5.34185	0.98190
H	-2.26616	-5.13587	2.60555
H	-3.26986	-4.78278	1.17785
C	-0.27679	-3.19730	2.10197
H	0.07725	-2.15789	2.20509
H	-0.17867	-3.68296	3.08952
H	0.39234	-3.72800	1.40590
C	-1.45294	-3.27009	-1.55164
C	-1.65498	-2.27578	-2.72096
H	-1.05741	-1.35816	-2.58668
H	-1.34229	-2.76437	-3.66174
H	-2.71342	-1.98594	-2.83151
C	0.04012	-3.65250	-1.44835
H	0.22003	-4.42834	-0.68594
H	0.36963	-4.06536	-2.41881
H	0.67780	-2.77900	-1.22678
C	-2.33030	-4.51674	-1.78871
H	-3.40283	-4.26745	-1.78853
H	-2.08233	-4.93308	-2.78193
H	-2.15556	-5.31005	-1.04784
C	-1.62804	3.30802	1.60954
C	-1.95758	2.34108	2.77246
H	-1.34981	1.42132	2.72747
H	-1.75267	2.85176	3.73095
H	-3.02088	2.04857	2.77041
C	-0.13523	3.70022	1.66527
H	0.12263	4.46536	0.91490
H	0.08503	4.12886	2.65948
H	0.53140	2.83118	1.52498
C	-2.53066	4.55453	1.71704
H	-3.59566	4.29793	1.60712
H	-2.39335	4.99936	2.71934
H	-2.27960	5.32819	0.97747
C	-1.56623	3.21470	-1.62242
C	-2.28482	2.38972	-2.71712
H	-3.38110	2.44381	-2.61994
H	-2.01345	2.80162	-3.70577
H	-1.98000	1.32866	-2.69219
C	-2.07716	4.66777	-1.64186
H	-1.49300	5.32468	-0.97780
H	-1.97141	5.06664	-2.66718
H	-3.14148	4.73818	-1.36583
C	-0.04121	3.16364	-1.87041
H	0.16880	3.59393	-2.86626
H	0.52744	3.75231	-1.13259
H	0.33933	2.12918	-1.86151
C	0.36399	0.00061	0.07862
H	0.87412	-0.03639	1.21104
C	1.64529	-0.00019	0.08475
C	3.07872	-0.00109	0.06135
C	3.78532	-1.22887	0.03208
C	3.78658	1.22624	0.05451
H	3.21412	-2.16192	0.03669
H	3.21622	2.15953	0.07453
C	5.18965	-1.24646	-0.00708
C	5.19100	1.24280	0.01461
C	5.85945	-0.00202	-0.01382
H	6.95016	-0.00236	-0.04386
C	5.94280	2.59205	0.00265
C	5.57923	3.38961	1.28381
C	5.51367	3.40223	-1.24999
H	5.76408	2.86185	-2.17863
H	4.42932	3.60547	-1.25875
H	6.03534	4.37462	-1.26939
H	4.49716	3.59465	1.34987
H	6.10273	4.36118	1.28656
H	5.87604	2.83962	2.19300
C	5.93981	-2.59622	-0.04272
C	5.50945	-3.38402	-1.30915
C	5.57554	-3.41552	1.22445
H	5.87316	-2.88181	2.14301
H	4.49320	-3.62032	1.28719
H	6.09783	-4.38764	1.21016
H	4.42490	-3.58600	-1.32107
H	6.03007	-4.35648	-1.34561
H	5.76017	-2.82787	-2.22834
C	7.47616	2.41061	-0.03760
H	7.85245	1.86556	0.84528
H	7.80663	1.87632	-0.94501

H 7.96274 3.40013 -0.04417
C 7.47338 -2.41596 -0.08025
H 7.80416 -1.86609 -0.97819
H 7.85062 -1.88707 0.81200
H 7.95874 -3.40579 -0.10451

TS(C-E)$_{O-Ar}$
SCF (BP86) Energy = -1775.59461421
Enthalpy 0K = -1774.717044
Enthalpy 298K = -1774.661456
Free Energy 298K = -1774.806629
Lowest Frequency = -629.9917 cm^{-1}
Second Frequency = 5.0932 cm^{-1}
SCF (BP86-D3BJ) Energy = -1775.854929
SCF (FB) Energy = -1775.6356
SCF (DFB) Energy = -1775.641791
SCF (BS2) Energy = -2445.310446

Rh -1.58438 -0.00000 -0.01117
P -1.91767 -2.29434 0.01510
P -1.91774 2.29433 0.01528
N -3.67579 -0.00003 -0.00600
C -4.37342 -1.17999 -0.01316
C -5.77438 -1.21801 -0.02592
H -6.28428 -2.18237 -0.02941
C -6.46652 -0.00008 -0.03222
H -7.56032 -0.00010 -0.04168
C -5.77442 1.21788 -0.02582
H -6.28435 2.18222 -0.02924
C -4.37346 1.17989 -0.01307
O -3.68487 -2.34353 -0.00662
O -3.68495 2.34346 -0.00644
C -1.58469 -3.27111 1.62767
C -2.33293 -2.50103 2.74190
H -3.42593 -2.54088 2.60881
H -2.09390 -2.97204 3.71191
H -2.02127 -1.44401 2.79355
C -2.08790 -4.72718 1.57061
H -1.49159 -5.34684 0.88261
H -1.98878 -5.17201 2.57709
H -3.14913 -4.79168 1.28130
C -0.06287 -3.22268 1.89757
H 0.33164 -2.19306 1.89588
H 0.12800 -3.65667 2.89530
H 0.51247 -3.81244 1.16696
C -1.56683 -3.23409 -1.61707
C -1.87243 -2.20471 -2.73295
H -1.23882 -1.30531 -2.64349
H -1.66189 -2.67016 -3.71271
H -2.93242 -1.89822 -2.73512
C -0.06431 -3.59272 -1.64088
H 0.17996 -4.40225 -0.93393
H 0.19634 -3.95227 -2.65246
H 0.57473 -2.71943 -1.42239
C -2.45059 -4.48245 -1.81406
H -3.52289 -4.24344 -1.73755
H -2.26607 -4.88035 -2.82828
H -2.21931 -5.28569 -1.09983
C -1.58480 3.27098 1.62793
C -2.33301 2.50078 2.74209
H -2.02132 1.44377 2.79365
H -2.09399 2.97171 3.71215
H -3.42602 2.54062 2.60901
C -0.06297 3.22257 1.89782
H 0.51235 3.81242 1.16726
H 0.12788 3.65648 2.89559
H 0.33157 2.19297 1.89603
C -2.08805 4.72704 1.57099
H -3.14928 4.79153 1.28169
H -1.98895 5.17178 2.57752
H -1.49176 5.34677 0.88305
C -1.56694 3.23423 -1.61681
C -1.87251 2.20493 -2.73278
H -2.93249 1.89841 -2.73497
H -1.66199 2.67047 -3.71250
H -1.23888 1.30554 -2.64339
C -2.45073 4.48258 -1.81369
H -2.21947 5.28577 -1.09941
H -2.26625 4.88056 -2.82788
H -3.52303 4.24353 -1.73719
C -0.06443 3.59290 -1.64060
H 0.19620 3.95255 -2.65216
H 0.17982 4.40238 -0.93358
H 0.57464 2.71961 -1.42219
C 0.37738 0.00002 -0.08646
H -0.64232 -0.00004 1.23596
C 1.62336 0.00002 -0.00572
C 3.04887 0.00002 -0.00687
C 3.76729 1.22306 -0.00496
C 3.76730 -1.22301 -0.00475
H 3.19889 2.15814 -0.00637
H 3.19890 -2.15809 -0.00599
C 5.17192 1.24136 -0.00201
C 5.17192 -1.24131 -0.00178
C 5.84648 0.00003 -0.00045
H 6.93747 0.00003 0.00129
C 5.92076 2.59305 -0.00177
C 5.52160 3.39851 1.26349
C 5.52620 3.39624 -1.26993
H 5.80361 2.85025 -2.18766
H 4.44168 3.59458 -1.31035
H 6.04550 4.37044 -1.28137
H 4.43687 3.59660 1.29967
H 6.04051 4.37291 1.27489
H 5.79601 2.85439 2.18324
C 5.92077 -2.59299 -0.00130
C 5.52624 -3.39640 -1.26934
C 5.52158 -3.39824 1.26408
H 5.79597 -2.85397 2.18375
H 4.43684 -3.59634 1.30027
H 6.04049 -4.37265 1.27566
H 4.44172 -3.59474 -1.30975
H 6.04553 -4.37060 -1.28061
H 5.80367 -2.85056 -2.18715
C 7.45541 2.41742 0.00115
H 7.80825 1.87823 0.89716
H 7.81144 1.87695 -0.89282
H 7.93980 3.40837 0.00127
C 7.45541 -2.41737 0.00163
H 7.81146 -1.87705 -0.89243
H 7.80823 -1.87801 0.89755
H 7.93981 -3.40831 0.00193

E$_{O-Ar}$
SCF (BP86) Energy = -1775.60047370
Enthalpy 0K = -1774.721048
Enthalpy 298K = -1774.665442

Free Energy 298K = -1774.809748
Lowest Frequency = 5.3868 cm^{-1}
Second Frequency = 14.0854 cm^{-1}
SCF (BP86-D3BJ) Energy = -1775.861389
SCF (FB) Energy = -1775.643132
SCF (DFB) Energy = -1775.649931
SCF (BS2) Energy = -2445.315253

Rh	-1.59081	0.00005	0.02325
P	-1.92091	-2.29453	0.03172
P	-1.92062	2.29462	0.03045
N	-3.68709	0.00013	-0.07165
C	-4.37910	-1.17941	-0.09063
C	-5.77941	-1.21851	-0.13949
H	-6.29005	-2.18242	-0.15552
C	-6.47047	0.00029	-0.16422
H	-7.56365	0.00036	-0.20163
C	-5.77925	1.21902	-0.14017
H	-6.28976	2.18298	-0.15672
C	-4.37894	1.17976	-0.09129
O	-3.68498	-2.34267	-0.06803
O	-3.68467	2.34295	-0.06935
C	-1.63704	-3.29764	1.63660
C	-2.49100	-2.61809	2.73225
H	-3.57029	-2.69480	2.52541
H	-2.29285	-3.12762	3.69178
H	-2.22935	-1.55426	2.86357
C	-2.04999	-4.77765	1.50408
H	-1.39356	-5.33374	0.81642
H	-1.96015	-5.25587	2.49590
H	-3.09482	-4.89240	1.17320
C	-0.13687	-3.16763	1.99099
H	0.19278	-2.11629	2.03004
H	0.02607	-3.61696	2.98689
H	0.50998	-3.70309	1.27848
C	-1.48512	-3.19908	-1.59921
C	-1.71385	-2.13863	-2.70442
H	-1.06311	-1.25693	-2.56448
H	-1.46075	-2.58366	-3.68361
H	-2.76543	-1.80836	-2.75485
C	0.01282	-3.57322	-1.54572
H	0.21022	-4.39514	-0.83862
H	0.32480	-3.92079	-2.54692
H	0.64631	-2.70897	-1.27921
C	-2.37188	-4.42981	-1.87673
H	-3.44348	-4.17630	-1.86066
H	-2.13061	-4.80929	-2.88609
H	-2.19614	-5.25083	-1.16706
C	-1.63661	3.29859	1.63477
C	-2.49050	2.61964	2.73086
H	-2.22884	1.55589	2.86276
H	-2.29230	3.12972	3.69008
H	-3.56981	2.69623	2.52404
C	-0.13642	3.16876	1.98913
H	0.51037	3.70386	1.27630
H	0.02658	3.61859	2.98479
H	0.19324	2.11744	2.02868
C	-2.04955	4.77853	1.50150
H	-3.09441	4.89312	1.17065
H	-1.95961	5.25729	2.49305
H	-1.39318	5.33424	0.81347
C	-1.48464	3.19813	-1.60101
C	-1.71331	2.13699	-2.70558
H	-2.76489	1.80671	-2.75588
H	-1.46012	2.58142	-3.68502
H	-1.06259	1.25538	-2.56504
C	-2.37135	4.42870	-1.87938
H	-2.19563	5.25017	-1.17021
H	-2.13001	4.80754	-2.88896
H	-3.44296	4.17524	-1.86320
C	0.01330	3.57225	-1.54761
H	0.32540	3.91917	-2.54900
H	0.21064	4.39462	-0.84102
H	0.64674	2.70816	-1.28047
C	0.36468	-0.00001	0.01686
H	-1.55059	0.00056	1.54282
C	1.61113	-0.00005	0.04177
C	3.03858	-0.00009	0.02218
C	3.75866	1.22168	0.01587
C	3.75861	-1.22188	0.01435
H	3.19074	2.15716	0.02333
H	3.19065	-2.15735	0.02066
C	5.16339	1.24053	0.00295
C	5.16334	-1.24076	0.00137
C	5.83886	-0.00013	-0.00443
H	6.92979	-0.00014	-0.01508
C	5.91158	2.59266	-0.00296
C	5.52673	3.39594	1.26808
C	5.50261	3.39821	-1.26499
H	5.77034	2.85410	-2.18674
H	4.41745	3.59520	-1.29290
H	6.02075	4.37306	-1.28047
H	4.44231	3.59295	1.31717
H	6.04524	4.37068	1.27548
H	5.81180	2.85008	2.18354
C	5.91148	-2.59292	-0.00624
C	5.50229	-3.39699	-1.26915
C	5.52676	-3.39765	1.26392
H	5.81197	-2.85286	2.17997
H	4.44235	-3.59468	1.31293
H	6.04524	-4.37242	1.27014
H	4.41712	-3.59391	-1.29715
H	6.02039	-4.37185	-1.28582
H	5.76993	-2.85183	-2.19030
C	7.44631	2.41818	-0.01780
H	7.80942	1.87763	0.87327
H	7.79235	1.87898	-0.91646
H	7.93027	3.40940	-0.02165
C	7.44621	-2.41849	-0.02110
H	7.79212	-1.87819	-0.91914
H	7.80948	-1.87905	0.87057
H	7.93012	-3.40972	-0.02625

$10_{o\text{-}Ar}$

SCF (BP86) Energy = -1775.61581242
Enthalpy 0K = -1774.734340
Enthalpy 298K = -1774.678732
Free Energy 298K = -1774.823642
Lowest Frequency = 8.1893 cm^{-1}
Second Frequency = 11.0302 cm^{-1}
SCF (BP86-D3BJ) Energy = -1775.878639
SCF (FB) Energy = -1775.655648
SCF (DFB) Energy = -1775.661348
SCF (BS2) Energy = -2445.329201

Rh	1.42529	-0.00078	0.25099
P	1.33826	2.32504	0.27074

P	2.16466	-2.19217	0.06726
N	3.42481	0.38984	-0.28637
C	3.86837	1.67864	-0.42504
C	5.19326	1.97520	-0.77647
H	5.50259	3.01649	-0.87601
C	6.07235	0.90508	-0.98630
H	7.11159	1.10732	-1.26196
C	5.64092	-0.42042	-0.84645
H	6.30405	-1.27259	-1.00113
C	4.30288	-0.64147	-0.49074
O	3.00139	2.69286	-0.22368
O	3.86715	-1.90990	-0.33536
C	1.32607	3.16895	1.99195
C	2.42796	2.44475	2.80235
H	3.43523	2.64675	2.40315
H	2.39900	2.81493	3.84281
H	2.26702	1.35260	2.82382
C	1.61698	4.68126	1.94437
H	0.78492	5.25209	1.50316
H	1.74740	5.04614	2.97926
H	2.54132	4.91196	1.39089
C	-0.05134	2.88844	2.63603
H	-0.29318	1.81287	2.64273
H	-0.02445	3.23881	3.68349
H	-0.87123	3.42357	2.13196
C	0.42699	3.27290	-1.12288
C	0.59051	2.37851	-2.37559
H	0.18821	1.36424	-2.21110
H	0.03833	2.83830	-3.21476
H	1.64657	2.28970	-2.68199
C	-1.06621	3.37501	-0.74149
H	-1.23656	4.07996	0.08817
H	-1.62571	3.75697	-1.61387
H	-1.50707	2.39900	-0.47398
C	1.02358	4.66666	-1.40979
H	2.10428	4.61790	-1.61473
H	0.52851	5.07611	-2.30869
H	0.85395	5.37878	-0.58959
C	2.42012	-3.26081	1.63782
C	2.78521	-2.24994	2.75166
H	1.99896	-1.48890	2.89074
H	2.90967	-2.79890	3.70246
H	3.73613	-1.73225	2.54035
C	1.07765	-3.94826	1.97410
H	0.83652	-4.75889	1.26777
H	1.15456	-4.40156	2.97855
H	0.23337	-3.23773	1.99431
C	3.55456	-4.29703	1.49657
H	4.50702	-3.82595	1.20852
H	3.70258	-4.78385	2.47732
H	3.32138	-5.08774	0.76927
C	1.61885	-3.15225	-1.49878
C	1.89583	-2.18953	-2.67842
H	2.97417	-2.01931	-2.82911
H	1.49455	-2.64183	-3.60294
H	1.39919	-1.21386	-2.53308
C	2.37725	-4.47669	-1.71068
H	2.10243	-5.23868	-0.96419
H	2.10612	-4.88217	-2.70224
H	3.47039	-4.33923	-1.69503
C	0.09626	-3.39790	-1.38543
H	-0.25754	-3.83580	-2.33597
H	-0.16144	-4.10635	-0.58283
H	-0.46296	-2.46360	-1.21366
C	-0.29691	-0.35629	0.80144
H	-1.49806	-1.00005	2.31915
C	-1.50610	-0.62657	1.27952
C	-2.83413	-0.47132	0.64616
C	-2.98135	-0.26399	-0.74426
C	-3.98458	-0.54615	1.45827
H	-2.08258	-0.23293	-1.37074
H	-3.85966	-0.71142	2.53429
C	-4.25579	-0.13274	-1.32669
C	-5.27522	-0.41220	0.91253
C	-5.38279	-0.20605	-0.47872
H	-6.37641	-0.10905	-0.91777
C	-6.50862	-0.50001	1.83854
C	-6.42415	0.61966	2.91039
C	-6.52513	-1.88444	2.54029
H	-6.58999	-2.70226	1.80251
H	-5.62011	-2.04935	3.14907
H	-7.39758	-1.96033	3.21240
H	-5.51566	0.53012	3.52972
H	-7.29535	0.56657	3.58635
H	-6.41665	1.61826	2.44096
C	-4.38635	0.06102	-2.85511
C	-3.75930	-1.15967	-3.58033
C	-3.63582	1.35057	-3.28011
H	-4.06544	2.23876	-2.78569
H	-2.56361	1.30298	-3.02353
H	-3.71296	1.49649	-4.37188
H	-2.69030	-1.27820	-3.33383
H	-3.84017	-1.03796	-4.67479
H	-4.27591	-2.09357	-3.30105
C	-7.83650	-0.33236	1.06752
H	-7.90229	0.64868	0.56608
H	-7.97598	-1.12111	0.30825
H	-8.68263	-0.39988	1.77183
C	-5.85676	0.18909	-3.31136
H	-6.44222	-0.71594	-3.07559
H	-6.35849	1.05689	-2.84981
H	-5.89304	0.32940	-4.40491

TS(B-10)'$_{o\text{-}Ar}$

SCF (BP86) Energy = -1775.51764068
Enthalpy 0K = -1774.637854
Enthalpy 298K = -1774.582764
Free Energy 298K = -1774.721335
Lowest Frequency = -273.8383 cm^{-1}
Second Frequency = 20.4939 cm^{-1}
SCF (BP86-D3BJ) Energy = -1775.806318
SCF (FB) Energy = -1775.570888
SCF (DFB) Energy = -1775.57623
SCF (BS2) Energy = -2445.24517

Rh	1.09642	-0.12009	-0.23801
P	0.58051	-2.31206	0.14689
P	2.17319	1.93371	-0.55880
N	2.87467	-0.53715	0.71806
C	3.09217	-1.80595	1.21893
C	4.29622	-2.13037	1.87737
H	4.42320	-3.14233	2.26463
C	5.28608	-1.15321	2.00183
H	6.22527	-1.39202	2.50953
C	5.09077	0.12812	1.46750
H	5.84576	0.91324	1.52582
C	3.87613	0.38967	0.82422

O	2.15513	-2.74005	1.08219
O	3.68923	1.61540	0.27047
C	0.94614	-3.54703	-1.32136
C	2.23510	-3.02939	-1.99970
H	3.10405	-3.08070	-1.32512
H	2.45070	-3.66563	-2.87735
H	2.12465	-1.98779	-2.34501
C	1.18910	-4.97579	-0.78939
H	0.26175	-5.45139	-0.43192
H	1.56546	-5.59183	-1.62622
H	1.94248	-5.00190	0.01201
C	-0.19853	-3.57776	-2.35648
H	-0.32857	-2.60875	-2.86200
H	0.05619	-4.32856	-3.12722
H	-1.16372	-3.86713	-1.91268
C	-0.59050	-3.02107	1.52917
C	-0.80261	-1.87854	2.54735
H	-1.35680	-1.03451	2.11309
H	-1.39174	-2.26947	3.39700
H	0.15474	-1.50420	2.94682
C	-1.93962	-3.46989	0.92802
H	-1.81835	-4.31416	0.22942
H	-2.58896	-3.82070	1.75079
H	-2.46241	-2.65584	0.40481
C	0.05151	-4.21215	2.28021
H	1.00880	-3.94296	2.74683
H	-0.64946	-4.51007	3.08072
H	0.21002	-5.09201	1.64203
C	2.88065	2.36308	-2.29685
C	3.19282	0.99563	-2.94982
H	2.29579	0.35698	-3.01441
H	3.57527	1.16594	-3.97270
H	3.96640	0.44210	-2.39174
C	1.78910	3.09002	-3.11203
H	1.60701	4.11411	-2.74808
H	2.12097	3.17044	-4.16274
H	0.82935	2.54359	-3.11367
C	4.17542	3.20104	-2.24379
H	4.94290	2.72556	-1.61390
H	4.58160	3.28055	-3.26845
H	4.00807	4.22355	-1.87670
C	1.62044	3.46812	0.45349
C	1.54346	2.96703	1.91555
H	2.54285	2.74338	2.32142
H	1.09310	3.75804	2.54186
H	0.92389	2.05748	2.00753
C	2.59408	4.66005	0.36883
H	2.58128	5.14037	-0.62250
H	2.28169	5.42447	1.10353
H	3.62857	4.36909	0.61116
C	0.21372	3.88402	-0.03194
H	-0.16777	4.68343	0.62892
H	0.22213	4.28646	-1.05749
H	-0.50157	3.04541	0.00323
C	-0.60162	0.13667	-1.45589
H	-0.71377	0.61830	-2.42662
C	-0.76144	-1.07100	-0.85765
C	-2.01780	0.02821	-0.57248
C	-3.19685	-0.28105	-1.31645
C	-2.11114	0.78782	0.62606
H	-3.08907	-0.87549	-2.22753
H	-1.17660	1.01483	1.14783
C	-4.45146	0.15625	-0.88481
C	-3.36348	1.21624	1.10479
C	-4.49797	0.89089	0.32906
H	-5.47735	1.22616	0.68625
C	-5.75409	-0.13567	-1.65707
C	-6.71670	-0.94475	-0.74648
C	-5.49458	-0.95074	-2.94263
H	-4.83501	-0.41418	-3.64689
H	-5.04769	-1.93650	-2.72499
H	-6.44951	-1.13213	-3.46255
H	-6.27127	-1.91030	-0.45244
H	-7.65659	-1.15286	-1.28538
H	-6.97825	-0.39673	0.17422
C	-3.54158	2.01567	2.41333
C	-2.19790	2.25648	3.13294
C	-4.47379	1.22409	3.37002
H	-5.47238	1.05537	2.93363
H	-4.04364	0.24034	3.62371
H	-4.61401	1.78711	4.30847
H	-1.69932	1.31035	3.40691
H	-2.37444	2.81716	4.06576
H	-1.50232	2.85204	2.51768
C	-6.42062	1.20976	-2.05196
H	-5.76229	1.80457	-2.70779
H	-7.36070	1.01764	-2.59647
H	-6.66827	1.82532	-1.17090
C	-4.18127	3.39241	2.08899
H	-3.53914	3.98214	1.41275
H	-5.16985	3.28844	1.61134
H	-4.32151	3.97106	3.01794

TS(B-10)"$_{\text{o-Ar}}$

SCF (BP86) Energy = -1775.54863066
Enthalpy 0K = -1774.669963
Enthalpy 298K = -1774.614420
Free Energy 298K = -1774.756536
Lowest Frequency = -321.7255 cm^{-1}
Second Frequency = 9.5419 cm^{-1}
SCF (BP86-D3BJ) Energy = -1775.82065
SCF (FB) Energy = -1775.587193
SCF (DFB) Energy = -1775.592631
SCF (BS2) Energy = -2445.261953

Rh	1.17143	-0.15463	0.20058
P	0.60346	-2.33443	-0.32425
P	2.40320	1.77023	0.50352
N	2.94678	-0.72760	-0.76702
C	3.10296	-1.99556	-1.25883
C	4.27158	-2.41763	-1.91072
H	4.33385	-3.44208	-2.28060
C	5.31478	-1.49720	-2.06046
H	6.23750	-1.79706	-2.56545
C	5.18334	-0.19449	-1.56409
H	5.97311	0.55248	-1.65603
C	3.98543	0.15052	-0.92334
O	2.09110	-2.87538	-1.11322
O	3.84574	1.40666	-0.44227
C	-0.59998	-2.73148	-1.77759
C	-0.53307	-1.48274	-2.68995
H	0.48136	-1.32284	-3.09297
H	-1.21353	-1.62943	-3.54874
H	-0.84113	-0.56746	-2.15659
C	-0.18623	-3.97813	-2.58780
H	-0.25295	-4.90787	-2.00406
H	-0.87615	-4.07620	-3.44581
H	0.83611	-3.89069	-2.98488

C	-2.03256	-2.89867	-1.22877
H	-2.35204	-2.04293	-0.61088
H	-2.73090	-2.96568	-2.08279
H	-2.14766	-3.82465	-0.64166
C	0.56104	-3.63012	1.09187
C	1.87762	-3.42024	1.87709
H	1.99059	-2.37107	2.20281
H	1.86051	-4.06007	2.77785
H	2.76089	-3.69995	1.28098
C	-0.63225	-3.28244	2.01008
H	-1.60491	-3.42557	1.51266
H	-0.61082	-3.95041	2.89008
H	-0.57136	-2.24292	2.37437
C	0.47236	-5.08789	0.60113
H	1.27593	-5.33233	-0.11189
H	0.58036	-5.76292	1.46972
H	-0.49895	-5.31505	0.13296
C	1.91633	3.38823	-0.40905
C	1.27703	2.90054	-1.73216
H	0.45999	2.17899	-1.55805
H	0.86884	3.77073	-2.27755
H	2.02160	2.41543	-2.38518
C	0.86912	4.13048	0.44994
H	1.31585	4.57170	1.35643
H	0.44396	4.96208	-0.14052
H	0.03405	3.47648	0.75501
C	3.10544	4.31296	-0.74357
H	3.90412	3.77542	-1.27763
H	2.74190	5.11946	-1.40618
H	3.53883	4.79111	0.14616
C	3.25256	2.05360	2.21144
C	4.00649	0.73718	2.51638
H	4.85522	0.58090	1.83167
H	4.40866	0.78881	3.54423
H	3.33763	-0.13902	2.45381
C	4.24322	3.23463	2.21836
H	3.73223	4.20899	2.16152
H	4.80567	3.21797	3.16967
H	4.97488	3.16735	1.39771
C	2.15785	2.26280	3.27985
H	2.64091	2.38576	4.26614
H	1.54377	3.15953	3.09740
H	1.49384	1.38332	3.34449
C	-0.54939	0.43151	1.09211
C	-0.76679	0.86770	2.28144
H	-1.02464	1.25666	3.25607
C	-2.03485	0.58648	0.63485
C	-2.37754	1.60987	-0.27933
C	-3.03686	-0.25400	1.17603
H	-1.59057	2.26026	-0.66521
H	-2.74293	-1.01529	1.90151
C	-3.70716	1.76162	-0.70637
C	-4.38305	-0.11377	0.78058
C	-4.68196	0.89289	-0.15842
H	-5.72253	1.01670	-0.47543
C	-5.51448	-0.99394	1.35481
C	-4.98904	-2.03777	2.36437
C	-6.21951	-1.74642	0.19481
H	-6.65546	-1.05299	-0.54337
H	-5.51523	-2.40827	-0.33779
H	-7.03976	-2.36941	0.59090
H	-4.26807	-2.73431	1.90131
H	-5.83041	-2.64138	2.74317
H	-4.50624	-1.56421	3.23691
C	-4.13410	2.83770	-1.72742
C	-4.77158	2.14717	-2.96285
C	-2.94315	3.69387	-2.20963
H	-2.46534	4.24075	-1.37809
H	-2.17454	3.08390	-2.71566
H	-3.29835	4.44419	-2.93537
H	-4.04987	1.47756	-3.46125
H	-5.09479	2.90651	-3.69552
H	-5.65715	1.54886	-2.69148
C	-5.17625	3.78008	-1.06607
H	-6.07760	3.23652	-0.73793
H	-4.74983	4.29095	-0.18601
H	-5.49758	4.55150	-1.78690
C	-6.54366	-0.08725	2.08225
H	-6.99134	0.65683	1.40275
H	-7.36455	-0.70002	2.49281
H	-6.07355	0.45793	2.91842

TS(10-F)$_{O\text{-}Ar}$

SCF (BP86) Energy = -1775.51764068
Enthalpy 0K = -1774.637854
Enthalpy 298K = -1774.582764
Free Energy 298K = -1774.721335
Lowest Frequency = -273.8383 cm^{-1}
Second Frequency = 20.4939 cm^{-1}
SCF (BP86-D3BJ) Energy = -1775.802628
SCF (FB) Energy = -1775.556636
SCF (DFB) Energy = -1775.562191
SCF (BS2) Energy = -2445.232566

Rh	0.71125	0.17249	-0.22619
P	2.46611	-1.40007	-0.49800
P	-0.21641	2.31439	0.14977
N	2.15415	0.94812	1.09323
C	3.19419	0.16592	1.52875
C	4.12938	0.61535	2.47013
H	4.92579	-0.05701	2.79204
C	4.02404	1.93558	2.92734
H	4.74531	2.31660	3.65621
C	3.01935	2.77751	2.43891
H	2.92018	3.81796	2.75128
C	2.10451	2.25047	1.51327
O	3.33179	-1.07319	1.01133
O	1.14949	3.05005	1.01416
C	3.82178	-0.82385	-1.77690
C	4.07338	0.68172	-1.52651
H	4.55218	0.87755	-0.55340
H	4.76306	1.04722	-2.30839
H	3.14267	1.26860	-1.59403
C	5.14658	-1.59172	-1.58401
H	5.07571	-2.64306	-1.90266
H	5.91516	-1.11400	-2.21830
H	5.50568	-1.55514	-0.54311
C	3.30591	-0.99366	-3.22266
H	2.37416	-0.43421	-3.39476
H	4.08029	-0.59811	-3.90498
H	3.13162	-2.04451	-3.49606
C	2.41840	-3.33070	-0.34577
C	1.15462	-3.67280	0.46625
H	0.23460	-3.37860	-0.06086
H	1.12318	-4.76656	0.61962
H	1.16764	-3.20159	1.46419
C	2.30013	-3.96235	-1.75040

H	3.22618	-3.86361	-2.33760
H	2.10845	-5.04311	-1.62432
H	1.46135	-3.53883	-2.32670
C	3.65424	-3.88038	0.40257
H	3.73926	-3.46769	1.41880
H	3.52498	-4.97421	0.49192
H	4.59990	-3.70334	-0.12694
C	-0.29941	3.56307	-1.32451
C	0.65244	3.00665	-2.40814
H	0.38389	1.98378	-2.71753
H	0.60087	3.66655	-3.29339
H	1.69993	3.00077	-2.06263
C	-1.74369	3.59514	-1.86854
H	-2.44441	4.08022	-1.17055
H	-1.75355	4.18112	-2.80496
H	-2.12645	2.58926	-2.10624
C	0.15923	4.98413	-0.93098
H	1.18384	4.99106	-0.52990
H	0.14954	5.60652	-1.84417
H	-0.50493	5.46375	-0.19831
C	-1.50748	2.67459	1.55066
C	-1.00454	1.87550	2.77704
H	-0.05367	2.26624	3.17348
H	-1.75688	1.96694	3.58107
H	-0.88778	0.80254	2.54965
C	-1.57163	4.17670	1.89820
H	-2.06557	4.76628	1.10941
H	-2.17888	4.29178	2.81457
H	-0.57842	4.60689	2.09996
C	-2.90834	2.16112	1.16358
H	-3.59794	2.40274	1.99318
H	-3.30662	2.64279	0.25780
H	-2.92914	1.07214	1.01700
C	0.03266	-0.71155	-1.85714
H	-0.18504	-1.65792	-3.95863
C	-0.03627	-1.23579	-2.98109
C	-1.30017	-0.68951	-0.44437
C	-2.43176	-0.27380	-1.18026
C	-1.46680	-1.51540	0.68336
H	-2.28878	0.32471	-2.08289
H	-0.59912	-1.83966	1.26016
C	-3.72263	-0.72056	-0.83556
C	-2.76300	-1.90370	1.10943
C	-3.86356	-1.51524	0.32310
H	-4.85991	-1.85004	0.61274
C	-4.92065	-0.39306	-1.75960
C	-4.69139	-1.09534	-3.12567
C	-5.03742	1.13518	-1.98668
H	-5.21465	1.66846	-1.03710
H	-4.13224	1.55578	-2.45621
H	-5.88440	1.35384	-2.65967
H	-3.76617	-0.74524	-3.61435
H	-5.53357	-0.88712	-3.80852
H	-4.61489	-2.18873	-3.00037
C	-2.92401	-2.76772	2.38251
C	-2.21967	-2.07998	3.58134
C	-2.28303	-4.16007	2.14116
H	-2.76055	-4.67457	1.29015
H	-1.20393	-4.08154	1.92902
H	-2.40273	-4.79563	3.03588
H	-1.13926	-1.93986	3.40537
H	-2.32803	-2.69699	4.49007
H	-2.66291	-1.09088	3.78832
C	-6.26203	-0.89239	-1.17614
H	-6.28006	-1.98917	-1.05820
H	-6.48398	-0.43295	-0.19739
H	-7.08298	-0.62429	-1.86204
C	-4.40839	-2.97851	2.75920
H	-4.93048	-2.02144	2.93051
H	-4.95747	-3.54064	1.98479
H	-4.47064	-3.56351	3.69209

F_{O-Ar}

SCF (BP86) Energy = -1775.55986685
Enthalpy 0K = -1774.679157
Enthalpy 298K = -1774.623400
Free Energy 298K = -1774.763408
Lowest Frequency = 18.9493 cm^{-1}
Second Frequency = 24.6728 cm^{-1}
SCF (BP86-D3BJ) Energy = -1775.850476
SCF (FB) Energy = -1775.600138
SCF (DFB) Energy = -1775.606079
SCF (BS2) Energy = -2445.274716

Rh	0.94821	0.02381	-0.51587
P	1.29335	-2.29675	-0.19559
P	1.08444	2.36746	-0.24267
N	1.47482	0.07588	1.52212
C	1.77370	-1.08146	2.18651
C	2.14716	-1.08455	3.53897
H	2.37145	-2.03151	4.03203
C	2.21913	0.14611	4.20426
H	2.50715	0.17321	5.25921
C	1.93960	1.34432	3.53298
H	2.00134	2.31797	4.02121
C	1.57411	1.27103	2.18138
O	1.70518	-2.26021	1.52469
O	1.30086	2.41617	1.51106
C	2.97161	-2.90565	-0.92922
C	3.87184	-1.65419	-1.01234
H	4.03155	-1.18038	-0.02851
H	4.86452	-1.95186	-1.39648
H	3.45416	-0.91675	-1.71751
C	3.67053	-3.96427	-0.05025
H	3.13759	-4.92333	-0.01744
H	4.66952	-4.15708	-0.48159
H	3.81506	-3.60925	0.98225
C	2.71460	-3.41905	-2.36461
H	2.18270	-2.67104	-2.97810
H	3.69182	-3.60748	-2.84495
H	2.15430	-4.36647	-2.38623
C	-0.03687	-3.69303	-0.19858
C	-1.03400	-3.41626	0.94737
H	-1.52555	-2.43843	0.85371
H	-1.81669	-4.19518	0.90677
H	-0.54867	-3.48012	1.93432
C	-0.75472	-3.59390	-1.56515
H	-0.08240	-3.78402	-2.41664
H	-1.54901	-4.36136	-1.59398
H	-1.22922	-2.61022	-1.70545
C	0.55563	-5.10334	0.00568
H	1.10398	-5.19323	0.95703
H	-0.28799	-5.81604	0.04484
H	1.20863	-5.42403	-0.81975
C	2.79615	3.06104	-0.80434
C	3.79058	1.89386	-0.62190
H	3.51502	1.03066	-1.24762

H	4.79414	2.22463	-0.94572
H	3.87567	1.56960	0.42921
C	2.70043	3.40951	-2.30685
H	2.07571	4.29677	-2.49511
H	3.71528	3.64064	-2.67808
H	2.31037	2.56531	-2.90214
C	3.28677	4.25738	0.03848
H	3.27055	4.03447	1.11715
H	4.33516	4.46352	-0.24402
H	2.71513	5.17758	-0.13710
C	-0.33242	3.65197	-0.47420
C	-1.43758	3.36652	0.56567
H	-1.07314	3.49859	1.59679
H	-2.24925	4.09752	0.39896
H	-1.86312	2.35943	0.46510
C	0.13301	5.11327	-0.30450
H	0.84649	5.43116	-1.07966
H	-0.75787	5.75957	-0.40237
H	0.56825	5.30352	0.68945
C	-0.87382	3.41831	-1.90473
H	-1.71502	4.11468	-2.07205
H	-0.12129	3.61668	-2.68437
H	-1.25029	2.39229	-2.03615
C	0.84327	-0.00294	-2.48217
H	1.00355	-0.02055	-4.78915
C	0.93239	-0.01382	-3.71595
C	-1.08218	-0.04159	-0.18030
C	-1.97065	-0.09947	-1.26450
C	-1.57241	-0.02248	1.14230
H	-1.58359	-0.11738	-2.28424
H	-0.88985	0.01826	1.98989
C	-3.37324	-0.13429	-1.04262
C	-2.96294	-0.05673	1.38980
C	-3.83806	-0.11055	0.28237
H	-4.91455	-0.13598	0.46814
C	-4.32267	-0.19800	-2.26200
C	-4.02271	-1.47991	-3.08329
C	-4.09670	1.04767	-3.15903
H	-4.30717	1.97874	-2.60543
H	-3.06206	1.09983	-3.53817
H	-4.76950	1.01299	-4.03344
H	-2.98580	-1.49457	-3.45959
H	-4.69434	-1.53643	-3.95745
H	-4.18039	-2.38693	-2.47486
C	-3.54173	-0.03680	2.82374
C	-4.44715	1.21313	2.99104
C	-2.44330	0.01385	3.90772
H	-1.77931	-0.86744	3.86510
H	-1.82264	0.92349	3.82603
H	-2.91056	0.02444	4.90666
H	-3.87129	2.14359	2.84793
H	-4.88240	1.23415	4.00528
H	-5.28073	1.21738	2.26972
C	-5.80917	-0.22895	-1.84102
H	-6.04611	-1.11397	-1.22575
H	-6.09816	0.67494	-1.27760
H	-6.44505	-0.27358	-2.74098
C	-4.38838	-1.31816	3.05087
H	-5.22077	-1.39501	2.33230
H	-3.77006	-2.22672	2.95049
H	-4.82249	-1.31173	4.06577

9_{NH}

SCF (BP86) Energy = -2537.88846550

Enthalpy 0K = -2536.549203
Enthalpy 298K = -2536.467549
Free Energy 298K = -2536.660105
Lowest Frequency = 14.1004 cm^{-1}
Second Frequency = 18.1482 cm^{-1}
SCF (BP86-D3BJ) Energy = -2538.34435
SCF (FB) Energy = -2538.015502
SCF (DFB) Energy = -2538.033086
SCF (BS2) Energy = -3877.0767

Rh	2.74235	-2.03509	1.21206
P	4.02904	-2.80345	-0.60374
P	1.95707	-1.69022	3.46091
N	4.08694	-3.33041	2.26012
C	1.20450	-1.40063	-0.23171
H	1.57347	-1.77281	-1.19777
C	1.86610	-0.25067	0.27109
H	2.71371	0.12487	-0.31939
C	1.16736	0.87470	1.01784
H	1.92460	1.52779	1.48388
H	0.53887	0.48444	1.83567
C	-0.26527	-1.73365	-0.05213
H	-0.59066	-1.57649	0.98820
H	-0.41984	-2.80658	-0.26402
C	5.17547	-3.88319	1.62906
C	6.08412	-4.73357	2.28750
H	6.93774	-5.14670	1.74523
C	5.86080	-5.03231	3.63417
H	6.55018	-5.69294	4.16806
C	4.75957	-4.48933	4.29945
H	4.56305	-4.70945	5.35133
C	3.89315	-3.63871	3.58364
N	5.33860	-3.55374	0.30176
N	2.78961	-3.07724	4.18039
C	3.33037	-4.32677	-1.61405
C	2.32859	-5.01520	-0.65774
H	2.81764	-5.36659	0.26617
H	1.89772	-5.89918	-1.16294
H	1.50595	-4.34267	-0.36437
C	4.44095	-5.33824	-1.97719
H	5.22661	-4.91303	-2.62092
H	3.98234	-6.17295	-2.53731
H	4.90989	-5.77905	-1.08246
C	2.60803	-3.87917	-2.90239
H	1.84034	-3.10778	-2.72261
H	2.09115	-4.75318	-3.33870
H	3.30836	-3.50424	-3.66585
C	5.05883	-1.58494	-1.70127
C	5.73404	-0.61408	-0.70384
H	4.99728	-0.09445	-0.06845
H	6.29811	0.14747	-1.27179
H	6.44223	-1.13655	-0.04140
C	4.13150	-0.79387	-2.65081
H	3.68251	-1.42749	-3.43014
H	4.73200	-0.02030	-3.16241
H	3.31970	-0.27460	-2.11670
C	6.14182	-2.30238	-2.53561
H	6.84067	-2.89256	-1.91911
H	6.75188	-1.53847	-3.05101
H	5.71574	-2.95448	-3.31440
C	0.18483	-2.11955	4.14923
C	-0.20237	-3.45108	3.46408
H	-0.18965	-3.37035	2.36496
H	-1.22454	-3.73278	3.77571

H	0.47759	-4.26831	3.75153
C	-0.84342	-1.02782	3.78592
H	-0.64685	-0.07273	4.29559
H	-1.84497	-1.37074	4.10271
H	-0.89363	-0.83766	2.70227
C	0.16951	-2.30947	5.68276
H	0.84933	-3.10518	6.03046
H	-0.84614	-2.62389	5.98485
H	0.39608	-1.38142	6.23101
C	2.78710	-0.21495	4.46593
C	3.99468	0.23338	3.60989
H	4.71920	-0.58476	3.46143
H	4.52108	1.05542	4.12937
H	3.68839	0.59181	2.61401
C	3.31251	-0.67927	5.84337
H	2.52219	-1.07140	6.50345
H	3.75465	0.19274	6.35812
H	4.11122	-1.43317	5.75345
C	1.81729	0.96739	4.67126
H	2.38497	1.82184	5.08265
H	1.02160	0.73181	5.39658
H	1.35044	1.30880	3.73451
C	-1.20450	1.40063	0.23171
H	-1.57347	1.77281	1.19777
C	-1.86610	0.25067	-0.27109
H	-2.71371	-0.12487	0.31939
C	-1.16736	-0.87470	-1.01784
H	-1.92460	-1.52779	-1.48388
H	-0.53887	-0.48444	-1.83567
C	0.26527	1.73365	0.05213
H	0.59066	1.57649	-0.98820
H	0.41984	2.80658	0.26402
Rh	-2.74235	2.03509	-1.21206
P	-4.02904	2.80345	0.60374
P	-1.95707	1.69022	-3.46091
N	-4.08694	3.33041	-2.26012
C	-5.17547	3.88319	-1.62906
C	-6.08412	4.73357	-2.28750
H	-6.93774	5.14670	-1.74523
C	-5.86080	5.03231	-3.63417
H	-6.55018	5.69294	-4.16806
C	-4.75957	4.48933	-4.29945
H	-4.56305	4.70945	-5.35133
C	-3.89315	3.63871	-3.58364
N	-5.33860	3.55374	-0.30176
N	-2.78961	3.07724	-4.18039
C	-3.33037	4.32677	1.61405
C	-2.32859	5.01520	0.65774
H	-2.81764	5.36659	-0.26617
H	-1.89772	5.89918	1.16294
H	-1.50595	4.34267	0.36437
C	-4.44095	5.33824	1.97719
H	-5.22661	4.91303	2.62092
H	-3.98234	6.17295	2.53731
H	-4.90989	5.77905	1.08246
C	-2.60803	3.87917	2.90239
H	-1.84034	3.10778	2.72261
H	-2.09115	4.75318	3.33870
H	-3.30836	3.50424	3.66585
C	-5.05883	1.58494	1.70127
C	-5.73404	0.61408	0.70384
H	-4.99728	0.09445	0.06845
H	-6.29811	-0.14747	1.27179
H	-6.44223	1.13655	0.04140
C	-4.13150	0.79387	2.65081
H	-3.68251	1.42749	3.43014
H	-4.73200	0.02030	3.16241
H	-3.31970	0.27460	2.11670
C	-6.14182	2.30238	2.53561
H	-6.84067	2.89256	1.91911
H	-6.75188	1.53847	3.05101
H	-5.71574	2.95448	3.31440
C	-0.18483	2.11955	-4.14923
C	0.20237	3.45108	-3.46408
H	0.18965	3.37035	-2.36496
H	1.22454	3.73278	-3.77571
H	-0.47759	4.26831	-3.75153
C	0.84342	1.02782	-3.78592
H	0.64685	0.07273	-4.29559
H	1.84497	1.37074	-4.10271
H	0.89363	0.83766	-2.70227
C	-0.16951	2.30947	-5.68276
H	-0.84933	3.10518	-6.03046
H	0.84614	2.62389	-5.98485
H	-0.39608	1.38142	-6.23101
C	-2.78710	0.21495	-4.46593
C	-3.99468	-0.23338	-3.60989
H	-4.71920	0.58476	-3.46143
H	-4.52108	-1.05542	-4.12937
H	-3.68839	-0.59181	-2.61401
C	-3.31251	0.67927	-5.84337
H	-2.52219	1.07140	-6.50345
H	-3.75465	-0.19274	-6.35812
H	-4.11122	1.43317	-5.75345
C	-1.81729	-0.96739	-4.67126
H	-2.38497	-1.82184	-5.08265
H	-1.02160	-0.73181	-5.39658
H	-1.35044	-1.30880	-3.73451
H	-6.07668	4.05577	0.19220
H	-2.74029	3.20078	-5.19217
H	6.07668	-4.05577	-0.19220
H	2.74029	-3.20078	5.19217

8_{NH}

SCF (BP86) Energy = -1424.98194552
Enthalpy 0K = -1424.224952
Enthalpy 298K = -1424.179849
Free Energy 298K = -1424.296869
Lowest Frequency = 18.7555 cm^{-1}
Second Frequency = 29.7453 cm^{-1}
SCF (BP86-D3BJ) Energy = -1425.222455
SCF (FB) Energy = -1425.024157
SCF (DFB) Energy = -1425.03031
SCF (BS2) Energy = -2094.613717

C	2.67483	4.48821	0.41572
H	3.68700	4.83002	0.66857
C	2.27335	4.63403	-0.86426
H	2.98567	5.08543	-1.56707
C	0.93717	4.22438	-1.45352
H	0.84271	4.66100	-2.46185
H	0.10790	4.65320	-0.85611
C	1.88265	3.87336	1.55377
H	0.87291	4.32615	1.60701
H	2.37685	4.11772	2.50899
C	-0.09168	2.14309	-0.39994
H	-1.14523	2.44023	-0.50145

C	0.35278	1.93675	0.92862
H	-0.40725	2.03380	1.71712
C	1.73256	2.31393	1.43793
H	1.88849	1.85525	2.42975
H	2.52643	1.93378	0.77570
C	0.73529	2.66982	-1.55442
H	1.71896	2.17999	-1.60307
H	0.21702	2.42848	-2.50040
Rh	-0.15855	-0.01488	0.05203
P	-2.48984	0.16230	0.10052
P	2.06257	-0.93081	-0.04772
N	-0.65409	-2.08080	-0.16066
C	-1.94660	-2.51588	0.00310
C	-2.31030	-3.87130	-0.11929
H	-3.35032	-4.17364	0.02367
C	-1.31426	-4.80194	-0.42824
H	-1.57092	-5.86049	-0.53139
C	0.00664	-4.38565	-0.60574
H	0.80118	-5.09473	-0.84967
C	0.30530	-3.01424	-0.46174
N	-2.87971	-1.54732	0.30264
N	1.58261	-2.53826	-0.62977
C	-3.40028	0.56642	-1.58380
C	-2.39373	0.17141	-2.68942
H	-2.12495	-0.89706	-2.63794
H	-2.85485	0.35372	-3.67779
H	-1.46016	0.75321	-2.62611
C	-4.68406	-0.27521	-1.76367
H	-5.43648	-0.09729	-0.97945
H	-5.15028	0.00134	-2.72658
H	-4.46849	-1.35511	-1.81529
C	-3.75353	2.06410	-1.70461
H	-2.89098	2.72857	-1.53161
H	-4.10928	2.26050	-2.73247
H	-4.56489	2.35978	-1.02029
C	-3.41597	0.89379	1.63666
C	-2.72247	0.25808	2.86479
H	-1.63850	0.46064	2.87704
H	-3.16341	0.68293	3.78456
H	-2.86224	-0.83442	2.89256
C	-3.25564	2.43059	1.68685
H	-3.79333	2.94175	0.87461
H	-3.67879	2.79633	2.63970
H	-2.20223	2.75105	1.65773
C	-4.91859	0.54062	1.65377
H	-5.10554	-0.54614	1.61378
H	-5.35354	0.89816	2.60488
H	-5.47764	1.02852	0.83959
C	3.40274	-0.58081	-1.42026
C	2.61057	-0.50970	-2.74698
H	1.82438	0.26168	-2.71872
H	3.30690	-0.25786	-3.56731
H	2.13330	-1.47290	-2.98806
C	4.13921	0.75443	-1.17579
H	4.76535	0.73505	-0.27142
H	4.81045	0.94362	-2.03304
H	3.46214	1.61936	-1.10395
C	4.45754	-1.70589	-1.51722
H	4.02155	-2.69641	-1.73204
H	5.13167	-1.47799	-2.36297
H	5.08594	-1.77960	-0.61570
C	2.90057	-1.42139	1.66677
C	1.76929	-1.32102	2.71641
H	0.92857	-1.99498	2.48021
H	2.16707	-1.61396	3.70595
H	1.36533	-0.29940	2.79453
C	3.42617	-2.87504	1.65837
H	4.19888	-3.05552	0.89372
H	3.89302	-3.08031	2.63875
H	2.61630	-3.61167	1.53043
C	4.05744	-0.47267	2.04365
H	4.36706	-0.68989	3.08238
H	4.94363	-0.62294	1.40622
H	3.77444	0.58979	2.00469
H	-3.85278	-1.85329	0.29622
H	2.30091	-3.25714	-0.72054

A_{NH}

SCF (BP86) Energy = -1112.91730227
Enthalpy 0K = -1112.338468
Enthalpy 298K = -1112.301753
Free Energy 298K = -1112.403195
Lowest Frequency = 15.6067 cm^{-1}
Second Frequency = 29.5735 cm^{-1}
SCF (BP86-D3BJ) Energy = -1113.092091
SCF (FB) Energy = -1112.968017
SCF (DFB) Energy = -1112.976433
SCF (BS2) Energy = -1782.479111

Rh	0.00003	-0.48544	0.08256
P	2.29812	-0.26780	0.03846
P	-2.29808	-0.26787	0.03837
N	0.00004	1.51514	-0.06516
C	1.18707	2.22164	-0.12610
C	1.20971	3.62334	-0.25002
H	2.16967	4.14313	-0.29568
C	0.00000	4.31855	-0.31122
H	-0.00001	5.40784	-0.40846
C	-1.20968	3.62330	-0.25027
H	-2.16966	4.14304	-0.29613
C	-1.18701	2.22158	-0.12645
N	2.35172	1.48700	-0.05253
N	-2.35165	1.48690	-0.05329
C	3.15615	-0.87912	-1.57649
C	2.49372	-0.08636	-2.72632
H	2.76479	0.98162	-2.70493
H	2.83499	-0.50311	-3.69090
H	1.39281	-0.16414	-2.68817
C	4.68351	-0.68222	-1.61510
H	5.20911	-1.30303	-0.87208
H	5.05856	-0.98023	-2.61117
H	4.97710	0.37083	-1.46380
C	2.79464	-2.37658	-1.72469
H	1.69955	-2.52605	-1.73015
H	3.18322	-2.74932	-2.68954
H	3.22931	-3.00460	-0.93096
C	3.31051	-0.62986	1.63767
C	2.37958	-0.21667	2.80200
H	1.43425	-0.78575	2.79183
H	2.89321	-0.41186	3.76095
H	2.12924	0.85668	2.76589
C	3.59986	-2.14434	1.71778
H	4.32933	-2.47678	0.96143
H	4.02880	-2.37684	2.70889
H	2.68263	-2.75027	1.61041
C	4.61989	0.18230	1.72416
H	4.43124	1.26937	1.71117

H	5.11168	-0.04042	2.68841
H	5.33740	-0.06404	0.92758
C	-3.15571	-0.87972	-1.57656
C	-2.49300	-0.08739	-2.72654
H	-1.39210	-0.16522	-2.68810
H	-2.83409	-0.50448	-3.69103
H	-2.76400	0.98061	-2.70555
C	-2.79423	-2.37724	-1.72414
H	-3.22908	-3.00497	-0.93027
H	-3.18261	-2.75032	-2.68894
H	-1.69914	-2.52677	-1.72933
C	-4.68307	-0.68275	-1.61562
H	-4.97661	0.37037	-1.46477
H	-5.05789	-0.98109	-2.61168
H	-5.20890	-1.30327	-0.87252
C	-3.31100	-0.62929	1.63739
C	-2.38033	-0.21588	2.80184
H	-2.12972	0.85740	2.76541
H	-2.89426	-0.41055	3.76074
H	-1.43512	-0.78517	2.79221
C	-4.62028	0.18311	1.72331
H	-5.33765	-0.06334	0.92663
H	-5.11232	-0.03924	2.68751
H	-4.43148	1.27015	1.71006
C	-3.60064	-2.14369	1.71792
H	-4.02989	-2.37579	2.70898
H	-4.32995	-2.47623	0.96147
H	-2.68350	-2.74981	1.61099
H	3.22378	2.01109	-0.11574
H	-3.22373	2.01096	-0.11653

B_{NH-Ar}

SCF (BP86) Energy = -1735.87141024
Enthalpy 0K = -1734.965595
Enthalpy 298K = -1734.909682
Free Energy 298K = -1735.051739
Lowest Frequency = 11.6033 cm^{-1}
Second Frequency = 16.5167 cm^{-1}
SCF (BP86-D3BJ) Energy = -1736.152509
SCF (FB) Energy = -1735.912782
SCF (DFB) Energy = -1735.91896
SCF (BS2) Energy = -2405.573751

Rh	-1.25596	0.14033	-0.30468
P	-0.82791	2.42482	0.10204
P	-2.22766	-1.98338	-0.47013
N	-2.99693	0.54752	0.81448
C	-3.25014	1.81435	1.28730
C	-4.40632	2.11661	2.03563
H	-4.57280	3.13366	2.39807
C	-5.32060	1.09220	2.29225
H	-6.22344	1.30311	2.87324
C	-5.09486	-0.19850	1.80580
H	-5.80455	-1.00886	1.98777
C	-3.92479	-0.43882	1.05862
N	-2.31492	2.77886	0.99353
N	-3.65644	-1.67873	0.52413
C	-0.98706	3.59460	-1.43046
C	-2.28923	3.15543	-2.13988
H	-3.18139	3.34755	-1.52157
H	-2.39614	3.73078	-3.07737
H	-2.26987	2.08157	-2.39232
C	-1.07730	5.09033	-1.06768
H	-0.13097	5.48344	-0.66383
H	-1.30078	5.66447	-1.98542
H	-1.88777	5.30910	-0.35095
C	0.21510	3.34802	-2.36903
H	0.32774	2.27990	-2.61691
H	0.04871	3.90039	-3.31168
H	1.16490	3.70525	-1.94230
C	0.48676	3.03161	1.39054
C	0.53605	1.91060	2.45382
H	0.87849	0.95770	2.02176
H	1.24557	2.20266	3.24964
H	-0.44787	1.74918	2.92674
C	1.86356	3.17596	0.70970
H	1.90552	4.05191	0.04201
H	2.63196	3.32538	1.48968
H	2.14882	2.27779	0.13749
C	0.09732	4.35426	2.08680
H	-0.83968	4.26347	2.66223
H	0.88771	4.60653	2.81690
H	0.01169	5.20574	1.39574
C	-3.04742	-2.53834	-2.13545
C	-3.55381	-1.23241	-2.79179
H	-2.73559	-0.52458	-2.99703
H	-4.04691	-1.47951	-3.74968
H	-4.29482	-0.71768	-2.15714
C	-1.98780	-3.21025	-3.03527
H	-1.71740	-4.21678	-2.67719
H	-2.40162	-3.32732	-4.05321
H	-1.06398	-2.61343	-3.11823
C	-4.25388	-3.48205	-1.93788
H	-5.06202	-3.00531	-1.35772
H	-4.67776	-3.72015	-2.93036
H	-3.98813	-4.43680	-1.46112
C	-1.38781	-3.43801	0.48336
C	-1.15034	-2.89099	1.91049
H	-2.09547	-2.73260	2.45490
H	-0.54986	-3.62333	2.47955
H	-0.60171	-1.93321	1.89383
C	-2.24433	-4.71800	0.55961
H	-2.34347	-5.21653	-0.41759
H	-1.74863	-5.43466	1.23972
H	-3.25328	-4.53754	0.96945
C	-0.03013	-3.75131	-0.18392
H	0.50080	-4.50090	0.43060
H	-0.14269	-4.17815	-1.19241
H	0.61358	-2.86086	-0.25529
C	-0.09353	-0.13969	-2.01709
H	-0.39413	-0.23921	-3.05506
C	0.75719	-0.29098	-1.07698
C	2.09495	-0.42238	-0.54883
C	3.18120	-0.08538	-1.39943
C	2.35421	-0.89894	0.75825
H	2.95817	0.28116	-2.40414
H	1.50432	-1.16213	1.39208
C	4.50910	-0.22536	-0.96433
C	3.67315	-1.05010	1.22509
C	4.72240	-0.70542	0.34727
H	5.75362	-0.81854	0.69813
C	5.71748	0.11905	-1.86218
C	6.56680	1.22402	-1.17911
C	5.28605	0.62961	-3.25455
H	4.70332	-0.12623	-3.80924
H	4.68505	1.55339	-3.18777
H	6.18060	0.86189	-3.85622

H	5.97834	2.14662	-1.03620
H	7.44207	1.47110	-1.80456
H	6.94222	0.90623	-0.19215
C	4.00351	-1.57774	2.63858
C	2.73379	-1.90211	3.45540
C	4.81766	-0.50541	3.41077
H	5.76278	-0.25792	2.89975
H	4.23985	0.42823	3.52195
H	5.07079	-0.87297	4.42039
H	2.09925	-1.01084	3.60457
H	3.02023	-2.27340	4.45366
H	2.12439	-2.68649	2.97364
C	4.84729	-2.87502	2.51678
H	4.29228	-3.66100	1.97660
H	5.79394	-2.70178	1.97883
H	5.09918	-3.26113	3.51981
C	6.58589	-1.15284	-2.05696
H	6.00966	-1.95606	-2.54701
H	7.45944	-0.92260	-2.69121
H	6.96422	-1.54510	-1.09830
H	-4.35231	-2.40468	0.69150
H	-2.49493	3.71028	1.36669

10_{NH-Ar}

SCF (BP86) Energy = -1735.87890945
Enthalpy 0K = -1734.973041
Enthalpy 298K = -1734.917054
Free Energy 298K = -1735.062180
Lowest Frequency = 7.5262 cm^{-1}
Second Frequency = 10.9294 cm^{-1}
SCF (BP86-D3BJ) Energy = -1736.15106
SCF (FB) Energy = -1735.921915
SCF (DFB) Energy = -1735.928453
SCF (BS2) Energy = -2405.581169

Rh	-1.48352	-0.01304	-0.24774
P	-1.60322	2.32208	-0.30479
P	-1.91757	-2.29626	-0.04284
N	-3.51424	0.15991	0.34436
C	-4.09025	1.39785	0.49735
C	-5.43660	1.54262	0.88733
H	-5.87398	2.53698	1.00231
C	-6.18611	0.38527	1.12155
H	-7.23314	0.47361	1.42698
C	-5.61721	-0.88351	0.96973
H	-6.19652	-1.79219	1.14855
C	-4.26782	-0.96600	0.57293
N	-3.27793	2.48626	0.25775
N	-3.63507	-2.17691	0.38216
C	-1.65790	3.13604	-2.05366
C	-2.72784	2.33584	-2.83304
H	-3.73854	2.47443	-2.41548
H	-2.74326	2.68990	-3.87951
H	-2.49901	1.25578	-2.84013
C	-2.03317	4.63098	-2.03227
H	-1.24303	5.25599	-1.58676
H	-2.17259	4.97756	-3.07238
H	-2.98116	4.82721	-1.50168
C	-0.28359	2.93468	-2.73044
H	0.02134	1.87594	-2.72784
H	-0.35590	3.26780	-3.78157
H	0.51562	3.52264	-2.25374
C	-0.65450	3.34393	1.02478
C	-0.65334	2.44450	2.28317
H	-0.15460	1.47952	2.09196
H	-0.11088	2.96279	3.09456
H	-1.67645	2.23881	2.64138
C	0.79370	3.57654	0.54495
H	0.84728	4.30435	-0.28080
H	1.38331	3.99062	1.38236
H	1.28754	2.64280	0.22637
C	-1.33556	4.68606	1.36749
H	-2.35579	4.54514	1.76327
H	-0.75338	5.18060	2.16586
H	-1.37614	5.38202	0.51650
C	-1.98680	-3.38970	-1.62844
C	-2.46504	-2.43739	-2.74955
H	-1.76612	-1.59744	-2.89625
H	-2.53408	-3.00383	-3.69611
H	-3.46366	-2.02061	-2.53450
C	-0.56699	-3.90428	-1.94926
H	-0.24079	-4.69161	-1.25056
H	-0.56855	-4.34716	-2.96152
H	0.18209	-3.09443	-1.93946
C	-2.97812	-4.56709	-1.51072
H	-4.01352	-4.22117	-1.35156
H	-2.97458	-5.12600	-2.46387
H	-2.71326	-5.27979	-0.71522
C	-1.15153	-3.17401	1.49363
C	-1.51356	-2.26703	2.69309
H	-2.59864	-2.24252	2.88564
H	-1.01842	-2.66102	3.59871
H	-1.16471	-1.23135	2.53524
C	-1.69450	-4.59741	1.72931
H	-1.37499	-5.30374	0.94663
H	-1.29767	-4.97546	2.68896
H	-2.79545	-4.62834	1.80602
C	0.38445	-3.20360	1.32779
H	0.83197	-3.58117	2.26477
H	0.71345	-3.87036	0.51632
H	0.79830	-2.20047	1.13644
C	0.25362	-0.18173	-0.82612
H	1.49077	-0.55600	-2.40374
C	1.47842	-0.32507	-1.32340
C	2.79829	-0.21283	-0.66642
C	3.96031	-0.34179	-1.45551
C	2.93209	0.01079	0.72310
H	3.84790	-0.51527	-2.53179
H	2.02521	0.10541	1.33151
C	5.24582	-0.25350	-0.88884
C	4.20011	0.10168	1.32597
C	5.33853	-0.03237	0.50089
H	6.32744	0.03474	0.95582
C	6.49023	-0.40151	-1.79236
C	6.47096	0.70926	-2.87644
C	6.46205	-1.79266	-2.48027
H	6.48036	-2.60456	-1.73327
H	5.56149	-1.92667	-3.10308
H	7.34212	-1.91159	-3.13614
H	5.56973	0.65141	-3.50994
H	7.35033	0.61284	-3.53694
H	6.49721	1.71208	-2.41684
C	4.31113	0.33624	2.85026
C	3.60061	-0.82037	3.60243
C	3.62827	1.68108	3.21477
H	4.11836	2.52496	2.69962
H	2.56096	1.68592	2.93468
H	3.69128	1.86109	4.30247

H	2.53189	-0.88724	3.33617
H	3.66551	-0.66480	4.69373
H	4.06937	-1.79106	3.36715
C	7.81062	-0.28093	-0.99994
H	7.90922	0.70245	-0.50863
H	7.90284	-1.06539	-0.22907
H	8.66535	-0.39283	-1.68816
C	5.77695	0.39507	3.33464
H	6.31584	-0.54656	3.13336
H	6.33508	1.22165	2.86249
H	5.79930	0.56189	4.42490
H	-4.19016	-3.01081	0.57267
H	-3.71300	3.40332	0.35547

9_S

SCF (BP86) Energy = -2357.31258953
Enthalpy 0K = -2356.032388
Enthalpy 298K = -2355.950099
Free Energy 298K = -2356.143423
Lowest Frequency = -6.4659 cm^{-1}
Second Frequency = 10.9800 cm^{-1}
SCF (BP86-D3BJ) Energy = -2357.800649
SCF (FB) Energy = -2357.436878
SCF (DFB) Energy = -2357.453655
SCF (BS2) Energy = -5247.449346

Rh	2.71433	-2.03695	1.20413
P	4.16181	-2.57080	-0.61338
P	1.82734	-1.65767	3.42551
N	3.92203	-3.61426	2.30150
C	1.07305	-1.52024	-0.13318
H	1.32579	-2.06208	-1.05219
C	1.84513	-0.34917	0.11439
H	2.59171	-0.11662	-0.65459
C	1.33105	0.92736	0.75935
H	2.19021	1.56834	1.02579
H	0.79209	0.72307	1.69703
C	-0.38492	-1.71358	0.23077
H	-0.58566	-1.37318	1.25794
H	-0.62713	-2.79057	0.20098
C	5.13761	-4.05441	1.83943
C	5.86897	-5.09680	2.43681
H	6.81383	-5.41573	1.99075
C	5.36422	-5.70959	3.58776
H	5.91309	-6.52078	4.07492
C	4.15356	-5.25278	4.11037
H	3.73647	-5.67038	5.02974
C	3.46832	-4.21466	3.44855
S	5.92161	-3.27858	0.45307
S	1.95341	-3.70450	4.19566
C	3.69859	-4.11675	-1.73916
C	3.33608	-5.25560	-0.76021
H	4.21518	-5.62650	-0.20966
H	2.93216	-6.10303	-1.34312
H	2.56548	-4.94530	-0.03324
C	4.85777	-4.56259	-2.65121
H	5.02724	-3.86570	-3.48740
H	4.59282	-5.53942	-3.09520
H	5.80141	-4.69946	-2.09859
C	2.45465	-3.79860	-2.60142
H	1.54314	-3.70386	-1.99048
H	2.28929	-4.64839	-3.28835
H	2.56769	-2.89676	-3.22329
C	5.11129	-1.17154	-1.61738
C	5.35221	-0.00231	-0.63403
H	4.42243	0.43405	-0.24013
H	5.90135	0.79464	-1.16744
H	5.97153	-0.31600	0.22208
C	4.24932	-0.71608	-2.81440
H	4.18468	-1.49279	-3.59349
H	4.72637	0.16793	-3.27508
H	3.22561	-0.42505	-2.52769
C	6.48996	-1.63382	-2.14737
H	7.19086	-1.89903	-1.33887
H	6.94322	-0.78310	-2.68823
H	6.42964	-2.47499	-2.85035
C	0.04484	-1.37139	4.26135
C	-0.89700	-2.52168	3.82676
H	-0.86539	-2.72739	2.74642
H	-1.93251	-2.23704	4.08845
H	-0.67917	-3.46398	4.35281
C	-0.56016	-0.02764	3.80360
H	0.08666	0.83636	4.01494
H	-1.50267	0.12631	4.35998
H	-0.80976	-0.02426	2.73083
C	0.13643	-1.37377	5.80438
H	0.62891	-2.27458	6.20411
H	-0.89368	-1.36057	6.20587
H	0.64965	-0.48584	6.20327
C	3.19028	-0.61137	4.41149
C	4.47154	-0.63143	3.54418
H	4.96405	-1.61514	3.55194
H	5.18868	0.10241	3.95616
H	4.26579	-0.35699	2.49125
C	3.52629	-1.16713	5.80786
H	2.68384	-1.11898	6.51157
H	4.34609	-0.55890	6.23208
H	3.87839	-2.20989	5.76442
C	2.69904	0.85060	4.51324
H	3.52613	1.46589	4.91165
H	1.85001	0.97047	5.20324
H	2.42599	1.27295	3.53112
C	-1.07305	1.52024	0.13318
H	-1.32579	2.06208	1.05219
C	-1.84513	0.34917	-0.11439
H	-2.59171	0.11662	0.65459
C	-1.33105	-0.92736	-0.75935
H	-2.19021	-1.56834	-1.02579
H	-0.79209	-0.72307	-1.69703
C	0.38492	1.71358	-0.23077
H	0.58566	1.37318	-1.25794
H	0.62713	2.79057	-0.20098
Rh	-2.71433	2.03695	-1.20413
P	-4.16181	2.57080	0.61338
P	-1.82734	1.65767	-3.42551
N	-3.92203	3.61426	-2.30150
C	-5.13761	4.05441	-1.83943
C	-5.86897	5.09680	-2.43681
H	-6.81383	5.41573	-1.99075
C	-5.36422	5.70959	-3.58776
H	-5.91309	6.52078	-4.07492
C	-4.15356	5.25278	-4.11037
H	-3.73647	5.67038	-5.02974
C	-3.46832	4.21466	-3.44855
S	-5.92161	3.27858	-0.45307
S	-1.95341	3.70450	-4.19566
C	-3.69859	4.11675	1.73916

C	-3.33608	5.25560	0.76021
H	-4.21518	5.62650	0.20966
H	-2.93216	6.10303	1.34312
H	-2.56548	4.94530	0.03324
C	-4.85777	4.56259	2.65121
H	-5.02724	3.86570	3.48740
H	-4.59282	5.53942	3.09520
H	-5.80141	4.69946	2.09859
C	-2.45465	3.79860	2.60142
H	-1.54314	3.70386	1.99048
H	-2.28929	4.64839	3.28835
H	-2.56769	2.89676	3.22329
C	-5.11129	1.17154	1.61738
C	-5.35221	0.00231	0.63403
H	-4.42243	-0.43405	0.24013
H	-5.90135	-0.79464	1.16744
H	-5.97153	0.31600	-0.22208
C	-4.24932	0.71608	2.81440
H	-4.18468	1.49279	3.59349
H	-4.72637	-0.16793	3.27508
H	-3.22561	0.42505	2.52769
C	-6.48996	1.63382	2.14737
H	-7.19086	1.89903	1.33887
H	-6.94322	0.78310	2.68823
H	-6.42964	2.47499	2.85035
C	-0.04484	1.37139	-4.26135
C	0.89700	2.52168	-3.82676
H	0.86539	2.72739	-2.74642
H	1.93251	2.23704	-4.08845
H	0.67917	3.46398	-4.35281
C	0.56016	0.02764	-3.80360
H	-0.08666	-0.83636	-4.01494
H	1.50267	-0.12631	-4.35998
H	0.80976	0.02426	-2.73083
C	-0.13643	1.37377	-5.80438
H	-0.62891	2.27458	-6.20411
H	0.89368	1.36057	-6.20587
H	-0.64965	0.48584	-6.20327
C	-3.19028	0.61137	-4.41149
C	-4.47154	0.63143	-3.54418
H	-4.96405	1.61514	-3.55194
H	-5.18868	-0.10241	-3.95616
H	-4.26579	0.35699	-2.49125
C	-3.52629	1.16713	-5.80786
H	-2.68384	1.11898	-6.51157
H	-4.34609	0.55890	-6.23208
H	-3.87839	2.20989	-5.76442
C	-2.69904	-0.85060	-4.51324
H	-3.52613	-1.46589	-4.91165
H	-1.85001	-0.97047	-5.20324
H	-2.42599	-1.27295	-3.53112

8_S

SCF (BP86) Energy = -1334.69800849
Enthalpy 0K = -1333.970218
Enthalpy 298K = -1333.924338
Free Energy 298K = -1334.043299
Lowest Frequency = 19.7071 cm^{-1}
Second Frequency = 33.4344 cm^{-1}
SCF (BP86-D3BJ) Energy = -1334.953874
SCF (FB) Energy = -1334.738192
SCF (DFB) Energy = -1334.743732
SCF (BS2) Energy = -2779.803757

C	2.77723	4.47378	0.53422
H	3.75575	4.80718	0.90389
C	2.55570	4.57585	-0.79347
H	3.37011	4.98533	-1.40532
C	1.30712	4.16990	-1.55371
H	1.36854	4.56794	-2.58024
H	0.41148	4.63791	-1.09851
C	1.83056	3.93163	1.58907
H	0.84257	4.42711	1.50857
H	2.22045	4.19415	2.58672
C	0.08750	2.17041	-0.58287
H	-0.92474	2.49774	-0.85535
C	0.32309	2.04475	0.81133
H	-0.53629	2.26890	1.45478
C	1.62295	2.37623	1.51768
H	1.58802	1.96189	2.54115
H	2.49050	1.92364	1.01450
C	1.08803	2.61561	-1.62452
H	2.05542	2.11103	-1.49696
H	0.71189	2.33710	-2.62592
Rh	-0.15004	0.07093	0.00396
P	-2.47348	0.42004	0.03498
P	2.11474	-0.81381	-0.01451
N	-0.72977	-2.10089	-0.11708
C	-1.95690	-2.55807	0.29300
C	-2.32587	-3.91784	0.27618
H	-3.32843	-4.20603	0.60100
C	-1.40767	-4.86685	-0.17595
H	-1.66624	-5.92974	-0.19160
C	-0.15447	-4.43089	-0.61407
H	0.60167	-5.13391	-0.97044
C	0.14208	-3.05508	-0.58339
S	-3.21385	-1.45317	0.87496
S	1.71604	-2.59356	-1.23796
C	-3.29620	0.45825	-1.74933
C	-2.70302	-0.75120	-2.50727
H	-3.05321	-1.71222	-2.09701
H	-3.03782	-0.70001	-3.55923
H	-1.59935	-0.73988	-2.49935
C	-4.83249	0.34717	-1.72716
H	-5.31636	1.28167	-1.40427
H	-5.18021	0.14391	-2.75643
H	-5.18765	-0.48000	-1.09086
C	-2.87109	1.74897	-2.48597
H	-1.78280	1.78819	-2.65036
H	-3.35194	1.74975	-3.48120
H	-3.19097	2.67002	-1.97297
C	-3.38621	1.58274	1.33001
C	-3.21400	3.06015	0.90844
H	-3.74677	3.28794	-0.02867
H	-3.65411	3.70147	1.69337
H	-2.16084	3.36147	0.79403
C	-4.89594	1.27664	1.46565
H	-5.10277	0.22167	1.71229
H	-5.28802	1.88180	2.30346
H	-5.47240	1.54512	0.57037
C	-2.72904	1.32442	2.70846
H	-1.63323	1.42110	2.69943
H	-3.12943	2.06182	3.42733
H	-2.96993	0.31934	3.08942
C	3.75634	-0.35716	-1.03443
C	3.34847	-0.18635	-2.51844
H	2.47277	0.46677	-2.65148

H	4.19588	0.27024	-3.06113
H	3.12572	-1.14903	-3.00491
C	4.39471	0.95460	-0.52436
H	4.69210	0.90562	0.53327
H	5.31503	1.12977	-1.11104
H	3.75714	1.84083	-0.66375
C	4.81121	-1.48318	-0.93382
H	4.42389	-2.46967	-1.23656
H	5.64063	-1.23371	-1.62085
H	5.24280	-1.57078	0.07511
C	2.60014	-1.55265	1.76173
C	1.30363	-1.51965	2.60447
H	0.54887	-2.22999	2.23236
H	1.54840	-1.80775	3.64379
H	0.84267	-0.51674	2.62259
C	3.12507	-3.00068	1.70407
H	4.04459	-3.10344	1.10972
H	3.35754	-3.32279	2.73582
H	2.37638	-3.69960	1.30003
C	3.65589	-0.64807	2.43641
H	3.78652	-0.99228	3.47875
H	4.64225	-0.71174	1.95169
H	3.34957	0.40863	2.48107

A_S

SCF (BP86) Energy = -1022.64568109
Enthalpy 0K = -1022.097358
Enthalpy 298K = -1022.060202
Free Energy 298K = -1022.162234
Lowest Frequency = 22.3343 cm^{-1}
Second Frequency = 31.0707 cm^{-1}
SCF (BP86-D3BJ) Energy = -1022.835715
SCF (FB) Energy = -1022.68902
SCF (DFB) Energy = -1022.695228
SCF (BS2) Energy = -2467.682424

Rh	0.08685	-0.36747	-0.00475
P	-2.23619	-0.35789	0.09953
P	2.34778	-0.34018	-0.07858
N	0.08081	1.66604	-0.01826
C	-1.02534	2.41355	0.34439
C	-1.03512	3.81927	0.30479
H	-1.94878	4.35154	0.57985
C	0.11398	4.50811	-0.08755
H	0.12903	5.60136	-0.10854
C	1.24363	3.77407	-0.46287
H	2.16429	4.27290	-0.77479
C	1.19796	2.37099	-0.44613
S	-2.52990	1.65322	0.91585
S	2.67438	1.56527	-1.07022
C	-2.99684	-1.42114	1.52784
C	-1.92919	-1.41206	2.64681
H	-1.75885	-0.39763	3.04290
H	-2.27653	-2.05006	3.47999
H	-0.95974	-1.80644	2.29128
C	-4.32422	-0.86027	2.07870
H	-5.12803	-0.84371	1.32823
H	-4.66063	-1.50664	2.90993
H	-4.20579	0.15620	2.49083
C	-3.19529	-2.86444	1.01373
H	-2.27968	-3.27897	0.55665
H	-3.45556	-3.51167	1.87041
H	-4.01830	-2.94220	0.28550
C	-3.26733	-0.38338	-1.54067
C	-2.74816	0.80084	-2.38652
H	-1.65137	0.76677	-2.50879
H	-3.20316	0.74289	-3.39165
H	-3.02530	1.77350	-1.94886
C	-2.91946	-1.70353	-2.26908
H	-3.26869	-2.59838	-1.73161
H	-3.41189	-1.70042	-3.25829
H	-1.83302	-1.79622	-2.44076
C	-4.78585	-0.25299	-1.32573
H	-5.04552	0.64932	-0.74658
H	-5.28053	-0.16455	-2.31011
H	-5.21788	-1.13391	-0.82441
C	3.54176	-0.35997	1.43312
C	3.13354	0.84273	2.31225
H	2.07045	0.79692	2.60325
H	3.74038	0.82427	3.23528
H	3.32280	1.80484	1.80908
C	3.28476	-1.67054	2.21152
H	3.57053	-2.57189	1.64604
H	3.89646	-1.65881	3.13141
H	2.22826	-1.76160	2.51734
C	5.01363	-0.23079	0.99589
H	5.18575	0.68924	0.41156
H	5.64930	-0.16875	1.89779
H	5.35928	-1.09411	0.40722
C	2.51739	-1.82877	-1.30642
C	2.22538	-1.33015	-2.73629
H	3.05950	-0.73156	-3.13646
H	2.09132	-2.20563	-3.39789
H	1.30839	-0.71855	-2.77820
C	3.81811	-2.64662	-1.29310
H	4.06819	-3.05338	-0.30110
H	3.71074	-3.50508	-1.98165
H	4.67148	-2.04835	-1.65139
C	1.31239	-2.67048	-0.78438
H	1.11911	-3.53087	-1.45410
H	1.45556	-3.06226	0.23444
H	0.31471	-2.10553	-0.86837

B_{S-Ar}

SCF (BP86) Energy = -1645.59264327
Enthalpy 0K = -1644.716481
Enthalpy 298K = -1644.659786
Free Energy 298K = -1644.805370
Lowest Frequency = 2.9759 cm^{-1}
Second Frequency = 12.8255 cm^{-1}
SCF (BP86-D3BJ) Energy = -1645.890171
SCF (FB) Energy = -1645.631464
SCF (DFB) Energy = -1645.636906
SCF (BS2) Energy = -3090.768764

Rh	-1.11733	0.01974	-0.43859
P	-1.40795	2.37507	-0.36554
P	-1.33703	-2.31930	-0.57983
N	-2.43952	-0.11315	1.28743
C	-3.14108	0.97911	1.74666
C	-3.87948	0.96889	2.94301
H	-4.38146	1.88087	3.27387
C	-3.95589	-0.21362	3.68621
H	-4.52595	-0.24748	4.61932
C	-3.30920	-1.35442	3.20891
H	-3.37771	-2.30863	3.73663

C	-2.56550	-1.27466	2.01470
S	-3.25055	2.48622	0.80739
S	-1.80417	-2.79810	1.50794
C	-2.05967	3.20084	-2.00550
C	-2.90214	2.12073	-2.72023
H	-3.78386	1.83254	-2.12363
H	-3.26717	2.53255	-3.67888
H	-2.31501	1.21365	-2.93475
C	-2.95119	4.43861	-1.76303
H	-2.42204	5.26341	-1.26584
H	-3.29561	4.81175	-2.74496
H	-3.85512	4.19622	-1.17884
C	-0.84680	3.58788	-2.88117
H	-0.12758	2.75996	-2.99650
H	-1.21163	3.85900	-3.88845
H	-0.31157	4.46441	-2.48317
C	-0.20553	3.53615	0.63867
C	-0.08110	2.88247	2.03219
H	0.23259	1.82751	1.96219
H	0.68964	3.42510	2.60817
H	-1.02361	2.93706	2.60101
C	1.17798	3.53470	-0.04951
H	1.16066	4.00508	-1.04391
H	1.87296	4.12216	0.57805
H	1.59726	2.52217	-0.14517
C	-0.72652	4.97794	0.78653
H	-1.75320	5.01720	1.18764
H	-0.07398	5.51259	1.50095
H	-0.68949	5.53613	-0.16229
C	-2.98126	-2.76955	-1.54646
C	-3.95147	-1.59303	-1.29156
H	-3.50441	-0.62196	-1.57143
H	-4.85822	-1.74283	-1.90611
H	-4.27104	-1.53898	-0.23833
C	-2.64324	-2.82721	-3.05308
H	-2.04947	-3.71625	-3.31795
H	-3.58802	-2.88561	-3.62372
H	-2.10611	-1.92631	-3.39656
C	-3.66025	-4.07504	-1.08968
H	-3.86414	-4.07572	-0.00650
H	-4.63153	-4.15924	-1.61086
H	-3.07947	-4.97476	-1.33483
C	0.07126	-3.63224	-0.90160
C	1.12233	-3.48809	0.21970
H	0.74659	-3.83672	1.19476
H	1.99285	-4.11490	-0.04634
H	1.48096	-2.45396	0.33420
C	-0.45901	-5.08102	-0.91518
H	-1.09094	-5.29162	-1.79175
H	0.40918	-5.76299	-0.97034
H	-1.02100	-5.34144	-0.00245
C	0.73599	-3.30289	-2.26025
H	1.53211	-4.04840	-2.43911
H	0.03655	-3.36423	-3.10769
H	1.19970	-2.30568	-2.25943
C	0.10246	0.16796	-2.14264
H	-0.08363	0.21172	-3.21049
C	0.90589	0.10099	-1.14884
C	2.18874	0.05482	-0.48580
C	3.35565	0.18634	-1.28037
C	2.31209	-0.12494	0.91143
H	3.24183	0.32851	-2.35963
H	1.39436	-0.22706	1.50049
C	4.63387	0.13845	-0.69824
C	3.57902	-0.18535	1.52483
C	4.71609	-0.04907	0.70012
H	5.70359	-0.09142	1.16135
C	3.68825	-0.40562	3.05076
C	3.01646	-1.75478	3.42237
C	2.96351	0.74758	3.79363
H	3.41702	1.72359	3.55019
H	1.89247	0.79443	3.53338
H	3.03495	0.60133	4.88547
H	1.94965	-1.77387	3.14089
H	3.07878	-1.92401	4.51152
H	3.51689	-2.59888	2.91788
C	5.88562	0.28868	-1.59195
C	5.83828	1.66403	-2.31006
C	5.89731	-0.84578	-2.65133
H	5.93623	-1.83799	-2.17011
H	5.00364	-0.81670	-3.29743
H	6.78279	-0.74796	-3.30297
H	4.94229	1.76736	-2.94531
H	6.72276	1.78442	-2.95931
H	5.83511	2.49256	-1.58133
C	5.15402	-0.44606	3.53714
H	5.72177	-1.27006	3.07190
H	5.68408	0.50016	3.33305
H	5.17545	-0.60669	4.62807
C	7.19887	0.20937	-0.78247
H	7.26937	1.01191	-0.02811
H	7.31123	-0.76156	-0.26986
H	8.05827	0.32259	-1.46428

$10_{S\text{-}Ar}$

SCF (BP86) Energy = -1645.60578491
Enthalpy 0K = -1644.729252
Enthalpy 298K = -1644.672617
Free Energy 298K = -1644.818899
Lowest Frequency = 8.1052 cm^{-1}
Second Frequency = 11.1223 cm^{-1}
SCF (BP86-D3BJ) Energy = -1645.893289
SCF (FB) Energy = -1645.645613
SCF (DFB) Energy = -1645.65129
SCF (BS2) Energy = -3090.782308

Rh	-1.47069	-0.02732	-0.19928
P	-1.59295	2.30962	-0.34536
P	-1.49362	-2.37040	-0.06711
N	-3.60411	-0.03752	0.32944
C	-4.28192	1.12400	0.62260
C	-5.64556	1.14780	0.97023
H	-6.13455	2.10308	1.17482
C	-6.34844	-0.05661	1.04748
H	-7.40641	-0.06411	1.32598
C	-5.68312	-1.25128	0.76263
H	-6.19762	-2.21338	0.81845
C	-4.32524	-1.20817	0.39522
S	-3.50050	2.72210	0.63662
S	-3.63698	-2.79183	-0.03173
C	-1.85320	2.99900	-2.14226
C	-3.06641	2.23259	-2.71551
H	-4.00538	2.49568	-2.20194
H	-3.18014	2.50186	-3.78105
H	-2.92235	1.13922	-2.65647
C	-2.11877	4.51509	-2.18109
H	-1.23228	5.10350	-1.89555

H	-2.37904	4.80180	-3.21627
H	-2.96560	4.80801	-1.53771
C	-0.60086	2.64042	-2.97486
H	-0.42450	1.55299	-2.98816
H	-0.77171	2.96866	-4.01620
H	0.31327	3.13729	-2.61661
C	-0.43889	3.39924	0.77025
C	-0.26546	2.59398	2.07746
H	0.16700	1.59730	1.88958
H	0.41650	3.14826	2.74739
H	-1.22312	2.46143	2.60846
C	0.92451	3.56788	0.06462
H	0.85533	4.22067	-0.82050
H	1.62292	4.05199	0.77063
H	1.37069	2.60597	-0.23460
C	-1.03797	4.78344	1.10198
H	-1.99121	4.70791	1.65166
H	-0.32829	5.31535	1.76137
H	-1.19206	5.41093	0.21223
C	-0.99896	-3.43206	-1.61656
C	-1.39376	-2.57882	-2.84278
H	-0.85617	-1.61715	-2.86427
H	-1.13978	-3.13905	-3.76098
H	-2.47676	-2.37046	-2.86606
C	0.52764	-3.66924	-1.60388
H	0.82981	-4.38360	-0.82148
H	0.81660	-4.11121	-2.57475
H	1.09979	-2.73680	-1.47464
C	-1.73856	-4.78692	-1.67876
H	-2.82999	-4.66443	-1.77753
H	-1.39238	-5.32664	-2.57890
H	-1.53223	-5.43050	-0.81082
C	-0.86184	-3.09214	1.61789
C	-1.63043	-2.32014	2.71406
H	-2.70773	-2.55364	2.71012
H	-1.22752	-2.61431	3.69990
H	-1.50307	-1.22798	2.60857
C	-1.10505	-4.60525	1.76750
H	-0.49309	-5.19979	1.07054
H	-0.81955	-4.91009	2.79079
H	-2.16632	-4.87338	1.63010
C	0.64373	-2.76252	1.73511
H	0.98566	-3.05403	2.74457
H	1.26245	-3.30799	1.00755
H	0.83870	-1.68476	1.61249
C	0.28824	-0.02893	-0.71658
H	1.52337	-0.14451	-2.31449
C	1.52135	-0.05242	-1.21249
C	2.85618	0.01047	-0.57903
C	3.03564	0.23558	0.80449
C	3.99104	-0.16312	-1.39972
H	2.15320	0.38437	1.43632
H	3.84311	-0.33320	-2.47226
C	4.32271	0.28068	1.37192
C	5.29383	-0.12477	-0.86902
C	5.43160	0.09638	0.51693
H	6.43432	0.12950	0.94454
C	6.50655	-0.32157	-1.80556
C	6.49900	0.78594	-2.89315
C	6.40735	-1.71286	-2.48673
H	6.41517	-2.52279	-1.73739
H	5.48636	-1.81448	-3.08552
H	7.26453	-1.86681	-3.16509
H	5.58010	0.75947	-3.50301
H	7.35634	0.65483	-3.57608
H	6.57455	1.78855	-2.43875
C	4.48669	0.53932	2.88750
C	3.72399	-0.55049	3.68637
C	3.90015	1.93402	3.23296
H	4.43045	2.73234	2.68621
H	2.82900	2.00051	2.97640
H	4.00013	2.13524	4.31399
H	2.64539	-0.55227	3.45371
H	3.83077	-0.37405	4.77100
H	4.12148	-1.55531	3.46324
C	7.85145	-0.24810	-1.04945
H	8.00049	0.73266	-0.56574
H	7.93533	-1.03281	-0.27788
H	8.68224	-0.39451	-1.76000
C	5.96533	0.51472	3.33471
H	6.44045	-0.46117	3.13560
H	6.56114	1.29888	2.83706
H	6.02498	0.69604	4.42114

$HCCNMe_2$

SCF (BP86) Energy = -211.293321810
Enthalpy 0K = -211.195618
Enthalpy 298K = -211.187833
Free Energy 298K = -211.225131
Lowest Frequency = 158.2611 cm^{-1}
Second Frequency = 180.2648 cm^{-1}
SCF (BP86-D3BJ) Energy = -211.3057554
SCF (FB) Energy = -211.2967408
SCF (DFB) Energy = -211.2974719
SCF (BS2) Energy = -211.3540515

C	0.99442	-0.00148	-0.08578
C	2.20683	-0.00057	0.08839
H	3.27750	-0.00104	0.13008
N	-0.34545	-0.00010	-0.27857
C	-1.05127	1.23987	0.07380
H	-2.05164	1.22815	-0.39171
H	-1.17214	1.36681	1.17046
H	-0.48839	2.09905	-0.32011
C	-1.05404	-1.23844	0.07394
H	-2.05437	-1.22456	-0.39161
H	-0.49312	-2.09895	-0.31987
H	-1.17525	-1.36500	1.17061

$TS(C\text{-}10)_{C\text{-}NMe2}$

SCF (BP86) Energy = -1292.13454000
Enthalpy 0K = -1291.436055
Enthalpy 298K = -1291.392318
Free Energy 298K = -1291.508778
Lowest Frequency = -754.6174 cm^{-1}
Second Frequency = 15.8377 cm^{-1}
SCF (BP86-D3BJ) Energy = -1292.349423
SCF (FB) Energy = -1292.175404
SCF (DFB) Energy = -1292.181271
SCF (BS2) Energy = -1961.73039

Rh	0.00568	-0.03306	0.03108
P	2.32323	-0.28015	-0.06863
P	-2.31099	-0.32647	0.09867
N	0.02177	-2.16467	-0.05470
C	1.17007	-2.84386	-0.38388

C	1.20592	-4.24611	-0.43435
H	2.14118	-4.74749	-0.69816
C	0.04615	-4.98239	-0.17026
H	0.05577	-6.07546	-0.21459
C	-1.12657	-4.29032	0.14994
H	-2.05356	-4.82766	0.36824
C	-1.11537	-2.88804	0.21293
C	2.39094	-2.04040	-0.75194
H	3.31459	-2.57611	-0.47399
H	2.41206	-1.92201	-1.85123
C	-2.35532	-2.13882	0.63072
H	-3.26467	-2.66311	0.29069
H	-2.39728	-2.11814	1.73553
C	3.19947	-0.38829	1.65387
C	2.49759	-1.53605	2.41765
H	2.69633	-2.52586	1.97319
H	2.87976	-1.56012	3.45441
H	1.40532	-1.38264	2.46027
C	4.71263	-0.67013	1.57710
H	5.27625	0.17339	1.14746
H	5.10044	-0.83173	2.59973
H	4.94681	-1.57839	0.99572
C	2.93365	0.93152	2.41302
H	1.85135	1.12961	2.49009
H	3.34128	0.84814	3.43703
H	3.41336	1.80038	1.93595
C	3.36341	0.69583	-1.37761
C	2.43960	0.87038	-2.60663
H	1.51040	1.40318	-2.34877
H	2.97626	1.45193	-3.37862
H	2.15850	-0.09431	-3.06405
C	3.71807	2.08855	-0.81392
H	4.45741	2.03437	0.00154
H	4.16305	2.70147	-1.61884
H	2.82232	2.61510	-0.44489
C	4.65102	-0.03854	-1.81368
H	4.44418	-1.02059	-2.27041
H	5.16086	0.56968	-2.58317
H	5.36285	-0.18487	-0.98818
C	-3.38146	0.51448	1.47720
C	-2.47680	0.58674	2.73037
H	-1.54664	1.14512	2.53525
H	-3.02750	1.09293	3.54433
H	-2.19016	-0.41184	3.10366
C	-3.75091	1.94773	1.03788
H	-4.48238	1.95529	0.21362
H	-4.21307	2.48014	1.88916
H	-2.86438	2.52310	0.72241
C	-4.66430	-0.27134	1.83030
H	-4.45043	-1.28925	2.19614
H	-5.18967	0.25718	2.64684
H	-5.36543	-0.34848	0.98667
C	-3.17305	-0.30174	-1.63440
C	-2.43201	-1.35744	-2.48865
H	-2.60728	-2.38770	-2.13561
H	-2.80397	-1.29959	-3.52773
H	-1.34417	-1.17113	-2.50366
C	-4.67800	-0.63091	-1.59919
H	-5.26931	0.15671	-1.10531
H	-5.05195	-0.71439	-2.63621
H	-4.89146	-1.59211	-1.10079
C	-2.93784	1.08794	-2.26907
H	-3.31941	1.08029	-3.30643
H	-3.46326	1.89260	-1.73095
H	-1.86319	1.33305	-2.29914
C	0.00366	1.87190	-0.00681
H	-0.27701	2.60729	1.14927
C	-0.00996	3.16592	0.04749
N	-0.00031	4.48555	-0.24146
C	1.09652	5.30980	0.29752
H	1.19149	6.22027	-0.31632
H	0.91450	5.61042	1.34874
H	2.03881	4.74669	0.24230
C	-1.29601	5.17877	-0.36315
H	-1.71700	5.45670	0.62384
H	-1.15105	6.09865	-0.95287
H	-2.00708	4.52888	-0.89270

The full Gaussian reference (g09, D.01):

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian 09 (Revision D.01); Gaussian Inc.: Wallingford, CT, 2009.