Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

A Computational Study on the Identity of the Active Catalyst Structure for Ru(II) Carboxylate Assisted C—H Activation in Acetonitrile

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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 and BS1
ΔH_{BS1}	Enthalpy at 0 K with BS1
ΔG_{BS1}	Free energy at 298 K and 1 atm with BS1
$\Delta G_{BS1/MeCN}$	Free energy corrected for acteonitrile solvent with BS1
$\Delta G_{BS1/MeCN+D3}$	Free energy corrected for acteonitrile and dispersion effects with BS1
ΔE_{BS2}	Single point SCF energy computed with the BP86 functional and BS2
ΔG_{393}	Free energy at 393.15 K and 1 atm with BS1
ΔG_{393+CC}	Free energy at 393.15 K and 1 M with BS1 (cratic correction applied)
ΔG_{MeCN}	Free energy corrected for basis set (BS2), dispersion effects, temperature, cratic and acetonitrile solvent
ΔG_{tol}	Free energy corrected for basis set (BS2), dispersion effects, temperature, cratic and toluene solvent
$\Delta G_{MeCN-298}$	Free energy corrected for basis set (BS2), dispersion effects and acetonitrile solvent at 292 K (no cratic correction)

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

Table S1 – Relative energies (in kcal mol^{-1}) for computed structures. Data in bold are those used in the main text. All energies are quoted relative to **A** at 0.0 kcal/mol. * single point at 393.15 K has negative frequency.

	ΔE_{BS1}	ΔH_{BS1}	ΔG_{BS1}	$\Delta G_{BS1/MeCN}$	$\Delta G_{BS1/MeCN+D3}$	ΔE_{BS2}	ΔG_{393}	ΔG_{393+CC}	ΔG_{MeCN}	ΔG_{tol}
Temperature [K]	0	298	298	298	298	0	393.15	393.15	393.15	393.15
Phase	[1 atm]	[1 atm]	[1 atm]	[1 atm]	[1 atm]	[1 atm]	[1 atm]	[1 M]	[1 M]	[1 M]
A	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	**0.0**	*0.0*
$[(C_6H_6)Ru(O^tBu)_2]$	13.9	14.5	11.7	9.4	-2.1	6.3	10.2	10.2	**-11.1**	*-7.4*
$[(C_6H_6)Ru(O^tBu)]^+$	150.5	147.8	136.1	144.7	48.5	136.1	132.6	135.3	**33.3**	*73.7*
$[(C_6H_6)Ru(OMes)_2]$	26.4	26.2	25.6	21.0	3.2	15.9	25.2	25.2	**-7.8**	*-2.5*
$[(C_6H_6)Ru(OMes)]^+$	136.3	134.5	121.8	132.4	47.2	124.0	117.9	120.7	**33.8**	*69.5*

[(toluene)Ru(OAc)$_2$]	-1.6	-1.5	-0.1	-1.1	-1.4	-1.8	0.4	0.4	**-1.2**	*-0.9*
[(*o*-xylene)Ru(OAc)$_2$]	-1.3	-1,5	-2.0	-3.9	-4.2	-1.6	-2.2	-2.2	**-4.8**	*-4.6*
[(*p*-cymene)Ru(OAc)$_2$]	-3.4	-3.3	-1.4	-4.3	-3.9	-3.5	-0.8	-0.8	**-3.5**	*-3.6*
[(Bn*)Ru(OAc)$_2$]	-5.9	-5.6	-2.4	-9.1	-10.0	-6.2	-1.3	-1.3	**-9.2**	*-8.5*
B$^+$	113.5	113.1	114.3	104.5	17.2	98.7	114.6	114.6	***2.8***	*37.5*
TS(**B**$^+$-**C**$^+$)	128.2	126.9	128.6	117.8	27.9	113.2	129.1	129.1	***13.4***	*49.6*
C$^+$	112.8	112.1	113.2	102.5	15.2	99.1	113.4	113.4	***1.7***	*36.5*
B·OAc	14.8	15.2	28.3	9.7	8.1	14.4	32.2	29.5	***8.9***	*9.7*
TS(**B**-**C**)1·OAc	28.0	27.1	39.4	17.9	18.0	26.6	43.1	40.4	***17.6***	*19.0*
INT(**B**-**C**)·OAc	24.0	22.6	35.1	18.0	13.6	23.8	38.8	36.1	***14.4***	*16.7*
TS(**B**-**C**)2·OAc	24.2	21.6	35.0	17.6	13.8	24.5	39.1	36.4	***15.6***	*17.5*
C·OAc	15.6	15.5	28.2	11.1	7.5	15.8	32.0	29.3	***8.8***	*10.6*
A·**a**-H	-3.7	-3.1	7.2	-1.1	1.8	-2.1	10.1	7.4	***3.6***	*2.1*
B	0.6	1.5	15.2	-2.8	-1.9	0.8	19.4	19.4	***-0.2***	*-0.5*
TS(**B**-**C**)	30.6	29.7	43.6	25.5	20.3	30.3	47.9	47.9	***21.6***	*24.6*
C	-13.4	-12.7	0.7	-30.6	-13.2	-11.6	4.7	4.7	***-10.0***	*-11.7*
B′	-2.0	-2.2	-0.1	-4.1	-3.6	1.8	0.6	0.6	***0.8***	*0.8*
TS(**B′**-**C′**)	19.9	18.8	20.1	16.8	14.6	22.3	20.6	20.6	***17.6***	*18.9*
C′	22.2	21.6	20.7	17.9	14.9	24.3	20.2	20.2	***16.5***	*18.8*
C′ (without HOAc)	31.9	30.4	18.9	20.8	15.3	31.0	15.2	17.9	***13.4***	*16.9*
D	-15.5	-15.8	-0.3	-25.0	-23.4	-11.2	4.5	7.8	***-17.0***	*-17.6*
TS(**D**-**E**)	6.3	3.5	18.9	-6.0	-3.1	10.7	23.6	20.9	***3.2***	*1.9*
E	-9.0	-8.3	6.1	-33.3	-13.0	-5.3	10.4	7.7	***-7.7***	*-10.4*
E (without HOAc)	-11.0	-11.2	-7.9	-25.0	-21.2	-9.8	-7.0	-7.0	***-19.0***	*-19.2*
D$^+$ (η^6)	110.3	109.8	110.6	97.8	14.0	96.0	110.7	110.7	***-0.2***	*31.4*
TS(**D**$^+$-**E**$^+$) (η^6)	124.5	123.1	125.1	110.8	25.0	109.9	125.7	125.7	***11.0***	*45.4*
E$^+$ (η^6)	108.8	108.1	110.1	96.5	13.1	95.6	110.6	110.6	***0.4***	*33.4*
D$^+$ (κ^2)	114.4	113.3	116.4	99.3	15.4	102.6	117.2	117.2	***4.5***	*37.8*

TS(**D**$^+$-**E**$^+$) (κ^2)	131.0	126.8	129.7	114.9	30.2	119.8	130.5	130.5	***19.9***	*52.8*
E$^+$ (κ^2)	121.8	120.9	122.8	104.0	16.9	110.2	123.1	123.1	***5.6***	*41.9*
D$^+$ (κ^1)	127.0	124.8	127.3	113.7	25.4	114.0	127.9	127.9	***13.1***	*49.1*
TS(**D**$^+$-**E**$^+$) (κ^1)	129.9	125.4	128.7	116.0	27.8	118.1	129.7	129.7	***17.0***	*52.3*
E$^+$ (κ^1)	127.3	125.4	128.2	114.8	28.6	115.9	128.9	128.9	***17.9***	*52.6*
^{3}**D**$^+$	65.8	69.0	110.9	60.5	-10.6	55.3	113.3	105.2	***-16.9***	*10.7*
INT(^{3}**D**$^+$)	79.3	82.2	115.0	74.7	4.2	70.1	127.5	119.4	***-0.6***	*26.4*
TS(^{3}**D**$^+$-^{3}**E**$^+$)	90.1	89.7	123.3	49.5	13.4	82.1	136.2	128.1	***10.2***	*36.8*
^{3}**E**$^+$	84.4	86.8	119.0	79.1	10.0	76.2	131.3	123.2	***6.0***	*32.5*
^{1}**A**	-9.9	-8.9	1.1	-5.8	-2.5	-4.3	5.0	2.3	***4.4***	*2.8*
^{1}**A**$^+$	118.9	118.2	114.9	115.7	24.8	103.0	114.6	114.6	***8.7***	*45.0*
^{6}**F**$^{2+}$	215.6	217.6	234.0	224.4	13.5	186.2	247.4*	239.3*	***-10.6****	*72.6**
^{3}**A**$^{2+}$	297.8	297.2	300.8	296.6	56.7	264.3	304.2	301.5	***23.9***	*119.9*
^{5}**F**$^+$ (κ^1)	54.4	57.1	79.8	68.7	-4.0	41.3	90.7	82.6	***-14.2***	*14.0*
^{4}**F**$^+$ (κ^2)	62.4	64.3	77.6	73.0	-2.5	50.2	85.0	79.6	***-12.7***	*16.6*
c-**4F** ($2\kappa^1$)	-39.3	-36.3	-9.6	-22.1	-6.0	-18.5	1.8	-6.3	***-13.7***	*-15.0*
t-**4F** ($2\kappa^1$)	-38.5	-35.5	-9.6	-21.8	-6.1	-18.2	1.5	-6.6	***-13.5***	*-14.9*
f-**3F** ($\kappa^2\kappa^1$)	-34.6	-32.3	-15.2	-21.2	-18.0	-31.6	-7.5	-12.9	***-12.7***	*-13.9*
m-**3F** ($\kappa^2\kappa^1$)	-30.0	-28.0	-13.4	-35.5	-17.7	-26.8	-6.7	-12.1	***-13.2***	*-13.2*
c-**2F** ($2\kappa^2$)	-25.1	-23.8	-16.8	-16.5	-13.6	-20.4	-13.0	-15.7	***-7.8***	*-9.0*
t-**2F** ($2\kappa^2$)	-23.2	-22.0	-17.7	-17.6	-16.6	-18.6	-10.8*	-13.5*	***-7.9****	*-8.0**
^{1}**B**$^+$ (*t*-N,*t*-O)	110.1	110.4	121.4	101.4	20.4	99.8	125.5	122.8	***11.5***	*43.3*
TS(^{1}**B**$^+$-^{1}**C**$^+$) (*t*-N,*t*-O)	127.1	126.1	137.5	119.9	37.1	115.7	141.8	139.1	***27.3***	*60.0*
^{1}**C**$^+$ (*t*-N,*t*-O)	103.8	103.9	115.0	95.0	12.1	93.1	119.1	116.4	***2.8***	*35.9*
^{1}**B**$^+$ (*t*-C_6H_6,*t*-O)	109.8	110.1	120.8	102.0	20.4	99.4	124.9	122.2	***11.4***	*43.5*
TS(^{1}**B**$^+$-^{1}**C**$^+$)1 (*t*-C_6H_6,*t*-O)	128.9	128.5	139.3	122.4	38.0	117.8	143.4	140.7	***28.3***	*62.2*
INT (^{1}**B**$^+$-^{1}**C**$^+$) (*t*-C_6H_6,*t*-O)	130.6	128.8	139.1	119.9	32.5	119.1	143.0	140.3	***22.1***	*57.9*
TS(^{1}**B**$^+$-^{1}**C**$^+$)2 (*t*-C_6H_6,*t*-O)	130.7	127.7	138.8	119.3	32.8	119.6	143.0	140.3	***23.1***	*58.4*

^{1}C$^+$ (*t*-C_6H_6,*t*-O)	119.9	119.4	129.5	110.0	25.8	109.2	133.2	130.5	***16.0***	*50.1*
^{1}B$^+$ (*t*-O,*t*-N)	108.9	109.1	120.8	102.9	20.9	98.4	125.1	122.4	***12.0***	*44.4*
TS(**^{1}B$^+$**-**^{1}C$^+$**) (*t*-O,*t*-N)	131.1	127.7	139.9	120.9	39.6	121.4	144.4	141.7	***31.8***	*63.8*
^{1}C$^+$ (*t*-O,*t*-N)	125.7	125.5	136.2	118.3	32.8	115.6	140.2	137.5	***23.9***	*58.8*
^{1}B$^+$ (*t*-O,*t*-C_6H_6)	114.9	114.8	126.1	108.3	25.8	104.5	130.3	127.6	***16.9***	*49.6*
TS(**^{1}B$^+$**-**^{1}C$^+$**) (*t*-O,*t*-C_6H_6)	129.8	126.4	137.9	120.2	39.0	119.9	142.3	139.6	***30.7***	*62.6*
^{1}C$^+$ (*t*-O,*t*-C_6H_6)	107.9	108.0	118.6	100.9	17.8	97.4	122.5	119.8	***8.6***	*41.8*
^{1}B$^+$ (*t*-O,*t*-O)	112.4	112.4	122.6	105.2	23.7	101.4	126.5	123.8	***13.8***	*45.9*
^{4}G$^+$ (κ^1)	59.6	62.6	89.9	65.9	-7.1	48.3	101.6	93.5	***-14.9***	*13.6*
^{3}G ($2\kappa^1$)	-35.5	-32.1	-1.1	-26.3	-20.7	-32.4	10.9	2.8	***-14.0***	*-16.2*
^{3}G$^+$ (κ^2)	75.3	76.6	94.6	78.5	1.3	63.3	102.5	97.1	***-8.3***	*22.1*
^{2}G$^+$ (κ^2)	84.4	84.8	92.7	84.1	4.8	72.0	96.7	94.0	***-6.3***	*24.8*
^{1}G ($2\kappa^2$)	-21.5	-20.3	-11.1	-19.4	-17.0	-16.6	-7.0	-9.7	***-10.7***	*-11.3*
^{2}G ($\kappa^2\kappa^1$)	-29.7	-28.8	-7.9	-25.1	-22.0	-27.4	0.2	-5.3	***-17.1***	*-18.2*
TS(**^{2}G**-**^{2}H**)	-27.9	-29.1	-7.4	-25.1	-20.4	-24.7	1.0	-4.4	***-14.2***	*-16.2*
^{2}H	-33.2	-31.6	-10.8	-50.7	-23.1	-29.8	-2.8	-8.2	***-17.1***	*-19.4*
^{1}G ($\kappa^2\kappa^1$)	-21.0	-21.2	-10.0	-20.1	-18.7	-17.2	-5.7	-8.5	***-13.4***	*-13.9*
TS(**^{1}G**-**^{1}H**)	-19.9	-22.1	-10.5	-20.9	-18.2	-15.4	-6.0	-8.7	***-11.8***	*-13.0*
^{1}H	-27.1	-26.4	-16.5	-26.6	-23.0	-22.2	-12.6	-15.3	***-17.1***	*-18.8*

A thermal correction uses the ideal gas law to convert from gas-phase [1 atm] to solution-phase [1 M] units. This cratic correction (CC) adjusts the free energy value when above the standard state temperature (298 K), and accounts for an increase in volume when a solution is heated.

Molar volume of gas at 1 atm at T: $V = \frac{1000 \times 8.315 \times T}{101300}$

To convert V from 1 atm to 1 dm^3 mol^{-1}: $\text{Cratic Correction } (\mathbf{CC}) = 1.98 \times \frac{T}{1000} \times \ln(V)$

From the data in Table S2, comparing the difference ($\Delta(G_{393}\text{-}G_{BS1})$; orange) in free energy between 298K (ΔG_{BS1}) and 393.15 K (ΔG_{393}) with the equivalent difference ($\Delta(G_{393+CC}\text{-}G_{BS1})$; blue) after the application of the cratic correction (ΔG_{393+CC}) there is a clear compensation when more individual computed species are required to balance the energies relative to complex **A**. Where the number of molecules to balance with **A** are equal (i.e. ratio is 1), there is no difference between the orange and blue values. If the ratio is less than 1, $\Delta(G_{393+CC}\text{-}G_{BS1})$ is negative (**C′** without HOAc). The largest increases in free energy (4 - 5 kcal mol^{-1}) with this thermal correction was observed for pathway **B** → **C** and ^{3}**D**$^+$ → ^{3}**E**$^+$, both have two acetates at the Ru centre during the C–H activation process. Another factor to consider when analysing these values is the impact of low frequencies, which are involved in computing free energies. For two species, ^{6}**F**$^{2+}$ and *t*-**2F** ($2\kappa^2$), calculating the single point free energy at 393.15 K made the lowest positive frequency (originally 1.7042 and 2.0102 cm^{-1} respectively) now a small negative frequency instead (-4.1196 and -1.9844 cm^{-1}), and therefore more prone to thermal correction variation.

Table S2 – Relative energies (in kcal mol^{-1}) for computed structures at 298 and 393.15 K. Data in bold are used in the main text. All energies are quoted relative to **A** at 0.0 kcal/mol. * single point at 393.15 K has negative frequency.

	ΔG_{BS1}	ΔG_{393}	$\Delta(G_{393}\text{-}G_{BS1})$	$\Delta(G_{393+CC}\text{-}G_{BS1})$	$\Delta G_{MeCN\text{-}298}$	ΔG_{MeCN}
Temperature [in K]	**298**	**393.15** (120 °C)		**+ CC**	**298**	**393.15 + CC** (120 °C)
A	0.0	0.0	-	-	0.0	***0.0***
B$^+$	114.3	114.6	*0.29*	*0.29*	2.5	***2.8***
TS(**B**$^+$-**C**$^+$)	128.6	129.1	*0.54*	*0.54*	12.9	***13.4***
C$^+$	113.2	113.4	*0.22*	*0.22*	1.5	***1.7***
B·OAc	28.3	32.2	*3.93*	*1.23*	7.7	***8.9***
TS(**B**-**C**)1·OAc	39.4	43.1	*3.72*	*1.01*	16.6	***17.6***
INT(**B**-**C**)·OAc	35.1	38.8	*3.72*	*1.02*	13.4	***14.4***

			Thermal (Cratic) Correction			
TS(**B**-**C**)2·OAc	35.0	39.1	*4.16*	*1.46*	14.1	***15.6***
C·OAc	28.2	32.0	*3.80*	*1.09*	7.7	***8.8***
A·**a**-H	7.2	10.1	*2.96*	*0.25*	3.4	***3.6***
B	15.2	19.4	*4.16*	*4.16*	-1.6	***-0.2***
TS(**B**-**C**)	43.6	47.9	*4.33*	*4.33*	20.0	***21.6***
C	0.7	4.7	*4.03*	*4.03*	-11.4	***-10.0***
B′	-0.1	0.6	*0.66*	*0.66*	0.2	***0.8***
TS(**B′**-**C′**)	20.1	20.6	*0.50*	*0.50*	17.1	***17.6***
C′	20.7	20.2	*-0.49*	*-0.49*	17.0	***16.5***
C′ (without HOAc)	18.9	15.2	*-3.71*	*-1.01*	14.4	***13.4***
D	-0.3	4.5	*4.79*	*2.08*	-19.0	***-17.0***
TS(**D**-**E**)	18.9	23.6	*4.71*	*2.01*	1.2	***3.2***
E	6.1	10.4	*4.31*	*1.60*	-9.3	***-7.7***
E (without HOAc)	-7.9	-7.0	*0.94*	*0.94*	-19.9	***-19.0***
D^{+} (η^6)	110.6	110.7	*0.09*	*0.09*	-0.3	***-0.2***
TS(**D**$^{+}$-**E**$^{+}$) (η^6)	125.1	125.7	*0.61*	*0.61*	10.4	***11.0***
E^{+} (η^6)	110.1	110.6	*0.51*	*0.51*	-0.1	***0.4***
D^{+} (κ^2)	116.4	117.2	*0.90*	*0.90*	3.6	***4.5***
TS(**D**$^{+}$-**E**$^{+}$) (κ^2)	129.7	130.5	*0.83*	*0.83*	19.0	***19.9***
E^{+} (κ^2)	122.8	123.1	*0.36*	*0.36*	5.3	***5.6***
D^{+} (κ^1)	127.3	127.9	*0.65*	*0.65*	12.4	***13.1***
TS(**D**$^{+}$-**E**$^{+}$) (κ^1)	128.7	129.7	*1.01*	*1.01*	16.0	***17.0***
E^{+} (κ^1)	128.2	128.9	*0.77*	*0.77*	17.1	***17.9***
^{3}**D**$^{+}$	110.9	113.3	*12.38*	*4.27*	-21.2	***-16.9***
INT(^{3}**D**$^{+}$)	115.0	127.5	*12.51*	*4.40*	-5.0	***-0.6***
TS(^{3}**D**$^{+}$-^{3}**E**$^{+}$)	123.3	136.2	*12.89*	*4.78*	5.4	***10.2***
^{3}**E**$^{+}$	119.0	131.3	*12.28*	*4.17*	1.8	***6.0***
^{1}**A**	1.1	5.0	*3.92*	*1.21*	3.2	***4.4***

^{1}**A**$^{+}$	20.8	114.6	*-0.29*	*-0.29*	9.0	***8.7***
^{6}**F**$^{2+}$	234.0	247.4*	*13.4*	*5.31*	-16.0	***-10.6***
^{3}**A**$^{2+}$	300.8	304.2	*3.41*	*0.70*	23.2	***23.9***
^{5}**F**$^{+}$ (κ^{1})	79.8	90.7	*10.90*	*2.79*	-17.0	***-14.2***
^{4}**F**$^{+}$ (κ^{2})	77.6	85.0	*7.40*	*2.00*	-12.0	***-12.7***
c-**4F** ($2\kappa^{1}$)	-9.6	1.8	*11.41*	*3.30*	-17.0	***-13.7***
t-**4F** ($2\kappa^{1}$)	-9.6	1.5	*11.15*	*3.04*	-16.5	***-13.5***
f-**3F** ($\kappa^{2}\kappa^{1}$)	-15.2	-7.5	*7.70*	*2.30*	-15.0	***-12.7***
m-**3F** ($\kappa^{2}\kappa^{1}$)	-13.4	-6.7	*6.68*	*1.27*	-14.5	***-13.2***
c-**2F** ($2\kappa^{2}$)	-16.8	-13.0	*3.8*	*1.09*	-8.9	***-7.8***
t-**2F** ($2\kappa^{2}$)	-17.7	-10.8*	*6.85*	*4.14*	-12.0	***-7.9***
^{1}**B**$^{+}$ (*t*-N,*t*-O)	121.4	125.5	*4.09*	*1.39*	10.1	***11.5***
TS(^{1}**B**$^{+}$-^{1}**C**$^{+}$) (*t*-N,*t*-O)	137.5	141.8	*4.32*	*1.62*	25.6	***27.3***
^{1}**C**$^{+}$ (*t*-N,*t*-O)	115.0	119.1	*4.11*	*1.41*	1.4	***2.8***
^{1}**B**$^{+}$ (*t*-C_6H_6,*t*-O)	120.8	124.9	*4.00*	*1.29*	10.1	***11.4***
TS(^{1}**B**$^{+}$-^{1}**C**$^{+}$)1 (*t*-C_6H_6,*t*-O)	139.3	143.4	*4.10*	*1.40*	26.9	***28.3***
INT (^{1}**B**$^{+}$-^{1}**C**$^{+}$) (*t*-C_6H_6,*t*-O)	139.1	143.0	*3.82*	*1.12*	21.0	***22.1***
TS(^{1}**B**$^{+}$-^{1}**C**$^{+}$)2 (*t*-C_6H_6,*t*-O)	138.8	143.0	*4.16*	*1.45*	21.7	***23.1***
^{1}**C**$^{+}$ (*t*-C_6H_6,*t*-O)	129.5	133.2	*3.73*	*1.03*	15.0	***16.0***
^{1}**B**$^{+}$ (*t*-O,*t*-N)	120.8	125.1	*4.35*	*1.65*	10.4	***12.0***
TS(^{1}**B**$^{+}$-^{1}**C**$^{+}$) (*t*-O,*t*-N)	139.9	144.4	*4.57*	*1.87*	29.9	***31.8***
^{1}**C**$^{+}$ (*t*-O,*t*-N)	136.2	140.2	*3.97*	*1.27*	22.6	***23.9***
^{1}**B**$^{+}$ (*t*-O,*t*-C_6H_6)	126.1	130.3	*4.21*	*1.50*	15.4	***16.9***
TS(^{1}**B**$^{+}$-^{1}**C**$^{+}$) (*t*-O,*t*-C_6H_6)	137.9	142.3	*4.32*	*1.61*	29.1	***30.7***
^{1}**C**$^{+}$ (*t*-O,*t*-C_6H_6)	118.6	122.5	*3.91*	*1.20*	7.4	***8.6***
^{1}**B**$^{+}$ (*t*-O,*t*-O)	122.6	126.5	*3.82*	*1.11*	12.7	***13.8***
^{4}**G**$^{+}$ (κ^{1})	89.9	101.6	*11.68*	*3.57*	-18.5	***-14.9***
^{3}**G** ($2\kappa^{1}$)	-1.1	10.9	*11.96*	*3.85*	-17.8	***-14.0***

				Thermal (Cratic) Correction		
^{3}**G**$^{+}$ (κ^2)	94.6	102.5	*7.93*	*2.52*	-10.8	***-8.3***
^{2}**G**$^{+}$ (κ^2)	92.7	96.7	*4.06*	*1.35*	-7.6	***-6.3***
^{1}**G** ($2\kappa^2$)	-11.1	-7.0	*4.09*	*1.38*	-12.0	***-10.7***
^{2}**G** ($\kappa^2\kappa^1$)	-7.9	0.2	*8.05*	*2.65*	-19.7	***-17.1***
TS(^{2}**G**-^{2}**H**)	-7.4	1.0	*8.42*	*3.01*	-17.2	***-14.2***
^{2}**H**	-10.8	-2.8	*8.01*	*2.60*	-19.8	***-17.1***
^{1}**G** ($\kappa^2\kappa^1$)	-10.0	-5.7	*4.27*	*1.56*	-15.0	***-13.4***
TS(^{1}**G**-^{1}**H**)	-10.5	-6.0	*4.51*	*1.81*	-13.6	***-11.8***
^{1}**H**	-16.5	-12.6	*3.83*	*1.13*	-18.2	***-17.1***

Three DFT functionals have been tested; B3LYP, PBE1PBE (a similar hybrid functional) and ωB97X-D (a similar formulation to B3LYP but equipped to describe dispersion better). M06L results have been omitted as over 23 out of the 80 optimisations failed and had to be run as single points. Likewise, for the three functionals tested, 5 B3LYP, 5 PBE1PBE and 15 ωB97X-D structures needed to be run as single points (i.e. not free to optimise / adjust geometry parameters) due to failure to converge or giving an unwanted low negative frequency (and therefore not a true minima) based on the BP86 optimised starting geometry. The majority of these issues stem for low positive frequencies in the optimised BP86 geometries. These are shown in Table S3 with * by their energy and free energy values. Additionally, three transition states were optimised to give a second low negative frequency, which are highlighted as yellow in the XYZ coordinates and energies pages. These were; B3LYP's TS(**B**-**C**)1·OAc, PBE1PBE's TS(**B**-**C**)2·OAc and ωB97X-D's TS(**^{1}B$^+$-^{1}C$^+$**)2 (*t*-C_6H_6,*t*-O), and denoted as ^.

B3LYP and PBE1PBE both stabilise the "B" species more than the associated transition states for each pathway, thereby increasing the barrier to C-H activation for the majority of pathways and mechanisms in the manuscript. The largest changes were seen from ωB97X-D, as this includes a dispersion description larger species were significantly stabilised. All three functionals did not capture the agostic nature of INT(**^{1}B$^+$-^{1}C$^+$**), leading to this species being much lower in energy than the equivalent BP86 geometry.

Ignoring the results of ωB97X-D due to the additional dispersion stabilisation the bulkiest of species receive, for all B3LYP and PBE1PBE pathways that are viable (based on the BP86 equivalent *final* energies and the change in free energies relative to **A**) the barrier height is increased by 0.5 to 3.6 kcal mol^{-1}. In some cases stabilisation of the preceding intermediate occurs, but in no way does that suggest the BP86 functional results are incorrect or favouring a different mechanism / pathway.

Table S3 – Relative energies (in kcal mol^{-1}) for computed optimised structures for different functionals. Data in bold are values from BP86 optimisations (see Table S1). All energies are quoted relative to **A** at 0.0 kcal/mol. Functionals; BP86 = **black**, B3LYP = navy, PBE1PBE = teal, ωB97XD = purple. The delta (Δ) columns represent the energy difference from each respective ΔE_{BS1} or ΔG_{BS1} to the BP86 equivalent energy for that structure. Not all optimisations were successful, those denoted with * are single point energies based on the BP86 geometry.

	BP86		**B3LYP**				**PBE1PBE**				**ωB97X-D**			
	ΔE_{BS1}	**ΔG_{BS1}**	**ΔE_{BS1}**	**Δ**	**ΔG_{BS1}**	**Δ**	**ΔE_{BS1}**	**Δ**	**ΔG_{BS1}**	**Δ**	**ΔE_{BS1}**	**Δ**	**ΔG_{BS1}**	**Δ**
A	**0.0**	**0.0**	0.0		0.0		0.0		0.0		0.0		0.0	
B$^+$	**113.5**	**114.3**	113.1	*-0.4*	114.2	*-0.8*	110.7	*-2.8*	112.3	*-2.0*	102.2	*-11.3*	104.1	*-10.3*
TS(**B$^+$-C$^+$**)	**128.2**	**128.6**	129.3	*1.1*	129.6	*1.1*	126.6	*-1.6*	127.14	*-1.5*	119.1	*-9.1*	119.7	*-8.9*
C$^+$	**112.8**	**113.2**	115.5	*2.7*	116.6	*3.4*	110.6	*-2.2*	111.5	*-1.7*	106.3	*-6.6*	107.5	*-5.6*

B·OAc	**14.8**	**28.3**	13.5	*-1.3*	26.9	*-1.4*	9.5	*-5.3*	23.2	*-5.1*	-4.6	*-19.4*	11.3	*-17.0*
TS(**B**-**C**)1·OAc	**28.0**	**39.4**	28.3	*0.3*	40.5^	*1.1*	28.7*	*0.7*	43.9*	*4.6*	18.5*	*-9.5*	33.6*	*-5.8*
INT(**B**-**C**)·OAc	**24.0**	**35.1**	26.9	*2.9*	38.2	*3.1*	22.5	*-1.5*	34.0	*-1.1*	13.9	*-10.1*	26.3	*-8.8*
TS(**B**-**C**)2·OAc	**24.2**	**35.0**	31.3	*7.1*	41.2	*6.3*	24.5	*0.3*	36.1^	*1.2*	19.1	*-5.1*	30.0	*-5.0*
C·OAc	**15.6**	**28.2**	19.1	*3.6*	31.4	*3.2*	12.1	*-3.5*	24.5	*-3.7*	5.2	*-10.3*	17.6	*-10.6*
A·**a**-H	**-3.7**	**7.2**	-5.2	*5.3*	-1.6	*-1.9*	-6.9	*-3.3*	4.3	*-2.8*	-16.0	*-12.3*	-2.5	*-9.6*
B	**0.6**	**15.2**	0.2	*-0.4*	14.4	*-0.8*	-3.6	*-4.1*	11.2	*-4.0*	-15.3	*-15.9*	-0.8	*-16.0*
TS(**B**-**C**)	**30.6**	**43.6**	34.5	*3.9*	47.1	*3.5*	29.0	*-1.6*	42.4	*-1.2*	20.2	*-10.4*	34.4	*-9.2*
C	**-13.4**	**0.7**	-11.2	*2.1*	2.7	*2.0*	-17.3	*-3.9*	-3.1	*-3.8*	-24.9	*-11.6*	-9.8	*-10.5*
B′	**-2.0**	**-0.1**	-6.3	*-4.3*	-5.8	*-5.8*	0.7	*2.7*	1.3	*1.4*	-2.4	*-0.5*	-2.6	*-2.5*
TS(**B′**-**C′**)	**19.9**	**20.1**	12.7	*-7.1*	13.2	*-7.0*	22.7	*2.8*	22.8	*2.7*	19.0	*-0.8*	18.6	*-1.5*
C′	**22.2**	**20.7**	13.2	*-8.9*	11.0	*-9.7*	22.7	*0.6*	21.4	*0.6*	17.8	*-4.3*	17.1	*-3.6*
C′ (no HOAc)	**31.9**	**18.9**	24.4	*-7.5*	10.6	*-8.4*	34.7	*2.9*	20.8	*1.8*	35.4	*3.5*	21.0	*2.0*
D	**-15.5**	**-0.3**	-18.5	*-3.0*	-4.0	*-3.7*	-15.6	*-0.1*	-1.2	*-0.9*	-30.6	*-15.1*	-16.1	*-15.8*
TS(**D**-**E**)	**6.3**	**18.9**	5.2	*-1.1*	16.9	*-2.0*	6.8	*0.5*	18.5	*-0.4*	-6.9	*-13.2*	4.9	*-14.0*
E	**-9.0**	**6.1**	-14.1	*-5.1*	0.3	*-5.9*	-11.8	*-2.8*	2.6	*-3.8*	-26.5	*-17.5*	-12.5	*-18.6*
E (without HOAc)	**-11.0**	**-7.9**	-11.6	*-0.5*	-9.9	*-2.0*	-8.3	*2.8*	-6.2	*1.7*	-14.0	*-2.9*	-12.7	*-4.7*
D$^+$ (η^6)	**110.3**	**110.6**	110.2	*-0.2*	110.6	*0.0*	112.4*	*2.1*	114.9*	*4.3*	94.8	*-15.6*	96.7	*-13.9*
TS(**D**$^+$-**E**$^+$) (η^6)	**124.5**	**125.1**	125.8	*1.3*	126.2	*1.0*	123.4	*-1.1*	123.7	*-1.4*	112.7	*-11.8*	113.4	*-11.7*
E$^+$ (η^6)	**108.8**	**110.1**	11.9	*3.0*	113.1	*3.0*	107.1	*-1.7*	108.3	*-1.8*	100.4	*-8.4*	101.2	*-8.9*
D$^+$ (κ^2)	**114.4**	**116.4**	110.3	*-4.0*	112.0	*-4.3*	115.4	*1.0*	116.9	*0.5*	105.0	*-9.3*	106.5	*-9.8*
TS(**D**$^+$-**E**$^+$) (κ^2)	**131.0**	**129.7**	131.3	*0.3*	129.4	*-0.3*	133.8	*2.8*	132.1	*2.4*	126.7	*-4.3*	124.8	*-4.9*
E$^+$ (κ^2)	**121.8**	**122.8**	116.8	*-5.0*	117.2	*-5.6*	121.6	*-0.3*	122.2	*-0.6*	113.0	*-8.9*	113.8	*-8.9*
D$^+$ (κ^1)	**127.0**	**127.3**	106.3	*-20.7*	108.2	*-19.1*	129.6	*2.6*	129.8	*2.8*	100.6	*-9.3*	106.5	*-9.8*
TS(**D**$^+$-**E**$^+$) (κ^1)	**129.9**	**128.7**	130.4	*0.5*	128.9	*0.2*	133.8	*3.9*	132.2	*3.5*	128.5	*-4.3*	124.8	*-4.9*
E$^+$ (κ^1)	**127.3**	**128.2**	124.8	*-2.6*	125.7	*-2.4*	128.7	*1.4*	129.5	*1.4*	121.7	*-8.9*	113.8	*-8.9*
^{3}**D**$^+$	**65.8**	**110.9**	64.7*	*-1.1*	109.6*	*8.7*	60.8	*-5.0*	98.9	*-2.0*	36.5	*-29.3*	75.9	*-25.0*
INT(^{3}**D**$^+$)	**79.3**	**115.0**	73.1	*-6.2*	109.7	*-5.3*	73.0	*-6.3*	110.5	*-4.5*	49.8	*-29.5*	88.4	*-26.6*

TS(^{3}**D**$^+$-^{3}**E**$^+$)	**90.1**	**123.3**	90.4	*0.3*	125.2	*1.9*	87.7	*-2.4*	122.9	*-0.4*	76.4*	*-13.6*	117.2*	*-6.1*
^{3}**E**$^+$	**84.4**	**119.0**	82.5	*-1.9*	118.6	*-0.4*	79.9	*-4.5*	116.4	*-2.5*	58.9	*-25.6*	97.5	*-21.5*
^{1}**A**	**-9.9**	**1.1**	-12.9	*-3.0*	-1.6	*-2.7*	-7.4	*2.5*	4.2	*3.1*	-5.2	*4.8*	10.3	*9.2*
^{1}**A**$^+$	**10.1**	**20.8**	118.7	*-0.2*	115.7	*0.9*	118.7	*-0.2*	115.8	*0.9*	121.5*	*2.6*	122.0*	*71*
^{6}**F**$^{2+}$	**215.6**	**234.0**	211.9*	*-3.8*	250.4*	*16.4*	216.4*	*0.7*	254.9*	*20.9*	217.9*	*2.3*	255.7*	*21.7*
^{3}**A**$^{2+}$	**297.8**	**300.8**	295.4	*-2.3*	302.1	*1.3*	293.6	*-4.1*	300.4	*-0.4*	294.9*	*-2.8*	306.8*	*6.0*
^{5}**F**$^+$ (κ^1)	**54.4**	**79.8**	52.3*	*-2.1*	92.1*	*12.3*	54.7	*0.3*	83.6	*3.8*	59.9*	*5.5*	99.4*	*19.5*
^{4}**F**$^+$ (κ^2)	**62.4**	**77.6**	57.9	*-4.5*	75.4	*-2.2*	62.0	*2.6*	82.7	*5.1*	71.1*	*8.7*	97.6*	*20.0*
c-**4F** ($2\kappa^1$)	**-39.3**	**-9.6**	-43.6	*-4.2*	-11.7	*-2.1*	-37.3	*2.0*	-5.2	*4.4*	-38.8	*0.6*	-5.4	*4.2*
t-**4F** ($2\kappa^1$)	**-38.5**	**-9.6**	-43.6	*-5.1*	-12.4	*-2.7*	-36.9	*1.6*	-5.5	*4.1*	-31.9*	*6.6*	8.9*	*18.5*
f-**3F** ($\kappa^2\kappa^1$)	**-34.6**	**-15.2**	-38.2	*-3.7*	-17.9	*-2.6*	-30.4	*4.2*	-9.6	*5.6*	-29.4	*5.1*	-8.6	*6.7*
m-**3F** ($\kappa^2\kappa^1$)	**-30.0**	**-13.4**	-36.8	*-6.8*	-17.1	*-3.7*	-28.5	*1.5*	-8.8	*4.6*	-19.8*	*10.2*	7.5*	*20.9*
c-**2F** ($2\kappa^2$)	**-25.1**	**-16.8**	-30.0	*-4.8*	-21.2	*-4.3*	-20.0	*5.1*	-11.2	*5.6*	-18.1	*7.1*	-10.0	*4.2*
t-**2F** ($2\kappa^2$)	**-23.2**	**-17.7**	-27.8*	*-4.6*	-13.1*	*4.6*	-16.9*	*6.3*	-2.4*	*15.3*	-18.9	*4.3*	-11.0	*19.5*
^{1}**B**$^+$ (*t*-N,*t*-O)	**110.1**	**121.4**	105.7	*-4.4*	117.5	*-3.9*	108.7	*-1.4*	120.7	*-0.7*	103.0*	*-7.1*	118.5*	*-2.9*
TS(^{1}**B**$^+$-^{1}**C**$^+$) (*t*-N,*t*-O)	**127.1**	**137.5**	124.2	*-2.9*	135.4	*-2.1*	127.9	*0.8*	139.2	*1.7*	119.7	*-7.3*	130.8	*-6.6*
^{1}**C**$^+$ (*t*-N,*t*-O)	**103.8**	**115.0**	103.7	*-0.2*	115.5	*0.5*	103.7	*-0.1*	115.8	*0.8*	96.2	*-7.6*	107.8	*-7.2*
^{1}**B**$^+$ (*t*-C_6H_6,*t*-O)	**109.8**	**120.8**	104.5	*-5.3*	115.9	*-5.0*	108.2	*-1.6*	120.1	*-0.8*	97.2	*-12.6*	109.2	*-11.7*
TS(^{1}**B**$^+$-^{1}**C**$^+$)1 (*t*-C_6H_6,*t*-O)	**128.9**	**139.3**	123.2	*-5.7*	133.9	*-5.4*	128.0	*-0.9*	138.9	*-0.4*	124.9*	*-4.1*	139.8*	*0.5*
INT (^{1}**B**$^+$-^{1}**C**$^+$) (*t*-C_6H_6,*t*-O)	**130.6**	**139.1**	108.5	*-22.1*	120.2	*-18.9*	111.4	*-19.1*	123.8	*-15.3*	122.7	*-7.9*	133.6	*-5.6*
TS(^{1}**B**$^+$-^{1}**C**$^+$)2 (*t*-C_6H_6,*t*-O)	**130.7**	**138.8**	131.2	*0.5*	138.8	*0.0*	133.0	*2.3*	141.3	*2.5*	125.2	*-5.4*	134.9^	*-3.9*
^{1}**C**$^+$ (*t*-C_6H_6,*t*-O)	**119.9**	**129.5**	117.6	*-2.3*	128.2	*-1.2*	118.4	*-1.5*	129.2	*-0.3*	115.6*	*-4.3*	130.0*	*0.6*
^{1}**B**$^+$ (*t*-O,*t*-N)	**108.9**	**120.8**	106.2	*-2.7*	118.1	*-2.7*	108.9	*0.0*	121.3	*0.5*	106.1*	*-2.9*	121.2*	*0.5*
TS(^{1}**B**$^+$-^{1}**C**$^+$) (*t*-O,*t*-N)	**131.1**	**139.9**	134.1	*3.1*	143.7	*3.8*	133.3	*2.2*	143.2	*3.3*	127.4	*-3.7*	137.4	*-2.4*
^{1}**C**$^+$ (*t*-O,*t*-N)	**125.7**	**136.2**	124.5	*-1.2*	135.7	*-0.4*	124.9	*-0.8*	136.5	*0.3*	117.6	*-8.2*	128.5	*-7.6*
^{1}**B**$^+$ (*t*-O,*t*-C_6H_6)	**114.9**	**126.1**	111.4	*-3.5*	123.2	*-2.9*	114.3	*-0.6*	126.9	*0.7*	104.3	*-10.6*	116.9	*-9.3*
TS(^{1}**B**$^+$-^{1}**C**$^+$) (*t*-O,*t*-C_6H_6)	**129.8**	**137.9**	130.8	*1.1*	139.3	*1.4*	131.7	*2.0*	141.1	*3.1*	125.9	*-3.9*	134.9	*-3.0*
^{1}**C**$^+$ (*t*-O,*t*-C_6H_6)	**107.9**	**118.6**	106.2	*-1.6*	117.9	*-0.7*	107.0	*-0.9*	119.0	*0.4*	100.7	*-7.2*	112.0	*-6.6*

^{1}**B**$^{+}$ (*t*-O,*t*-O)	**112.4**	**122.6**	105.8	*-6.5*	117.7	*-4.9*	110.9	*-1.4*	122.8	*0.2*	100.9	*-115.*	112.0	*-10.6*
^{4}**G**$^{+}$ (κ^{1})	**59.6**	**89.9**	54.4	*-5.2*	87.2	*-2.7*	57.8	*-1.8*	89.9	*-0.1*	47.5	*-12.1*	80.8	*-9.1*
^{3}**G** ($2\kappa^{1}$)	**-35.5**	**-1.1**	-40.1	*-4.8*	-4.5	*-3.5*	-36.3	*-1.0*	-0.3	*0.7*	-47.9	*-12.6*	-10.8	*-9.8*
^{3}**G**$^{+}$ (κ^{2})	**75.3**	**94.6**	71.2	*-4.1*	92.4	*-2.2*	75.2	*-0.1*	96.3	*1.7*	76.5*	*1.1*	104.4*	*9.8*
^{2}**G**$^{+}$ (κ^{2})	**84.4**	**92.7**	80.2	*-4.3*	89.8	*-2.9*	86.1	*1.7*	95.5	*2.9*	83.6	*-0.8*	91.8	*-0.9*
^{1}**G** ($2\kappa^{2}$)	**-21.5**	**-11.1**	-27.3*	*-5.8*	-10.9*	*0.2*	-17.4*	*4.1*	-1.4*	*9.6*	-22.3*	*-0.7*	-6.3*	*4.7*
^{2}**G** ($\kappa^{2}\kappa^{1}$)	**-29.7**	**-7.9**	-31.2	*-1.5*	-8.5	*-0.6*	-27.1	*2.6*	-4.5	*3.4*	-31.0	*-1.3*	-10.0	*-2.1*
TS(^{2}**G**-^{2}**H**)	**-27.9**	**-7.4**	-25.2	*2.7*	-4.3	*3.0*	-23.7	*4.2*	-2.8	*4.6*	-25.4	*2.5*	-4.4	*3.0*
^{2}**H**	**-33.2**	**-10.8**	-33.6	*-0.4*	-10.5	*0.3*	-31.8	*1.4*	-8.7	*2.1*	-34.8	*1.6*	-11.1	*-0.4*
^{1}**G** ($\kappa^{2}\kappa^{1}$)	**-21.0**	**-10.0**	-22.7	*-1.7*	-11.6	*-1.5*	-17.0	*4.0*	-6.1	*3.9*	-19.2	*1.8*	-8.6	*1.4*
TS(^{1}**G**-^{1}**H**)	**-19.9**	**-10.5**	-18.0	*1.9*	-8.9	*1.6*	-14.6	*5.4*	-5.5	*4.9*	-14.3	*5.6*	-5.8	*4.6*
^{1}**H**	**-27.1**	**-16.5**	-28.5	*-1.5*	-17.9	*-1.5*	-24.7	*2.4*	-14.3	*2.1*	-25.5	*1.6*	-15.1	*1.3*

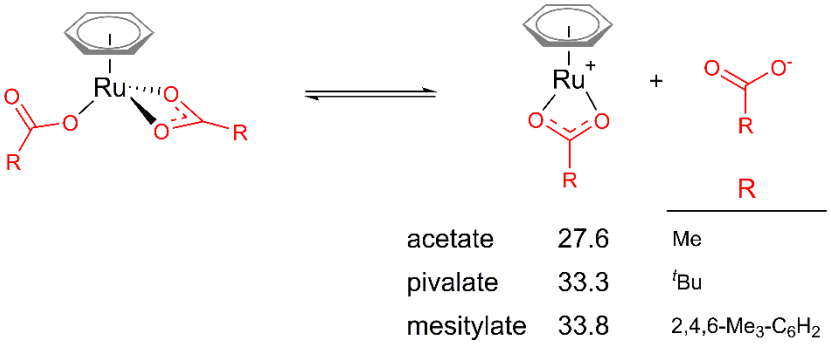

Figure S1 – BP86-D3BJ(BS2,MeCN)//BP86(BS1) free energy values for different carboxylate ($^{-}O_2CR$) dissociations from **A**, $[(C_6H_6)Ru(O_2CR)_2]$, in kcal mol^{-1}

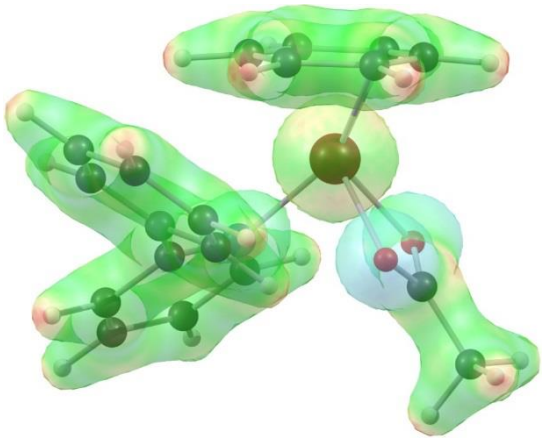

Figure S2 – Electrostatic potential surface of **B**$^{+}$ to find potential acetate anion coordination "sites" / areas

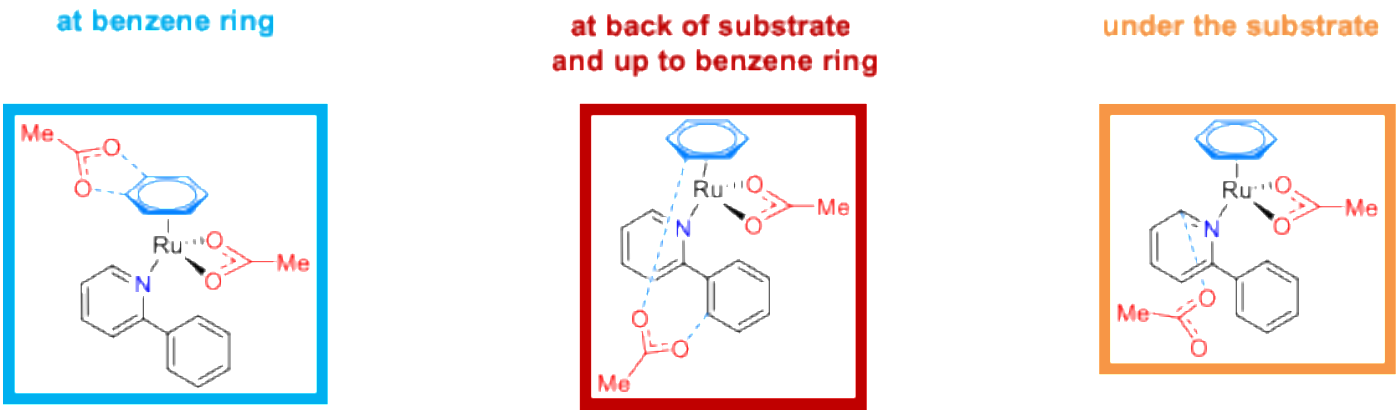

Figure S3 – Three ion-pair binding sites were identified in **B**$^{+}$, at the benzene ring (six isomers; a – f), at the "back" of the **a**-H substrate, and "under" the substrate. Computed values can be found for all eight isomers in the cartesian coordinates and energies section.

$^{-}$OAc
SCF (BP86) Energy = -228.501360689
Enthalpy 0K = -228.454943
Enthalpy 298K = -228.449433
Free Energy 298K = -228.482845
Lowest Frequency = 29.1085 cm^{-1}
Second Frequency = 394.2040 cm^{-1}
SCF (BP86-D3BJ) Energy = -228.506682590
SCF (MeCN) Energy = -228.601950143
SCF (Toluene) Energy = -228.560110356
SCF (BS2) Energy = -228.606540536

O 0.69867 1.17860 0.00046
C 0.22375 0.00215 -0.00211
O 0.81598 -1.11868 0.00049
C -1.36311 -0.05746 -0.00077
H -1.76086 0.42591 0.91393
H -1.77069 0.51960 -0.85439
H -1.74949 -1.09295 -0.04983

AcOH
SCF (BP86) Energy = -229.088708932
Enthalpy 0K = -229.028635
Enthalpy 298K = -229.023037
Free Energy 298K = -229.056000
Lowest Frequency = 62.3881 cm^{-1}
Second Frequency = 405.1869 cm^{-1}
SCF (BP86-D3BJ) Energy = -229.094744166
SCF (MeCN) Energy = -229.094701290
SCF (Toluene) Energy = -229.091705970
SCF (BS2) Energy = -229.166189272

C 1.40382 -0.10154 -0.00001
H 1.92101 0.86628 -0.00014
H 1.69796 -0.68621 -0.88713
H 1.69816 -0.68609 0.88713
C -0.09248 0.12615 0.00017
O -0.65936 1.20853 -0.00004
O -0.77354 -1.06295 -0.00004
H -1.72193 -0.80631 -0.00013

a-H, 2-phenylpyridine
SCF (BP86) Energy = -479.337880864
Enthalpy 0K = -479.173096
Enthalpy 298K = -479.163059
Free Energy 298K = -479.208174
Lowest Frequency = 40.8265 cm^{-1}
Second Frequency = 91.4535 cm^{-1}
SCF (BP86-D3BJ) Energy = -479.377089966
SCF (MeCN) Energy = -479.343317783
SCF (Toluene) Energy = -479.340265969
SCF (BS2) Energy = -479.454661331

N -1.36753 -1.17191 -0.17495
C -2.71055 -1.21710 -0.18210
C -3.53632 -0.09266 -0.02278
H -3.15281 -2.21232 -0.32607
H -4.62575 -0.19223 -0.04405
C 0.72646 0.03168 -0.00419
C 1.47889 1.21545 -0.17705
C 2.82036 -1.22025 0.17294
C 2.88039 1.18198 -0.16888
H 0.97157 2.17082 -0.34574
C 3.55776 -0.03504 0.01029
H 3.34001 -2.17469 0.30982
H 3.44504 2.10951 -0.31122
H 4.65256 -0.05996 0.01751
C -0.76446 0.03302 0.00011
C -2.91551 1.14941 0.17447
H -3.51173 2.05619 0.32210
C -1.51758 1.21508 0.19240
H -1.01757 2.17046 0.37490
C 1.42054 -1.18858 0.16256
H 0.83156 -2.10225 0.28074

Benzene (C_6H_6)
SCF (BP86) Energy = -232.242069991
Enthalpy 0K = -232.144359
Enthalpy 298K = -232.138884
Free Energy 298K = -232.171901
Lowest Frequency = 397.4291 cm^{-1}
Second Frequency = 397.4496 cm^{-1}
SCF (BP86-D3BJ) Energy = -232.258991055
SCF (MeCN) Energy = -232.244669833
SCF (Toluene) Energy = =
SCF (BS2) Energy = -232.299996216

C -0.00852 1.40478 0.00000
C -1.22083 0.69500 0.00000
C -1.21231 -0.70976 0.00000
C 0.00852 -1.40477 0.00000
C 1.22083 -0.69500 0.00000
C 1.21230 0.70977 0.00000
H -2.17273 1.23691 0.00000
H -2.15756 -1.26318 0.00000
H 0.01517 -2.50009 0.00000
H 2.17273 -1.23691 0.00000
H 2.15756 1.26318 0.00000
H -0.01517 2.49996 0.00000

MeCN
SCF (BP86) Energy = -132.751073424
Enthalpy 0K = -132.706992
Enthalpy 298K = -132.702405
Free Energy 298K = -132.730016
Lowest Frequency = 373.9643 cm^{-1}
Second Frequency = 373.9650 cm^{-1}
SCF (BP86-D3BJ) Energy = -132.755185372
SCF (MeCN) Energy = -132.758518000
SCF (Toluene) Energy = -132.754759633
SCF (BS2) Energy = -132.790873881

C 0.00000 0.00000 -1.18538
H 0.00000 -1.03346 -1.56891
H 0.89501 0.51673 -1.56891
H -0.89501 0.51673 -1.56891
C 0.00000 0.00000 0.27726
N 0.00000 0.00000 1.45077

A

SCF (BP86) Energy = -784.308941980
Enthalpy 0K = -784.109005
Enthalpy 298K = -784.091970
Free Energy 298K = -784.154847
Lowest Frequency = 8.5076 cm^{-1}
Second Frequency = 52.9194 cm^{-1}
SCF (BP86-D3BJ) Energy = -784.361136777
SCF (MeCN) Energy = -784.322848319
SCF (Toluene) Energy = -784.315480649
SCF (BS2) Energy = -784.216159690

C	1.74819	-0.95076	1.42935
C	2.51360	0.03836	0.70675
C	2.50983	0.03301	-0.71694
C	1.74286	-0.96256	-1.42923
C	1.01242	-1.95553	-0.71575
C	1.01490	-1.94982	0.72696
Ru	0.42692	0.04258	-0.00087
O	-0.17123	1.79950	-1.09835
C	-0.47086	2.39897	0.00138
C	-1.16735	3.73253	0.00259
H	2.99563	0.84329	-1.26725
H	0.34152	-2.62622	1.25466
O	-1.60638	-0.19648	-0.00574
C	-2.25143	-1.35538	0.00024
O	-1.74441	-2.48688	0.00915
O	-0.17525	1.79558	1.10012
C	-3.76885	-1.15049	-0.00459
H	-4.07482	-0.56912	0.88086
H	-4.07016	-0.57255	-0.89383
H	-4.27716	-2.12467	-0.00374
H	-2.25781	3.56333	-0.00030
H	-0.90834	4.30023	0.90854
H	-0.90419	4.30402	-0.89978
H	1.65933	-0.87544	2.51696
H	0.33694	-2.63609	-1.23540
H	1.65039	-0.89634	-2.51710
H	3.00248	0.85238	1.24869

$[(C_6H_6)Ru(OAc)]^+$
SCF (BP86) Energy = -555.552331451
Enthalpy 0K = -555.402417
Enthalpy 298K = -555.390582
Free Energy 298K = -555.440931
Lowest Frequency = 30.6721 cm^{-1}
Second Frequency = 46.2829 cm^{-1}
SCF (BP86-D3BJ) Energy = -555.588306393
SCF (MeCN) Energy = -555.632258049
SCF (Toluene) Energy = -555.597739758
SCF (BS2) Energy = -555.383426681

C	1.75665	-1.44628	0.19123
C	1.38699	-0.72314	1.37541
C	1.38699	0.72308	1.37544
C	1.75666	1.44627	0.19129
C	2.03601	0.72200	-0.99762
C	2.03601	-0.72196	-0.99765
Ru	0.10122	0.00000	-0.17310
O	-1.65481	1.09577	0.02265
C	-2.35963	0.00000	-0.01163
H	1.03130	1.26338	2.25781
H	2.16439	-1.25883	-1.94240
O	-1.65481	-1.09576	0.02265
H	1.67634	-2.53636	0.16743
H	2.16441	1.25891	-1.94235
H	1.67635	2.53635	0.16753
H	1.03130	-1.26347	2.25775
C	-3.84441	-0.00000	-0.05740
H	-4.21429	-0.90905	-0.55386
H	-4.22402	-0.00003	0.98156
H	-4.21430	0.90906	-0.55382

$^-$OtBu
SCF (BP86) Energy = -346.450213517
Enthalpy 0K = -346.321651
Enthalpy 298K = -346.313239
Free Energy 298K = -346.352484
Lowest Frequency = -27.1798 cm^{-1}
Second Frequency = 205.8424 cm^{-1}
SCF (BP86-D3BJ) Energy = -346.471301993
SCF (MeCN) Energy = -346.541159640
SCF (Toluene) Energy = -346.502381228
SCF (BS2) Energy = -346.574851177

O	-1.61207	-1.14713	-0.03947
C	-1.07240	0.00007	-0.05642
O	-1.61214	1.14724	-0.03947
C	0.54322	0.00004	-0.01674
C	1.09211	-1.27045	-0.68659
H	0.93136	-1.23965	-1.78107
H	2.18050	-1.40979	-0.50988
H	0.53120	-2.13737	-0.30050
C	1.09227	1.27150	-0.68461
H	0.53153	2.13793	-0.29718
H	2.18069	1.41036	-0.50773
H	0.93144	1.24245	-1.77912
C	0.92422	-0.00120	1.48034
H	0.50278	-0.89437	1.97639
H	2.02450	-0.00156	1.63689
H	0.50319	0.89136	1.97784

$[(C_6H_6)Ru(OtBu)_2]$
SCF (BP86) Energy = -1020.18455813
Enthalpy 0K = -1019.819295
Enthalpy 298K = -1019.794047
Free Energy 298K = -1019.875552
Lowest Frequency = 8.8353 cm^{-1}
Second Frequency = 16.5328 cm^{-1}
SCF (BP86-D3BJ) Energy = -1020.27192980
SCF (MeCN) Energy = -1020.19744502
SCF (Toluene) Energy = -1020.19029340
SCF (BS2) Energy = -1020.14281408

C	-0.41960	-2.60729	-1.50164
C	-1.65456	-2.61766	-0.75190
C	-1.62140	-2.70033	0.66908
C	-0.35043	-2.76210	1.35183
C	0.86727	-2.78001	0.61202
C	0.83107	-2.70262	-0.82794
Ru	-0.33416	-1.03330	0.01771
O	-1.27106	0.45960	1.25667
C	-1.63552	1.12475	0.21443
H	-2.54589	-2.60385	1.24457
H	1.76943	-2.57738	-1.36936
O	1.13195	0.39916	0.02316
C	2.43726	0.17611	-0.02027
O	2.98989	-0.93397	-0.07515
O	-1.39141	0.59076	-0.93327
H	-0.44450	-2.43495	-2.58143
H	1.83128	-2.71181	1.11722
H	-0.32150	-2.70563	2.44385
H	-2.60533	-2.45654	-1.26717
C	-2.31414	2.47646	0.33215
H	-2.50000	2.63326	1.41100
C	-1.36810	3.58237	-0.18789
H	-1.83915	4.57209	-0.06288
H	-0.41181	3.58276	0.35953
H	-1.15049	3.43228	-1.25806
C	-3.66533	2.48593	-0.42459
H	-4.07309	3.51257	-0.36967
H	-3.46853	2.28120	-1.49281
C	-4.69777	1.48853	0.12116
H	-5.65013	1.56255	-0.43032

```
H  -4.34061  0.44814  0.02717
H  -4.91190  1.67408  1.18839
C   3.26058  1.49986  0.00791
C   2.94462  2.25535  1.32165
H   3.51068  3.20348  1.36077
H   1.86957  2.48304  1.39612
H   3.22925  1.65607  2.20438
C   2.85251  2.37110 -1.20457
H   3.42017  3.31911 -1.19947
H   3.06818  1.85465 -2.15653
H   1.77667  2.60405 -1.17758
C   4.76347  1.16843 -0.06151
H   5.00827  0.62022 -0.98551
H   5.35592  2.10057 -0.03981
H   5.07204  0.53760  0.78749
```

$[(C_6H_6)Ru(OtBu)]^+$

```
SCF (BP86) Energy = -673.494518023
Enthalpy 0K = -673.262135
Enthalpy 298K = -673.246174
Free Energy 298K = -673.306141
Lowest Frequency = 10.9134 cm-1
Second Frequency = 38.1474 cm-1
SCF (BP86-D3BJ) Energy = -673.547145247
SCF (MeCN) Energy = -673.569789385
SCF (Toluene) Energy = -673.537047121
SCF (BS2) Energy = -673.351017571

C  -2.51715  1.44601  0.16286
C  -2.17948  0.72311  1.35604
C  -2.17943 -0.72308  1.35607
C  -2.51704 -1.44605  0.16292
C  -2.76173 -0.72199 -1.03377
C  -2.76179  0.72189 -1.03380
Ru -0.84991  0.00001 -0.15677
O   0.89509 -1.09401  0.04956
C   1.61016  0.00002  0.00177
H  -1.84957 -1.26329  2.24836
H  -2.86528  1.25883 -1.98146
O   0.89510  1.09406  0.04953
H  -2.43759  2.53612  0.14164
H  -2.86513 -1.25897 -1.98141
H  -2.43738 -2.53615  0.14173
H  -1.84966  1.26339  2.24831
C   3.11304  0.00003 -0.04403
C   3.62494 -1.27872 -0.74607
H   3.32265 -1.30373 -1.80600
H   4.72604 -1.29000 -0.70723
H   3.25347 -2.19183 -0.25575
C   3.62502  1.27936 -0.74489
H   3.25372  2.19205 -0.25367
H   4.72614  1.29046 -0.70613
H   3.32266  1.30542 -1.80477
C   3.56062 -0.00070  1.45763
H   3.20415 -0.89962  1.98590
H   4.66290 -0.00074  1.48072
H   3.20421  0.89776  1.98674
```

^-OMes

```
SCF (BP86) Energy = -538.202534223
Enthalpy 0K = -538.023840
Enthalpy 298K = -538.010464
Free Energy 298K = -538.062679
Lowest Frequency = 40.9704 cm-1
Second Frequency = 76.0093 cm-1
SCF (BP86-D3BJ) Energy = -538.242672971
SCF (MeCN) Energy = -538.289235123
SCF (Toluene) Energy = -538.251220410
SCF (BS2) Energy = -538.367686377

O  -2.71489  0.75466  0.87067
C  -2.17084  0.00076  0.00714
O  -2.72492 -0.75171 -0.85105
C  -0.61382 -0.00028  0.00159
C   0.11664 -1.21994  0.07278
C   0.11655  1.21883 -0.08025
C   1.52454 -1.20068  0.07386
C   1.52423  1.19897 -0.09611
C   2.25413 -0.00088 -0.01161
H   2.06861 -2.15572  0.13216
H   2.06776  2.15319 -0.16995
C  -0.61498  2.54417 -0.15307
H  -1.09730  2.68302 -1.13969
H  -1.43158  2.53627  0.58884
H   0.07278  3.39385  0.01084
C  -0.61453 -2.54582  0.13859
H  -1.08802 -2.69418  1.12813
H  -1.43773 -2.53077 -0.59592
H   0.07188 -3.39385 -0.03914
C   3.76979  0.00130  0.01983
H   4.16867  0.09061  1.05059
H   4.18576 -0.93140 -0.40264
H   4.18744  0.84668 -0.55673
```

$[(C_6H_6)Ru(OMes)_2]$

```
SCF (BP86) Energy = -1403.66917957
Enthalpy 0K = -1403.205117
Enthalpy 298K = -1403.171310
Free Energy 298K = -1403.273704
Lowest Frequency = 10.8509 cm-1
Second Frequency = 15.4577 cm-1
SCF (BP86-D3BJ) Energy = -1403.79835972
SCF (MeCN) Energy = -1403.68375095
SCF (Toluene) Energy = -1403.67558344
SCF (BS2) Energy = -1403.71317397

C   0.05828 -3.82693  1.39774
C   1.32536 -3.95451  0.71441
C   1.37693 -3.96178 -0.70922
C   0.15651 -3.79667 -1.46055
C  -1.09992 -3.68765 -0.79448
C  -1.14365 -3.70157  0.64666
Ru  0.29280 -2.16405 -0.02151
O   1.36649 -0.73979 -1.19962
C   1.84507 -0.17211 -0.13922
H   2.34147 -3.96936 -1.22350
H  -2.08966 -3.47832  1.14193
O  -0.95984 -0.54140  0.12944
C  -2.28267 -0.57220  0.07260
O  -2.98871 -1.58324 -0.08862
O   1.58148 -0.76757  0.98056
H   0.03573 -3.73222  2.48681
H  -2.01080 -3.45526 -1.34685
H   0.20606 -3.67015 -2.54614
H   2.25440 -3.95332  1.29125
C  -2.90010  0.80706  0.20547
C  -3.81909  1.24483 -0.78480
C  -2.60162  1.63251  1.32129
C  -4.40555  2.51572 -0.64991
C  -3.23231  2.88630  1.42192
C  -4.12725  3.35427  0.44402
H  -5.10751  2.85595 -1.42193
H  -3.01374  3.51623  2.29364
C   2.64222  1.07700 -0.20492
C   3.71912  1.28083  0.70728
C   2.32441  2.06746 -1.18149
C   4.46595  2.46670  0.60927
C   3.09405  3.24276 -1.21457
C   4.16866  3.46422 -0.33580
H   5.30671  2.61529  1.29796
H   2.84272  4.01085 -1.95614
C  -4.17970  0.38061 -1.97615
H  -3.28299  0.06816 -2.54036
H  -4.68222 -0.54463 -1.65132
```

H -4.84298 0.92640 -2.66679
C -1.65271 1.19075 2.41756
H -1.94986 0.21493 2.84157
H -0.62655 1.06591 2.03661
H -1.64074 1.92524 3.23948
C -4.75439 4.72816 0.55288
H -4.13238 5.49407 0.05264
H -5.74945 4.75805 0.07789
H -4.86795 5.03922 1.60493
C 4.10705 0.26909 1.76680
H 3.35998 0.23099 2.57667
H 4.17331 -0.75346 1.36002
H 5.08322 0.53287 2.20526
C 1.18008 1.92165 -2.16329
H 1.41050 1.17364 -2.94003
H 0.25664 1.58085 -1.66852
H 0.98133 2.88624 -2.65798
C 4.96251 4.75110 -0.38577
H 4.50491 5.52347 0.26007
H 5.99676 4.60310 -0.03355
H 5.00125 5.16357 -1.40759

$[(C_6H_6)Ru(OMes)]^+$
SCF (BP86) Energy = -865.249489758
Enthalpy 0K = -864.967005
Enthalpy 298K = -864.947082
Free Energy 298K = -865.016888
Lowest Frequency = 20.1591 cm^{-1}
Second Frequency = 27.7342 cm^{-1}
SCF (BP86-D3BJ) Energy = -865.321718849
SCF (MeCN) Energy = -865.313119253
SCF (Toluene) Energy = -865.286081042
SCF (BS2) Energy = -865.147858194

C 3.57009 -1.44425 0.06350
C 3.39394 -0.71769 1.28309
C 3.39540 0.72738 1.27751
C 3.57193 1.44381 0.05226
C 3.64588 0.71655 -1.16848
C 3.64568 -0.72712 -1.16290
Ru 1.87125 0.00016 -0.07315
O 0.14868 1.09737 0.05495
C -0.59258 0.00003 0.04079
H 3.18909 1.27086 2.20400
H 3.62326 -1.26896 -2.11281
O 0.14867 -1.09737 0.05169
H 3.48691 -2.53409 0.05854
H 3.62352 1.25091 -2.12265
H 3.49019 2.53367 0.03846
H 3.18670 -1.25358 2.21380
C -2.03341 0.00006 0.01638
C -2.75534 -1.25487 0.00850
C -2.75521 1.25499 0.00819
C -4.15241 -1.21070 -0.00292
C -4.15237 1.21094 -0.00336
C -4.87571 0.00019 -0.01220
H -4.70462 -2.15670 -0.00334
H -4.70451 2.15696 -0.00429
C -2.09800 -2.61632 0.01612
H -1.45500 -2.76703 -0.86648
H -1.45212 -2.75585 0.89842
H -2.86855 -3.40208 0.02173
C -2.09783 2.61641 0.01519
H -1.45311 2.75682 0.89819
H -1.45364 2.76618 -0.86671
H -2.86834 3.40223 0.01897
C -6.38020 -0.00012 -0.05683
H -6.72790 -0.01227 -1.10728
H -6.80232 -0.89138 0.43388
H -6.80260 0.90146 0.41411

Toluene (tol)
SCF (BP86) Energy = -271.559258208
Enthalpy 0K = -271.434921
Enthalpy 298K = -271.427571
Free Energy 298K = -271.465906
Lowest Frequency = 28.8277 cm^{-1}
Second Frequency = 202.7218 cm^{-1}
SCF (BP86-D3BJ) Energy = -271.581062971
SCF (MeCN) Energy = -271.561882000
SCF (Toluene) Energy = -271.560395742
SCF (BS2) Energy = -271.625271803

C -0.92053 0.00019 -0.01166
C -0.19611 1.20978 -0.00912
C 1.20745 1.21254 0.00223
C 1.91518 -0.00010 0.00874
C 1.20713 -1.21270 0.00223
C -0.19629 -1.20969 -0.00912
H 1.74913 2.16470 0.00119
H 1.74878 -2.16489 0.00120
H 3.01022 -0.00030 0.01415
C -2.43505 0.00007 0.00930
H -2.84739 -0.88826 -0.49773
H -2.82119 -0.00848 1.04567
H -2.84733 0.89648 -0.48326
H -0.74124 2.16125 -0.01840
H -0.74170 -2.16101 -0.01841

$[(tol)Ru(OAc)_2]$
SCF (BP86) Energy = -823.628702029
Enthalpy 0K = -823.402023
Enthalpy 298K = -823.383196
Free Energy 298K = -823.449027
Lowest Frequency = 24.7333 cm^{-1}
Second Frequency = 54.4412 cm^{-1}
SCF (BP86-D3BJ) Energy = -823.687423812
SCF (MeCN) Energy = -823.643044922
SCF (Toluene) Energy = -823.635287216
SCF (BS2) Energy = -823.544299887

C 0.34933 -2.03279 1.09089
C 0.38594 -2.22353 -0.33270
C 1.33295 -1.52259 -1.13241
H -0.46814 -2.46660 1.66770
H -0.41736 -2.79483 -0.80066
H 1.27999 -1.59127 -2.22301
C 1.28492 -1.12992 1.68877
C 2.28371 -0.46172 0.89818
C 2.28685 -0.61450 -0.52448
H 1.19172 -0.88268 2.75084
Ru 0.24907 -0.07062 0.10805
O 0.28174 1.84944 -0.88370
C -0.15389 2.41879 0.18568
O -0.24959 1.69063 1.24362
C -0.56664 3.86594 0.19205
H 0.01396 4.43424 -0.54971
H -1.63389 3.93154 -0.08081
H -0.43920 4.29798 1.19561
O -1.72829 0.12183 -0.39754
C -2.64277 -0.83110 -0.27552
C -4.03454 -0.32617 -0.66768
H -4.40695 0.36249 0.10990
H -3.99496 0.23697 -1.61352
H -4.72739 -1.17466 -0.75710
O -2.45837 -1.99137 0.12087
C 3.22648 0.18441 -1.39299
H 3.59981 1.07580 -0.86560
H 4.09508 -0.43503 -1.68227
H 2.72239 0.51645 -2.31463
H 2.94771 0.27185 1.36425

o-xylene (*o*-xyl)
SCF (BP86) Energy = -310.876056618

Enthalpy 0K = -310.724572
Enthalpy 298K = -310.715838
Free Energy 298K = -310.756261
Lowest Frequency = 132.8543 cm^{-1}
Second Frequency = 155.6289 cm^{-1}
SCF (BP86-D3BJ) Energy = -310.903701384
SCF (MeCN) Energy = -310.878807439
SCF (Toluene) Energy = -310.877237271
SCF (BS2) Energy = -310.949972732

C	0.48160	0.71045	0.00000
C	-0.75001	1.39259	0.00000
C	-1.97137	0.70092	0.00000
C	-1.97138	-0.70092	0.00000
C	-0.75001	-1.39259	0.00000
C	0.48159	-0.71046	0.00000
H	-2.91540	1.25611	0.00000
H	-0.74711	-2.48926	0.00000
C	1.78295	-1.48324	0.00000
H	-2.91540	-1.25610	0.00000
H	2.40099	-1.24585	0.88567
H	1.60141	-2.57003	-0.00016
H	2.40114	-1.24562	-0.88550
C	1.78295	1.48324	0.00000
H	2.40106	1.24575	0.88559
H	2.40107	1.24572	-0.88558
H	1.60141	2.57003	-0.00002
H	-0.74710	2.48926	0.00000

[(*o*-xyl)Ru(OAc)$_2$]
SCF (BP86) Energy = -862.944926979
Enthalpy 0K = -862.691562
Enthalpy 298K = -862.670810
Free Energy 298K = -862.742334
Lowest Frequency = 5.2173 cm^{-1}
Second Frequency = 53.0388 cm^{-1}
SCF (BP86-D3BJ) Energy = -863.010885089
SCF (MeCN) Energy = -862.959552984
SCF (Toluene) Energy = -862.951647539
SCF (BS2) Energy = -862.868680272

C	0.10292	-2.07046	-0.99455
C	-0.00117	-2.26331	0.42456
C	0.93449	-1.64039	1.29509
C	2.00861	-0.81087	0.78036
C	2.15115	-0.64060	-0.64137
C	1.15795	-1.24881	-1.49796
Ru	0.07554	-0.10740	-0.01530
O	-1.92840	0.24622	0.25828
C	-2.89678	-0.63535	0.05190
O	-2.76404	-1.81598	-0.30383
O	0.15187	1.78792	1.02988
C	-0.10965	2.41168	-0.06543
O	-0.13687	1.71632	-1.14895
C	-0.40712	3.88735	-0.07537
C	-4.27848	-0.01630	0.28533
H	-4.30476	0.52776	1.24299
H	-4.49446	0.71422	-0.51280
H	-5.04668	-0.80219	0.27318
H	-1.49059	4.03082	0.07729
H	0.12528	4.39264	0.74416
H	-0.13324	4.32950	-1.04467
H	0.78999	-1.70290	2.37785
H	-0.69194	-2.43456	-1.64636
H	1.17243	-1.00026	-2.56477
H	-0.88388	-2.76580	0.82288
C	2.92260	-0.10552	1.75605
H	3.02019	0.96617	1.52168
H	2.53348	-0.18765	2.78243
H	3.93298	-0.55269	1.73432
C	3.24304	0.20908	-1.24859
H	3.46360	1.10143	-0.64283
H	4.17995	-0.37188	-1.33759
H	2.95808	0.54593	-2.25766

p-cymene (*p*-cym)
SCF (BP86) Energy = -389.500963444
Enthalpy 0K = -389.294560
Enthalpy 298K = -389.282766
Free Energy 298K = -389.331806
Lowest Frequency = 27.5335 cm^{-1}
Second Frequency = 39.1086 cm^{-1}
SCF (BP86-D3BJ) Energy = -389.538808507
SCF (MeCN) Energy = -389.503525007
SCF (Toluene) Energy = -389.502062924
SCF (BS2) Energy = -389.592347940

C	0.21782	1.34626	0.00880
C	-0.63077	0.22312	0.00387
C	-0.02574	-1.05185	-0.01100
C	1.36824	-1.19298	-0.01922
C	2.21724	-0.06636	-0.01057
C	1.61461	1.20576	0.00059
C	-2.14898	0.38600	0.00847
H	-0.65273	-1.95130	-0.02077
C	3.72322	-0.22432	0.01049
H	2.24790	2.10115	0.00118
H	-0.22349	2.35057	0.01492
H	1.80879	-2.19736	-0.03467
H	4.23031	0.68736	-0.34624
H	4.09272	-0.42601	1.03323
H	4.05168	-1.06628	-0.62247
H	-2.35703	1.47386	0.02431
C	-2.79155	-0.19235	-1.27228
C	-2.78799	-0.22881	1.27383
H	-3.87835	-0.05489	1.28625
H	-2.62379	-1.32018	1.31289
H	-2.35873	0.20705	2.19142
H	-3.88200	-0.01845	-1.27673
H	-2.36486	0.26980	-2.17812
H	-2.62700	-1.28207	-1.34302

[(*p*-cym)Ru(OAc)$_2$]
SCF (BP86) Energy = -941.573231537
Enthalpy 0K = -941.264458
Enthalpy 298K = -941.241076
Free Energy 298K = -941.316954
Lowest Frequency = 23.7871 cm^{-1}
Second Frequency = 38.7196 cm^{-1}
SCF (BP86-D3BJ) Energy = -941.651020035
SCF (MeCN) Energy = -941.586490428
SCF (Toluene) Energy = -941.579377161
SCF (BS2) Energy = -941.514155902

Ru	0.19383	-0.26148	0.18626
O	1.47195	1.13945	-0.59538
C	1.55210	2.40725	-0.21658
C	2.65062	3.15286	-0.98080
C	-1.97767	0.12686	0.01133
O	0.86365	2.96970	0.64842
O	2.02459	-1.41266	0.12992
C	1.86940	-1.62624	-1.13028
C	2.94745	-2.28363	-1.95052
O	0.76889	-1.22987	-1.66661
H	3.63772	2.74578	-0.70359
H	2.53178	3.00838	-2.06681
H	2.61613	4.22361	-0.73563
H	3.61129	-1.50137	-2.35689
H	3.55051	-2.95773	-1.32441
H	2.50631	-2.83365	-2.79505
C	-1.74446	-1.26288	0.35228
C	-0.95376	-1.63012	1.47839
C	-1.38091	1.11822	0.84803
C	-0.55846	0.76086	1.97341

```
C  -0.31494 -0.61480  2.28633
H  -1.42069  2.17080  0.55869
H  -0.72098 -2.68470  1.65481
C  -2.81044  0.54120 -1.19631
H  -2.46915  1.55692 -1.47344
H  -0.01017  1.55113  2.48937
H  -2.09846 -2.04879 -0.32087
C   0.63051 -1.00605  3.39508
H   0.06013 -1.23921  4.31296
H   1.21626 -1.89778  3.12045
H   1.33028 -0.18782  3.62501
C  -4.29923  0.63567 -0.78336
H  -4.91053  0.99177 -1.63018
H  -4.68678 -0.35305 -0.47952
H  -4.44345  1.33083  0.06069
C  -2.62585 -0.36981 -2.42515
H  -3.15447  0.06119 -3.29209
H  -1.56132 -0.48516 -2.68425
H  -3.05171 -1.37517 -2.25657
```

C_6Me_6 (Bn*)
SCF (BP86) Energy = -468.126901047
Enthalpy 0K = -467.867928
Enthalpy 298K = -467.851887
Free Energy 298K = -467.910997
Lowest Frequency = 39.4803 cm^{-1}
Second Frequency = 54.8645 cm^{-1}
SCF (BP86-D3BJ) Energy = -468.179037098
SCF (MeCN) Energy = -468.129608459
SCF (Toluene) Energy = -468.128025243
SCF (BS2) Energy = -468.232580905

```
C   0.06877 -1.41549  0.00986
C  -1.19138 -0.76729 -0.00996
C  -1.26015  0.64811  0.01006
C  -0.06879  1.41546 -0.00990
C   1.19134  0.76726  0.00997
C   1.26012 -0.64815 -0.00997
C   0.14260 -2.93319  0.07354
H  -0.72304 -3.36056  0.60280
H   0.16887 -3.39830 -0.93159
H   1.04215 -3.27425  0.60897
C   2.61162 -1.34256 -0.07351
H   3.02864 -1.54993  0.93168
H   2.54905 -2.30708 -0.60065
H   3.35594 -0.73466 -0.61084
C  -2.46905 -1.58969 -0.07371
H  -2.31443 -2.54052 -0.60680
H  -2.86037 -1.84253  0.93141
H  -3.27094 -1.05435 -0.60527
C  -2.61152  1.34278  0.07380
H  -3.02790  1.55181 -0.93132
H  -3.35633  0.73438  0.60984
H  -2.54887  2.30651  0.60239
C   2.46908  1.58957  0.07361
H   3.27059  1.05457  0.60611
H   2.86099  1.84133 -0.93154
H   2.31433  2.54093  0.60570
C  -0.14269  2.93314 -0.07377
H  -0.16844  3.39846  0.93128
H   0.72266  3.36043 -0.60358
H  -1.04256  3.27406 -0.60877
```

[(Bn*)Ru(OAc)$_2$]
SCF (BP86) Energy = -1020.20321509
Enthalpy 0K = -1019.841450
Enthalpy 298K = -1019.814071
Free Energy 298K = -1019.897732
Lowest Frequency = 26.4238 cm^{-1}
Second Frequency = 45.3947 cm^{-1}
SCF (BP86-D3BJ) Energy = -1020.30133902
SCF (MeCN) Energy = -1020.21860888
SCF (Toluene) Energy = -1020.20993497
SCF (BS2) Energy = -1020.15863897

```
C  -0.47135 -1.54500 -1.26527
C  -0.15387 -2.03802  0.04735
C  -0.84913 -1.54578  1.21868
C  -1.48897 -0.51268 -1.40648
C  -2.27509 -0.08914 -0.27406
C  -1.87607 -0.53596  1.04763
Ru -0.08389  0.18699  0.09084
O  -0.11475  2.12128  1.06084
C   0.39841  2.66924  0.01457
O   0.53916  1.93289 -1.03113
C   0.84960  4.10688  0.02679
H   0.22750  4.69903  0.71452
H   1.89275  4.15107  0.38421
H   0.81397  4.53076 -0.98763
O   1.86787  0.25589  0.78510
C   2.88402 -0.14452  0.04315
C   4.23824  0.14507  0.69976
H   4.61309  1.11461  0.32788
H   4.15815  0.20704  1.79545
H   4.96477 -0.62863  0.40898
O   2.81947 -0.67697 -1.07853
C  -2.52071  0.09767  2.26491
H  -3.34553 -0.53360  2.64565
H  -1.79058  0.23432  3.07552
H  -2.92856  1.09053  2.03248
C  -3.42353  0.89387 -0.43149
H  -4.24149  0.64292  0.26292
H  -3.12195  1.93620 -0.22735
H  -3.84157  0.85756 -1.44798
C  -1.69569  0.13396 -2.76123
H  -2.34151 -0.49182 -3.40527
H  -2.15749  1.12647 -2.67049
H  -0.73263  0.27416 -3.27341
C   0.29653 -2.07256 -2.45982
H  -0.16761 -1.77691 -3.41062
H   1.33421 -1.69755 -2.43019
H   0.32653 -3.17563 -2.43536
C   0.97017 -3.04302  0.18593
H   0.63103 -4.03542 -0.16651
H   1.83519 -2.73368 -0.41949
H   1.30297 -3.15266  1.22630
C  -0.46960 -2.06790  2.59258
H  -0.51187 -3.17096  2.60792
H   0.55311 -1.76578  2.87463
H  -1.15315 -1.70695  3.37265
```

B$^+$

SCF (BP86) Energy = -1034.96464167
Enthalpy 0K = -1034.646883
Enthalpy 298K = -1034.624860
Free Energy 298K = -1034.697996
Lowest Frequency = 26.7530 cm^{-1}
Second Frequency = 39.6295 cm^{-1}
SCF (BP86-D3BJ) Energy = -1035.06637398
SCF (MeCN) Energy = -1035.02251539
SCF (Toluene) Energy = -1034.99853602
SCF (BS2) Energy = -1034.90693552

C	-0.21819	2.19516	0.80183
C	-2.82350	1.44584	-1.91348
C	-3.88326	1.88636	-1.10133
C	-4.14580	1.23904	0.11816
C	-2.26433	-0.27171	-0.27429
C	-1.42260	-3.79348	0.85045
O	1.09415	0.17151	-1.89536
C	2.10835	-0.61945	-1.79947
O	2.56487	-0.79370	-0.60133
C	2.70409	-1.30986	-2.98702
H	-1.94363	-4.73456	1.04987
H	2.52298	-0.72406	-3.89982
H	3.78258	-1.46479	-2.83563
H	2.23033	-2.29943	-3.11146
H	-4.97611	1.56951	0.74978
H	-4.51283	2.72103	-1.42490
H	-2.63322	1.92929	-2.87691
C	0.58485	-2.47133	0.72347
H	1.66590	-2.35016	0.81569
C	-0.03177	-3.69328	0.99506
H	0.57818	-4.54222	1.31396
C	-1.46512	-1.44831	0.16699
Ru	1.04765	0.45053	0.23399
C	2.36643	1.36614	1.70998
H	3.34570	0.96662	1.99038
C	2.26603	2.27251	0.59906
H	3.16187	2.57104	0.04958
C	0.97160	2.64534	0.13011
H	0.87988	3.21906	-0.79682
C	1.19660	0.91145	2.39870
H	1.28318	0.19406	3.21815
C	-0.09221	1.32821	1.92602
H	-0.99510	0.90360	2.37342
H	-1.20487	2.44157	0.40388
C	-2.13100	-2.66424	0.43018
H	-3.21208	-2.70334	0.27401
C	-3.35023	0.15619	0.52381
H	-3.56371	-0.35534	1.46915
N	-0.10368	-1.36032	0.32838
C	-2.01297	0.37556	-1.50494
H	-1.19376	0.03366	-2.14270

TS(**B$^+$**–**C$^+$**)

SCF (BP86) Energy = -1034.94113282
Enthalpy 0K = -1034.624885
Enthalpy 298K = -1034.603321
Free Energy 298K = -1034.675315
Lowest Frequency = -100.9920 cm^{-1}
Second Frequency = 28.4528 cm^{-1}
SCF (BP86-D3BJ) Energy = -1035.04430926
SCF (MeCN) Energy = -1035.00319665
SCF (Toluene) Energy = -1034.97699319
SCF (BS2) Energy = -1034.88392504

C	0.10375	2.68553	-0.52549
N	0.53067	1.42284	-0.27049
C	1.84584	1.19800	0.04503
C	2.76659	2.26266	0.05003
C	2.33517	3.55899	-0.25098
C	0.97698	3.77629	-0.53197
Ru	-0.79734	-0.22475	-0.38828
C	-2.57627	-1.44370	-0.95168
C	-2.47856	-0.24158	-1.74208
C	-1.27741	0.04715	-2.47293
C	-0.16723	-0.87437	-2.43755
C	-0.24994	-2.02660	-1.61921
C	-1.45263	-2.30146	-0.86246
H	-1.19086	0.98857	-3.02354
C	2.19153	-0.18812	0.41211
C	3.45038	-0.75870	0.13727
C	3.71001	-2.09223	0.49222
C	2.72444	-2.86922	1.13093
C	1.46788	-2.31145	1.41171
C	1.19724	-0.97747	1.04967
H	-1.46669	-3.13603	-0.15688
O	-1.91076	1.04580	0.85042
C	-2.08910	0.46716	2.02313
O	-1.59227	-0.65075	2.28740
C	-2.91251	1.25463	3.02324
H	-2.24053	1.64726	3.80514
H	-3.44256	2.09427	2.55274
H	-3.62853	0.57984	3.51682
H	4.21919	-0.17284	-0.37685
H	4.68868	-2.52824	0.26975
H	0.70420	-2.88530	1.94566
H	2.94595	-3.90044	1.42232
H	3.80631	2.06547	0.32345
H	0.28136	-0.52083	1.49721
H	-3.45280	-1.61882	-0.32386
H	0.62674	-2.66500	-1.48674
H	-3.28651	0.49439	-1.71415
H	0.76466	-0.63152	-2.95505
H	0.58935	4.77462	-0.74919
H	3.04371	4.39229	-0.24485
H	-0.96618	2.79801	-0.71266

C$^+$

SCF (BP86) Energy = -1034.96564411
Enthalpy 0K = -1034.648482
Enthalpy 298K = -1034.626399
Free Energy 298K = -1034.699841
Lowest Frequency = 22.7322 cm^{-1}
Second Frequency = 23.9055 cm^{-1}
SCF (BP86-D3BJ) Energy = -1035.06869494
SCF (MeCN) Energy = -1035.02349528
SCF (Toluene) Energy = -1034.99949265
SCF (BS2) Energy = -1034.90637128

C	0.40471	2.73165	-0.03461
N	0.60472	1.40614	-0.25033
C	1.87946	0.93347	-0.46556
C	2.96447	1.83212	-0.50765
C	2.75119	3.19927	-0.31562
C	1.44748	3.65943	-0.06273
Ru	-0.94982	0.00526	-0.21935
C	-3.07382	-0.69899	-0.01615
C	-3.20028	0.72823	-0.20931
C	-2.53645	1.33880	-1.28790
C	-1.74274	0.53519	-2.19309
C	-1.71507	-0.88664	-2.06205
C	-2.40815	-1.51703	-0.96835
H	-2.56963	2.42497	-1.41420
C	1.95161	-0.52229	-0.58683
C	3.14327	-1.23342	-0.84143
C	3.13129	-2.63297	-0.89087
C	1.92917	-3.32567	-0.67246
C	0.73428	-2.62189	-0.42449
C	0.70697	-1.20638	-0.38755
H	-2.36583	-2.59984	-0.83223
O	-0.81945	0.23503	1.91944
C	-0.16545	-0.38526	2.79847
O	0.67610	-1.36863	2.53436

```
C  -0.30403 -0.04608  4.25503
H   0.67627  0.25981  4.65644
H  -1.03548  0.75960  4.39287
H  -0.61560 -0.94331  4.81481
H   4.08530 -0.69880 -1.00308
H   4.05616 -3.18165 -1.09011
H  -0.18409 -3.19394 -0.25243
H   1.91486 -4.42026 -0.69746
H   3.97299  1.44897 -0.68096
H   0.71822 -1.50103  1.53710
H  -3.50867 -1.15900  0.87585
H  -1.12231 -1.48723 -2.75633
H  -3.73334  1.33212  0.52941
H  -1.17049  1.01585 -2.99105
H   1.23459  4.71729  0.10903
H   3.59131  3.89888 -0.35154
H  -0.62608  3.03250  0.16572
```

B·OAc

SCF (BP86) Energy = -1263.62317136
Enthalpy 0K = -1263.257959
Enthalpy 298K = -1263.229825
Free Energy 298K = -1263.317921
Lowest Frequency = 25.6024 cm^{-1}
Second Frequency = 37.4299 cm^{-1}
SCF (BP86-D3BJ) Energy = -1263.74415414
SCF (MeCN) Energy = -1263.64507734
SCF (Toluene) Energy = -1263.63339724
SCF (BS2) Energy = -1263.64784484

```
C  -0.46161 -1.76693  1.51405
N  -0.24142 -0.52532  0.99936
C  -1.09453  0.49047  1.33635
C  -2.16626  0.25235  2.21940
C  -2.37928 -1.01938  2.75623
C  -1.50538 -2.05168  2.39359
Ru  1.28668 -0.41104 -0.48730
C   2.51627 -0.70733 -2.29770
C   1.49504 -1.72436 -2.20492
C   0.11463 -1.37159 -2.09993
C  -0.25311  0.01589 -2.03318
C   0.74369  1.03348 -2.06852
C   2.13413  0.66300 -2.19486
H  -0.71204 -2.08420 -1.88362
C  -0.91977  1.86356  0.77906
C  -1.96168  2.40288 -0.00948
C  -1.85237  3.71383 -0.50028
C  -0.72478  4.49678 -0.19821
C   0.30488  3.96259  0.59558
C   0.21174  2.65002  1.08462
H   2.90935  1.43224 -2.12033
O   2.41315 -1.65165  0.87383
C   2.87205 -0.61774  1.49326
O   2.53753  0.53438  1.03040
C   3.73074 -0.75858  2.72133
H   4.39110  0.11433  2.82880
H   3.08352 -0.81466  3.61387
H   4.32235 -1.68453  2.66940
H  -2.80200  1.75040 -0.28240
H  -2.65255  4.12251 -1.12655
H   1.18202  4.57050  0.84194
H  -0.64919  5.52170 -0.57746
H  -2.82381  1.08958  2.46518
H   1.01665  2.23273  1.69595
H   3.57374 -0.98453 -2.31664
H   0.47114  2.07996 -1.90745
H   1.79636 -2.77468 -2.13353
H  -1.32727  0.19775 -1.78225
H  -1.63343 -3.07349  2.75849
H  -3.21674 -1.20284  3.43625
H   0.23300 -2.54297  1.19017
O  -2.42767 -2.41964 -1.07886
C  -3.25082 -1.45930 -0.94474
C  -4.69609 -1.82118 -0.52833
H  -4.78361 -2.88282 -0.25024
H  -5.02652 -1.18383  0.30997
H  -5.38056 -1.61558 -1.37032
O  -3.02804 -0.21126 -1.13702
```

TS(**B**–**C**)1·OAc

SCF (BP86) Energy = -1263.60220672
Enthalpy 0K = -1263.238938
Enthalpy 298K = -1263.211039
Free Energy 298K = -1263.300286
Lowest Frequency = -98.0070 cm^{-1}
Second Frequency = 14.9814 cm^{-1}
SCF (BP86-D3BJ) Energy = -1263.72302944
SCF (MeCN) Energy = -1263.62618544
SCF (Toluene) Energy = -1263.61358679
SCF (BS2) Energy = -1263.62848166

```
C  -1.49738 -0.90450  1.51044
N  -0.64116 -0.00742  0.96830
C  -0.77849  1.32488  1.25593
C  -1.79338  1.76882  2.11751
C  -2.67940  0.84125  2.68149
C  -2.52449 -0.51513  2.37868
Ru  0.82754 -0.64569 -0.41941
C   1.90495 -1.78381 -1.98488
C   0.62325 -2.37601 -1.68194
C  -0.57901 -1.59451 -1.75320
C  -0.51344 -0.20648 -2.14428
C   0.74881  0.38981 -2.39842
C   1.95899 -0.39822 -2.30058
H  -1.57684 -1.93525 -1.37723
C   0.20697  2.23233  0.63415
C  -0.14380  3.52405  0.19141
C   0.81285  4.34017 -0.43134
C   2.13154  3.88294 -0.61476
C   2.49121  2.59929 -0.17752
C   1.53360  1.77247  0.43891
H   2.93303  0.09233 -2.38813
O   1.30458 -1.95113  1.16773
C   2.50462 -1.67542  1.61426
O   3.20413 -0.74177  1.15270
C   2.99001 -2.54747  2.76348
H   2.82009 -2.01244  3.71379
H   2.45051 -3.50486  2.80302
H   4.07241 -2.72007  2.66669
H  -1.17675  3.87063  0.29605
H   0.52553  5.33622 -0.78329
H   3.51775  2.23539 -0.28680
H   2.87475  4.53152 -1.08990
H  -1.86586  2.83443  2.34943
H   1.90210  0.83483  0.90961
H   2.82815 -2.34930 -1.83710
H   0.82527  1.46785 -2.56322
H   0.58385 -3.39738 -1.29153
H  -1.47156  0.34931 -2.03512
H  -3.20039 -1.27611  2.77416
H  -3.47686  1.17714  3.35118
H  -1.34550 -1.94651  1.23511
O  -3.24944 -1.70733 -0.60796
C  -3.79558 -0.57311 -0.85909
C  -5.31827 -0.48356 -0.61425
H  -5.84788 -0.72317 -1.55400
H  -5.64540 -1.20966  0.14709
H  -5.61026  0.53834 -0.32277
O  -3.22693  0.47049 -1.31213
```

INT(**B**–**C**)·OAc

SCF (BP86) Energy = -1263.60859226
Enthalpy 0K = -1263.246053
Enthalpy 298K = -1263.217946

Free Energy 298K = -1263.307081
Lowest Frequency = 16.8261 cm^{-1}
Second Frequency = 20.6744 cm^{-1}
SCF (BP86-D3BJ) Energy = -1263.72734511
SCF (MeCN) Energy = -1263.63483730
SCF (Toluene) Energy = -1263.62081428
SCF (BS2) Energy = -1263.63294424

C	-1.47077	1.40945	0.67366
N	-0.22043	1.08108	0.26945
C	0.74123	2.04610	0.09029
C	0.44228	3.39484	0.33857
C	-0.84613	3.74923	0.76432
C	-1.80840	2.74772	0.93030
Ru	0.29891	-0.90401	-0.13812
C	0.77529	-2.91730	-1.02702
C	-0.49888	-2.96658	-0.39519
C	-1.52957	-2.01962	-0.72837
C	-1.26932	-0.99975	-1.69802
C	0.00642	-0.94031	-2.35541
C	1.02508	-1.87113	-1.98661
H	-2.47004	-1.92948	-0.16499
C	2.05064	1.53671	-0.34281
C	3.00290	2.32126	-1.02123
C	4.21999	1.75726	-1.43123
C	4.50477	0.40515	-1.15967
C	3.56492	-0.38463	-0.48495
C	2.31824	0.15592	-0.08898
H	2.03237	-1.75623	-2.39766
O	-0.11153	-1.18362	1.89064
C	0.76751	-0.91393	2.82273
O	1.92392	-0.47454	2.62014
C	0.26297	-1.15152	4.24073
H	-0.16535	-0.20940	4.62375
H	-0.52490	-1.91765	4.26003
H	1.10175	-1.43565	4.89253
H	2.78273	3.36791	-1.25629
H	4.95118	2.37454	-1.96281
H	3.80181	-1.42232	-0.22668
H	5.46571	-0.02348	-1.46250
H	1.22348	4.14987	0.21761
H	1.91872	-0.29489	0.93486
H	1.57404	-3.60242	-0.73249
H	0.23202	-0.13167	-3.05540
H	-0.66143	-3.66624	0.43009
H	-2.04409	-0.19810	-1.80452
H	-2.83168	2.97710	1.23651
H	-1.08989	4.79804	0.96101
H	-2.21980	0.59437	0.74148
O	-3.82410	-0.41084	0.31395
C	-4.22540	0.35402	-0.63298
C	-5.74749	0.59359	-0.72609
H	-6.22508	-0.28838	-1.18969
H	-6.18578	0.70618	0.27904
H	-5.97567	1.47462	-1.34571
O	-3.49036	0.91937	-1.50965

TS(**B**–**C**)2·OAc
SCF (BP86) Energy = -1263.60826342
Enthalpy 0K = -1263.247706
Enthalpy 298K = -1263.220274
Free Energy 298K = -1263.307321
Lowest Frequency = -254.6594 cm^{-1}
Second Frequency = 17.4118 cm^{-1}
SCF (BP86-D3BJ) Energy = -1263.72730471
SCF (MeCN) Energy = -1263.63363514
SCF (Toluene) Energy = -1263.62006693
SCF (BS2) Energy = -1263.63182435

C	-1.47326	1.43725	0.63003
N	-0.22675	1.09516	0.22399
C	0.73527	2.05311	0.00423
C	0.43699	3.40967	0.20813
C	-0.84786	3.77866	0.63187
C	-1.80835	2.78372	0.84335
Ru	0.29010	-0.89714	-0.12900
C	0.74283	-2.93705	-0.96854
C	-0.51580	-2.97029	-0.30046
C	-1.56755	-2.05175	-0.64137
C	-1.33569	-1.05539	-1.63793
C	-0.07359	-1.00222	-2.32515
C	0.95992	-1.92095	-1.96529
H	-2.49595	-1.95738	-0.05991
C	2.03800	1.51856	-0.41353
C	3.02460	2.28689	-1.06014
C	4.23677	1.69686	-1.44637
C	4.47866	0.33552	-1.17979
C	3.50181	-0.43607	-0.53725
C	2.25485	0.12461	-0.15716
H	1.95311	-1.81540	-2.41160
O	-0.03498	-1.11966	1.93456
C	0.88508	-0.80369	2.79000
O	2.01966	-0.33506	2.47711
C	0.54573	-1.03012	4.25268
H	0.64394	-0.07780	4.79817
H	-0.47347	-1.42271	4.36576
H	1.27243	-1.73429	4.68962
H	2.83815	3.34172	-1.28879
H	4.99679	2.29978	-1.95345
H	3.71167	-1.48284	-0.28964
H	5.43470	-0.11632	-1.46477
H	1.21549	4.16124	0.05291
H	1.95104	-0.24581	1.01005
H	1.55011	-3.61413	-0.67900
H	0.12768	-0.21112	-3.05217
H	-0.65121	-3.64656	0.54920
H	-2.11805	-0.26346	-1.75203
H	-2.82852	3.02366	1.15173
H	-1.09050	4.83392	0.79240
H	-2.22135	0.62480	0.73840
O	-3.83108	-0.40512	0.42871
C	-4.27110	0.31799	-0.53376
C	-5.79887	0.53472	-0.58902
H	-6.27867	-0.37172	-1.00025
H	-6.20740	0.68386	0.42394
H	-6.05827	1.38629	-1.23693
O	-3.57105	0.85888	-1.45321

C·OAc
SCF (BP86) Energy = -1263.62198852
Enthalpy 0K = -1263.257396
Enthalpy 298K = -1263.229328
Free Energy 298K = -1263.318043
Lowest Frequency = 13.2243 cm^{-1}
Second Frequency = 26.8130 cm^{-1}
SCF (BP86-D3BJ) Energy = -1263.74066362
SCF (MeCN) Energy = -1263.64702057
SCF (Toluene) Energy = -1263.63384899
SCF (BS2) Energy = -1263.64567358

C	-1.45480	1.51994	0.41280
N	-0.22655	1.11216	0.00571
C	0.74124	2.02803	-0.34493
C	0.45747	3.40247	-0.29801
C	-0.81174	3.83592	0.11029
C	-1.77198	2.88558	0.47469
Ru	0.25983	-0.91440	-0.14336
C	0.49765	-3.09846	-0.63849
C	-0.69269	-2.94896	0.15269
C	-1.75549	-2.08106	-0.23400
C	-1.57851	-1.25154	-1.38187
C	-0.39182	-1.36502	-2.18912
C	0.63997	-2.28881	-1.80974
H	-2.63063	-1.87411	0.39770

```
C   2.02641  1.41571 -0.70061
C   3.15744  2.14208 -1.12788
C   4.36239  1.47870 -1.39450
C   4.44408  0.08612 -1.22033
C   3.31601 -0.64357 -0.80352
C   2.07272 -0.01078 -0.54602
H   1.57062 -2.32622 -2.38414
O   0.42599 -0.86021  2.01105
C   1.32934 -0.41853  2.75879
O   2.47522  0.08088  2.31843
C   1.17657 -0.42402  4.25578
H   1.17312  0.61481  4.62600
H   0.23800 -0.91863  4.53526
H   2.03574 -0.93459  4.72002
H   3.10097  3.22885 -1.25666
H   5.23722  2.04596 -1.72748
H   3.40686 -1.72849 -0.67023
H   5.38806 -0.43575 -1.41350
H   1.23137  4.12369 -0.57399
H   2.45733  0.03854  1.30783
H   1.29852 -3.77216 -0.32404
H  -0.24813 -0.71232 -3.05420
H  -0.75303 -3.47442  1.11178
H  -2.34858 -0.46333 -1.55867
H  -2.77983  3.17047  0.78531
H  -1.04255  4.90572  0.14028
H  -2.20917  0.74434  0.66491
O  -3.87019 -0.21526  0.79994
C  -4.41826  0.33211 -0.22268
C  -5.94623  0.54879 -0.14801
H  -6.45835 -0.40723 -0.36007
H  -6.24747  0.85826  0.86632
H  -6.28095  1.28960 -0.89077
O  -3.82912  0.69548 -1.29261
```

A·**a**–H
SCF (BP86) Energy = -1263.65263818
Enthalpy 0K = -1263.287059
Enthalpy 298K = -1263.258636
Free Energy 298K = -1263.351606
Lowest Frequency = 10.1944 cm^{-1}
Second Frequency = 12.9810 cm^{-1}
SCF (BP86-D3BJ) Energy = -1263.75713265
SCF (MeCN) Energy = -1263.66744502
SCF (Toluene) Energy = -1263.65942668
SCF (BS2) Energy = -1263.67410493

C	-2.03846	-1.22732	-2.06263
C	-0.67425	-0.80322	-1.89221
C	-0.37019	0.59361	-1.88843
C	2.38988	1.57040	0.68609
C	2.48394	2.97064	0.69290
H	1.64958	3.56056	1.08688
C	2.19012	-1.42497	0.38612
H	1.25795	-0.90274	0.62018
O	-2.11006	-1.12039	1.10758
C	-1.91672	-3.08199	2.41688
H	-2.90567	-2.82531	2.82656
H	-1.82889	-4.16907	2.27923
H	-1.15878	-2.75558	3.14993
C	-1.67107	-2.36804	1.08539
O	-1.09674	-2.93429	0.13937
O	-3.29578	1.27713	0.90001
C	-2.30886	1.65572	1.63302
O	-1.12260	1.39318	1.20024
H	1.48218	1.10878	1.08672
C	-2.52737	2.34399	2.95226
H	-2.60499	1.57836	3.74322
H	-1.67803	3.00128	3.18994
H	-3.46603	2.91724	2.93428
C	3.63827	3.60917	0.21138
H	3.70910	4.70215	0.21935
C	3.45416	0.77960	0.19184
C	4.61441	1.43488	-0.28218
H	5.43588	0.81526	-0.65227
C	4.70434	2.83231	-0.27388
H	5.61156	3.31896	-0.64842
N	4.54648	-1.35383	-0.15676
C	2.18847	-2.82378	0.30164
H	1.25049	-3.36895	0.45375
C	3.38865	-0.71175	0.14994
C	3.38829	-3.48228	-0.00648
H	3.43915	-4.57277	-0.08425
C	4.53129	-2.69615	-0.22403
H	5.49122	-3.17060	-0.47065
Ru	-1.94388	0.23995	-0.42319
C	-1.40078	1.57546	-2.10618
H	-1.16942	2.64118	-2.03550
C	-2.75123	1.14086	-2.24356
H	-3.55789	1.87935	-2.26458
C	-3.07631	-0.26733	-2.23548
H	-4.12176	-0.58560	-2.26184
H	0.64169	0.92424	-1.63295
H	0.08783	-1.53933	-1.63447
H	-2.27799	-2.28240	-1.91935

B
SCF (BP86) Energy = -1263.64592625
Enthalpy 0K = -1263.279761
Enthalpy 298K = -1263.251863
Free Energy 298K = -1263.338799
Lowest Frequency = 28.1817 cm^{-1}
Second Frequency = 34.0115 cm^{-1}
SCF (BP86-D3BJ) Energy = -1263.76603215
SCF (MeCN) Energy = -1263.66375545
SCF (Toluene) Energy = -1263.65386872
SCF (BS2) Energy = -1263.66950286

C	-0.70198	-2.16360	1.92181
Ru	-0.66456	-0.35118	-0.46770
C	-1.07950	0.11547	-2.60737
C	-1.99360	-0.87897	-2.13138
C	-0.11568	-2.28331	-1.35706
C	0.82404	-1.31783	-1.83587
H	-1.45852	1.06613	-2.98583
H	-3.06123	-0.64779	-2.14376
H	0.22397	-3.14071	-0.77257
H	1.89369	-1.44694	-1.66016
C	-0.55159	-2.27819	3.44325
H	-0.54699	-3.33702	3.74069
H	0.35741	-1.77320	3.80634
H	-1.41630	-1.78424	3.91909
O	-0.24440	-1.00721	1.46686
O	-1.22069	-3.07445	1.25826
C	1.61869	1.65797	0.49498
C	-0.54221	2.54942	0.29883
N	0.28796	1.47051	0.21492
O	-2.33054	0.25335	0.64802
C	-3.35271	0.92941	0.16474
O	-3.40142	1.50389	-0.94164
C	-4.53329	0.96650	1.14017
H	-4.19460	1.25267	2.14874
H	-5.29667	1.67115	0.78090
H	-4.97475	-0.04133	1.22163
C	2.64040	0.58788	0.27365
C	3.67156	0.84976	-0.65772
C	2.67019	-0.61587	1.00885
C	4.69224	-0.08859	-0.87838
H	3.66265	1.79054	-1.21978
C	3.70137	-1.54347	0.79563
H	1.86110	-0.82245	1.71377
C	4.70979	-1.28898	-0.14985
H	5.47463	0.12235	-1.61486
H	3.71564	-2.47314	1.37431
H	5.50873	-2.01970	-0.31383
C	-0.11829	3.81610	0.71007
C	2.09192	2.91540	0.92762
C	1.22464	4.00410	1.05512
H	3.15499	3.01028	1.16431
H	1.59393	4.97556	1.39854
H	-0.84539	4.63162	0.74942
H	-1.57014	2.38013	-0.02757
C	-1.52744	-2.09092	-1.52653
H	-2.21968	-2.79072	-1.05763
C	0.32301	-0.10341	-2.41426
H	1.02938	0.69706	-2.65754

TS(**B**–**C**)
SCF (BP86) Energy = -1263.59805874
Enthalpy 0K = -1263.234743
Enthalpy 298K = -1263.207363
Free Energy 298K = -1263.293555
Lowest Frequency = -86.5861 cm^{-1}
Second Frequency = 23.6734 cm^{-1}
SCF (BP86-D3BJ) Energy = -1263.71826892
SCF (MeCN) Energy = -1263.62573482
SCF (Toluene) Energy = -1263.61056740
SCF (BS2) Energy = -1263.62251906

C	-3.63878	-0.24066	-1.12482
Ru	0.07863	-0.48231	0.64200
C	0.72938	-1.44397	2.47749
C	-0.22640	-2.29404	1.83782
C	-1.85136	-0.42478	1.74875
C	-0.90610	0.41728	2.44530
H	1.73925	-1.81673	2.67077
H	0.09337	-3.28146	1.50028
H	-2.76575	-0.00279	1.26393
H	-1.13611	1.47634	2.58774

```
C  -4.72810 -0.84764 -2.03461
H  -4.46677 -1.88536 -2.30205
H  -5.71713 -0.82024 -1.55241
H  -4.77395 -0.27827 -2.97962
O  -2.43195 -0.36876 -1.51498
O  -4.03596  0.35849 -0.06171
C   1.98426  1.52964 -0.55319
C   4.25899 -0.07240 -0.57634
C   3.03908 -0.52624 -0.06727
H   2.89153 -1.55194  0.28484
N   1.93412  0.26314 -0.03313
O   0.31038 -1.53802 -1.12362
C   0.93319 -2.69754 -1.20655
O   1.56725 -3.26179 -0.29209
C   0.78408 -3.32496 -2.59216
H   0.87308 -2.56255 -3.38082
H   1.53471 -4.11646 -2.72808
H  -0.22434 -3.76408 -2.67856
H   5.12234 -0.74263 -0.57520
C   0.73565  2.30157 -0.48175
C   0.76578  3.70726 -0.34787
C  -0.51670  1.62308 -0.43351
C  -0.41886  4.43069 -0.15942
H   1.72742  4.23133 -0.34616
C  -1.70412  2.36011 -0.22599
H  -0.76497  0.59560 -0.88726
C  -1.65021  3.75434 -0.08550
H  -0.37729  5.51967 -0.05170
H  -2.65992  1.80550 -0.18926
H  -2.57620  4.31792  0.07107
C   3.18709  2.02499 -1.09670
C   4.33502  1.22822 -1.09869
H   5.27033  1.60794 -1.52137
H   3.19780  3.02544 -1.53653
C  -1.52243 -1.77958  1.47657
H  -2.19806 -2.37584  0.85970
C   0.37852 -0.07752  2.79553
H   1.12643  0.59176  3.23112
```

C

SCF (BP86) Energy = -1263.66809038
Enthalpy 0K = -1263.302391
Enthalpy 298K = -1263.274400
Free Energy 298K = -1263.361925
Lowest Frequency = 23.7692 cm^{-1}
Second Frequency = 26.8672 cm^{-1}
SCF (BP86-D3BJ) Energy = -1263.78697393
SCF (MeCN) Energy = -1263.68201499
SCF (Toluene) Energy = -1263.67428098
SCF (BS2) Energy = -1263.68923639

```
C   3.91368  0.23167  0.77064
Ru -0.25241 -0.62654 -0.67274
C  -1.10035 -2.55583 -1.68266
C   0.13337 -2.90782 -1.10830
C   1.24148 -0.99437 -2.27530
C  -0.02863 -0.62411 -2.84797
H  -2.00320 -3.12211 -1.43536
H   0.18915 -3.72076 -0.38223
H   2.13914 -0.39817 -2.44782
H  -0.11066  0.26579 -3.47771
C   5.25584  0.81882  1.17759
H   6.01224  0.58568  0.41668
H   5.16700  1.91159  1.29576
H   5.56669  0.41358  2.15462
O   2.96902  0.47088  1.69296
O   3.73208 -0.38181 -0.28458
C  -4.14668 -0.38660  1.30416
C  -2.95250 -0.83569  0.73629
H  -2.68525 -1.89288  0.69688
N  -2.01942  0.01551  0.23953
O   0.60026 -0.60063  1.27746
C   0.21046 -1.52637  2.15256
O  -0.60752 -2.42692  1.91566
C   0.84058 -1.35588  3.53492
H   0.27141 -0.59255  4.09367
H   0.78360 -2.30530  4.08609
H   1.88286 -1.00764  3.47102
H  -4.86950 -1.11340  1.68345
C  -1.08200  2.16230 -0.14140
C  -1.03554  3.57486 -0.11436
C   0.02815  1.39058 -0.60568
C   0.11865  4.24462 -0.53043
H  -1.89802  4.15242  0.23841
C   1.19327  2.09470 -0.98237
H   2.06969  0.06536  1.41897
C   1.23599  3.49882 -0.95222
H   0.15669  5.33849 -0.51337
H   2.08933  1.54071 -1.28060
H   2.15237  4.01768 -1.25738
C  -2.21130  1.37556  0.34312
C  -4.37807  0.99794  1.38386
C  -3.40099  1.87667  0.91311
H  -5.30334  1.38484  1.82257
H  -3.54317  2.95787  0.98882
C   1.29223 -2.07708 -1.35629
H   2.22529 -2.24351 -0.81275
C  -1.19887 -1.37235 -2.51181
H  -2.17354 -1.05357 -2.89256
```

B′

SCF (BP86) Energy = -1031.40787653
Enthalpy 0K = -1031.141235
Enthalpy 298K = -1031.119573
Free Energy 298K = -1031.191217
Lowest Frequency = 35.8311 cm^{-1}
Second Frequency = 58.8947 cm^{-1}
SCF (BP86-D3BJ) Energy = -1031.48880480
SCF (MeCN) Energy = -1031.42375148
SCF (Toluene) Energy = -1031.41487867
SCF (BS2) Energy = -1031.36802683

```
C  -2.71121 -0.43588 -1.03110
Ru -0.37956 -0.32950 -0.11546
C  -4.08873 -0.65733 -1.60325
H  -4.84834 -0.19809 -0.95350
H  -4.15342 -0.24901 -2.62272
H  -4.28862 -1.74180 -1.65353
O  -1.67699 -0.38276 -1.81009
O  -2.51674 -0.33065  0.23303
C   1.96413  0.91396 -0.27000
C   2.41518 -1.16519 -1.30036
N   1.53682 -0.30390 -0.73354
O  -0.45802 -2.42798  0.24114
C   0.02091 -2.25497  1.42784
O   0.33403 -1.05143  1.76869
C   0.16390 -3.40462  2.38891
H   0.35857 -4.33891  1.84142
H   0.97077 -3.20371  3.10899
H  -0.77904 -3.52569  2.95025
C   0.75023  1.60225  0.25738
C   0.70826  2.23014  1.55008
C  -0.33094  1.83766 -0.68891
C  -0.38792  2.98530  1.92312
H   1.54578  2.07713  2.23810
C  -1.42992  2.66016 -0.25708
H  -0.14861  1.73978 -1.76552
C  -1.47480  3.19103  1.01877
H  -0.42146  3.43906  2.91916
H  -2.22489  2.88628 -0.97590
H  -2.32719  3.80332  1.33007
C   3.77377 -0.82973 -1.40229
C   3.30372  1.29482 -0.32252
C   4.22823  0.40005 -0.90133
```

H 3.61262 2.26681 0.07258
H 5.28792 0.66499 -0.96294
H 4.46597 -1.53998 -1.86339
H 2.00577 -2.11816 -1.64562

TS(**B′-C′**)
SCF (BP86) Energy = -1031.37308205
Enthalpy 0K = -1031.107767
Enthalpy 298K = -1031.086471
Free Energy 298K = -1031.159065
Lowest Frequency = -64.5937 cm^{-1}
Second Frequency = 11.4914 cm^{-1}
SCF (BP86-D3BJ) Energy = -1031.45281755
SCF (MeCN) Energy = -1031.39332066
SCF (Toluene) Energy = -1031.38220072
SCF (BS2) Energy = -1031.33529765

C -3.01850 0.67584 -0.55252
Ru -0.38980 -0.32167 0.01316
C -4.48273 0.99259 -0.25078
H -5.05316 1.06909 -1.18777
H -4.92561 0.22789 0.40606
H -4.54724 1.96025 0.27757
O -2.51430 0.93237 -1.66986
O -2.35727 0.16504 0.45804
C 2.35840 0.33274 -0.12604
C 3.54441 -2.10320 -0.67492
C 2.15418 -1.96460 -0.61193
H 1.47157 -2.80024 -0.78634
N 1.56312 -0.77408 -0.32295
O -1.12205 -2.16447 -0.61001
C -1.13921 -2.58834 0.61171
O -0.64940 -1.76212 1.47632
C -1.70613 -3.92085 0.99718
H -1.17689 -4.32031 1.87539
H -2.77017 -3.79602 1.26287
H -1.63949 -4.62272 0.15264
H 3.97493 -3.08134 -0.90704
C 1.55261 1.54687 0.10914
C 1.97271 2.59545 0.96096
C 0.28422 1.66423 -0.56913
C 1.18627 3.74030 1.11492
H 2.91195 2.49225 1.51465
C -0.48258 2.85213 -0.42201
H 0.04883 1.02177 -1.47958
C -0.04176 3.86813 0.42576
H 1.52162 4.54046 1.78271
H -1.42184 2.91909 -0.97770
H -0.64847 4.76954 0.55885
C 3.75590 0.25206 -0.16811
C 4.36256 -0.98584 -0.43825
H 5.45216 -1.07282 -0.47729
H 4.35334 1.15366 -0.00526

C′
SCF (BP86) Energy = -1031.36947647
Enthalpy 0K = -1031.103291
Enthalpy 298K = -1031.080737
Free Energy 298K = -1031.158098
Lowest Frequency = 12.1067 cm^{-1}
Second Frequency = 23.0969 cm^{-1}
SCF (BP86-D3BJ) Energy = -1031.44848936
SCF (MeCN) Energy = -1031.39104658
SCF (Toluene) Energy = -1031.37844569
SCF (BS2) Energy = -1031.33217274

C 2.84591 -1.11596 -2.19038
Ru -0.18920 1.11335 1.01187
C 2.86279 -2.11458 -3.33204
H 3.81512 -2.66035 -3.33209
H 2.02684 -2.82459 -3.21705
H 2.71979 -1.59751 -4.29476
O 1.73100 -0.35235 -2.21485
O 3.73394 -1.01655 -1.34547
C -3.05799 1.88151 -2.14104
C -2.00920 2.00901 -1.22748
H -1.42866 2.93300 -1.14011
N -1.63906 1.00625 -0.38551
O 1.52961 1.33831 -0.05065
C 2.30741 1.31644 1.02251
O 1.69748 1.19728 2.13157
C 3.79071 1.40387 0.85937
H 4.05970 2.34919 0.35811
H 4.28267 1.34676 1.83989
H 4.11089 0.57404 0.20202
H -3.31079 2.72315 -2.79122
C -1.74685 -1.21259 0.44966
C -2.25127 -2.51753 0.62660
C -0.56990 -0.78519 1.15983
C -1.58906 -3.41841 1.47066
H -3.16300 -2.83390 0.10591
C 0.09451 -1.72125 1.98943
H 1.74720 0.25840 -1.42254
C -0.41713 -3.01882 2.14570
H -1.98177 -4.43135 1.60418
H 1.00147 -1.41873 2.52344
H 0.09816 -3.72731 2.80443
C -2.31279 -0.20809 -0.45152
C -3.76646 0.66877 -2.19536
C -3.38247 -0.37666 -1.34586
H -4.59894 0.53798 -2.89308
H -3.90582 -1.33654 -1.37605

C′ (without HOAc)
SCF (BP86) Energy = -802.265265896
Enthalpy 0K = -802.060614
Enthalpy 298K = -802.044223
Free Energy 298K = -802.104940
Lowest Frequency = 33.6601 cm^{-1}
Second Frequency = 44.0195 cm^{-1}
SCF (BP86-D3BJ) Energy = -802.330766802
SCF (MeCN) Energy = -802.284698570
SCF (Toluene) Energy = -802.273223401
SCF (BS2) Energy = -802.155279837

Ru 0.75517 -0.50025 -0.60981
C -2.85794 -2.73856 0.22009
C -1.53469 -2.39269 -0.06329
H -0.76614 -3.15053 -0.24592
N -1.10869 -1.10208 -0.13789
O 1.90389 -1.18140 0.91677
C 3.00253 -0.65249 0.43747
O 2.89223 -0.00775 -0.65962
C 4.29237 -0.78436 1.19771
H 4.31699 -1.73330 1.75404
H 5.14494 -0.71850 0.50625
H 4.37114 0.04093 1.92722
H -3.14070 -3.79372 0.26370
C -1.39932 1.24305 0.07997
C -2.08414 2.46356 0.25424
C 0.02769 1.22927 -0.11177
C -1.37454 3.67122 0.27449
H -3.17415 2.47439 0.37423
C 0.72449 2.46189 -0.06490
C 0.02724 3.66587 0.11848
H -1.90880 4.61671 0.41163
H 1.81201 2.46876 -0.19518
H 0.57825 4.61346 0.13389
C -2.02170 -0.08105 0.10606
C -3.79611 -1.71431 0.43638
C -3.36541 -0.38230 0.38149
H -4.84273 -1.94986 0.65106
H -4.06908 0.43585 0.56004

D⁺ (κ^1)
SCF (BP86) Energy = -1282.03894895
Enthalpy 0K = -1281.656984
Enthalpy 298K = -1281.630229
Free Energy 298K = -1281.713656
Lowest Frequency = 29.3841 cm^{-1}
Second Frequency = 36.3951 cm^{-1}
SCF (BP86-D3BJ) Energy = -1282.16898642
SCF (MeCN) Energy = -1282.10115295
SCF (Toluene) Energy = -1282.07357931
SCF (BS2) Energy = -1282.03733615

Ru	0.09253	-0.09352	-0.19539
O	0.43432	-1.67319	2.37151
C	-0.38260	-0.75653	2.55087
C	-1.09612	-0.53950	3.87541
O	-0.74945	0.13094	1.62178
H	-1.87700	-1.31088	3.98358
H	-0.37643	-0.67570	4.69665
H	-1.56702	0.45159	3.93731
C	-2.91313	-0.23821	-0.52291
C	-4.20733	-0.55597	-0.06671
C	-1.92120	-1.25767	-0.53412
C	-4.50891	-1.85900	0.35732
H	-4.97341	0.22288	-0.00169
C	-2.22871	-2.56237	-0.11125
C	-3.52326	-2.86114	0.34162
H	-5.51748	-2.09056	0.71249
H	-1.46340	-3.34294	-0.14235
H	-3.76464	-3.87489	0.67451
H	-1.00885	-1.17015	-1.23516
C	-2.51693	1.12102	-0.91881
C	-2.94542	3.35157	-1.79164
H	-3.64008	4.10861	-2.16632
C	-3.41447	2.09654	-1.39331
H	-4.47611	1.84923	-1.47167
C	-0.71630	2.61817	-1.24124
H	0.36261	2.77374	-1.16490
C	-1.56698	3.61395	-1.72214
H	-1.14945	4.57391	-2.03577
N	-1.16875	1.39935	-0.83703
C	2.86964	-0.68416	-0.62246
C	3.88387	-1.08549	-1.51184
C	1.70386	-1.51256	-0.45040
C	3.78062	-2.30579	-2.19594
H	4.74617	-0.43464	-1.68900
C	1.64213	-2.75895	-1.12436
C	2.66299	-3.14096	-2.00351
H	4.57604	-2.60903	-2.88307
H	0.79766	-3.42964	-0.93881
H	2.59787	-4.09676	-2.53199
H	1.11170	-1.47401	0.58361
C	2.89762	0.58038	0.12945
C	3.92245	2.44354	1.29415
H	4.81221	2.99920	1.60361
C	4.04879	1.29049	0.50938
H	5.03270	0.91865	0.21218
C	1.52739	2.12957	1.28401
H	0.50671	2.39328	1.57121
C	2.64330	2.86138	1.69891
H	2.50487	3.74056	2.33309
N	1.64979	1.02933	0.49710

TS(**D⁺**–**E⁺**) (κ^1)
SCF (BP86) Energy = -1282.03427438
Enthalpy 0K = -1281.656041
Enthalpy 298K = -1281.629732
Free Energy 298K = -1281.711410
Lowest Frequency = -890.9595 cm^{-1}
Second Frequency = 33.0578 cm^{-1}
SCF (BP86-D3BJ) Energy = -1282.16481909
SCF (MeCN) Energy = -1282.09444711
SCF (Toluene) Energy = -1282.06804171
SCF (BS2) Energy = -1282.03076453

Ru	0.07521	-0.02339	-0.24294
O	0.86069	-1.81485	1.96941
C	-0.03657	-1.02648	2.40651
C	-0.51266	-1.12958	3.83314
O	-0.59485	-0.10493	1.67118
H	-1.00119	-2.10753	3.97580
H	0.35581	-1.09572	4.50969
H	-1.21922	-0.32574	4.07805
C	-2.96157	-0.31961	-0.40755
C	-4.19971	-0.74891	0.10998
C	-1.91577	-1.27269	-0.55840
C	-4.39993	-2.09406	0.45515
H	-5.00108	-0.02349	0.28149
C	-2.12469	-2.62114	-0.21817
C	-3.36503	-3.03109	0.29561
H	-5.36685	-2.40990	0.85808
H	-1.32514	-3.35259	-0.36639
H	-3.52660	-4.08013	0.56082
H	-1.05005	-1.08222	-1.29321
C	-2.68715	1.09061	-0.73240
C	-3.33265	3.32345	-1.44582
H	-4.10066	4.04109	-1.74826
C	-3.68272	2.01135	-1.11193
H	-4.72308	1.68159	-1.17083
C	-1.03314	2.74270	-1.02094
H	0.03227	2.98504	-0.97386
C	-1.97874	3.69486	-1.40693
H	-1.65375	4.70389	-1.67276
N	-1.36525	1.46923	-0.67866
C	2.86046	-0.53576	-0.71436
C	3.93662	-0.97931	-1.50643
C	1.64695	-1.31378	-0.61447
C	3.85622	-2.20862	-2.17542
H	4.83253	-0.35977	-1.61990
C	1.61850	-2.56821	-1.28082
C	2.69918	-3.00244	-2.06086
H	4.69667	-2.55056	-2.78656
H	0.73935	-3.21372	-1.18053
H	2.64490	-3.96538	-2.57846
H	1.05330	-1.43640	0.70044
C	2.86850	0.72515	0.03747
C	3.85063	2.61515	1.20326
H	4.72697	3.20037	1.49633
C	3.99927	1.47781	0.40115
H	4.98970	1.15156	0.07398
C	1.47131	2.21422	1.24294
H	0.44879	2.44594	1.55160
C	2.56760	2.98104	1.64545
H	2.41154	3.84609	2.29468
N	1.61246	1.12888	0.43830

E⁺ (κ^1)
SCF (BP86) Energy = -1282.03838938
Enthalpy 0K = -1281.656057
Enthalpy 298K = -1281.629390
Free Energy 298K = -1281.712200
Lowest Frequency = 31.1643 cm^{-1}
Second Frequency = 35.4231 cm^{-1}
SCF (BP86-D3BJ) Energy = -1282.16847171
SCF (MeCN) Energy = -1282.09698916
SCF (Toluene) Energy = -1282.07155918
SCF (BS2) Energy = -1282.03431484

Ru	0.10213	-0.02252	-0.24892
O	0.80292	-1.80572	2.09943
C	-0.11706	-0.95552	2.47060
C	-0.60300	-1.03172	3.88572
O	-0.60255	-0.08325	1.67509
H	-1.05862	-2.02066	4.05985

```
H   0.25230 -0.94129  4.57491
H  -1.33836 -0.24200  4.08470
C  -2.95515 -0.34335 -0.42630
C  -4.18764 -0.79328  0.08812
C  -1.89445 -1.28054 -0.57738
C  -4.36979 -2.14141  0.43164
H  -5.00009 -0.07949  0.25682
C  -2.08700 -2.63314 -0.24075
C  -3.32119 -3.06293  0.27184
H  -5.33317 -2.47173  0.83161
H  -1.27880 -3.35393 -0.39508
H  -3.46801 -4.11524  0.53296
H  -1.03019 -1.07515 -1.30700
C  -2.70781  1.07465 -0.74740
C  -3.39991  3.28892 -1.47076
H  -4.17985  3.98638 -1.78964
C  -3.72177  1.96663 -1.14783
H  -4.75116  1.60871 -1.23205
C  -1.09614  2.76640 -0.99663
H  -0.03827  3.03742 -0.92764
C  -2.05785  3.69644 -1.39901
H  -1.75495  4.71543 -1.65312
N  -1.39875  1.48403 -0.66600
C   2.87807 -0.53704 -0.72879
C   3.97296 -1.02109 -1.47149
C   1.63807 -1.28009 -0.64719
C   3.89073 -2.26676 -2.10820
H   4.88732 -0.42560 -1.56786
C   1.61195 -2.54948 -1.28901
C   2.71178 -3.03129 -2.01382
H   4.74461 -2.64408 -2.67868
H   0.71062 -3.17043 -1.22889
H   2.65348 -4.00579 -2.50960
H   1.00513 -1.57761  1.08811
C   2.89413  0.73177  0.00778
C   3.87817  2.64540  1.13614
H   4.75386  3.24287  1.40549
C   4.02250  1.50173  0.34236
H   5.00985  1.18642 -0.00437
C   1.50412  2.22403  1.21855
H   0.48375  2.45781  1.53376
C   2.59954  3.00453  1.59649
H   2.44563  3.87661  2.23679
N   1.64000  1.12693  0.42845
```

D⁺ (κ^2)

```
SCF (BP86) Energy = -1282.05904449
Enthalpy 0K = -1281.675413
Enthalpy 298K = -1281.648838
Free Energy 298K = -1281.731036
Lowest Frequency = 24.2476 cm-1
Second Frequency = 42.6875 cm-1
SCF (BP86-D3BJ) Energy = -1282.19464727
SCF (MeCN) Energy = -1282.11432978
SCF (Toluene) Energy = -1282.09121296
SCF (BS2) Energy = -1282.05543093
```

```
Ru  0.29314  0.66968  0.00749
O   1.18783  2.21322  1.19213
C   1.21741  3.02292  0.18251
C   1.71957  4.43153  0.32559
O   0.76787  2.56814 -0.93938
H   2.15987  4.78028 -0.62005
H   0.87294  5.09638  0.57125
H   2.45091  4.49713  1.14409
C  -2.49699 -0.00069  0.82367
C  -3.87420 -0.20093  0.60755
C  -1.85554  1.11707  0.20223
C  -4.60121  0.69710 -0.18917
H  -4.38026 -1.07015  1.03954
C  -2.59793  2.02780 -0.58388
C  -3.96845  1.80890 -0.78223
H  -5.67021  0.52965 -0.35122
H  -2.09303  2.88952 -1.03025
H  -4.54889  2.50556 -1.39479
H  -0.98109  1.59582  0.82157
C  -1.64098 -0.86921  1.64159
C  -1.21634 -2.43491  3.45265
H  -1.58003 -3.11108  4.23134
C  -2.11624 -1.74676  2.63404
H  -3.19418 -1.85528  2.77908
C   0.58382 -1.34768  2.26645
H   1.64214 -1.14413  2.09033
C   0.15962 -2.21205  3.27727
H   0.90281 -2.69647  3.91574
N  -0.28205 -0.70516  1.43863
C   1.95692 -1.14397 -0.91779
C   2.68584 -2.08955 -0.15236
C   2.42149  0.20953 -1.00995
C   3.81961 -1.68781  0.55620
H   2.34354 -3.12846 -0.11351
C   3.56539  0.59339 -0.25258
C   4.24361 -0.33644  0.53314
H   4.38438 -2.42308  1.13835
H   3.94029  1.61771 -0.33602
H   5.13010 -0.03494  1.09877
H   2.09824  0.84775 -1.83912
C   0.76520 -1.52005 -1.71756
C  -0.51763 -2.76643 -3.33603
H  -0.61823 -3.59087 -4.04754
C   0.67204 -2.59238 -2.61096
H   1.52856 -3.25857 -2.74635
C  -1.41586 -0.81185 -2.22070
H  -2.21026 -0.08598 -2.03823
C  -1.56440 -1.85262 -3.14559
H  -2.49946 -1.93756 -3.70531
N  -0.27377 -0.65331 -1.50490
```

TS(**D⁺**–**E⁺**) (κ^2)

```
SCF (BP86) Energy = -1282.03247462
Enthalpy 0K = -1281.653789
Enthalpy 298K = -1281.627216
Free Energy 298K = -1281.709781
Lowest Frequency = -995.2539 cm-1
Second Frequency = 22.6898 cm-1
SCF (BP86-D3BJ) Energy = -1282.16646981
SCF (MeCN) Energy = -1282.08697163
SCF (Toluene) Energy = -1282.06426013
SCF (BS2) Energy = -1282.02796959
```

```
Ru  0.00554  0.61643 -0.02447
O   0.87964  2.38051 -1.30127
C   0.51982  3.20024 -0.30894
C   0.64584  4.67416 -0.53067
O   0.07923  2.67666  0.75460
H   0.31175  5.22713  0.35705
H   1.69514  4.92327 -0.76189
H   0.04712  4.97042 -1.40843
C   2.52131 -0.81396 -0.53146
C   3.85397 -1.23573 -0.35914
C   2.03777  0.35183  0.15242
C   4.71936 -0.51570  0.47767
H   4.22193 -2.13571 -0.86283
C   2.93022  1.05617  1.00054
C   4.25933  0.62765  1.15564
H   5.75294 -0.85033  0.60607
H   2.57894  1.94197  1.54084
H   4.93646  1.18437  1.81155
H   1.47682  1.42206 -0.73992
C   1.53387 -1.50402 -1.36584
C   0.79128 -3.09411 -3.05133
H   1.00439 -3.90904 -3.74883
C   1.80905 -2.55602 -2.25851
H   2.83096 -2.93490 -2.33926
```

```
C  -0.73188 -1.52019 -2.03869
H  -1.72108 -1.07295 -1.91897
C  -0.50156 -2.55621 -2.94624
H  -1.32832 -2.92878 -3.55622
N   0.24828 -1.00192 -1.25162
C  -2.64105 -0.24713  0.60563
C  -3.56957 -0.98879 -0.16148
C  -2.51685  1.15454  0.38876
C  -4.31790 -0.35770 -1.16349
H  -3.67855 -2.06371  0.01589
C  -3.25993  1.76965 -0.64491
C  -4.14396  1.01653 -1.42739
H  -5.03559 -0.93905 -1.75092
H  -3.17747  2.85048 -0.79620
H  -4.72593  1.49910 -2.21819
H  -2.00100  1.78072  1.12338
C  -1.79430 -0.89771  1.63532
C  -1.37715 -2.30596  3.56211
H  -1.73313 -2.97814  4.34773
C  -2.27169 -1.76320  2.62882
H  -3.34201 -1.98347  2.67001
C   0.40641 -1.09872  2.45743
H   1.45159 -0.80771  2.34330
C  -0.02108 -1.95691  3.47425
H   0.71390 -2.34462  4.18435
N  -0.45989 -0.57862  1.54428
```

E⁺ (κ^2)

SCF (BP86) Energy = -1282.04711192
Enthalpy 0K = -1281.663206
Enthalpy 298K = -1281.636011
Free Energy 298K = -1281.720797
Lowest Frequency = 26.6433 cm^{-1}
Second Frequency = 31.9963 cm^{-1}
SCF (BP86-D3BJ) Energy = -1282.18394412
SCF (MeCN) Energy = -1282.10889181
SCF (Toluene) Energy = -1282.08099710
SCF (BS2) Energy = -1282.04337397

```
Ru -0.22933 -0.27729 -0.42564
O  -2.38417 -2.16086 -2.12950
C  -1.36485 -2.86282 -1.62823
C  -1.29782 -4.28588 -2.09328
O  -0.52219 -2.37038 -0.83576
H  -0.40458 -4.77621 -1.68690
H  -2.20465 -4.82587 -1.77290
H  -1.28029 -4.31601 -3.19557
C  -2.38727  1.55498  0.13447
C  -3.70057  2.01229  0.36328
C  -2.07836  0.15288  0.16949
C  -4.72241  1.10292  0.67200
H  -3.93390  3.08134  0.31555
C  -3.12410 -0.73599  0.53237
C  -4.43023 -0.26777  0.77170
H  -5.73913  1.46410  0.85116
H  -2.92209 -1.80908  0.64165
H  -5.22015 -0.97827  1.03736
H  -2.45034 -1.30311 -1.62767
C  -1.23456  2.43732 -0.08112
C  -0.08743  4.57485 -0.26128
H  -0.11268  5.66824 -0.27803
C  -1.26856  3.84232 -0.10360
H  -2.22607  4.35720  0.00651
C   1.10967  2.48450 -0.38018
H   2.02762  1.90692 -0.49477
C   1.12497  3.88131 -0.39472
H   2.07602  4.40580 -0.51495
N  -0.03407  1.76171 -0.23643
C   2.80587 -0.42690  0.21297
C   4.05206  0.22276  0.36746
C   2.30965 -0.63006 -1.09879
C   4.77933  0.64499 -0.75504
H   4.43663  0.43356  1.37019
C   3.03758 -0.20123 -2.22177
C   4.27577  0.43728 -2.05193
H   5.74097  1.14833 -0.61573
H   2.64315 -0.38421 -3.22608
H   4.84895  0.76683 -2.92360
H   1.42490 -1.27933 -1.26618
C   2.01309 -0.83826  1.39145
C   1.85329 -1.63730  3.69110
H   2.33143 -1.96585  4.61787
C   2.62359 -1.25532  2.58967
H   3.71486 -1.30103  2.62907
C  -0.11473 -1.18866  2.36728
H  -1.19445 -1.13179  2.23078
C   0.45577 -1.60115  3.57056
H  -0.20012 -1.88869  4.39624
N   0.63502 -0.80811  1.28974
```

D

SCF (BP86) Energy = -1510.76736972
Enthalpy 0K = -1510.336047
Enthalpy 298K = -1510.303881
Free Energy 298K = -1510.399816
Lowest Frequency = 23.7201 cm^{-1}
Second Frequency = 32.4862 cm^{-1}
SCF (BP86-D3BJ) Energy = -1510.92042404
SCF (MeCN) Energy = -1510.78690618
SCF (Toluene) Energy = -1510.77585526
SCF (BS2) Energy = -1510.84332074

```
Ru  0.91517 -0.03275 -0.45023
O   2.13513  1.03385 -1.89904
C   1.59032  0.37074 -2.85606
C   2.08710  0.49742 -4.27503
O   0.62742 -0.43754 -2.56589
H   1.26539  0.33234 -4.98789
H   2.54627  1.48383 -4.43617
H   2.85505 -0.27508 -4.45362
C  -2.60168  0.23686 -0.77240
C  -3.64932 -0.05912  0.12745
C  -2.38046 -0.61868 -1.87386
C  -4.45253 -1.19375 -0.06114
H  -3.82326  0.59957  0.98530
C  -3.19761 -1.74241 -2.06664
C  -4.23416 -2.03424 -1.16458
H  -5.25279 -1.41705  0.65221
H  -3.02350 -2.39147 -2.93155
H  -4.86993 -2.91221 -1.32078
H  -1.56583 -0.40020 -2.56980
C  -1.86166  1.52525 -0.64705
C  -2.01198  3.96471 -0.59168
H  -2.60959  4.88103 -0.55810
C  -2.62809  2.71037 -0.59641
H  -3.71757  2.61906 -0.59751
C   0.09625  2.80783 -0.68519
H   1.18567  2.79432 -0.73486
C  -0.61387  4.00953 -0.66305
H  -0.06673  4.95577 -0.69213
N  -0.48993  1.57541 -0.64672
C   0.14154  0.26078  2.41833
C  -0.21118  0.93756  3.60208
C   1.11648  0.81956  1.52795
C   0.41232  2.14765  3.93765
H  -0.99137  0.53086  4.25572
C   1.75621  2.02481  1.90780
C   1.40188  2.68528  3.09246
H   0.13298  2.66832  4.85927
H   2.55977  2.41966  1.27691
H   1.90518  3.61903  3.36663
H   1.94198  0.05441  1.00815
C  -0.44128 -1.01053  1.98821
C  -1.56337 -3.14478  2.29801
```

H -2.09823 -3.85653 2.93414
C -1.13632 -1.91596 2.81066
H -1.30843 -1.65782 3.85943
C -0.58729 -2.52084 0.17798
H -0.33265 -2.70386 -0.86824
C -1.27016 -3.45466 0.95835
H -1.56445 -4.40984 0.51535
N -0.19647 -1.31066 0.66108
O 2.28036 -1.57337 -0.64656
C 3.27322 -1.67524 0.20472
C 4.27641 -2.77614 -0.12822
O 3.44209 -0.94271 1.20547
H 3.84712 -3.52260 -0.81205
H 5.15638 -2.31974 -0.61370
H 4.62130 -3.25787 0.79929

TS(**D**-**E**)
SCF (BP86) Energy = -1510.73262187
Enthalpy 0K = -1510.305297
Enthalpy 298K = -1510.272928
Free Energy 298K = -1510.369216
Lowest Frequency = -1053.6258 cm^{-1}
Second Frequency = 27.1991 cm^{-1}
SCF (BP86-D3BJ) Energy = -1510.88592214
SCF (MeCN) Energy = -1510.75027871
SCF (Toluene) Energy = -1510.74035627
SCF (BS2) Energy = -1510.80850232

Ru -0.67874 -0.39619 -0.58591
O -1.41339 -2.14641 -1.60745
C -0.67409 -1.92356 -2.64051
C -0.81795 -2.78504 -3.87475
O 0.15246 -0.94087 -2.61094
H 0.13226 -2.82933 -4.42730
H -1.15386 -3.79670 -3.60278
H -1.57962 -2.33844 -4.53737
C 2.79465 -0.33263 0.09351
C 3.60805 0.49877 0.89517
C 2.88149 -0.22849 -1.31273
C 4.48050 1.42548 0.30599
H 3.53982 0.42772 1.98610
C 3.76710 0.68981 -1.89633
C 4.56783 1.51888 -1.09262
H 5.09477 2.07238 0.94107
H 3.83281 0.75327 -2.98777
H 5.25868 2.23269 -1.55384
H 2.24647 -0.85921 -1.94151
C 1.99103 -1.41452 0.72636
C 2.01901 -3.39758 2.16090
H 2.54363 -4.06459 2.85169
C 2.65798 -2.27824 1.62258
H 3.70642 -2.06738 1.84987
C 0.07681 -2.76251 0.88581
H -0.94794 -2.92100 0.55017
C 0.70218 -3.65516 1.75455
H 0.14991 -4.53134 2.10504
N 0.67012 -1.62667 0.39984
C -1.21459 0.79936 2.06467
C -1.63771 0.88273 3.40433
C -1.73042 -0.21958 1.19537
C -2.60141 -0.01197 3.89549
H -1.21618 1.64025 4.07528
C -2.71795 -1.09238 1.71415
C -3.14938 -0.99118 3.04775
H -2.92970 0.05981 4.93759
H -3.15619 -1.85146 1.05454
H -3.91329 -1.67839 3.42885
H -2.23766 0.24585 -0.12469
C -0.26332 1.71809 1.43109
C 1.02381 3.77085 1.23161
H 1.39549 4.70703 1.65938
C 0.22036 2.91387 1.99010
H -0.06548 3.18023 3.01154
C 0.83374 2.20822 -0.59606
H 1.04698 1.87696 -1.61489
C 1.31961 3.41685 -0.09478
H 1.92207 4.06127 -0.73995
N 0.08456 1.35269 0.14458
O -2.50483 0.54486 -1.41150
C -2.73764 1.87509 -1.53832
C -3.51572 2.17356 -2.81485
O -2.39463 2.73411 -0.73259
H -2.90661 1.89817 -3.69230
H -4.43333 1.56448 -2.85268
H -3.76832 3.24205 -2.85810

E
SCF (BP86) Energy = -1510.75701342
Enthalpy 0K = -1510.324023
Enthalpy 298K = -1510.291288
Free Energy 298K = -1510.389520
Lowest Frequency = 19.9446 cm^{-1}
Second Frequency = 23.3709 cm^{-1}
SCF (BP86-D3BJ) Energy = -1510.90941903
SCF (MeCN) Energy = -1510.77098542
SCF (Toluene) Energy = -1510.76331717
SCF (BS2) Energy = -1510.83394144

Ru 0.59777 0.44011 0.22597
O 1.45701 1.64602 1.76321
C 0.71123 2.69429 1.62086
C 0.92855 3.87842 2.54440
O -0.19851 2.71898 0.72631
H 0.06781 3.97020 3.22889
H 1.84715 3.75638 3.13582
H 0.97855 4.80989 1.95799
C -2.79359 -0.22256 0.55325
C -3.68928 -1.08431 -0.11723
C -2.86315 1.16736 0.30628
C -4.62409 -0.57325 -1.03049
H -3.63545 -2.16299 0.06555
C -3.81014 1.67444 -0.59734
C -4.69029 0.80884 -1.27052
H -5.30199 -1.25650 -1.55285
H -3.86212 2.75470 -0.77065
H -5.42777 1.21028 -1.97381
H -2.16982 1.84465 0.81451
C -1.90405 -0.75880 1.61964
C -1.76329 -1.97441 3.73923
H -2.23081 -2.57834 4.52261
C -2.49795 -1.54043 2.63223
H -3.56522 -1.76184 2.54519
C 0.12801 -0.81888 2.79083
H 1.16923 -0.50060 2.81685
C -0.42243 -1.57382 3.82460
H 0.20770 -1.84401 4.67657
N -0.56178 -0.44151 1.66583
C 1.58974 -2.12495 -0.77327
C 2.41400 -3.26538 -0.87125
C 1.82673 -1.11345 0.21661
C 3.50536 -3.42011 -0.00526
H 2.21469 -4.03445 -1.62774
C 2.95658 -1.28724 1.05599
C 3.78133 -2.42169 0.94823
H 4.14520 -4.30526 -0.08067
H 3.19443 -0.51865 1.80340
H 4.64668 -2.52985 1.61341
H 2.96919 1.04919 -0.93293
C 0.48555 -1.81437 -1.68129
C -0.90538 -2.10731 -3.66041
H -1.20065 -2.69050 -4.53828
C 0.10022 -2.56944 -2.80506
H 0.61405 -3.51247 -3.01274
C -1.11742 -0.17594 -2.22933

H -1.59254 0.76582 -1.94414
C -1.51550 -0.87531 -3.37167
H -2.30218 -0.45960 -4.00681
N -0.15086 -0.61700 -1.37953
O 2.06438 1.38200 -1.13193
C 2.19489 2.53139 -1.92437
C 0.86132 3.12814 -2.27136
O 3.30312 2.91435 -2.24436
H 0.30710 3.34862 -1.34153
H 1.01868 4.03482 -2.86988
H 0.26497 2.39652 -2.84126

E (without HOAc)
SCF (BP86) Energy = -1281.67152225
Enthalpy 0K = -1281.299998
Enthalpy 298K = -1281.273548
Free Energy 298K = -1281.355919
Lowest Frequency = 30.2586 cm^{-1}
Second Frequency = 35.7505 cm^{-1}
SCF (BP86-D3BJ) Energy = -1281.80135597
SCF (MeCN) Energy = -1281.68662640
SCF (Toluene) Energy = -1281.67802521
SCF (BS2) Energy = -1281.67489536

Ru -0.22894 -0.62481 -0.26816
O -0.71342 -2.74463 -0.17993
C -1.06624 -2.71587 -1.42148
C -1.64287 -3.93672 -2.09438
O -0.93430 -1.60467 -2.05870
H -1.45321 -3.90269 -3.17746
H -1.21959 -4.85334 -1.65674
H -2.73562 -3.95513 -1.93800
C 2.77863 -0.22385 0.51801
C 4.01832 0.44564 0.41382
C 2.30448 -0.94617 -0.60684
C 4.76737 0.38541 -0.77028
H 4.37839 1.05413 1.24999
C 3.06056 -1.01050 -1.79107
C 4.29049 -0.34007 -1.87763
H 5.72141 0.91886 -0.83397
H 2.67772 -1.58376 -2.64112
H 4.87626 -0.38134 -2.80169
H 1.45341 -1.66543 -0.48999
C 1.94756 -0.13779 1.73566
C 1.71295 0.10759 4.15090
H 2.15613 0.23341 5.14296
C 2.51839 0.02983 3.01174
H 3.60783 0.07370 3.09617
C -0.19968 -0.17699 2.70138
H -1.27379 -0.26784 2.52685
C 0.32194 0.00212 3.98074
H -0.36437 0.05162 4.83090
N 0.57481 -0.25241 1.57421
C -2.41873 1.27695 -0.09895
C -3.70985 1.77789 0.17894
C -2.07712 -0.08622 0.18096
C -4.68455 0.94134 0.73439
H -3.95820 2.82417 -0.03656
C -3.08516 -0.91062 0.74206
C -4.36659 -0.40330 1.01336
H -5.68527 1.32979 0.94919
H -2.85717 -1.95996 0.96145
H -5.12963 -1.06272 1.44479
C -1.33388 2.06354 -0.67851
C -0.31112 4.05276 -1.64739
H -0.37724 5.09895 -1.96195
C -1.41505 3.41077 -1.08011
H -2.35920 3.94631 -0.94784
C 0.91650 1.99114 -1.39138
H 1.81920 1.38846 -1.50423
C 0.87821 3.32297 -1.80967
H 1.77158 3.77061 -2.25358
N -0.14920 1.35366 -0.83373

D⁺ (η^6)
SCF (BP86) Energy = -1282.06544575
Enthalpy 0K = -1281.680956
Enthalpy 298K = -1281.654034
Free Energy 298K = -1281.740246
Lowest Frequency = 9.2286 cm^{-1}
Second Frequency = 16.3393 cm^{-1}
SCF (BP86-D3BJ) Energy = -1282.19423018
SCF (MeCN) Energy = -1282.12052189
SCF (Toluene) Energy = -1282.09744342
SCF (BS2) Energy = -1282.06590930

Ru -0.23790 1.09414 -0.39988
O 0.03493 2.60704 1.08282
C -1.24020 2.74565 1.23950
C -1.82148 3.73387 2.20376
O -1.97817 1.99869 0.48913
H -1.14004 3.88894 3.05287
H -1.95406 4.70287 1.69116
H -2.80750 3.39498 2.55334
C -2.01899 -1.74109 0.38725
C -1.95434 -3.00707 -0.24002
C -3.10704 -0.88573 0.10362
C -2.93795 -3.39483 -1.16294
H -1.12498 -3.68460 -0.00736
C -4.09705 -1.28675 -0.80713
C -4.01164 -2.53459 -1.44862
H -2.87080 -4.37262 -1.64990
H -4.94616 -0.62503 -1.00563
H -4.78719 -2.84259 -2.15676
H -3.18302 0.08263 0.60457
C -0.98070 -1.38727 1.39616
C 0.19838 -1.97516 3.45326
H 0.34981 -2.64871 4.30204
C -0.77341 -2.25597 2.48851
H -1.40922 -3.14123 2.57035
C 0.72393 0.02131 2.21507
H 1.29886 0.93637 2.06170
C 0.96280 -0.80915 3.31093
H 1.73752 -0.53498 4.03133
N -0.22120 -0.25001 1.26851
C 1.53896 0.24032 -1.47871
C 0.34880 -0.51029 -1.80561
C 1.47581 1.66866 -1.61276
C -0.82255 0.12466 -2.30585
H 0.30224 -1.57832 -1.57736
C 0.32043 2.32613 -2.16045
C -0.83396 1.55576 -2.47182
H -1.73050 -0.45888 -2.47352
H 0.28934 3.41702 -2.21753
H -1.76297 2.05904 -2.75459
H 2.32442 2.24686 -1.23568
C 2.76812 -0.39854 -0.92806
C 4.26498 -2.27954 -0.66278
H 4.53195 -3.32434 -0.84889
C 3.07044 -1.75284 -1.17649
H 2.41026 -2.37689 -1.78619
C 4.72893 -0.10265 0.26080
H 5.36966 0.58748 0.82299
C 5.11300 -1.44285 0.07452
H 6.05608 -1.81048 0.48845
N 3.58808 0.41891 -0.22265

TS(**D⁺**–**E⁺**) (η^6)
SCF (BP86) Energy = -1282.04288362
Enthalpy 0K = -1281.659807
Enthalpy 298K = -1281.633420
Free Energy 298K = -1281.717072
Lowest Frequency = -102.1103 cm^{-1}
Second Frequency = 14.3036 cm^{-1}

SCF (BP86-D3BJ) Energy = -1282.17401029
SCF (MeCN) Energy = -1282.10129106
SCF (Toluene) Energy = -1282.07638517
SCF (BS2) Energy = -1282.04374955

Ru	0.38477	-0.79916	-0.26668
O	0.23698	-1.80645	1.56642
C	1.37966	-2.40745	1.82723
C	1.41721	-3.21714	3.10909
O	2.37217	-2.29795	1.07034
H	2.01876	-2.67226	3.85633
H	0.41143	-3.38925	3.51674
H	1.92204	-4.17678	2.91981
C	2.00712	1.82987	0.13439
C	2.55922	2.95072	-0.51832
C	2.59006	0.55241	-0.07160
C	3.67099	2.79671	-1.36149
H	2.10651	3.93919	-0.38883
C	3.71133	0.40610	-0.91067
C	4.25049	1.52855	-1.55753
H	4.08914	3.67190	-1.86810
H	4.17418	-0.57989	-1.01674
H	5.13013	1.42316	-2.19990
H	2.34464	-0.31932	0.58230
C	0.82916	1.92366	1.01767
C	-0.53866	3.00599	2.70784
H	-0.74425	3.85609	3.36491
C	0.56640	3.02773	1.84994
H	1.25462	3.87682	1.83983
C	-1.06139	0.80088	1.87784
H	-1.66856	-0.10681	1.84593
C	-1.36101	1.86907	2.72822
H	-2.22470	1.79922	3.39397
N	-0.00408	0.83543	1.02865
C	-1.51553	-0.66326	-1.38155
C	-0.51178	0.08843	-2.10883
C	-1.21680	-2.02740	-1.01801
C	0.71982	-0.51701	-2.45720
H	-0.65923	1.15266	-2.30832
C	0.01142	-2.65807	-1.42555
C	0.98748	-1.89501	-2.10926
H	1.50901	0.08649	-2.91194
H	0.24368	-3.67049	-1.08684
H	1.97806	-2.31843	-2.29247
H	-1.93302	-2.54788	-0.37704
C	-2.82357	-0.07053	-0.98019
C	-4.63087	1.51178	-1.26617
H	-5.08047	2.36920	-1.77600
C	-3.36268	1.04818	-1.64770
H	-2.82830	1.52925	-2.47180
C	-4.69225	-0.25674	0.37087
H	-5.19455	-0.80431	1.17742
C	-5.31264	0.85049	-0.23659
H	-6.30564	1.17415	0.08767
N	-3.47961	-0.71570	0.01684

E^{+} (η^6)
SCF (BP86) Energy = -1282.06784697
Enthalpy 0K = -1281.683613
Enthalpy 298K = -1281.656854
Free Energy 298K = -1281.740959
Lowest Frequency = 17.7254 cm^{-1}
Second Frequency = 25.9548 cm^{-1}
SCF (BP86-D3BJ) Energy = -1282.19791784
SCF (MeCN) Energy = -1282.12231427
SCF (Toluene) Energy = -1282.09955152
SCF (BS2) Energy = -1282.06666601

Ru	0.30062	-0.79240	-0.05539
O	0.87855	-0.71141	2.01976
C	2.00616	-0.64927	2.57398
C	2.14132	-0.68036	4.06977
O	3.14836	-0.55892	1.91450
H	2.62467	0.24863	4.41484
H	1.15617	-0.78912	4.53969
H	2.79888	-1.51473	4.36430
C	2.22176	1.31104	-0.89417
C	3.35354	1.90359	-1.49260
C	2.09862	-0.11441	-0.78848
C	4.39130	1.10266	-1.98557
H	3.42923	2.99296	-1.57744
C	3.17459	-0.89349	-1.28039
C	4.30474	-0.29450	-1.87030
H	5.26687	1.56521	-2.44996
H	3.14080	-1.98602	-1.20336
H	5.11725	-0.92675	-2.24340
H	2.94928	-0.50701	0.92913
C	1.11790	2.06883	-0.30504
C	-0.04494	4.04547	0.50068
H	-0.10415	5.13147	0.61886
C	1.04624	3.46780	-0.15393
H	1.85593	4.09298	-0.53825
C	-0.94465	1.83249	0.83510
H	-1.70249	1.13813	1.21177
C	-1.05308	3.21362	1.01639
H	-1.91545	3.62059	1.54988
N	0.10086	1.27536	0.17377
C	-1.98360	-1.23534	-0.57750
C	-1.10415	-1.03394	-1.71941
C	-1.58605	-2.16059	0.41435
C	0.03625	-1.86917	-1.92953
H	-1.32862	-0.25040	-2.44776
C	-0.36344	-2.90587	0.25769
C	0.40484	-2.84354	-0.93868
H	0.66229	-1.71928	-2.81285
H	-0.02949	-3.55351	1.07392
H	1.29200	-3.46769	-1.06435
H	-2.18440	-2.24543	1.32440
C	-3.25062	-0.46804	-0.42156
C	-5.19827	0.63687	-1.33854
H	-5.78993	0.98215	-2.19182
C	-3.97763	-0.02314	-1.54479
H	-3.61892	-0.21749	-2.55979
C	-4.85121	0.35792	1.03046
H	-5.16801	0.49419	2.07164
C	-5.64852	0.83320	-0.02647
H	-6.59556	1.33944	0.18040
N	-3.67881	-0.27693	0.85255

^{3}D^{+}
SCF (BP86) Energy = -1680.38957212
Enthalpy 0K = -1679.866976
Enthalpy 298K = -1679.825220
Free Energy 298K = -1679.945706
Lowest Frequency = 4.7782 cm^{-1}
Second Frequency = 23.1364 cm^{-1}
SCF (BP86-D3BJ) Energy = -1680.57298956
SCF (MeCN) Energy = -1680.44675564
SCF (Toluene) Energy = -1680.42140955
SCF (BS2) Energy = -1680.50344097

Ru	-0.00128	0.85694	0.49393
C	2.05486	-1.58709	-1.24131
C	1.26945	-2.68544	-0.83566
C	3.45866	-1.66149	-1.09170
C	1.86914	-3.81778	-0.26210
H	0.18896	-2.67477	-1.00014
C	4.05364	-2.78866	-0.50767
C	3.26081	-3.87111	-0.09058
H	1.24530	-4.66742	0.03319
H	5.14141	-2.82612	-0.39008
H	3.72754	-4.75794	0.34982
H	4.07189	-0.81340	-1.41082
C	1.47460	-0.46077	-2.03499

```
C   1.39825  0.58356 -4.25061
H   1.75013  0.64536 -5.28469
C   1.91980 -0.36765 -3.37343
H   2.67443 -1.08374 -3.70791
C   0.00654  1.31656 -2.43475
H  -0.75550  1.97967 -2.02524
C   0.39733  1.43569 -3.76701
H  -0.07529  2.19154 -4.40008
N   0.52931  0.41295 -1.55269
C  -2.76485 -1.38915 -0.24817
C  -2.34434 -1.25426 -1.58815
C  -4.14656 -1.29096  0.03989
C  -3.27699 -1.01963 -2.60959
H  -1.28521 -1.34820 -1.83452
C  -5.07820 -1.05056 -0.98162
C  -4.64562 -0.91559 -2.31217
H  -2.93295 -0.93669 -3.64550
H  -6.14437 -0.98699 -0.73959
H  -5.37232 -0.74679 -3.11321
H  -4.48867 -1.40025  1.07477
C  -1.83017 -1.78675  0.84576
C  -1.37058 -3.42727  2.60514
H  -1.65871 -4.31682  3.17365
C  -2.19122 -2.93433  1.58806
H  -3.11973 -3.44629  1.32291
C   0.14956 -1.63183  2.09251
H   1.08825 -1.08741  2.23398
C  -0.16397 -2.76153  2.84978
H   0.54082 -3.10408  3.61220
N  -0.65861 -1.11848  1.11763
O   1.89779  0.36561  1.18515
C   3.04327  0.85665  0.72938
C   4.21766  0.50454  1.64611
O   3.19726  1.51397 -0.31089
H   4.32027 -0.59052  1.72301
H   5.14737  0.93258  1.24603
H   4.04063  0.89017  2.66408
N   0.66056  2.69809  0.12871
C   1.11567  3.75903 -0.06419
C   1.82082  5.00730 -0.32012
H   1.77896  5.66759  0.56170
H   2.87555  4.77315 -0.54464
H   1.38061  5.53917 -1.17942
N  -0.35434  1.38911  2.38080
C  -0.50414  1.69987  3.50115
C  -0.67740  2.08888  4.89568
H  -1.51293  2.80125  4.99788
H  -0.89307  1.20325  5.51631
H   0.24152  2.56687  5.27444
N  -1.84732  1.46671  0.03486
C  -2.88394  1.98714 -0.15725
C  -4.19401  2.58138 -0.39359
H  -4.46056  3.27155  0.42459
H  -4.19858  3.14587 -1.34111
H  -4.95574  1.78627 -0.45631
```

INT(^{3}D$^+$)

```
SCF (BP86) Energy = -1680.36814747
Enthalpy 0K = -1679.845892
Enthalpy 298K = -1679.804142
Free Energy 298K = -1679.923247
Lowest Frequency = 23.3854 cm-1
Second Frequency = 25.3254 cm-1
SCF (BP86-D3BJ) Energy = -1680.55136469
SCF (MeCN) Energy = -1680.42432126
SCF (Toluene) Energy = -1680.39986533
SCF (BS2) Energy = -1680.47990859
```

```
Ru  0.31823  0.80251  0.23477
C  -2.19621 -0.87730 -1.52878
C  -1.57757 -1.98012 -2.13395
C  -1.54465  0.39310 -1.58060
C  -0.33594 -1.84790 -2.79646
H  -2.09498 -2.94423 -2.11714
C  -0.29417  0.51918 -2.23115
C   0.30481 -0.61311 -2.85227
H   0.10239 -2.71857 -3.29513
H   0.10287  1.51991 -2.42219
H   1.24631 -0.49869 -3.39829
H  -2.03261  1.31149 -1.23032
C  -3.52883 -1.04100 -0.88695
C  -5.73940 -0.22289 -0.30836
H  -6.49887  0.56590 -0.31496
C  -4.47996  0.00507 -0.87952
H  -4.24693  0.96741 -1.34418
C  -5.01108 -2.45996  0.19856
H  -5.18851 -3.45736  0.62034
C  -6.01757 -1.48218  0.24541
H  -6.98960 -1.70826  0.69303
N  -3.79508 -2.26127 -0.34665
C   2.96435 -1.63827  0.13562
C   2.86097 -2.92657 -0.43244
C   3.07718 -1.51554  1.53632
C   2.83423 -4.06571  0.38642
H   2.79413 -3.03114 -1.52032
C   3.05929 -2.65532  2.35289
C   2.93272 -3.93275  1.78209
H   2.75570 -5.05909 -0.06743
H   3.16253 -2.54847  3.43764
H   2.93136 -4.82219  2.42021
H   3.19774 -0.52365  1.97885
C   3.13564 -0.45137 -0.75186
C   4.58423  0.64048 -2.39402
H   5.46179  0.62551 -3.04744
C   4.26445 -0.46415 -1.60094
H   4.90128 -1.35259 -1.59223
C   2.64527  1.72362 -1.46406
H   1.97065  2.57796 -1.35543
C   3.76427  1.77127 -2.29733
H   3.97105  2.68477 -2.86129
N   2.29219  0.63321 -0.72201
O   0.42333  2.84695 -0.19595
C  -0.61755  3.63541 -0.44489
C  -0.22368  5.11099 -0.52299
O  -1.79664  3.27445 -0.58607
H  -0.99104  5.67274 -1.07374
H  -0.15653  5.52255  0.49924
H   0.76124  5.24580 -0.99609
N  -1.40000  1.08343  1.20560
C  -2.36480  1.26371  1.84222
C  -3.59383  1.55753  2.56605
H  -3.48044  1.33697  3.64006
H  -3.84827  2.62377  2.44250
H  -4.41877  0.94818  2.16045
N   1.22400  1.29087  1.88551
C   1.72390  1.71073  2.85997
C   2.35703  2.23538  4.06378
H   3.44616  2.32573  3.91470
H   1.95419  3.23448  4.30071
H   2.17294  1.56797  4.92224
N   0.08805 -1.13952  0.66518
C  -0.32815 -2.21124  0.89608
C  -0.92434 -3.52136  1.11266
H  -1.00395 -3.73932  2.19056
H  -1.93576 -3.51026  0.65949
H  -0.30980 -4.30442  0.63999
```

TS(^{3}D$^+$–^{3}E$^+$)

```
SCF (BP86) Energy = -1680.35096196
Enthalpy 0K = -1679.833884
Enthalpy 298K = -1679.792700
Free Energy 298K = -1679.909989
Lowest Frequency = -873.7643 cm-1
Second Frequency = 18.1391 cm-1
```

SCF (BP86-D3BJ) Energy = =
SCF (MeCN) Energy = =
SCF (Toluene) Energy = -1680.38153973
SCF (BS2) Energy = =

Ru	-0.12571	-0.95127	0.26623
C	1.60818	1.17565	-1.49899
C	1.50708	2.23366	-2.43050
C	0.69277	0.07205	-1.55544
C	0.58961	2.18614	-3.48877
H	2.19875	3.07738	-2.33875
C	-0.19435	0.04524	-2.67313
C	-0.24502	1.06334	-3.63272
H	0.55071	3.00343	-4.21635
H	-0.86277	-0.81471	-2.79231
H	-0.93536	0.99055	-4.47958
H	1.28444	-1.16706	-1.49218
C	2.80065	1.24038	-0.59432
C	4.97744	0.38762	0.05944
H	5.76410	-0.37279	-0.00145
C	3.77243	0.21391	-0.63521
H	3.59793	-0.67874	-1.24219
C	4.14552	2.51897	0.79649
H	4.26149	3.45475	1.35889
C	5.17432	1.56484	0.79772
H	6.10465	1.75189	1.34220
N	2.98772	2.38308	0.11633
C	-2.63922	1.74475	0.15204
C	-1.78313	2.54316	-0.63407
C	-3.27150	2.31856	1.27851
C	-1.56838	3.88844	-0.29888
H	-1.30756	2.11829	-1.52048
C	-3.04527	3.66123	1.61791
C	-2.19998	4.45350	0.82195
H	-0.91461	4.49956	-0.92886
H	-3.54610	4.09277	2.49069
H	-2.04371	5.50899	1.06796
H	-3.94863	1.70812	1.88611
C	-3.05737	0.37970	-0.28554
C	-4.95937	-0.97258	-1.03663
H	-6.02618	-1.07309	-1.25817
C	-4.43701	0.23142	-0.56330
H	-5.07995	1.10428	-0.42470
C	-2.72010	-1.84363	-0.92442
H	-2.00669	-2.66202	-1.03727
C	-4.06729	-2.03380	-1.23171
H	-4.39634	-3.00531	-1.61025
N	-2.19096	-0.67470	-0.45075
O	-0.06948	-2.86875	-0.65539
C	0.90952	-3.16334	-1.43801
C	1.01716	-4.58070	-1.95137
O	1.78170	-2.30505	-1.82199
H	2.06310	-4.91984	-1.89827
H	0.36570	-5.25710	-1.38199
H	0.72389	-4.60196	-3.01488
N	1.60940	-1.43024	1.08384
C	2.56314	-1.77333	1.67399
C	3.76526	-2.18663	2.38570
H	3.55892	-2.30071	3.46304
H	4.13102	-3.15079	1.99437
H	4.55490	-1.42789	2.25293
N	-1.04032	-1.81116	1.85736
C	-1.57027	-2.33455	2.76344
C	-2.23395	-2.99073	3.88405
H	-3.32792	-2.88260	3.79667
H	-1.98788	-4.06565	3.89932
H	-1.91240	-2.54166	4.83850
N	0.01829	0.76794	1.23588
C	0.29805	1.72741	1.84682
C	0.66735	2.96046	2.52623
H	1.17401	2.74274	3.48107
H	1.35787	3.51229	1.86511
H	-0.22823	3.57168	2.71959

$^3E^+$
SCF (BP86) Energy = -1680.35995727
Enthalpy 0K = -1679.838641
Enthalpy 298K = -1679.796672
Free Energy 298K = -1679.916885
Lowest Frequency = 18.9765 cm^{-1}
Second Frequency = 22.0693 cm^{-1}
SCF (BP86-D3BJ) Energy = -1680.54251887
SCF (MeCN) Energy = -1680.41391658
SCF (Toluene) Energy = -1680.39021319
SCF (BS2) Energy = -1680.47016172

Ru	0.16883	-0.84851	-0.34114
C	-1.80478	0.87234	1.53322
C	-2.15274	1.38188	2.81383
C	-0.62106	0.07185	1.36780
C	-1.38220	1.13404	3.95365
H	-3.05267	2.00162	2.89902
C	0.10745	-0.18615	2.57198
C	-0.24428	0.32383	3.82995
H	-1.67437	1.55431	4.92100
H	0.99961	-0.81923	2.51806
H	0.37121	0.08923	4.70556
H	-1.69278	-1.54392	1.57463
C	-2.81971	1.20684	0.47192
C	-5.15915	1.19496	-0.21825
H	-6.20210	0.90155	-0.05635
C	-4.16123	0.79740	0.68082
H	-4.40860	0.18407	1.55291
C	-3.44302	2.33854	-1.44956
H	-3.12417	2.96635	-2.29268
C	-4.79505	1.98877	-1.31696
H	-5.53514	2.33989	-2.04236
N	-2.46913	1.97441	-0.58884
C	2.62561	1.86015	0.22252
C	1.66888	2.49517	1.04159
C	3.32947	2.63381	-0.73102
C	1.41381	3.86752	0.89654
H	1.13966	1.92005	1.80355
C	3.06988	4.00510	-0.87440
C	2.11039	4.62714	-0.05698
H	0.67555	4.34615	1.54738
H	3.62999	4.58958	-1.61202
H	1.91790	5.70055	-0.15388
H	4.08511	2.15291	-1.36213
C	3.06630	0.44828	0.43846
C	4.98919	-0.97414	0.98674
H	6.04964	-1.08533	1.23200
C	4.43900	0.28446	0.74432
H	5.05482	1.18467	0.81258
C	2.79142	-1.86964	0.60386
H	2.10495	-2.71459	0.53596
C	4.13291	-2.08038	0.91903
H	4.48567	-3.09846	1.10481
N	2.23278	-0.64451	0.35845
O	0.02690	-2.78631	0.61771
C	-0.91090	-3.24391	1.32032
C	-0.95736	-4.69079	1.72548
O	-1.91681	-2.50992	1.76871
H	-0.74205	-4.77297	2.80470
H	-1.96905	-5.09603	1.56649
H	-0.21813	-5.27139	1.15925
N	-1.61432	-1.21007	-1.10529
C	-2.62722	-1.48110	-1.63420
C	-3.90316	-1.79399	-2.26477
H	-3.83690	-1.66155	-3.35775
H	-4.19273	-2.83756	-2.05569
H	-4.68543	-1.12147	-1.87424
N	1.03139	-1.87616	-1.98585
C	1.49427	-2.43934	-2.90522

```
C   2.07359 -3.13865 -4.04714
H   1.57051 -2.83305 -4.97953
H   3.14734 -2.90348 -4.13459
H   1.96098 -4.22910 -3.92786
N   0.24732  0.80865 -1.36330
C   0.18508  1.76606 -2.03364
C   0.09106  3.00223 -2.79458
H  -0.29058  2.81143 -3.81153
H  -0.59445  3.69011 -2.27178
H   1.08181  3.47997 -2.86497
```

^{6}F^{2+}

SCF (BP86) Energy = -891.226975638
Enthalpy 0K = -890.949934
Enthalpy 298K = -890.919875
Free Energy 298K = -891.024473
Lowest Frequency = 1.7042 cm^{-1}
Second Frequency = 5.4741 cm^{-1}
SCF (BP86-D3BJ) Energy = -891.288170342
SCF (MeCN) Energy = -891.417842274
SCF (Toluene) Energy = -891.340482156
SCF (BS2) Energy = -891.151556051

N	1.43112	-0.00292	-1.42559
C	2.25978	-0.00335	-2.25087
N	-1.39683	0.40783	-1.40113
C	-2.20755	0.64311	-2.21055
N	0.29175	1.97818	0.28630
C	0.46273	3.12333	0.45115
N	-1.43167	0.00404	1.42509
C	-2.26154	0.00746	2.24915
C	3.29159	-0.00380	-3.27832
H	4.23435	0.39646	-2.86946
H	3.46800	-1.03105	-3.63859
H	2.97914	0.62303	-4.13014
C	0.67660	4.54893	0.65652
H	0.16386	5.12685	-0.13041
H	0.27897	4.85475	1.63861
H	1.75445	4.77967	0.62184
C	-3.29476	0.01199	3.27516
H	-3.84169	0.96947	3.25854
H	-4.00959	-0.80876	3.09749
H	-2.84098	-0.12108	4.27141
C	-3.21755	0.93611	-3.21767
H	-2.73589	1.16648	-4.18259
H	-3.88346	0.06725	-3.35115
H	-3.82319	1.80360	-2.90646
N	1.39503	-0.40884	1.40252
C	2.20162	-0.64655	2.21534
C	3.20557	-0.94264	3.22761
H	2.85993	-1.76553	3.87536
H	4.15210	-1.24187	2.74731
H	3.38943	-0.05216	3.85163
Ru	-0.00004	-0.00002	-0.00003
N	-0.28960	-1.97844	-0.28724
C	-0.45528	-3.12405	-0.45426
C	-0.66100	-4.55036	-0.66311
H	0.24937	-5.10911	-0.38886
H	-1.49854	-4.90817	-0.04131
H	-0.89444	-4.74893	-1.72247

^{3}A^{2+}

SCF (BP86) Energy = -725.084942129
Enthalpy 0K = -724.846559
Enthalpy 298K = -724.825534
Free Energy 298K = -724.899859
Lowest Frequency = 14.8400 cm^{-1}
Second Frequency = 18.9807 cm^{-1}
SCF (BP86-D3BJ) Energy = -725.143825219
SCF (MeCN) Energy = -725.302227226
SCF (Toluene) Energy = -725.214329131
SCF (BS2) Energy = -724.954581954

C	2.17914	1.42683	0.11105
C	2.18034	0.79409	-1.18871
C	2.17990	-0.62011	-1.28848
C	2.17846	-1.42941	-0.09064
C	2.17744	-0.80866	1.18397
C	2.17775	0.63334	1.28591
Ru	0.44921	-0.00017	0.00044
H	2.11973	-1.09756	-2.27047
H	2.11617	1.11182	2.26730
H	2.11839	2.51597	0.18839
H	2.11541	-1.42026	2.08840
H	2.11730	-2.51857	-0.16707
H	2.12080	1.40486	-2.09385
N	-0.81401	-0.11819	1.60734
C	-1.52268	-0.18682	2.53533
C	-2.39329	-0.27234	3.69707
H	-3.44914	-0.21058	3.38406
H	-2.23021	-1.22985	4.22046
H	-2.17679	0.55673	4.39204
N	-0.81165	-1.33358	-0.90730
N	-0.81104	1.45217	-0.70254
C	-1.51729	2.29172	-1.10805
C	-1.51855	-2.10372	-1.43194
C	-2.38666	-3.06820	-2.08862
H	-2.24992	-4.06610	-1.63817
H	-3.44147	-2.76595	-1.97616
H	-2.14278	-3.12416	-3.16324
C	-2.38441	3.34319	-1.61553
H	-3.43506	3.00772	-1.59987
H	-2.28731	4.24650	-0.98942
H	-2.10438	3.59478	-2.65268

^{5}F^{+} (κ^{1})

SCF (BP86) Energy = -987.234219222
Enthalpy 0K = -986.953661
Enthalpy 298K = -986.922819
Free Energy 298K = -987.022968
Lowest Frequency = 9.5290 cm^{-1}
Second Frequency = 17.4976 cm^{-1}
SCF (BP86-D3BJ) Energy = -987.299667163
SCF (MeCN) Energy = -987.297866185
SCF (Toluene) Energy = -987.270113235
SCF (BS2) Energy = -987.198114781

N	1.31371	1.34007	0.99706
C	1.87447	2.11376	1.67233
N	1.27801	-1.49468	0.79309
C	1.81932	-2.36896	1.35144
N	1.54098	0.10091	-1.61949
C	2.26930	0.15757	-2.53712
N	-0.89229	-1.32329	-1.02214
C	-1.63630	-2.06488	-1.53361
C	2.56027	3.07683	2.52412
H	2.48081	4.09012	2.09679
H	2.10620	3.08060	3.52903
H	3.62742	2.81617	2.61832
C	3.17532	0.22757	-3.67764
H	4.17144	0.57429	-3.35565
H	3.28286	-0.76597	-4.14403
H	2.78636	0.93016	-4.43343
C	-2.63974	-2.94733	-2.11093
H	-2.41185	-3.99978	-1.87541
H	-3.62596	-2.69080	-1.68819
H	-2.67724	-2.82999	-3.20633
C	2.48156	-3.45773	2.05810
H	3.57154	-3.29371	2.08417
H	2.10679	-3.51723	3.09351
H	2.28103	-4.41791	1.55459
O	-2.95521	-0.00287	0.51847
C	-2.27262	-0.08782	1.54936
C	-2.91402	-0.23048	2.93303
H	-2.32530	0.28227	3.70860
H	-3.93991	0.16381	2.90735
H	-2.96163	-1.29988	3.20275
O	-0.94630	-0.09934	1.62126
Ru	0.25526	0.00428	-0.05925
N	-0.85904	1.48528	-0.81580
C	-1.58766	2.31091	-1.20620
C	-2.57320	3.29109	-1.63832
H	-3.56379	2.99259	-1.25520
H	-2.32361	4.29040	-1.24573
H	-2.61439	3.34310	-2.73861

^{4}F$^+$ (κ^2)
SCF (BP86) Energy = -854.470356594
Enthalpy 0K = -854.235272
Enthalpy 298K = -854.209710
Free Energy 298K = -854.296524
Lowest Frequency = 15.8938 cm^{-1}
Second Frequency = 16.6417 cm^{-1}
SCF (BP86-D3BJ) Energy = -854.521763404
SCF (MeCN) Energy = -854.531114858
SCF (Toluene) Energy = -854.505329434
SCF (BS2) Energy = -854.393081696

N	-1.99534	0.15915	0.00008
C	-3.16103	0.26959	0.00010
N	-0.01428	-1.30936	-1.42330
C	-0.02229	-2.07131	-2.31474
N	-0.01418	-1.30942	1.42328
C	-0.02208	-2.07144	2.31466
N	1.99445	0.12070	-0.00005
C	3.16261	0.20213	-0.00009
C	-4.61049	0.41528	0.00012
H	-4.93611	0.96855	0.89674
H	-4.93600	0.96988	-0.89572
H	-5.09553	-0.57488	-0.00065
C	-0.03187	-2.99444	3.44283
H	-0.93616	-3.62490	3.41504
H	0.85396	-3.65033	3.40991
H	-0.02122	-2.43453	4.39317
C	4.61532	0.31134	-0.00016
H	5.07512	-0.69081	0.00147
H	4.95510	0.85522	-0.89729
H	4.95496	0.85805	0.89530
C	-0.03228	-2.99421	-3.44299
H	-0.93014	-3.63344	-3.40809
H	-0.03464	-2.43409	-4.39326
H	0.86015	-3.64144	-3.41733
O	0.01233	1.89410	1.09994
C	0.02205	2.57410	0.00005
C	0.07099	4.07406	0.00007
H	-0.41237	4.47121	-0.90441
H	-0.41156	4.47117	0.90498
H	1.12375	4.40614	-0.00043
O	0.01228	1.89413	-1.09986
Ru	-0.00105	0.07865	0.00002

f-**^{3}F** ($\kappa^2\kappa^1$)
SCF (BP86) Energy = -950.375149815
Enthalpy 0K = -950.137086
Enthalpy 298K = -950.110719
Free Energy 298K = -950.197295
Lowest Frequency = 22.9867 cm^{-1}
Second Frequency = 36.3143 cm^{-1}
SCF (BP86-D3BJ) Energy = -950.430470073
SCF (MeCN) Energy = -950.403661510
SCF (Toluene) Energy = -950.388479371
SCF (BS2) Energy = -950.339062014

Ru	-0.31674	0.06719	-0.00001
N	-1.96920	-1.00933	-0.00006
C	-2.97688	-1.61811	-0.00005
N	0.52523	-1.01995	1.38779
C	1.08016	-1.60540	2.24032
N	0.52524	-1.01991	-1.38785
C	1.08020	-1.60534	-2.24036
C	-4.23327	-2.35841	0.00013
H	-4.83187	-2.10927	-0.89326
H	-4.04581	-3.44598	-0.00193
H	-4.82986	-2.11230	0.89570
C	1.87863	-2.26053	3.26768
H	1.64180	-1.85498	4.26626
H	1.69327	-3.34795	3.28102
H	2.94959	-2.08890	3.06232
C	1.87888	-2.26039	-3.26762
H	1.64162	-1.85539	-4.26632
H	2.94977	-2.08806	-3.06252
H	1.69416	-3.34793	-3.28048
O	-1.30450	1.61228	-1.10489
C	-1.60903	2.20258	0.00001
O	-1.30452	1.61224	1.10489
C	-2.26598	3.55926	0.00002
H	-2.87879	3.68890	0.90454
H	-1.48150	4.33558	0.00004
H	-2.87878	3.68893	-0.90450
O	1.24711	1.40652	0.00002
C	2.52328	1.07002	-0.00000
O	2.99980	-0.07672	-0.00007
C	3.42918	2.31193	0.00001
H	3.22190	2.93427	0.88673
H	4.48604	2.00827	-0.00005
H	3.22182	2.93435	-0.88664

m-**^{3}F** ($\kappa^2\kappa^1$)
SCF (BP86) Energy = -950.367950845
Enthalpy 0K = -950.130302
Enthalpy 298K = -950.103601
Free Energy 298K = -950.194307
Lowest Frequency = 3.2056 cm^{-1}
Second Frequency = 21.8810 cm^{-1}
SCF (BP86-D3BJ) Energy = -950.422541032
SCF (MeCN) Energy = -950.399823277
SCF (Toluene) Energy = -950.382742275
SCF (BS2) Energy = -950.331397239

Ru	0.16572	-0.09906	-0.19254
N	2.06604	0.12468	0.28736
C	3.18403	0.24493	0.62418
N	0.24209	1.39304	-1.43367
C	0.28425	2.29706	-2.18662
N	-1.74835	-0.37712	-0.58162
C	-2.88943	-0.57358	-0.76009
C	4.56586	0.39271	1.06314
H	4.82265	1.45994	1.17366
H	4.71138	-0.10142	2.03892
H	5.25975	-0.06085	0.33483
C	0.34436	3.38163	-3.15932
H	1.34407	3.84920	-3.15468
H	0.14357	3.00845	-4.17921
H	-0.39909	4.16244	-2.92258
C	-4.33292	-0.76505	-0.78073
H	-4.58855	-1.80031	-1.06198
H	-4.73195	-0.56030	0.22807
H	-4.81114	-0.08014	-1.50071
O	0.64334	-1.87689	-1.35619
C	0.50431	-2.59770	-0.29728
O	0.20940	-2.00815	0.80808
C	0.64878	-4.10028	-0.35577
H	1.07756	-4.47764	0.58488
H	-0.34727	-4.55940	-0.48042
H	1.27604	-4.39298	-1.21052
O	-0.19895	1.32805	1.28177
C	-1.19313	1.18548	2.13936
O	-2.06252	0.30150	2.14941
C	-1.15867	2.26939	3.23068
H	-0.68169	3.19617	2.87670
H	-2.18231	2.47475	3.57952
H	-0.57771	1.89273	4.09094

c-**^{2}F** ($2\kappa^2$)
SCF (BP86) Energy = -817.609089806
Enthalpy 0K = -817.416617
Enthalpy 298K = -817.395373
Free Energy 298K = -817.469800
Lowest Frequency = 20.7944 cm^{-1}

Second Frequency = 23.8982 cm^{-1}
SCF (BP86-D3BJ) Energy = -817.650885546
SCF (MeCN) Energy = -817.630707906
SCF (Toluene) Energy = -1083.15017290
SCF (BS2) Energy = -817.530437528

Ru	-0.00009	0.08090	-0.00002
N	1.21586	-1.25343	-0.68751
C	1.97403	-2.03597	-1.13762
N	-1.21556	-1.25404	0.68715
C	-1.97335	-2.03699	1.13719
C	2.88545	-2.98878	-1.75984
H	3.61970	-2.46190	-2.39400
H	3.43946	-3.56435	-0.99792
H	2.33125	-3.70111	-2.39601
C	-2.88384	-2.99061	1.75953
H	-3.67365	-2.45998	2.31936
H	-3.36995	-3.62863	1.00102
H	-2.34246	-3.64421	2.46601
O	1.45983	1.62660	-0.27466
C	1.89116	1.42929	0.92403
C	2.95257	2.31261	1.52856
H	3.46686	1.78984	2.34808
H	3.67301	2.62330	0.75684
H	2.47853	3.22215	1.93681
O	1.35418	0.47351	1.60418
O	-1.35434	0.47363	-1.60413
C	-1.89168	1.42904	-0.92373
O	-1.46054	1.62607	0.27508
C	-2.95324	2.31226	-1.52812
H	-3.67360	2.62289	-0.75631
H	-2.47933	3.22184	-1.93645
H	-3.46759	1.78945	-2.34758

t-^{2}**F** ($2\kappa^{2}$)
SCF (BP86) Energy = -817.605958375
Enthalpy 0K = -817.413625
Enthalpy 298K = -817.392185
Free Energy 298K = -817.471124
Lowest Frequency = 2.0102 cm^{-1}
Second Frequency = 5.2030 cm^{-1}
SCF (BP86-D3BJ) Energy = -817.648207278
SCF (MeCN) Energy = -817.630534346
SCF (Toluene) Energy = -1083.14941919
SCF (BS2) Energy = -817.527583962

Ru	0.00696	0.00112	-0.00002
N	1.96342	-0.00102	-0.00015
C	3.14019	-0.00336	-0.00014
N	-1.94935	0.00161	-0.00003
C	-3.12639	0.00069	0.00003
C	4.59753	-0.00874	0.00023
H	4.98533	-0.52282	0.89676
H	4.98571	-0.52692	-0.89376
H	4.98718	1.02368	-0.00207
C	-4.58377	-0.00326	0.00021
H	-4.97284	1.02944	0.00100
H	-4.97264	-0.51822	-0.89539
H	-4.97242	-0.51949	0.89518
O	0.00796	-1.84598	1.09921
C	0.00146	-2.51543	-0.00003
C	-0.04659	-4.02455	-0.00003
H	0.43958	-4.42114	-0.90371
H	0.43895	-4.42113	0.90399
H	-1.09829	-4.36000	-0.00042
O	0.00789	-1.84598	-1.09926
O	0.01058	1.84820	1.09922
C	0.00506	2.51761	-0.00003
O	0.01051	1.84819	-1.09927
C	-0.04083	4.02682	-0.00002
H	0.44501	4.42271	-0.90419
H	-1.09202	4.36383	0.00064
H	0.44609	4.42272	0.90357

c-^{4}**F** ($2\kappa^{1}$)
SCF (BP86) Energy = -1083.13381665
Enthalpy 0K = -1082.850419
Enthalpy 298K = -1082.818734
Free Energy 298K = -1082.918388
Lowest Frequency = 30.7870 cm^{-1}
Second Frequency = 31.9477 cm^{-1}
SCF (BP86-D3BJ) Energy = -1083.20308512
SCF (MeCN) Energy = -1083.16910722
SCF (Toluene) Energy = -1083.15017290
SCF (BS2) Energy = -1083.14000703

N	1.04128	1.68810	-0.05506
C	1.68289	2.65771	0.07375
N	-1.24719	0.74965	-1.48665
C	-2.04304	1.19269	-2.22636
N	-1.04118	-1.68806	-0.05479
C	-1.68289	-2.65759	0.07420
C	2.57315	3.78965	0.29002
H	2.17714	4.44670	1.08231
H	3.56393	3.41596	0.60065
H	2.68998	4.38307	-0.63216
C	-3.13402	1.72845	-3.03036
H	-2.94832	2.78386	-3.29230
H	-3.25708	1.15543	-3.96508
H	-4.07282	1.66801	-2.45268
C	-2.57337	-3.78930	0.29070
H	-2.17843	-4.44529	1.08440
H	-3.56459	-3.41522	0.59949
H	-2.68893	-4.38394	-0.63086
O	3.20437	-0.15768	0.68239
C	2.43395	-0.70178	1.49410
O	1.12532	-0.81254	1.41107
C	2.96950	-1.33204	2.79155
H	2.65804	-0.72003	3.65546
H	2.54819	-2.33955	2.94089
H	4.06788	-1.38291	2.76232
O	-1.12533	0.81286	1.41081
C	-2.43396	0.70205	1.49381
O	-3.20434	0.15773	0.68221
C	-2.96957	1.33235	2.79123
H	-2.54655	2.33894	2.94186
H	-4.06784	1.38514	2.76105
H	-2.66007	0.71900	3.65490
Ru	0.00007	-0.00001	-0.13699
N	1.24733	-0.74992	-1.48648
C	2.04307	-1.19314	-2.22621
C	3.13382	-1.72915	-3.03037
H	3.25693	-1.15606	-3.96504
H	4.07273	-1.66904	-2.45282
H	2.94777	-2.78447	-3.29240

t-^{4}**F** ($2\kappa^{1}$)
SCF (BP86) Energy = -1083.13257282
Enthalpy 0K = -1082.849270
Enthalpy 298K = -1082.817441
Free Energy 298K = -1082.918392
Lowest Frequency = 22.4094 cm^{-1}
Second Frequency = 24.9524 cm^{-1}
SCF (BP86-D3BJ) Energy = -1083.20127459
SCF (MeCN) Energy = -1083.16801488
SCF (Toluene) Energy = -1083.14941919
SCF (BS2) Energy = -1083.13832420

N	1.05172	1.46052	-0.82666
C	1.69937	2.30059	-1.32220
N	1.09143	-1.32425	-0.98924
C	1.75910	-2.08318	-1.58003
N	-1.05167	-1.46079	0.82657
C	-1.69956	-2.30079	1.32190

```
C   2.59992  3.30051 -1.87959
H   2.56741  3.28464 -2.98203
H   2.31910  4.31099 -1.53825
H   3.63269  3.09101 -1.55149
C   2.68131 -2.98753 -2.25322
H   2.64005 -2.84520 -3.34626
H   3.71088 -2.79030 -1.90794
H   2.42915 -4.03780 -2.03003
C  -2.60049 -3.30058  1.87890
H  -2.57048 -3.28283  2.98138
H  -3.63270 -3.09249  1.54815
H  -2.31804 -4.31139  1.53990
O   3.24671  0.00979  0.55628
C   2.56563 -0.06423  1.59477
O   1.25468 -0.07788  1.69446
C   3.24435 -0.18803  2.97171
H   2.72347  0.41937  3.72898
H   3.20350 -1.23876  3.30894
H   4.29922  0.11611  2.90016
O  -1.25442  0.07747 -1.69449
C  -2.56536  0.06424 -1.59479
O  -3.24648 -0.00981 -0.55632
C  -3.24467  0.19022 -2.97121
H  -2.71171 -0.39754 -3.73541
H  -4.29370 -0.13465 -2.90413
H  -3.22507  1.24581 -3.29505
Ru  0.00009 -0.00014  0.00000
N  -1.09125  1.32392  0.98928
C  -1.75893  2.08276  1.58017
C  -2.68125  2.98696  2.25342
H  -2.64147  2.84308  3.34631
H  -2.42796  4.03733  2.03201
H  -3.71055  2.79101  1.90661
```

^{1}A

SCF (BP86) Energy = -917.075823895
Enthalpy 0K = -916.830211
Enthalpy 298K = -916.808205
Free Energy 298K = -916.883155
Lowest Frequency = 8.0025 cm^{-1}
Second Frequency = 42.9121 cm^{-1}
SCF (BP86-D3BJ) Energy = -917.142477672
SCF (MeCN) Energy = -917.091989194
SCF (Toluene) Energy = -917.083363353
SCF (BS2) Energy = -917.013804146

```
Ru  0.25672  0.02914 -0.09363
O   1.40150  0.84278  1.53467
C   1.85571  1.76416  0.75653
C   2.73288  2.87000  1.28088
C  -1.02505 -1.83843  0.15046
C  -0.59810 -1.34082  1.43752
C  -1.57065 -0.69617  2.28559
C  -2.87753 -0.53777  1.86833
O   1.49793  1.72569 -0.48223
H   2.10027  3.72426  1.57869
H   3.29198  2.52909  2.16470
H   3.42336  3.21313  0.49593
C  -3.30747 -1.05730  0.60518
C  -2.41273 -1.70885 -0.22035
H  -2.74949 -2.15628 -1.16126
H  -3.60327 -0.03885  2.51954
H  -0.43094 -2.59871 -0.36734
H  -1.25685 -0.34525  3.27404
C  -1.54777  1.12182 -1.42143
O  -1.36766  1.41656 -0.18261
O  -0.81060  0.18084 -1.91843
C  -2.53269  1.87078 -2.27903
H  -2.83352  1.26043 -3.14286
H  -3.41277  2.15384 -1.68239
H  -2.06018  2.79636 -2.65149
H   0.31420 -1.73008  1.90354
H  -4.35960 -0.96469  0.31441
N   1.71181 -1.18393 -0.45689
C   2.61542 -1.90135 -0.70401
C   3.73741 -2.75110 -1.08696
H   4.32325 -2.27701 -1.89410
H   4.40964 -2.92799 -0.22959
H   3.37953 -3.72966 -1.45106
```

^{1}A$^+$

SCF (BP86) Energy = -688.369203652
Enthalpy 0K = -688.172671
Enthalpy 298K = -688.156154
Free Energy 298K = -688.218994
Lowest Frequency = 14.5816 cm^{-1}
Second Frequency = 20.6417 cm^{-1}
SCF (BP86-D3BJ) Energy = -688.418244771
SCF (MeCN) Energy = -688.434832348
SCF (Toluene) Energy = -688.407692434
SCF (BS2) Energy = -688.236303071

```
C   1.97900 -0.42422  1.43435
C   2.28864  0.78205  0.70186
C   2.28603  0.77224 -0.71909
C   1.97489 -0.44377 -1.43457
C   1.70483 -1.63847 -0.71220
C   1.70728 -1.62908  0.72964
Ru  0.35148 -0.01553  0.00002
O  -0.82251  1.38037 -1.09232
C  -1.28684  1.89340 -0.00003
C  -2.30737  2.98729 -0.00009
H   2.42145  1.70631 -1.27086
H   1.40689 -2.52383  1.28095
O  -0.82236  1.38061  1.09229
H  -3.31923  2.54584 -0.00018
H  -2.20274  3.60433  0.90434
H  -2.20259  3.60439 -0.90447
H   1.89384 -0.39504  2.52381
H   1.40205 -2.54042 -1.25037
H   1.88724 -0.42964 -2.52409
H   2.42658  1.72336  1.24048
N  -1.32682 -1.16329  0.00024
C  -2.31924 -1.78292 -0.00000
C  -3.54858 -2.56142 -0.00010
H  -4.12787 -2.34935  0.91401
H  -4.15939 -2.29936 -0.88008
H  -3.31641 -3.63875 -0.03428
```

^{1}B$^+$ (*t*-O,*t*-N)
SCF (BP86) Energy = -1167.72294599
Enthalpy 0K = -1167.360368
Enthalpy 298K = -1167.333315
Free Energy 298K = -1167.417720
Lowest Frequency = 34.6334 cm^{-1}
Second Frequency = 35.6536 cm^{-1}
SCF (BP86-D3BJ) Energy = -1167.84105962
SCF (MeCN) Energy = -1167.77977010
SCF (Toluene) Energy = -1167.75581339
SCF (BS2) Energy = -1167.69840730

Ru	0.38913	-0.31209	-0.30093
O	1.45495	-2.11947	-0.83740
C	1.36237	-1.80915	-2.08272
C	1.90602	-2.68086	-3.17491
C	0.57286	-1.09144	1.90360
C	1.91867	-1.31025	2.34945
C	2.65967	-0.26444	2.87591
C	2.09679	1.04283	2.98262
O	0.73616	-0.70251	-2.35687
H	2.29835	-2.06260	-3.99633
H	2.68930	-3.34313	-2.77973
H	1.09266	-3.30486	-3.58475
C	-2.65477	-0.05081	0.01040
C	-3.88509	-0.22327	0.67752
C	-1.82616	-1.18916	-0.19278
C	-4.28335	-1.49696	1.11131
H	-4.52087	0.64173	0.89036
C	-2.23418	-2.46731	0.23514
C	-3.46237	-2.61902	0.89569
H	-5.23992	-1.61349	1.62949
H	-1.59876	-3.33524	0.03297
H	-3.78486	-3.60834	1.23320
H	-1.08087	-1.17411	-1.05356
C	0.79712	1.28068	2.56419
C	0.00632	0.21875	2.01257
H	-1.07868	0.34826	1.97625
H	2.68128	1.84729	3.44124
H	-0.07791	-1.96116	1.77586
H	3.67252	-0.44726	3.25006
C	-2.15228	1.26535	-0.42012
C	-2.44395	3.57781	-1.11805
H	-3.09232	4.42725	-1.35000
C	-2.99076	2.35859	-0.70797
H	-4.07363	2.23198	-0.63087
C	-0.25932	2.56721	-0.94958
H	0.82773	2.59751	-1.03850
C	-1.04927	3.68051	-1.24065
H	-0.57022	4.60768	-1.56537
N	-0.78234	1.37838	-0.54499
H	2.33449	-2.32107	2.30597
H	0.34216	2.26658	2.70488
N	2.11269	0.59634	-0.26213
C	3.18150	1.07786	-0.31319
C	4.51198	1.66943	-0.36306
H	5.25496	0.96768	0.05182
H	4.78966	1.89986	-1.40528
H	4.54109	2.60195	0.22486

TS(**^{1}B$^+$**-**^{1}C$^+$**) (*t*-O,*t*-N)
SCF (BP86) Energy = -1167.68769362
Enthalpy 0K = -1167.330650
Enthalpy 298K = -1167.303913
Free Energy 298K = -1167.387313
Lowest Frequency = -844.5664 cm^{-1}
Second Frequency = 27.1368 cm^{-1}
SCF (BP86-D3BJ) Energy = -1167.80750834
SCF (MeCN) Energy = -1167.74353548
SCF (Toluene) Energy = -1167.72013087
SCF (BS2) Energy = -1167.66167829

Ru	0.31812	-0.29543	-0.12650
O	1.04593	-2.33784	-0.43548
C	0.51405	-2.52671	-1.56260
C	0.81133	-3.69059	-2.45143
C	0.77970	-0.68856	2.05279
C	2.15210	-1.03259	2.31999
C	3.10398	-0.04206	2.47397
C	2.74623	1.34215	2.37178
O	-0.36413	-1.61012	-2.00134
H	1.20807	-3.32826	-3.41495
H	1.53825	-4.36136	-1.97482
H	-0.12225	-4.23416	-2.67376
C	-2.59477	0.22607	0.13738
C	-3.94287	0.07560	0.51834
C	-1.66543	-0.85831	0.27878
C	-4.39225	-1.14744	1.03747
H	-4.64686	0.90966	0.43039
C	-2.15405	-2.07872	0.80878
C	-3.50079	-2.22460	1.18281
H	-5.43958	-1.25848	1.33369
H	-1.47224	-2.93046	0.92181
H	-3.85533	-3.17678	1.59044
H	-1.01714	-1.28358	-1.04366
C	1.44097	1.70782	2.11095
C	0.42172	0.70050	1.92615
H	-0.62154	0.99727	2.07635
H	3.50764	2.10879	2.54903
H	0.00561	-1.42866	2.27760
H	4.13664	-0.31154	2.71946
C	-2.02923	1.47519	-0.38568
C	-2.11325	3.75196	-1.24422
H	-2.68670	4.63591	-1.53749
C	-2.76627	2.61491	-0.76068
H	-3.85585	2.59610	-0.68017
C	-0.02066	2.58609	-0.96966
H	1.06701	2.51988	-1.02591
C	-0.71268	3.73767	-1.34873
H	-0.15643	4.60315	-1.71733
N	-0.65198	1.47329	-0.50926
H	2.41921	-2.08548	2.45019
H	1.15090	2.76353	2.10364
N	2.20486	0.32121	-0.69854
C	3.27083	0.57916	-1.11856
C	4.59768	0.88891	-1.63651
H	5.29828	0.07092	-1.39881
H	4.56338	1.01591	-2.73160
H	4.97901	1.82012	-1.18551

^{1}C$^+$ (*t*-O,*t*-N)
SCF (BP86) Energy = -1167.69618736
Enthalpy 0K = -1167.334234
Enthalpy 298K = -1167.306763
Free Energy 298K = -1167.393179
Lowest Frequency = 18.7163 cm^{-1}
Second Frequency = 31.3377 cm^{-1}
SCF (BP86-D3BJ) Energy = -1167.81435769
SCF (MeCN) Energy = -1167.75863580
SCF (Toluene) Energy = -1167.73069997
SCF (BS2) Energy = -1167.67099141

Ru	-0.29762	0.16134	-0.11291
O	-1.24784	2.09525	-0.39326
C	-0.79392	2.95122	-1.19348
C	-1.59116	4.14556	-1.62642
C	-0.87114	0.59922	1.98870
C	-2.29044	0.78118	2.19636
C	-3.11961	-0.30897	2.35088
C	-2.59044	-1.64648	2.31913
O	0.42406	2.87325	-1.73128
H	-1.62866	4.18868	-2.72738
H	-2.60564	4.09741	-1.21196
H	-1.08832	5.06669	-1.28669

C 2.61028 -0.10600 0.01986
C 3.97139 0.21777 0.19398
C 1.56748 0.84043 0.31435
C 4.33542 1.47664 0.69223
H 4.75534 -0.50920 -0.04429
C 1.97897 2.09013 0.84719
C 3.33855 2.40860 1.02611
H 5.39163 1.72464 0.83135
H 1.22726 2.83940 1.12758
H 3.61886 3.38616 1.43255
H 0.93988 2.17091 -1.23426
C -1.24457 -1.86348 2.12259
C -0.34161 -0.74521 1.93601
H 0.71847 -0.90626 2.16023
H -3.26266 -2.49131 2.50214
H -0.20230 1.42696 2.24654
H -4.18664 -0.16194 2.54758
C 2.14171 -1.42083 -0.42801
C 2.36741 -3.71981 -1.19857
H 2.99751 -4.56074 -1.50270
C 2.94895 -2.50568 -0.82133
H 4.03521 -2.38792 -0.83191
C 0.20295 -2.74374 -0.79129
H -0.88735 -2.77630 -0.75248
C 0.96795 -3.84508 -1.17872
H 0.47128 -4.77796 -1.45643
N 0.76402 -1.55534 -0.44003
H -2.68677 1.79744 2.27766
H -0.83033 -2.87530 2.17646
N -2.13481 -0.57196 -0.86282
C -3.12757 -0.87750 -1.41302
C -4.36475 -1.25330 -2.08654
H -5.10152 -0.43586 -2.01485
H -4.17387 -1.46305 -3.15245
H -4.79554 -2.15618 -1.62237

^{1}B$^+$ (*t*-O,*t*-C_6H_6)
SCF (BP86) Energy = -1167.71349134
Enthalpy 0K = -1167.351221
Enthalpy 298K = -1167.324016
Free Energy 298K = -1167.409183
Lowest Frequency = 30.6796 cm^{-1}
Second Frequency = 32.7008 cm^{-1}
SCF (BP86-D3BJ) Energy = -1167.83151821
SCF (MeCN) Energy = -1167.77124339
SCF (Toluene) Energy = -1167.74671985
SCF (BS2) Energy = -1167.68864116

Ru -0.42558 0.00216 -0.14150
O -1.81753 1.59465 -0.43850
C -1.99935 1.25643 -1.66745
C -2.92923 2.00624 -2.57578
C -1.80941 -1.36197 1.21976
C -2.59698 -0.59318 2.14148
C -3.81921 -0.06535 1.75718
C -4.32580 -0.31003 0.45057
O -1.34169 0.21630 -2.08206
H -3.93067 1.54430 -2.53143
H -3.02017 3.05306 -2.25150
H -2.57618 1.95092 -3.61613
C 2.53779 0.42494 -0.49721
C 3.74641 1.03883 -0.11588
C 1.41688 1.25221 -0.79479
C 3.83190 2.43855 -0.03955
H 4.61399 0.42983 0.15669
C 1.50513 2.65748 -0.70612
C 2.71590 3.24969 -0.32429
H 4.77786 2.90223 0.25733
H 0.63165 3.26979 -0.94689
H 2.79840 4.33842 -0.25547
H 0.63689 0.83250 -1.49951
C -3.58994 -1.05468 -0.46201
C -2.31437 -1.57698 -0.09775
H -1.85247 -2.29940 -0.77546
H -5.31453 0.07201 0.17677
H -1.01086 -1.99484 1.62016
H -4.41572 0.51287 2.46925
C 2.34412 -1.03446 -0.52568
C 3.15866 -3.31779 -0.74136
H 3.97523 -4.02683 -0.90286
C 3.40195 -1.94187 -0.72243
H 4.41070 -1.55306 -0.88371
C 0.82669 -2.82043 -0.37154
H -0.20413 -3.14570 -0.22286
C 1.84057 -3.76212 -0.55780
H 1.58787 -4.82553 -0.56171
N 1.04355 -1.47681 -0.35892
H -2.23557 -0.45644 3.16497
H -3.98971 -1.27502 -1.45598
N 0.29866 0.38892 1.65593
C 0.73692 0.70217 2.69920
C 1.24921 1.13652 3.99330
H 0.65236 1.98239 4.37490
H 1.20345 0.31327 4.72560
H 2.29825 1.46246 3.89805

TS(**^{1}B$^+$**–**^{1}C$^+$**) (*t*-O,*t*-C_6H_6)
SCF (BP86) Energy = -1167.68971637
Enthalpy 0K = -1167.332733
Enthalpy 298K = -1167.305764
Free Energy 298K = -1167.390367
Lowest Frequency = -1005.5325 cm^{-1}
Second Frequency = 19.5884 cm^{-1}
SCF (BP86-D3BJ) Energy = -1167.80768527
SCF (MeCN) Energy = -1167.74528082
SCF (Toluene) Energy = -1167.72200053
SCF (BS2) Energy = -1167.66414526

Ru -0.33741 -0.01695 0.08001
O -1.75618 1.59931 0.23340
C -1.68187 1.99128 -0.96596
C -2.56165 3.04250 -1.56136
C -2.15204 -1.73246 0.48706
C -3.20855 -1.18456 1.26590
C -4.24398 -0.47927 0.65353
C -4.25540 -0.31336 -0.75141
O -0.75149 1.41993 -1.74231
H -3.11232 2.62229 -2.41915
H -3.26812 3.42093 -0.81081
H -1.94114 3.86676 -1.95173
C 2.50679 0.63107 -0.40565
C 3.72694 1.33356 -0.37304
C 1.29510 1.27042 0.01787
C 3.76589 2.65462 0.09789
H 4.65851 0.85245 -0.68792
C 1.37034 2.59263 0.52514
C 2.59353 3.28090 0.55742
H 4.71852 3.19230 0.12047
H 0.45898 3.08693 0.87855
H 2.63448 4.30494 0.94210
H 0.28268 1.37428 -1.02515
C -3.22095 -0.83264 -1.53202
C -2.15110 -1.53914 -0.92089
H -1.44591 -2.07267 -1.56473
H -5.09330 0.20517 -1.22876
H -1.46411 -2.44106 0.95838
H -5.06262 -0.07542 1.25678
C 2.38665 -0.78641 -0.76278
C 3.23848 -2.94362 -1.50521
H 4.04665 -3.55842 -1.91117
C 3.42898 -1.57771 -1.28216
H 4.39107 -1.11147 -1.50799
C 0.98495 -2.67934 -0.69120
H 0.00779 -3.09060 -0.43186

```
C   1.99411 -3.50834 -1.18498
H   1.79584 -4.57508 -1.31595
N   1.14366 -1.34096 -0.50774
H  -3.22190 -1.35135  2.34735
H  -3.24234 -0.73135 -2.62147
N   0.06489 -0.40417  1.92555
C   0.34748 -0.57951  3.05265
C   0.67351 -0.75803  4.46224
H  -0.01215 -0.16450  5.09059
H   0.58784 -1.81877  4.75189
H   1.70593 -0.42325  4.65872
```

^{1}C$^+$ (*t*-O,*t*-C_6H_6)
SCF (BP86) Energy = -1167.72465820
Enthalpy 0K = -1167.362087
Enthalpy 298K = -1167.334562
Free Energy 298K = -1167.421173
Lowest Frequency = 22.4661 cm^{-1}
Second Frequency = 30.7549 cm^{-1}
SCF (BP86-D3BJ) Energy = -1167.84257878
SCF (MeCN) Energy = -1167.78315921
SCF (Toluene) Energy = -1167.75798196
SCF (BS2) Energy = -1167.69989919

```
Ru -0.29339 -0.36696  0.25964
O  -2.32477  0.25795  0.54126
C  -2.75394  1.39532  0.84699
C  -4.17619  1.63264  1.26110
C  -1.76770 -2.99872 -0.07342
C  -3.08510 -2.67700 -0.39506
C  -3.36820 -1.75819 -1.43878
C  -2.32807 -1.14670 -2.13361
O  -1.99710  2.49414  0.81829
H  -4.71554  0.67965  1.32239
H  -4.20311  2.14849  2.23490
H  -4.66842  2.29743  0.53136
C   1.93932  0.94379 -1.08911
C   2.62960  1.87367 -1.89804
C   0.51640  1.00419 -0.95947
C   1.92419  2.85728 -2.59988
H   3.72001  1.82313 -1.99016
C  -0.17812  1.97563 -1.71417
C   0.52144  2.89717 -2.51729
H   2.46069  3.57735 -3.22416
H  -1.27305  2.00929 -1.70881
H  -0.03924  3.64512 -3.08812
H  -1.10080  2.23942  0.47372
C  -0.96954 -1.43004 -1.80372
C  -0.68294 -2.38886 -0.78130
H   0.30743 -2.85175 -0.73610
H  -2.54389 -0.46732 -2.96456
H  -1.55740 -3.76609  0.67882
H  -4.40748 -1.55232 -1.71275
C   2.57252 -0.16557 -0.38161
C   4.40916 -1.56221  0.39085
H   5.47891 -1.78577  0.43775
C   3.95156 -0.45111 -0.32154
H   4.65781  0.20628 -0.83493
C   2.12173 -2.06061  0.96068
H   1.35478 -2.65921  1.46177
C   3.47682 -2.38376  1.04936
H   3.78776 -3.26038  1.62282
N   1.66882 -0.98806  0.25964
H  -3.90898 -3.16573  0.13485
H  -0.17891 -1.10327 -2.48472
N   0.21090  0.67331  1.85058
C   0.56782  1.22562  2.82723
C   0.98865  1.89907  4.04835
H   0.43202  2.84268  4.17833
H   0.80103  1.25603  4.92521
H   2.06621  2.13013  4.00510
```

^{1}B$^+$ (*t*-O,*t*-O)
SCF (BP86) Energy = -1167.71744568
Enthalpy 0K = -1167.355100
Enthalpy 298K = -1167.327720
Free Energy 298K = -1167.414767
Lowest Frequency = 20.6209 cm^{-1}
Second Frequency = 21.5538 cm^{-1}
SCF (BP86-D3BJ) Energy = -1167.83491764
SCF (MeCN) Energy = -1167.77357241
SCF (Toluene) Energy = -1167.75010664
SCF (BS2) Energy = -1167.69351956

```
Ru  0.45795  0.24801 -0.20921
O   2.13773  1.19257  0.59431
C   2.92405  0.66020 -0.29732
C   4.38622  0.99133 -0.33977
C   0.93100 -1.20804  1.81094
C   0.45576 -2.05251  0.77173
C   1.36617 -2.91217  0.08974
C   2.70806 -2.93441  0.45090
O   2.36631 -0.14016 -1.13071
H   4.62349  1.50009 -1.28898
H   4.66428  1.63777  0.50403
H   4.97488  0.06060 -0.31111
C  -2.54023 -0.65286 -0.27279
C  -3.61451 -1.56766 -0.21951
C  -1.51045 -0.88606 -1.22227
C  -3.66792 -2.66068 -1.09732
H  -4.39769 -1.44960  0.53548
C  -1.56145 -1.98315 -2.09891
C  -2.64530 -2.87299 -2.03833
H  -4.50869 -3.35821 -1.03689
H  -0.76239 -2.12422 -2.83293
H  -2.69427 -3.72586 -2.72182
H  -0.78647 -0.07303 -1.54947
C   3.17628 -2.11087  1.50874
C   2.30570 -1.25742  2.17999
H   2.66286 -0.64194  3.01051
H   3.40271 -3.60860 -0.05951
H   0.22452 -0.68556  2.46221
H   0.99081 -3.57801 -0.69308
C  -2.41060  0.45892  0.68888
C  -3.29010  2.04389  2.31392
H  -4.13335  2.47617  2.85991
C  -3.49799  1.01248  1.39315
H  -4.50661  0.63963  1.19833
C  -0.93988  1.94877  1.78390
H   0.09702  2.28126  1.88943
C  -1.98323  2.51738  2.51649
H  -1.76814  3.32099  3.22533
N  -1.13705  0.94132  0.89032
H  -0.61567 -2.22562  0.65949
H   4.22621 -2.16957  1.81414
N   0.33062  1.84359 -1.34453
C   0.30260  2.80589 -2.01651
C   0.26995  3.99166 -2.86210
H   0.80940  4.82149 -2.37547
H   0.74747  3.78065 -3.83382
H  -0.77212  4.30526 -3.04087
```

^{1}B$^+$ (*t*-C_6H_6,*t*-O)
SCF (BP86) Energy = -1167.72161570
Enthalpy 0K = -1167.358734
Enthalpy 298K = -1167.331363
Free Energy 298K = -1167.417585
Lowest Frequency = 21.7265 cm^{-1}
Second Frequency = 28.6031 cm^{-1}
SCF (BP86-D3BJ) Energy = =
SCF (MeCN) Energy = =
SCF (Toluene) Energy = -1167.75425489
SCF (BS2) Energy = =

```
Ru -0.29300 -0.16535  0.18402
O  -1.25858 -1.93542  0.70640
C  -1.74137 -2.07331 -0.49625
C  -2.60966 -3.23664 -0.86379
C  -2.24315  0.75084  1.34752
C  -1.85309  1.67946  0.33731
C  -2.68877  1.83881 -0.81220
C  -3.84576  1.08642 -0.95635
O  -1.41837 -1.14641 -1.32772
H  -2.28971 -3.65484 -1.83119
H  -2.57583 -4.00864 -0.08199
H  -3.65024 -2.88976 -0.97928
C   1.91916  0.93876 -0.90024
C   2.63660  2.02392 -0.33578
C   0.77955  1.19457 -1.72525
C   2.22459  3.33637 -0.57273
H   3.51452  1.82073  0.28563
C   0.40551  2.53941 -1.97885
C   1.10394  3.59699 -1.39476
H   2.78383  4.16926 -0.13513
H  -0.41444  2.73917 -2.67437
H   0.80971  4.63048 -1.60152
H   0.35385  0.39516 -2.33925
C  -4.23155  0.16361  0.05439
C  -3.45257  0.00558  1.19290
H  -3.77120 -0.66447  1.99672
H  -4.48475  1.22744 -1.83358
H  -1.77430  0.77893  2.33409
H  -2.43031  2.59105 -1.56257
C   2.37028 -0.46570 -0.72335
C   3.90679 -2.32756 -0.75786
H   4.90115 -2.74220 -0.94654
C   3.65813 -0.96062 -0.96125
H   4.43858 -0.28348 -1.31898
C   1.59973 -2.59755 -0.07629
H   0.75869 -3.17962  0.30682
C   2.86199 -3.15354 -0.31516
H   3.01647 -4.22206 -0.14462
N   1.36655 -1.27751 -0.27851
H  -1.09184  2.43760  0.54993
H  -5.17037 -0.39041 -0.04992
N   0.60836  0.39632  1.84408
C   1.11823  0.67485  2.86677
C   1.72951  1.00003  4.15007
H   1.41725  0.27214  4.91821
H   2.82932  0.97569  4.07177
H   1.42445  2.00821  4.47736
```

TS(^{1}**B**$^+$–^{1}**C**$^+$)1 (t-C_6H_6,t-O)
SCF (BP86) Energy = -1167.69108449
Enthalpy 0K = -1167.329320
Enthalpy 298K = -1167.302354
Free Energy 298K = -1167.388168
Lowest Frequency = -91.3696 cm^{-1}
Second Frequency = 23.8225 cm^{-1}
SCF (BP86-D3BJ) Energy = -1167.80766931
SCF (MeCN) Energy = -1167.75184805
SCF (Toluene) Energy = -1167.72541215
SCF (BS2) Energy = -1167.66737436

```
C   2.90523 -0.37778 -0.31224
N   1.76673  0.34486 -0.15008
C   1.82303  1.71390 -0.11501
C   3.05632  2.38019 -0.20973
C   4.23434  1.63812 -0.36035
C   4.15476  0.23753 -0.42332
Ru -0.06980 -0.49386  0.21027
C  -2.94686 -1.57842 -0.80545
C  -2.05871 -1.84101  0.27882
C  -2.13432 -1.02156  1.44581
C  -3.12437  0.00083  1.53146
C  -4.01016  0.20437  0.47644
C  -3.90879 -0.57401 -0.70424
H  -1.62841 -1.33005  2.36521
C   0.51161  2.38319 -0.01441
C   0.34669  3.62192  0.63927
C  -0.90617  4.25064  0.64933
C  -2.00653  3.65714  0.00246
C  -1.85877  2.41985 -0.63879
C  -0.61582  1.75561 -0.62816
H  -4.61172 -0.40897 -1.52686
O   0.52089 -2.00295 -1.00574
C   0.26250 -1.72120 -2.28101
O  -0.28679 -0.66337 -2.63775
C   0.68992 -2.80622 -3.25001
H   1.36817 -2.36907 -4.00054
H   1.18534 -3.64589 -2.74238
H  -0.19744 -3.17561 -3.78963
H   1.19727  4.08900  1.14582
H  -1.02359  5.21354  1.15574
H  -2.69891  1.96586 -1.16945
H  -2.97347  4.16926 -0.00962
H   3.07572  3.47291 -0.19362
H  -0.47044  0.91630 -1.36428
H  -2.90715 -2.21006 -1.69735
H  -4.79772  0.96002  0.56151
H  -1.49988 -2.78073  0.29113
H  -3.21487  0.58450  2.45269
H   5.04688 -0.37862 -0.56106
H   5.19947  2.14579 -0.44433
H   2.77061 -1.46068 -0.35863
N   0.68400 -1.54381  1.63134
C   1.18408 -2.18179  2.48399
C   1.79465 -2.96120  3.55364
H   2.75407 -3.38758  3.21520
H   1.98300 -2.32682  4.43653
H   1.13047 -3.79069  3.84993
```

INT(^{1}**B**$^+$–^{1}**C**$^+$) (t-C_6H_6,t-O)
SCF (BP86) Energy = -1167.68848672
Enthalpy 0K = -1167.328946
Enthalpy 298K = -1167.301412
Free Energy 298K = -1167.388459
Lowest Frequency = 19.9654 cm^{-1}
Second Frequency = 25.7067 cm^{-1}
SCF (BP86-D3BJ) Energy = -1167.80874890
SCF (MeCN) Energy = -1167.75404375
SCF (Toluene) Energy = -1167.72465319
SCF (BS2) Energy = -1167.66542208

```
C   1.64481 -1.41816 -1.65674
N   0.54143 -1.01832 -0.96576
C  -0.65636 -1.68931 -1.13446
C  -0.73398 -2.74840 -2.06009
C   0.38960 -3.13851 -2.79150
C   1.60404 -2.46535 -2.57654
Ru  0.62056  0.47928  0.36017
C  -1.44778  3.05905  0.62629
C  -0.27300  2.65924 -0.07087
C  -0.38934  1.99229 -1.33315
C  -1.68616  1.72552 -1.85347
C  -2.82553  2.11501 -1.15084
C  -2.70575  2.78469  0.09123
H   0.47193  1.90842 -2.00149
C  -1.74805 -1.23684 -0.27418
C  -3.09585 -1.60003 -0.46114
C  -4.07472 -1.14369  0.43246
C  -3.71814 -0.31973  1.51580
C  -2.38130  0.06162  1.70088
C  -1.37797 -0.37285  0.80451
H  -3.60692  3.11220  0.61866
O   1.95670 -0.56797  1.49294
C   1.53492 -1.46850  2.37274
O   0.33522 -1.75762  2.54700
```

```
C   2.65073 -2.14371  3.14684
H   2.96674 -3.04803  2.59871
H   3.52293 -1.48263  3.25027
H   2.27926 -2.45385  4.13350
H  -3.39098 -2.22988 -1.30639
H  -5.11826 -1.44036  0.29034
H  -2.10083  0.66214  2.57156
H  -4.48274  0.01163  2.22543
H  -1.68342 -3.27617 -2.17788
H  -0.38782 -0.70864  1.42569
H  -1.35354  3.61555  1.56408
H  -3.81768  1.92930 -1.57263
H   0.68093  3.11684  0.22182
H  -1.78266  1.26042 -2.83966
H   2.51858 -2.74794 -3.10377
H   0.32678 -3.96516 -3.50456
H   2.56235 -0.87029 -1.44192
N   2.32454  1.33325 -0.30042
C   3.33654  1.85308 -0.59116
C   4.60204  2.48752 -0.93489
H   4.71985  2.54746 -2.02974
H   4.64103  3.50841 -0.51912
H   5.44015  1.90498 -0.51702
```

TS(**^{1}B$^+$**–**^{1}C$^+$**)2 (*t*-C_6H_6,*t*-O)
SCF (BP86) Energy = -1167.68832136
Enthalpy 0K = -1167.330581
Enthalpy 298K = -1167.303609
Free Energy 298K = -1167.389004
Lowest Frequency = -240.3499 cm^{-1}
Second Frequency = 20.8773 cm^{-1}
SCF (BP86-D3BJ) Energy = -1167.80894582
SCF (MeCN) Energy = -1167.75245138
SCF (Toluene) Energy = -1167.72386138
SCF (BS2) Energy = -1167.66463484

```
C   1.60758 -1.40774 -1.69698
N   0.51795 -1.00290 -0.98796
C  -0.69791 -1.63832 -1.16986
C  -0.80541 -2.66767 -2.12596
C   0.30535 -3.06393 -2.87335
C   1.53732 -2.42714 -2.64589
Ru  0.63102  0.46048  0.37334
C  -1.38173  3.07778  0.63456
C  -0.19831  2.66307 -0.03868
C  -0.29662  2.01174 -1.31083
C  -1.58625  1.77556 -1.86465
C  -2.73426  2.17628 -1.18360
C  -2.63156  2.83048  0.06852
H   0.57765  1.92421 -1.96157
C  -1.76906 -1.17730 -0.28994
C  -3.12435 -1.52150 -0.45610
C  -4.08069 -1.05547  0.45651
C  -3.69111 -0.24230  1.53680
C  -2.34556  0.11826  1.69922
C  -1.35560 -0.32764  0.78890
H  -3.53890  3.16752  0.57901
O   1.91724 -0.67477  1.49574
C   1.43256 -1.56741  2.33135
O   0.20249 -1.78877  2.46125
C   2.45755 -2.33632  3.13574
H   2.51438 -3.36644  2.74493
H   3.45040 -1.87142  3.07183
H   2.12792 -2.39958  4.18370
H  -3.44355 -2.14369 -1.29854
H  -5.13110 -1.33538  0.33199
H  -2.04647  0.71427  2.56754
H  -4.43824  0.09966  2.26013
H  -1.76878 -3.16643 -2.25683
H  -0.39931 -0.80656  1.46984
H  -1.29966  3.62266  1.58031
H  -3.71961  2.01244 -1.62975
H   0.75755  3.09753  0.28185
H  -1.66800  1.32437 -2.85861
H   2.44175 -2.71590 -3.18700
H   0.21895 -3.86713 -3.61041
H   2.53829 -0.88570 -1.47338
N   2.38774  1.28639 -0.23452
C   3.41964  1.78564 -0.49065
C   4.70895  2.39380 -0.79151
H   4.83979  2.50438 -1.88091
H   4.77758  3.39083 -0.32480
H   5.52350  1.76375 -0.39666
```

^{1}C$^+$ (*t*-C_6H_6,*t*-O)
SCF (BP86) Energy = -1167.70548939
Enthalpy 0K = -1167.343933
Enthalpy 298K = -1167.316334
Free Energy 298K = -1167.403907
Lowest Frequency = 15.4518 cm^{-1}
Second Frequency = 25.6287 cm^{-1}
SCF (BP86-D3BJ) Energy = -1167.82603599
SCF (MeCN) Energy = -1167.76600865
SCF (Toluene) Energy = -1167.73940155
SCF (BS2) Energy = -1167.68120831

```
C  -1.16821 -0.64425  2.32558
N  -0.23062 -0.48890  1.35256
C   1.07763 -0.88368  1.57914
C   1.42628 -1.42869  2.83181
C   0.46534 -1.58151  3.83273
C  -0.85973 -1.18746  3.57249
Ru -0.66527  0.29587 -0.43917
C   0.85747  2.96859 -1.41404
C  -0.34950  2.54932 -0.77617
C  -0.36947  2.35296  0.64785
C   0.84345  2.55339  1.38199
C   2.01550  2.92046  0.73205
C   2.02148  3.13745 -0.67184
H  -1.31540  2.36581  1.19682
C   1.95434 -0.69939  0.42841
C   3.32048 -1.05233  0.39904
C   4.05790 -0.88454 -0.77968
C   3.42889 -0.37190 -1.92917
C   2.07016 -0.00356 -1.89733
C   1.29012 -0.14472 -0.71982
H   2.94232  3.46369 -1.16476
O  -1.44548 -1.56851 -1.05272
C  -0.89071 -2.59572 -1.53663
O   0.40458 -2.70819 -1.75258
C  -1.70550 -3.79608 -1.92436
H  -1.31678 -4.68920 -1.40837
H  -2.76124 -3.64028 -1.67108
H  -1.60010 -3.97743 -3.00712
H   3.81159 -1.46651  1.28660
H   5.11526 -1.16324 -0.80850
H   1.61198  0.40566 -2.80622
H   4.00105 -0.25160 -2.85541
H   2.46150 -1.73332  3.00541
H   0.85805 -1.84468 -1.48918
H   0.85076  3.17983 -2.48811
H   2.93177  3.08448  1.30747
H  -1.29773  2.68006 -1.31765
H   0.82601  2.46700  2.47324
H  -1.64911 -1.29637  4.32022
H   0.74023 -2.00534  4.80284
H  -2.17655 -0.31879  2.06331
N  -2.74584  0.73222 -0.22708
C  -3.89970  0.95686 -0.24737
C  -5.33218  1.22573 -0.28111
H  -5.56653  2.13256  0.30077
H  -5.66669  1.37778 -1.32112
H  -5.89001  0.37631  0.14723
```

^{1}B$^+$ (*t*-N,*t*-O)
SCF (BP86) Energy = -1167.72106216
Enthalpy 0K = -1167.358285
Enthalpy 298K = -1167.330997
Free Energy 298K = -1167.416737
Lowest Frequency = 22.3268 cm^{-1}
Second Frequency = 25.8824 cm^{-1}
SCF (BP86-D3BJ) Energy = -1167.84260003
SCF (MeCN) Energy = -1167.77625682
SCF (Toluene) Energy = -1167.75323488
SCF (BS2) Energy = -1167.69612388

Ru	-0.61908	-0.25270	-0.02815
O	-1.13757	-2.28328	0.02042
C	-1.43997	-2.28641	-1.24154
C	-1.97443	-3.50840	-1.92164
C	-0.51821	-0.51883	2.26218
C	0.35109	-1.57330	2.70811
C	1.70087	-1.33907	2.89904
C	2.24178	-0.03279	2.69462
O	-1.27160	-1.16549	-1.85525
H	-1.61898	-3.54836	-2.96232
H	-1.67484	-4.41474	-1.37553
H	-3.07734	-3.46389	-1.94175
C	1.16670	1.66682	-0.96689
C	1.63474	2.86211	-0.37550
C	-0.15364	1.62846	-1.52350
C	0.79686	3.97850	-0.27916
H	2.65211	2.90070	0.02612
C	-0.98807	2.77322	-1.40175
C	-0.52938	3.92593	-0.76187
H	1.17210	4.89832	0.18056
H	-1.98089	2.75411	-1.86163
H	-1.17615	4.80421	-0.67528
H	-0.40600	0.87354	-2.27356
C	1.42399	1.00365	2.28094
C	0.02851	0.78480	2.01352
H	-0.63159	1.65711	1.95500
H	3.29683	0.15548	2.91769
H	-1.59218	-0.64586	2.42518
H	2.35143	-2.14104	3.26307
C	2.00128	0.43895	-0.99132
C	4.00618	-0.86319	-1.35194
H	5.05140	-0.93949	-1.66507
C	3.34577	0.37461	-1.38062
H	3.85160	1.28153	-1.72324
C	1.96813	-1.86910	-0.52673
H	1.37809	-2.71279	-0.16120
C	3.30364	-1.99990	-0.92383
H	3.78060	-2.98281	-0.88947
N	1.33023	-0.67334	-0.55480
H	-0.08210	-2.55221	2.93394
H	1.82268	2.01846	2.20030
N	-2.51919	0.25892	0.32790
C	-3.64993	0.51543	0.51484
C	-5.05227	0.84854	0.73337
H	-5.14036	1.80972	1.26702
H	-5.57944	0.93163	-0.23193
H	-5.54308	0.06594	1.33576

TS(**^{1}B$^+$**-**^{1}C$^+$**) (*t*-N,*t*-O)
SCF (BP86) Energy = -1167.69403568
Enthalpy 0K = -1167.333210
Enthalpy 298K = -1167.306433
Free Energy 298K = -1167.391158
Lowest Frequency = -115.9398 cm^{-1}
Second Frequency = 24.5883 cm^{-1}
SCF (BP86-D3BJ) Energy = -1167.81164970
SCF (MeCN) Energy = -1167.75221893
SCF (Toluene) Energy = -1167.72769431
SCF (BS2) Energy = -1167.67084546

C	-2.14377	-1.32936	0.86487
N	-1.43885	-0.23236	0.49145
C	-2.03126	1.00588	0.56476
C	-3.37970	1.14344	0.93057
C	-4.11761	0.00360	1.27539
C	-3.48210	-1.24817	1.26234
Ru	0.54178	-0.17601	-0.13007
C	0.60988	-1.93878	-1.64835
C	-0.40960	-2.94075	-1.52420
C	-1.68521	-2.72226	-2.02260
C	-1.99971	-1.49653	-2.68296
C	-1.03735	-0.50862	-2.83313
C	0.28823	-0.70504	-2.31778
H	-2.44545	-3.50621	-1.95049
C	-1.11054	2.12405	0.29005
C	-1.51393	3.33412	-0.30845
C	-0.57747	4.35111	-0.54523
C	0.77555	4.17910	-0.19043
C	1.19820	2.98553	0.40679
C	0.27238	1.93709	0.62708
H	1.09474	-0.07240	-2.70858
O	0.92752	-1.75210	1.08504
C	1.24877	-1.36495	2.31729
O	1.27399	-0.17336	2.67602
C	1.59958	-2.51464	3.24179
H	1.08199	-2.37272	4.20327
H	1.33813	-3.49093	2.80951
H	2.68375	-2.49077	3.44323
H	-2.55833	3.47282	-0.60611
H	-0.90323	5.28645	-1.01034
H	2.23664	2.85774	0.72538
H	1.49274	4.98611	-0.36831
H	-3.82522	2.14053	0.97992
H	0.56711	1.14691	1.40607
H	1.65104	-2.24112	-1.51000
H	-1.26359	0.40817	-3.38646
H	-0.14985	-3.90225	-1.07054
H	-3.00006	-1.35313	-3.10393
H	-4.01065	-2.15726	1.56040
H	-5.16516	0.09396	1.57685
H	-1.59643	-2.27230	0.83741
N	2.49421	0.01100	-0.52317
C	3.65353	0.08575	-0.69469
C	5.09468	0.19922	-0.87899
H	5.58145	0.42543	0.08475
H	5.50734	-0.74659	-1.26767
H	5.32994	1.00663	-1.59255

^{1}C$^+$ (*t*-N,*t*-O)
SCF (BP86) Energy = -1167.73105755
Enthalpy 0K = -1167.368547
Enthalpy 298K = -1167.341278
Free Energy 298K = -1167.426913
Lowest Frequency = 23.6952 cm^{-1}
Second Frequency = 33.5991 cm^{-1}
SCF (BP86-D3BJ) Energy = -1167.85256029
SCF (MeCN) Energy = -1167.78934120
SCF (Toluene) Energy = -1167.76422473
SCF (BS2) Energy = -1167.70680159

C	-2.15475	0.11488	-1.87378
N	-1.40328	-0.18468	-0.78434
C	-1.84463	-1.14881	0.09657
C	-3.07969	-1.79195	-0.11573
C	-3.85455	-1.46795	-1.23306
C	-3.37984	-0.50197	-2.13667
Ru	0.48970	0.57010	-0.41674
C	-1.35214	3.13919	-0.63482
C	-2.55131	2.86899	0.01363
C	-2.55603	2.22185	1.28182
C	-1.36178	1.86249	1.89076
C	-0.10521	2.10334	1.24029

```
C  -0.10729  2.74933 -0.04371
H  -3.50659  2.04914  1.79601
C  -0.90267 -1.41835  1.18559
C  -1.13161 -2.34588  2.22470
C  -0.16809 -2.54985  3.22066
C   1.03545 -1.82475  3.18573
C   1.27909 -0.89090  2.15971
C   0.32609 -0.67805  1.13561
H   0.81215  3.21564 -0.41924
O   1.17859 -0.80203 -1.83401
C   1.75161 -1.91878 -1.72364
O   1.96996 -2.51523 -0.56239
C   2.22991 -2.67307 -2.92900
H   1.66305 -3.61508 -3.01987
H   2.09472 -2.06959 -3.83513
H   3.29034 -2.94520 -2.80321
H  -2.06896 -2.91134  2.26124
H  -0.35413 -3.27048  4.02205
H   2.21514 -0.32308  2.16063
H   1.79093 -1.97936  3.96337
H  -3.42101 -2.55243  0.59108
H   1.57539 -1.95720  0.17322
H  -1.34542  3.69270 -1.57974
H   0.80292  2.08369  1.84980
H  -3.49877  3.18687 -0.43327
H  -1.36410  1.42854  2.89528
H  -3.94457 -0.22597 -3.03054
H  -4.81238 -1.96799 -1.40404
H  -1.74179  0.87555 -2.54171
N   2.37041  1.15331 -0.11037
C   3.48630  1.51147  0.00658
C   4.87303  1.93911  0.14531
H   5.51729  1.08075  0.40098
H   5.23519  2.38096 -0.79855
H   4.96427  2.69530  0.94309
```

$^4G^+$ (κ^1)
SCF (BP86) Energy = -1333.81273065
Enthalpy 0K = -1333.411050
Enthalpy 298K = -1333.374809
Free Energy 298K = -1333.485025
Lowest Frequency = 9.4832 cm^{-1}
Second Frequency = 16.5330 cm^{-1}
SCF (BP86-D3BJ) Energy = -1333.93437337
SCF (MeCN) Energy = -1333.87498497
SCF (Toluene) Energy = -1333.84744571
SCF (BS2) Energy = -1333.85086793

N	-2.14833	-1.66299	-0.65023
C	-2.96908	-2.47395	-0.85076
N	-1.76481	0.96345	-1.54307
C	-2.35908	1.62624	-2.30512
C	-3.10493	2.45420	-3.24457
H	-3.27091	1.91006	-4.18924
H	-4.08447	2.72610	-2.81693
H	-2.54732	3.37954	-3.46549
C	-4.00356	-3.47390	-1.08606
H	-3.56026	-4.48175	-1.14503
H	-4.73880	-3.45822	-0.26420
H	-4.52997	-3.26578	-2.03234
O	-0.79106	0.46059	2.95486
C	-1.91951	0.57835	2.45804
C	-3.14901	0.90928	3.30708
H	-3.72855	-0.01290	3.48670
H	-2.83336	1.32000	4.27636
H	-3.81536	1.61755	2.79041
O	-2.22837	0.43328	1.16995
N	-0.05138	-1.48430	1.10689
C	0.26895	-2.30359	1.87718
C	0.67167	-3.23506	2.92097
H	1.72506	-3.53172	2.78691
H	0.55634	-2.75083	3.90561
H	0.04613	-4.14248	2.89593
N	0.38105	1.50312	0.23972
C	-0.37476	2.61576	0.47592
C	1.73978	1.66499	0.16066
C	0.15091	3.90301	0.58423
H	-1.44448	2.42744	0.58606
C	2.31978	2.94991	0.22898
C	1.53110	4.08487	0.43162
H	-0.52273	4.74065	0.78346
H	3.40795	3.02577	0.15783
H	1.98524	5.07826	0.49469
C	2.67967	0.50785	0.08756
C	3.56757	0.37954	-1.00259
C	2.82839	-0.34472	1.20139
C	4.56026	-0.61316	-0.99805
H	3.48204	1.06865	-1.85019
C	3.82993	-1.32855	1.20631
H	2.17797	-0.19987	2.06864
C	4.69118	-1.47254	0.10634
H	5.25164	-0.69637	-1.84357
H	3.96146	-1.96557	2.08751
H	5.47918	-2.23216	0.12041
Ru	-0.83313	-0.21796	-0.22284
N	0.39387	-0.89085	-1.66499
C	1.06044	-1.34774	-2.51525
C	1.92633	-1.90702	-3.54536
H	2.97775	-1.83732	-3.21889
H	1.68001	-2.96690	-3.72483
H	1.80957	-1.35438	-4.49253

^3G ($2\kappa^1$)
SCF (BP86) Energy = -1429.71423530
Enthalpy 0K = -1429.309801
Enthalpy 298K = -1429.272739
Free Energy 298K = -1429.382864
Lowest Frequency = 18.7966 cm^{-1}
Second Frequency = 29.6347 cm^{-1}
SCF (BP86-D3BJ) Energy = -1429.83953150
SCF (MeCN) Energy = -1429.74439008
SCF (Toluene) Energy = -1429.72764261
SCF (BS2) Energy = -1429.79512584

N	-0.75508	0.82633	1.34184
C	-1.55069	1.29558	2.06574
N	1.70198	1.85610	0.56963
C	2.31375	2.83062	0.78467
C	-2.58642	1.92909	2.87051
H	-2.72089	2.97454	2.54327
H	-3.54305	1.39538	2.74003
H	-2.31817	1.92551	3.94062
C	2.96648	4.11949	0.96995
H	3.16913	4.31028	2.03714
H	3.92288	4.15393	0.42168
H	2.30680	4.91627	0.58515
O	3.60793	-1.58875	-0.27666
C	3.28675	-0.79648	-1.18965
O	2.16126	-0.13549	-1.30561
C	4.24520	-0.52171	-2.35770
H	3.70640	-0.56166	-3.31786
H	4.66144	0.49628	-2.26247
H	5.07056	-1.24868	-2.35289
O	-0.13655	1.17347	-1.52785
C	-0.46341	2.45056	-1.55898
O	-0.50371	3.24606	-0.60497
C	-0.79782	2.91469	-2.98713
H	-1.45720	2.19531	-3.50086
H	-1.26948	3.90817	-2.96318
H	0.13237	2.97160	-3.57858
N	-0.27521	-1.63917	-0.38390
C	-1.60370	-1.98727	-0.44940
C	0.64394	-2.63692	-0.56925
C	-1.99310	-3.32162	-0.70362
C	0.30580	-3.96636	-0.83232
H	1.69419	-2.34470	-0.45613
C	-1.04441	-4.32630	-0.90532
H	-3.06298	-3.53865	-0.76330
H	1.10840	-4.69611	-0.97116
H	-1.35340	-5.35541	-1.11515
C	-2.71504	-1.00777	-0.26071
C	-2.88493	0.10445	-1.10987
C	-3.70671	-1.28960	0.70708
C	-4.01540	0.92534	-0.97810
H	-2.10946	0.32855	-1.84620
C	-4.83501	-0.46516	0.83718
H	-3.58372	-2.15746	1.36469
C	-4.99331	0.64567	-0.00949
H	-4.13309	1.78757	-1.64241
H	-5.59483	-0.69813	1.59149
H	-5.87786	1.28538	0.08156
Ru	0.68222	0.22548	0.13429
N	1.57837	-0.74544	1.60134
C	2.15904	-1.31075	2.45138
C	3.03964	-2.05983	3.33865
H	3.44504	-1.41088	4.13329
H	2.50516	-2.89844	3.81604
H	3.87857	-2.46109	2.74340

^1G ($2\kappa^2$)
SCF (BP86) Energy = -1164.19014654
Enthalpy 0K = -1163.877080
Enthalpy 298K = -1163.850076
Free Energy 298K = -1163.938791
Lowest Frequency = 2.3128 cm^{-1}
Second Frequency = 30.5548 cm^{-1}
SCF (BP86-D3BJ) Energy = -1164.28137607
SCF (MeCN) Energy = -1164.21057055
SCF (Toluene) Energy = -1164.19895034
SCF (BS2) Energy = -1164.18808245

```
Ru -0.96422  0.11027 -0.20165
N  -2.62762 -0.88204 -0.09697
C  -3.63760 -1.48828 -0.03921
C  -4.88678 -2.23601  0.03404
H  -4.82740 -3.14967 -0.58270
H  -5.10203 -2.53971  1.07366
H  -5.73412 -1.62943 -0.33174
O  -1.98415  1.92872  0.31291
C  -1.80771  1.71145  1.56977
C  -2.36276  2.64913  2.61408
H  -1.70983  2.66272  3.49967
H  -2.47052  3.66271  2.20074
H  -3.35979  2.29718  2.93156
O  -1.16796  0.64519  1.89777
O  -0.80988 -0.31590 -2.28837
C  -0.17821 -1.41333 -2.04155
O   0.05167 -1.69030 -0.80840
C   0.24133 -2.34368 -3.15299
H   1.15992 -2.88015 -2.87238
H  -0.55181 -3.09157 -3.32697
H   0.39353 -1.78024 -4.08551
N   0.79820  1.22459 -0.42176
C   0.60542  2.39751 -1.09796
C   2.09103  0.86265 -0.11524
C   1.64187  3.23098 -1.51675
H  -0.43987  2.63973 -1.30123
C   3.17428  1.67796 -0.51489
C   2.96371  2.86192 -1.22490
H   1.40543  4.14974 -2.06047
H   4.18328  1.37062 -0.22746
H   3.80815  3.48890 -1.52791
C   2.38178 -0.37534  0.65616
C   3.45877 -1.19918  0.25660
C   1.66199 -0.71006  1.82391
C   3.80252 -2.33831  0.99751
H   4.01047 -0.95870 -0.65901
C   2.01619 -1.84596  2.56630
H   0.83351 -0.07706  2.15071
C   3.08147 -2.66452  2.15755
H   4.62996 -2.97397  0.66466
H   1.45205 -2.09108  3.47234
H   3.34914 -3.55283  2.73972
```

$^2G^+$ (κ^2)

SCF (BP86) Energy = -1068.27102324
Enthalpy 0K = -1067.961742
Enthalpy 298K = -1067.935718
Free Energy 298K = -1068.020632
Lowest Frequency = 19.2404 cm^{-1}
Second Frequency = 23.0511 cm^{-1}
SCF (BP86-D3BJ) Energy = -1068.36092796
SCF (MeCN) Energy = -1068.32837445
SCF (Toluene) Energy = -1068.30435561
SCF (BS2) Energy = -1068.23131615

```
Ru  0.69568 -0.18817  0.10478
N  -0.15594 -1.66385 -0.92977
C  -0.59201 -2.55135 -1.55736
C  -1.12944 -3.66120 -2.33272
H  -2.23125 -3.65559 -2.29357
H  -0.81176 -3.57931 -3.38551
H  -0.76601 -4.61972 -1.92604
O   2.23605 -1.59125  0.67627
C   2.89626 -1.27876 -0.37972
O   2.35362 -0.38997 -1.16015
C   4.23613 -1.87446 -0.70089
H   5.02346 -1.30903 -0.17283
H   4.27872 -2.91669 -0.35152
H   4.43471 -1.81909 -1.78081
N  -0.51900  1.22878 -0.76357
C  -1.84114  1.31180 -0.39092
C  -0.02776  2.09069 -1.69112
C  -2.67607  2.29455 -0.95654
C  -0.81827  3.07590 -2.28669
H   1.02613  1.95093 -1.94762
C  -2.16719  3.18300 -1.90911
H  -3.71701  2.36563 -0.63100
H  -0.37729  3.74393 -3.03078
H  -2.81105  3.95015 -2.34859
C  -2.27985  0.31122  0.59678
C  -1.28730 -0.36697  1.35885
C  -3.62645 -0.07694  0.74926
C  -1.63794 -1.39792  2.24908
H  -0.28649  0.14392  1.60943
C  -3.97425 -1.10003  1.64459
H  -4.40619  0.39421  0.14261
C  -2.98496 -1.76558  2.39036
H  -0.85767 -1.89236  2.83543
H  -5.02467 -1.38709  1.75224
H  -3.26419 -2.56348  3.08501
N   1.69611  1.23802  1.07488
C   2.33467  2.05103  1.62928
C   3.12739  3.04989  2.33332
H   3.64838  2.58740  3.18849
H   3.87879  3.48905  1.65605
H   2.47697  3.85668  2.71033
```

$^3G^+$ (κ^2)

SCF (BP86) Energy = -1201.03658210
Enthalpy 0K = -1200.681669
Enthalpy 298K = -1200.650483
Free Energy 298K = -1200.747576
Lowest Frequency = 19.0768 cm^{-1}
Second Frequency = 24.1061 cm^{-1}
SCF (BP86-D3BJ) Energy = -1201.14204377
SCF (MeCN) Energy = -1201.09804878
SCF (Toluene) Energy = -1201.07132453
SCF (BS2) Energy = -1201.03610409

```
N  -1.39003  0.75911 -1.52943
C  -1.90097  1.08669 -2.53010
N  -1.83323  1.08482  1.22297
C  -2.65607  1.60253  1.87885
C  -3.69136  2.22771  2.69214
H  -4.20690  3.01559  2.11804
H  -4.43552  1.47377  2.99965
H  -3.25240  2.68126  3.59644
C  -2.54050  1.41721 -3.79558
H  -2.69958  0.49256 -4.37588
H  -3.51630  1.89908 -3.61942
H  -1.90699  2.10239 -4.38256
O  -1.38500 -2.15854 -1.83647
C  -2.08350 -2.23807 -0.80487
C  -3.14251 -3.32550 -0.64270
H  -3.92207 -3.03437  0.07607
H  -3.58821 -3.55694 -1.62133
H  -2.65884 -4.24554 -0.27081
O  -1.97725 -1.44789  0.24627
N   0.91825  1.56798  0.00282
C   0.65100  2.88768  0.18582
C   2.18190  1.19411 -0.38994
C   1.60615  3.88810 -0.00307
H  -0.37012  3.12160  0.49556
C   3.17918  2.16536 -0.60974
C   2.89767  3.52022 -0.41362
H   1.33367  4.93373  0.16175
H   4.16556  1.84769 -0.95672
H   3.66766  4.27723 -0.58783
C   2.41197 -0.25332 -0.55132
C   3.69541 -0.81530 -0.38043
C   1.31771 -1.12884 -0.79590
C   3.88790 -2.20200 -0.46469
H   4.54625 -0.16889 -0.14360
```

```
C   1.51460 -2.51960 -0.87554
H   0.32842 -0.82897 -1.28556
C   2.79993 -3.05706 -0.71029
H   4.89248 -2.61540 -0.33134
H   0.65334 -3.14722 -1.11854
H   2.95527 -4.13765 -0.78594
Ru -0.54868  0.07058  0.15318
N   0.19522 -0.69484  1.84179
C   0.56845 -1.19078  2.83411
C   1.03104 -1.82584  4.06102
H   1.82475 -2.55612  3.83223
H   1.43351 -1.07277  4.75863
H   0.19653 -2.35463  4.55093
```

^{1}G ($\kappa^2\kappa^1$)

SCF (BP86) Energy = -1164.18926447
Enthalpy 0K = -1163.878437
Enthalpy 298K = -1163.851793
Free Energy 298K = -1163.937094
Lowest Frequency = 21.4406 cm^{-1}
Second Frequency = 31.2131 cm^{-1}
SCF (BP86-D3BJ) Energy = -1164.28335477
SCF (MeCN) Energy = -1164.21125998
SCF (Toluene) Energy = -1164.19927038
SCF (BS2) Energy = -1164.18914090

```
Ru -0.68338  0.20175 -0.05184
N   0.01902  1.88700 -0.79434
C   0.40070  2.90424 -1.24419
C   0.86532  4.17226 -1.79348
H   1.92560  4.33520 -1.53618
H   0.76830  4.18136 -2.89278
H   0.27674  5.01180 -1.38478
O  -2.38867  1.29119  0.74067
C  -3.02229  1.06253 -0.35196
O  -2.39329  0.45664 -1.30611
C  -4.47081  1.44990 -0.51621
H  -5.10525  0.60455 -0.19836
H  -4.70923  2.31710  0.11711
H  -4.69416  1.66800 -1.57123
O  -1.69959 -1.49809  0.53386
C  -1.36668 -2.11325  1.64418
O  -0.41666 -1.78972  2.39148
C  -2.27737 -3.28428  2.00308
H  -2.66789 -3.77685  1.10000
H  -1.73494 -4.00461  2.63237
H  -3.13779 -2.90243  2.57971
N   0.62293 -0.97079 -1.06449
C   1.94952 -0.99144 -0.68131
C   0.20667 -1.77343 -2.07958
C   2.86790 -1.81887 -1.35510
C   1.08142 -2.61027 -2.77446
H  -0.85952 -1.70703 -2.31238
C   2.43953 -2.63124 -2.40970
H   3.91154 -1.83337 -1.02884
H   0.69753 -3.23487 -3.58554
H   3.14917 -3.27922 -2.93297
C   2.25537 -0.11377  0.45190
C   1.12855  0.38333  1.18239
C   3.55685  0.30366  0.79509
C   1.35190  1.27450  2.25609
H   0.21081 -0.38087  1.42232
C   3.75517  1.19532  1.85824
H   4.41774 -0.04251  0.21196
C   2.65149  1.68287  2.58541
H   0.49293  1.62758  2.83548
H   4.76946  1.51530  2.11809
H   2.81032  2.37786  3.41717
```

TS(**^{1}G**–**^{1}H**)

SCF (BP86) Energy = -1164.18761053
Enthalpy 0K = -1163.879960
Enthalpy 298K = -1163.853689
Free Energy 298K = -1163.937821
Lowest Frequency = -656.6399 cm^{-1}
Second Frequency = 22.8723 cm^{-1}
SCF (BP86-D3BJ) Energy = -1164.28226882
SCF (MeCN) Energy = -1164.20737032
SCF (Toluene) Energy = -1164.19658039
SCF (BS2) Energy = -1164.18618920

```
Ru -0.70253  0.12661 -0.08331
N  -0.18756  1.87637 -0.78845
C   0.09070  2.93561 -1.21726
C   0.42308  4.25276 -1.74616
H   1.46567  4.51387 -1.49727
H   0.31152  4.27388 -2.84405
H  -0.23883  5.02327 -1.31424
O  -2.49084  1.00830  0.76411
C  -3.13890  0.75760 -0.31945
O  -2.50359  0.23952 -1.31308
C  -4.62231  1.02937 -0.41086
H  -5.17326  0.12326 -0.10458
H  -4.90569  1.84945  0.26533
H  -4.90597  1.26725 -1.44695
O  -1.52522 -1.70314  0.49107
C  -1.08165 -2.23289  1.58163
O  -0.14607 -1.72441  2.27864
C  -1.73551 -3.51950  2.04786
H  -2.39265 -3.93184  1.26988
H  -0.96239 -4.25296  2.32515
H  -2.33101 -3.31152  2.95286
N   0.73515 -0.86638 -1.11854
C   2.04843 -0.75984 -0.69877
C   0.43524 -1.65363 -2.18509
C   3.06734 -1.44510 -1.38901
C   1.41196 -2.35384 -2.89549
H  -0.62557 -1.68873 -2.44896
C   2.75552 -2.24385 -2.49343
H   4.09986 -1.35827 -1.03908
H   1.11845 -2.97191 -3.74826
H   3.54488 -2.77998 -3.02922
C   2.21801  0.08570  0.48423
C   0.99818  0.45188  1.15060
C   3.46229  0.57181  0.93442
C   1.09746  1.31490  2.27101
H   0.19610 -0.57447  1.50715
C   3.52423  1.42204  2.04624
H   4.38437  0.31213  0.40115
C   2.33870  1.79540  2.71041
H   0.18096  1.59137  2.80396
H   4.49214  1.79890  2.39260
H   2.38856  2.46318  3.57802
```

^{1}H

SCF (BP86) Energy = -1164.19893635
Enthalpy 0K = -1163.886803
Enthalpy 298K = -1163.859793
Free Energy 298K = -1163.947262
Lowest Frequency = 18.0371 cm^{-1}
Second Frequency = 19.6736 cm^{-1}
SCF (BP86-D3BJ) Energy = -1164.29321973
SCF (MeCN) Energy = -1164.21743860
SCF (Toluene) Energy = -1164.20740040
SCF (BS2) Energy = -1164.19712912

```
Ru  0.66175  0.16617  0.11254
N   0.58480  2.06510 -0.17026
C   0.56071  3.22957 -0.35086
C   0.55160  4.67198 -0.56059
H  -0.46125  5.01807 -0.82994
H   0.86801  5.20658  0.35252
H   1.23757  4.95114 -1.37951
O   2.52959  0.06864 -0.94804
```

```
C   3.23638  0.24531  0.12401
O   2.65721  0.40780  1.24933
C   4.74839  0.28676  0.01004
H   5.20964 -0.12664  0.91959
H   5.08772 -0.26548 -0.87879
H   5.07788  1.33589 -0.08858
O   1.00238 -1.87537  0.58830
C   0.70349 -2.87649 -0.10410
O   0.01098 -2.80980 -1.23236
C   1.12002 -4.26573  0.29894
H   1.64291 -4.23404  1.26315
H   0.23597 -4.92061  0.36518
H   1.78422 -4.68941 -0.47284
N  -0.95968  0.16824  1.35237
C  -2.21500  0.05771  0.77738
C  -0.85052  0.23934  2.70422
C  -3.36281  0.01970  1.59291
C  -1.96047  0.20405  3.55200
H   0.17366  0.32644  3.07960
C  -3.24268  0.09302  2.98460
H  -4.34766 -0.07221  1.12566
H  -1.81571  0.26440  4.63410
H  -4.13409  0.06301  3.61908
C  -2.16956 -0.01252 -0.68344
C  -0.83393 -0.01060 -1.22640
C  -3.30675 -0.05294 -1.51637
C  -0.72611 -0.02111 -2.64359
H  -0.22611 -1.83526 -1.37782
C  -3.15598 -0.08567 -2.90947
H  -4.31517 -0.04926 -1.08414
C  -1.86381 -0.06525 -3.46909
H   0.27271  0.00638 -3.09722
H  -4.03850 -0.11947 -3.55652
H  -1.74398 -0.07731 -4.55911
```

^{2}G ($\kappa^2\kappa^1$)

SCF (BP86) Energy = -1296.95420395
Enthalpy 0K = -1296.597601
Enthalpy 298K = -1296.565701
Free Energy 298K = -1296.663759
Lowest Frequency = 29.5860 cm^{-1}
Second Frequency = 32.8386 cm^{-1}
SCF (BP86-D3BJ) Energy = -1297.06313633
SCF (MeCN) Energy = -1296.98097139
SCF (Toluene) Energy = -1296.96637380
SCF (BS2) Energy = -1296.99614684

```
N   1.90057 -1.02015  0.87780
C   2.79413 -1.61156  1.35244
C   3.95949 -2.30561  1.88338
H   4.25579 -1.87207  2.85344
H   3.74765 -3.37798  2.03202
H   4.80372 -2.20594  1.17973
O   3.27357 -0.14223 -1.60367
C   2.83568  1.00848 -1.45737
O   1.71749  1.36846 -0.85084
C   3.60141  2.23142 -1.98793
H   2.94331  2.87064 -2.59955
H   3.95569  2.84471 -1.14205
H   4.46364  1.90340 -2.58616
O   0.64533  1.42071  1.65805
C   0.12873  1.16281  2.83433
O  -0.53682  0.14442  3.13095
C   0.36862  2.26291  3.86807
H   1.30666  2.80125  3.66663
H  -0.46024  2.99044  3.81784
H   0.37970  1.83109  4.87973
N  -1.15667  1.22731 -0.52511
C  -2.42296  0.69088 -0.45888
C  -0.98741  2.51885 -0.90443
C  -3.54162  1.47947 -0.79337
C  -2.06584  3.33667 -1.25032
H   0.05597  2.84717 -0.92935
C  -3.36677  2.80776 -1.19358
H  -4.54335  1.04891 -0.71250
H  -1.88304  4.37184 -1.55130
H  -4.23354  3.42632 -1.44686
C  -2.47655 -0.70860 -0.01610
C  -1.30727 -1.23599  0.62237
C  -3.57675 -1.55197 -0.27150
C  -1.29823 -2.59901  0.99883
H  -0.70257 -0.55905  1.41693
C  -3.54163 -2.90215  0.10265
H  -4.45427 -1.16169 -0.79899
C  -2.39723 -3.42606  0.73409
H  -0.42202 -2.99413  1.52207
H  -4.40155 -3.54736 -0.10405
H  -2.37062 -4.48101  1.02847
Ru  0.42406  0.06150  0.10367
N   0.42841 -1.05951 -1.53761
C   0.50858 -1.69133 -2.52123
C   0.71464 -2.44656 -3.74994
H   0.48185 -3.51379 -3.59751
H   0.07252 -2.06153 -4.56004
H   1.76946 -2.35404 -4.06052
```

TS(**^{2}G–^{2}H**)

SCF (BP86) Energy = -1296.95136606
Enthalpy 0K = -1296.598151
Enthalpy 298K = -1296.566695
Free Energy 298K = -1296.662937
Lowest Frequency = -789.9563 cm^{-1}
Second Frequency = 33.6814 cm^{-1}
SCF (BP86-D3BJ) Energy = -1297.06107808
SCF (MeCN) Energy = -1296.97556370
SCF (Toluene) Energy = -1296.96229320
SCF (BS2) Energy = -1296.99187977

```
N   1.85109 -1.25936  0.62320
C   2.73246 -1.98055  0.90523
C   3.90511 -2.79534  1.19388
H   4.18231 -2.71109  2.25831
H   3.71686 -3.85859  0.96749
H   4.75450 -2.44746  0.58070
O   3.40235  0.39160 -1.33440
C   2.93944  1.43754 -0.84983
O   1.78378  1.58720 -0.23381
C   3.72548  2.75884 -0.91677
H   3.12007  3.54558 -1.39789
H   3.96028  3.10943  0.10256
H   4.65942  2.61577 -1.47938
O   0.50452  0.80395  2.09302
C  -0.18243  0.20085  2.99770
O  -0.92156 -0.81464  2.76355
C  -0.11168  0.74304  4.41233
H   0.62409  1.55564  4.48344
H  -1.10568  1.11621  4.71020
H   0.15268 -0.06970  5.10776
N  -1.12838  1.34148 -0.21961
C  -2.38782  0.80732 -0.39071
C  -0.95232  2.68651 -0.22876
C  -3.49195  1.66393 -0.57892
C  -2.01687  3.57179 -0.41443
H   0.08769  3.00305 -0.09803
C  -3.31029  3.04983 -0.59246
H  -4.49026  1.23313 -0.69412
H  -1.83018  4.64917 -0.41517
H  -4.16727  3.71658 -0.73200
C  -2.43539 -0.65825 -0.34598
C  -1.24938 -1.31352  0.14002
C  -3.53743 -1.40534 -0.81085
C  -1.24393 -2.73250  0.12059
H  -0.82525 -0.93278  1.38944
C  -3.49539 -2.80540 -0.80979
```

```
H  -4.42258 -0.89451 -1.20750
C  -2.34128 -3.46737 -0.34746
H  -0.36214 -3.25931  0.50212
H  -4.35345 -3.37914 -1.17483
H  -2.30443 -4.56296 -0.34960
Ru  0.42049  0.02610  0.14408
N   0.55852 -0.50585 -1.74725
C   0.71280 -0.79089 -2.87331
C   1.01865 -1.10430 -4.26271
H   0.80738 -2.16437 -4.48208
H   0.41846 -0.48063 -4.94659
H   2.08802 -0.90828 -4.45215
H   2.54019  1.15120 -4.22001
```

^{2}H

SCF (BP86) Energy = -1296.95983161
Enthalpy 0K = -1296.602109
Enthalpy 298K = -1296.570100
Free Energy 298K = -1296.668324
Lowest Frequency = 29.1953 cm^{-1}
Second Frequency = 29.9636 cm^{-1}
SCF (BP86-D3BJ) Energy = -1297.06923639
SCF (MeCN) Energy = -1296.98323969
SCF (Toluene) Energy = -1296.97041092
SCF (BS2) Energy = -1297.00011140

```
N   1.68269 -1.53945 -0.03311
C   2.50761 -2.37404 -0.10333
C   3.66969 -3.24830 -0.19975
H   3.86162 -3.75058  0.76368
H   3.52441 -4.02473 -0.97006
H   4.55567 -2.64479 -0.46532
O   3.57243  0.70356 -0.74449
C   3.10179  1.43369  0.14836
O   1.89463  1.38127  0.66190
C   3.95980  2.55107  0.77420
H   3.49700  3.53612  0.58927
H   4.01571  2.42288  1.86849
H   4.97397  2.54098  0.34836
O   0.27136 -0.28612  2.18051
C  -0.35854 -1.18678  2.78214
O  -1.10406 -2.09301  2.16655
C  -0.31841 -1.30612  4.28259
H   0.35799 -0.54882  4.69871
H  -1.33284 -1.17203  4.69359
H   0.01908 -2.31563  4.56898
N  -1.04112  1.43474  0.21697
C  -2.33269  1.09674 -0.13287
C  -0.76036  2.67918  0.67632
C  -3.35953  2.05644 -0.01122
C  -1.74676  3.65956  0.81240
H   0.29696  2.83331  0.92233
C  -3.07025  3.34016  0.46029
H  -4.38347  1.78495 -0.28238
H  -1.47768  4.65077  1.18763
H  -3.86825  4.08378  0.55593
C  -2.48213 -0.28372 -0.60568
C  -1.28422 -1.08731 -0.54383
C  -3.69186 -0.79667 -1.12089
C  -1.39431 -2.40804 -1.05816
H  -1.08720 -1.84702  1.17580
C  -3.75735 -2.11286 -1.59545
H  -4.58819 -0.16620 -1.16804
C  -2.60157 -2.91576 -1.56677
H  -0.50621 -3.05246 -1.05378
H  -4.69804 -2.50780 -1.99276
H  -2.64342 -3.94326 -1.94830
Ru  0.38731 -0.05549  0.05924
N   0.71791  0.34511 -1.80814
C   0.98591  0.60356 -2.92076
C   1.45166  0.97019 -4.25160
H   1.24672  0.16684 -4.97939
H   0.95199  1.88975 -4.60101
```

B·OAc (back)
SCF (BP86) Energy = -1263.61755175
Enthalpy 0K = -1263.252431
Enthalpy 298K = -1263.224193
Free Energy 298K = -1263.312746
Lowest Frequency = 17.3975 cm^{-1}
Second Frequency = 28.7966 cm^{-1}
SCF (BP86-D3BJ) Energy = -1263.73742642
SCF (MeCN) Energy = -1263.64064955
SCF (Toluene) Energy = -1263.62818423
SCF (BS2) Energy = -1263.64417376

C	-0.07768	-1.97782	1.42682
N	-0.05249	-0.69014	0.97628
C	-1.09177	0.14432	1.29555
C	-2.18410	-0.33791	2.04896
C	-2.20621	-1.65742	2.50120
C	-1.12338	-2.49199	2.19108
Ru	1.41958	-0.29344	-0.52617
C	2.60342	-0.39066	-2.39071
C	1.61889	-1.44709	-2.35698
C	0.23451	-1.14378	-2.18758
C	-0.17492	0.22007	-1.99489
C	0.78924	1.26535	-1.96557
C	2.18586	0.95194	-2.16216
H	-0.54523	-1.90448	-2.07362
C	-1.08181	1.57679	0.88906
C	-2.23397	2.10902	0.26328
C	-2.26059	3.46775	-0.08902
C	-1.16712	4.30491	0.19452
C	-0.03401	3.77881	0.83962
C	0.01323	2.41900	1.18538
H	2.93949	1.73700	-2.04690
O	2.72373	-1.51471	0.68307
C	3.09294	-0.49410	1.38122
O	2.62184	0.64890	1.02932
C	4.00276	-0.64495	2.56942
H	4.58020	0.27748	2.72847
H	3.39371	-0.83013	3.47133
H	4.67731	-1.50236	2.42863
H	-3.07263	1.41975	0.04443
H	-3.14684	3.87528	-0.58765
H	0.81271	4.42922	1.08488
H	-1.20113	5.36652	-0.07459
H	-3.00802	0.34448	2.25712
H	0.89404	2.01280	1.69050
H	3.66734	-0.63216	-2.46006
H	0.48744	2.28266	-1.70391
H	1.95086	-2.48951	-2.39013
H	-1.23427	0.34501	-1.71863
H	-1.08567	-3.53509	2.51656
H	-3.05940	-2.02966	3.07566
H	0.77786	-2.59426	1.14496
O	-2.51680	-1.13081	-1.27699
C	-3.70755	-1.13297	-0.80289
C	-4.59622	-2.33084	-1.21487
H	-4.69977	-2.36058	-2.31372
H	-4.11533	-3.27917	-0.91580
H	-5.59527	-2.26637	-0.75686
O	-4.21882	-0.26020	-0.03688

B·OAc (a) – "**B**·OAc" in figure
SCF (BP86) Energy = -1263.62317136
Enthalpy 0K = -1263.257959
Enthalpy 298K = -1263.229825
Free Energy 298K = -1263.317921
Lowest Frequency = 25.6024 cm^{-1}
Second Frequency = 37.4299 cm^{-1}
SCF (BP86-D3BJ) Energy = -1263.74415414
SCF (MeCN) Energy = -1263.64507734
SCF (Toluene) Energy = -1263.63339724
SCF (BS2) Energy = -1263.64784484

C	-0.46161	-1.76693	1.51405
N	-0.24142	-0.52532	0.99936
C	-1.09453	0.49047	1.33635
C	-2.16626	0.25235	2.21940
C	-2.37928	-1.01938	2.75623
C	-1.50538	-2.05168	2.39359
Ru	1.28668	-0.41104	-0.48730
C	2.51627	-0.70733	-2.29770
C	1.49504	-1.72436	-2.20492
C	0.11463	-1.37159	-2.09993
C	-0.25311	0.01589	-2.03318
C	0.74369	1.03348	-2.06852
C	2.13413	0.66300	-2.19486
H	-0.71204	-2.08420	-1.88362
C	-0.91977	1.86356	0.77906
C	-1.96168	2.40288	-0.00948
C	-1.85237	3.71383	-0.50028
C	-0.72478	4.49678	-0.19821
C	0.30488	3.96259	0.59558
C	0.21174	2.65002	1.08462
H	2.90935	1.43224	-2.12033
O	2.41315	-1.65165	0.87383
C	2.87205	-0.61774	1.49326
O	2.53753	0.53438	1.03040
C	3.73074	-0.75858	2.72133
H	4.39110	0.11433	2.82880
H	3.08352	-0.81466	3.61387
H	4.32235	-1.68453	2.66940
H	-2.80200	1.75040	-0.28240
H	-2.65255	4.12251	-1.12655
H	1.18202	4.57050	0.84194
H	-0.64919	5.52170	-0.57746
H	-2.82381	1.08958	2.46518
H	1.01665	2.23273	1.69595
H	3.57374	-0.98453	-2.31664
H	0.47114	2.07996	-1.90745
H	1.79636	-2.77468	-2.13353
H	-1.32727	0.19775	-1.78225
H	-1.63343	-3.07349	2.75849
H	-3.21674	-1.20284	3.43625
H	0.23300	-2.54297	1.19017
O	-2.42767	-2.41964	-1.07886
C	-3.25082	-1.45930	-0.94474
C	-4.69609	-1.82118	-0.52833
H	-4.78361	-2.88282	-0.25024
H	-5.02652	-1.18383	0.30997
H	-5.38056	-1.61558	-1.37032
O	-3.02804	-0.21126	-1.13702

B·OAc (b)
SCF (BP86) Energy = -1263.61961761
Enthalpy 0K = -1263.254889
Enthalpy 298K = -1263.226765
Free Energy 298K = -1263.315320
Lowest Frequency = 16.4969 cm^{-1}
Second Frequency = 32.4630 cm^{-1}
SCF (BP86-D3BJ) Energy = -1263.73537216
SCF (MeCN) Energy = -1263.64571925
SCF (Toluene) Energy = -1263.63184926
SCF (BS2) Energy = -1263.64431141

C	-0.77298	2.05946	0.03924
N	0.30583	1.22260	0.05652
C	1.57013	1.75377	-0.00645
C	1.75186	3.15106	-0.02512
C	0.64900	4.01279	-0.00124
C	-0.63248	3.45171	0.01141
Ru	-0.21653	-0.84822	0.07120
C	-1.11575	-2.82953	-0.35670
C	-1.80008	-1.79898	-1.09269
C	-1.06164	-0.92810	-1.95636

```
C   0.36658 -1.05424 -2.04214
C   1.06526 -2.03753 -1.27605
C   0.30878 -2.91344 -0.41439
H  -1.61510 -0.07912 -2.37613
C   2.77439  0.87927 -0.13281
C   3.62449  1.07603 -1.24542
C   4.78882  0.30816 -1.40156
C   5.13055 -0.65291 -0.43623
C   4.30119 -0.83990  0.68268
C   3.12833 -0.08409  0.83668
H   0.84249 -3.58922  0.26153
O  -1.54361 -0.25578  1.66715
C  -0.64158 -0.45917  2.55694
O   0.49131 -0.91895  2.14376
C  -0.88560 -0.14552  4.00865
H  -0.28423 -0.80612  4.65053
H  -0.58871  0.89811  4.21188
H  -1.95515 -0.24955  4.24265
H   3.35864  1.82678 -1.99787
H   5.42903  0.46412 -2.27596
H   4.57000 -1.57593  1.44774
H   6.04286 -1.24736 -0.55134
H   2.77342  3.53959 -0.05217
H   2.48493 -0.23829  1.70643
H  -1.66896 -3.44923  0.35471
H   2.15749 -2.06636 -1.27300
H  -2.89082 -1.54511 -0.92990
H   0.94653 -0.31484 -2.60356
H  -1.53619  4.06574 -0.01816
H   0.79327  5.09801 -0.01068
H  -1.76939  1.58952 -0.05874
O  -4.47556 -0.78474 -0.76485
C  -4.26892  0.46472 -0.86334
C  -5.43417  1.40464 -0.48467
H  -6.37883  0.84980 -0.37731
H  -5.20645  1.90202  0.47570
H  -5.54719  2.19949 -1.24104
O  -3.17817  1.03222 -1.23558
```

B·OAc (c)

SCF (BP86) Energy = -1263.61961756
Enthalpy 0K = -1263.254889
Enthalpy 298K = -1263.226765
Free Energy 298K = -1263.315322
Lowest Frequency = 16.5031 cm^{-1}
Second Frequency = 32.4711 cm^{-1}
SCF (BP86-D3BJ) Energy = -1263.73537003
SCF (MeCN) Energy = -1263.64572011
SCF (Toluene) Energy = -1263.63184947
SCF (BS2) Energy = -1263.64431247

```
C  -0.77285  2.05950  0.03911
N   0.30593  1.22261  0.05645
C   1.57024  1.75375 -0.00641
C   1.75201  3.15102 -0.02498
C   0.64918  4.01279 -0.00115
C  -0.63232  3.45175  0.01136
Ru -0.21653 -0.84818  0.07119
C  -1.80019 -1.79890 -1.09262
C  -1.06181 -0.92796 -1.95627
C   0.36641 -1.05414 -2.04222
C   1.06515 -2.03747 -1.27624
C   0.30874 -2.91341 -0.41456
C  -1.11579 -2.82951 -0.35676
H   0.94632 -0.31474 -2.60365
C   2.77447  0.87921 -0.13275
C   3.62480  1.07623 -1.24517
C   4.78911  0.30832 -1.40131
C   5.13061 -0.65301 -0.43618
C   4.30106 -0.84027  0.68252
C   3.12822 -0.08444  0.83652
H  -1.66893 -3.44927  0.35463
O  -1.54357 -0.25579  1.66723
C  -0.64149 -0.45920  2.55694
O   0.49143 -0.91884  2.14367
C  -0.88534 -0.14589  4.00878
H  -0.28737 -0.80985  4.65040
H  -0.58360  0.89607  4.21342
H  -1.95549 -0.24542  4.24189
H   3.35911  1.82719 -1.99747
H   5.42948  0.46448 -2.27557
H   4.56967 -1.57653  1.44741
H   6.04291 -1.24749 -0.55131
H   2.77357  3.53952 -0.05191
H   2.48464 -0.23884  1.70612
H  -2.89093 -1.54509 -0.92985
H   0.84248 -3.58928  0.26127
H  -1.61537 -0.07894 -2.37581
H   2.15739 -2.06630 -1.27330
H  -1.53601  4.06579 -0.01822
H   0.79346  5.09801 -0.01050
H  -1.76930  1.58958 -0.05883
O  -4.47576 -0.78471 -0.76497
C  -4.26919  0.46479 -0.86329
C  -5.43462  1.40461 -0.48492
H  -6.37909  0.84958 -0.37685
H  -5.20673  1.90289  0.47491
H  -5.54816  2.19881 -1.24193
O  -3.17841  1.03243 -1.23524
```

B·OAc (d)

SCF (BP86) Energy = -1263.61507137
Enthalpy 0K = -1263.249889
Enthalpy 298K = -1263.222304
Free Energy 298K = -1263.308311
Lowest Frequency = 17.6901 cm^{-1}
Second Frequency = 31.3655 cm^{-1}
SCF (BP86-D3BJ) Energy = -1263.73110743
SCF (MeCN) Energy = -1263.64376079
SCF (Toluene) Energy = -1263.62829778
SCF (BS2) Energy = -1263.63891540

```
C   1.74835 -2.53872 -0.31222
N   1.61726 -1.18249 -0.24002
C   2.68431 -0.40218 -0.61047
C   3.89759 -1.00089 -1.01634
C   4.03298 -2.39075 -1.05616
C   2.92693 -3.17641 -0.70257
Ru -0.22253 -0.52138  0.65635
C  -1.97221 -0.26146  1.97350
C  -1.01000 -1.14066  2.59037
C   0.34519 -0.72505  2.78241
C   0.75038  0.57617  2.31139
C  -0.19432  1.44445  1.68937
C  -1.56067  1.01779  1.50558
H   1.08360 -1.41890  3.19362
C   2.58867  1.08320 -0.60344
C   3.62335  1.83745 -0.00290
C   3.59063  3.23960 -0.02917
C   2.53479  3.90526 -0.67391
C   1.51219  3.16235 -1.28806
C   1.53125  1.75959 -1.25270
H  -2.32374  1.57014  0.87830
O  -1.14316 -2.12245 -0.40331
C  -1.46140 -1.32916 -1.38027
O  -0.94104 -0.14984 -1.33434
C  -2.45166 -1.72402 -2.41940
H  -3.42114 -1.39485 -1.97978
H  -2.27352 -1.18691 -3.36244
H  -2.45981 -2.81305 -2.57255
H   4.44547  1.31946  0.50390
H   4.39009  3.81084  0.45368
H   0.68985  3.67344 -1.79860
H   2.51093  4.99949 -0.70068
```

```
H    4.71743 -0.34740 -1.32561
H    0.73060  1.18905 -1.73110
H   -2.96442 -0.59983  1.63616
H    0.14564  2.39275  1.26525
H   -1.29139 -2.17130  2.82971
H    1.80555  0.86250  2.35214
H    2.96245 -4.26868 -0.72869
H    4.97423 -2.84980 -1.37378
H    0.85370 -3.10592 -0.04678
O   -3.76776  1.98539 -0.04132
C   -4.31879  0.93577 -0.50566
C   -5.45457  1.14824 -1.53383
H   -5.83868  2.17949 -1.49829
H   -5.06824  0.95933 -2.55246
H   -6.27399  0.43152 -1.35877
O   -4.02082 -0.28014 -0.23052
```

B·OAc (e)

SCF (BP86) Energy = -1263.61424113
Enthalpy 0K = -1263.249268
Enthalpy 298K = -1263.221303
Free Energy 298K = -1263.308786
Lowest Frequency = 19.8544 cm^{-1}
Second Frequency = 37.7138 cm^{-1}
SCF (BP86-D3BJ) Energy = -1263.73026114
SCF (MeCN) Energy = -1263.64295556
SCF (Toluene) Energy = -1263.62741353
SCF (BS2) Energy = -1263.63837944

```
C    2.85683 -1.36773 -0.44090
N    1.95136 -0.36456 -0.24295
C    2.32473  0.92472 -0.54816
C    3.61754  1.17645 -1.06785
C    4.53802  0.14533 -1.25493
C    4.14766 -1.16083 -0.92617
Ru   0.08848 -1.05151  0.59895
C   -1.12625 -2.22019  2.01117
C    0.18231 -1.97377  2.58147
C    0.66530 -0.63554  2.67912
C   -0.13780  0.46402  2.19860
C   -1.41135  0.20586  1.61632
C   -1.92412 -1.14197  1.54567
H    1.68699 -0.45692  3.02877
C    1.42271  2.08266 -0.31684
C    1.96566  3.23963  0.29653
C    1.16031  4.36163  0.53513
C   -0.19628  4.34537  0.16541
C   -0.74480  3.20923 -0.45174
C    0.06318  2.08819 -0.70064
H   -2.86207 -1.23727  0.94492
O    0.32437 -2.74623 -0.72436
C   -0.27074 -2.11267 -1.68327
O   -0.64615 -0.91265 -1.43208
C   -0.55082 -2.76339 -3.00796
H   -1.58846 -3.13969 -3.00236
H   -0.46831 -2.02386 -3.81843
H    0.13151 -3.60814 -3.18041
H    3.01328  3.24282  0.61807
H    1.59018  5.24210  1.02449
H   -1.81322  3.13158 -0.68903
H   -0.82836  5.21633  0.36866
H    3.86677  2.20511 -1.33939
H   -0.37830  1.21836 -1.19162
H   -1.44460 -3.25318  1.83984
H   -2.03519  0.96403  1.06762
H    0.82549 -2.81080  2.86929
H    0.27856  1.47437  2.18606
H    4.81853 -2.01505 -1.04921
H    5.53348  0.35367 -1.65921
H    2.50087 -2.37132 -0.20096
O   -3.26263  1.58013 -0.12384
C   -3.99561  0.66621 -0.64905
C   -4.91582  1.13677 -1.79885
H   -5.49443  2.02210 -1.48457
H   -4.30065  1.44716 -2.66244
H   -5.60192  0.33664 -2.11627
O   -4.04142 -0.56370 -0.33288
```

B·OAc (f)

SCF (BP86) Energy = -1263.62317092
Enthalpy 0K = -1263.257959
Enthalpy 298K = -1263.229825
Free Energy 298K = -1263.317921
Lowest Frequency = 25.5920 cm^{-1}
Second Frequency = 37.5366 cm^{-1}
SCF (BP86-D3BJ) Energy = -1263.74415430
SCF (MeCN) Energy = -1263.64507472
SCF (Toluene) Energy = -1263.63339571
SCF (BS2) Energy = -1263.64784417

```
C   -0.46220 -1.76645  1.51423
N   -0.24161 -0.52500  0.99931
C   -1.09438  0.49113  1.33615
C   -2.16606  0.25355  2.21941
C   -2.37944 -1.01800  2.75653
C   -1.50596 -2.05068  2.39393
Ru   1.28671 -0.41145 -0.48720
C    2.13457  0.66170 -2.19511
C    2.51626 -0.70879 -2.29745
C    1.49469 -1.72547 -2.20436
C    0.11440 -1.37223 -2.09948
C   -0.25289  0.01540 -2.03321
C    0.74423  1.03266 -2.06888
H    1.79567 -2.77586 -2.13265
C   -0.91939  1.86403  0.77842
C   -1.96123  2.40319 -0.01035
C   -1.85178  3.71396 -0.50158
C   -0.72413  4.49691 -0.19974
C    0.30544  3.96289  0.59428
C    0.21216  2.65049  1.08378
H    0.47202  2.07927 -1.90809
O    2.41271 -1.65167  0.87475
C    2.87155 -0.61756  1.49384
O    2.53736  0.53441  1.03033
C    3.72977 -0.75773  2.72232
H    4.39586  0.11144  2.82496
H    3.08252 -0.80432  3.61539
H    4.31527 -1.68777  2.67514
H   -2.80161  1.75070 -0.28304
H   -2.65190  4.12250 -1.12803
H    1.18262  4.57080  0.84048
H   -0.64842  5.52170 -0.57932
H   -2.82330  1.09104  2.46509
H    1.01701  2.23333  1.69527
H    2.91003  1.43072 -2.12084
H   -1.32698  0.19767 -1.78239
H    3.57364 -0.98634 -2.31634
H   -0.71249 -2.08454 -1.88291
H   -1.63433 -3.07238  2.75901
H   -3.21684 -1.20104  3.43671
H    0.23211 -2.54279  1.19042
O   -2.42795 -2.41989 -1.07841
C   -3.25088 -1.45933 -0.94443
C   -4.69622 -1.82078 -0.52793
H   -5.38107 -1.61289 -1.36903
H   -4.78447 -2.88283 -0.25167
H   -5.02553 -1.18471  0.31181
O   -3.02775 -0.21136 -1.13673
```

B·OAc (under)

SCF (BP86) Energy = -1263.60508082
Enthalpy 0K = -1263.239992
Enthalpy 298K = -1263.212332
Free Energy 298K = -1263.297578

Lowest Frequency = 29.9419 cm^{-1}
Second Frequency = 40.0174 cm^{-1}
SCF (BP86-D3BJ) Energy = -1263.72755546
SCF (MeCN) Energy = -1263.63052978
SCF (Toluene) Energy = -1263.61629427
SCF (BS2) Energy = -1263.63187008

C	1.46540	-0.49254	1.71408
N	0.48803	0.13376	1.00247
C	0.44055	1.50961	1.03440
C	1.19187	2.22877	1.97207
C	2.08132	1.55791	2.82693
C	2.24676	0.18566	2.66567
Ru	-1.00535	-1.09811	0.09648
C	-2.74898	-2.36498	-0.44821
C	-2.47019	-2.44293	0.95979
C	-2.43740	-1.26530	1.77765
C	-2.61089	0.01195	1.14947
C	-2.84074	0.12210	-0.25401
C	-2.87409	-1.07619	-1.05003
H	-2.18365	-1.33475	2.83780
C	-0.38673	2.24317	0.04087
C	-1.34125	3.20046	0.44706
C	-2.09220	3.90539	-0.50872
C	-1.88047	3.67169	-1.87827
C	-0.90186	2.74652	-2.28689
C	-0.15280	2.03603	-1.33768
H	-2.92801	-0.99407	-2.13971
O	0.47285	-2.61009	-0.00748
C	0.90961	-2.16845	-1.14925
O	0.24469	-1.17419	-1.63715
C	2.10772	-2.75220	-1.80758
H	2.12067	-2.51202	-2.88038
H	2.96932	-2.26154	-1.29167
H	2.14747	-3.84001	-1.64426
H	-1.49948	3.38598	1.51616
H	-2.83781	4.63885	-0.18368
H	-0.70703	2.59104	-3.35339
H	-2.46070	4.22505	-2.62445
H	1.11869	3.31913	1.97114
H	0.65291	1.35566	-1.62851
H	-2.71278	-3.26488	-1.06668
H	-2.88638	1.10528	-0.72765
H	-2.21063	-3.41005	1.40109
H	-2.46691	0.92457	1.73373
H	2.98258	-0.38222	3.23967
H	2.67080	2.11484	3.56210
H	1.51523	-1.57460	1.60967
O	3.35416	-0.82996	0.02891
C	3.57182	0.28824	-0.57974
C	4.81562	0.29413	-1.50616
H	5.65967	-0.23426	-1.03265
H	4.58164	-0.24217	-2.44437
H	5.10820	1.32411	-1.76255
O	2.88166	1.34083	-0.51457

$^{-}$OAc
SCF (BP86) Energy = -228.501360687
Free Energy 393K = -228.493848
Lowest Frequency = 29.2221 cm^{-1}
Second Frequency = 394.1986 cm^{-1}

AcOH
SCF (BP86) Energy = -229.088709027
Free Energy 393K = -229.066909
Lowest Frequency = 61.5916 cm^{-1}
Second Frequency = 405.1411 cm^{-1}

a–H, 2-phenylpyridine
SCF (BP86) Energy = -479.337880864
Free Energy 393K = -479.223488
Lowest Frequency = 40.8265 cm^{-1}
Second Frequency = 91.4534 cm^{-1}

Benzene (C_6H_6)
SCF (BP86) Energy = -232.242069547
Free Energy 393K = -232.182907
Lowest Frequency = 397.4291 cm^{-1}
Second Frequency = 397.4511 cm^{-1}

MeCN
SCF (BP86) Energy = -132.751073488
Free Energy 393K = -132.740469
Lowest Frequency = 373.9505 cm^{-1}
Second Frequency = 373.9931 cm^{-1}

A
SCF (BP86) Energy = -784.308941980
Free Energy 393K = -784.176317
Lowest Frequency = 8.5090 cm^{-1}
Second Frequency = 52.9166 cm^{-1}

B^{+}
SCF (BP86) Energy = -1034.96464164
Free Energy 393K = -1034.723316
Lowest Frequency = 26.7464 cm^{-1}
Second Frequency = 39.6376 cm^{-1}

TS(**B**$^{+}$–**C**$^{+}$)
SCF (BP86) Energy = -1034.94113282
Free Energy 393K = -1034.700230
Lowest Frequency = -100.9914 cm^{-1}
Second Frequency = 28.4602 cm^{-1}

C^{+}
SCF (BP86) Energy = -1034.96564411
Free Energy 393K = -1034.725270
Lowest Frequency = 22.7345 cm^{-1}
Second Frequency = 23.9119 cm^{-1}

B·OAc
SCF (BP86) Energy = -1263.62317136
Free Energy 393K = -1263.348440
Lowest Frequency = 25.6019 cm^{-1}
Second Frequency = 37.4342 cm^{-1}

TS(**B**–**C**)1·OAc
SCF (BP86) Energy = -1263.60220672
Free Energy 393K = -1263.331145
Lowest Frequency = -98.0066 cm^{-1}
Second Frequency = 14.9802 cm^{-1}

INT(**B**–**C**)·OAc
SCF (BP86) Energy = -1263.60859226
Free Energy 393K = -1263.337931
Lowest Frequency = 16.8307 cm^{-1}
Second Frequency = 20.6795 cm^{-1}

TS(**B**–**C**)2·OAc
SCF (BP86) Energy = -1263.60826342
Free Energy 393K = -1263.337475
Lowest Frequency = -254.6588 cm^{-1}
Second Frequency = 17.4296 cm^{-1}

C·OAc
SCF (BP86) Energy = -1263.62198851
Free Energy 393K = -1263.348779
Lowest Frequency = 13.2167 cm^{-1}
Second Frequency = 26.7650 cm^{-1}

A·**a**–H
SCF (BP86) Energy = -1263.65263818
Free Energy 393K = -1263.383678
Lowest Frequency = 10.1879 cm^{-1}
Second Frequency = 12.9851 cm^{-1}

B
SCF (BP86) Energy = -1263.64592624
Free Energy 393K = -1263.368954
Lowest Frequency = 28.1806 cm^{-1}
Second Frequency = 34.0089 cm^{-1}

TS(**B**–**C**)
SCF (BP86) Energy = -1263.59805873
Free Energy 393K = -1263.323436
Lowest Frequency = -86.5875 cm^{-1}
Second Frequency = 23.6666 cm^{-1}

C
SCF (BP86) Energy = -1263.66809038
Free Energy 393K = -1263.392280
Lowest Frequency = 23.7543 cm^{-1}
Second Frequency = 26.8449 cm^{-1}

B′
SCF (BP86) Energy = -1031.40787653
Free Energy 393K = -1031.215943
Lowest Frequency = 35.8296 cm^{-1}
Second Frequency = 58.8576 cm^{-1}

TS(**B′**–**B′**)
SCF (BP86) Energy = -1031.37308205
Free Energy 393K = -1031.184045
Lowest Frequency = -64.5915 cm^{-1}
Second Frequency = 11.5338 cm^{-1}

C′
SCF (BP86) Energy = -1031.36947647
Free Energy 393K = -1031.184656
Lowest Frequency = 12.1013 cm^{-1}
Second Frequency = 23.0938 cm^{-1}

C′ (without HOAc)
SCF (BP86) Energy = -802.265265895
Free Energy 393K = -802.125733
Lowest Frequency = 33.6630 cm^{-1}
Second Frequency = 44.0278 cm^{-1}

D^{+} (κ^1)
SCF (BP86) Energy = -1282.03894895
Free Energy 393K = -1281.742706
Lowest Frequency = 29.3843 cm^{-1}
Second Frequency = 36.3944 cm^{-1}

TS(**D**$^{+}$–**E**$^{+}$) (κ^1)
SCF (BP86) Energy = -1282.03427439

Free Energy 393K = -1281.739891
Lowest Frequency = -890.9421 cm^{-1}
Second Frequency = 33.0601 cm^{-1}

E$^+$ (κ^1)
SCF (BP86) Energy = -1282.03838937
Free Energy 393K = -1281.741054
Lowest Frequency = 31.1664 cm^{-1}
Second Frequency = 35.4221 cm^{-1}

D$^+$ (κ^2)
SCF (BP86) Energy = -1282.05904449
Free Energy 393K = -1281.759698
Lowest Frequency = 24.2483 cm^{-1}
Second Frequency = 42.6874 cm^{-1}

TS(**D$^+$**–**E$^+$**) (κ^2)
SCF (BP86) Energy = -1282.03247464
Free Energy 393K = -1281.738554
Lowest Frequency = -995.2545 cm^{-1}
Second Frequency = 22.6884 cm^{-1}

E$^+$ (κ^2)
SCF (BP86) Energy = -1282.04711192
Free Energy 393K = -1281.750307
Lowest Frequency = 26.6438 cm^{-1}
Second Frequency = 31.9960 cm^{-1}

D
SCF (BP86) Energy = -1510.76736972
Free Energy 393K = -1510.433281
Lowest Frequency = 23.7201 cm^{-1}
Second Frequency = 32.4861 cm^{-1}

TS(**D**–**E**)
SCF (BP86) Energy = -1510.73262187
Free Energy 393K = -1510.402800
Lowest Frequency = -1053.6288 cm^{-1}
Second Frequency = 27.2003 cm^{-1}

E
SCF (BP86) Energy = -1510.75701343
Free Energy 393K = -1510.423749
Lowest Frequency = 19.9444 cm^{-1}
Second Frequency = 23.3707 cm^{-1}

E (without HOAc)
SCF (BP86) Energy = -1281.67152225
Free Energy 393K = -1281.384617
Lowest Frequency = 30.2612 cm^{-1}
Second Frequency = 35.7530 cm^{-1}

D$^+$ (η^6)
SCF (BP86) Energy = -1282.06544576
Free Energy 393K = -1281.770188
Lowest Frequency = 9.2296 cm^{-1}
Second Frequency = 16.3692 cm^{-1}

TS(**D$^+$**–**E$^+$**) (η^6)
SCF (BP86) Energy = -1282.04288362
Free Energy 393K = -1281.746182
Lowest Frequency = -102.1099 cm^{-1}
Second Frequency = 14.3031 cm^{-1}

E$^+$ (η^6)
SCF (BP86) Energy = -1282.06784697
Free Energy 393K = -1281.770237
Lowest Frequency = 17.7257 cm^{-1}
Second Frequency = 25.9568 cm^{-1}

^{3}D$^+$
SCF (BP86) Energy = -1680.38957213
Free Energy 393K = -1679.987415
Lowest Frequency = 5.7842 cm^{-1}
Second Frequency = 23.1450 cm^{-1}

INT(**^{3}D$^+$**)
SCF (BP86) Energy = -1680.36814747
Free Energy 393K = -1679.964754
Lowest Frequency = 23.3930 cm^{-1}
Second Frequency = 25.4866 cm^{-1}

TS(**^{3}D$^+$**–**^{3}E$^+$**)
SCF (BP86) Energy = -1680.35096198
Free Energy 393K = -1679.950878
Lowest Frequency = -873.7813 cm^{-1}
Second Frequency = 18.3071 cm^{-1}

^{3}E$^+$
SCF (BP86) Energy = -1680.35995727
Free Energy 393K = -1679.958757
Lowest Frequency = 18.9857 cm^{-1}
Second Frequency = 22.0690 cm^{-1}

^{6}F^{2+}
SCF (BP86) Energy = -891.226975652
Free Energy 393K = -891.054235
Lowest Frequency = -4.1196 cm^{-1}
Second Frequency = 3.7482 cm^{-1}

^{3}A^{2+}
SCF (BP86) Energy = -725.084942003
Free Energy 393K = -724.925239
Lowest Frequency = 14.6220 cm^{-1}
Second Frequency = 18.9704 cm^{-1}

^{5}F$^+$ (κ^1)
SCF (BP86) Energy = -987.234219220
Free Energy 393K = -987.057303
Lowest Frequency = 8.9474 cm^{-1}
Second Frequency = 17.0147 cm^{-1}

^{4}F$^+$ (κ^2)
SCF (BP86) Energy = -854.470356597
Free Energy 393K = -854.325986
Lowest Frequency = 16.3263 cm^{-1}
Second Frequency = 17.1735 cm^{-1}

f–**^{3}F** ($\kappa^2\kappa^1$)
SCF (BP86) Energy = -950.375149816
Free Energy 393K = -950.226828
Lowest Frequency = 23.1768 cm^{-1}
Second Frequency = 36.3363 cm^{-1}

m–**^{3}F** ($\kappa^2\kappa^1$)
SCF (BP86) Energy = -950.367950843
Free Energy 393K = -950.225475
Lowest Frequency = 2.5503 cm^{-1}
Second Frequency = 21.5824 cm^{-1}

c–**^{2}F** ($2\kappa^2$)
SCF (BP86) Energy = -817.609089806
Free Energy 393K = -817.495110
Lowest Frequency = 20.8094 cm^{-1}
Second Frequency = 23.7247 cm^{-1}

t–**^{2}F** ($2\kappa^2$)
SCF (BP86) Energy = -817.605958390
Free Energy 393K = -817.491575
Lowest Frequency = -1.9844 cm^{-1}

Second Frequency = 5.9946 cm^{-1}

c-**^{4}F** ($2\kappa^1$)
SCF (BP86) Energy = -1083.13381667
Free Energy 393K = -1082.952470
Lowest Frequency = 30.7708 cm^{-1}
Second Frequency = 31.9410 cm^{-1}

t-**^{4}F** ($2\kappa^1$)
SCF (BP86) Energy = -1083.13257282
Free Energy 393K = -1082.952891
Lowest Frequency = 22.3020 cm^{-1}
Second Frequency = 24.9120 cm^{-1}

^{1}A
SCF (BP86) Energy = -917.075823895
Free Energy 393K = -916.908832
Lowest Frequency = 8.0027 cm^{-1}
Second Frequency = 42.9119 cm^{-1}

^{1}A$^+$
SCF (BP86) Energy = -688.369203651
Free Energy 393K = -688.240375
Lowest Frequency = 14.5765 cm^{-1}
Second Frequency = 20.7538 cm^{-1}

^{1}B$^+$ (*t*-O,*t*-N)
SCF (BP86) Energy = -1167.72294598
Free Energy 393K = -1167.447011
Lowest Frequency = 34.4425 cm^{-1}
Second Frequency = 35.4414 cm^{-1}

TS(**^{1}B$^+$**–**^{1}C$^+$**) (*t*-O,*t*-N)
SCF (BP86) Energy = -1167.68769362
Free Energy 393K = -1167.416256
Lowest Frequency = -844.6082 cm^{-1}
Second Frequency = 27.2943 cm^{-1}

^{1}C$^+$ (*t*-O,*t*-N)
SCF (BP86) Energy = -1167.69618734
Free Energy 393K = -1167.423078
Lowest Frequency = 19.2265 cm^{-1}
Second Frequency = 31.3465 cm^{-1}

^{1}B$^+$ (*t*-O,*t*-C_6H_6)
SCF (BP86) Energy = -1167.71349134
Free Energy 393K = -1167.438709
Lowest Frequency = 30.5581 cm^{-1}
Second Frequency = 32.7017 cm^{-1}

TS(**^{1}B$^+$**–**^{1}C$^+$**) (*t*-O,*t*-C_6H_6)
SCF (BP86) Energy = -1167.68971633
Free Energy 393K = -1167.419716
Lowest Frequency = -1005.5333 cm^{-1}
Second Frequency = 19.3865 cm^{-1}

^{1}C$^+$ (*t*-O,*t*-C_6H_6)
SCF (BP86) Energy = -1167.72465823
Free Energy 393K = -1167.451178
Lowest Frequency = 22.4613 cm^{-1}
Second Frequency = 30.5848 cm^{-1}

^{1}B$^+$ (*t*-O,*t*-O)
SCF (BP86) Energy = -1167.71744568
Free Energy 393K = -1167.444915
Lowest Frequency = 20.4934 cm^{-1}
Second Frequency = 21.4590 cm^{-1}

^{1}B$^+$ (*t*-C_6H_6,*t*-O)
SCF (BP86) Energy = -1167.72161567
Free Energy 393K = -1167.447448
Lowest Frequency = 21.8185 cm^{-1}
Second Frequency = 28.6002 cm^{-1}

TS(**^{1}B$^+$**–**^{1}C$^+$**)1 (*t*-C_6H_6,*t*-O)
SCF (BP86) Energy = -1167.69108447
Free Energy 393K = -1167.417865
Lowest Frequency = -91.3713 cm^{-1}
Second Frequency = 23.8054 cm^{-1}

INT(**^{1}B$^+$**–**^{1}C$^+$**) (*t*-C_6H_6,*t*-O)
SCF (BP86) Energy = -1167.68848672
Free Energy 393K = -1167.418594
Lowest Frequency = 19.9603 cm^{-1}
Second Frequency = 25.7070 cm^{-1}

TS(**^{1}B$^+$**–**^{1}C$^+$**)2 (*t*-C_6H_6,*t*-O)
SCF (BP86) Energy = -1167.68832141
Free Energy 393K = -1167.418609
Lowest Frequency = -240.3765 cm^{-1}
Second Frequency = 20.2290 cm^{-1}

^{1}C$^+$ (*t*-C_6H_6,*t*-O)
SCF (BP86) Energy = -1167.70548939
Free Energy 393K = -1167.434191
Lowest Frequency = 15.7244 cm^{-1}
Second Frequency = 25.6284 cm^{-1}

^{1}B$^+$ (*t*-N,*t*-O)
SCF (BP86) Energy = -1167.72106214
Free Energy 393K = -1167.446449
Lowest Frequency = 22.3355 cm^{-1}
Second Frequency = 25.9615 cm^{-1}

TS(**^{1}B$^+$**–**^{1}C$^+$**) (*t*-N,*t*-O)
SCF (BP86) Energy = -1167.69403569
Free Energy 393K = -1167.420498
Lowest Frequency = -115.9387 cm^{-1}
Second Frequency = 24.5977 cm^{-1}

^{1}C$^+$ (*t*-N,*t*-O)
SCF (BP86) Energy = -1167.73105755
Free Energy 393K = -1167.456594
Lowest Frequency = 23.6990 cm^{-1}
Second Frequency = 33.5988 cm^{-1}

^{4}G$^+$ (κ^1)
SCF (BP86) Energy = -1333.81273065
Free Energy 393K = -1333.522977
Lowest Frequency = 9.4918 cm^{-1}
Second Frequency = 17.2099 cm^{-1}

^{3}G ($2\kappa^1$)
SCF (BP86) Energy = -1429.71423532
Free Energy 393K = -1429.420933
Lowest Frequency = 18.7942 cm^{-1}
Second Frequency = 29.6300 cm^{-1}

^{1}G ($2\kappa^2$)
SCF (BP86) Energy = -1164.19014654
Free Energy 393K = -1163.968504
Lowest Frequency = 4.3996 cm^{-1}
Second Frequency = 30.5514 cm^{-1}

^{2}G$^+$ (κ^2)
SCF (BP86) Energy = -1068.27102327
Free Energy 393K = -1068.049841
Lowest Frequency = 19.4187 cm^{-1}
Second Frequency = 23.0992 cm^{-1}

^{3}G^{+} (κ^2)
SCF (BP86) Energy = -1201.03658211
Free Energy 393K = -1200.781064
Lowest Frequency = 18.9178 cm^{-1}
Second Frequency = 23.9391 cm^{-1}

^{1}G ($\kappa^2\kappa^1$)
SCF (BP86) Energy = -1164.18926443
Free Energy 393K = -1163.966520
Lowest Frequency = 21.5009 cm^{-1}
Second Frequency = 31.2083 cm^{-1}

TS(**^{1}G–^{1}H**)
SCF (BP86) Energy = -1164.18761054
Free Energy 393K = -1163.966856
Lowest Frequency = -656.6522 cm^{-1}
Second Frequency = 23.0147 cm^{-1}

^{1}H
SCF (BP86) Energy = -1164.19893635
Free Energy 393K = -1163.977379
Lowest Frequency = 18.0223 cm^{-1}
Second Frequency = 19.6428 cm^{-1}

^{2}G ($\kappa^2\kappa^1$)
SCF (BP86) Energy = -1296.95420397
Free Energy 393K = -1296.697602
Lowest Frequency = 29.6859 cm^{-1}
Second Frequency = 32.8414 cm^{-1}

TS(**^{2}G–^{2}H**)
SCF (BP86) Energy = -1296.95136610
Free Energy 393K = -1296.696199
Lowest Frequency = -789.9532 cm^{-1}
Second Frequency = 33.6754 cm^{-1}

^{2}H
SCF (BP86) Energy = -1296.95983158
Free Energy 393K = -1296.702236
Lowest Frequency = 29.1975 cm^{-1}
Second Frequency = 29.9685 cm^{-1}

$^{-}$OMes
SCF (BP86) Energy = -538.202534223
Free Energy 393K = -538.080444
Lowest Frequency = 40.8103 cm^{-1}
Second Frequency = 76.0025 cm^{-1}

$[(C_6H_6)Ru(OMes)]^{+}$
SCF (BP86) Energy = -865.249489757
Free Energy 393K = -865.040896
Lowest Frequency = 20.1617 cm^{-1}
Second Frequency = 27.7357 cm^{-1}

$[(C_6H_6)Ru(OMes)_2]$
SCF (BP86) Energy = -1403.66917957
Free Energy 393K = -1403.309293
Lowest Frequency = 10.8485 cm^{-1}
Second Frequency = 15.4587 cm^{-1}

$^{-}$O^{t}Bu
SCF (BP86) Energy = -346.450213517
Free Energy 393K = -346.365698
Lowest Frequency = -27.2251 cm^{-1}
Second Frequency = 205.8483 cm^{-1}

$[(C_6H_6)Ru(O^tBu)]^{+}$
SCF (BP86) Energy = -673.494518023
Free Energy 393K = -673.326655
Lowest Frequency = 10.9105 cm^{-1}
Second Frequency = 38.1463 cm^{-1}

$[(C_6H_6)Ru(O^tBu)_2]$
SCF (BP86) Energy = -1020.18455813
Free Energy 393K = -1019.903725
Lowest Frequency = 8.8349 cm^{-1}
Second Frequency = 16.5325 cm^{-1}

$[(C_6H_6)Ru(OAc)]$
SCF (BP86) Energy = -555.552331451
Free Energy 393K = -555.457985
Lowest Frequency = 30.6692 cm-1
Second Frequency = 46.2171 cm-1

Toluene (tol)
SCF (BP86) Energy = -271.559258208
Free Energy 393K = -271.478745
Lowest Frequency = 28.9236 cm^{-1}
Second Frequency = 202.7212 cm^{-1}

$[(tol)Ru(OAc)_2]$
SCF (BP86) Energy = -823.628702031
Free Energy 393K = -823.471582
Lowest Frequency = 24.7351 cm^{-1}
Second Frequency = 54.4596 cm^{-1}

o-xylene (*o*-xyl)
SCF (BP86) Energy = -310.876056618
Free Energy 393K = -310.769909
Lowest Frequency = 132.8541 cm^{-1}
Second Frequency = 155.6287 cm^{-1}

$[(o\text{-xyl})Ru(OAc)_2]$
SCF (BP86) Energy = -862.944926979
Free Energy 393K = -862.766848
Lowest Frequency = 5.2150 cm-1
Second Frequency = 53.0386 cm-1

p-cymene (*p*-cym)
SCF (BP86) Energy = -389.500963444
Free Energy 393K = -389.348456
Lowest Frequency = 27.5360 cm^{-1}
Second Frequency = 39.1081 cm^{-1}

$[(p\text{-cym})Ru(OAc)_2]$
SCF (BP86) Energy = -941.573231536
Free Energy 393K = -941.343107
Lowest Frequency = 23.7827 cm^{-1}
Second Frequency = 38.7127 cm^{-1}

C_6Me_6 (Bn*)
SCF (BP86) Energy = -468.126900997
Free Energy 393K = -467.931152
Lowest Frequency = 39.6292 cm^{-1}
Second Frequency = 54.9209 cm^{-1}

$[(Bn^*)Ru(OAc)_2]$

SCF (BP86) Energy = -1020.20321510
Free Energy 393K = -1019.926679
Lowest Frequency = 26.4277 cm^{-1}
Second Frequency = 45.4342 cm^{-1}

$^{-}$OAc (* single point)
SCF (B3LYP) Energy = -228.496852530
Enthalpy 0K = -228.448903
Enthalpy 298K = -228.443902
Free Energy 298K = -228.475153
Lowest Frequency = 257.5981 cm^{-1}
Second Frequency = 432.8976 cm^{-1}

AcOH
SCF (B3LYP) Energy = -229.087408880
Enthalpy 0K = -229.025401
Enthalpy 298K = -229.019902
Free Energy 298K = -229.052543
Lowest Frequency = 77.3824 cm^{-1}
Second Frequency = 419.5733 cm^{-1}

O	-0.77943	-1.04551	-0.00011
H	-1.72070	-0.80361	-0.00036
C	-0.09256	0.12511	0.00041
O	-0.64408	1.20247	-0.00010
C	1.39696	-0.11065	-0.00001
H	1.68318	-0.69263	0.88110
H	1.68270	-0.69285	-0.88114
H	1.91652	0.84661	-0.00028

a-H, 2-phenylpyridine
SCF (B3LYP) Energy = -479.348941685
Enthalpy 0K = -479.179008
Enthalpy 298K = -479.169290
Free Energy 298K = -479.213774
Lowest Frequency = 45.3882 cm^{-1}
Second Frequency = 95.9752 cm^{-1}

N	-1.36715	-1.15785	-0.20136
C	-2.70085	-1.20482	-0.20910
C	-3.51897	-0.08968	-0.02298
H	-3.14130	-2.18704	-0.37525
H	-4.59963	-0.18653	-0.04448
C	0.72524	0.02777	-0.00462
C	1.47063	1.20195	-0.20138
C	2.81013	-1.20765	0.19767
C	2.86456	1.17246	-0.19297
H	0.96559	2.14449	-0.38839
C	3.54063	-0.03163	0.01074
H	3.32759	-2.15018	0.35353
H	3.42238	2.09068	-0.35381
H	4.62666	-0.05409	0.01818
C	-0.76305	0.03000	-0.00072
C	-2.89916	1.13895	0.20044
H	-3.48889	2.03582	0.36832
C	-1.50905	1.20172	0.21782
H	-1.01093	2.14328	0.41951
C	1.41778	-1.17972	0.18651
H	0.84139	-2.08753	0.32347

Benzene (C6H6)
SCF (B3LYP) Energy = -232.252444239
Enthalpy 0K = -232.152638
Enthalpy 298K = -232.147379
Free Energy 298K = -232.180078
Lowest Frequency = 432.6362 cm^{-1}
Second Frequency = 432.6589 cm^{-1}

C	0.00000	1.40481	0.00000
C	-1.21659	0.70239	0.00000
C	-1.21659	-0.70239	0.00000
C	0.00000	-1.40480	0.00000
C	1.21659	-0.70239	0.00000
C	1.21658	0.70240	0.00000
H	-2.16519	1.25006	0.00000
H	-2.16518	-1.25007	0.00000
H	0.00001	-2.50014	0.00000
H	2.16519	-1.25006	0.00000
H	2.16518	1.25007	0.00000
H	-0.00001	2.50001	0.00000

MeCN
SCF (B3LYP) Energy = -132.755637557
Enthalpy 0K = -132.710201
Enthalpy 298K = -132.705658
Free Energy 298K = -132.734217
Lowest Frequency = 387.0631 cm^{-1}
Second Frequency = 387.0843 cm^{-1}

C	0.00001	-1.18046	0.00000
H	-1.02585	-1.55954	0.00000
H	0.51294	-1.55953	0.88842
H	0.51294	-1.55953	-0.88842
C	0.00000	0.28001	0.00000
N	-0.00001	1.44019	0.00000

A
SCF (B3LYP) Energy = -784.206320951
Enthalpy 0K = -783.999965
Enthalpy 298K = -783.983254
Free Energy 298K = -784.045019
Lowest Frequency = 14.9029 cm^{-1}
Second Frequency = 59.3099 cm^{-1}

C	1.87318	-0.72673	1.41961
C	2.49806	0.34739	0.70106
C	2.49534	0.34199	-0.71029
C	1.86981	-0.73828	-1.41927
C	1.27544	-1.80537	-0.71153
C	1.27695	-1.79975	0.72211
Ru	0.40909	0.10709	-0.00083
O	-0.40928	1.77397	-1.08827
C	-0.78777	2.31782	0.00130
C	-1.66960	3.53212	0.00225
H	2.87959	1.19561	-1.25702
H	0.71140	-2.55811	1.24571
O	-1.57444	-0.41053	-0.00575
C	-2.05459	-1.63010	0.00006
O	-1.40050	-2.67317	0.00813
O	-0.41297	1.76963	1.09003
C	-3.57931	-1.64702	-0.00382
H	-3.95987	-1.11807	0.87521
H	-3.95578	-1.12179	-0.88680
H	-3.94157	-2.67565	-0.00226
H	-2.71403	3.20264	-0.00055
H	-1.49850	4.12645	0.90173
H	-1.49498	4.13036	-0.89396
H	1.78912	-0.67080	2.49937
H	0.70845	-2.56779	-1.22765
H	1.78369	-0.69123	-2.49926
H	2.88463	1.20486	1.24003

B^{+}
SCF (B3LYP) Energy = -1034.87824638
Enthalpy 0K = -1034.550636
Enthalpy 298K = -1034.529100
Free Energy 298K = -1034.601619
Lowest Frequency = 20.1662 cm^{-1}
Second Frequency = 40.2229 cm^{-1}

C	-0.07344	-2.30152	-0.68524
C	-2.81859	-1.43876	1.93136
C	-3.84290	-1.93324	1.11914
C	-4.09547	-1.33871	-0.11965
C	-2.27605	0.22945	0.25660

```
C  -1.52248  3.73283 -0.92697
O   1.07992 -0.08398  1.90223
C   2.06296  0.72407  1.79669
O   2.52804  0.88107  0.61335
C   2.61878  1.46473  2.97025
H  -2.06271  4.64982 -1.13989
H   2.42227  0.91604  3.89257
H   3.69032  1.62724  2.83969
H   2.13225  2.44415  3.03949
H  -4.89757 -1.70937 -0.75034
H  -4.45133 -2.76682  1.45620
H  -2.63554 -1.88111  2.90597
C   0.50297  2.46970 -0.78394
H   1.57744  2.37806 -0.87680
C  -0.13831  3.66497 -1.07471
H   0.44420  4.51629 -1.40830
C  -1.50425  1.41535 -0.20614
Ru  1.06658 -0.42667 -0.21423
C   2.37118 -1.31995 -1.75063
H   3.29599 -0.87449 -2.10191
C   2.39475 -2.18072 -0.60890
H   3.33171 -2.39571 -0.10874
C   1.17286 -2.64116 -0.06973
H   1.17401 -3.19844  0.86101
C   1.14727 -0.98272 -2.37933
H   1.13578 -0.30416 -3.22409
C  -0.07479 -1.47759 -1.83200
H  -1.02111 -1.15421 -2.24975
H  -1.00842 -2.61265 -0.23599
C  -2.19874  2.60101 -0.48745
H  -3.27158  2.61779 -0.33426
C  -3.32518 -0.25461 -0.54332
H  -3.53471  0.21584 -1.50051
N  -0.15235  1.35840 -0.36739
C  -2.03458 -0.36546  1.50517
H  -1.24345  0.01338  2.14161
```

TS (B^+-C^+)

SCF (B3LYP) Energy = -1034.85234568
Enthalpy 0K = -1034.526184
Enthalpy 298K = -1034.504951
Free Energy 298K = -1034.577054
Lowest Frequency = -69.6633 cm^{-1}
Second Frequency = 25.8127 cm^{-1}

```
C   0.36172  2.69270 -0.51792
N   0.67025  1.40602 -0.26623
C   1.94151  1.06895  0.07462
C   2.94886  2.03823  0.10638
C   2.63935  3.36230 -0.19121
C   1.31988  3.69866 -0.49692
Ru -0.79231 -0.14133 -0.40704
C  -2.67947 -1.19313 -1.00402
C  -2.45896 -0.01494 -1.78829
C  -1.24191  0.14414 -2.50919
C  -0.23960 -0.88064 -2.47486
C  -0.43634 -1.99948 -1.65078
C  -1.65861 -2.15272 -0.90707
H  -1.06224  1.05854 -3.06457
C   2.15781 -0.34476  0.44235
C   3.31627 -1.04526  0.08304
C   3.45300 -2.39166  0.42812
C   2.44265 -3.05306  1.13621
C   1.28728 -2.36277  1.50395
C   1.14259 -1.01337  1.15942
H  -1.76289 -2.97787 -0.21213
O  -1.76636  1.12656  0.91281
C  -2.07895  0.53049  2.04134
O  -1.75977 -0.63982  2.28024
C  -2.82674  1.39807  3.03020
H  -2.11915  2.07726  3.51770
H  -3.57776  2.01039  2.52617
H  -3.29228  0.77207  3.79177
H   4.09945 -0.55011 -0.48314
H   4.35308 -2.92760  0.14317
H   0.50757 -2.84548  2.08482
H   2.56783 -4.09532  1.41229
H   3.95345  1.75071  0.39492
H   0.30549 -0.46971  1.61149
H  -3.56890 -1.28102 -0.39157
H   0.36192 -2.72046 -1.51749
H  -3.18914  0.78633 -1.77745
H   0.70007 -0.74164 -2.99717
H   1.02953  4.72087 -0.71102
H   3.41149  4.12438 -0.16373
H  -0.68056  2.90076 -0.72727
```

C^+

SCF (B3LYP) Energy = -1034.87433790
Enthalpy 0K = -1034.547080
Enthalpy 298K = -1034.525448
Free Energy 298K = -1034.597821
Lowest Frequency = 27.3950 cm^{-1}
Second Frequency = 32.2787 cm^{-1}

```
C   0.44938  2.74317  0.11881
N   0.62901  1.43921 -0.17116
C   1.88343  0.96634 -0.42170
C   2.97729  1.84278 -0.41082
C   2.78550  3.19052 -0.13522
C   1.49684  3.65295  0.14347
Ru -0.94649  0.03928 -0.20408
C  -3.07306 -0.74043 -0.03780
C  -3.23761  0.68876 -0.02952
C  -2.65390  1.45412 -1.03670
C  -1.87233  0.80837 -2.05774
C  -1.80432 -0.60421 -2.12655
C  -2.43453 -1.39086 -1.11065
H  -2.73333  2.53589 -1.02117
C   1.93945 -0.47808 -0.65068
C   3.12160 -1.17200 -0.94751
C   3.10129 -2.55525 -1.11192
C   1.89869 -3.24830 -0.96981
C   0.71353 -2.55853 -0.67912
C   0.69754 -1.16078 -0.52458
H  -2.36395 -2.47151 -1.13084
O  -0.69618  0.04833  1.95062
C  -0.09579 -0.66654  2.77055
O   0.66422 -1.68560  2.43540
C  -0.18987 -0.42506  4.24636
H   0.80505 -0.19392  4.63920
H  -0.87296  0.39717  4.45260
H  -0.52958 -1.33708  4.74563
H   4.06310 -0.64102 -1.05121
H   4.01775 -3.08856 -1.34180
H  -0.20396 -3.13116 -0.57379
H   1.87593 -4.32796 -1.08661
H   3.97180  1.46278 -0.61103
H   0.71276 -1.76563  1.45287
H  -3.47038 -1.32631  0.78398
H  -1.24237 -1.08386 -2.91913
H  -3.75766  1.16532  0.79391
H  -1.35792  1.40622 -2.80189
H   1.30233  4.69358  0.37603
H   3.62984  3.87236 -0.12877
H  -0.56706  3.04739  0.33832
```

B•OAc

SCF (B3LYP) Energy = -1263.53369533
Enthalpy 0K = -1263.156538

Enthalpy 298K = -1263.128981
Free Energy 298K = -1263.215992
Lowest Frequency = 28.4306 cm^{-1}
Second Frequency = 39.5624 cm^{-1}

C	-0.48864	-1.70153	1.57788
N	-0.25958	-0.48546	1.03312
C	-1.09976	0.53790	1.33512
C	-2.17126	0.33621	2.21377
C	-2.39449	-0.91190	2.78090
C	-1.53207	-1.95463	2.45472
Ru	1.28675	-0.43601	-0.46679
C	2.51532	-0.77604	-2.28866
C	1.51478	-1.79572	-2.17289
C	0.14156	-1.46118	-2.08456
C	-0.24509	-0.08716	-2.06859
C	0.73133	0.93321	-2.13678
C	2.11642	0.58038	-2.24064
H	-0.65780	-2.18056	-1.87625
C	-0.91352	1.89203	0.73990
C	-1.92675	2.40543	-0.08689
C	-1.80367	3.69346	-0.61212
C	-0.68838	4.47879	-0.30892
C	0.31348	3.97092	0.52219
C	0.20429	2.68195	1.04676
H	2.87276	1.35771	-2.19988
O	2.40701	-1.61567	0.94600
C	2.86305	-0.56872	1.51792
O	2.53801	0.55563	1.01696
C	3.71419	-0.66502	2.75140
H	4.35869	0.21137	2.83770
H	3.06339	-0.70392	3.63191
H	4.31020	-1.57933	2.72886
H	-2.76091	1.76020	-0.35423
H	-2.58246	4.08162	-1.26254
H	1.17889	4.57947	0.76936
H	-0.60185	5.48326	-0.71428
H	-2.82064	1.17558	2.43241
H	0.98785	2.28723	1.68371
H	3.56709	-1.03807	-2.30397
H	0.44518	1.97297	-2.02984
H	1.82571	-2.83140	-2.07668
H	-1.31042	0.10184	-1.85120
H	-1.66856	-2.95616	2.84572
H	-3.22993	-1.06872	3.45621
H	0.19495	-2.48695	1.28567
O	-2.43076	-2.41828	-0.99902
C	-3.25625	-1.46936	-0.92293
C	-4.69444	-1.81453	-0.49092
H	-4.78984	-2.86880	-0.22159
H	-4.99454	-1.18629	0.35515
H	-5.38510	-1.58818	-1.31090
O	-3.03963	-0.24259	-1.17376

TS(**B-C**)1•OAc
SCF (B3LYP) Energy = -1263.51018151
Enthalpy 0K = -1263.134741
Enthalpy 298K = -1263.108223
Free Energy 298K = -1263.194298
Lowest Frequency = -61.0679 cm^{-1}
Second Frequency = -7.2365 cm^{-1}

C	-1.39333	-1.17752	1.51778
N	-0.66461	-0.17837	0.99725
C	-0.95749	1.10778	1.31377
C	-2.00773	1.41029	2.17801
C	-2.76498	0.37407	2.72188
C	-2.44929	-0.93943	2.39283
Ru	0.87227	-0.55354	-0.43006
C	2.04182	-1.57642	-2.02582
C	0.81224	-2.26330	-1.74773
C	-0.43227	-1.57908	-1.83725
C	-0.46743	-0.19353	-2.20685
C	0.74117	0.49200	-2.41346
C	2.00104	-0.20087	-2.31865
H	-1.39352	-2.00694	-1.50642
C	-0.08556	2.13771	0.71067
C	-0.60919	3.32348	0.17833
C	0.23944	4.25195	-0.42566
C	1.61629	4.01234	-0.50628
C	2.14563	2.83388	0.01924
C	1.30015	1.89812	0.62625
H	2.92839	0.35691	-2.38956
O	1.62093	-1.72843	1.12869
C	2.81044	-1.37496	1.52811
O	3.42500	-0.39943	1.07454
C	3.38717	-2.24796	2.62986
H	2.83426	-2.07227	3.55857
H	3.27501	-3.30633	2.38013
H	4.43866	-2.00598	2.78776
H	-1.68084	3.49381	0.19969
H	-0.17686	5.16359	-0.84423
H	3.21222	2.63431	-0.01624
H	2.26862	4.74570	-0.97114
H	-2.21236	2.44591	2.42400
H	1.76567	1.04380	1.12508
H	2.99391	-2.07298	-1.87906
H	0.73986	1.56702	-2.55683
H	0.84197	-3.28637	-1.38834
H	-1.44857	0.29283	-2.11224
H	-3.02035	-1.77713	2.77456
H	-3.58807	0.59339	3.39481
H	-1.12023	-2.17964	1.22062
O	-3.12355	-1.86927	-0.74302
C	-3.69259	-0.74481	-0.88005
C	-5.19833	-0.68664	-0.55833
H	-5.74013	-0.23119	-1.39352
H	-5.60362	-1.67976	-0.35193
H	-5.36280	-0.04179	0.31333
O	-3.16014	0.34523	-1.23608

INT(**B-C**)•OAc
SCF (B3LYP) Energy = -1263.51241253
Enthalpy 0K = -1263.136403
Enthalpy 298K = -1263.108424
Free Energy 298K = -1263.197922
Lowest Frequency = 18.7437 cm^{-1}
Second Frequency = 27.6727 cm^{-1}

C	-1.57721	1.22997	1.07742
N	-0.33113	1.08380	0.59428
C	0.56085	2.10701	0.65993
C	0.20041	3.33030	1.22163
C	-1.09084	3.49484	1.72643
C	-1.98510	2.43408	1.65441
Ru	0.29522	-0.73848	-0.29687
C	0.92312	-2.42947	-1.63628
C	-0.30848	-2.74585	-1.02792
C	-1.40705	-1.83081	-1.09780
C	-1.27557	-0.61575	-1.83675
C	-0.04585	-0.30279	-2.47994
C	1.05600	-1.18073	-2.32656
H	-2.32671	-1.95404	-0.52712
C	1.90695	1.83079	0.10996
C	2.62397	2.79365	-0.61387
C	3.86964	2.48001	-1.15937
C	4.42024	1.20395	-0.99538
C	3.71853	0.23785	-0.27562
C	2.46933	0.54839	0.27430
H	2.03236	-0.88488	-2.69613

O 0.18009 -1.37598 1.67785
C 1.10636 -2.19108 2.12040
O 2.12703 -2.49748 1.49654
C 0.81464 -2.72926 3.51256
H 0.65902 -1.90070 4.20946
H -0.11079 -3.31308 3.49694
H 1.64097 -3.35360 3.85373
H 2.19461 3.77790 -0.77429
H 4.41160 3.23469 -1.72186
H 4.13151 -0.75177 -0.10719
H 5.39344 0.97323 -1.41793
H 0.93160 4.12887 1.27908
H 2.03415 -0.17677 0.96989
H 1.78901 -3.06033 -1.47910
H 0.08271 0.64977 -2.98118
H -0.38195 -3.62753 -0.40055
H -2.10964 0.10806 -1.76809
H -3.00239 2.51919 2.01823
H -1.38614 4.44133 2.16910
H -2.26662 0.38887 0.95808
O -3.80081 -0.65459 0.23568
C -4.28853 0.26622 -0.49097
C -5.81493 0.44341 -0.43901
H -6.29071 -0.37652 -0.98997
H -6.17127 0.38189 0.59371
H -6.12022 1.38999 -0.89074
O -3.63947 1.03599 -1.25472

TS(**B**–**C**)2•OAc
SCF (B3LYP) Energy = -1263.50531182
Enthalpy 0K = -1263.133583
Enthalpy 298K = -1263.106547
Free Energy 298K = -1263.193083
Lowest Frequency = -925.8672 cm^{-1}
Second Frequency = 17.9574 cm^{-1}

C -1.46030 1.45766 0.65195
N -0.23146 1.10837 0.23064
C 0.72009 2.05497 -0.01002
C 0.43373 3.40586 0.18857
C -0.83565 3.78016 0.62863
C -1.79101 2.79707 0.86109
Ru 0.28930 -0.90073 -0.10919
C 0.69478 -2.97244 -0.92744
C -0.54643 -2.98183 -0.24641
C -1.58675 -2.07014 -0.59051
C -1.36442 -1.11359 -1.61291
C -0.11938 -1.08427 -2.31054
C 0.90422 -1.99540 -1.94863
H -2.50651 -1.97236 -0.01594
C 2.01633 1.52140 -0.45508
C 2.95784 2.28557 -1.15431
C 4.15766 1.70772 -1.56933
C 4.42897 0.36566 -1.28346
C 3.49106 -0.39816 -0.59017
C 2.26155 0.14896 -0.17274
H 1.87944 -1.91816 -2.41660
O 0.06029 -1.09808 1.97683
C 0.99212 -0.77165 2.78312
O 2.10043 -0.28983 2.41187
C 0.74520 -0.98125 4.25925
H 0.84617 -0.02450 4.77931
H -0.24751 -1.39588 4.43229
H 1.50935 -1.65283 4.66118
H 2.74975 3.32283 -1.40008
H 4.88265 2.30524 -2.11414
H 3.72442 -1.42940 -0.33589
H 5.37214 -0.07584 -1.59281
H 1.20363 4.14923 0.01661
H 2.02380 -0.20226 1.05561
H 1.49187 -3.64746 -0.63899
H 0.06907 -0.32688 -3.06286
H -0.67684 -3.63800 0.60810
H -2.14138 -0.34166 -1.75647
H -2.79650 3.04093 1.18340
H -1.06979 4.82896 0.78486
H -2.19990 0.66077 0.77891
O -3.85238 -0.39696 0.44236
C -4.30095 0.30670 -0.51553
C -5.81336 0.58882 -0.50656
H -6.34890 -0.31503 -0.82080
H -6.15280 0.82494 0.50648
H -6.06964 1.39960 -1.19247
O -3.62872 0.78118 -1.47404

C•OAc
SCF (B3LYP) Energy = -1263.52476102
Enthalpy 0K = -1263.147983
Enthalpy 298K = -1263.120362
Free Energy 298K = -1263.208788
Lowest Frequency = 11.1401 cm^{-1}
Second Frequency = 24.4206 cm^{-1}

C -1.46894 1.52022 0.49711
N -0.26171 1.12748 0.04795
C 0.68364 2.04888 -0.30144
C 0.40460 3.41312 -0.19939
C -0.84426 3.82889 0.25907
C -1.78952 2.87258 0.61371
Ru 0.25301 -0.90444 -0.14513
C 0.41287 -3.13071 -0.55046
C -0.76001 -2.93441 0.24497
C -1.79147 -2.06454 -0.15938
C -1.61341 -1.29721 -1.34468
C -0.45928 -1.47577 -2.16050
C 0.54993 -2.39988 -1.75623
H -2.65759 -1.82919 0.45795
C 1.95578 1.46037 -0.73913
C 3.05364 2.21601 -1.17392
C 4.24200 1.58504 -1.53825
C 4.33761 0.19481 -1.45776
C 3.23965 -0.56238 -1.03093
C 2.01665 0.03903 -0.67444
H 1.45537 -2.49806 -2.34528
O 0.64491 -0.80610 1.99962
C 1.61477 -0.47586 2.69121
O 2.77288 -0.08301 2.19625
C 1.56108 -0.49420 4.19116
H 1.69914 0.52326 4.56968
H 0.60118 -0.88569 4.52419
H 2.38058 -1.10281 4.58374
H 2.98906 3.29894 -1.23205
H 5.08903 2.17505 -1.87486
H 3.34426 -1.64375 -0.97489
H 5.26454 -0.30378 -1.72913
H 1.15942 4.14075 -0.47414
H 2.71672 -0.07797 1.20825
H 1.19717 -3.80255 -0.22123
H -0.32665 -0.88504 -3.05953
H -0.82410 -3.42690 1.21080
H -2.37115 -0.52559 -1.55362
H -2.77990 3.14304 0.96057
H -1.07111 4.88844 0.33331
H -2.20780 0.74983 0.74095
O -3.93327 -0.20665 0.84114
C -4.47049 0.32668 -0.18062
C -5.97785 0.62248 -0.08035
H -6.53639 -0.31081 -0.22136
H -6.23067 1.00021 0.91489
H -6.29368 1.33193 -0.84892

O -3.89448 0.61888 -1.26420

A•a–H
SCF (B3LYP) Energy = -1263.56358218
Enthalpy 0K = -1263.186380
Enthalpy 298K = -1263.158587
Free Energy 298K = -1263.250416
Lowest Frequency = 9.1340 cm^{-1}
Second Frequency = 11.9010 cm^{-1}

C 1.87413 1.34051 -2.07956
C 0.58767 0.73528 -1.92762
C 0.47858 -0.67736 -1.92500
C -2.14121 -1.59981 0.71203
C -2.00545 -2.98875 0.73127
H -1.09968 -3.42421 1.14314
C -2.39564 1.36666 0.33165
H -1.39745 1.00224 0.54154
O 1.88757 1.27394 1.11431
C 1.41466 3.19847 2.39008
H 2.44337 3.17048 2.75825
H 1.08786 4.23077 2.25836
H 0.78412 2.71570 3.14429
C 1.29766 2.43988 1.07286
O 0.68334 2.91295 0.11242
O 3.42292 -0.93694 0.94440
C 2.49943 -1.44673 1.65861
O 1.30624 -1.37485 1.20912
H -1.33521 -1.00109 1.12194
C 2.79523 -2.07269 2.98976
H 2.73987 -1.29516 3.75912
H 2.05659 -2.84167 3.22336
H 3.80307 -2.49189 2.99698
C -3.02530 -3.80444 0.23756
H -2.91971 -4.88570 0.25517
C -3.30140 -0.99835 0.19231
C -4.32425 -1.83157 -0.29297
H -5.22265 -1.36667 -0.68250
C -4.18664 -3.21765 -0.27184
H -4.98891 -3.84263 -0.65477
N -4.70809 0.93540 -0.14482
C -2.60867 2.73985 0.23620
H -1.76779 3.41501 0.36305
C -3.46994 0.48168 0.13545
C -3.89418 3.20182 -0.04378
H -4.11237 4.26180 -0.12792
C -4.90245 2.25367 -0.22455
H -5.92043 2.57069 -0.44857
Ru 1.96148 -0.11173 -0.40477
C 1.63322 -1.50134 -2.11412
H 1.54922 -2.57988 -2.05069
C 2.90181 -0.89037 -2.23631
H 3.79551 -1.50460 -2.25413
C 3.02745 0.53975 -2.23130
H 4.01034 0.99590 -2.25733
H -0.47599 -1.14052 -1.69756
H -0.26804 1.35647 -1.70278
H 1.96082 2.41147 -1.95166

B
SCF (B3LYP) Energy = -1263.55502336
Enthalpy 0K = -1263.177229
Enthalpy 298K = -1263.149902
Free Energy 298K = -1263.235846
Lowest Frequency = 27.7019 cm^{-1}
Second Frequency = 32.4273 cm^{-1}

C -0.68596 -2.09601 1.98820
Ru -0.67309 -0.36172 -0.44768
C -1.10070 0.00948 -2.62023
C -2.00545 -0.95988 -2.10899
C -0.13453 -2.32997 -1.31043
C 0.79290 -1.38720 -1.82298
H -1.47917 0.93459 -3.03452
H -3.06459 -0.73482 -2.12870
H 0.20751 -3.16603 -0.71407
H 1.85557 -1.51540 -1.66301
C -0.55309 -2.16170 3.50770
H -0.66884 -3.19106 3.85059
H 0.40649 -1.75697 3.84166
H -1.33988 -1.54566 3.95592
O -0.24045 -0.96825 1.49527
O -1.17869 -3.03046 1.35478
C 1.64053 1.68312 0.44983
C -0.50068 2.57491 0.26805
N 0.31855 1.50217 0.18587
O -2.33319 0.30264 0.63787
C -3.35007 0.94635 0.13875
O -3.40319 1.46292 -0.98466
C -4.52581 1.03659 1.10694
H -4.19304 1.42914 2.07207
H -5.30813 1.67353 0.69178
H -4.92636 0.03426 1.28970
C 2.64599 0.59676 0.24535
C 3.63696 0.79280 -0.73081
C 2.69030 -0.55751 1.03976
C 4.63381 -0.16309 -0.93536
H 3.62048 1.69499 -1.33681
C 3.69668 -1.50385 0.84155
H 1.91581 -0.71671 1.77935
C 4.66572 -1.31521 -0.14735
H 5.38580 -0.00305 -1.70266
H 3.72242 -2.39349 1.46438
H 5.44428 -2.05750 -0.29815
C -0.07085 3.83900 0.65502
C 2.12663 2.93499 0.85504
C 1.27006 4.02299 0.97449
H 3.18390 3.03005 1.07506
H 1.64545 4.99038 1.29452
H -0.78720 4.65213 0.69618
H -1.52669 2.40918 -0.02768
C -1.53756 -2.13727 -1.46433
H -2.22165 -2.82131 -0.98161
C 0.29276 -0.20160 -2.43539
H 0.99204 0.57717 -2.72247

TS(**B–C**)
SCF (B3LYP) Energy = -1263.50020833
Enthalpy 0K = -1263.126081
Enthalpy 298K = -1263.099347
Free Energy 298K = -1263.183714
Lowest Frequency = -120.4490 cm^{-1}
Second Frequency = 25.1675 cm^{-1}

C -3.16774 0.45715 -1.47807
Ru -0.08618 -0.40274 0.72953
C 0.24991 -1.66617 2.50419
C -1.01534 -2.00145 1.95775
C -1.69730 0.34580 2.07491
C -0.44761 0.69397 2.67885
H 1.01493 -2.42857 2.58614
H -1.16957 -3.00903 1.59391
H -2.40243 1.10417 1.75863
H -0.21391 1.73185 2.88397
C -4.28443 -0.08654 -2.38081
H -4.27648 -1.18262 -2.33677
H -5.26234 0.25839 -2.03601
H -4.12211 0.20402 -3.42165
O -2.02410 0.57116 -2.02033
O -3.45938 0.72179 -0.27837

C 2.20478 0.95907 -0.65525
C 3.94913 -1.18077 -0.79209
C 2.70633 -1.27924 -0.17808
H 2.33296 -2.21333 0.22653
N 1.86525 -0.22957 -0.09496
O -0.30595 -1.53299 -0.98093
C -0.02156 -2.80419 -1.04681
O 0.46891 -3.48790 -0.13814
C -0.32123 -3.39848 -2.41647
H 0.52652 -3.20095 -3.08208
H -0.45098 -4.47890 -2.33229
H -1.20309 -2.93056 -2.85761
H 4.59630 -2.04974 -0.83138
C 1.21585 2.03660 -0.50980
C 1.63918 3.36761 -0.36229
C -0.15943 1.70949 -0.40120
C 0.71729 4.37768 -0.10107
H 2.69750 3.60710 -0.41248
C -1.07184 2.75171 -0.14088
H -0.75563 0.86051 -0.97071
C -0.64178 4.06604 0.01773
H 1.05819 5.40242 0.01575
H -2.12689 2.48617 -0.11679
H -1.36447 4.85379 0.21191
C 3.43850 1.10832 -1.30321
C 4.32052 0.03649 -1.36483
H 5.27659 0.14269 -1.86836
H 3.67945 2.05541 -1.77163
C -1.99828 -0.99252 1.73840
H -2.91188 -1.18671 1.19060
C 0.52871 -0.30663 2.86678
H 1.51504 -0.03838 3.23149

C
SCF (B3LYP) Energy = -1263.57310428
Enthalpy 0K = -1263.195767
Enthalpy 298K = -1263.168358
Free Energy 298K = -1263.254567
Lowest Frequency = 27.1882 cm^{-1}
Second Frequency = 30.8684 cm^{-1}

C 3.88176 0.26177 0.80833
Ru -0.24187 -0.65544 -0.64867
C -1.05724 -2.64484 -1.62593
C 0.14734 -2.97205 -1.00617
C 1.28862 -1.12954 -2.21231
C 0.04458 -0.78132 -2.83061
H -1.96047 -3.19692 -1.38804
H 0.18197 -3.75337 -0.25759
H 2.18683 -0.55351 -2.39161
H -0.01179 0.06747 -3.50254
C 5.20628 0.89182 1.18286
H 5.96938 0.61146 0.45729
H 5.10104 1.98085 1.21082
H 5.50408 0.57111 2.18543
O 2.93385 0.53400 1.70105
O 3.71706 -0.40905 -0.20024
C -4.16802 -0.28847 1.25169
C -2.98640 -0.77067 0.70475
H -2.75511 -1.82733 0.68244
N -2.03526 0.04344 0.20934
O 0.55284 -0.55374 1.32187
C 0.14224 -1.42192 2.22240
O -0.66366 -2.32691 2.01042
C 0.73197 -1.19222 3.60848
H 0.22858 -0.33644 4.07174
H 0.57166 -2.07428 4.22969
H 1.79637 -0.95121 3.55470
H -4.90706 -0.98372 1.63355
C -1.04923 2.15419 -0.22105
C -0.99396 3.55854 -0.23187
C 0.04546 1.36840 -0.66708
C 0.15288 4.20790 -0.67350
H -1.84173 4.14775 0.10803
C 1.20095 2.05349 -1.07775
H 2.04915 0.12302 1.45336
C 1.25351 3.44938 -1.08693
H 0.19643 5.29290 -0.68472
H 2.08388 1.49432 -1.37191
H 2.16156 3.95010 -1.41487
C -2.19224 1.39631 0.28057
C -4.36070 1.09429 1.30693
C -3.36586 1.93612 0.82974
H -5.27094 1.50905 1.72989
H -3.48488 3.01175 0.88465
C 1.31060 -2.16281 -1.25500
H 2.22276 -2.32171 -0.69307
C -1.12807 -1.50354 -2.50048
H -2.08028 -1.20933 -2.92841

B′
SCF (B3LYP) Energy = -1031.31280320
Enthalpy 0K = -1031.037737
Enthalpy 298K = -1031.016322
Free Energy 298K = -1031.087994
Lowest Frequency = 34.5891 cm^{-1}
Second Frequency = 53.7190 cm^{-1}

C -2.73975 -0.29836 -1.07481
Ru -0.42677 -0.35225 -0.10071
C -4.11400 -0.41793 -1.67775
H -4.85524 0.04815 -1.02574
H -4.13680 0.03344 -2.67160
H -4.36533 -1.47952 -1.77800
O -1.70171 -0.26864 -1.82483
O -2.57423 -0.25815 0.18511
C 1.99644 0.83614 -0.32008
C 2.35173 -1.27799 -1.25727
N 1.52379 -0.37174 -0.71486
O -0.56221 -2.43383 0.25737
C -0.09813 -2.28454 1.44078
O 0.25625 -1.11300 1.79571
C -0.01770 -3.44828 2.38853
H 0.15210 -4.37605 1.83849
H 0.77297 -3.28572 3.12326
H -0.97109 -3.53685 2.92093
C 0.86632 1.64103 0.22353
C 0.91307 2.21788 1.52328
C -0.22520 1.94972 -0.64252
C -0.11820 3.01892 1.96428
H 1.75742 1.99531 2.16818
C -1.26341 2.78872 -0.15538
H -0.15547 1.76230 -1.70846
C -1.22326 3.29650 1.12617
H -0.08355 3.43948 2.96506
H -2.08212 3.04539 -0.82096
H -2.02733 3.93011 1.48775
C 3.71019 -1.00270 -1.41425
C 3.33967 1.16892 -0.43098
C 4.21218 0.22740 -0.98974
H 3.68837 2.14010 -0.09630
H 5.26820 0.45552 -1.09508
H 4.35983 -1.75082 -1.85570
H 1.90471 -2.22303 -1.54613

TS(**B′-C′**)
SCF (B3LYP) Energy = -1031.28251738
Enthalpy 0K = -1031.007987
Enthalpy 298K = -1030.987177
Free Energy 298K = -1031.057744

Lowest Frequency = -59.8195 cm^{-1}
Second Frequency = 39.7253 cm^{-1}

C	-2.89170	1.17750	-0.56025
Ru	-0.50030	-0.26292	0.07579
C	-4.33791	1.61068	-0.36454
H	-4.59152	2.40889	-1.06412
H	-4.99640	0.75614	-0.55565
H	-4.51090	1.93495	0.66488
O	-2.27317	1.45716	-1.60010
O	-2.39406	0.49756	0.42814
C	2.39629	-0.03241	-0.17576
C	3.11034	-2.64688	-0.63803
C	1.78216	-2.26063	-0.49656
H	0.96663	-2.96905	-0.58103
N	1.42379	-0.98366	-0.25608
O	-1.42512	-1.98914	-0.63613
C	-1.56305	-2.42346	0.56002
O	-1.01047	-1.71915	1.46969
C	-2.34675	-3.66072	0.87166
H	-1.95083	-4.14403	1.76703
H	-3.38669	-3.37673	1.06535
H	-2.32921	-4.34581	0.02185
H	3.34712	-3.68784	-0.82961
C	1.87308	1.32895	0.04912
C	2.52729	2.25922	0.86934
C	0.63261	1.68617	-0.54730
C	1.96944	3.51730	1.08909
H	3.45642	1.98315	1.35906
C	0.08518	2.96121	-0.32296
H	0.20535	1.10135	-1.39207
C	0.74673	3.86605	0.50262
H	2.48275	4.22517	1.73326
H	-0.85356	3.20147	-0.80872
H	0.31718	4.84595	0.68729
C	3.74716	-0.35596	-0.30585
C	4.11280	-1.68157	-0.53313
H	5.15809	-1.95324	-0.64028
H	4.49293	0.42927	-0.24690

C′
SCF (B3LYP) Energy = -1031.28177048
Enthalpy 0K = -1031.006881
Enthalpy 298K = -1030.984779
Free Energy 298K = -1031.061183
Lowest Frequency = 11.4717 cm^{-1}
Second Frequency = 23.3156 cm^{-1}

C	2.55168	1.95342	1.67357
Ru	-0.15470	-1.49744	-0.49697
C	2.45355	3.34518	2.25390
H	3.36793	3.89760	2.04039
H	1.59531	3.86531	1.81733
H	2.28685	3.29215	3.33364
O	1.48356	1.20633	1.98540
O	3.48646	1.55625	1.00155
C	-3.38099	-0.87113	2.35834
C	-2.30294	-1.40055	1.66054
H	-1.84813	-2.34320	1.94928
N	-1.75054	-0.78867	0.59509
O	1.47133	-1.23022	0.72325
C	2.32626	-1.65008	-0.17265
O	1.83947	-2.03563	-1.26766
C	3.78784	-1.63281	0.13924
H	3.98042	-2.22781	1.03760
H	4.35718	-2.02947	-0.70154
H	4.07684	-0.59869	0.35627
H	-3.78655	-1.40446	3.21073
C	-1.53551	0.98209	-0.96808
C	-1.88474	2.17889	-1.61084
C	-0.40491	0.22905	-1.39940
C	-1.11708	2.64971	-2.67328
H	-2.75458	2.74625	-1.28925
C	0.35807	0.72907	-2.46925
H	1.56661	0.32338	1.54903
C	0.00285	1.92428	-3.09845
H	-1.38834	3.57666	-3.16959
H	1.22946	0.17565	-2.80776
H	0.60132	2.29428	-3.92730
C	-2.25678	0.41474	0.17248
C	-3.91397	0.34761	1.93257
C	-3.34584	0.98930	0.83716
H	-4.75753	0.79333	2.45066
H	-3.73765	1.94071	0.49605

C′ (without HOAc)
SCF (B3LYP) Energy = -802.176544706
Enthalpy 0K = -801.965271
Enthalpy 298K = -801.949242
Free Energy 298K = -802.009320
Lowest Frequency = 37.1505 cm^{-1}
Second Frequency = 43.7642 cm^{-1}

Ru	0.75132	-0.57729	-0.64043
C	-3.01656	-2.59174	0.19725
C	-1.69475	-2.32017	-0.13276
H	-0.99637	-3.11480	-0.37689
N	-1.19109	-1.07107	-0.16828
O	1.83691	-1.15688	0.99447
C	2.94882	-0.70382	0.51593
O	2.91423	-0.17444	-0.63274
C	4.20381	-0.78551	1.33600
H	4.20773	-1.69821	1.93554
H	5.07991	-0.74611	0.68697
H	4.23681	0.06878	2.02123
H	-3.36942	-3.61690	0.21146
C	-1.31844	1.28237	0.09655
C	-1.93948	2.51857	0.32885
C	0.07497	1.21137	-0.19640
C	-1.19313	3.69354	0.28560
H	-3.00451	2.57156	0.54103
C	0.80691	2.41214	-0.22873
C	0.17842	3.63657	0.00734
H	-1.67526	4.64971	0.46585
H	1.87119	2.38051	-0.44541
H	0.75899	4.55540	-0.02732
C	-2.00534	-0.00958	0.14010
C	-3.85892	-1.52057	0.50331
C	-3.34634	-0.22773	0.47498
H	-4.89879	-1.69141	0.76449
H	-3.97977	0.61784	0.71787

D⁺ (K^1)
SCF (B3LYP) Energy = -1281.98552893
Enthalpy 0K = -1281.589326
Enthalpy 298K = -1281.563235
Free Energy 298K = -1281.644939
Lowest Frequency = 30.8995 cm^{-1}
Second Frequency = 36.8516 cm^{-1}

Ru	0.05481	-0.49549	-0.15393
O	-0.01933	-2.56510	-0.75652
C	-0.63826	-2.84659	0.32147
C	-1.12983	-4.22748	0.62588
O	-0.85003	-1.87220	1.13526
H	-2.13961	-4.34258	0.21663
H	-0.48406	-4.97076	0.15512
H	-1.18165	-4.38580	1.70456
C	-2.66167	0.77821	0.28513
C	-3.98860	0.67075	0.72564

C -2.24909 -0.03101 -0.79142
C -4.87475 -0.20204 0.09428
H -4.32699 1.23959 1.58520
C -3.13438 -0.90788 -1.42234
C -4.45449 -0.99221 -0.97915
H -5.89774 -0.27270 0.45026
H -2.79230 -1.50814 -2.25952
H -5.15198 -1.66596 -1.46640
H -1.29743 0.19559 -1.33497
C -1.68137 1.64876 0.96335
C -1.11336 3.55141 2.34653
H -1.40750 4.43339 2.90591
C -2.06524 2.78695 1.68384
H -3.11034 3.07134 1.70667
C 0.55041 2.03894 1.52701
H 1.57767 1.70813 1.44843
C 0.22402 3.16201 2.27355
H 1.00679 3.71720 2.77809
N -0.36477 1.29102 0.87519
C 2.13031 0.61290 -1.24110
C 2.27059 2.01032 -1.40451
C 1.37256 -0.12842 -2.19075
C 1.63811 2.66077 -2.45196
H 2.87911 2.57146 -0.70188
C 0.74260 0.56201 -3.25563
C 0.85512 1.93788 -3.37202
H 1.75323 3.73400 -2.56772
H 0.20285 -0.00922 -4.00495
H 0.37173 2.45625 -4.19402
H 1.46621 -1.20777 -2.24505
C 2.80578 -0.10802 -0.12625
C 4.59817 -0.82867 1.29414
H 5.64956 -0.83635 1.56257
C 4.15851 -0.08321 0.19625
H 4.84860 0.49201 -0.41137
C 2.33059 -1.53741 1.67156
H 1.56085 -2.06668 2.22151
C 3.67511 -1.56678 2.03552
H 3.98425 -2.15690 2.89090
N 1.91717 -0.81430 0.61749

TS(**D**$^{+}$**-E**$^{+}$) (K^{1})
SCF (B3LYP) Energy = -1281.94712078
Enthalpy 0K = -1281.556574
Enthalpy 298K = -1281.530819
Free Energy 298K = -1281.611939
Lowest Frequency = -1168.9487 cm^{-1}
Second Frequency = 32.3953 cm^{-1}

Ru 0.08925 -0.00606 -0.27818
O 0.88612 -1.73961 1.97905
C -0.04487 -0.98535 2.38139
C -0.54770 -1.11029 3.79323
O -0.60588 -0.10469 1.62932
H -1.05265 -2.07512 3.90242
H 0.30011 -1.10619 4.48250
H -1.24221 -0.30671 4.03648
C -2.96669 -0.37585 -0.39721
C -4.14549 -0.80077 0.22929
C -1.97710 -1.33677 -0.68946
C -4.33340 -2.14671 0.54588
H -4.90612 -0.07670 0.50291
C -2.16774 -2.68396 -0.37669
C -3.34879 -3.09098 0.24573
H -5.25140 -2.45777 1.03450
H -1.40735 -3.41349 -0.63436
H -3.50366 -4.13750 0.48742
H -1.13492 -1.09306 -1.38231
C -2.72024 1.04434 -0.71360
C -3.45177 3.25117 -1.37209
H -4.24460 3.94501 -1.63211
C -3.75090 1.93482 -1.03887
H -4.77504 1.58098 -1.05707
C -1.13836 2.72841 -1.05398
H -0.08818 2.99870 -1.05357
C -2.11623 3.65591 -1.38771
H -1.83155 4.66697 -1.65614
N -1.42099 1.45456 -0.71078
C 2.90370 -0.52442 -0.66056
C 3.99423 -0.96067 -1.42231
C 1.72557 -1.32631 -0.53968
C 3.95163 -2.20540 -2.04905
H 4.86940 -0.32968 -1.54580
C 1.73003 -2.58818 -1.16733
C 2.82262 -3.02053 -1.91916
H 4.79941 -2.54123 -2.63766
H 0.87482 -3.24774 -1.04871
H 2.79967 -3.99397 -2.39960
H 1.13268 -1.41528 0.73309
C 2.87584 0.76365 0.04505
C 3.82283 2.68086 1.16375
H 4.68480 3.26893 1.46179
C 3.99224 1.52063 0.41531
H 4.98373 1.18108 0.13970
C 1.45904 2.28714 1.14165
H 0.43822 2.53141 1.41128
C 2.53527 3.06517 1.54701
H 2.36304 3.94787 2.15219
N 1.62106 1.17960 0.38969

E^{+} (K^{1})
SCF (B3LYP) Energy = -1281.95609085
Enthalpy 0K = -1281.560645
Enthalpy 298K = -1281.534418
Free Energy 298K = -1281.616949
Lowest Frequency = 30.0574 cm^{-1}
Second Frequency = 34.5416 cm^{-1}

Ru 0.11874 0.01862 -0.32560
O 0.87634 -1.77785 2.10416
C -0.07906 -0.95153 2.42663
C -0.58677 -1.03980 3.83013
O -0.56067 -0.12362 1.61649
H -1.00493 -2.03694 3.99855
H 0.24597 -0.91494 4.52812
H -1.34787 -0.28163 4.00735
C -2.96542 -0.45239 -0.38741
C -4.11186 -0.94263 0.25247
C -1.93883 -1.36217 -0.71585
C -4.23513 -2.30078 0.54791
H -4.89964 -0.25781 0.54969
C -2.06730 -2.72271 -0.42705
C -3.21614 -3.19429 0.21031
H -5.12963 -2.66105 1.04637
H -1.28348 -3.41437 -0.71667
H -3.32022 -4.25157 0.43191
H -1.12163 -1.06796 -1.41853
C -2.79837 0.98540 -0.68484
C -3.66028 3.15338 -1.30912
H -4.49220 3.80381 -1.55937
C -3.88211 1.81633 -0.99698
H -4.88391 1.40353 -1.02288
C -1.32104 2.75813 -0.99810
H -0.28795 3.08983 -0.99598
C -2.35079 3.63512 -1.31629
H -2.12583 4.66563 -1.56734
N -1.52628 1.46592 -0.67578
C 2.94979 -0.48085 -0.66936
C 4.10254 -0.99330 -1.27877
C 1.72032 -1.21574 -0.65672

C 4.07589 -2.25861 -1.86221
H 5.01899 -0.41129 -1.31366
C 1.74447 -2.49741 -1.24587
C 2.89847 -3.01218 -1.84142
H 4.96985 -2.65669 -2.33157
H 0.84594 -3.10951 -1.24421
H 2.88090 -4.00030 -2.29220
H 1.12296 -1.60109 1.13856
C 2.90390 0.82158 0.00391
C 3.81258 2.78725 1.07623
H 4.66350 3.39920 1.35770
C 4.00350 1.61217 0.35772
H 5.00225 1.29094 0.08690
C 1.45841 2.35093 1.05611
H 0.43229 2.58956 1.31133
C 2.51758 3.15902 1.44670
H 2.32670 4.05526 2.02577
N 1.63941 1.22413 0.33759

D⁺ (K^2)
SCF (B3LYP) Energy = -1281.97908724
Enthalpy 0K = -1281.583204
Enthalpy 298K = -1281.557188
Free Energy 298K = -1281.638843
Lowest Frequency = 28.7604 cm^{-1}
Second Frequency = 36.9089 cm^{-1}

Ru -0.00293 0.89418 -0.00159
O 0.16806 2.75061 1.07048
C -0.01234 3.42055 -0.00607
C -0.05395 4.91824 -0.00183
O -0.18131 2.74592 -1.08134
H 0.24961 5.30924 -0.97416
H -1.08021 5.24755 0.19571
H 0.58437 5.31173 0.79109
C -2.36047 -0.75836 0.93644
C -3.47967 -1.55512 0.66278
C -2.30721 0.53981 0.38442
C -4.52123 -1.05744 -0.12261
H -3.53267 -2.57222 1.03750
C -3.35300 1.03992 -0.40072
C -4.46415 0.23578 -0.65503
H -5.38303 -1.68586 -0.32474
H -3.29398 2.04852 -0.79663
H -5.28410 0.61329 -1.25744
H -1.62634 1.29615 0.85935
C -1.21390 -1.22031 1.73909
C -0.22697 -2.54285 3.50252
H -0.31264 -3.29019 4.28452
C -1.33367 -2.19323 2.73711
H -2.29998 -2.64571 2.92671
C 1.04578 -0.93985 2.25366
H 1.96576 -0.41214 2.04069
C 0.98402 -1.89579 3.25993
H 1.87187 -2.11644 3.84166
N -0.01723 -0.60679 1.49270
C 2.36943 -0.73979 -0.93421
C 3.49431 -1.52665 -0.65525
C 2.30605 0.56096 -0.38948
C 4.53135 -1.01674 0.12831
H 3.55529 -2.54535 -1.02437
C 3.34709 1.07323 0.39412
C 4.46406 0.27890 0.65368
H 5.39769 -1.63752 0.33461
H 3.27988 2.08357 0.78418
H 5.28068 0.66583 1.25465
H 1.61896 1.30884 -0.86728
C 1.22719 -1.21486 -1.73551
C 0.25334 -2.55233 -3.49493
H 0.34625 -3.30148 -4.27436
C 1.35638 -2.19004 -2.73012
H 2.32694 -2.63423 -2.91763
C -1.03459 -0.95676 -2.25215
H -1.95949 -0.43679 -2.04149
C -0.96358 -1.91545 -3.25519
H -1.84906 -2.14607 -3.83669
N 0.02485 -0.61150 -1.49167

TS(**D⁺-E⁺**) (K^2)
SCF (B3LYP) Energy = -1281.94568989
Enthalpy 0K = -1281.555135
Enthalpy 298K = -1281.529197
Free Energy 298K = -1281.611175
Lowest Frequency = -1248.3163 cm^{-1}
Second Frequency = 14.8030 cm^{-1}

Ru 0.07459 0.65888 -0.06207
O 1.08899 2.30174 -1.35125
C 0.73728 3.18287 -0.42837
C 0.94857 4.63194 -0.72159
O 0.23271 2.74879 0.63160
H 0.61940 5.24328 0.11811
H 2.00824 4.81011 -0.92889
H 0.39556 4.90516 -1.62582
C 2.50010 -0.95110 -0.50231
C 3.77161 -1.48979 -0.27315
C 2.11907 0.27308 0.11814
C 4.67653 -0.82595 0.55634
H 4.06162 -2.43534 -0.72067
C 3.04765 0.91756 0.95843
C 4.31754 0.37580 1.17236
H 5.66060 -1.25110 0.72632
H 2.77477 1.85123 1.44307
H 5.02393 0.88795 1.81876
H 1.63949 1.33503 -0.75285
C 1.47491 -1.60134 -1.32752
C 0.66279 -3.20058 -2.94789
H 0.83562 -4.03949 -3.61408
C 1.70185 -2.68722 -2.18064
H 2.69569 -3.11250 -2.25335
C -0.77111 -1.53524 -1.99364
H -1.73032 -1.04273 -1.89407
C -0.59784 -2.60887 -2.85731
H -1.43606 -2.96436 -3.44575
N 0.22912 -1.04025 -1.23641
C -2.71771 -0.14789 0.60423
C -3.68354 -0.93889 -0.03940
C -2.55569 1.19680 0.20837
C -4.44550 -0.40894 -1.07961
H -3.81680 -1.97432 0.25926
C -3.31490 1.71397 -0.85168
C -4.25139 0.91220 -1.50131
H -5.18956 -1.02951 -1.56975
H -3.19505 2.75438 -1.13778
H -4.84587 1.31613 -2.31447
H -1.94967 1.87253 0.80605
C -1.86313 -0.71119 1.67539
C -1.51063 -1.95210 3.71253
H -1.89332 -2.53653 4.54279
C -2.37245 -1.46959 2.73111
H -3.44006 -1.65211 2.78265
C 0.30030 -0.90315 2.53653
H 1.34640 -0.65482 2.41683
C -0.15177 -1.65559 3.61348
H 0.55873 -1.99916 4.35688
N -0.53115 -0.44251 1.57646

E⁺ (K^2)
SCF (B3LYP) Energy = -1281.96870492
Enthalpy 0K = -1281.572473

Enthalpy 298K = -1281.545738
Free Energy 298K = -1281.630548
Lowest Frequency = 23.4937 cm^{-1}
Second Frequency = 28.7144 cm^{-1}

Ru	-0.21535	-0.29147	-0.45898
O	-2.27040	-2.52684	-2.03453
C	-1.18528	-3.06834	-1.50131
C	-0.98493	-4.50851	-1.85433
O	-0.40159	-2.43726	-0.77611
H	-0.05112	-4.87351	-1.42986
H	-1.82562	-5.09785	-1.47520
H	-0.97819	-4.62211	-2.94259
C	-2.41548	1.51832	0.05933
C	-3.71765	1.96381	0.32329
C	-2.09668	0.12925	0.08155
C	-4.72515	1.05209	0.63657
H	-3.95632	3.02290	0.29664
C	-3.12852	-0.76192	0.43726
C	-4.42701	-0.30939	0.70438
H	-5.73124	1.40394	0.83982
H	-2.92399	-1.82631	0.53435
H	-5.20221	-1.02300	0.96927
H	-2.42074	-1.63539	-1.65620
C	-1.28854	2.41932	-0.21142
C	-0.21433	4.55982	-0.54078
H	-0.26780	5.64235	-0.59718
C	-1.35967	3.81442	-0.28300
H	-2.31168	4.31144	-0.14086
C	1.01472	2.50899	-0.65214
H	1.92973	1.95014	-0.79946
C	0.99781	3.89555	-0.73069
H	1.91552	4.43329	-0.93945
N	-0.09037	1.77922	-0.39464
C	2.78144	-0.34808	0.32014
C	3.88748	0.50976	0.44288
C	2.47481	-0.88157	-0.94664
C	4.65467	0.83828	-0.67454
H	4.12905	0.94341	1.40840
C	3.24166	-0.54027	-2.06559
C	4.33030	0.32203	-1.93325
H	5.50469	1.50455	-0.56382
H	3.00033	-0.97032	-3.03290
H	4.93085	0.58060	-2.79951
H	1.70436	-1.64384	-1.04321
C	1.95439	-0.67191	1.50649
C	1.74429	-1.25432	3.84588
H	2.19476	-1.47573	4.80780
C	2.53939	-0.94888	2.74681
H	3.62048	-0.94568	2.82557
C	-0.17321	-0.99815	2.42916
H	-1.24038	-0.99299	2.25764
C	0.36055	-1.28174	3.67836
H	-0.30776	-1.51663	4.49913
N	0.59727	-0.69113	1.35915

D
SCF (B3LYP) Energy = -1510.68131982
Enthalpy 0K = -1510.235172
Enthalpy 298K = -1510.203567
Free Energy 298K = -1510.298882
Lowest Frequency = 23.5008 cm^{-1}
Second Frequency = 28.7376 cm^{-1}

Ru	0.96019	0.05676	-0.40635
O	2.12876	1.25235	-1.81208
C	1.71295	0.51599	-2.76018
C	2.25922	0.65047	-4.15535
O	0.83347	-0.37481	-2.49157
H	1.50348	0.36910	-4.89158
H	2.60740	1.66983	-4.33181
H	3.11154	-0.02894	-4.26413
C	-2.57606	0.06174	-0.93250
C	-3.63364	-0.31822	-0.09139
C	-2.22167	-0.77428	-2.00232
C	-4.31622	-1.51616	-0.30510
H	-3.91443	0.32477	0.73829
C	-2.91798	-1.96293	-2.22202
C	-3.96443	-2.33853	-1.37682
H	-5.12548	-1.80177	0.36089
H	-2.64090	-2.59638	-3.06006
H	-4.50358	-3.26512	-1.55282
H	-1.39891	-0.49524	-2.65033
C	-1.95137	1.40435	-0.76996
C	-2.29122	3.80781	-0.72732
H	-2.95166	4.66949	-0.74812
C	-2.80562	2.51911	-0.78773
H	-3.87236	2.34998	-0.88115
C	-0.11602	2.81972	-0.63177
H	0.96189	2.89426	-0.58245
C	-0.90834	3.95907	-0.66583
H	-0.43942	4.93670	-0.63903
N	-0.60482	1.55717	-0.65774
C	-0.08296	0.17668	2.43836
C	-0.73397	0.78373	3.52042
C	0.94746	0.87349	1.76418
C	-0.34983	2.05314	3.95169
H	-1.55759	0.27596	4.01438
C	1.34339	2.13482	2.22680
C	0.69315	2.72756	3.30900
H	-0.86138	2.51457	4.79136
H	2.18088	2.63271	1.74754
H	1.00442	3.70729	3.66028
H	1.79369	0.30119	1.21968
C	-0.43869	-1.15262	1.92592
C	-1.27672	-3.40729	2.12609
H	-1.74070	-4.19564	2.71071
C	-1.04740	-2.15645	2.68748
H	-1.30412	-1.95764	3.72193
C	-0.28230	-2.60259	0.09705
H	0.05295	-2.72184	-0.92606
C	-0.87814	-3.63583	0.80742
H	-1.02053	-4.59968	0.33125
N	-0.08114	-1.38034	0.62937
O	2.51240	-1.31605	-0.48962
C	3.49294	-1.28150	0.36397
C	4.62069	-2.25608	0.04547
O	3.56287	-0.53297	1.34789
H	4.22155	-3.22055	-0.27868
H	5.21883	-1.85332	-0.77927
H	5.26461	-2.38448	0.91679

TS(**D-E**)
SCF (B3LYP) Energy = -1510.64344920
Enthalpy 0K = -1510.202365
Enthalpy 298K = -1510.170809
Free Energy 298K = -1510.265568
Lowest Frequency = -1259.3908 cm^{-1}
Second Frequency = 27.4181 cm^{-1}

Ru	-0.64116	-0.47938	-0.57291
O	-1.21550	-2.35011	-1.48667
C	-0.46594	-2.14925	-2.49955
C	-0.50551	-3.09964	-3.67002
O	0.28434	-1.12139	-2.51772
H	0.44716	-3.09158	-4.20296
H	-0.74885	-4.10954	-3.33378
H	-1.28944	-2.77460	-4.36291
C	2.83670	-0.17680	0.15191
C	3.55722	0.75554	0.91516

```
C   2.94982 -0.14651 -1.24680
C   4.36291  1.71016  0.29475
H   3.47362  0.73941  1.99828
C   3.76914  0.80082 -1.86203
C   4.47618  1.73110 -1.09679
H   4.90466  2.43258  0.89851
H   3.85520  0.80803 -2.94499
H   5.11347  2.46572 -1.58103
H   2.38756 -0.85272 -1.84689
C   2.09621 -1.27316  0.83381
C   2.22897 -3.15493  2.36595
H   2.78599 -3.75486  3.07910
C   2.81063 -2.04866  1.76188
H   3.84091 -1.78151  1.96741
C   0.25903 -2.67514  1.09684
H  -0.75422 -2.89631  0.79377
C   0.92514 -3.48560  2.00368
H   0.41830 -4.35235  2.41364
N   0.79898 -1.56364  0.53464
C  -1.34629  0.88422  1.97151
C  -1.74561  1.01722  3.30656
C  -1.80752 -0.20547  1.18205
C  -2.63371  0.09713  3.86549
H  -1.36435  1.82796  3.92150
C  -2.71884 -1.10272  1.76628
C  -3.12959 -0.95730  3.09356
H  -2.94324  0.20753  4.90089
H  -3.11482 -1.91793  1.16437
H  -3.83399 -1.66258  3.52692
H  -2.27047  0.11471 -0.13244
C  -0.45493  1.82686  1.28290
C   0.65240  3.94968  0.96888
H   0.91569  4.94022  1.32730
C  -0.10891  3.09619  1.75833
H  -0.46781  3.42013  2.72850
C   0.68963  2.24363 -0.71042
H   0.98107  1.85638 -1.67910
C   1.04872  3.51993 -0.29772
H   1.62630  4.15484 -0.96000
N  -0.02102  1.40152  0.06017
O  -2.54303  0.29465 -1.41648
C  -2.82922  1.56989 -1.71044
C  -3.52148  1.69749 -3.05592
O  -2.58936  2.52205 -0.98989
H  -2.85155  1.34472 -3.84660
H  -4.41195  1.06273 -3.07966
H  -3.79621  2.73692 -3.23872
```

E

SCF (B3LYP) Energy = -1510.67425458
Enthalpy 0K = -1510.227323
Enthalpy 298K = -1510.195321
Free Energy 298K = -1510.292089
Lowest Frequency = 22.7985 cm^{-1}
Second Frequency = 24.8135 cm^{-1}

```
Ru  0.60273  0.47507  0.12259
O   1.41065  2.00809  1.38319
C   0.66871  2.98163  1.00749
C   0.84782  4.33323  1.66546
O  -0.21122  2.81177  0.11574
H   0.01196  4.51230  2.35061
H   1.78178  4.37470  2.22790
H   0.82598  5.12343  0.91059
C  -2.82892 -0.07725  0.52877
C  -3.69112 -1.07752  0.05333
C  -2.88939  1.20402 -0.04260
C  -4.58423 -0.81189 -0.98515
H  -3.64888 -2.07157  0.48966
C  -3.79469  1.46877 -1.07186
C  -4.64157  0.46448 -1.54836
H  -5.23615 -1.60048 -1.35001
H  -3.83941  2.46712 -1.49811
H  -5.34506  0.67660 -2.34866
H  -2.22407  1.98469  0.30954
C  -1.97590 -0.34107  1.71947
C  -1.90874 -1.00455  4.05594
H  -2.40439 -1.37874  4.94639
C  -2.61202 -0.82901  2.87116
H  -3.67572 -1.03243  2.82143
C   0.02273 -0.19315  2.89839
H   1.06672  0.07965  2.87098
C  -0.56064 -0.65521  4.06865
H   0.04484 -0.73967  4.96458
N  -0.64011 -0.06265  1.71992
C   1.62013 -2.24776 -0.25153
C   2.43596 -3.37622 -0.07342
C   1.83197 -1.05117  0.49187
C   3.49477 -3.33816  0.83044
H   2.25670 -4.28627 -0.64123
C   2.93016 -1.03976  1.37685
C   3.74659 -2.16159  1.54576
H   4.12624 -4.21101  0.96800
H   3.14900 -0.13442  1.94114
H   4.58454 -2.12088  2.23846
H   3.00615  0.86414 -1.06638
C   0.54219 -2.16139 -1.23642
C  -0.79056 -2.92719 -3.10708
H  -1.05782 -3.69905 -3.82282
C   0.19262 -3.16219 -2.15427
H   0.70996 -4.11447 -2.12575
C  -1.04897 -0.73330 -2.18371
H  -1.53049  0.23622 -2.14460
C  -1.41783 -1.67999 -3.13151
H  -2.18775 -1.44119 -3.85672
N  -0.10599 -0.95171 -1.24623
O   2.12063  1.11158 -1.38731
C   2.26844  2.09679 -2.34813
C   0.95322  2.56815 -2.89077
O   3.37149  2.46820 -2.65961
H   0.35420  2.98065 -2.07235
H   1.13621  3.31658 -3.66108
H   0.40115  1.72199 -3.30999
```

E (without HOAc)

SCF (B3LYP) Energy = -1281.58282267
Enthalpy 0K = -1281.199599
Enthalpy 298K = -1281.173620
Free Energy 298K = -1281.255785
Lowest Frequency = 28.0921 cm^{-1}
Second Frequency = 35.4198 cm^{-1}

```
Ru -0.24054 -0.65374 -0.21135
O  -0.58416 -2.79417  0.08730
C  -0.95212 -2.90231 -1.13151
C  -1.45996 -4.21512 -1.66836
O  -0.90749 -1.86799 -1.87442
H  -1.29814 -4.27426 -2.74632
H  -0.97298 -5.04953 -1.15934
H  -2.53717 -4.28299 -1.47992
C   2.78731 -0.10372  0.54018
C   3.92452  0.68759  0.30889
C   2.45942 -1.09746 -0.40003
C   4.70637  0.49392 -0.82960
H   4.17690  1.48237  1.00429
C   3.24054 -1.28669 -1.54202
C   4.36626 -0.49093 -1.76113
H   5.57671  1.12220 -0.99569
H   2.96583 -2.05880 -2.25406
H   4.97416 -0.63604 -2.64915
```

```
H    1.64215 -1.79776 -0.19475
C    1.93921  0.11708  1.73489
C    1.71098  0.65444  4.08503
H    2.15071  0.91329  5.04296
C    2.51204  0.45713  2.96630
H    3.59090  0.53921  3.03674
C   -0.18233  0.14872  2.70086
H   -1.24551  0.01304  2.55019
C    0.33278  0.49424  3.94201
H   -0.34528  0.62941  4.77792
N    0.58639 -0.04007  1.59992
C   -2.46199  1.20554 -0.21624
C   -3.75128  1.70980  0.02328
C   -2.09862 -0.10922  0.19249
C   -4.70266  0.92372  0.66539
H   -4.01797  2.71666 -0.28916
C   -3.08532 -0.88380  0.83530
C   -4.36451 -0.37519  1.06826
H   -5.69897  1.31453  0.85018
H   -2.84183 -1.89500  1.15176
H   -5.10790 -0.99456  1.56582
C   -1.40376  1.94993 -0.89446
C   -0.45166  3.82589 -2.09395
H   -0.54667  4.82091 -2.51832
C   -1.52470  3.23628 -1.43824
H   -2.46800  3.76312 -1.35031
C    0.81581  1.84462 -1.64237
H    1.72098  1.25306 -1.70687
C    0.74424  3.11243 -2.20431
H    1.60860  3.52325 -2.71462
N   -0.21681  1.26558 -0.99547
```

D⁺ (η^6)
SCF (B3LYP) Energy = -1281.97936970
Enthalpy 0K = -1281.582734
Enthalpy 298K = -1281.556522
Free Energy 298K = -1281.641109
Lowest Frequency = 9.0290 cm^{-1}
Second Frequency = 20.6904 cm^{-1}

```
Ru -0.40824  1.11941 -0.42013
O  -0.53602  2.67632  1.03244
C  -1.80447  2.54171  1.13078
C  -2.62258  3.39431  2.04780
O  -2.33044  1.65246  0.37906
H  -2.03822  3.67905  2.92449
H  -2.90855  4.31020  1.51858
H  -3.53354  2.87107  2.34265
C  -1.60509 -2.02359  0.40296
C  -1.25823 -3.26216 -0.16480
C  -2.82301 -1.42468  0.04423
C  -2.09549 -3.87353 -1.09898
H  -0.32782 -3.74405  0.12391
C  -3.66413 -2.04813 -0.87947
C  -3.30120 -3.26679 -1.45859
H  -1.81188 -4.82640 -1.53522
H  -4.61251 -1.58524 -1.13560
H  -3.96056 -3.74844 -2.17409
H  -3.11602 -0.48292  0.49270
C  -0.70919 -1.43313  1.43577
C   0.45330 -1.70948  3.54866
H   0.69217 -2.30846  4.42179
C  -0.38955 -2.20634  2.56155
H  -0.83255 -3.19130  2.65238
C   0.62737  0.29965  2.26384
H   1.01025  1.29927  2.10692
C   0.97321 -0.42631  3.39451
H   1.63529  0.01589  4.13029
N  -0.19205 -0.18005  1.29692
C   1.48766  0.45088 -1.46445
C   0.38548 -0.37673 -1.87587
C   1.33131  1.85806 -1.56289
C  -0.79502  0.18437 -2.40362
H   0.41818 -1.44525 -1.70345
C   0.15176  2.43772 -2.13004
C  -0.91040  1.60715 -2.53533
H  -1.63668 -0.45590 -2.63875
H   0.04313  3.51603 -2.15607
H  -1.84595  2.04352 -2.86730
H   2.11423  2.48714 -1.15580
C   2.73743 -0.11832 -0.88800
C   4.36413 -1.87296 -0.65685
H   4.72377 -2.87081 -0.88780
C   3.16136 -1.41638 -1.19763
H   2.58977 -2.04846 -1.86874
C   4.59546  0.25795  0.41239
H   5.14275  0.95420  1.04363
C   5.09731 -1.02423  0.16795
H   6.03922 -1.33663  0.60584
N   3.44709  0.70705 -0.09838
```

TS(**D⁺-E⁺**) (η^6)
SCF (B3LYP) Energy = -1281.95443523
Enthalpy 0K = -1281.559105
Enthalpy 298K = -1281.533277
Free Energy 298K = -1281.616294
Lowest Frequency = -75.3638 cm^{-1}
Second Frequency = 13.5234 cm^{-1}

```
Ru  0.39575 -0.78111 -0.25359
O   0.45900 -1.78576  1.56205
C   1.60441 -2.39521  1.75068
C   1.69944 -3.18540  3.03819
O   2.54208 -2.30666  0.94736
H   2.55394 -3.86109  2.99570
H   1.83816 -2.49290  3.87529
H   0.77869 -3.74364  3.22227
C   1.91355  1.89849  0.11292
C   2.31709  3.00461 -0.64678
C   2.62031  0.68463 -0.00929
C   3.40176  2.89490 -1.51913
H   1.77412  3.94225 -0.57376
C   3.70851  0.58181 -0.88370
C   4.09852  1.68702 -1.64078
H   3.70563  3.75617 -2.10607
H   4.25683 -0.35361 -0.93651
H   4.95022  1.61772 -2.31020
H   2.44662 -0.15273  0.67505
C   0.75591  1.95116  1.02910
C  -0.58818  2.98563  2.74345
H  -0.80420  3.82479  3.39698
C   0.48213  3.04532  1.85520
H   1.12988  3.91375  1.81757
C  -1.04730  0.77115  1.94669
H  -1.61446 -0.15153  1.94326
C  -1.35974  1.82489  2.79778
H  -2.18978  1.72728  3.48815
N  -0.02902  0.84309  1.06858
C  -1.52384 -0.72360 -1.36117
C  -0.56665  0.03562 -2.12201
C  -1.18790 -2.06319 -0.98591
C   0.66957 -0.53472 -2.46706
H  -0.75151  1.07873 -2.34718
C   0.04196 -2.66135 -1.40446
C   0.97827 -1.89279 -2.11275
H   1.42708  0.07668 -2.94373
H   0.30120 -3.65697 -1.06407
H   1.96555 -2.29182 -2.31326
H  -1.87586 -2.59866 -0.34324
C  -2.84000 -0.15793 -0.95117
```

C -4.68855 1.35179 -1.24092
H -5.17222 2.17057 -1.76416
C -3.42587 0.91102 -1.64027
H -2.93325 1.37250 -2.48888
C -4.65429 -0.34472 0.45055
H -5.11455 -0.87127 1.28333
C -5.31806 0.71617 -0.17443
H -6.30169 1.02264 0.16484
N -3.44792 -0.77630 0.07756

E^{+} (η^6)
SCF (B3LYP) Energy = -1281.97664136
Enthalpy 0K = -1281.580168
Enthalpy 298K = -1281.553993
Free Energy 298K = -1281.637126
Lowest Frequency = 17.1472 cm^{-1}
Second Frequency = 29.1475 cm^{-1}

Ru 0.28871 -0.77697 -0.06200
O 0.94031 -0.68196 2.00549
C 2.04571 -0.67564 2.57084
C 2.16935 -0.69220 4.06425
O 3.19537 -0.65777 1.93161
H 2.69134 0.21079 4.39511
H 1.18374 -0.74474 4.52365
H 2.77831 -1.54755 4.37127
C 2.24998 1.28338 -0.89557
C 3.39599 1.85341 -1.46900
C 2.09218 -0.12882 -0.81499
C 4.41430 1.03985 -1.96082
H 3.50193 2.93221 -1.53508
C 3.14527 -0.92185 -1.30566
C 4.29137 -0.34735 -1.87158
H 5.29936 1.48471 -2.40362
H 3.08243 -2.00574 -1.25403
H 5.08488 -0.98879 -2.24427
H 3.04061 -0.60723 0.95814
C 1.15835 2.06675 -0.31445
C 0.04417 4.06772 0.45416
H 0.01303 5.14718 0.56337
C 1.12386 3.46049 -0.17548
H 1.94589 4.05890 -0.54954
C -0.90995 1.89637 0.78701
H -1.68296 1.23330 1.16001
C -0.98927 3.27276 0.95493
H -1.84223 3.70366 1.46648
N 0.12464 1.31075 0.15365
C -2.02899 -1.23323 -0.55885
C -1.16848 -1.03784 -1.70467
C -1.62380 -2.14889 0.42110
C -0.04832 -1.87542 -1.93038
H -1.40321 -0.26823 -2.43044
C -0.41697 -2.90178 0.24700
C 0.32362 -2.84700 -0.95214
H 0.55394 -1.74007 -2.82113
H -0.08664 -3.55594 1.04724
H 1.19295 -3.47697 -1.09458
H -2.20627 -2.24020 1.32958
C -3.28941 -0.46136 -0.39161
C -5.22909 0.64889 -1.28107
H -5.82527 0.99091 -2.12123
C -4.02538 -0.02213 -1.49971
H -3.68757 -0.22442 -2.51032
C -4.85085 0.38667 1.07000
H -5.14797 0.53248 2.10606
C -5.65419 0.86021 0.02786
H -6.58449 1.37455 0.24379
N -3.69712 -0.25679 0.87544

^{3}D^{+} (* single point)
SCF (B3LYP) Energy = -1680.31867788
Enthalpy 0K = -1679.780517
Enthalpy 298K = -1679.743169
Free Energy 298K = -1679.845397
Lowest Frequency = 50.8627 cm^{-1}
Second Frequency = 51.2231 cm^{-1}

INT(**^{3}D^{+}**)
SCF (B3LYP) Energy = -1680.30531939
Enthalpy 0K = -1679.767003
Enthalpy 298K = -1679.725842
Free Energy 298K = -1679.845129
Lowest Frequency = 17.3653 cm^{-1}
Second Frequency = 19.4605 cm^{-1}

Ru 0.38035 0.82714 0.27366
C -2.33289 -0.89408 -1.53895
C -1.72442 -2.00480 -2.12693
C -1.69118 0.36232 -1.63271
C -0.50216 -1.88420 -2.80495
H -2.22757 -2.96487 -2.07546
C -0.46070 0.47874 -2.29314
C 0.13182 -0.65304 -2.89110
H -0.06759 -2.75706 -3.28348
H -0.04532 1.46653 -2.45722
H 1.06481 -0.55141 -3.43670
H -2.14474 1.26978 -1.24939
C -3.64248 -1.04170 -0.85147
C -5.82925 -0.22027 -0.24679
H -6.59403 0.55058 -0.27505
C -4.60418 -0.01774 -0.87923
H -4.40620 0.90417 -1.41524
C -5.05298 -2.39522 0.37546
H -5.19868 -3.35681 0.86369
C -6.06465 -1.43461 0.39855
H -7.00656 -1.64008 0.89604
N -3.87091 -2.21529 -0.22574
C 2.96535 -1.69241 0.11154
C 2.77645 -2.98304 -0.40532
C 3.15564 -1.53523 1.49129
C 2.74521 -4.08947 0.44454
H 2.64858 -3.11754 -1.47540
C 3.13136 -2.64183 2.33977
C 2.92116 -3.92124 1.82045
H 2.60222 -5.08340 0.03033
H 3.29444 -2.50876 3.40530
H 2.91464 -4.78347 2.48054
H 3.34166 -0.54601 1.89323
C 3.12610 -0.53935 -0.81868
C 4.49162 0.44974 -2.56793
H 5.32291 0.39143 -3.26363
C 4.19723 -0.61277 -1.72278
H 4.80851 -1.50791 -1.72258
C 2.64661 1.60440 -1.57415
H 2.01019 2.47319 -1.46315
C 3.70653 1.59463 -2.47095
H 3.89696 2.47276 -3.07816
N 2.32024 0.55909 -0.77488
O 0.55323 2.86166 -0.17317
C -0.44704 3.65558 -0.48125
C -0.03400 5.11909 -0.57540
O -1.61097 3.30545 -0.68160
H -0.86736 5.72094 -0.93843
H 0.27477 5.48132 0.41064
H 0.82512 5.23528 -1.24274
N -1.35540 1.19727 1.24999
C -2.32707 1.46634 1.81403
C -3.57198 1.85798 2.45981
H -3.48224 1.78698 3.54711
H -3.80862 2.89007 2.18412

H -4.38267 1.20589 2.12264
N 1.33604 1.29829 1.92571
C 1.86320 1.70272 2.87345
C 2.53622 2.21699 4.05992
H 3.61975 2.21200 3.90955
H 2.21464 3.24438 4.25391
H 2.29648 1.60015 4.93074
N 0.06993 -1.13550 0.73957
C -0.36282 -2.18281 0.97535
C -0.96568 -3.48498 1.21944
H -1.02784 -3.67938 2.29389
H -1.97290 -3.47701 0.78444
H -0.36225 -4.26818 0.75373

TS(^{3}D$^+$–^{3}E$^+$)
SCF (B3LYP) Energy = -1680.27776349
Enthalpy 0K = -1679.744648
Enthalpy 298K = -1679.704202
Free Energy 298K = -1679.820409
Lowest Frequency = -1158.6118 cm^{-1}
Second Frequency = 18.2623 cm^{-1}

Ru -0.10692 -0.93836 0.27381
C 1.61355 1.20736 -1.52295
C 1.49447 2.26916 -2.43477
C 0.72167 0.09870 -1.58178
C 0.57069 2.22332 -3.47721
H 2.16996 3.11464 -2.34537
C -0.17230 0.07690 -2.68082
C -0.24847 1.10060 -3.62221
H 0.51527 3.04133 -4.18977
H -0.82636 -0.78188 -2.80459
H -0.94257 1.03039 -4.45493
H 1.31820 -1.15877 -1.51253
C 2.80649 1.27463 -0.62167
C 5.00211 0.47443 -0.01691
H 5.81147 -0.24381 -0.11937
C 3.81618 0.30251 -0.72764
H 3.68065 -0.54766 -1.38686
C 4.08386 2.50045 0.85605
H 4.15796 3.39161 1.47720
C 5.14492 1.59737 0.79948
H 6.05583 1.78240 1.35959
N 2.94464 2.36063 0.16372
C -2.71790 1.67963 0.13877
C -1.90349 2.51524 -0.63704
C -3.33975 2.20405 1.28343
C -1.71581 3.84884 -0.27225
H -1.43469 2.13009 -1.53348
C -3.14217 3.53538 1.65268
C -2.33541 4.36439 0.86873
H -1.09394 4.48772 -0.89193
H -3.63477 3.92851 2.53727
H -2.20090 5.40789 1.13882
H -3.98831 1.56853 1.88032
C -3.09616 0.31178 -0.32248
C -4.93286 -1.07400 -1.11603
H -5.98224 -1.19955 -1.36400
C -4.45616 0.13668 -0.63444
H -5.12039 0.98428 -0.51227
C -2.69140 -1.88628 -0.94232
H -1.96568 -2.68179 -1.03865
C -4.01820 -2.10983 -1.28050
H -4.31386 -3.08208 -1.65944
N -2.20784 -0.71118 -0.46545
O -0.00233 -2.86798 -0.63872
C 0.96788 -3.14308 -1.41234
C 1.12532 -4.55599 -1.91186
O 1.80574 -2.26796 -1.80792
H 2.17609 -4.85147 -1.86785
H 0.51012 -5.24505 -1.33328
H 0.82209 -4.59596 -2.96341
N 1.66923 -1.38374 1.10851
C 2.62796 -1.70223 1.67352
C 3.84893 -2.09224 2.36631
H 3.65142 -2.24169 3.43163
H 4.23762 -3.02427 1.94573
H 4.60206 -1.30826 2.24803
N -1.01644 -1.82540 1.89481
C -1.53210 -2.35563 2.78590
C -2.18655 -3.02848 3.90192
H -3.27295 -2.95233 3.80075
H -1.90778 -4.08599 3.91864
H -1.88789 -2.56853 4.84817
N 0.00288 0.81624 1.26080
C 0.26271 1.77426 1.85409
C 0.61357 3.00721 2.54363
H 1.16152 2.78489 3.46375
H 1.25154 3.59308 1.87565
H -0.28903 3.57228 2.78513

^{3}E$^+$
SCF (B3LYP) Energy = -1680.29030330
Enthalpy 0K = -1679.752582
Enthalpy 298K = -1679.711334
Free Energy 298K = -1679.830992
Lowest Frequency = 18.0340 cm^{-1}
Second Frequency = 19.2569 cm^{-1}

Ru 0.16027 -0.83648 -0.34226
C -1.81024 0.87349 1.55273
C -2.15184 1.38130 2.82607
C -0.63656 0.07770 1.37841
C -1.38288 1.13117 3.95658
H -3.04400 1.99535 2.91732
C 0.08822 -0.18280 2.57339
C -0.25494 0.32268 3.82701
H -1.66867 1.54588 4.91840
H 0.97269 -0.81034 2.51865
H 0.35773 0.08598 4.69314
H -1.71408 -1.61764 1.61476
C -2.82589 1.21044 0.49615
C -5.14418 1.15529 -0.21347
H -6.17160 0.83112 -0.07122
C -4.14959 0.76217 0.67822
H -4.38709 0.12587 1.52471
C -3.46192 2.37701 -1.38633
H -3.15629 3.03519 -2.19865
C -4.79582 1.98595 -1.27929
H -5.53288 2.33455 -1.99553
N -2.49591 2.01321 -0.53140
C 2.65386 1.85868 0.22623
C 1.71898 2.49592 1.05321
C 3.32391 2.61578 -0.75077
C 1.44973 3.85606 0.89283
H 1.21456 1.93557 1.82927
C 3.05074 3.97454 -0.91084
C 2.11147 4.59939 -0.08607
H 0.72875 4.33605 1.54742
H 3.58327 4.54633 -1.66564
H 1.90850 5.66061 -0.19670
H 4.06448 2.13618 -1.38514
C 3.09498 0.45010 0.45070
C 4.99430 -0.96934 1.00720
H 6.04416 -1.08580 1.25741
C 4.45706 0.28593 0.76387
H 5.07450 1.17377 0.83327
C 2.80837 -1.84730 0.61043
H 2.12735 -2.68359 0.53898
C 4.13964 -2.06570 0.93122

```
H    4.48547 -3.07705  1.11542
N    2.26407 -0.62784  0.36717
O    0.02298 -2.79857  0.61954
C   -0.88880 -3.28196  1.30917
C   -0.91906 -4.73316  1.68647
O   -1.89731 -2.57838  1.77827
H   -0.71543 -4.82813  2.75822
H   -1.91586 -5.14525  1.50969
H   -0.17100 -5.28743  1.12139
N   -1.64533 -1.22254 -1.12587
C   -2.64146 -1.49937 -1.65005
C   -3.90752 -1.82805 -2.29293
H   -3.79790 -1.80526 -3.38109
H   -4.23547 -2.82790 -1.99384
H   -4.66775 -1.10023 -1.99642
N    1.04685 -1.86849 -2.03085
C    1.51283 -2.41406 -2.94076
C    2.10506 -3.09980 -4.08405
H    1.65333 -2.74199 -5.01354
H    3.18139 -2.90904 -4.11974
H    1.94052 -4.17808 -4.00399
N    0.22041  0.85029 -1.37913
C    0.13952  1.80741 -2.02166
C    0.01004  3.04550 -2.77433
H   -0.47749  2.86104 -3.73600
H   -0.59240  3.74751 -2.19099
H    0.99513  3.48494 -2.94807
```

$^{6}F^{2+}$ (* single point)
SCF (B3LYP) Energy = -891.156384704
Enthalpy 0K = -890.868490
Enthalpy 298K = -890.842903
Free Energy 298K = -890.920942
Lowest Frequency = 67.6506 cm^{-1}
Second Frequency = 67.6534 cm^{-1}

$^{3}A^{2+}$
SCF (B3LYP) Energy = -725.008746480
Enthalpy 0K = -724.763198
Enthalpy 298K = -724.742420
Free Energy 298K = -724.815952
Lowest Frequency = 21.9834 cm^{-1}
Second Frequency = 23.3816 cm^{-1}

```
C    2.20883  1.34073  0.46975
C    2.20901  1.06471 -0.94014
C    2.20856 -0.26480 -1.39606
C    2.20815 -1.34781 -0.45208
C    2.20796 -1.07786  0.92727
C    2.20819  0.28115  1.39319
Ru   0.44093 -0.00012  0.00002
H    2.16019 -0.47363 -2.45934
H    2.15937  0.48860  2.45673
H    2.16066  2.36601  0.82047
H    2.15903 -1.89423  1.63977
H    2.15935 -2.37258 -0.80420
H    2.16091  1.88209 -1.65156
N   -0.83306 -0.52701  1.54354
C   -1.53145 -0.82481  2.41600
C   -2.40218 -1.20167  3.52006
H   -3.44915 -1.09151  3.22201
H   -2.21686 -2.24340  3.79958
H   -2.20581 -0.55844  4.38341
N   -0.83284 -1.07313 -1.22852
N   -0.83210  1.60081 -0.31541
C   -1.52976  2.50584 -0.49374
C   -1.53107 -1.67972 -1.92289
C   -2.40161 -2.44735 -2.80156
H   -2.21456 -3.51715 -2.66662
H   -3.44864 -2.23422 -2.56618
H   -2.20674 -2.17805 -3.84424
C   -2.39955  3.65114 -0.71935
H   -3.44662  3.33623 -0.67946
H   -2.22336  4.40807  0.05116
H   -2.19324  4.08548 -1.70243
```

$^{5}F^{+}$ (κ^{1}) (* single point)
SCF (B3LYP) Energy = -987.151886450
Enthalpy 0K = -986.860491
Enthalpy 298K = -986.834007
Free Energy 298K = -986.914118
Lowest Frequency = 64.8194 cm^{-1}
Second Frequency = 66.9460 cm^{-1}

$^{4}F^{+}$ (κ^{2})
SCF (B3LYP) Energy = -854.387330262
Enthalpy 0K = -854.145119
Enthalpy 298K = -854.119784
Free Energy 298K = -854.206442
Lowest Frequency = 15.0798 cm^{-1}
Second Frequency = 15.7827 cm^{-1}

```
N    2.02733  0.16357 -0.00021
C    3.17732  0.28623 -0.00001
N    0.01622 -1.33828  1.44686
C    0.02510 -2.08675  2.33033
N    0.01590 -1.33831 -1.44686
C    0.02451 -2.08698 -2.33016
N   -2.02685  0.12010  0.00015
C   -3.17975  0.21219  0.00008
C    4.62496  0.45184 -0.00036
H    4.93606  1.00558 -0.89082
H    4.93632  1.00680  0.88925
H    5.11650 -0.52506  0.00024
C    0.03555 -3.01109 -3.45748
H    0.93463 -3.63305 -3.42618
H   -0.84382 -3.66037 -3.42133
H    0.02443 -2.45209 -4.39778
C   -4.63140  0.33832  0.00025
H   -5.09597 -0.65169 -0.00115
H   -4.95787  0.88250  0.89110
H   -4.95785  0.88501 -0.88908
C    0.03619 -3.01074  3.45774
H    0.92900 -3.64129  3.41955
H    0.03773 -2.45152  4.39797
H   -0.84960 -3.65158  3.42861
O   -0.01493  1.90200 -1.09062
C   -0.02462  2.57148 -0.00006
C   -0.07556  4.06945 -0.00007
H    0.40280  4.46418  0.89790
H    0.40189  4.46415 -0.89853
H   -1.12213  4.39336  0.00048
O   -0.01470  1.90204  1.09053
Ru   0.00097  0.07908 -0.00002
```

f-**^{3}F** ($\kappa^{2}\kappa^{1}$)
SCF (B3LYP) Energy = -950.281732021
Enthalpy 0K = -950.036092
Enthalpy 298K = -950.010118
Free Energy 298K = -950.096046
Lowest Frequency = 16.2282 cm^{-1}
Second Frequency = 30.3767 cm^{-1}

```
Ru -0.35307  0.04678  0.00013
N  -1.99196 -1.11003  0.00040
C  -2.96962 -1.73579  0.00042
N   0.56974 -1.02443  1.40373
C   1.22179 -1.54213  2.20788
N   0.56959 -1.02479 -1.40330
```

```
C   1.22161 -1.54269 -2.20734
C  -4.20499 -2.50988 -0.00073
H  -4.79978 -2.27426 -0.88861
H  -3.98474 -3.58168 -0.00293
H  -4.79915 -2.27779  0.88849
C   2.13732 -2.12492  3.17825
H   1.93398 -1.73655  4.18065
H   2.04371 -3.21458  3.19772
H   3.16119 -1.86070  2.89509
C   2.13656 -2.12482 -3.17865
H   1.93220 -1.73635 -4.18079
H   3.16054 -1.86018 -2.89627
H   2.04346 -3.21452 -3.19825
O  -1.40837  1.55790 -1.09553
C  -1.72528  2.13010 -0.00006
O  -1.40824  1.55818  1.09552
C  -2.42024  3.46465 -0.00019
H  -3.03108  3.57642  0.89787
H  -1.66131  4.25443 -0.00035
H  -3.03122  3.57617 -0.89818
O   1.18889  1.42516 -0.00010
C   2.46204  1.15468  0.00003
O   2.98986  0.03754  0.00019
C   3.32064  2.42258 -0.00044
H   3.08949  3.03125  0.87951
H   4.38073  2.16291 -0.00050
H   3.08927  3.03076 -0.88067
```

m-**^{3}F** ($\kappa^2\kappa^1$)
SCF (B3LYP) Energy = -950.279416573
Enthalpy 0K = -950.034003
Enthalpy 298K = -950.007816
Free Energy 298K = -950.094853
Lowest Frequency = 19.1623 cm^{-1}
Second Frequency = 30.5962 cm^{-1}

```
Ru -0.33017  0.11951 -0.09198
N  -1.69360 -1.34044  0.07484
C  -2.48094 -2.17373  0.23912
N   0.71009 -0.91805 -1.42402
C   1.37807 -1.50520 -2.16631
N   1.04065  1.58313 -0.15168
C   1.90175  2.35374 -0.12001
C  -3.47064 -3.21947  0.46327
H  -2.97595 -4.18717  0.58858
H  -4.04612 -3.00218  1.36806
H  -4.15929 -3.28295 -0.38454
C   2.28815 -2.23460 -3.03837
H   1.89581 -3.23252 -3.25563
H   2.42797 -1.70209 -3.98407
H   3.25879 -2.33765 -2.54282
C   3.05033  3.24335 -0.03310
H   2.86824  4.03184  0.70279
H   3.92272  2.66013  0.27786
H   3.25626  3.70659 -1.00233
O  -1.75955  1.36229 -1.18194
C  -2.17317  1.84712 -0.07862
O  -1.65053  1.43210  1.00807
C  -3.23621  2.91668 -0.05598
H  -3.86202  2.80838  0.83249
H  -2.75601  3.90042 -0.01156
H  -3.84385  2.86976 -0.96144
O   0.68658 -0.82907  1.45347
C   1.97885 -0.96303  1.53461
O   2.82256 -0.61218  0.70403
C   2.40584 -1.63257  2.84531
H   1.89139 -2.59071  2.96789
H   3.48608 -1.78827  2.85509
H   2.11883 -1.00349  3.69425
```

c-**^{2}F** ($2\kappa^2$)
SCF (B3LYP) Energy = -817.512920900
Enthalpy 0K = -817.314290
Enthalpy 298K = -817.293360
Free Energy 298K = -817.367116
Lowest Frequency = 22.2612 cm^{-1}
Second Frequency = 22.4648 cm^{-1}

```
Ru -0.00000  0.08418 -0.00001
N   1.25056 -1.27852 -0.69044
C   2.00738 -2.04019 -1.13292
N  -1.25054 -1.27856  0.69042
C  -2.00733 -2.04025  1.13290
C   2.94971 -2.98454 -1.72000
H   3.67596 -2.45343 -2.34313
H   3.49141 -3.52483 -0.93754
H   2.42155 -3.71111 -2.34531
C  -2.94962 -2.98464  1.72000
H  -3.67842 -2.45310  2.33976
H  -3.48831 -3.52795  0.93757
H  -2.42188 -3.70861  2.34867
O   1.47424  1.62257 -0.26314
C   1.89599  1.42768  0.92513
C   2.95392  2.31412  1.52506
H   3.48125  1.79160  2.32515
H   3.65333  2.64299  0.75361
H   2.47355  3.20289  1.94873
O   1.36979  0.48348  1.60398
O  -1.36979  0.48349 -1.60398
C  -1.89606  1.42762 -0.92510
O  -1.47428  1.62254  0.26315
C  -2.95397  2.31408 -1.52504
H  -3.65336  2.64299 -0.75358
H  -2.47359  3.20282 -1.94875
H  -3.48133  1.79154 -2.32510
```

t-**^{2}F** ($2\kappa^2$) (* single point)
SCF (B3LYP) Energy = -817.509393243
Enthalpy 0K = -817.309749
Enthalpy 298K = -817.291262
Free Energy 298K = -817.354200
Lowest Frequency = 67.5790 cm^{-1}
Second Frequency = 73.4840 cm^{-1}

c-**^{4}F** ($2\kappa^1$)
SCF (B3LYP) Energy = -1083.04584900
Enthalpy 0K = -1082.753417
Enthalpy 298K = -1082.722254
Free Energy 298K = -1082.820521
Lowest Frequency = 25.3315 cm^{-1}
Second Frequency = 25.6705 cm^{-1}

```
N  -1.05756  1.71300  0.08764
C  -1.74971  2.62224 -0.08021
N   1.29770  0.74781  1.53069
C   2.17040  1.16018  2.16949
N   1.05757 -1.71303  0.08727
C   1.74966 -2.62229 -0.08075
C  -2.69956  3.69326 -0.34294
H  -2.32486  4.34901 -1.13402
H  -3.64563  3.24785 -0.66616
H  -2.87356  4.28930  0.55741
C   3.35545  1.65705  2.85407
H   3.23585  2.71077  3.12226
H   3.54982  1.08284  3.76462
H   4.21013  1.55496  2.17750
C   2.69944 -3.69329 -0.34383
H   2.32459 -4.34888 -1.13497
H   3.64547 -3.24785 -0.66713
H   2.87358 -4.28948  0.55639
```

```
O  -3.23108 -0.16399 -0.66820
C  -2.44926 -0.70454 -1.46116
O  -1.15874 -0.80431 -1.35720
C  -2.97645 -1.34812 -2.74837
H  -2.58291 -0.80956 -3.61670
H  -2.62675 -2.38207 -2.82775
H  -4.06762 -1.32245 -2.76725
O   1.15865  0.80467 -1.35713
C   2.44917  0.70496 -1.46115
O   3.23104  0.16430 -0.66833
C   2.97628  1.34876 -2.74829
H   2.62673  2.38279 -2.82736
H   4.06744  1.32295 -2.76732
H   2.58254  0.81048 -3.61669
Ru  0.00005 -0.00002  0.17863
N  -1.29751 -0.74821  1.53059
C  -2.17032 -1.16069  2.16917
C  -3.35537 -1.65773  2.85363
H  -3.54978 -1.08371  3.76429
H  -4.21002 -1.55548  2.17703
H  -3.23577 -2.71150  3.12160
```

t-**^{4}F** ($2\kappa^1$)
SCF (B3LYP) Energy = -1083.04588883
Enthalpy 0K = -1082.753547
Enthalpy 298K = -1082.722202
Free Energy 298K = -1082.821544
Lowest Frequency = 27.0707 cm^{-1}
Second Frequency = 31.9921 cm^{-1}

```
N  -1.10380 -1.41252 -0.91360
C  -1.80629 -2.17945 -1.41727
N  -1.10344  1.41339 -0.91282
C  -1.80566  2.18084 -1.41609
N   1.10380  1.41264  0.91366
C   1.80639  2.17955  1.41721
C  -2.76376 -3.10638 -2.00363
H  -2.76418 -3.01805 -3.09389
H  -2.51345 -4.13699 -1.73601
H  -3.76463 -2.87458 -1.62641
C  -2.76290  3.10788 -2.00266
H  -2.76235  3.02031 -3.09298
H  -3.76402  2.87557 -1.62645
H  -2.51309  4.13837 -1.73411
C   2.76352  3.10659  2.00395
H   2.76368  3.01811  3.09421
H   3.76452  2.87501  1.62696
H   2.51309  4.13718  1.73640
O  -3.26002 -0.00053  0.60704
C  -2.56024 -0.00059  1.62612
O  -1.26291 -0.00039  1.69102
C  -3.21417 -0.00035  3.01356
H  -2.89290 -0.88003  3.58070
H  -2.89378  0.88015  3.57993
H  -4.30175 -0.00088  2.92076
O   1.26292  0.00046 -1.69094
C   2.56025  0.00042 -1.62606
O   3.26004  0.00013 -0.60699
C   3.21417  0.00030 -3.01350
H   2.89305  0.88013 -3.58049
H   4.30175  0.00061 -2.92072
H   2.89359 -0.88004 -3.58002
Ru -0.00002  0.00006  0.00004
N   1.10353 -1.41328  0.91286
C   1.80594 -2.18066  1.41594
C   2.76294 -3.10826  2.00202
H   2.76308 -3.02061  3.09234
H   2.51239 -4.13862  1.73367
H   3.76398 -2.87652  1.62523
```

^{1}A$^+$
SCF (B3LYP) Energy = -688.275901402
Enthalpy 0K = -688.073328
Enthalpy 298K = -688.057032
Free Energy 298K = -688.119677
Lowest Frequency = 16.5271 cm^{-1}
Second Frequency = 17.4999 cm^{-1}

```
C   2.00892 -0.42944  1.42387
C   2.30679  0.77166  0.69648
C   2.30435  0.76224 -0.71312
C   2.00485 -0.44820 -1.42410
C   1.73136 -1.63113 -0.70846
C   1.73368 -1.62205  0.72510
Ru  0.34553 -0.00892  0.00001
O  -0.83068  1.38429 -1.08263
C  -1.29129  1.88905 -0.00022
C  -2.31835  2.97357 -0.00032
H   2.44733  1.68651 -1.26168
H   1.44930 -2.51414  1.27145
O  -0.83032  1.38484  1.08229
H  -3.31711  2.52321 -0.00015
H  -2.21947  3.58584  0.89764
H  -2.21964  3.58552 -0.89853
H   1.93851 -0.40319  2.50543
H   1.44473 -2.53016 -1.24217
H   1.93195 -0.43638 -2.50572
H   2.45216  1.70291  1.23241
N  -1.35984 -1.17627  0.00051
C  -2.34163 -1.78656  0.00056
C  -3.57678 -2.55714  0.00020
H  -4.14802 -2.34029  0.90747
H  -4.17762 -2.29187 -0.87449
H  -3.34975 -3.62649 -0.03274
```

^{1}A
SCF (B3LYP) Energy = -916.982589580
Enthalpy 0K = -916.729340
Enthalpy 298K = -916.707553
Free Energy 298K = -916.781811
Lowest Frequency = 16.4674 cm^{-1}
Second Frequency = 37.8833 cm^{-1}

```
Ru  0.26546  0.04970 -0.09898
O   1.42088  0.79890  1.56325
C   1.89684  1.71218  0.81172
C   2.79048  2.78853  1.36181
C  -1.09836 -1.87282  0.15096
C  -0.68837 -1.40236  1.42713
C  -1.64501 -0.74977  2.26538
C  -2.93776 -0.56632  1.83734
O   1.56094  1.70681 -0.42112
H   2.17212  3.63823  1.67128
H   3.33368  2.42235  2.23496
H   3.48455  3.13442  0.59325
C  -3.35189 -1.05196  0.56795
C  -2.45870 -1.70172 -0.25006
H  -2.77893 -2.10727 -1.20490
H  -3.65700 -0.06497  2.47874
H  -0.48778 -2.58316 -0.39581
H  -1.33523 -0.41076  3.24915
C  -1.52215  1.18600 -1.41472
O  -1.33715  1.46360 -0.18501
O  -0.82091  0.24539 -1.92396
C  -2.49749  1.96524 -2.25199
H  -2.80948  1.38086 -3.11918
H  -3.36271  2.25190 -1.65057
H  -2.01100  2.88116 -2.60486
H   0.23449 -1.75609  1.87558
```

```
H  -4.38589 -0.92735  0.25823
N   1.73373 -1.21454 -0.48506
C   2.62245 -1.91369 -0.75236
C   3.74010 -2.77260 -1.12468
H   4.46004 -2.21126 -1.72833
H   4.25001 -3.14850 -0.23253
H   3.38566 -3.62611 -1.71066
```

$^1B^+$ (t-O,t-N)
SCF (B3LYP) Energy = -1167.64483201
Enthalpy 0K = -1167.271109
Enthalpy 298K = -1167.244242
Free Energy 298K = -1167.329644
Lowest Frequency = 26.1097 cm^{-1}
Second Frequency = 31.1038 cm^{-1}

```
Ru  0.40693 -0.30510 -0.33978
O   1.49816 -2.10994 -0.83643
C   1.37550 -1.83717 -2.07357
C   1.91493 -2.72330 -3.15302
C   0.58138 -1.05743  2.02045
C   1.92239 -1.27488  2.43197
C   2.67257 -0.22749  2.92932
C   2.11594  1.06916  3.02867
O   0.73221 -0.75867 -2.36570
H   2.37096 -2.11950 -3.94103
H   2.63879 -3.42639 -2.73972
H   1.09000 -3.28524 -3.60422
C  -2.65574 -0.07783  0.00862
C  -3.81594 -0.22044  0.78282
C  -1.89929 -1.23157 -0.28516
C  -4.20970 -1.47970  1.23855
H  -4.39785  0.65320  1.05846
C  -2.29476 -2.49237  0.17150
C  -3.45304 -2.61650  0.93927
H  -5.10926 -1.57199  1.83898
H  -1.70807 -3.36778 -0.08904
H  -3.76933 -3.59132  1.29582
H  -1.15441 -1.20209 -1.10867
C   0.81336  1.29919  2.63050
C   0.02475  0.23501  2.12038
H  -1.04417  0.37637  2.01885
H   2.70543  1.87635  3.45405
H  -0.05438 -1.91475  1.83126
H   3.68711 -0.40379  3.27515
C  -2.17063  1.24125 -0.44487
C  -2.52166  3.52500 -1.15328
H  -3.18626  4.35170 -1.38156
C  -3.03479  2.30499 -0.72742
H  -4.10457  2.15786 -0.63535
C  -0.33064  2.56649 -1.00777
H   0.74502  2.62091 -1.11450
C  -1.14041  3.65690 -1.29602
H  -0.69046  4.58380 -1.63339
N  -0.81968  1.38180 -0.58609
H   2.33697 -2.27623  2.38065
H   0.36804  2.28240  2.75032
N   2.14097  0.63736 -0.31508
C   3.19485  1.11535 -0.35554
C   4.52410  1.71042 -0.39788
H   5.26916  0.97741 -0.07492
H   4.76126  2.02957 -1.41693
H   4.57006  2.57816  0.26634
```

TS(**$^1B^+$-$^1C^+$**) (t-O,t-N)
SCF (B3LYP) Energy = -1167.60031917
Enthalpy 0K = -1167.232189
Enthalpy 298K = -1167.205837
Free Energy 298K = -1167.288934
Lowest Frequency = -1120.7126 cm^{-1}
Second Frequency = 26.6841 cm^{-1}

```
Ru  0.31788 -0.31609 -0.15065
O   1.02588 -2.39777 -0.42534
C   0.48782 -2.55558 -1.53621
C   0.73033 -3.71547 -2.44215
C   0.83579 -0.61290  2.13686
C   2.20347 -0.93367  2.38411
C   3.14115  0.06842  2.49216
C   2.76231  1.43069  2.35570
O  -0.35518 -1.60743 -1.95424
H   1.11552 -3.35454 -3.40110
H   1.43869 -4.40897 -1.98995
H  -0.21832 -4.22115 -2.64779
C  -2.59418  0.22005  0.14573
C  -3.91728  0.11027  0.59177
C  -1.69369 -0.87644  0.26717
C  -4.36904 -1.08600  1.15005
H  -4.59955  0.95219  0.52693
C  -2.18137 -2.06724  0.83655
C  -3.50453 -2.17594  1.27330
H  -5.39568 -1.16428  1.49361
H  -1.51963 -2.92514  0.93435
H  -3.85970 -3.10474  1.70957
H  -1.04772 -1.30890 -1.02434
C   1.45037  1.76449  2.11095
C   0.45739  0.74429  1.98785
H  -0.58668  1.02320  2.07317
H   3.50844  2.20949  2.48438
H   0.08094 -1.36957  2.31636
H   4.17467 -0.17823  2.71800
C  -2.03360  1.45668 -0.41756
C  -2.14922  3.70032 -1.31471
H  -2.72885  4.56799 -1.61257
C  -2.78311  2.57706 -0.79802
H  -3.86163  2.55675 -0.69848
C  -0.06209  2.55455 -1.06309
H   1.01528  2.49475 -1.14707
C  -0.75959  3.69105 -1.44824
H  -0.22069  4.54373 -1.84545
N  -0.67273  1.46008 -0.56461
H   2.48483 -1.97173  2.52883
H   1.14737  2.80615  2.06275
N   2.23906  0.29166 -0.74443
C   3.30190  0.52886 -1.14079
C   4.64240  0.81988 -1.63365
H   4.61846  0.99377 -2.71332
H   5.04012  1.71100 -1.13973
H   5.30613 -0.02453 -1.42629
```

$^1C^+$ (t-O,t-N)
SCF (B3LYP) Energy = -1167.61567440
Enthalpy 0K = -1167.242254
Enthalpy 298K = -1167.215114
Free Energy 298K = -1167.301555
Lowest Frequency = 15.1499 cm^{-1}
Second Frequency = 31.7977 cm^{-1}

```
Ru -0.28206  0.13994 -0.14816
O  -1.36073  2.03772 -0.40002
C  -1.02311  2.99731 -1.10849
C  -1.96556  4.10170 -1.47537
C  -0.94830  0.51974  2.01014
C  -2.37058  0.59599  2.18250
C  -3.11355 -0.54731  2.32535
C  -2.48374 -1.82807  2.31132
O   0.19390  3.14018 -1.61118
H  -1.97659  4.23042 -2.56158
H  -2.96635  3.88066 -1.10817
```

H -1.60757 5.04193 -1.04417
C 2.63090 0.02629 0.00173
C 3.96583 0.41863 0.17336
C 1.54973 0.91139 0.29517
C 4.26529 1.68932 0.66241
H 4.78052 -0.26067 -0.05972
C 1.89453 2.17369 0.81828
C 3.22868 2.56281 0.99404
H 5.29945 1.98939 0.79630
H 1.11366 2.87554 1.10668
H 3.45582 3.54663 1.39507
H 0.80520 2.48785 -1.20122
C -1.12654 -1.93455 2.14902
C -0.32169 -0.75685 1.98693
H 0.74385 -0.83291 2.17297
H -3.08518 -2.71817 2.47248
H -0.35489 1.40394 2.21358
H -4.18515 -0.48364 2.49050
C 2.23979 -1.31852 -0.43719
C 2.61633 -3.59353 -1.17027
H 3.29553 -4.39146 -1.45312
C 3.11505 -2.34948 -0.80329
H 4.18348 -2.17111 -0.80000
C 0.40787 -2.75018 -0.80648
H -0.66981 -2.85183 -0.78580
C 1.23516 -3.80353 -1.16833
H 0.80428 -4.76003 -1.44116
N 0.88700 -1.53743 -0.45846
H -2.84120 1.57187 2.23993
H -0.63855 -2.90285 2.20283
N -2.12620 -0.70811 -0.92248
C -3.09977 -1.06004 -1.44506
C -4.32925 -1.50077 -2.09284
H -5.09377 -0.72279 -2.01210
H -4.14480 -1.70696 -3.15112
H -4.70077 -2.41167 -1.61472

$^1B^+$ (t-O,t-C6H6)
SCF (B3LYP) Energy = -1167.63658643
Enthalpy 0K = -1167.263015
Enthalpy 298K = -1167.236125
Free Energy 298K = -1167.321485
Lowest Frequency = 30.4592 cm^{-1}
Second Frequency = 31.5336 cm^{-1}

Ru 0.41063 -0.02712 -0.14757
O 1.78663 -1.60977 -0.57015
C 1.95863 -1.18325 -1.75981
C 2.87656 -1.87066 -2.72405
C 1.94597 1.29909 1.27701
C 2.69246 0.45613 2.14581
C 3.89542 -0.08061 1.73548
C 4.40559 0.22218 0.45431
O 1.31705 -0.12084 -2.09064
H 3.88344 -1.45325 -2.61577
H 2.92667 -2.93856 -2.50444
H 2.54614 -1.70148 -3.75031
C -2.58007 -0.36266 -0.49814
C -3.77965 -0.94076 -0.06553
C -1.52461 -1.21442 -0.89053
C -3.91676 -2.33046 -0.03172
H -4.59806 -0.31452 0.27502
C -1.65914 -2.60681 -0.84293
C -2.86098 -3.16622 -0.41178
H -4.85374 -2.76464 0.30369
H -0.83251 -3.23691 -1.15375
H -2.98089 -4.24423 -0.37832
H -0.71608 -0.79791 -1.53219
C 3.69868 1.04185 -0.40652
C 2.45765 1.58432 -0.00521
H 1.98750 2.31767 -0.64928
H 5.36895 -0.17940 0.15432
H 1.13019 1.88355 1.68868
H 4.46555 -0.71696 2.40480
C -2.34863 1.09416 -0.48392
C -3.11170 3.38267 -0.63544
H -3.90704 4.10647 -0.77948
C -3.38352 2.01968 -0.65972
H -4.39051 1.66115 -0.83873
C -0.80938 2.83058 -0.27119
H 0.21991 3.12470 -0.11350
C -1.79530 3.79535 -0.43359
H -1.52543 4.84506 -0.40727
N -1.05792 1.50501 -0.29578
H 2.32051 0.26210 3.14658
H 4.09771 1.29610 -1.38288
N -0.30085 -0.48145 1.68445
C -0.70927 -0.83288 2.71040
C -1.20599 -1.30330 3.99784
H -0.60495 -2.14988 4.34298
H -1.15225 -0.50345 4.74192
H -2.24656 -1.62605 3.90173

TS(**$^1B^+$–$^1C^+$**) (t-O,t-C6H6)
SCF (B3LYP) Energy = -1167.60555158
Enthalpy 0K = -1167.237625
Enthalpy 298K = -1167.211006
Free Energy 298K = -1167.295862
Lowest Frequency = -1267.0782 cm^{-1}
Second Frequency = 17.0267 cm^{-1}

Ru -0.31066 0.01678 0.08187
O -1.70028 1.69461 0.18587
C -1.60383 2.01204 -1.01829
C -2.45213 3.04248 -1.68602
C -2.30203 -1.70219 0.47462
C -3.26613 -1.10626 1.31452
C -4.30530 -0.36461 0.76936
C -4.40290 -0.20913 -0.62283
O -0.68458 1.38611 -1.74420
H -2.98670 2.58672 -2.52464
H -3.16081 3.46910 -0.97677
H -1.81179 3.82694 -2.10148
C 2.55565 0.57254 -0.37581
C 3.79971 1.20662 -0.27864
C 1.36878 1.26866 -0.01136
C 3.88216 2.52131 0.18279
H 4.71389 0.68116 -0.53590
C 1.48324 2.58356 0.47801
C 2.72863 3.20881 0.56791
H 4.85154 3.00463 0.25292
H 0.58872 3.12283 0.77680
H 2.80032 4.22688 0.93854
H 0.35834 1.35552 -1.03367
C -3.45378 -0.78171 -1.46228
C -2.39475 -1.53048 -0.91796
H -1.72063 -2.05075 -1.58983
H -5.23421 0.34812 -1.04475
H -1.58562 -2.39614 0.90197
H -5.05351 0.08069 1.41740
C 2.39263 -0.83626 -0.75762
C 3.17426 -2.98109 -1.55850
H 3.96175 -3.60587 -1.96702
C 3.41225 -1.64074 -1.28159
H 4.38704 -1.20948 -1.47468
C 0.92934 -2.66116 -0.79321
H -0.06398 -3.03540 -0.58101
C 1.90829 -3.50655 -1.29757
H 1.67383 -4.54853 -1.48324
N 1.14309 -1.35360 -0.54207

H -3.20751 -1.25462 2.38829
H -3.54006 -0.68127 -2.53984
N 0.08797 -0.42536 1.95767
C 0.35288 -0.61977 3.06970
C 0.67418 -0.83852 4.47469
H -0.09365 -0.38559 5.10892
H 0.72664 -1.90928 4.69183
H 1.63987 -0.38249 4.71175

$^1C^+$ (t-O,t-C6H6)
SCF (B3LYP) Energy = -1167.64474056
Enthalpy 0K = -1167.270874
Enthalpy 298K = -1167.243773
Free Energy 298K = -1167.330027
Lowest Frequency = 20.5885 cm^{-1}
Second Frequency = 27.0640 cm^{-1}

Ru -0.27348 -0.29703 0.37278
O -2.33071 0.34580 0.53226
C -2.81454 1.47886 0.64408
C -4.24962 1.71719 0.99698
C -1.89335 -3.00915 0.34316
C -3.16002 -2.70466 -0.13088
C -3.31688 -1.95802 -1.31527
C -2.20510 -1.50759 -2.00866
O -2.11415 2.58772 0.44824
H -4.73967 0.77285 1.22738
H -4.31491 2.39841 1.85006
H -4.75389 2.20423 0.15615
C 1.93154 0.72661 -1.23496
C 2.61204 1.47928 -2.20574
C 0.52433 0.84457 -1.07706
C 1.91297 2.34782 -3.03856
H 3.68775 1.38352 -2.32209
C -0.16212 1.70081 -1.95296
C 0.52505 2.44846 -2.91709
H 2.44170 2.92908 -3.78671
H -1.24581 1.77479 -1.91998
H -0.03101 3.10531 -3.58035
H -1.20959 2.35080 0.15957
C -0.90263 -1.79506 -1.53632
C -0.74556 -2.56137 -0.35969
H 0.22218 -2.98610 -0.11841
H -2.32334 -0.95937 -2.93833
H -1.77425 -3.63475 1.22284
H -4.31356 -1.75505 -1.69511
C 2.57724 -0.25137 -0.36111
C 4.42467 -1.49884 0.57651
H 5.48580 -1.72227 0.62141
C 3.94912 -0.53658 -0.30472
H 4.63485 -0.00052 -0.95002
C 2.17493 -1.85048 1.30898
H 1.43280 -2.33713 1.93429
C 3.52155 -2.17072 1.40573
H 3.84855 -2.92556 2.11156
N 1.70579 -0.92576 0.44701
H -4.03681 -3.06849 0.39640
H -0.04911 -1.58778 -2.17166
N 0.23483 1.03974 1.75416
C 0.57927 1.76994 2.58961
C 1.00214 2.68193 3.64453
H 0.36559 3.57178 3.65167
H 0.93182 2.18907 4.61897
H 2.03826 2.99098 3.47846

$^1B^+$ (t-O,t-O)
SCF (B3LYP) Energy = -1167.64539468
Enthalpy 0K = -1167.271537
Enthalpy 298K = -1167.244743
Free Energy 298K = -1167.330211
Lowest Frequency = 24.0913 cm^{-1}
Second Frequency = 31.3675 cm^{-1}

Ru -0.47559 0.24327 0.33969
O -2.26385 0.69753 -0.60675
C -2.96237 0.44014 0.44627
C -4.45119 0.59825 0.43667
C -0.25214 -1.95381 -1.02148
C -0.91569 -2.33519 0.15892
C -2.28686 -2.67658 0.10952
C -2.97027 -2.62079 -1.09312
O -2.31920 0.03950 1.46540
H -4.83646 0.61375 1.45681
H -4.73129 1.51123 -0.09391
H -4.89562 -0.24704 -0.09856
C 2.57674 -0.44981 0.37194
C 3.67785 -1.31891 0.40524
C 1.64712 -0.51106 1.43148
C 3.85151 -2.20617 1.46787
H 4.38656 -1.33071 -0.41637
C 1.82088 -1.40016 2.49494
C 2.92603 -2.25256 2.51328
H 4.70913 -2.87136 1.47305
H 1.10345 -1.40851 3.30972
H 3.06752 -2.94317 3.33827
H 0.91446 0.31353 1.62121
C -2.31009 -2.21961 -2.27345
C -0.96642 -1.89443 -2.24198
H -0.44518 -1.62735 -3.15611
H -4.01652 -2.90963 -1.13662
H 0.82867 -1.88765 -1.03681
H -2.78834 -3.00246 1.01461
C 2.32555 0.44285 -0.77755
C 3.01470 1.70943 -2.71705
H 3.79470 2.07658 -3.37612
C 3.33745 0.91045 -1.62546
H 4.37016 0.65913 -1.41435
C 0.71485 1.55672 -2.06500
H -0.34019 1.77729 -2.18835
C 1.67639 2.03344 -2.94659
H 1.37678 2.64812 -3.78789
N 1.02654 0.78330 -1.00529
H -0.35372 -2.52236 1.06662
H -2.85554 -2.19179 -3.21173
N -0.45939 2.11761 1.01429
C -0.51273 3.20294 1.41538
C -0.58439 4.56223 1.93506
H -1.12082 5.20530 1.23143
H -1.11239 4.56539 2.89319
H 0.42323 4.96077 2.08390

$^1B^+$ (t-C6H6,t-O)
SCF (B3LYP) Energy = -1167.64758119
Enthalpy 0K = -1167.273583
Enthalpy 298K = -1167.246541
Free Energy 298K = -1167.333188
Lowest Frequency = 16.5467 cm^{-1}
Second Frequency = 29.1225 cm^{-1}

Ru -0.32762 -0.17649 0.20763
O -1.36671 -1.91214 0.70106
C -1.79104 -2.05029 -0.50812
C -2.69435 -3.17852 -0.89312
C -2.42495 0.88505 1.27914
C -1.94273 1.77708 0.30071
C -2.66868 1.94404 -0.90455
C -3.83128 1.22895 -1.12412
O -1.40325 -1.16565 -1.33811
H -2.44855 -3.52759 -1.89830
H -2.62040 -3.99420 -0.17226

H -3.72763 -2.81660 -0.90602
C 2.08310 0.85687 -0.92539
C 2.90650 1.85512 -0.37304
C 0.97518 1.23022 -1.72014
C 2.62300 3.19893 -0.59257
H 3.76292 1.56838 0.22995
C 0.71143 2.59315 -1.94205
C 1.51962 3.57166 -1.37351
H 3.26560 3.96219 -0.16441
H -0.10939 2.87468 -2.59346
H 1.31469 4.62194 -1.55557
H 0.42313 0.48028 -2.27766
C -4.31162 0.33738 -0.14244
C -3.62261 0.16903 1.04577
H -4.00612 -0.49098 1.81699
H -4.39053 1.36926 -2.04392
H -1.98328 0.86114 2.26814
H -2.32352 2.66117 -1.64179
C 2.38353 -0.57959 -0.70294
C 3.79354 -2.52870 -0.69764
H 4.74820 -3.00708 -0.89099
C 3.62389 -1.16731 -0.94766
H 4.43039 -0.56183 -1.34627
C 1.50824 -2.61895 0.03522
H 0.64821 -3.13196 0.44778
C 2.71790 -3.26403 -0.20059
H 2.80708 -4.32375 0.01047
N 1.34733 -1.30475 -0.21322
H -1.13922 2.46792 0.53755
H -5.24277 -0.19566 -0.31165
N 0.52989 0.41980 1.92661
C 1.00181 0.71387 2.94489
C 1.57966 1.07180 4.23459
H 1.22912 0.38007 5.00643
H 2.67128 1.02233 4.18650
H 1.28458 2.08828 4.51086

TS($^1B^+$–$^1C^+$)1 (t-C6H6,t-O)
SCF (B3LYP) Energy = -1167.61764800
Enthalpy 0K = -1167.244715
Enthalpy 298K = -1167.218074
Free Energy 298K = -1167.304485
Lowest Frequency = -59.7924 cm^{-1}
Second Frequency = 17.0569 cm^{-1}

C 2.92325 -0.47494 -0.17795
N 1.82410 0.29124 -0.02489
C 1.94027 1.64530 0.01851
C 3.19686 2.25259 -0.05047
C 4.33551 1.46331 -0.18386
C 4.19527 0.07646 -0.25952
Ru -0.06233 -0.49343 0.21078
C -3.08316 -1.25072 -0.95391
C -2.26717 -1.72291 0.09934
C -2.35247 -1.10806 1.36604
C -3.25881 -0.04716 1.57682
C -4.07618 0.37929 0.53948
C -3.98292 -0.21750 -0.73095
H -1.84716 -1.54485 2.22002
C 0.66714 2.38680 0.09574
C 0.55438 3.60399 0.78080
C -0.66065 4.28880 0.79600
C -1.77366 3.77194 0.12604
C -1.67567 2.55728 -0.55215
C -0.46966 1.84711 -0.55629
H -4.63182 0.11745 -1.53451
O 0.44537 -1.89670 -1.15267
C 0.24468 -1.53328 -2.40444
O -0.20781 -0.43352 -2.72541
C 0.59107 -2.60810 -3.41322
H 1.50601 -3.13369 -3.13072
H -0.21694 -3.34667 -3.44784
H 0.69842 -2.15924 -4.40112
H 1.41023 4.01037 1.31078
H -0.73730 5.23201 1.32782
H -2.52386 2.16218 -1.09834
H -2.70913 4.32243 0.12445
H 3.26674 3.33399 -0.03014
H -0.36115 1.01898 -1.29333
H -3.02986 -1.72638 -1.92739
H -4.80003 1.17050 0.71081
H -1.70811 -2.64229 -0.03336
H -3.34561 0.39766 2.56322
H 5.05381 -0.57310 -0.38705
H 5.31607 1.92378 -0.24723
H 2.74601 -1.54099 -0.24490
N 0.57553 -1.79613 1.53965
C 0.98209 -2.56760 2.30408
C 1.48783 -3.53770 3.26699
H 1.87061 -4.41853 2.74312
H 2.29479 -3.09610 3.85904
H 0.68500 -3.84996 3.94133

INT($^1B^+$–$^1C^+$) (t-C6H6,t-O)
SCF (B3LYP) Energy = -1167.64118254
Enthalpy 0K = -1167.267532
Enthalpy 298K = -1167.240626
Free Energy 298K = -1167.326273
Lowest Frequency = 22.2156 cm^{-1}
Second Frequency = 29.2309 cm^{-1}

C 0.57234 -2.82199 -0.00809
N -0.12970 -1.68612 0.18920
C -1.44034 -1.77992 0.56137
C -2.04297 -3.03246 0.73393
C -1.31552 -4.19637 0.51730
C 0.02208 -4.08770 0.13724
Ru 0.78372 0.20349 0.13229
C -0.51944 2.54347 -1.92877
C 0.40546 1.47428 -2.00790
C -0.05526 0.17617 -2.31416
C -1.43534 -0.03660 -2.54953
C -2.32374 1.02061 -2.47814
C -1.86317 2.31663 -2.16352
H 0.64631 -0.61114 -2.56586
C -2.16877 -0.51655 0.78800
C -3.56054 -0.42209 0.64334
C -4.21194 0.79336 0.85111
C -3.49004 1.94189 1.18871
C -2.10462 1.86851 1.32750
C -1.45347 0.64799 1.13118
H -2.56740 3.14224 -2.12896
O 1.75202 0.17350 1.99609
C 2.16036 1.38924 1.86213
O 1.82087 1.98891 0.79215
C 2.96509 2.04947 2.93811
H 2.30126 2.33122 3.76263
H 3.70548 1.35149 3.33557
H 3.44980 2.94675 2.55189
H -4.13850 -1.28982 0.34284
H -5.29080 0.84547 0.74168
H -1.52984 2.74408 1.61113
H -4.00597 2.88254 1.35220
H -3.07376 -3.08362 1.06351
H -0.43705 0.55811 1.57083
H -0.15603 3.54429 -1.71871
H -3.37732 0.86045 -2.68467
H 1.46466 1.70422 -2.02045
H -1.78245 -1.02656 -2.82972
H 0.63790 -4.96327 -0.03448

H -1.77809 -5.16800 0.65596
H 1.61014 -2.69212 -0.28670
N 2.49068 -0.35418 -0.71071
C 3.53528 -0.60098 -1.14911
C 4.85100 -0.90851 -1.69553
H 4.75113 -1.48093 -2.62228
H 5.39070 0.01886 -1.90897
H 5.42737 -1.49575 -0.97461

TS(^{1}B$^+$-^{1}C$^+$)2 (t-C6H6,t-O)
SCF (B3LYP) Energy = -1167.60501540
Enthalpy 0K = -1167.236929
Enthalpy 298K = -1167.210097
Free Energy 298K = -1167.296732
Lowest Frequency = -892.8741 cm^{-1}
Second Frequency = 13.5112 cm^{-1}

C 1.66775 -1.37920 -1.71912
N 0.57764 -1.02681 -1.00397
C -0.59677 -1.71209 -1.16792
C -0.67015 -2.74863 -2.10756
C 0.44449 -3.09398 -2.86034
C 1.63988 -2.40043 -2.65682
Ru 0.62038 0.45374 0.37219
C -1.49721 3.17128 0.63117
C -0.35448 2.80416 -0.10649
C -0.49652 2.11610 -1.33209
C -1.78771 1.80056 -1.79989
C -2.90740 2.16777 -1.06481
C -2.76190 2.85347 0.15208
H 0.35635 1.97476 -1.98680
C -1.68783 -1.29517 -0.28495
C -3.02415 -1.65646 -0.49099
C -4.00517 -1.22863 0.40342
C -3.65961 -0.43337 1.49961
C -2.32994 -0.05907 1.69871
C -1.31608 -0.47074 0.81486
H -3.64376 3.15249 0.71015
O 1.95535 -0.61847 1.50168
C 1.52005 -1.51446 2.32269
O 0.30011 -1.78453 2.44399
C 2.54375 -2.24702 3.15041
H 2.53221 -3.30533 2.87258
H 3.54201 -1.83754 2.99925
H 2.26487 -2.18576 4.20542
H -3.31250 -2.25821 -1.34749
H -5.03894 -1.52142 0.24813
H -2.06621 0.52474 2.57641
H -4.42435 -0.11787 2.20312
H -1.59970 -3.29315 -2.22208
H -0.34951 -0.95171 1.53834
H -1.38442 3.73208 1.55395
H -3.90018 1.93857 -1.43841
H 0.61090 3.20804 0.18475
H -1.90377 1.30217 -2.75740
H 2.54140 -2.64673 -3.20604
H 0.38898 -3.90099 -3.58353
H 2.56867 -0.81652 -1.51495
N 2.35635 1.40141 -0.26298
C 3.35375 1.93784 -0.51114
C 4.61333 2.60588 -0.81213
H 4.66579 2.85338 -1.87623
H 4.69445 3.52802 -0.22917
H 5.45106 1.95114 -0.55515

^{1}C$^+$ (t-C6H6,t-O)
SCF (B3LYP) Energy = -1167.62670799
Enthalpy 0K = -1167.253590
Enthalpy 298K = -1167.226336
Free Energy 298K = -1167.313556
Lowest Frequency = 17.8716 cm^{-1}
Second Frequency = 24.6047 cm^{-1}

C -1.20721 -0.79971 2.29185
N -0.26426 -0.60324 1.34713
C 1.01406 -1.05607 1.54809
C 1.33482 -1.70497 2.74902
C 0.36568 -1.89774 3.72421
C -0.93449 -1.44041 3.49127
Ru -0.63741 0.32661 -0.41590
C 0.77591 3.16527 -1.25445
C -0.35955 2.72834 -0.52924
C -0.23397 2.40656 0.84478
C 1.03412 2.52366 1.46614
C 2.13591 2.93919 0.73882
C 2.00646 3.26192 -0.62681
H -1.11574 2.29042 1.46488
C 1.92077 -0.81024 0.42874
C 3.26866 -1.19881 0.41152
C 4.04840 -0.95489 -0.71707
C 3.47878 -0.32756 -1.82829
C 2.13594 0.07200 -1.80684
C 1.31891 -0.14486 -0.67979
H 2.87293 3.60855 -1.18128
O -1.42162 -1.49129 -1.17303
C -0.92310 -2.46577 -1.76873
O 0.34998 -2.57816 -2.06279
C -1.76821 -3.61768 -2.22023
H -1.37504 -4.54676 -1.79748
H -2.80258 -3.47127 -1.91414
H -1.70712 -3.70723 -3.30921
H 3.71646 -1.69691 1.26686
H 5.08951 -1.26043 -0.73474
H 1.72633 0.57167 -2.68257
H 4.08107 -0.14526 -2.71413
H 2.34694 -2.05814 2.90679
H 0.84936 -1.78410 -1.74486
H 0.66595 3.45553 -2.29497
H 3.10088 3.04075 1.22545
H -1.34556 2.86577 -0.96645
H 1.12638 2.32330 2.52927
H -1.72540 -1.57576 4.22004
H 0.61616 -2.40089 4.65258
H -2.19546 -0.42623 2.05495
N -2.76487 0.79015 -0.17341
C -3.90457 1.00761 -0.17085
C -5.33782 1.27488 -0.17313
H -5.56510 2.11857 0.48467
H -5.67066 1.51656 -1.18674
H -5.88336 0.39395 0.17707

^{1}B$^+$ (t-N,t-O)
SCF (B3LYP) Energy = -1167.64565238
Enthalpy 0K = -1167.271623
Enthalpy 298K = -1167.244674
Free Energy 298K = -1167.330544
Lowest Frequency = 23.1807 cm^{-1}
Second Frequency = 24.6171 cm^{-1}

Ru -0.70707 -0.18865 -0.03070
O -1.49770 -2.12236 -0.05367
C -1.76188 -2.04206 -1.30823
C -2.44490 -3.15214 -2.04071
C -0.62070 -0.52128 2.37439
C 0.19970 -1.60702 2.78574
C 1.55181 -1.42090 2.98409
C 2.13161 -0.14239 2.80082
O -1.42755 -0.95001 -1.87956
H -2.12026 -3.17016 -3.08275
H -2.24319 -4.10895 -1.55603

H -3.52686 -2.98034 -2.02394
C 1.49889 1.47683 -0.98886
C 2.20867 2.53532 -0.39855
C 0.23447 1.73537 -1.56992
C 1.65641 3.81290 -0.34739
H 3.18486 2.34777 0.03774
C -0.31655 3.02750 -1.49579
C 0.38171 4.05818 -0.87450
H 2.21729 4.62222 0.11029
H -1.27388 3.22202 -1.96954
H -0.04200 5.05638 -0.82785
H -0.22587 1.00396 -2.22444
C 1.35008 0.92501 2.41076
C -0.04107 0.75221 2.16677
H -0.66905 1.63271 2.07345
H 3.18795 0.00206 3.00714
H -1.69623 -0.63447 2.44184
H 2.17132 -2.24678 3.32129
C 2.05255 0.09940 -0.98216
C 3.79053 -1.53415 -1.31242
H 4.79982 -1.79384 -1.61515
C 3.35911 -0.20949 -1.36158
H 4.01360 0.58154 -1.71056
C 1.61742 -2.14435 -0.49993
H 0.89155 -2.86364 -0.13982
C 2.90323 -2.51751 -0.87692
H 3.19564 -3.56028 -0.82494
N 1.19996 -0.86520 -0.54711
H -0.25947 -2.57197 2.97530
H 1.78025 1.91642 2.32387
N -2.56779 0.57197 0.32652
C -3.64131 0.97695 0.48903
C -4.99058 1.49223 0.68521
H -4.95540 2.44098 1.22840
H -5.47218 1.65574 -0.28325
H -5.58536 0.77700 1.26058

TS(^{1}**B**$^+$–^{1}**C**$^+$) (t-N,t-O)
SCF (B3LYP) Energy = -1167.61617449
Enthalpy 0K = -1167.243686
Enthalpy 298K = -1167.217229
Free Energy 298K = -1167.302091
Lowest Frequency = -94.1102 cm^{-1}
Second Frequency = 23.4579 cm^{-1}

C -2.07489 -1.36965 0.97388
N -1.44398 -0.26499 0.53360
C -2.09432 0.93145 0.55996
C -3.43030 1.01723 0.95591
C -4.09348 -0.13468 1.37222
C -3.39828 -1.34399 1.39974
Ru 0.54186 -0.15644 -0.13226
C 0.68002 -2.11427 -1.54862
C -0.32872 -3.09340 -1.34078
C -1.58126 -2.94021 -1.90187
C -1.87505 -1.80338 -2.69224
C -0.91125 -0.83996 -2.91839
C 0.38645 -0.98354 -2.35302
H -2.33812 -3.70616 -1.76324
C -1.25807 2.09458 0.20551
C -1.75396 3.21259 -0.47693
C -0.90637 4.27608 -0.78966
C 0.44524 4.24139 -0.42770
C 0.95512 3.13738 0.25288
C 0.11717 2.05351 0.55964
H 1.19166 -0.36303 -2.73478
O 1.04509 -1.58605 1.20424
C 1.39765 -1.10886 2.38043
O 1.39133 0.09388 2.65284
C 1.84312 -2.16913 3.36418
H 1.67933 -1.81198 4.38190
H 1.31954 -3.11284 3.19961
H 2.91522 -2.35058 3.23199
H -2.79628 3.24511 -0.77909
H -1.30171 5.13718 -1.31929
H 1.99181 3.11486 0.57255
H 1.09126 5.08065 -0.66494
H -3.92327 1.98260 0.97233
H 0.48371 1.32357 1.33010
H 1.70192 -2.35383 -1.28097
H -1.11882 0.00572 -3.56673
H -0.08739 -3.98205 -0.76603
H -2.85591 -1.70695 -3.14813
H -3.86649 -2.25676 1.75057
H -5.12805 -0.08410 1.69600
H -1.48491 -2.27584 0.98131
N 2.52101 0.11518 -0.56261
C 3.66114 0.25333 -0.71480
C 5.09650 0.43817 -0.88501
H 5.54209 0.75731 0.06184
H 5.56176 -0.50144 -1.19624
H 5.29157 1.20004 -1.64519

^{1}**C**$^+$ (t-N,t-O)
SCF (B3LYP) Energy = -1167.64883446
Enthalpy 0K = -1167.275024
Enthalpy 298K = -1167.248103
Free Energy 298K = -1167.333812
Lowest Frequency = 19.1859 cm^{-1}
Second Frequency = 29.7834 cm^{-1}

C -2.17146 -0.01133 -1.86032
N -1.40687 -0.27059 -0.78316
C -1.80458 -1.22026 0.11371
C -3.01509 -1.90096 -0.07230
C -3.80590 -1.62026 -1.18008
C -3.37516 -0.66081 -2.09947
Ru 0.47577 0.56024 -0.42771
C -1.39229 3.18133 -0.69261
C -2.61364 2.90019 -0.10818
C -2.67291 2.26614 1.15335
C -1.51030 1.92497 1.81761
C -0.24208 2.19181 1.23470
C -0.18646 2.82391 -0.03191
H -3.63763 2.07710 1.61407
C -0.85338 -1.44022 1.20708
C -1.06692 -2.34371 2.25896
C -0.11008 -2.50401 3.25910
C 1.06906 -1.75762 3.21238
C 1.29320 -0.84806 2.17038
C 0.34511 -0.67087 1.14698
H 0.74631 3.25456 -0.38514
O 1.22262 -0.84018 -1.80608
C 1.82709 -1.92152 -1.69702
O 2.08072 -2.49907 -0.54274
C 2.31870 -2.67367 -2.89451
H 1.78767 -3.62846 -2.96295
H 2.15291 -2.09201 -3.79983
H 3.38130 -2.90306 -2.77597
H -1.98233 -2.92630 2.30541
H -0.28264 -3.20594 4.06824
H 2.21059 -0.26643 2.16568
H 1.81847 -1.87735 3.98983
H -3.32672 -2.65208 0.64371
H 1.68830 -1.97544 0.19619
H -1.34430 3.71649 -1.63652
H 0.64291 2.12133 1.85632
H -3.53380 3.19351 -0.60473
H -1.55465 1.48118 2.80698
H -3.95446 -0.41814 -2.98296

H -4.74265 -2.14754 -1.33023
H -1.79331 0.74336 -2.54122
N 2.37431 1.22220 -0.10999
C 3.46535 1.60239 0.00913
C 4.83763 2.07103 0.15965
H 5.49143 1.23893 0.43744
H 5.19369 2.50065 -0.78145
H 4.89102 2.83673 0.93908

^{4}G$^+$ (κ^1)
SCF (B3LYP) Energy = -1333.74184339
Enthalpy 0K = -1333.327868
Enthalpy 298K = -1333.292114
Free Energy 298K = -1333.401393
Lowest Frequency = 13.0004 cm^{-1}
Second Frequency = 22.3243 cm^{-1}

N 2.05964 -1.86430 0.34598
C 2.86340 -2.69486 0.38723
N 1.32115 0.30936 2.06919
C 1.70269 0.67675 3.09783
C 2.19248 1.14717 4.38760
H 2.24403 0.31712 5.09788
H 3.19181 1.57651 4.27173
H 1.52233 1.91324 4.78791
C 3.89025 -3.72883 0.43044
H 3.63121 -4.54654 -0.24802
H 4.85269 -3.30782 0.12574
H 3.98373 -4.12762 1.44447
O 1.66355 1.44470 -2.50403
C 2.54646 1.31316 -1.65746
C 3.96354 1.82376 -1.90260
H 4.66319 0.98190 -1.93055
H 4.00872 2.36510 -2.84812
H 4.28236 2.47696 -1.08487
O 2.41167 0.75791 -0.47359
N 0.34564 -0.90868 -1.67648
C 0.30917 -1.13411 -2.80833
C 0.31426 -1.27883 -4.25590
H -0.70643 -1.34199 -4.64314
H 0.80675 -0.39439 -4.67281
H 0.86268 -2.17628 -4.55425
N -0.46916 1.50354 0.12787
C 0.28339 2.61827 0.29391
C -1.81842 1.66262 0.05170
C -0.23976 3.89845 0.40452
H 1.35033 2.44828 0.33470
C -2.40392 2.93246 0.17078
C -1.61994 4.06474 0.34943
H 0.43385 4.73930 0.52746
H -3.48253 3.00918 0.09606
H -2.07453 5.04703 0.43160
C -2.75306 0.52338 -0.18153
C -3.72925 0.22601 0.78232
C -2.78441 -0.15035 -1.40930
C -4.69792 -0.74835 0.53431
H -3.73182 0.76574 1.72536
C -3.75276 -1.12428 -1.65658
H -2.06569 0.11437 -2.17511
C -4.70914 -1.42954 -0.68590
H -5.45613 -0.95802 1.28377
H -3.77654 -1.62973 -2.61764
H -5.47205 -2.17560 -0.88752
Ru 0.75565 -0.31147 0.21749
N -0.68599 -1.50405 1.03509
C -1.41032 -2.27000 1.51412
C -2.34192 -3.22216 2.10534
H -3.36695 -2.89359 1.91467
H -2.19857 -4.21280 1.66428
H -2.18060 -3.29017 3.18501

^{3}G ($2\kappa^1$)
SCF (B3LYP) Energy = -1429.63366227
Enthalpy 0K = -1429.216413
Enthalpy 298K = -1429.180039
Free Energy 298K = -1429.288572
Lowest Frequency = 20.1982 cm^{-1}
Second Frequency = 26.9951 cm^{-1}

N 0.81680 -0.83762 1.37204
C 1.62657 -1.33218 2.03533
N -1.62289 -1.96052 0.57381
C -2.10966 -2.99932 0.70976
C 2.67352 -2.00068 2.79481
H 2.84943 -2.99218 2.36603
H 3.60028 -1.42316 2.73862
H 2.38300 -2.11313 3.84352
C -2.61413 -4.36181 0.79809
H -2.78093 -4.64966 1.83996
H -3.55603 -4.45840 0.25060
H -1.87110 -5.03233 0.35476
O -3.67517 1.51163 -0.24981
C -3.33848 0.70429 -1.13348
O -2.20625 0.08828 -1.23762
C -4.30543 0.37179 -2.27195
H -3.80365 0.48291 -3.23744
H -4.61972 -0.67460 -2.19300
H -5.18424 1.01767 -2.22831
O 0.18605 -1.15811 -1.51050
C 0.56870 -2.39887 -1.58174
O 0.66299 -3.21152 -0.65493
C 0.91939 -2.81818 -3.01384
H 1.64040 -2.12363 -3.45752
H 1.32766 -3.83052 -3.02480
H 0.01970 -2.77948 -3.63680
N 0.23502 1.68689 -0.35597
C 1.53651 2.07980 -0.43188
C -0.71564 2.63674 -0.54436
C 1.87676 3.41623 -0.69842
C -0.43370 3.96971 -0.81871
H -1.74422 2.31168 -0.43709
C 0.89363 4.37567 -0.90056
H 2.92770 3.67417 -0.76359
H -1.25641 4.66244 -0.96002
H 1.15958 5.40618 -1.11746
C 2.67831 1.13903 -0.24021
C 2.89473 0.05568 -1.10128
C 3.63575 1.42847 0.74598
C 4.03893 -0.73136 -0.96436
H 2.14878 -0.17619 -1.85083
C 4.77784 0.63789 0.88300
H 3.47980 2.27437 1.41018
C 4.98299 -0.44512 0.02411
H 4.19274 -1.57047 -1.63649
H 5.51024 0.87566 1.65004
H 5.87614 -1.05655 0.12023
Ru -0.66923 -0.24759 0.16388
N -1.63477 0.69076 1.65776
C -2.32837 1.24560 2.40062
C -3.32443 1.97457 3.17194
H -3.76866 1.33455 3.93971
H -2.88312 2.85013 3.65675
H -4.10398 2.29790 2.47418

^{1}G ($2\kappa^2$) (* single point)
SCF (B3LYP) Energy = -1164.10195520
Enthalpy 0K = -1163.779266
Enthalpy 298K = -1163.755188
Free Energy 298K = -1163.830240
Lowest Frequency = 53.6712 cm^{-1}

Second Frequency = 59.2192 cm^{-1}

$^2G^+$ (κ^2)
SCF (B3LYP) Energy = -1068.18950621
Enthalpy 0K = -1067.870343
Enthalpy 298K = -1067.844720
Free Energy 298K = -1067.928884
Lowest Frequency = 22.6219 cm^{-1}
Second Frequency = 25.6038 cm^{-1}

Ru	0.71566	-0.19935	0.10548
N	-0.15956	-1.72477	-0.89726
C	-0.59044	-2.62603	-1.48053
C	-1.12777	-3.76716	-2.20968
H	-2.22084	-3.75057	-2.18044
H	-0.79939	-3.73286	-3.25239
H	-0.77476	-4.69790	-1.75630
O	2.27392	-1.58075	0.69306
C	2.91548	-1.28124	-0.36156
O	2.36701	-0.41725	-1.14517
C	4.25611	-1.86781	-0.68388
H	5.03944	-1.21384	-0.28526
H	4.35869	-2.84857	-0.21695
H	4.39139	-1.93796	-1.76472
N	-0.52013	1.20753	-0.80609
C	-1.82613	1.30958	-0.43330
C	-0.02950	2.03031	-1.75431
C	-2.65282	2.27856	-1.01503
C	-0.80808	2.99971	-2.37307
H	1.01345	1.87846	-2.01106
C	-2.14434	3.12945	-1.99058
H	-3.68146	2.37050	-0.68668
H	-0.37029	3.63635	-3.13354
H	-2.77906	3.88450	-2.44296
C	-2.29115	0.34303	0.58079
C	-1.35627	-0.26198	1.44674
C	-3.62966	-0.06698	0.65888
C	-1.74385	-1.24380	2.36034
H	-0.35350	0.20103	1.62973
C	-4.01984	-1.04112	1.57889
H	-4.36706	0.34841	-0.02040
C	-3.08192	-1.63490	2.42759
H	-1.00396	-1.68375	3.02127
H	-5.06111	-1.34445	1.62563
H	-3.39263	-2.39229	3.14006
N	1.71885	1.27089	1.07618
C	2.34440	2.07675	1.62425
C	3.13504	3.08140	2.32303
H	3.64766	2.62492	3.17479
H	3.88104	3.50806	1.64641
H	2.48630	3.88307	2.68730

$^3G^+$ (κ^2)
SCF (B3LYP) Energy = -1200.95937148
Enthalpy 0K = -1200.593182
Enthalpy 298K = -1200.562427
Free Energy 298K = -1200.658955
Lowest Frequency = 22.4675 cm^{-1}
Second Frequency = 23.9783 cm^{-1}

N	-1.43559	0.77593	-1.55226
C	-1.95483	1.03628	-2.55178
N	-1.83016	1.14843	1.25156
C	-2.63671	1.66249	1.90350
C	-3.66387	2.29206	2.72375
H	-4.19491	3.05303	2.14477
H	-4.38245	1.53752	3.05705
H	-3.21286	2.76507	3.60073
C	-2.61268	1.29718	-3.82418
H	-2.79456	0.34567	-4.33301
H	-3.56833	1.80266	-3.65993
H	-1.98083	1.92631	-4.45714
O	-1.46377	-2.17607	-1.76131
C	-2.13825	-2.21636	-0.72423
C	-3.21691	-3.26915	-0.51650
H	-4.14826	-2.80440	-0.18174
H	-3.38433	-3.82269	-1.44088
H	-2.90380	-3.96620	0.26786
O	-2.00015	-1.40220	0.28736
N	0.96177	1.57406	-0.03374
C	0.72322	2.89108	0.12868
C	2.20754	1.16933	-0.40723
C	1.69485	3.86439	-0.06087
H	-0.28642	3.15318	0.42189
C	3.22517	2.10785	-0.62683
C	2.97352	3.46311	-0.45019
H	1.44716	4.90961	0.08657
H	4.19936	1.76724	-0.95705
H	3.75671	4.19414	-0.62319
C	2.42252	-0.28379	-0.56084
C	3.67618	-0.86080	-0.30776
C	1.35183	-1.13599	-0.90286
C	3.85555	-2.24112	-0.40499
H	4.50989	-0.23605	-0.00349
C	1.52994	-2.51834	-0.99504
H	0.39520	-0.77709	-1.34608
C	2.78642	-3.07276	-0.74772
H	4.83438	-2.66729	-0.20693
H	0.68124	-3.12534	-1.28934
H	2.93419	-4.14502	-0.82998
Ru	-0.56120	0.09652	0.15363
N	0.22326	-0.68348	1.85415
C	0.60448	-1.19277	2.81958
C	1.08157	-1.85291	4.02775
H	1.89610	-2.53903	3.77906
H	1.44724	-1.11325	4.74548
H	0.26750	-2.42204	4.48563

^1G ($\kappa^2\kappa^1$)
SCF (B3LYP) Energy = -1164.09455274
Enthalpy 0K = -1163.772754
Enthalpy 298K = -1163.746505
Free Energy 298K = -1163.831341
Lowest Frequency = 22.1427 cm^{-1}
Second Frequency = 26.0904 cm^{-1}

Ru	-0.68988	0.25458	-0.03294
N	0.15305	1.92503	-0.75716
C	0.58486	2.91439	-1.18269
C	1.12207	4.16446	-1.70569
H	2.17890	4.26198	-1.44008
H	1.03031	4.19338	-2.79569
H	0.57686	5.01546	-1.28601
O	-2.34675	1.45244	0.72712
C	-2.96052	1.24127	-0.36289
O	-2.34365	0.60253	-1.28907
C	-4.38279	1.68603	-0.56713
H	-5.05137	0.87440	-0.26051
H	-4.59856	2.56095	0.04887
H	-4.56879	1.90154	-1.62129
O	-1.80102	-1.39101	0.55112
C	-1.54686	-2.03805	1.65023
O	-0.59888	-1.81238	2.41404
C	-2.55768	-3.13411	1.96491
H	-2.78784	-3.71646	1.06880
H	-2.17613	-3.78495	2.75287
H	-3.49146	-2.67324	2.30465
N	0.55623	-1.01271	-1.05949
C	1.86411	-1.12420	-0.69042
C	0.07467	-1.78573	-2.05319

```
C   2.71155 -2.02314 -1.34904
C   0.87262 -2.68973 -2.74184
H  -0.97747 -1.64803 -2.27615
C   2.21760 -2.80934 -2.38409
H   3.74244 -2.11689 -1.02688
H   0.44148 -3.28904 -3.53618
H   2.86668 -3.51324 -2.89568
C   2.27290 -0.25671  0.42501
C   1.26021  0.23785  1.27930
C   3.59836  0.15350  0.62299
C   1.59190  1.10853  2.32235
H   0.29480 -0.36083  1.44841
C   3.91696  1.02892  1.66083
H   4.38029 -0.18499 -0.05082
C   2.91468  1.50958  2.50978
H   0.80824  1.45173  2.99033
H   4.94767  1.34009  1.80450
H   3.16812  2.18654  3.32065
```

TS(**^{1}G-^{1}H**)
SCF (B3LYP) Energy = -1164.08713356
Enthalpy 0K = -1163.769691
Enthalpy 298K = -1163.743915
Free Energy 298K = -1163.827140
Lowest Frequency = -1074.7533 cm^{-1}
Second Frequency = 19.4648 cm^{-1}

```
Ru -0.71518  0.12417 -0.08210
N  -0.19547  1.92108 -0.75585
C   0.06301  2.98051 -1.15151
C   0.37876  4.31655 -1.64113
H   1.40151  4.58850 -1.36369
H   0.28867  4.35585 -2.73101
H  -0.30707  5.05043 -1.20682
O  -2.52395  0.97992  0.76294
C  -3.15298  0.73944 -0.31847
O  -2.51258  0.24895 -1.30679
C  -4.63557  0.99354 -0.41732
H  -5.17025  0.08292 -0.12578
H  -4.93141  1.79639  0.26068
H  -4.91294  1.23623 -1.44512
O  -1.50870 -1.73657  0.48394
C  -1.06916 -2.25705  1.55773
O  -0.13715 -1.74183  2.24545
C  -1.70373 -3.53956  2.04341
H  -2.32804 -3.98178  1.26650
H  -0.92928 -4.24247  2.35950
H  -2.32325 -3.31707  2.91842
N   0.75148 -0.84989 -1.14790
C   2.04345 -0.75530 -0.71298
C   0.46131 -1.60334 -2.22649
C   3.06520 -1.43076 -1.39439
C   1.43624 -2.29083 -2.93724
H  -0.58743 -1.63065 -2.50287
C   2.76469 -2.19985 -2.51229
H   4.08419 -1.36310 -1.03039
H   1.15516 -2.88398 -3.80050
H   3.55203 -2.72861 -3.04095
C   2.21514  0.07531  0.48364
C   1.02047  0.39903  1.18941
C   3.45433  0.58917  0.89048
C   1.13694  1.24384  2.30910
H   0.22133 -0.63778  1.54437
C   3.53319  1.42440  2.00306
H   4.35658  0.36451  0.32739
C   2.37124  1.75384  2.71068
H   0.24145  1.48542  2.87604
H   4.49500  1.82100  2.31550
H   2.43348  2.40506  3.57889
```

^{1}H
SCF (B3LYP) Energy = -1164.10394730
Enthalpy 0K = -1163.781607
Enthalpy 298K = -1163.755077
Free Energy 298K = -1163.841488
Lowest Frequency = 17.0325 cm^{-1}
Second Frequency = 26.3616 cm^{-1}

```
Ru  0.63519  0.21568  0.11031
N   0.57857  2.08286 -0.45413
C   0.57519  3.19336 -0.79695
C   0.58467  4.58633 -1.22576
H  -0.43418  4.92833 -1.43237
H   1.01510  5.22496 -0.44774
H   1.17927  4.70034 -2.13773
O   2.53834 -0.04817 -0.86853
C   3.21663  0.27797  0.17075
O   2.62561  0.60339  1.23885
C   4.72723  0.29713  0.08156
H   5.16803  0.13846  1.06752
H   5.07975 -0.45969 -0.62250
H   5.05302  1.27687 -0.28562
O   0.91186 -1.77507  0.87317
C   0.82013 -2.85031  0.27131
O   0.34783 -2.96727 -0.95520
C   1.24934 -4.14944  0.88980
H   1.56076 -3.98385  1.92014
H   0.42913 -4.87157  0.84971
H   2.08110 -4.56586  0.31295
N  -1.04172  0.39051  1.30907
C  -2.25399  0.12418  0.73104
C  -0.97898  0.69511  2.61854
C  -3.42217  0.16524  1.50527
C  -2.10626  0.75252  3.42905
H   0.01806  0.88977  3.00099
C  -3.35211  0.48019  2.85736
H  -4.37847 -0.05246  1.04279
H  -2.00397  1.00231  4.47943
H  -4.25566  0.51199  3.45907
C  -2.16603 -0.18024 -0.69900
C  -0.83451 -0.18521 -1.21926
C  -3.27802 -0.41598 -1.52039
C  -0.70273 -0.40700 -2.60722
H   0.06118 -2.07415 -1.26994
C  -3.10377 -0.65711 -2.88212
H  -4.28465 -0.40684 -1.10827
C  -1.81391 -0.64618 -3.42335
H   0.29130 -0.38560 -3.05153
H  -3.96492 -0.84323 -3.51723
H  -1.67465 -0.81979 -4.48816
```

^{2}G
SCF (B3LYP) Energy = -1296.86375774
Enthalpy 0K = -1296.494884
Enthalpy 298K = -1296.463403
Free Energy 298K = -1296.560764
Lowest Frequency = 30.8547 cm^{-1}
Second Frequency = 32.6806 cm^{-1}

```
N  -1.94276  1.03553  0.84222
C  -2.85298  1.60689  1.26841
C  -4.03426  2.29772  1.76573
H  -4.36586  1.84827  2.70628
H  -3.81679  3.35540  1.94077
H  -4.84024  2.21807  1.02997
O  -3.15422  0.26979 -1.77721
C  -2.76366 -0.88758 -1.62033
O  -1.70861 -1.28295 -0.95871
C  -3.53446 -2.06731 -2.21847
H  -2.87049 -2.69186 -2.82423
```

H -3.92592 -2.69775 -1.41362
H -4.36064 -1.70336 -2.83137
O -0.70863 -1.46611 1.60280
C -0.41420 -1.18681 2.83546
O 0.10889 -0.13456 3.23181
C -0.76526 -2.30213 3.81545
H -1.82966 -2.54448 3.74020
H -0.21001 -3.20989 3.55869
H -0.52297 -2.00108 4.83560
N 1.17411 -1.25118 -0.51819
C 2.43823 -0.76353 -0.38949
C 0.98201 -2.51904 -0.92802
C 3.54233 -1.57074 -0.68967
C 2.04155 -3.36009 -1.24721
H -0.05761 -2.81913 -0.99686
C 3.34524 -2.87707 -1.12489
H 4.54358 -1.17809 -0.55392
H 1.84174 -4.37448 -1.57498
H 4.19605 -3.51218 -1.35258
C 2.54557 0.62935 0.08380
C 1.47884 1.18433 0.82856
C 3.63747 1.44282 -0.25041
C 1.53756 2.51988 1.24015
H 0.76743 0.54659 1.44899
C 3.68117 2.77615 0.15624
H 4.44314 1.04418 -0.85998
C 2.62972 3.31801 0.90086
H 0.72936 2.91619 1.84635
H 4.53348 3.39298 -0.11365
H 2.66835 4.35482 1.22275
Ru -0.42347 -0.06460 0.08995
N -0.31311 1.15099 -1.51593
C -0.39426 1.80580 -2.46685
C -0.60416 2.59749 -3.67087
H -0.42695 3.65828 -3.47126
H 0.06967 2.27345 -4.46937
H -1.63878 2.46504 -4.00261

TS(**^{2}G-^{2}H**)
SCF (B3LYP) Energy = -1296.85431990
Enthalpy 0K = -1296.489895
Enthalpy 298K = -1296.459021
Free Energy 298K = -1296.554073
Lowest Frequency = -1133.9072 cm^{-1}
Second Frequency = 28.8952 cm^{-1}

N 1.87341 -1.24210 0.72539
C 2.79893 -1.88376 0.99105
C 4.02567 -2.61984 1.26130
H 4.31807 -2.50388 2.30898
H 3.89549 -3.68508 1.04926
H 4.82250 -2.22341 0.62409
O 3.42364 0.35478 -1.28643
C 2.94728 1.40256 -0.83764
O 1.79682 1.55468 -0.24950
C 3.73162 2.71581 -0.93766
H 3.13791 3.47410 -1.45860
H 3.93777 3.10251 0.06567
H 4.67178 2.55742 -1.46885
O 0.43118 0.86698 2.10636
C -0.27482 0.30773 2.99853
O -1.01594 -0.70018 2.76951
C -0.24341 0.87031 4.40100
H 0.47573 1.68634 4.47401
H -1.24140 1.23100 4.66825
H 0.01452 0.07683 5.10805
N -1.15082 1.32717 -0.29462
C -2.39016 0.78527 -0.47221
C -0.97757 2.66049 -0.35604
C -3.48886 1.62083 -0.71853
C -2.03276 3.53014 -0.60333
H 0.04649 2.98909 -0.21148
C -3.31140 2.99782 -0.78603
H -4.47537 1.18693 -0.83481
H -1.85180 4.59870 -0.64540
H -4.16059 3.64924 -0.97073
C -2.44273 -0.68051 -0.37489
C -1.31175 -1.32268 0.21191
C -3.50762 -1.42960 -0.89512
C -1.32289 -2.73037 0.24948
H -0.92086 -0.88704 1.45723
C -3.48134 -2.82176 -0.84165
H -4.34808 -0.93233 -1.37229
C -2.38307 -3.47257 -0.27001
H -0.48690 -3.24704 0.71448
H -4.30896 -3.39589 -1.24823
H -2.36006 -4.55872 -0.22632
Ru 0.40273 0.02562 0.17005
N 0.59204 -0.59778 -1.72125
C 0.84334 -0.90131 -2.80879
C 1.26746 -1.24267 -4.15918
H 1.13129 -2.31130 -4.34859
H 0.69118 -0.67914 -4.89873
H 2.32748 -0.99216 -4.26716

^{2}H
SCF (B3LYP) Energy = -1296.86759061
Enthalpy 0K = -1296.498211
Enthalpy 298K = -1296.466778
Free Energy 298K = -1296.563807
Lowest Frequency = 23.6217 cm^{-1}
Second Frequency = 27.9328 cm^{-1}

N 1.67590 -1.58707 -0.18809
C 2.61680 -2.24618 -0.33696
C 3.91758 -2.87312 -0.51914
H 4.17768 -3.49143 0.34487
H 3.93330 -3.49844 -1.41636
H 4.65079 -2.06563 -0.62292
O 3.65224 0.63244 -0.54574
C 3.14810 1.26805 0.39294
O 1.93015 1.19618 0.82516
C 4.00643 2.27618 1.17162
H 3.58560 3.28275 1.07099
H 3.99855 2.03213 2.23890
H 5.03331 2.27557 0.80093
O 0.12430 -0.57726 2.12883
C -0.47959 -1.52773 2.63527
O -1.19752 -2.39147 1.94091
C -0.45402 -1.79194 4.11352
H 0.18473 -1.06160 4.60805
H -1.47062 -1.73578 4.51435
H -0.08522 -2.80474 4.30052
N -1.04459 1.43536 0.31844
C -2.32811 1.17021 -0.06830
C -0.73168 2.61494 0.88438
C -3.32285 2.14067 0.12526
C -1.68150 3.60745 1.09548
H 0.31450 2.71696 1.15828
C -3.00070 3.36159 0.70617
H -4.34318 1.93189 -0.17531
H -1.38999 4.54560 1.55516
H -3.77067 4.11286 0.85708
C -2.51943 -0.15871 -0.66386
C -1.35620 -0.99532 -0.68714
C -3.74265 -0.58196 -1.20524
C -1.51646 -2.25706 -1.30145
H -1.20057 -2.09403 0.99246
C -3.85740 -1.84314 -1.78639
H -4.61246 0.07046 -1.18665

```
C  -2.73795 -2.67888 -1.83598
H  -0.65811 -2.92378 -1.36553
H  -4.80696 -2.16796 -2.20179
H  -2.81706 -3.66123 -2.29686
Ru  0.34193 -0.09123  0.03837
N   0.76756  0.51496 -1.78379
C   1.13719  0.89260 -2.81435
C   1.70286  1.38621 -4.06222
H   1.53370  0.67306 -4.87445
H   1.24928  2.34291 -4.33807
H   2.78041  1.52975 -3.93291
```

$^{-}$OAc (* single point)
SCF (PBE1PBE) Energy = -228.245942673
Enthalpy 0K = -228.197670
Enthalpy 298K = -228.192698
Free Energy 298K = -228.223892
Lowest Frequency = 270.2044 cm^{-1}
Second Frequency = 435.2273 cm^{-1}

AcOH
SCF (PBE1PBE) Energy = -228.836379514
Enthalpy 0K = -228.773762
Enthalpy 298K = -228.768283
Free Energy 298K = -228.800882
Lowest Frequency = 77.3662 cm^{-1}
Second Frequency = 421.5018 cm^{-1}

O	-0.77050	-1.04286	0.00002
H	-1.70831	-0.80144	0.00003
C	-0.09268	0.12222	-0.00001
O	-0.64661	1.19474	-0.00001
C	1.39014	-0.10487	-0.00001
H	1.67772	-0.68605	0.88051
H	1.67771	-0.68611	-0.88049
H	1.90505	0.85443	-0.00004

a-H, 2-phenylpyridine
SCF (PBE1PBE) Energy = -478.784925840
Enthalpy 0K = -478.613658
Enthalpy 298K = -478.603964
Free Energy 298K = -478.648377
Lowest Frequency = 47.5470 cm^{-1}
Second Frequency = 95.6566 cm^{-1}

N	-1.35932	-1.15297	-0.20610
C	-2.68788	-1.20060	-0.21381
C	-3.50571	-0.09023	-0.02348
H	-3.12753	-2.18254	-0.38408
H	-4.58623	-0.18827	-0.04542
C	0.72198	0.02869	-0.00552
C	1.46408	1.19877	-0.20674
C	2.79835	-1.20446	0.20283
C	2.85440	1.16843	-0.19724
H	0.95813	2.14023	-0.39978
C	3.52724	-0.03234	0.01220
H	3.31545	-2.14646	0.36293
H	3.41348	2.08510	-0.36250
H	4.61329	-0.05538	0.02062
C	-0.76067	0.02975	-0.00187
C	-2.88881	1.13473	0.20572
H	-3.47949	2.03005	0.37889
C	-1.50228	1.19800	0.22304
H	-1.00228	2.13778	0.43088
C	1.40959	-1.17550	0.19024
H	0.82870	-2.08125	0.32893

Benzene (C_6H_6)
SCF (PBE1PBE) Energy = -231.969040346
Enthalpy 0K = -231.868678
Enthalpy 298K = -231.863433
Free Energy 298K = -231.896112
Lowest Frequency = 437.0575 cm^{-1}
Second Frequency = 437.0837 cm^{-1}

C	0.00000	1.40481	0.00000
C	-1.21659	0.70239	0.00000
C	-1.21659	-0.70239	0.00000
C	0.00000	-1.40480	0.00000
C	1.21659	-0.70239	0.00000
C	1.21658	0.70240	0.00000
H	-2.16519	1.25006	0.00000
H	-2.16518	-1.25007	0.00000
H	0.00001	-2.50014	0.00000
H	2.16519	-1.25006	0.00000
H	2.16518	1.25007	0.00000
H	-0.00001	2.50001	0.00000

MeCN
SCF (PBE1PBE) Energy = -132.592559640
Enthalpy 0K = -132.546833
Enthalpy 298K = -132.542300
Free Energy 298K = -132.570835
Lowest Frequency = 391.5366 cm^{-1}
Second Frequency = 391.5799 cm^{-1}

C	0.00000	-1.17638	0.00000
H	-1.02582	-1.55384	0.00000
H	0.51292	-1.55385	0.88839
H	0.51292	-1.55385	-0.88839
C	0.00000	0.27754	0.00000
N	-0.00001	1.43637	0.00000

A
SCF (PBE1PBE) Energy = -783.402744060
Enthalpy 0K = -783.194298
Enthalpy 298K = -783.177869
Free Energy 298K = -783.239119
Lowest Frequency = 12.2221 cm^{-1}
Second Frequency = 59.3681 cm^{-1}

C	1.79241	-0.82810	1.41653
C	2.48248	0.20156	0.69996
C	2.47940	0.19633	-0.70940
C	1.78826	-0.83937	-1.41643
C	1.12653	-1.86366	-0.70992
C	1.12844	-1.85819	0.72030
Ru	0.42536	0.07505	-0.00092
O	-0.27881	1.76824	-1.08437
C	-0.62779	2.32720	0.00132
C	-1.44319	3.57787	0.00227
H	2.90328	1.03228	-1.25481
H	0.50145	-2.56938	1.24195
O	-1.57374	-0.29807	-0.00603
C	-2.13423	-1.47462	0.00038
O	-1.55731	-2.55771	0.00935
O	-0.28287	1.76398	1.08615
C	-3.64801	-1.38524	-0.00397
H	-3.98883	-0.82948	0.87418
H	-3.98454	-0.83393	-0.88651
H	-4.08244	-2.38508	-0.00222
H	-2.50120	3.29717	-0.00073
H	-1.24427	4.16178	0.90223
H	-1.24028	4.16571	-0.89423
H	1.69853	-0.75874	2.49506
H	0.49786	-2.57881	-1.22412
H	1.69174	-0.77876	-2.49523
H	2.90898	1.04118	1.23760

B^{+}
SCF (PBE1PBE) Energy = -1033.76535648
Enthalpy 0K = -1033.434761
Enthalpy 298K = -1033.413588
Free Energy 298K = -1033.484657
Lowest Frequency = 33.4217 cm^{-1}
Second Frequency = 43.1431 cm^{-1}

C	-0.27432	-2.16634	-0.76662
C	-2.79482	-1.37929	1.91522
C	-3.82327	-1.84185	1.09513
C	-4.06750	-1.22178	-0.12881
C	-2.22877	0.30313	0.27500

```
C  -1.36120  3.78411 -0.85511
O   1.08137 -0.14083  1.87116
C   2.09071  0.62296  1.75192
O   2.54791  0.75830  0.56846
C   2.68558  1.34000  2.91094
H  -1.86569  4.72537 -1.05021
H   2.48901  0.79548  3.83532
H   3.75816  1.47375  2.76160
H   2.22679  2.33141  2.99021
H  -4.87584 -1.56854 -0.76534
H  -4.44390 -2.67294  1.41624
H  -2.61916 -1.84301  2.88134
C   0.60810  2.44166 -0.74836
H   1.67809  2.30540 -0.85183
C   0.01436  3.66321 -1.01535
H   0.62794  4.49525 -1.34228
C  -1.42626  1.46611 -0.17201
Ru  1.02704 -0.46546 -0.22777
C   2.31650 -1.44179 -1.66328
H   3.30144 -1.07847 -1.93953
C   2.18153 -2.30757 -0.54127
H   3.05669 -2.61687  0.01843
C   0.88478 -2.63463 -0.08375
H   0.76924 -3.17985  0.84764
C   1.17736 -0.96633 -2.36018
H   1.29071 -0.27241 -3.18514
C  -0.11515 -1.33190 -1.89469
H  -0.99449 -0.89035 -2.35166
H  -1.26378 -2.37276 -0.37483
C  -2.07732  2.67609 -0.42811
H  -3.14814  2.72929 -0.26511
C  -3.28267 -0.14433 -0.53144
H  -3.48300  0.34842 -1.47997
N  -0.08611  1.35806 -0.34321
C  -1.99603 -0.31404  1.50960
H  -1.19497  0.04017  2.14945
```

TS(**B**$^{+}$-**C**$^{+}$)
SCF (PBE1PBE) Energy = -1033.73990959
Enthalpy 0K = -1033.410800
Enthalpy 298K = -1033.389901
Free Energy 298K = -1033.461070
Lowest Frequency = -93.4009 cm^{-1}
Second Frequency = 27.7703 cm^{-1}

```
C   1.57663  2.38279 -0.34774
N   1.27456  1.09844 -0.13313
C   2.21152  0.25104  0.33917
C   3.52112  0.66554  0.54946
C   3.84929  1.99426  0.29739
C   2.86090  2.86936 -0.14298
Ru -0.57739  0.15690 -0.49101
C  -2.63302  0.02783 -1.26022
C  -1.88683  1.02378 -1.96192
C  -0.65560  0.67381 -2.57730
C  -0.15975 -0.66166 -2.51086
C  -0.87394 -1.61102 -1.75712
C  -2.12509 -1.27491 -1.14592
H  -0.05728  1.44597 -3.05147
C   1.67362 -1.09332  0.62754
C   2.29769 -2.27283  0.21805
C   1.68382 -3.49718  0.47192
C   0.44538 -3.56394  1.12016
C  -0.17592 -2.39702  1.54566
C   0.43283 -1.15516  1.30569
H  -2.62626 -1.98697 -0.50135
O  -1.12823  1.45096  1.00184
C  -2.08502  1.06238  1.81735
O  -2.59420 -0.05255  1.79208
C  -2.49317  2.12908  2.80338
H  -1.61834  2.50316  3.34147
H  -2.92991  2.97845  2.26986
H  -3.22108  1.72537  3.50638
H   3.24663 -2.23419 -0.30907
H   2.17450 -4.41392  0.15753
H  -1.11898 -2.41671  2.08335
H  -0.01237 -4.52951  1.31161
H   4.25501 -0.03647  0.93059
H   0.05726 -0.27327  1.82292
H  -3.51675  0.30412 -0.69717
H  -0.43989 -2.58992 -1.57941
H  -2.22376  2.05445 -1.96718
H   0.80606 -0.90985 -2.93633
H   3.07431  3.91648 -0.32609
H   4.86255  2.34730  0.46139
H   0.76411  3.01842 -0.68253
```

C^{+}
SCF (PBE1PBE) Energy = -1033.76540400
Enthalpy 0K = -1033.435183
Enthalpy 298K = -1033.413849
Free Energy 298K = -1033.485920
Lowest Frequency = 19.3940 cm^{-1}
Second Frequency = 28.7907 cm^{-1}

```
C   0.40294  2.72122  0.02005
N   0.59740  1.41651 -0.22649
C   1.85170  0.95115 -0.45194
C   2.93484  1.83386 -0.46685
C   2.72838  3.18494 -0.23973
C   1.43739  3.64104  0.01870
Ru -0.95297  0.02124 -0.21263
C  -3.04758 -0.66875  0.04289
C  -3.15581  0.75312 -0.10196
C  -2.53288  1.37759 -1.18152
C  -1.79135  0.59833 -2.13070
C  -1.77143 -0.81163 -2.03412
C  -2.42890 -1.45816 -0.94388
H  -2.55227  2.45902 -1.27323
C   1.92107 -0.49588 -0.62228
C   3.10508 -1.18987 -0.88900
C   3.09361 -2.57542 -0.99226
C   1.89834 -3.26722 -0.81871
C   0.71231 -2.57549 -0.55873
C   0.68655 -1.17548 -0.46444
H  -2.38884 -2.53560 -0.83571
O  -0.71665  0.15230  1.91720
C  -0.09616 -0.51680  2.75561
O   0.66992 -1.53039  2.45702
C  -0.17893 -0.21188  4.21218
H   0.81735  0.04351  4.58462
H  -0.86744  0.61222  4.38908
H  -0.50462 -1.10409  4.75398
H   4.04278 -0.65667 -1.01753
H   4.01317 -3.11302 -1.19919
H  -0.20144 -3.14895 -0.42361
H   1.88315 -4.35131 -0.88715
H   3.93408  1.45550 -0.64822
H   0.70676 -1.64565  1.47771
H  -3.45146 -1.14499  0.93041
H  -1.20736 -1.39526 -2.75302
H  -3.64729  1.33928  0.66660
H  -1.24672  1.09030 -2.92920
H   1.23049  4.68653  0.21675
H   3.56550  3.87587 -0.25349
H  -0.61809  3.01967  0.22867
```

B.OAc
SCF (PBE1PBE) Energy = -1262.17247458
Enthalpy 0K = -1261.791919

Enthalpy 298K = -1261.764768
Free Energy 298K = -1261.850468
Lowest Frequency = 28.9137 cm^{-1}
Second Frequency = 37.9768 cm^{-1}

C	-0.54621	-1.80002	1.39878
N	-0.28403	-0.55507	0.96040
C	-1.10586	0.45359	1.32505
C	-2.19250	0.21260	2.16700
C	-2.44917	-1.06783	2.63070
C	-1.60621	-2.09786	2.23600
Ru	1.27327	-0.40531	-0.48272
C	2.54257	-0.56866	-2.25532
C	1.54860	-1.59542	-2.25671
C	0.17288	-1.27835	-2.16445
C	-0.22186	0.08203	-2.02490
C	0.74750	1.10828	-1.97879
C	2.13245	0.77311	-2.08536
H	-0.62669	-2.01596	-2.02425
C	-0.88357	1.83466	0.82969
C	-1.87623	2.42155	0.03500
C	-1.71321	3.72996	-0.41410
C	-0.57891	4.46034	-0.06404
C	0.40133	3.87801	0.73793
C	0.25289	2.56813	1.18557
H	2.88279	1.54395	-1.93806
O	2.31330	-1.73329	0.82448
C	2.76653	-0.75993	1.50608
O	2.48986	0.40998	1.10330
C	3.55902	-0.99200	2.75101
H	4.21662	-0.14397	2.94673
H	2.86903	-1.09697	3.59480
H	4.13447	-1.91523	2.66613
H	-2.72515	1.81213	-0.27294
H	-2.47621	4.17752	-1.04478
H	1.28306	4.44582	1.02174
H	-0.46022	5.48298	-0.41181
H	-2.82767	1.04839	2.43700
H	1.02245	2.11047	1.79831
H	3.59645	-0.82350	-2.26030
H	0.45291	2.13040	-1.76614
H	1.86441	-2.63431	-2.23464
H	-1.29357	0.24160	-1.79337
H	-1.77169	-3.12448	2.54115
H	-3.29891	-1.25921	3.27894
H	0.12634	-2.57409	1.05228
O	-2.38584	-2.29050	-1.17129
C	-3.21045	-1.35758	-1.01612
C	-4.62905	-1.73582	-0.57846
H	-4.72341	-2.81057	-0.41086
H	-4.89483	-1.19259	0.33473
H	-5.34259	-1.42362	-1.34794
O	-3.00562	-0.12025	-1.18616

TS(**B**–**C**)1.OAc (* single point)
SCF (PBE1PBE) Energy = -1262.14185881
Enthalpy 0K = -1261.765705
Enthalpy 298K = -1261.740805
Free Energy 298K = -1261.817507
Lowest Frequency = -70.4683 cm^{-1}
Second Frequency = 40.8335 cm^{-1}

INT(**B**–**C**).OAc
SCF (PBE1PBE) Energy = -1262.15188720
Enthalpy 0K = -1261.772677
Enthalpy 298K = -1261.745163
Free Energy 298K = -1261.833370
Lowest Frequency = 17.2424 cm^{-1}
Second Frequency = 27.7331 cm^{-1}

C	-1.57024	1.21592	1.02241
N	-0.32353	1.06542	0.55977
C	0.57142	2.07653	0.63774
C	0.21659	3.29796	1.19715
C	-1.07810	3.47062	1.67996
C	-1.97755	2.42007	1.59155
Ru	0.29984	-0.73524	-0.30210
C	0.95082	-2.39629	-1.60835
C	-0.27770	-2.72227	-1.00457
C	-1.38452	-1.82186	-1.08231
C	-1.25817	-0.60367	-1.80517
C	-0.02801	-0.27612	-2.44020
C	1.07419	-1.14854	-2.29690
H	-2.30342	-1.94791	-0.50827
C	1.91190	1.78033	0.10585
C	2.69509	2.74980	-0.52613
C	3.93744	2.41234	-1.05521
C	4.41967	1.10592	-0.96374
C	3.64907	0.13140	-0.33911
C	2.39966	0.46420	0.18592
H	2.05099	-0.83906	-2.65534
O	0.07700	-1.36736	1.65297
C	1.02175	-2.10853	2.15473
O	2.09672	-2.34063	1.59883
C	0.68589	-2.66251	3.52096
H	0.45824	-1.84230	4.20714
H	-0.21159	-3.28416	3.45767
H	1.52057	-3.24923	3.90442
H	2.31898	3.76334	-0.63089
H	4.53320	3.17539	-1.54771
H	4.00851	-0.88634	-0.21923
H	5.39599	0.85668	-1.36838
H	0.95433	4.08962	1.27019
H	1.95253	-0.29576	0.86031
H	1.82271	-3.01837	-1.44432
H	0.09863	0.68586	-2.92448
H	-0.34162	-3.59886	-0.36819
H	-2.09583	0.12127	-1.72520
H	-3.00054	2.51231	1.93753
H	-1.37325	4.41845	2.12015
H	-2.26241	0.37444	0.89540
O	-3.77887	-0.64871	0.19905
C	-4.25435	0.28120	-0.51442
C	-5.77101	0.46529	-0.47078
H	-6.24724	-0.36497	-1.00374
H	-6.12777	0.42447	0.56236
H	-6.07124	1.40376	-0.94099
O	-3.59621	1.05710	-1.25592

TS(**B**–**C**)2.OAc
SCF (PBE1PBE) Energy = -1262.14864379
Enthalpy 0K = -1261.773369
Enthalpy 298K = -1261.747610
Free Energy 298K = -1261.829954
Lowest Frequency = -660.2145 cm^{-1}
Second Frequency = -7.2970 cm^{-1}

C	-1.46009	1.42677	0.62322
N	-0.22622	1.08939	0.22624
C	0.72312	2.03505	0.01669
C	0.43319	3.37993	0.22041
C	-0.84420	3.74531	0.63324
C	-1.79916	2.76005	0.83509
Ru	0.29231	-0.89258	-0.12581
C	0.77455	-2.88837	-0.97470
C	-0.46697	-2.95178	-0.30656
C	-1.52547	-2.05335	-0.62897
C	-1.32155	-1.05983	-1.61379
C	-0.07273	-0.97634	-2.29789
C	0.96649	-1.87272	-1.96012

H -2.44682 -1.98416 -0.05009
C 2.02407 1.50530 -0.40042
C 2.98241 2.26670 -1.07115
C 4.18724 1.68678 -1.45476
C 4.44678 0.34697 -1.16394
C 3.49195 -0.41401 -0.49870
C 2.25712 0.13673 -0.12211
H 1.94780 -1.74499 -2.40510
O -0.04485 -1.10832 1.91941
C 0.85411 -0.79859 2.76693
O 1.97747 -0.33799 2.45374
C 0.52451 -1.01121 4.21910
H 0.62500 -0.06140 4.75064
H -0.48612 -1.40035 4.33750
H 1.24927 -1.70478 4.65388
H 2.78256 3.30555 -1.31873
H 4.92850 2.28250 -1.97932
H 3.71235 -1.44629 -0.23666
H 5.39756 -0.09573 -1.44714
H 1.20697 4.12524 0.07358
H 1.93615 -0.24471 1.04842
H 1.59099 -3.54320 -0.69230
H 0.10912 -0.17907 -3.01016
H -0.58298 -3.62850 0.53421
H -2.11308 -0.29110 -1.72842
H -2.81325 2.99767 1.13473
H -1.08569 4.79203 0.79290
H -2.19792 0.62127 0.72938
O -3.80612 -0.43818 0.37532
C -4.25302 0.29116 -0.55668
C -5.75844 0.55942 -0.54790
H -6.28492 -0.35066 -0.85615
H -6.09665 0.79394 0.46542
H -6.02211 1.36621 -1.23472
O -3.57882 0.80381 -1.48744

C.OAc
SCF (PBE1PBE) Energy = -1262.16835417
Enthalpy 0K = -1261.788226
Enthalpy 298K = -1261.760991
Free Energy 298K = -1261.848377
Lowest Frequency = 13.1943 cm^{-1}
Second Frequency = 22.6385 cm^{-1}

C -1.42528 1.55217 0.31532
N -0.21008 1.12149 -0.05382
C 0.76913 2.00167 -0.38870
C 0.51635 3.37027 -0.37119
C -0.74567 3.82851 -0.00881
C -1.72455 2.91088 0.34358
Ru 0.24163 -0.90602 -0.14761
C 0.49976 -3.05958 -0.62166
C -0.64449 -2.91760 0.20943
C -1.73159 -2.08072 -0.14396
C -1.62770 -1.28614 -1.30593
C -0.47553 -1.37998 -2.14321
C 0.57800 -2.26846 -1.79878
H -2.57882 -1.89030 0.51276
C 2.04739 1.36452 -0.70827
C 3.19079 2.06615 -1.10161
C 4.37994 1.38679 -1.33873
C 4.42894 0.00470 -1.17072
C 3.28555 -0.69689 -0.78588
C 2.06069 -0.04693 -0.55702
H 1.48067 -2.28941 -2.40110
O 0.42755 -0.75569 1.99655
C 1.32315 -0.35131 2.74100
O 2.49335 0.06114 2.32185
C 1.14377 -0.29778 4.22226
H 1.21252 0.74210 4.55452
H 0.17364 -0.70978 4.49435
H 1.94903 -0.85077 4.71287
H 3.16044 3.14543 -1.22592
H 5.26673 1.93388 -1.64411
H 3.35157 -1.77570 -0.65722
H 5.35938 -0.53065 -1.34168
H 1.30215 4.06860 -0.63658
H 2.51383 0.00353 1.33418
H 1.32026 -3.70576 -0.33135
H -0.37960 -0.73875 -3.01245
H -0.65436 -3.42117 1.17201
H -2.41673 -0.53021 -1.48070
H -2.72684 3.21540 0.62163
H -0.95627 4.89411 -0.00341
H -2.18334 0.79985 0.57522
O -3.82867 -0.18304 0.80615
C -4.42346 0.31885 -0.19258
C -5.92453 0.56879 -0.03379
H -6.45390 -0.38868 -0.09579
H -6.13962 0.98887 0.95280
H -6.30186 1.22613 -0.81986
O -3.90022 0.61512 -1.29616

A.a-H
SCF (PBE1PBE) Energy = -1262.19873619
Enthalpy 0K = -1261.818124
Enthalpy 298K = -1261.790685
Free Energy 298K = -1261.880574
Lowest Frequency = 12.3166 cm^{-1}
Second Frequency = 17.5785 cm^{-1}

C 1.96546 1.45649 -1.98695
C 0.59445 1.07568 -1.86740
C 0.22331 -0.28117 -1.93531
C -1.90710 -1.64216 0.72649
C -1.74713 -3.02459 0.74118
H -0.82650 -3.44138 1.13882
C -2.22224 1.30803 0.39502
H -1.22974 0.95296 0.65093
O 1.39881 1.07683 1.20932
C 0.95385 2.89320 2.62293
H 1.81999 2.61332 3.22733
H 0.84901 3.97804 2.59201
H 0.06965 2.45708 3.09883
C 1.09088 2.34179 1.21718
O 0.89479 3.04928 0.23130
O 3.40106 -0.65117 0.83238
C 2.62417 -1.41594 1.48291
O 1.44971 -1.57988 1.02601
H -1.10310 -1.03120 1.12448
C 3.06130 -2.06814 2.75253
H 2.81103 -1.40226 3.58458
H 2.53388 -3.01225 2.89778
H 4.14103 -2.22444 2.74853
C -2.75484 -3.85402 0.25591
H -2.63033 -4.93336 0.26999
C -3.07833 -1.06306 0.21790
C -4.08799 -1.90885 -0.26133
H -4.99560 -1.45473 -0.64466
C -3.92746 -3.28876 -0.24252
H -4.72167 -3.92714 -0.62000
N -4.50010 0.83689 -0.17042
C -2.45589 2.67377 0.28648
H -1.63619 3.37021 0.44246
C -3.27133 0.40857 0.15716
C -3.73390 3.11108 -0.04543
H -3.96691 4.16668 -0.14193
C -4.71424 2.14620 -0.26020
H -5.72858 2.44402 -0.52355
Ru 1.79870 -0.06348 -0.43756

```
C   1.22644 -1.28249 -2.13549
H   0.95286 -2.33048 -2.07451
C   2.58075 -0.91783 -2.28684
H   3.34753 -1.68131 -2.35351
C   2.94768  0.45975 -2.18296
H   3.99837  0.73008 -2.15733
H  -0.80015 -0.57700 -1.73028
H  -0.13231  1.82728 -1.58738
H   2.24367  2.48499 -1.79686
```

B

SCF (PBE1PBE) Energy = -1262.19334428
Enthalpy 0K = -1261.812037
Enthalpy 298K = -1261.785142
Free Energy 298K = -1261.869723
Lowest Frequency = 28.3654 cm^{-1}
Second Frequency = 36.0027 cm^{-1}

```
C  -0.67718 -2.08210  1.95656
Ru -0.64831 -0.36432 -0.45674
C  -1.05432  0.03898 -2.58341
C  -1.94798 -0.94896 -2.09591
C  -0.07262 -2.29197 -1.28159
C   0.84673 -1.33294 -1.77284
H  -1.44437  0.96843 -2.97832
H  -3.00968 -0.73171 -2.11592
H   0.27213 -3.11821 -0.67152
H   1.90858 -1.43934 -1.58615
C  -0.55173 -2.15212  3.46805
H  -0.67792 -3.18030  3.80933
H   0.40884 -1.75425  3.80624
H  -1.33505 -1.52931  3.91154
O  -0.22613 -0.96049  1.47290
O  -1.16876 -3.00942  1.32025
C   1.58731  1.67672  0.47668
C  -0.55180  2.54032  0.26449
N   0.27884  1.48344  0.19198
O  -2.31262  0.25609  0.61331
C  -3.32462  0.89016  0.11117
O  -3.36538  1.42417 -1.00065
C  -4.50940  0.94946  1.05648
H  -4.19548  1.33792  2.02903
H  -5.29770  1.57528  0.63696
H  -4.89099 -0.06206  1.22503
C   2.60160  0.60881  0.26577
C   3.58147  0.82592 -0.71088
C   2.65800 -0.55045  1.04462
C   4.57960 -0.11897 -0.93541
H   3.55249  1.73671 -1.30431
C   3.66579 -1.48530  0.82666
H   1.88517 -0.72273  1.78470
C   4.62275 -1.27863 -0.16555
H   5.32486  0.05509 -1.70622
H   3.70130 -2.38342  1.43681
H   5.40338 -2.01517 -0.33328
C  -0.14478  3.80279  0.66959
C   2.05373  2.92468  0.90081
C   1.18410  3.99851  1.01641
H   3.10733  3.02664  1.13705
H   1.54192  4.96718  1.35262
H  -0.87109  4.60745  0.70232
H  -1.56990  2.36312 -0.05936
C  -1.47297 -2.12326 -1.45657
H  -2.15156 -2.81341 -0.97318
C   0.33743 -0.15331 -2.38194
H   1.02809  0.64523 -2.63634
```

TS(**B-C**)
SCF (PBE1PBE) Energy = -1262.14151667
Enthalpy 0K = -1261.763085
Enthalpy 298K = -1261.736786
Free Energy 298K = -1261.819954
Lowest Frequency = -36.3555 cm^{-1}
Second Frequency = 32.1050 cm^{-1}

```
C  -3.36812  0.13857 -1.29528
Ru -0.03097 -0.42175  0.67549
C   0.38797 -1.66413  2.38681
C  -0.84312 -2.08628  1.82216
C  -1.69796  0.19625  1.96352
C  -0.48824  0.63226  2.57831
H   1.21087 -2.36629  2.44959
H  -0.90825 -3.09499  1.43239
H  -2.46052  0.88908  1.61738
H  -0.32867  1.68531  2.78015
C  -4.48405 -0.51921 -2.10813
H  -4.44215 -1.60464 -1.95825
H  -5.46523 -0.16963 -1.77940
H  -4.34736 -0.33090 -3.17554
O  -2.23585  0.19438 -1.84233
O  -3.66682  0.54463 -0.13672
C   2.13037  1.19162 -0.59804
C   4.08920 -0.74230 -0.67092
C   2.83992 -0.97832 -0.11860
H   2.54501 -1.95259  0.26030
N   1.89555 -0.02635 -0.06563
O  -0.03021 -1.54917 -1.02922
C   0.37367 -2.78127 -1.06605
O   0.88077 -3.40444 -0.12866
C   0.19180 -3.40679 -2.43222
H   0.97531 -3.03578 -3.10099
H   0.27154 -4.49212 -2.36099
H  -0.76766 -3.10987 -2.86029
H   4.82507 -1.53837 -0.68817
C   1.02629  2.14862 -0.50022
C   1.28337  3.51644 -0.35330
C  -0.30129  1.67552 -0.44820
C   0.23895  4.41099 -0.15470
H   2.30835  3.87699 -0.35534
C  -1.34339  2.59029 -0.24808
H  -0.74459  0.71544 -0.92452
C  -1.07458  3.94557 -0.09440
H   0.45186  5.46977 -0.03755
H  -2.35989  2.19061 -0.24277
H  -1.89225  4.64485  0.05640
C   3.36490  1.48120 -1.18479
C   4.35531  0.51206 -1.21266
H   5.31704  0.72516 -1.66955
H   3.52209  2.45445 -1.63586
C  -1.89428 -1.15629  1.61000
H  -2.79017 -1.40245  1.05159
C   0.55773 -0.29514  2.76621
H   1.52359  0.04625  3.12613
```

C

SCF (PBE1PBE) Energy = -1262.21517174
Enthalpy 0K = -1261.834278
Enthalpy 298K = -1261.807264
Free Energy 298K = -1261.892398
Lowest Frequency = 26.4011 cm^{-1}
Second Frequency = 31.9636 cm^{-1}

```
C   3.82114  0.17498  0.82572
Ru -0.24727 -0.64957 -0.66598
C  -1.14500 -2.52307 -1.64003
C   0.03115 -2.92045 -1.00592
C   1.27924 -1.12822 -2.17414
C   0.06642 -0.71206 -2.80569
H  -2.08100 -3.02194 -1.40918
H   0.00796 -3.69701 -0.25165
```

H 2.20628 -0.58726 -2.31620
H 0.05996 0.15902 -3.45178
C 5.14394 0.79161 1.19807
H 5.91158 0.48235 0.48979
H 5.05123 1.88177 1.19360
H 5.42365 0.49704 2.21303
O 2.88115 0.45281 1.71157
O 3.65365 -0.49095 -0.18164
C -4.13584 -0.21747 1.22846
C -2.96764 -0.71701 0.67653
H -2.75541 -1.77829 0.64328
N -2.00304 0.07922 0.19360
O 0.52155 -0.59043 1.29460
C 0.08278 -1.45527 2.17446
O -0.74181 -2.33279 1.94452
C 0.66366 -1.25927 3.55992
H 0.17455 -0.39902 4.02869
H 0.47886 -2.14509 4.16809
H 1.73291 -1.03899 3.51738
H -4.88973 -0.90139 1.60163
C -0.96784 2.16025 -0.20055
C -0.87456 3.55805 -0.18981
C 0.10141 1.34958 -0.64741
C 0.29088 4.17826 -0.61326
H -1.70823 4.16618 0.15277
C 1.27635 2.00505 -1.03905
H 1.99241 0.05709 1.45513
C 1.36905 3.39501 -1.02768
H 0.36655 5.26151 -0.60919
H 2.14529 1.42337 -1.33380
H 2.29394 3.87357 -1.34150
C -2.12809 1.42709 0.28424
C -4.29691 1.16457 1.30165
C -3.28451 1.98736 0.83831
H -5.19789 1.59435 1.72970
H -3.37603 3.06520 0.90806
C 1.23458 -2.17379 -1.23336
H 2.12656 -2.37185 -0.65009
C -1.14419 -1.38119 -2.51058
H -2.07483 -1.02712 -2.94122

B′
SCF (PBE1PBE) Energy = -1030.21745469
Enthalpy 0K = -1029.939789
Enthalpy 298K = -1029.918745
Free Energy 298K = -1029.989243
Lowest Frequency = 37.0192 cm^{-1}
Second Frequency = 59.0084 cm^{-1}

C -2.68783 -0.42992 -1.02842
Ru -0.38090 -0.34290 -0.12104
C -4.06055 -0.63226 -1.59111
H -4.80833 -0.19158 -0.92985
H -4.12939 -0.20593 -2.59327
H -4.25612 -1.70718 -1.66175
O -1.67558 -0.36237 -1.80223
O -2.49510 -0.35340 0.22060
C 1.93434 0.92417 -0.27167
C 2.43506 -1.11159 -1.29279
N 1.54918 -0.28207 -0.73782
O -0.42433 -2.42188 0.22963
C 0.05800 -2.24337 1.39377
O 0.36563 -1.05833 1.73369
C 0.21745 -3.38688 2.34393
H 0.41409 -4.31036 1.79668
H 1.01769 -3.18047 3.05622
H -0.71686 -3.51233 2.90087
C 0.72088 1.59707 0.25499
C 0.67169 2.17657 1.55708
C -0.34667 1.84052 -0.66782
C -0.42532 2.89746 1.94787
H 1.50188 2.01055 2.23693
C -1.45265 2.62168 -0.22251
H -0.18776 1.72255 -1.73649
C -1.50512 3.11265 1.05569
H -0.46740 3.31414 2.95006
H -2.24837 2.84308 -0.92812
H -2.36139 3.69540 1.38151
C 3.77639 -0.75254 -1.39010
C 3.25431 1.33926 -0.31508
C 4.19123 0.47715 -0.88824
H 3.53516 2.30948 0.08085
H 5.23604 0.76677 -0.94568
H 4.48280 -1.43840 -1.84523
H 2.05132 -2.06556 -1.63916

TS(**B′-C′**)
SCF (PBE1PBE) Energy = -1030.18248425
Enthalpy 0K = -1029.905652
Enthalpy 298K = -1029.885038
Free Energy 298K = -1029.955070
Lowest Frequency = -65.8309 cm^{-1}
Second Frequency = 39.8148 cm^{-1}

C -2.91933 0.95020 -0.57922
Ru -0.44856 -0.27916 0.05281
C -4.38594 1.27701 -0.39126
H -4.69191 2.05767 -1.08925
H -4.97734 0.37847 -0.59627
H -4.58950 1.57900 0.63856
O -2.33469 1.22646 -1.63480
O -2.36632 0.36172 0.42856
C 2.36783 0.11615 -0.16830
C 3.26870 -2.41878 -0.67533
C 1.91680 -2.13192 -0.55195
H 1.15029 -2.89082 -0.66516
N 1.47312 -0.89366 -0.29006
O -1.29033 -2.04904 -0.59407
C -1.36922 -2.45817 0.61012
O -0.83305 -1.70624 1.48353
C -2.06949 -3.72225 0.97244
H -1.62166 -4.15998 1.86617
H -3.11612 -3.48787 1.19160
H -2.04092 -4.42498 0.13812
H 3.58312 -3.43507 -0.88673
C 1.72541 1.41764 0.07090
C 2.27769 2.38301 0.92064
C 0.48212 1.68237 -0.56204
C 1.61923 3.58695 1.13132
H 3.20978 2.17152 1.43704
C -0.16494 2.90923 -0.34727
H 0.12581 1.07234 -1.43130
C 0.39684 3.84809 0.50497
H 2.05258 4.32455 1.80049
H -1.10460 3.07970 -0.86165
H -0.11280 4.78984 0.68472
C 3.73694 -0.10242 -0.27450
C 4.19586 -1.39110 -0.52554
H 5.25947 -1.58775 -0.61636
H 4.42295 0.73258 -0.17888

C′
SCF (PBE1PBE) Energy = -1030.18243994
Enthalpy 0K = -1029.904858
Enthalpy 298K = -1029.883087
Free Energy 298K = -1029.957335
Lowest Frequency = 21.1932 cm^{-1}
Second Frequency = 29.4385 cm^{-1}

C 2.10518 1.59034 1.75897

```
Ru -0.13355 -1.41161 -0.72033
C   1.90743  3.04620  2.07158
H   2.86341  3.56656  2.02610
H   1.23003  3.46909  1.32228
H   1.44200  3.17483  3.05125
O   1.04761  0.85720  2.10473
O   3.10045  1.13451  1.23294
C  -3.88758 -1.09561  1.39617
C  -2.71645 -1.57031  0.82850
H  -2.42163 -2.61140  0.92363
N  -1.87288 -0.78958  0.13585
O   1.17183 -1.56302  0.83285
C   2.17243 -1.87302  0.06269
O   1.91876 -1.98661 -1.16136
C   3.52786 -2.03832  0.64941
H   3.47698 -2.66274  1.54485
H   4.20813 -2.47036 -0.08422
H   3.87055 -1.04121  0.94883
H  -4.53265 -1.77063  1.94729
C  -1.14289  1.26507 -0.76258
C  -1.21031  2.62675 -1.07456
C  -0.02165  0.48301 -1.14694
C  -0.16540  3.23321 -1.76077
H  -2.07562  3.21912 -0.78615
C   1.02190  1.11878 -1.83551
H   1.17091 -0.05250  1.74944
C   0.94749  2.47634 -2.13766
H  -0.21637  4.28999 -2.00557
H   1.89574  0.54358 -2.12897
H   1.76577  2.95256 -2.67224
C  -2.16287  0.53569 -0.01955
C  -4.20064  0.25265  1.23754
C  -3.33140  1.06740  0.52762
H  -5.10952  0.66363  1.66640
H  -3.54886  2.12174  0.39774
```

C′ (without HOAc)
SCF (PBE1PBE) Energy = -801.326920706
Enthalpy 0K = -801.113664
Enthalpy 298K = -801.097786
Free Energy 298K = -801.157419
Lowest Frequency = 39.2484 cm^{-1}
Second Frequency = 45.1589 cm^{-1}

```
Ru  0.71454 -0.63516 -0.64410
C  -3.11365 -2.44951  0.20967
C  -1.78667 -2.24044 -0.12960
H  -1.12801 -3.06757 -0.37820
N  -1.22624 -1.02167 -0.16939
O   1.74162 -1.15289  1.02606
C   2.86691 -0.76734  0.53941
O   2.86609 -0.31500 -0.63814
C   4.10196 -0.83105  1.37706
H   4.05089 -1.67495  2.06714
H   4.98435 -0.90267  0.73989
H   4.17359  0.08755  1.96879
H  -3.51400 -3.45702  0.22673
C  -1.23692  1.32262  0.09007
C  -1.78640  2.58624  0.32989
C   0.14009  1.17270 -0.22516
C  -0.98070  3.71579  0.26991
H  -2.84343  2.69581  0.56148
C   0.93323  2.32927 -0.27549
C   0.37692  3.58253 -0.03266
H  -1.40584  4.69749  0.45598
H   1.99024  2.23816 -0.51241
H   1.00578  4.46850 -0.08092
C  -1.98339  0.07165  0.14354
C  -3.89962 -1.34248  0.52198
C  -3.32704 -0.07951  0.48901
H  -4.94428 -1.46369  0.79202
H  -3.91522  0.79734  0.73637
```

D^{+} (K^{1})
SCF (PBE1PBE) Energy = -1280.55114205
Enthalpy 0K = -1280.152928
Enthalpy 298K = -1280.126955
Free Energy 298K = -1280.208958
Lowest Frequency = 28.1803 cm^{-1}
Second Frequency = 37.5341 cm^{-1}

```
Ru  0.11441 -0.09757 -0.20753
O   0.19926 -1.70697  2.29433
C  -0.57359 -0.76643  2.44895
C  -1.37697 -0.57497  3.70843
O  -0.80989  0.15249  1.54086
H  -2.35708 -1.04278  3.57027
H  -0.87340 -1.06586  4.54155
H  -1.53796  0.48288  3.92323
C  -2.85494 -0.24078 -0.56297
C  -4.12102 -0.52754 -0.05084
C  -1.90541 -1.27539 -0.63723
C  -4.43013 -1.81799  0.36970
H  -4.85714  0.26266  0.06067
C  -2.21470 -2.56515 -0.21565
C  -3.48156 -2.83600  0.29393
H  -5.41708 -2.02747  0.77043
H  -1.47430 -3.35458 -0.29017
H  -3.72984 -3.83869  0.62670
H  -0.99665 -1.16966 -1.30193
C  -2.45062  1.11326 -0.95417
C  -2.87852  3.32696 -1.80230
H  -3.56761  4.08205 -2.16679
C  -3.34539  2.08064 -1.41436
H  -4.39891  1.83616 -1.48981
C  -0.67068  2.58901 -1.27126
H   0.40111  2.73978 -1.20126
C  -1.51148  3.58500 -1.73625
H  -1.09695  4.53895 -2.04205
N  -1.12217  1.38460 -0.87936
C   2.89272 -0.66897 -0.53416
C   3.90131 -1.00625 -1.43777
C   1.79526 -1.55002 -0.34886
C   3.84137 -2.21185 -2.13015
H   4.72346 -0.31977 -1.61791
C   1.76488 -2.77071 -1.03592
C   2.77765 -3.09314 -1.93192
H   4.63026 -2.46659 -2.83096
H   0.95901 -3.47216 -0.84295
H   2.74796 -4.03629 -2.46829
H   1.15844 -1.49381  0.61257
C   2.87741  0.58856  0.22427
C   3.84015  2.42741  1.42750
H   4.70716  2.97882  1.77719
C   4.00367  1.28745  0.65074
H   4.99185  0.91807  0.39982
C   1.47096  2.10863  1.31104
H   0.44495  2.36279  1.55391
C   2.55476  2.83822  1.77379
H   2.38863  3.70787  2.39958
N   1.63283  1.02494  0.53631
```

TS(**D**$^{+}$**-E**$^{+}$) (K^{1})
SCF (PBE1PBE) Energy = -1280.54433543
Enthalpy 0K = -1280.150367
Enthalpy 298K = -1280.124898
Free Energy 298K = -1280.205195
Lowest Frequency = -1053.6222 cm^{-1}
Second Frequency = 33.9850 cm^{-1}

Ru	0.08581	-0.01202	-0.29579
O	0.80468	-1.76605	1.93319
C	-0.10796	-0.99900	2.32661
C	-0.65073	-1.12895	3.71453
O	-0.63147	-0.09505	1.58011
H	0.17134	-1.27303	4.41799
H	-1.24732	-0.25913	3.98777
H	-1.28103	-2.02267	3.75647
C	-2.91323	-0.38006	-0.40712
C	-4.09306	-0.81454	0.19940
C	-1.89505	-1.31895	-0.65395
C	-4.25720	-2.15375	0.54117
H	-4.87449	-0.10064	0.44147
C	-2.06315	-2.65936	-0.31635
C	-3.24588	-3.07751	0.28755
H	-5.17898	-2.47602	1.01550
H	-1.28063	-3.37788	-0.53621
H	-3.38136	-4.12164	0.55110
H	-1.05882	-1.08706	-1.37637
C	-2.67748	1.03251	-0.73324
C	-3.39789	3.22952	-1.40320
H	-4.18695	3.92511	-1.67080
C	-3.70297	1.91920	-1.06601
H	-4.72813	1.56680	-1.08697
C	-1.09333	2.70260	-1.07263
H	-0.04048	2.96656	-1.06828
C	-2.06428	3.62939	-1.41411
H	-1.77539	4.63844	-1.68597
N	-1.38370	1.43713	-0.72804
C	2.88713	-0.49582	-0.63328
C	3.99068	-0.90576	-1.38290
C	1.71676	-1.30422	-0.55097
C	3.96672	-2.13343	-2.03554
H	4.86291	-0.26506	-1.47736
C	1.73853	-2.54848	-1.20255
C	2.84380	-2.95553	-1.94316
H	4.82617	-2.45140	-2.61733
H	0.88524	-3.21535	-1.11427
H	2.83500	-3.91796	-2.44595
H	1.08000	-1.40413	0.68296
C	2.83506	0.77211	0.09687
C	3.73175	2.66508	1.27696
H	4.57947	3.25518	1.61059
C	3.93274	1.52668	0.50928
H	4.93422	1.20121	0.25151
C	1.38014	2.24801	1.18646
H	0.34818	2.47034	1.43610
C	2.43432	3.02633	1.63539
H	2.23754	3.89296	2.25632
N	1.57512	1.16526	0.41729

E⁺ (K^1)
SCF (PBE1PBE) Energy = -1280.55257042
Enthalpy 0K = -1280.153782
Enthalpy 298K = -1280.127886
Free Energy 298K = -1280.209444
Lowest Frequency = 32.3578 cm^{-1}
Second Frequency = 35.4663 cm^{-1}

Ru	0.10618	0.02275	-0.34645
O	0.82011	-1.81557	2.00078
C	-0.11480	-0.99191	2.34835
C	-0.63589	-1.11843	3.73527
O	-0.57786	-0.12889	1.56876
H	-1.13077	-2.08876	3.83949
H	0.19600	-1.10038	4.44371
H	-1.34238	-0.31894	3.95136
C	-2.90880	-0.46670	-0.38507
C	-4.04815	-0.97343	0.24368
C	-1.85029	-1.34724	-0.67699
C	-4.13702	-2.32489	0.56429
H	-4.85840	-0.30391	0.51643
C	-1.94576	-2.70143	-0.36304
C	-3.08827	-3.19110	0.26449
H	-5.02897	-2.70184	1.05519
H	-1.13717	-3.37698	-0.62154
H	-3.16426	-4.24625	0.50763
H	-1.04575	-1.06019	-1.41516
C	-2.76378	0.96450	-0.69125
C	-3.63321	3.11706	-1.32307
H	-4.46747	3.76328	-1.57722
C	-3.84971	1.78390	-1.00589
H	-4.84947	1.36465	-1.03036
C	-1.29802	2.73452	-1.01030
H	-0.26450	3.06804	-1.00968
C	-2.32893	3.60337	-1.33188
H	-2.10848	4.63369	-1.58805
N	-1.50001	1.44851	-0.68465
C	2.93158	-0.43872	-0.64043
C	4.09852	-0.91726	-1.24030
C	1.71422	-1.18280	-0.66985
C	4.09632	-2.16090	-1.86113
H	5.00823	-0.32300	-1.24110
C	1.76179	-2.43977	-1.29948
C	2.92896	-2.92263	-1.88774
H	5.00277	-2.53576	-2.32587
H	0.86889	-3.05940	-1.33896
H	2.92917	-3.89508	-2.37194
H	1.06934	-1.59462	1.04002
C	2.85494	0.84188	0.06096
C	3.70656	2.78193	1.20532
H	4.54129	3.39572	1.52902
C	3.93289	1.63020	0.46630
H	4.94299	1.32389	0.21953
C	1.36616	2.32100	1.10124
H	0.32818	2.53715	1.33177
C	2.39996	3.12914	1.54391
H	2.18077	4.00790	2.13972
N	1.58351	1.22060	0.36309

D⁺ (K^2)
SCF (PBE1PBE) Energy = -1280.57375894
Enthalpy 0K = -1280.174445
Enthalpy 298K = -1280.148658
Free Energy 298K = -1280.229621
Lowest Frequency = 25.1148 cm^{-1}
Second Frequency = 41.9699 cm^{-1}

Ru	0.27532	0.70843	0.02432
O	1.12183	2.26500	1.18904
C	1.14744	3.04874	0.18270
C	1.63197	4.45388	0.31008
O	0.71796	2.58668	-0.92344
H	2.07215	4.79103	-0.62960
H	0.78038	5.10429	0.53632
H	2.34780	4.53714	1.12890
C	-2.45746	-0.07281	0.86837
C	-3.79869	-0.36927	0.62025
C	-1.90444	1.09731	0.30516
C	-4.57273	0.49441	-0.15082
H	-4.23945	-1.28396	1.00526
C	-2.68607	1.96978	-0.45657
C	-4.02331	1.66095	-0.68762
H	-5.61504	0.25461	-0.33715
H	-2.24062	2.87329	-0.86104
H	-4.64033	2.32885	-1.28056
H	-1.02004	1.57923	0.86370
C	-1.55594	-0.91579	1.65868
C	-1.05875	-2.48434	3.41420

H -1.38385 -3.17780 4.18309
C -1.98903 -1.81320 2.63487
H -3.05163 -1.95086 2.80098
C 0.66455 -1.33356 2.22071
H 1.70431 -1.09415 2.03041
C 0.29433 -2.22497 3.21458
H 1.05802 -2.69815 3.82170
N -0.22927 -0.70930 1.43801
C 1.96241 -1.11227 -0.98554
C 2.67080 -2.09152 -0.27266
C 2.42347 0.22507 -0.99154
C 3.79208 -1.73571 0.46120
H 2.32521 -3.12102 -0.28789
C 3.54223 0.56779 -0.20676
C 4.21236 -0.39959 0.52224
H 4.34325 -2.49828 1.00402
H 3.90335 1.59136 -0.21544
H 5.08324 -0.13228 1.11216
H 2.06880 0.92571 -1.74388
C 0.75401 -1.44008 -1.76789
C -0.53180 -2.62462 -3.39854
H -0.63455 -3.41126 -4.13924
C 0.65961 -2.46668 -2.69763
H 1.51584 -3.10760 -2.87935
C -1.41930 -0.75309 -2.18844
H -2.21420 -0.05334 -1.96067
C -1.57903 -1.74554 -3.14676
H -2.51832 -1.82012 -3.68343
N -0.27772 -0.60933 -1.50040

TS(**D**$^{+}$**-E**$^{+}$) (K^2)
SCF (PBE1PBE) Energy = -1280.54432862
Enthalpy 0K = -1280.150194
Enthalpy 298K = -1280.124542
Free Energy 298K = -1280.205364
Lowest Frequency = -1174.0832 cm^{-1}
Second Frequency = 20.9745 cm^{-1}

Ru 0.01228 0.65025 -0.01468
O 0.84839 2.38970 -1.23491
C 0.53466 3.19441 -0.24107
C 0.67502 4.65771 -0.45525
O 0.12470 2.67937 0.81765
H 0.37975 5.20563 0.43863
H 1.71227 4.88697 -0.71671
H 0.05828 4.96165 -1.30628
C 2.47033 -0.81722 -0.57496
C 3.76257 -1.31044 -0.38854
C 2.04781 0.35778 0.09847
C 4.65046 -0.64042 0.44800
H 4.08348 -2.22545 -0.87785
C 2.96051 1.01345 0.93985
C 4.25287 0.52022 1.10989
H 5.65471 -1.02825 0.58725
H 2.65305 1.91252 1.46813
H 4.94921 1.03862 1.76251
H 1.47619 1.42569 -0.72315
C 1.46091 -1.45848 -1.41631
C 0.68372 -2.97652 -3.11760
H 0.87168 -3.77448 -3.82883
C 1.71015 -2.48886 -2.32351
H 2.71338 -2.88828 -2.41789
C -0.77544 -1.39563 -2.07781
H -1.74232 -0.92203 -1.95200
C -0.58274 -2.41094 -3.00031
H -1.41291 -2.74314 -3.61346
N 0.20964 -0.93456 -1.29074
C -2.60955 -0.27174 0.64721
C -3.54147 -0.99959 -0.10416
C -2.49413 1.11826 0.44944
C -4.30779 -0.36040 -1.07136
H -3.64073 -2.06971 0.05459
C -3.25315 1.74365 -0.54833
C -4.14699 1.00651 -1.31481
H -5.02913 -0.93092 -1.64897
H -3.17078 2.81742 -0.68779
H -4.74251 1.49532 -2.07937
H -1.94228 1.72834 1.16108
C -1.73510 -0.93570 1.63375
C -1.27746 -2.37780 3.49444
H -1.60968 -3.06732 4.26386
C -2.18833 -1.82392 2.60261
H -3.24738 -2.05188 2.66018
C 0.45334 -1.13701 2.39505
H 1.48623 -0.83598 2.26997
C 0.06251 -2.02006 3.39050
H 0.80819 -2.41794 4.06977
N -0.42536 -0.60887 1.52634

E^{+} (K^2)
SCF (PBE1PBE) Energy = -1280.56389991
Enthalpy 0K = -1280.164202
Enthalpy 298K = -1280.137813
Free Energy 298K = -1280.221142
Lowest Frequency = 28.6330 cm^{-1}
Second Frequency = 34.1189 cm^{-1}

Ru -0.21497 -0.30151 -0.48150
O -2.40275 -2.22764 -2.08665
C -1.41789 -2.91197 -1.54504
C -1.38958 -4.35067 -1.92306
O -0.58256 -2.40250 -0.78799
H -0.51905 -4.83775 -1.48762
H -2.30628 -4.83668 -1.57615
H -1.37260 -4.44242 -3.01286
C -2.25016 1.65678 0.08929
C -3.50266 2.19885 0.38748
C -2.04181 0.25245 0.06852
C -4.57353 1.36515 0.69130
H -3.65378 3.27467 0.39517
C -3.13499 -0.55983 0.41740
C -4.38529 -0.01361 0.71682
H -5.54508 1.79038 0.92109
H -3.01570 -1.64055 0.48287
H -5.21187 -0.66988 0.97511
H -2.45330 -1.34185 -1.67219
C -1.05956 2.46319 -0.17693
C 0.17841 4.50881 -0.47652
H 0.21541 5.59325 -0.50733
C -1.01728 3.85672 -0.21485
H -1.92347 4.42592 -0.04382
C 1.22369 2.37024 -0.65772
H 2.08566 1.74060 -0.84025
C 1.32270 3.75129 -0.70555
H 2.27894 4.21357 -0.92236
N 0.07113 1.73174 -0.39384
C 2.70866 -0.50553 0.34308
C 3.88993 0.22933 0.49954
C 2.33490 -0.91919 -0.94563
C 4.67151 0.54801 -0.60668
H 4.17992 0.58348 1.48439
C 3.11615 -0.58989 -2.05279
C 4.28544 0.14653 -1.88560
H 5.58345 1.12146 -0.47077
H 2.81952 -0.92879 -3.04083
H 4.89967 0.39836 -2.74439
H 1.49641 -1.61176 -1.07599
C 1.85534 -0.80968 1.50626
C 1.57074 -1.42978 3.81856
H 1.98854 -1.69609 4.78403

C 2.40125 -1.14302 2.74549
H 3.47975 -1.20014 2.84339
C -0.29551 -1.04494 2.37237
H -1.35781 -0.97852 2.17823
C 0.19509 -1.38074 3.62282
H -0.50229 -1.59730 4.42434
N 0.50914 -0.75796 1.33067

D$^+$ (η^6) (* single point)
SCF (PBE1PBE) Energy = -1280.57851221
Enthalpy 0K = -1280.181870
Enthalpy 298K = -1280.157430
Free Energy 298K = -1280.232828
Lowest Frequency = 46.1586 cm^{-1}
Second Frequency = 57.7623 cm^{-1}

TS(**D$^+$-E$^+$**) (η^6)
SCF (PBE1PBE) Energy = -1280.56094936
Enthalpy 0K = -1280.162167
Enthalpy 298K = -1280.136657
Free Energy 298K = -1280.218720
Lowest Frequency = -98.7464 cm^{-1}
Second Frequency = 16.3866 cm^{-1}

Ru 0.41886 -0.76436 -0.27009
O 0.32607 -1.84791 1.48533
C 1.46657 -2.43497 1.70120
C 1.53207 -3.28533 2.93994
O 2.43463 -2.27605 0.94856
H 1.74488 -2.64140 3.79953
H 0.57993 -3.78525 3.12590
H 2.33862 -4.01305 2.84810
C 1.86314 1.88254 0.21347
C 2.28159 2.99008 -0.52724
C 2.57986 0.67740 0.11806
C 3.39574 2.88815 -1.35703
H 1.72739 3.92306 -0.47348
C 3.69924 0.58317 -0.70995
C 4.10568 1.68937 -1.45068
H 3.71443 3.75121 -1.93377
H 4.25568 -0.34891 -0.74141
H 4.98294 1.62834 -2.08745
H 2.38137 -0.16495 0.79482
C 0.67538 1.90972 1.08137
C -0.75413 2.88491 2.74676
H -1.01906 3.71003 3.40058
C 0.34492 2.98518 1.90343
H 0.97172 3.87027 1.89924
C -1.11916 0.67280 1.91257
H -1.65640 -0.26831 1.87560
C -1.49175 1.70524 2.76032
H -2.34410 1.57688 3.41788
N -0.07545 0.78602 1.07917
C -1.42013 -0.65180 -1.41568
C -0.44693 0.17753 -2.06900
C -1.07960 -2.00870 -1.13005
C 0.81209 -0.34308 -2.40018
H -0.63596 1.23630 -2.20594
C 0.17983 -2.55100 -1.52414
C 1.13023 -1.71327 -2.12400
H 1.58321 0.31906 -2.77883
H 0.45194 -3.55845 -1.23059
H 2.14050 -2.07355 -2.28291
H -1.78208 -2.59282 -0.54559
C -2.75121 -0.13622 -1.00615
C -4.60431 1.36345 -1.24100
H -5.08694 2.20988 -1.71977
C -3.32985 0.96662 -1.63623
H -2.82099 1.48800 -2.44010
C -4.58800 -0.44027 0.32588
H -5.06208 -1.02948 1.10769
C -5.24897 0.65072 -0.23886
H -6.24484 0.92126 0.09559
N -3.37160 -0.83004 -0.04333

E$^+$ (η^6)
SCF (PBE1PBE) Energy = -1280.58694547
Enthalpy 0K = -1280.186823
Enthalpy 298K = -1280.161003
Free Energy 298K = -1280.243214
Lowest Frequency = 17.8592 cm^{-1}
Second Frequency = 28.1246 cm^{-1}

Ru 0.28788 -0.79295 -0.04973
O 0.91519 -0.65003 1.99866
C 2.02413 -0.59430 2.54683
C 2.16032 -0.57431 4.03112
O 3.15673 -0.55084 1.89799
H 2.64160 0.35921 4.33675
H 1.18304 -0.66332 4.50180
H 2.81353 -1.39136 4.34937
C 2.18987 1.28880 -0.90766
C 3.31454 1.87792 -1.49287
C 2.06453 -0.12018 -0.80301
C 4.34771 1.08376 -1.97498
H 3.39258 2.95833 -1.57628
C 3.13295 -0.89256 -1.28502
C 4.25921 -0.30090 -1.86249
H 5.22030 1.54243 -2.42858
H 3.09861 -1.97700 -1.21136
H 5.06766 -0.92839 -2.22711
H 2.98346 -0.52195 0.92698
C 1.08614 2.04716 -0.32878
C -0.06586 4.01618 0.44050
H -0.12442 5.09513 0.54553
C 1.01988 3.43594 -0.19675
H 1.82404 4.05239 -0.58149
C -0.95454 1.82718 0.79230
H -1.70464 1.14315 1.17755
C -1.06825 3.19832 0.95629
H -1.92603 3.60778 1.47753
N 0.08215 1.27021 0.14913
C -1.95981 -1.24611 -0.54585
C -1.10210 -1.07727 -1.69181
C -1.55966 -2.13337 0.46093
C 0.03037 -1.90362 -1.87984
H -1.33133 -0.32097 -2.43425
C -0.34943 -2.87891 0.31564
C 0.40342 -2.84281 -0.87463
H 0.65136 -1.77175 -2.75903
H -0.01031 -3.49825 1.14005
H 1.28955 -3.45633 -0.98529
H -2.14702 -2.19281 1.36999
C -3.22003 -0.47840 -0.40012
C -5.15117 0.60246 -1.32060
H -5.74297 0.92837 -2.17044
C -3.94498 -0.06297 -1.51883
H -3.59657 -0.28036 -2.52311
C -4.79103 0.37660 1.03033
H -5.09798 0.53443 2.06196
C -5.58684 0.82960 -0.02171
H -6.52215 1.34101 0.17944
N -3.63650 -0.26052 0.85532

D
SCF (PBE1PBE) Energy = -1509.02838442
Enthalpy 0K = -1508.578787
Enthalpy 298K = -1508.547570
Free Energy 298K = -1508.641739
Lowest Frequency = 23.9221 cm^{-1}

Second Frequency = 29.7182 cm^{-1}

Ru	0.95128	-0.04731	-0.39167
O	2.21251	0.89905	-1.86195
C	1.75286	0.11753	-2.74641
C	2.33060	0.08520	-4.12713
O	0.80439	-0.66888	-2.42508
H	1.56631	-0.19188	-4.85531
H	2.77321	1.05015	-4.37861
H	3.11888	-0.67404	-4.15463
C	-2.50937	0.07598	-0.93255
C	-3.55916	-0.18059	-0.04411
C	-2.21437	-0.85847	-1.93100
C	-4.29440	-1.35813	-0.14134
H	-3.78949	0.54300	0.73371
C	-2.96448	-2.02562	-2.03560
C	-4.00384	-2.27981	-1.14380
H	-5.09874	-1.55138	0.56270
H	-2.73358	-2.73967	-2.82128
H	-4.58650	-3.19275	-1.22975
H	-1.39141	-0.67110	-2.61274
C	-1.82475	1.39184	-0.90421
C	-2.04562	3.79164	-1.11162
H	-2.66266	4.67924	-1.21512
C	-2.62318	2.53459	-1.02956
H	-3.69838	2.40695	-1.09329
C	0.07349	2.71166	-0.93650
H	1.15591	2.73011	-0.90794
C	-0.65966	3.87729	-1.08578
H	-0.14204	4.82658	-1.17056
N	-0.47826	1.48772	-0.81991
C	-0.07041	0.50820	2.34813
C	-0.60674	1.29983	3.36567
C	0.98716	1.00101	1.55026
C	-0.07943	2.56086	3.62222
H	-1.45193	0.94176	3.94785
C	1.53046	2.25563	1.84847
C	0.99480	3.03487	2.86835
H	-0.50093	3.17183	4.41504
H	2.39477	2.60082	1.28803
H	1.42168	4.00986	3.08687
H	1.81664	0.24855	1.13476
C	-0.55778	-0.82629	2.01010
C	-1.61665	-2.93824	2.46013
H	-2.16817	-3.59885	3.12217
C	-1.27481	-1.65896	2.87024
H	-1.52888	-1.30672	3.86410
C	-0.51323	-2.49507	0.38427
H	-0.17236	-2.76951	-0.60767
C	-1.22005	-3.36717	1.19547
H	-1.45020	-4.36419	0.83655
N	-0.20435	-1.24719	0.76862
O	2.35870	-1.54135	-0.32615
C	3.29955	-1.51710	0.56025
C	4.34305	-2.60037	0.38369
O	3.39685	-0.69178	1.47383
H	3.88536	-3.53172	0.04371
H	5.05544	-2.28050	-0.38387
H	4.88518	-2.75661	1.31708

TS(**D-E**)
SCF (PBE1PBE) Energy = -1508.99269745
Enthalpy 0K = -1508.547618
Enthalpy 298K = -1508.516357
Free Energy 298K = -1508.610252
Lowest Frequency = -1188.5342 cm^{-1}
Second Frequency = 29.4066 cm^{-1}

Ru	-0.69346	-0.36846	-0.60655
O	-1.43697	-2.06784	-1.67242
C	-0.69684	-1.82164	-2.67553
C	-0.83731	-2.63260	-3.92999
O	0.13202	-0.86474	-2.61007
H	0.10093	-2.64307	-4.48686
H	-1.15770	-3.64870	-3.69356
H	-1.60572	-2.17244	-4.55983
C	2.75775	-0.36429	0.06724
C	3.54198	0.44078	0.90099
C	2.85089	-0.20834	-1.32022
C	4.39484	1.39723	0.35980
H	3.46788	0.32597	1.97926
C	3.71793	0.73892	-1.85685
C	4.49009	1.54370	-1.02199
H	4.98792	2.02529	1.01837
H	3.78949	0.84554	-2.93571
H	5.16581	2.28103	-1.44646
H	2.23263	-0.81762	-1.97181
C	1.95991	-1.46854	0.64962
C	1.98189	-3.48859	1.98465
H	2.50202	-4.18880	2.63127
C	2.62815	-2.36877	1.48821
H	3.67414	-2.18402	1.70740
C	0.04791	-2.76739	0.78789
H	-0.97900	-2.89099	0.46994
C	0.66302	-3.70135	1.60250
H	0.10382	-4.57113	1.92951
N	0.65377	-1.64723	0.33622
C	-1.18002	0.72826	2.07804
C	-1.53650	0.74262	3.42707
C	-1.74564	-0.21986	1.18817
C	-2.48624	-0.15578	3.90481
H	-1.07469	1.44569	4.11564
C	-2.71815	-1.09532	1.69274
C	-3.08557	-1.06720	3.03646
H	-2.76466	-0.13913	4.95464
H	-3.19486	-1.79982	1.01374
H	-3.83982	-1.75536	3.40931
H	-2.21796	0.28610	-0.07280
C	-0.23486	1.66028	1.46390
C	1.04900	3.69139	1.33237
H	1.42336	4.60456	1.78527
C	0.25054	2.82376	2.06096
H	-0.02998	3.05854	3.08179
C	0.84165	2.20527	-0.52488
H	1.04464	1.90939	-1.54785
C	1.33815	3.38396	0.00633
H	1.93985	4.03934	-0.61306
N	0.09826	1.34714	0.18494
O	-2.49547	0.62990	-1.33424
C	-2.67733	1.94386	-1.44260
C	-3.40932	2.30369	-2.71401
O	-2.32436	2.76600	-0.62174
H	-2.80632	2.00604	-3.57721
H	-4.34984	1.74921	-2.77132
H	-3.60132	3.37627	-2.74590

E
SCF (PBE1PBE) Energy = -1509.02242773
Enthalpy 0K = -1508.571572
Enthalpy 298K = -1508.539858
Free Energy 298K = -1508.636072
Lowest Frequency = 21.2879 cm^{-1}
Second Frequency = 21.9380 cm^{-1}

Ru	0.61390	0.45687	0.17297
O	1.49754	1.76001	1.59976
C	0.75504	2.77468	1.39349
C	0.97176	4.01790	2.21431
O	-0.15685	2.73287	0.52446
H	0.12979	4.14388	2.90232

H 1.89703 3.95272 2.78769
H 0.99234 4.89495 1.56273
C -2.75910 -0.13966 0.60532
C -3.63830 -1.04723 0.00498
C -2.82619 1.21356 0.25303
C -4.55645 -0.61682 -0.94811
H -3.58579 -2.09914 0.27327
C -3.75739 1.64177 -0.68942
C -4.62121 0.73051 -1.29498
H -5.22312 -1.33478 -1.41724
H -3.80779 2.69591 -0.94788
H -5.34619 1.07015 -2.02953
H -2.14009 1.92367 0.70488
C -1.87101 -0.58717 1.70335
C -1.71867 -1.60898 3.89276
H -2.17900 -2.12542 4.72948
C -2.46392 -1.25607 2.77915
H -3.52865 -1.45775 2.73198
C 0.15985 -0.60555 2.81298
H 1.20185 -0.31845 2.78795
C -0.37654 -1.25072 3.91326
H 0.26231 -1.46878 4.76221
N -0.54461 -0.30080 1.69975
C 1.53797 -2.18515 -0.61928
C 2.33033 -3.33810 -0.64009
C 1.80974 -1.10852 0.26507
C 3.42837 -3.44191 0.20464
H 2.10256 -4.15751 -1.31853
C 2.94624 -1.23587 1.08475
C 3.74059 -2.38109 1.05723
H 4.04553 -4.33543 0.19054
H 3.21290 -0.41796 1.75390
H 4.61196 -2.45001 1.70504
H 2.95802 0.97820 -1.03622
C 0.42335 -1.93523 -1.52420
C -1.00997 -2.38909 -3.41214
H -1.33559 -3.04307 -4.21581
C 0.00191 -2.78414 -2.55189
H 0.48810 -3.74505 -2.68018
C -1.14850 -0.34872 -2.17913
H -1.59513 0.61876 -1.97785
C -1.59017 -1.13620 -3.23068
H -2.38258 -0.77270 -3.87543
N -0.17804 -0.72440 -1.33120
O 2.06277 1.27182 -1.27014
C 2.16370 2.35516 -2.10654
C 0.82928 2.88465 -2.50913
O 3.24669 2.75870 -2.43589
H 0.26803 3.16401 -1.61069
H 0.97066 3.73853 -3.17019
H 0.26424 2.10035 -3.02090

E (without HOAc)
SCF (PBE1PBE) Energy = -1280.18036574
Enthalpy 0K = -1279.793669
Enthalpy 298K = -1279.768044
Free Energy 298K = -1279.848829
Lowest Frequency = 31.8652 cm^{-1}
Second Frequency = 37.9891 cm^{-1}

Ru -0.23832 -0.67661 -0.17699
O -0.71659 -2.74550 0.23584
C -1.05235 -2.90469 -0.98155
C -1.63403 -4.20435 -1.44909
O -0.91160 -1.93105 -1.78205
H -1.44453 -4.34490 -2.51441
H -1.22668 -5.03502 -0.86998
H -2.71791 -4.17988 -1.29485
C 2.72027 -0.14948 0.58170
C 3.90153 0.55987 0.33636
C 2.32191 -1.13092 -0.33901
C 4.66357 0.29433 -0.79691
H 4.20389 1.35359 1.01357
C 3.08514 -1.39477 -1.47416
C 4.25721 -0.68025 -1.70759
H 5.57216 0.86149 -0.97742
H 2.75469 -2.15763 -2.17242
H 4.85146 -0.88007 -2.59433
H 1.48223 -1.80781 -0.09924
C 1.87430 0.15324 1.74966
C 1.61292 0.82153 4.05240
H 2.03728 1.12652 5.00374
C 2.43091 0.55067 2.96628
H 3.51010 0.61836 3.05260
C -0.25676 0.26845 2.66337
H -1.31953 0.13989 2.49402
C 0.23864 0.67486 3.89045
H -0.45341 0.86709 4.70338
N 0.52909 0.00863 1.59756
C -2.35673 1.27022 -0.31039
C -3.61926 1.84487 -0.11787
C -2.06679 -0.04240 0.14162
C -4.62025 1.12765 0.52188
H -3.82769 2.85436 -0.46534
C -3.10247 -0.74674 0.78120
C -4.35631 -0.17051 0.96782
H -5.59985 1.57179 0.67202
H -2.91377 -1.75818 1.13424
H -5.14069 -0.73741 1.46507
C -1.24867 1.93189 -0.98419
C -0.18142 3.70904 -2.22110
H -0.21428 4.69339 -2.67863
C -1.29228 3.20099 -1.56802
H -2.20836 3.77856 -1.51298
C 0.96183 1.68146 -1.68386
H 1.83426 1.03934 -1.71569
C 0.97008 2.92847 -2.28735
H 1.86436 3.27146 -2.79611
N -0.10595 1.18386 -1.03755

$^3D^+$
SCF (PBE1PBE) Energy = -1678.43837997
Enthalpy 0K = -1677.895058
Enthalpy 298K = -1677.854617
Free Energy 298K = -1677.970804
Lowest Frequency = 20.0565 cm^{-1}
Second Frequency = 21.7603 cm^{-1}

Ru -0.00091 0.82408 0.54213
C 1.96771 -1.52775 -1.34098
C 1.17021 -2.63776 -1.05299
C 3.35071 -1.61675 -1.14129
C 1.73693 -3.80021 -0.53688
H 0.10560 -2.61165 -1.25898
C 3.91336 -2.77495 -0.61604
C 3.10791 -3.86991 -0.31005
H 1.10387 -4.65753 -0.32761
H 4.98667 -2.82606 -0.45749
H 3.55033 -4.77932 0.08576
H 3.97380 -0.75919 -1.37672
C 1.41820 -0.34792 -2.06221
C 1.35964 0.81422 -4.19015
H 1.69936 0.92536 -5.21522
C 1.85385 -0.19668 -3.38524
H 2.57765 -0.90873 -3.76546
C 0.02872 1.47768 -2.33087
H -0.69756 2.13879 -1.87651
C 0.40500 1.66542 -3.64769
H -0.04019 2.47012 -4.22279
N 0.51843 0.51119 -1.52563

C -2.75680 -1.32276 -0.30185
C -2.37722 -1.05777 -1.62051
C -4.11089 -1.21938 0.04313
C -3.32551 -0.68377 -2.56784
H -1.33797 -1.14929 -1.91027
C -5.05845 -0.83898 -0.90229
C -4.66773 -0.56993 -2.21290
H -3.01464 -0.49674 -3.59165
H -6.10486 -0.76836 -0.61899
H -5.40832 -0.29253 -2.95750
H -4.41955 -1.43361 1.06309
C -1.79931 -1.83086 0.71288
C -1.29789 -3.61612 2.27246
H -1.55962 -4.55736 2.74640
C -2.13443 -3.04340 1.32757
H -3.05349 -3.53477 1.02771
C 0.16756 -1.76327 1.93174
H 1.09176 -1.22513 2.11780
C -0.11401 -2.95822 2.57345
H 0.59815 -3.35699 3.28763
N -0.64923 -1.18382 1.02699
O 1.89387 0.30726 1.19175
C 3.02773 0.78788 0.76868
C 4.19386 0.38389 1.65148
O 3.19667 1.48092 -0.23189
H 4.28356 -0.70640 1.66525
H 5.12006 0.82174 1.27812
H 4.02004 0.70911 2.68149
N 0.69773 2.68346 0.28957
C 1.28044 3.66747 0.13621
C 2.13336 4.81709 -0.08051
H 2.16263 5.45122 0.80905
H 3.13865 4.44007 -0.29419
H 1.77941 5.40797 -0.92892
N -0.35119 1.23031 2.47017
C -0.48707 1.45260 3.59600
C -0.64439 1.73060 5.01107
H -1.04286 2.73834 5.15581
H -1.33173 1.01016 5.46255
H 0.32397 1.65807 5.51368
N -1.85104 1.48006 0.12310
C -2.87572 1.99397 -0.04032
C -4.16966 2.61455 -0.25027
H -4.13538 3.67185 0.02634
H -4.45854 2.52484 -1.30069
H -4.92429 2.10859 0.35766

INT($^3D^+$)
SCF (PBE1PBE) Energy = -1678.41891901
Enthalpy 0K = -1677.875945
Enthalpy 298K = -1677.835411
Free Energy 298K = -1677.952220
Lowest Frequency = 17.7199 cm^{-1}
Second Frequency = 23.9745 cm^{-1}

Ru 0.30649 0.78833 0.23455
C -2.13962 -0.89691 -1.52805
C -1.51197 -1.99739 -2.09424
C -1.50537 0.36770 -1.59899
C -0.27030 -1.86968 -2.73524
H -2.01472 -2.95936 -2.06029
C -0.26148 0.49043 -2.22894
C 0.35398 -0.64112 -2.80756
H 0.18244 -2.74063 -3.20061
H 0.13634 1.48229 -2.41744
H 1.29845 -0.53117 -3.33250
H -2.00065 1.27773 -1.26477
C -3.46731 -1.05292 -0.89266
C -5.67005 -0.24471 -0.36691
H -6.43455 0.52579 -0.41344
C -4.42320 -0.02978 -0.94195
H -4.20149 0.90403 -1.44824
C -4.91533 -2.42188 0.25047
H -5.07840 -3.39117 0.71806
C -5.92798 -1.46665 0.24737
H -6.88929 -1.68277 0.70159
N -3.71578 -2.23233 -0.29892
C 2.95709 -1.59092 0.12954
C 2.83349 -2.85797 -0.44917
C 3.06907 -1.48477 1.51837
C 2.78645 -3.99618 0.35046
H 2.76689 -2.94809 -1.52987
C 3.02911 -2.62288 2.31679
C 2.88186 -3.88073 1.73616
H 2.69403 -4.97578 -0.11010
H 3.13071 -2.53104 3.39430
H 2.86352 -4.76998 2.35948
H 3.20339 -0.50677 1.96739
C 3.13119 -0.39851 -0.73604
C 4.56535 0.71318 -2.33903
H 5.44111 0.71732 -2.98078
C 4.25838 -0.39472 -1.56519
H 4.90014 -1.26903 -1.56114
C 2.62065 1.74914 -1.42101
H 1.93967 2.58715 -1.31384
C 3.73454 1.82102 -2.24137
H 3.92958 2.73401 -2.79338
N 2.28501 0.65980 -0.69873
O 0.37507 2.82175 -0.17919
C -0.65166 3.59156 -0.42094
C -0.27849 5.05814 -0.50306
O -1.81320 3.22294 -0.57430
H -1.14751 5.65175 -0.78608
H 0.09949 5.39975 0.46525
H 0.52402 5.20843 -1.23084
N -1.43967 1.03898 1.18408
C -2.42274 1.23754 1.75344
C -3.67727 1.54621 2.40846
H -3.55995 1.52770 3.49483
H -4.00143 2.54346 2.09671
H -4.43652 0.81666 2.11376
N 1.18673 1.28520 1.90980
C 1.66810 1.70143 2.87431
C 2.28181 2.22807 4.07835
H 3.37127 2.18335 3.99510
H 1.98358 3.27032 4.22153
H 1.96856 1.64615 4.94932
N 0.09841 -1.16323 0.67428
C -0.29203 -2.22831 0.89485
C -0.85043 -3.54682 1.11140
H -0.87862 -3.77874 2.17925
H -1.86816 -3.54668 0.70037
H -0.24009 -4.29692 0.60291

TS($^3D^+$-$^3E^+$)
SCF (PBE1PBE) Energy = -1678.39560433
Enthalpy 0K = -1677.857883
Enthalpy 298K = -1677.817922
Free Energy 298K = -1677.932553
Lowest Frequency = -1085.5166 cm^{-1}
Second Frequency = 19.6719 cm^{-1}

Ru -0.14687 -0.95167 0.27150
C 1.56940 1.12618 -1.54080
C 1.46909 2.16441 -2.47560
C 0.66351 0.03638 -1.57424
C 0.54814 2.10559 -3.51525
H 2.15867 3.00068 -2.40295
C -0.22723 -0.00420 -2.66932

```
C  -0.28735  0.99518 -3.63238
H   0.50511  2.90595 -4.24846
H  -0.89252 -0.85866 -2.76873
H  -0.98274  0.91618 -4.46313
H   1.21933 -1.20635 -1.44837
C   2.75275  1.19182 -0.63935
C   4.90117  0.33744  0.02259
H   5.68413 -0.41440 -0.03854
C   3.71858  0.17757 -0.68951
H   3.55229 -0.69611 -1.31124
C   4.05806  2.43281  0.78270
H   4.16284  3.35084  1.35929
C   5.07991  1.48874  0.78427
H   5.99223  1.66548  1.34486
N   2.92590  2.30601  0.08714
C  -2.53333  1.79907  0.14971
C  -1.65718  2.54785 -0.63895
C  -3.10787  2.38835  1.28243
C  -1.35845  3.86296 -0.29605
H  -1.22456  2.10832 -1.52944
C  -2.80085  3.70107  1.62866
C  -1.92985  4.44443  0.83372
H  -0.68418  4.43607 -0.92542
H  -3.25868  4.14918  2.50599
H  -1.70718  5.47687  1.08812
H  -3.80426  1.81587  1.88997
C  -3.01242  0.46074 -0.27981
C  -4.94969 -0.80329 -1.01086
H  -6.00984 -0.86088 -1.23791
C  -4.38315  0.37685 -0.56181
H  -4.98227  1.27285 -0.44310
C  -2.77088 -1.76061 -0.86209
H  -2.09922 -2.60485 -0.95666
C  -4.11274 -1.89922 -1.17137
H  -4.48028 -2.85603 -1.52611
N  -2.20261 -0.61713 -0.41984
O  -0.15874 -2.86004 -0.63543
C   0.80836 -3.17561 -1.39353
C   0.88895 -4.58098 -1.90911
O   1.69493 -2.34730 -1.75335
H   1.91848 -4.94007 -1.85000
H   0.22091 -5.24017 -1.35548
H   0.60706 -4.58481 -2.96675
N   1.60054 -1.47114  1.06850
C   2.55881 -1.82007  1.61191
C   3.77615 -2.24718  2.27291
H   3.56516 -2.55220  3.30134
H   4.21530 -3.09285  1.73638
H   4.49362 -1.42201  2.28248
N  -1.06385 -1.77546  1.88155
C  -1.60111 -2.27329  2.77607
C  -2.28026 -2.90290  3.89287
H  -3.36252 -2.79528  3.78085
H  -2.03375 -3.96748  3.92952
H  -1.97453 -2.43527  4.83259
N   0.06223  0.77276  1.24764
C   0.36797  1.71293  1.84432
C   0.76766  2.91625  2.54423
H   1.44732  2.66763  3.36369
H   1.28539  3.56209  1.82955
H  -0.11095  3.43061  2.93892
```

$^{3}E^{+}$

SCF (PBE1PBE) Energy = -1678.40794139
Enthalpy 0K = -1677.865639
Enthalpy 298K = -1677.824893
Free Energy 298K = -1677.942802
Lowest Frequency = 18.7146 cm^{-1}
Second Frequency = 20.8932 cm^{-1}

```
Ru  0.19059 -0.84729 -0.35341
C  -1.74906  0.84046  1.54378
C  -2.07317  1.35441  2.81419
C  -0.58348  0.04487  1.35680
C  -1.29336  1.10598  3.93353
H  -2.96312  1.97191  2.91169
C   0.14641 -0.22395  2.54285
C  -0.17830  0.28606  3.79518
H  -1.56400  1.52753  4.89681
H   1.02375 -0.86278  2.47805
H   0.43976  0.04461  4.65617
H  -1.64620 -1.60743  1.54061
C  -2.78101  1.15450  0.50566
C  -5.10368  1.05101 -0.15538
H  -6.12401  0.71672  0.01242
C  -4.09148  0.69662  0.72618
H  -4.30217  0.07959  1.59445
C  -3.46055  2.25616 -1.38694
H  -3.17754  2.89635 -2.22209
C  -4.78461  1.85333 -1.24738
H  -5.53827  2.17511 -1.95915
N  -2.47872  1.93005 -0.54315
C   2.53561  1.90210  0.22386
C   1.57194  2.50894  1.03322
C   3.19145  2.67232 -0.74662
C   1.25704  3.85361  0.85722
H   1.07858  1.93638  1.80875
C   2.87452  4.01606 -0.92010
C   1.90362  4.61073 -0.11603
H   0.51014  4.31183  1.49840
H   3.39801  4.60148 -1.67099
H   1.66460  5.66339 -0.23754
H   3.95671  2.21219 -1.36682
C   3.02259  0.51499  0.45011
C   4.96506 -0.82649  1.01866
H   6.01324 -0.90259  1.29101
C   4.37930  0.40597  0.79011
H   4.95296  1.32074  0.88916
C   2.83477 -1.78589  0.55172
H   2.18937 -2.64853  0.44604
C   4.16406 -1.95430  0.89535
H   4.54993 -2.95430  1.06127
N   2.24506 -0.59009  0.33016
O   0.10369 -2.78273  0.60719
C  -0.81263 -3.26106  1.28845
C  -0.82731 -4.69673  1.69299
O  -1.83166 -2.56496  1.71929
H  -0.64241 -4.76449  2.76968
H  -1.81441 -5.12721  1.50845
H  -0.06096 -5.25121  1.15396
N  -1.60827 -1.24285 -1.09299
C  -2.62371 -1.50672 -1.58121
C  -3.90832 -1.81968 -2.17692
H  -3.77310 -2.39420 -3.09733
H  -4.51112 -2.40632 -1.47810
H  -4.44033 -0.89200 -2.40358
N   1.06135 -1.84462 -2.01861
C   1.53692 -2.37873 -2.92820
C   2.13766 -3.04692 -4.06804
H   1.74870 -2.62535 -4.99872
H   3.22303 -2.91690 -4.04892
H   1.90948 -4.11579 -4.04159
N   0.20857  0.82297 -1.37578
C   0.09956  1.78094 -2.00947
C  -0.06918  3.01533 -2.74630
H  -0.59549  2.83124 -3.68688
H  -0.65135  3.70668 -2.13055
H   0.90422  3.46387 -2.95738
```

$^{6}F^{2+}$ (*single point)

SCF (PBE1PBE) Energy = -890.152369530
Enthalpy 0K = -889.862603
Enthalpy 298K = -889.837463
Free Energy 298K = -889.914009
Lowest Frequency = 74.6860 cm^{-1}
Second Frequency = 74.6901 cm^{-1}

$^{3}A^{2+}$
SCF (PBE1PBE) Energy = -724.220592864
Enthalpy 0K = -723.972960
Enthalpy 298K = -723.952525
Free Energy 298K = -724.025050
Lowest Frequency = 23.3578 cm^{-1}
Second Frequency = 25.4738 cm^{-1}

C	2.16662	1.40270	-0.21259
C	2.16690	0.50134	-1.32675
C	2.16715	-0.88510	-1.10771
C	2.16697	-1.39931	0.22996
C	2.16674	-0.51641	1.32116
C	2.16671	0.89916	1.09765
Ru	0.45535	0.00020	0.00011
H	2.10436	-1.56611	-1.95024
H	2.10373	1.58097	1.93952
H	2.10336	2.47283	-0.38105
H	2.10351	-0.90562	2.33214
H	2.10428	-2.46931	0.39942
H	2.10389	0.88947	-2.33815
N	-0.81279	0.24870	1.59011
C	-1.51387	0.39038	2.49664
C	-2.38462	0.56898	3.63912
H	-3.43009	0.52760	3.32010
H	-2.20202	-0.22288	4.37178
H	-2.19043	1.53972	4.10507
N	-0.81221	-1.50150	-0.57967
N	-0.81259	1.25273	-1.01062
C	-1.51349	1.96679	-1.58703
C	-1.51238	-2.35812	-0.91032
C	-2.38216	-3.43763	-1.32687
H	-2.19577	-4.32254	-0.71094
H	-3.42794	-3.13713	-1.21488
H	-2.19064	-3.68438	-2.37549
C	-2.38414	2.86660	-2.31344
H	-3.42943	2.60073	-2.13126
H	-2.21324	3.89544	-1.98260
H	-2.17834	2.79637	-3.38577

$^{5}F^{+}$ (κ^{1})
SCF (PBE1PBE) Energy = -986.063406307
Enthalpy 0K = -985.771833
Enthalpy 298K = -985.741698
Free Energy 298K = -985.839992
Lowest Frequency = 8.0544 cm^{-1}
Second Frequency = 19.3268 cm^{-1}

N	1.32200	1.44565	0.85500
C	1.84810	2.27560	1.46047
N	1.32499	-1.40696	0.91288
C	1.85340	-2.21022	1.55145
N	1.58033	-0.03221	-1.64156
C	2.30182	-0.05070	-2.54504
N	-0.86016	-1.42404	-0.91451
C	-1.66911	-2.15577	-1.28684
C	2.49630	3.31863	2.23142
H	2.45587	4.26694	1.68903
H	1.98720	3.43717	3.19178
H	3.54240	3.05878	2.41354
C	3.20510	-0.07413	-3.68011
H	4.19617	0.27637	-3.37959
H	3.29331	-1.09216	-4.06909
H	2.82667	0.57554	-4.47395
C	-2.75612	-3.02080	-1.69412
H	-2.57335	-4.04682	-1.36518
H	-3.67469	-2.64993	-1.22908
H	-2.87010	-3.00913	-2.78094
C	2.50458	-3.21916	2.36411
H	3.55898	-2.96760	2.50541
H	2.01825	-3.27488	3.34181
H	2.43528	-4.19562	1.87743
O	-2.92300	0.00791	0.49984
C	-2.23209	0.02875	1.51527
C	-2.85985	0.05529	2.89694
H	-2.52930	0.94352	3.44287
H	-3.94693	0.05630	2.81583
H	-2.53368	-0.81463	3.47416
O	-0.92915	0.03095	1.56809
Ru	0.28848	-0.00138	-0.08384
N	-0.86268	1.38443	-0.97144
C	-1.67307	2.09925	-1.37242
C	-2.76186	2.94533	-1.81335
H	-3.67929	2.59228	-1.33247
H	-2.58031	3.98418	-1.52671
H	-2.87710	2.88921	-2.89865

$^{4}F^{+}$ (κ^{2})
SCF (PBE1PBE) Energy = -853.454432539
Enthalpy 0K = -853.210143
Enthalpy 298K = -853.185109
Free Energy 298K = -853.270675
Lowest Frequency = 17.3498 cm^{-1}
Second Frequency = 18.1497 cm^{-1}

N	2.00348	0.16724	0.00024
C	3.15117	0.29463	0.00003
N	0.01658	-1.32265	1.42331
C	0.02570	-2.07637	2.29991
N	0.01694	-1.32277	-1.42323
C	0.02584	-2.07712	-2.29930
N	-2.00306	0.12175	-0.00032
C	-3.15387	0.21757	-0.00042
C	4.59071	0.46518	-0.00015
H	4.89886	1.02014	-0.89041
H	4.89893	1.02136	0.88933
H	5.08574	-0.50950	0.00050
C	0.03775	-3.00557	-3.41347
H	0.93700	-3.62629	-3.37662
H	-0.84108	-3.65460	-3.37216
H	0.02664	-2.45381	-4.35759
C	-4.59769	0.34749	-0.00061
H	-5.06485	-0.64086	-0.00212
H	-4.92192	0.89265	0.89000
H	-4.92145	0.89513	-0.88988
C	0.03689	-3.00419	3.41462
H	0.92987	-3.63349	3.37169
H	0.03784	-2.45175	4.35842
H	-0.84838	-3.64481	3.38014
O	-0.01551	1.88139	-1.08675
C	-0.02617	2.54683	-0.00014
C	-0.07747	4.03718	-0.00020
H	0.39907	4.43209	0.89814
H	0.39860	4.43200	-0.89882
H	-1.12417	4.35854	0.00008
O	-0.01580	1.88149	1.08654
Ru	0.00102	0.07912	-0.00002

f-**^{3}F** ($\kappa^{2}\kappa^{1}$)
SCF (PBE1PBE) Energy = -949.259776610
Enthalpy 0K = -949.011846
Enthalpy 298K = -948.986205
Free Energy 298K = -949.070867

Lowest Frequency = 21.5146 cm^{-1}
Second Frequency = 31.3245 cm^{-1}

Ru	-0.36187	0.04232	0.00000
N	-1.96261	-1.12108	-0.00001
C	-2.93070	-1.75813	-0.00002
N	0.57364	-1.00314	1.37894
C	1.24814	-1.51114	2.16782
N	0.57365	-1.00313	-1.37894
C	1.24816	-1.51112	-2.16782
C	-4.14936	-2.54562	-0.00004
H	-4.74690	-2.31799	-0.88756
H	-3.91338	-3.61356	-0.00197
H	-4.74512	-2.32081	0.88940
C	2.19432	-2.07456	3.10922
H	2.00689	-1.69470	4.11734
H	2.12731	-3.16567	3.12463
H	3.20226	-1.78236	2.79852
C	2.19429	-2.07454	-3.10927
H	2.00662	-1.69490	-4.11744
H	3.20223	-1.78211	-2.79879
H	2.12746	-3.16566	-3.12447
O	-1.42289	1.52275	-1.09152
C	-1.74238	2.08911	0.00001
O	-1.42289	1.52274	1.09153
C	-2.44517	3.41105	0.00002
H	-3.05539	3.51797	0.89845
H	-1.69071	4.20424	0.00001
H	-3.05541	3.51797	-0.89841
O	1.14830	1.43006	0.00001
C	2.41632	1.16887	0.00002
O	2.95093	0.05922	0.00002
C	3.26099	2.43605	0.00003
H	3.02277	3.04174	0.87944
H	4.32285	2.18560	0.00003
H	3.02277	3.04176	-0.87936

m-**^{3}F** ($\kappa^2\kappa^1$)
SCF (PBE1PBE) Energy = -949.256795661
Enthalpy 0K = -949.009154
Enthalpy 298K = -948.983255
Free Energy 298K = -949.069528
Lowest Frequency = 19.0306 cm^{-1}
Second Frequency = 30.1009 cm^{-1}

Ru	-0.33790	0.12011	-0.08955
N	-1.67618	-1.33210	0.07362
C	-2.45717	-2.16955	0.23436
N	0.70397	-0.89980	-1.39637
C	1.38806	-1.48412	-2.12294
N	1.01230	1.57328	-0.14626
C	1.87698	2.33695	-0.11224
C	-3.43560	-3.21765	0.45197
H	-2.93230	-4.17551	0.60994
H	-4.03677	-2.98871	1.33638
H	-4.09967	-3.30557	-0.41244
C	2.32316	-2.20574	-2.96274
H	1.95680	-3.21558	-3.16697
H	2.46825	-1.68738	-3.91481
H	3.28480	-2.27584	-2.44505
C	3.03030	3.20834	-0.02206
H	2.86112	3.99014	0.72317
H	3.89357	2.60727	0.27924
H	3.23794	3.67801	-0.98716
O	-1.75248	1.33391	-1.17765
C	-2.17153	1.81722	-0.08156
O	-1.65366	1.41068	1.00404
C	-3.23585	2.87469	-0.06756
H	-3.86319	2.76627	0.81917
H	-2.76004	3.85985	-0.02473
H	-3.83829	2.82107	-0.97554
O	0.68406	-0.81659	1.43392
C	1.97172	-0.93654	1.49762
O	2.79998	-0.57409	0.66232
C	2.41783	-1.60422	2.79299
H	1.90699	-2.56295	2.92024
H	3.49826	-1.75575	2.78803
H	2.13905	-0.97755	3.64570

c-**^{2}F** ($2\kappa^2$)
SCF (PBE1PBE) Energy = -816.650758309
Enthalpy 0K = -816.450256
Enthalpy 298K = -816.429565
Free Energy 298K = -816.502605
Lowest Frequency = 24.0897 cm^{-1}
Second Frequency = 24.3216 cm^{-1}

Ru	0.00000	0.08767	-0.00000
N	1.23371	-1.25834	-0.68103
C	1.99141	-2.02037	-1.11636
N	-1.23370	-1.25835	0.68103
C	-1.99141	-2.02035	1.11637
C	2.93233	-2.96342	-1.69067
H	3.65952	-2.43517	-2.31427
H	3.47102	-3.49692	-0.90219
H	2.40674	-3.69394	-2.31262
C	-2.93235	-2.96338	1.69070
H	-3.65887	-2.43523	2.31516
H	-3.47182	-3.49610	0.90223
H	-2.40666	-3.69455	2.31179
O	1.45902	1.61172	-0.27441
C	1.88482	1.41165	0.90558
C	2.94455	2.28729	1.49917
H	3.47126	1.76166	2.29694
H	3.64107	2.61403	0.72492
H	2.46862	3.17688	1.92440
O	1.36223	0.47106	1.58239
O	-1.36223	0.47105	-1.58239
C	-1.88484	1.41162	-0.90558
O	-1.45902	1.61172	0.27440
C	-2.94456	2.28726	-1.49919
H	-3.64104	2.61406	-0.72493
H	-2.46862	3.17682	-1.92448
H	-3.47131	1.76160	-2.29691

t-**^{2}F** ($2\kappa^2$) (* single point)
SCF (PBE1PBE) Energy = -816.645728159
Enthalpy 0K = -816.444756
Enthalpy 298K = -816.426585
Free Energy 298K = -816.488453
Lowest Frequency = 76.6675 cm^{-1}
Second Frequency = 80.4370 cm^{-1}

c-**^{4}F** ($2\kappa^1$)
SCF (PBE1PBE) Energy = -1081.86334470
Enthalpy 0K = -1081.568290
Enthalpy 298K = -1081.537495
Free Energy 298K = -1081.634667
Lowest Frequency = 25.6858 cm^{-1}
Second Frequency = 26.0715 cm^{-1}

N	-1.06191	1.68358	0.09362
C	-1.77510	2.57366	-0.07593
N	1.28402	0.74278	1.51156
C	2.16757	1.15439	2.13216
N	1.06171	-1.68372	0.08886
C	1.77464	-2.57356	-0.08306
C	-2.75288	3.60891	-0.34022

H -2.40301 4.26815 -1.13895
H -3.68362 3.12672 -0.65428
H -2.94104 4.20548 0.55617
C 3.36629 1.64549 2.78105
H 3.26354 2.70310 3.03824
H 3.57758 1.07939 3.69218
H 4.19907 1.52475 2.08085
C 2.75206 -3.60846 -0.35008
H 2.40192 -4.26549 -1.15049
H 3.68300 -3.12585 -0.66290
H 2.94004 -4.20741 0.54477
O -3.20919 -0.16812 -0.63580
C -2.43265 -0.70175 -1.43264
O -1.14795 -0.79790 -1.33936
C -2.96300 -1.33965 -2.71139
H -2.57190 -0.79907 -3.57878
H -2.61074 -2.37188 -2.79351
H -4.05382 -1.31525 -2.72610
O 1.14777 0.80216 -1.33708
C 2.43242 0.70596 -1.43084
O 3.20893 0.16968 -0.63576
C 2.96278 1.34777 -2.70765
H 2.61101 2.38044 -2.78629
H 4.05358 1.32290 -2.72270
H 2.57119 0.81022 -3.57671
Ru -0.00002 -0.00016 0.18415
N -1.28367 -0.74703 1.50967
C -2.16681 -1.16058 2.12957
C -3.36495 -1.65392 2.77785
H -3.57642 -1.08969 3.69009
H -4.19807 -1.53258 2.07818
H -3.26122 -2.71191 3.03308

t-**^{4}F** ($2\kappa^1$)
SCF (PBE1PBE) Energy = -1081.86277701
Enthalpy 0K = -1081.567831
Enthalpy 298K = -1081.536831
Free Energy 298K = -1081.635158
Lowest Frequency = 26.4601 cm^{-1}
Second Frequency = 30.5174 cm^{-1}

N -1.10397 -1.39527 -0.89070
C -1.81990 -2.15605 -1.38030
N -1.10385 1.39594 -0.88977
C -1.81970 2.15708 -1.37893
N 1.10395 1.39526 0.89071
C 1.81991 2.15602 1.38031
C -2.79460 -3.06845 -1.94323
H -2.80666 -2.99101 -3.03370
H -2.55919 -4.09957 -1.66656
H -3.78469 -2.81212 -1.55458
C -2.79428 3.07003 -1.94118
H -2.80632 2.99341 -3.03171
H -3.78442 2.81352 -1.55275
H -2.55875 4.10091 -1.66373
C 2.79469 3.06837 1.94320
H 2.80659 2.99113 3.03369
H 3.78478 2.81180 1.55471
H 2.55948 4.09947 1.66629
O -3.22521 -0.00000 0.59406
C -2.53054 -0.00048 1.61161
O -1.24010 -0.00064 1.68133
C -3.18394 -0.00098 2.98990
H -2.86220 -0.88058 3.55568
H -2.86225 0.87824 3.55628
H -4.27098 -0.00098 2.89586
O 1.24009 0.00063 -1.68130
C 2.53053 0.00053 -1.61160
O 3.22522 0.00009 -0.59405
C 3.18391 0.00107 -2.98990
H 2.86245 0.88089 -3.55549
H 4.27095 0.00072 -2.89587
H 2.86193 -0.87792 -3.55647
Ru -0.00001 -0.00000 0.00001
N 1.10385 -1.39595 0.88978
C 1.81973 -2.15709 1.37891
C 2.79427 -3.07009 1.94114
H 2.80650 -2.99332 3.03166
H 2.55858 -4.10097 1.66385
H 3.78437 -2.81375 1.55250

^{1}A
SCF (PBE1PBE) Energy = -916.007063194
Enthalpy 0K = -915.751446
Enthalpy 298K = -915.730036
Free Energy 298K = -915.803251
Lowest Frequency = 17.4093 cm^{-1}
Second Frequency = 42.3731 cm^{-1}

Ru 0.25092 0.03873 -0.09927
O 1.39013 0.84658 1.50974
C 1.82318 1.75865 0.73827
C 2.68418 2.86564 1.25781
C -1.00423 -1.84188 0.16349
C -0.58655 -1.34705 1.42992
C -1.54759 -0.70121 2.26962
C -2.84237 -0.54713 1.85606
O 1.47294 1.72196 -0.48323
H 2.04094 3.69881 1.55910
H 3.24694 2.53208 2.13102
H 3.35695 3.22051 0.47525
C -3.26597 -1.06423 0.60260
C -2.37767 -1.71027 -0.21300
H -2.70587 -2.14534 -1.15222
H -3.56181 -0.04696 2.49821
H -0.40256 -2.57720 -0.36282
H -1.23221 -0.34290 3.24489
C -1.56431 1.08280 -1.40033
O -1.37798 1.38858 -0.18370
O -0.83497 0.16412 -1.89901
C -2.57544 1.80113 -2.23530
H -2.83959 1.20719 -3.11107
H -3.46187 2.02183 -1.63754
H -2.14795 2.75175 -2.57004
H 0.33530 -1.70252 1.88299
H -4.30754 -0.96752 0.30828
N 1.73988 -1.16947 -0.46332
C 2.64550 -1.85034 -0.71050
C 3.78172 -2.68495 -1.05357
H 4.49448 -2.11611 -1.65775
H 4.28824 -3.03304 -0.14893
H 3.45328 -3.55519 -1.62896

^{1}A$^+$
SCF (PBE1PBE) Energy = -687.560237308
Enthalpy 0K = -687.355771
Enthalpy 298K = -687.339750
Free Energy 298K = -687.401571
Lowest Frequency = 16.1291 cm^{-1}
Second Frequency = 20.0299 cm^{-1}

C 1.96698 -0.43900 1.42060
C 2.28196 0.75471 0.69522
C 2.27935 0.74518 -0.71203
C 1.96267 -0.45796 -1.42083
C 1.67580 -1.63629 -0.70647
C 1.67823 -1.62714 0.72339
Ru 0.35899 -0.01410 0.00000

O -0.79700 1.36974 -1.07893
C -1.25493 1.87090 -0.00011
C -2.27691 2.94973 -0.00016
H 2.41901 1.67101 -1.25970
H 1.36841 -2.51069 1.27059
O -0.79672 1.37012 1.07874
H -3.27440 2.49792 -0.00006
H -2.17933 3.56119 0.89804
H -2.17943 3.56101 -0.89850
H 1.88077 -0.40840 2.50139
H 1.36358 -2.52685 -1.24086
H 1.87386 -0.44201 -2.50169
H 2.42417 1.68758 1.23008
N -1.34642 -1.14607 0.00035
C -2.33741 -1.73768 0.00028
C -3.57978 -2.48148 0.00008
H -4.14611 -2.25378 0.90742
H -4.17516 -2.20462 -0.87440
H -3.37225 -3.55442 -0.03303

$^1B^+$ (t-O,t-N)
SCF (PBE1PBE) Energy = -1166.36074779
Enthalpy 0K = -1165.983792
Enthalpy 298K = -1165.957420
Free Energy 298K = -1166.041172
Lowest Frequency = 25.5551 cm^{-1}
Second Frequency = 28.0283 cm^{-1}

Ru 0.39104 -0.31483 -0.30649
O 1.46409 -2.10309 -0.79255
C 1.36847 -1.82076 -2.02572
C 1.92629 -2.69827 -3.09198
C 0.55503 -1.04828 1.92525
C 1.89523 -1.24240 2.35911
C 2.62158 -0.18605 2.85238
C 2.04904 1.10602 2.93007
O 0.73813 -0.74430 -2.32332
H 2.38662 -2.09120 -3.87422
H 2.64846 -3.39718 -2.66964
H 1.11078 -3.26503 -3.55288
C -2.63205 -0.06951 -0.00466
C -3.81469 -0.21635 0.72493
C -1.84589 -1.21014 -0.24873
C -4.20424 -1.47206 1.18304
H -4.41887 0.65285 0.96678
C -2.23942 -2.46771 0.20736
C -3.42100 -2.59777 0.93072
H -5.12431 -1.57077 1.75075
H -1.62945 -3.33723 -0.01916
H -3.73596 -3.57220 1.29007
H -1.09737 -1.19202 -1.08211
C 0.75634 1.31674 2.51508
C -0.01757 0.23933 2.00277
H -1.09379 0.35853 1.93957
H 2.62277 1.92291 3.35905
H -0.07637 -1.91991 1.78506
H 3.63198 -0.34720 3.21791
C -2.13878 1.24066 -0.45298
C -2.45464 3.51863 -1.16665
H -3.10613 4.35241 -1.40756
C -2.98686 2.30769 -0.74992
H -4.05981 2.16975 -0.67623
C -0.28244 2.53905 -0.98226
H 0.79625 2.57971 -1.06969
C -1.07330 3.63544 -1.28428
H -0.60746 4.55737 -1.61395
N -0.79117 1.36596 -0.57163
H 2.31960 -2.24074 2.32954
H 0.29579 2.29425 2.62592
N 2.11989 0.60187 -0.26876
C 3.17702 1.06770 -0.30190
C 4.50592 1.64553 -0.32440
H 5.23718 0.90194 0.00477
H 4.76021 1.96751 -1.33794
H 4.55098 2.50808 0.34606

TS(**$^1B^+$–$^1C^+$**) (t-O,t-N)
SCF (PBE1PBE) Energy = -1166.32186597
Enthalpy 0K = -1165.950398
Enthalpy 298K = -1165.924475
Free Energy 298K = -1166.006272
Lowest Frequency = -1051.6454 cm^{-1}
Second Frequency = 26.8299 cm^{-1}

Ru 0.31193 -0.31890 -0.13686
O 1.00944 -2.37287 -0.40302
C 0.49657 -2.51692 -1.52412
C 0.75152 -3.66580 -2.42739
C 0.78173 -0.63216 2.06556
C 2.15011 -0.94520 2.32430
C 3.07847 0.05635 2.43915
C 2.69644 1.41705 2.30149
O -0.32551 -1.56628 -1.94917
H 1.15902 -3.29959 -3.37449
H 1.44490 -4.36725 -1.96518
H -0.19568 -4.16219 -2.65849
C -2.57482 0.22782 0.13319
C -3.89944 0.11876 0.56070
C -1.67831 -0.86449 0.26031
C -4.35622 -1.07842 1.10364
H -4.58043 0.96205 0.49228
C -2.17100 -2.05763 0.81034
C -3.49616 -2.16741 1.22829
H -5.38689 -1.15940 1.43471
H -1.50885 -2.91588 0.90893
H -3.85822 -3.09904 1.65304
H -1.02991 -1.27808 -1.02263
C 1.39129 1.74625 2.04851
C 0.40086 0.72391 1.91219
H -0.64372 0.99983 2.02284
H 3.43851 2.19812 2.44137
H 0.02733 -1.38473 2.27310
H 4.11077 -0.18667 2.67533
C -2.00129 1.45749 -0.41768
C -2.08187 3.70013 -1.29831
H -2.64735 4.57736 -1.59607
C -2.73329 2.58477 -0.79564
H -3.81321 2.57583 -0.70437
C -0.01783 2.52862 -1.03426
H 1.06039 2.45370 -1.10453
C -0.69490 3.67392 -1.41783
H -0.14096 4.52236 -1.80353
N -0.64636 1.44394 -0.55289
H 2.43374 -1.98211 2.47437
H 1.08388 2.78730 2.00703
N 2.22137 0.27353 -0.68995
C 3.29269 0.50836 -1.05821
C 4.64116 0.79666 -1.50635
H 5.03526 1.66627 -0.97347
H 5.28843 -0.06219 -1.30828
H 4.64713 1.00434 -2.57985

$^1C^+$ (t-O,t-N)
SCF (PBE1PBE) Energy = -1166.33525988
Enthalpy 0K = -1165.958488
Enthalpy 298K = -1165.931789
Free Energy 298K = -1166.016940
Lowest Frequency = 13.6482 cm^{-1}

Second Frequency = 33.4685 cm^{-1}

Ru	-0.28427	0.15444	-0.14613
O	-1.28885	2.05879	-0.39779
C	-0.88987	2.98682	-1.11183
C	-1.76146	4.13337	-1.49039
C	-0.89101	0.56019	1.94911
C	-2.30952	0.66677	2.13674
C	-3.07463	-0.45534	2.27759
C	-2.47638	-1.74976	2.25184
O	0.32746	3.04999	-1.60414
H	-1.76033	4.25209	-2.57738
H	-2.77427	3.97514	-1.12475
H	-1.34947	5.05483	-1.06808
C	2.60435	-0.05280	-0.00323
C	3.94765	0.28719	0.17856
C	1.55540	0.86306	0.28799
C	4.28721	1.54046	0.67581
H	4.73886	-0.42068	-0.05247
C	1.93982	2.10616	0.81979
C	3.28210	2.44533	1.00554
H	5.33027	1.80384	0.81844
H	1.18130	2.83497	1.10403
H	3.54160	3.41813	1.41396
H	0.89388	2.37025	-1.17479
C	-1.12904	-1.88836	2.07956
C	-0.29533	-0.73070	1.91148
H	0.76678	-0.83178	2.11666
H	-3.09721	-2.62570	2.41837
H	-0.27472	1.42458	2.17753
H	-4.14275	-0.36691	2.45476
C	2.16411	-1.37547	-0.44487
C	2.44709	-3.65553	-1.17727
H	3.09242	-4.48009	-1.46378
C	2.99558	-2.43559	-0.81351
H	4.07049	-2.29800	-0.81439
C	0.28205	-2.72675	-0.80313
H	-0.79965	-2.78258	-0.77336
C	1.06235	-3.81012	-1.16759
H	0.59203	-4.74890	-1.43714
N	0.81074	-1.53929	-0.46178
H	-2.75606	1.65332	2.20775
H	-0.66328	-2.86799	2.13391
N	-2.14199	-0.62661	-0.86648
C	-3.14441	-0.94744	-1.34864
C	-4.40755	-1.34773	-1.93811
H	-5.13793	-0.54040	-1.83699
H	-4.27357	-1.57355	-2.99954
H	-4.79191	-2.23760	-1.43219

$^1B^+$ (t-O,t-C6H6)
SCF (PBE1PBE) Energy = -1166.35216908
Enthalpy 0K = -1165.975289
Enthalpy 298K = -1165.948921
Free Energy 298K = -1166.032274
Lowest Frequency = 33.3282 cm^{-1}
Second Frequency = 33.9038 cm^{-1}

Ru	0.43522	0.01153	-0.15209
O	1.82137	-1.54517	-0.51651
C	2.01154	-1.13719	-1.70359
C	2.95632	-1.82207	-2.63053
C	1.77701	1.31323	1.29742
C	2.53120	0.50672	2.19572
C	3.74137	-0.01730	1.81489
C	4.26788	0.26606	0.53534
O	1.36502	-0.09380	-2.06549
H	3.96334	-1.42686	-2.46102
H	2.97786	-2.89377	-2.42622
H	2.68124	-1.62928	-3.66824
C	-2.49507	-0.41665	-0.52891
C	-3.66632	-1.03743	-0.09253
C	-1.40661	-1.22142	-0.91398
C	-3.74281	-2.42806	-0.04950
H	-4.50978	-0.44267	0.24524
C	-1.48073	-2.61410	-0.85702
C	-2.65466	-3.21879	-0.42159
H	-4.66046	-2.90034	0.28866
H	-0.62588	-3.20982	-1.16027
H	-2.72867	-4.30076	-0.37832
H	-0.61982	-0.77075	-1.56760
C	3.56330	1.04617	-0.35033
C	2.29666	1.56690	0.01199
H	1.85424	2.30816	-0.64456
H	5.24655	-0.11876	0.26373
H	0.96501	1.91484	1.69596
H	4.31404	-0.62548	2.50809
C	-2.31649	1.04201	-0.51388
C	-3.15400	3.29542	-0.66052
H	-3.97142	3.99387	-0.80760
C	-3.37942	1.92769	-0.69234
H	-4.37200	1.53332	-0.87980
C	-0.84327	2.81734	-0.28226
H	0.17425	3.14645	-0.11185
C	-1.85680	3.74793	-0.44592
H	-1.62121	4.80573	-0.41040
N	-1.04664	1.49013	-0.31810
H	2.15290	0.33671	3.19884
H	3.97498	1.29428	-1.32335
N	-0.32765	-0.46178	1.62667
C	-0.77970	-0.83196	2.62485
C	-1.33345	-1.32519	3.87122
H	-0.71881	-2.14542	4.25286
H	-1.36314	-0.52642	4.61718
H	-2.34968	-1.69306	3.70565

TS(**$^1B^+$-$^1C^+$**) (t-O,t-C6H6)
SCF (PBE1PBE) Energy = -1166.32433074
Enthalpy 0K = -1165.952882
Enthalpy 298K = -1165.926782
Free Energy 298K = -1166.009629
Lowest Frequency = -1178.8908 cm^{-1}
Second Frequency = 18.9449 cm^{-1}

Ru	-0.34843	-0.01512	0.05354
O	-1.75995	1.60643	0.19156
C	-1.69430	1.92472	-1.01030
C	-2.57589	2.92918	-1.65623
C	-2.11227	-1.73186	0.52004
C	-3.10429	-1.17873	1.35831
C	-4.15903	-0.46867	0.81843
C	-4.25634	-0.30106	-0.57205
O	-0.78089	1.32294	-1.74978
H	-3.12826	2.45374	-2.47179
H	-3.26946	3.35008	-0.92924
H	-1.96362	3.71861	-2.10204
C	2.48000	0.64325	-0.38034
C	3.69548	1.32129	-0.27735
C	1.26884	1.28952	-0.02786
C	3.72211	2.63758	0.17469
H	4.63178	0.82991	-0.52412
C	1.32612	2.60797	0.44953
C	2.54232	3.28008	0.54485
H	4.67108	3.15958	0.24937
H	0.40757	3.11200	0.73888
H	2.57177	4.30267	0.90920
H	0.26468	1.32872	-1.05236
C	-3.28667	-0.82323	-1.40860
C	-2.19826	-1.53670	-0.86940

H -1.53014 -2.05168 -1.55250
H -5.10808 0.22705 -0.99120
H -1.40077 -2.43484 0.94299
H -4.92645 -0.05845 1.46728
C 2.36961 -0.76776 -0.75252
C 3.23941 -2.88351 -1.51661
H 4.05379 -3.48357 -1.90971
C 3.42260 -1.53561 -1.25419
H 4.38229 -1.06812 -1.44099
C 0.98297 -2.63621 -0.77899
H 0.00362 -3.04875 -0.56933
C 1.99491 -3.45024 -1.25960
H 1.80039 -4.50300 -1.43080
N 1.14185 -1.32273 -0.54745
H -3.04992 -1.34380 2.43004
H -3.37089 -0.71698 -2.48593
N 0.10901 -0.40946 1.90527
C 0.41692 -0.57315 3.00868
C 0.79161 -0.75203 4.39836
H 0.79160 -1.81370 4.65978
H 1.79237 -0.34566 4.56897
H 0.08348 -0.22717 5.04582

$^1C^+$ (t-O,t-C6H6)
SCF (PBE1PBE) Energy = -1166.36378221
Enthalpy 0K = -1165.986536
Enthalpy 298K = -1165.959860
Free Energy 298K = -1166.044786
Lowest Frequency = 20.0576 cm^{-1}
Second Frequency = 28.1597 cm^{-1}

Ru -0.28975 -0.37428 0.28703
O -2.31423 0.27746 0.54412
C -2.74399 1.40845 0.78466
C -4.15419 1.65849 1.19305
C -1.72349 -3.01042 0.04692
C -3.03233 -2.69288 -0.26107
C -3.32313 -1.81419 -1.32141
C -2.29932 -1.23542 -2.04257
O -2.00829 2.49617 0.68929
H -4.67571 0.71388 1.33512
H -4.17598 2.24878 2.11293
H -4.65516 2.24982 0.42052
C 1.89880 0.88997 -1.12181
C 2.57185 1.77369 -1.97318
C 0.48961 0.93561 -0.98795
C 1.86007 2.70525 -2.71659
H 3.65339 1.73047 -2.06955
C -0.20910 1.85365 -1.78416
C 0.46948 2.73286 -2.63025
H 2.38216 3.39131 -3.37540
H -1.29653 1.87277 -1.77930
H -0.09639 3.43764 -3.23350
H -1.12475 2.25487 0.34666
C -0.94910 -1.51678 -1.72616
C -0.65810 -2.43581 -0.69358
H 0.33259 -2.87404 -0.62699
H -2.52025 -0.58131 -2.88109
H -1.50679 -3.74653 0.81588
H -4.35701 -1.60922 -1.58194
C 2.54781 -0.17294 -0.36714
C 4.39528 -1.48946 0.44685
H 5.46045 -1.69269 0.49647
C 3.92125 -0.42765 -0.30578
H 4.60938 0.21040 -0.84841
C 2.14041 -1.98999 1.04376
H 1.39125 -2.57571 1.56887
C 3.48812 -2.28960 1.14076
H 3.81349 -3.12896 1.74472
N 1.67532 -0.96818 0.30710
H -3.84421 -3.15262 0.29478
H -0.16816 -1.20136 -2.41026
N 0.21621 0.78080 1.81193
C 0.56837 1.40723 2.72169
C 0.99805 2.18848 3.86441
H 0.40221 3.10260 3.93923
H 0.87490 1.60862 4.78367
H 2.05137 2.46105 3.75511

$^1B^+$ (t-O,t-O)
SCF (PBE1PBE) Energy = -1166.35750361
Enthalpy 0K = -1165.980583
Enthalpy 298K = -1165.954069
Free Energy 298K = -1166.038766
Lowest Frequency = 25.3136 cm^{-1}
Second Frequency = 27.3551 cm^{-1}

Ru -0.46834 0.25045 0.19771
O -2.12002 1.16829 -0.63057
C -2.90705 0.63782 0.23422
C -4.36911 0.92131 0.21690
C -0.92156 -1.22150 -1.80707
C -0.37527 -2.03030 -0.79787
C -1.21267 -2.91320 -0.07662
C -2.55405 -2.99350 -0.37878
O -2.37309 -0.13852 1.07779
H -4.74951 0.98652 1.23795
H -4.57782 1.83952 -0.33317
H -4.88173 0.09080 -0.27847
C 2.51943 -0.61975 0.29446
C 3.56042 -1.54920 0.19923
C 1.52271 -0.83537 1.26176
C 3.61128 -2.64515 1.05582
H 4.31827 -1.44128 -0.57057
C 1.57066 -1.93278 2.11702
C 2.62012 -2.84186 2.01537
H 4.42566 -3.35703 0.96388
H 0.79404 -2.06368 2.86424
H 2.66695 -3.69801 2.68090
H 0.80317 -0.03331 1.56388
C -3.09417 -2.20462 -1.41299
C -2.29589 -1.32694 -2.11642
H -2.70892 -0.73161 -2.92409
H -3.19451 -3.68272 0.16278
H -0.27122 -0.65813 -2.46907
H -0.78065 -3.54861 0.69019
C 2.39187 0.49433 -0.65823
C 3.27592 2.07675 -2.24548
H 4.11688 2.51755 -2.77129
C 3.48007 1.05359 -1.33163
H 4.48107 0.69493 -1.12020
C 0.94069 1.95134 -1.76069
H -0.09111 2.26768 -1.88279
C 1.97913 2.53163 -2.46994
H 1.76956 3.32717 -3.17621
N 1.13722 0.95716 -0.87790
H 0.69930 -2.13994 -0.71451
H -4.14482 -2.30687 -1.67044
N -0.37789 1.85859 1.33889
C -0.38415 2.80639 2.00158
C -0.39732 3.98908 2.83919
H -0.93505 4.79654 2.33462
H -0.89531 3.76799 3.78738
H 0.62609 4.31601 3.04219

$^1B^+$ (t-C6H6,t-O)
SCF (PBE1PBE) Energy = -1166.36191943
Enthalpy 0K = -1165.984679

Enthalpy 298K = -1165.958095
Free Energy 298K = -1166.043075
Lowest Frequency = 14.4552 cm^{-1}
Second Frequency = 29.1331 cm^{-1}

Ru	-0.30239	-0.16181	0.19261
O	-1.28405	-1.89352	0.73504
C	-1.75124	-2.04033	-0.45113
C	-2.64146	-3.18114	-0.79764
C	-2.25392	0.81131	1.31982
C	-1.84868	1.70803	0.31264
C	-2.64809	1.84517	-0.84961
C	-3.79378	1.09882	-1.00161
O	-1.41596	-1.15445	-1.29434
H	-2.41754	-3.53824	-1.80473
H	-2.53878	-3.98611	-0.06890
H	-3.67859	-2.83155	-0.78891
C	1.92968	0.89225	-0.91969
C	2.66502	1.94414	-0.34642
C	0.81998	1.18061	-1.74297
C	2.29238	3.25796	-0.57451
H	3.52647	1.71550	0.27460
C	0.47844	2.52178	-1.98460
C	1.19436	3.54976	-1.39459
H	2.86482	4.06675	-0.13025
H	-0.33116	2.74475	-2.67175
H	0.92691	4.58330	-1.59198
H	0.34842	0.39265	-2.32412
C	-4.19652	0.20265	0.00937
C	-3.44665	0.06581	1.15599
H	-3.77309	-0.59228	1.95474
H	-4.40703	1.21912	-1.88939
H	-1.78756	0.83524	2.29842
H	-2.37047	2.57254	-1.60490
C	2.33636	-0.51716	-0.72790
C	3.82097	-2.39173	-0.76287
H	4.79455	-2.82735	-0.96427
C	3.59912	-1.03537	-0.98357
H	4.37904	-0.38604	-1.36690
C	1.54570	-2.59514	-0.03559
H	0.70602	-3.14843	0.36955
C	2.77906	-3.18127	-0.28639
H	2.91439	-4.24096	-0.10060
N	1.33907	-1.29039	-0.25628
H	-1.07150	2.44178	0.51191
H	-5.12279	-0.35353	-0.10504
N	0.61328	0.42355	1.85721
C	1.12476	0.71169	2.85556
C	1.75097	1.06086	4.11650
H	1.45382	0.34811	4.89106
H	2.83956	1.03922	4.01640
H	1.44450	2.06468	4.42339

TS(^{1}**B**$^+$-^{1}**C**$^+$)1 (t-C6H6,t-O)
SCF (PBE1PBE) Energy = -1166.33033028
Enthalpy 0K = -1165.954147
Enthalpy 298K = -1165.927914
Free Energy 298K = -1166.013100
Lowest Frequency = -71.6655 cm^{-1}
Second Frequency = 12.6476 cm^{-1}

C	2.90042	-0.15729	-0.27127
N	1.73054	0.47644	-0.09545
C	1.69092	1.82645	-0.04835
C	2.86067	2.57719	-0.14018
C	4.07626	1.92569	-0.30163
C	4.09548	0.53560	-0.37936
Ru	-0.03424	-0.49735	0.21943
C	-2.83272	-1.63376	-0.88202
C	-1.95410	-1.96095	0.17505
C	-2.07286	-1.27617	1.40168
C	-3.08096	-0.30159	1.57072
C	-3.95595	-0.02975	0.53722
C	-3.82441	-0.68868	-0.69710
H	-1.54146	-1.63197	2.27847
C	0.34302	2.40514	0.05306
C	0.09566	3.59503	0.74309
C	-1.18509	4.13665	0.75843
C	-2.22688	3.50537	0.07888
C	-1.99258	2.31523	-0.60115
C	-0.72030	1.74158	-0.59850
H	-4.51986	-0.47130	-1.50246
O	0.63984	-1.87578	-1.06904
C	0.37532	-1.58008	-2.31813
O	-0.22395	-0.56193	-2.65463
C	0.83734	-2.61836	-3.30492
H	0.04209	-3.35875	-3.44026
H	1.02742	-2.14478	-4.26875
H	1.72659	-3.14191	-2.95011
H	0.90211	4.09279	1.27368
H	-1.36975	5.06228	1.29495
H	-2.78816	1.83292	-1.15721
H	-3.21696	3.95069	0.07172
H	2.80277	3.65975	-0.11681
H	-0.51836	0.92126	-1.32895
H	-2.75323	-2.16239	-1.82621
H	-4.75630	0.69042	0.68044
H	-1.32730	-2.84289	0.09065
H	-3.19516	0.18913	2.53237
H	5.02061	-0.01000	-0.52778
H	4.99595	2.49610	-0.38481
H	2.84120	-1.23791	-0.33439
N	0.79934	-1.61437	1.56934
C	1.33470	-2.28338	2.34792
C	2.00027	-3.12158	3.32602
H	1.27818	-3.47907	4.06545
H	2.45402	-3.98445	2.83040
H	2.78069	-2.55355	3.84001

INT(^{1}**B**$^+$-^{1}**C**$^+$) (t-C6H6,t-O)
SCF (PBE1PBE) Energy = -1166.35673734
Enthalpy 0K = -1165.979847
Enthalpy 298K = -1165.953456
Free Energy 298K = -1166.037100
Lowest Frequency = 28.7446 cm^{-1}
Second Frequency = 29.2028 cm^{-1}

C	0.59278	-2.79009	0.03489
N	-0.11909	-1.66261	0.19988
C	-1.42568	-1.75853	0.55942
C	-2.02035	-3.00671	0.75526
C	-1.28303	-4.16581	0.57186
C	0.05372	-4.05416	0.20268
Ru	0.75963	0.21092	0.10817
C	-0.47791	2.46570	-1.89210
C	0.43668	1.38356	-1.93581
C	-0.04163	0.07949	-2.18823
C	-1.42838	-0.11908	-2.41120
C	-2.29708	0.94649	-2.37511
C	-1.81818	2.24721	-2.11063
H	0.64516	-0.71355	-2.46750
C	-2.15382	-0.49668	0.74713
C	-3.54383	-0.40885	0.62887
C	-4.18657	0.81305	0.79675
C	-3.45746	1.97081	1.06641
C	-2.07310	1.90154	1.17799
C	-1.42879	0.67604	1.01845
H	-2.51256	3.08209	-2.10496
O	1.70516	0.20560	1.97275

```
C   2.10910  1.41284  1.81656
O   1.77350  1.99097  0.73843
C   2.90468  2.09406  2.87538
H   2.23324  2.40639  3.68186
H   3.63186  1.40111  3.30335
H   3.40156  2.97535  2.46923
H  -4.12907 -1.28815  0.37831
H  -5.26776  0.86335  0.70999
H  -1.49018  2.78691  1.41110
H  -3.96904  2.91867  1.20070
H  -3.05414 -3.05749  1.07719
H  -0.41880  0.59906  1.49699
H  -0.09944  3.46937 -1.72593
H  -3.35368  0.79385 -2.57233
H   1.49550  1.61051 -2.01202
H  -1.78916 -1.11295 -2.65978
H   0.67886 -4.92787  0.05637
H  -1.73839 -5.13842  0.72801
H   1.63268 -2.65520 -0.23642
N   2.46780 -0.34975 -0.69106
C   3.51749 -0.59583 -1.11211
C   4.83519 -0.90205 -1.63358
H   4.75009 -1.46990 -2.56414
H   5.37918  0.02550 -1.83314
H   5.39713 -1.49283 -0.90477
```

TS(**^{1}B$^+$**-**^{1}C$^+$**)2 (t-C6H6,t-O)
SCF (PBE1PBE) Energy = -1166.32241687
Enthalpy 0K = -1165.950784
Enthalpy 298K = -1165.924429
Free Energy 298K = -1166.009205
Lowest Frequency = -613.9506 cm^{-1}
Second Frequency = 18.5132 cm^{-1}

```
C   0.59285 -2.79012  0.03441
N  -0.11906 -1.66269  0.19958
C  -1.42563 -1.75872  0.55919
C  -2.02023 -3.00694  0.75495
C  -1.28286 -4.16599  0.57138
C   0.05386 -4.05423  0.20210
Ru  0.75957  0.21090  0.10820
C  -0.47761  2.46612 -1.89178
C   0.43683  1.38385 -1.93560
C  -0.04166  0.07987 -2.18817
C  -1.42845 -0.11848 -2.41115
C  -2.29699  0.94721 -2.37495
C  -1.81790  2.24784 -2.11034
H   0.64503 -0.71321 -2.46757
C  -2.15381 -0.49691  0.74705
C  -3.54381 -0.40911  0.62876
C  -4.18658  0.81276  0.79671
C  -3.45750  1.97052  1.06645
C  -2.07314  1.90127  1.17807
C  -1.42880  0.67579  1.01849
H  -2.51217  3.08282 -2.10460
O   1.70499  0.20524  1.97283
C   2.10895  1.41250  1.81688
O   1.77343  1.99084  0.73884
C   2.90443  2.09353  2.87591
H   2.23276  2.40652  3.68196
H   3.63099  1.40029  3.30443
H   3.40199  2.97445  2.46978
H  -4.12902 -1.28842  0.37812
H  -5.26777  0.86305  0.70992
H  -1.49024  2.78663  1.41128
H  -3.96910  2.91836  1.20078
H  -3.05399 -3.05780  1.07693
H  -0.41884  0.59880  1.49706
H  -0.09900  3.46972 -1.72550
H  -3.35361  0.79475 -2.57219
H   1.49567  1.61067 -2.01182
H  -1.78936 -1.11226 -2.65985
H   0.67902 -4.92789  0.05564
H  -1.73816 -5.13864  0.72746
H   1.63271 -2.65516 -0.23697
N   2.46777 -0.34959 -0.69111
C   3.51745 -0.59558 -1.11221
C   4.83516 -0.90167 -1.63375
H   4.75009 -1.47035 -2.56380
H   5.37871  0.02594 -1.83422
H   5.39752 -1.49160 -0.90457
```

^{1}C$^+$ (t-C6H6,t-O)
SCF (PBE1PBE) Energy = -1166.34557397
Enthalpy 0K = -1165.969282
Enthalpy 298K = -1165.942413
Free Energy 298K = -1166.028603
Lowest Frequency = 17.3483 cm^{-1}
Second Frequency = 22.1878 cm^{-1}

```
C  -1.20686 -0.71112  2.26599
N  -0.26322 -0.53056  1.32699
C   1.01652 -0.94184  1.55587
C   1.34319 -1.53442  2.77935
C   0.37249 -1.71231  3.75055
C  -0.93256 -1.29733  3.48855
Ru -0.64592  0.32091 -0.44414
C   0.77916  3.04778 -1.29822
C  -0.38467  2.61848 -0.61435
C  -0.31430  2.31754  0.76840
C   0.93057  2.44786  1.43436
C   2.05556  2.84410  0.74493
C   1.97965  3.14768 -0.62830
H  -1.22029  2.25108  1.36301
C   1.91960 -0.71957  0.43594
C   3.27025 -1.08309  0.43102
C   4.03850 -0.86943 -0.70669
C   3.45314 -0.29994 -1.83686
C   2.10781  0.07542 -1.82562
C   1.30146 -0.10953 -0.68881
H   2.86823  3.48396 -1.15359
O  -1.38122 -1.52760 -1.12698
C  -0.84135 -2.52088 -1.64282
O   0.43461 -2.62077 -1.88338
C  -1.64338 -3.71034 -2.04685
H  -1.25867 -4.59793 -1.53689
H  -2.69345 -3.56042 -1.80362
H  -1.52431 -3.88026 -3.12074
H   3.72896 -1.54058  1.30362
H   5.08512 -1.15621 -0.71828
H   1.68408  0.53022 -2.71928
H   4.04836 -0.14374 -2.73256
H   2.36317 -1.85533  2.95728
H   0.90060 -1.79445 -1.60060
H   0.70908  3.32783 -2.34521
H   3.00183  2.95153  1.26613
H  -1.35494  2.77974 -1.08308
H   0.98024  2.27267  2.50512
H  -1.72770 -1.42348  4.21451
H   0.62576 -2.17249  4.70043
H  -2.20096 -0.36888  2.00397
N  -2.75333  0.73989 -0.22964
C  -3.89394  0.94282 -0.23882
C  -5.32285  1.19081 -0.25605
H  -5.56450  2.04449  0.38281
H  -5.65029  1.40780 -1.27661
H  -5.85928  0.31021  0.10762
```

^{1}B$^+$ (t-N,t-O)
SCF (PBE1PBE) Energy = -1166.36111494

Enthalpy 0K = -1165.983953
Enthalpy 298K = -1165.957420
Free Energy 298K = -1166.042056
Lowest Frequency = 21.3440 cm^{-1}
Second Frequency = 23.5493 cm^{-1}

Ru	-0.62030	-0.25093	-0.02920
O	-1.13539	-2.25860	-0.00870
C	-1.42485	-2.23619	-1.25382
C	-1.95030	-3.43848	-1.95496
C	-0.52044	-0.54601	2.26582
C	0.33730	-1.61133	2.66291
C	1.68079	-1.39494	2.83372
C	2.22377	-0.09947	2.65348
O	-1.25812	-1.12364	-1.84590
H	-1.60459	-3.44990	-2.99008
H	-1.64634	-4.34745	-1.43412
H	-3.04444	-3.39590	-1.96504
C	1.16728	1.66999	-0.94098
C	1.63914	2.83116	-0.31296
C	-0.12193	1.67226	-1.52235
C	0.82419	3.94820	-0.20305
H	2.64182	2.84270	0.10404
C	-0.93784	2.81010	-1.38648
C	-0.47933	3.93013	-0.71225
H	1.20016	4.84159	0.28679
H	-1.91570	2.81558	-1.85849
H	-1.11037	4.80820	-0.61616
H	-0.39611	0.90930	-2.24471
C	1.41362	0.94337	2.28258
C	0.02374	0.74043	2.04108
H	-0.62605	1.61027	1.98265
H	3.27678	0.07363	2.85524
H	-1.58873	-0.67726	2.40187
H	2.32652	-2.20636	3.15719
C	1.98683	0.43886	-0.97850
C	3.97226	-0.84874	-1.34383
H	5.00960	-0.92384	-1.65452
C	3.31968	0.38004	-1.36666
H	3.82235	1.28148	-1.70076
C	1.95061	-1.84478	-0.53431
H	1.36194	-2.68328	-0.17864
C	3.27605	-1.97787	-0.92548
H	3.74879	-2.95332	-0.89581
N	1.32512	-0.66158	-0.55870
H	-0.09663	-2.58638	2.85999
H	1.81509	1.94847	2.21593
N	-2.54060	0.25696	0.33068
C	-3.65616	0.51060	0.50216
C	-5.05427	0.83448	0.71058
H	-5.14407	1.78116	1.25028
H	-5.56370	0.92481	-0.25278
H	-5.53782	0.04666	1.29460

TS(^{1}**B**$^+$–^{1}**C**$^+$) (t-N,t-O)
SCF (PBE1PBE) Energy = -1166.33052596
Enthalpy 0K = -1165.954992
Enthalpy 298K = -1165.928942
Free Energy 298K = -1166.012635
Lowest Frequency = -94.6243 cm^{-1}
Second Frequency = 24.6145 cm^{-1}

C	-1.94954	-1.84612	0.53363
N	-1.32470	-0.66259	0.55845
C	-1.98705	0.43733	0.97861
C	-3.31989	0.37763	1.36667
C	-3.97179	-0.85150	1.34337
C	-3.27492	-1.98010	0.92466
Ru	0.62056	-0.25087	0.02915
C	0.52024	-0.54598	-2.26586
C	-0.33840	-1.61055	-2.66300
C	-1.68170	-1.39297	-2.83385
C	-2.22357	-0.09705	-2.65358
C	-1.41251	0.94511	-2.28270
C	-0.02283	0.74094	-2.04117
H	-2.32814	-2.20382	-3.15735
C	-1.16823	1.66896	0.94165
C	-1.64083	2.83014	0.31422
C	-0.82659	3.94776	0.20488
C	0.47695	3.93025	0.71401
C	0.93620	2.81014	1.38763
C	0.12100	1.67174	1.52295
H	0.62772	1.61020	-1.98273
O	1.13658	-2.25827	0.00812
C	1.42611	-2.23605	1.25325
O	1.25879	-1.12375	1.84561
C	1.95249	-3.43822	1.95386
H	1.61546	-3.44509	2.99184
H	1.64055	-4.34755	1.43832
H	3.04686	-3.40040	1.95405
H	-2.64351	2.84123	-0.10281
H	-1.20315	4.84116	-0.28449
H	1.91409	2.81599	1.85958
H	1.10742	4.80877	0.61837
H	-3.82307	1.27868	1.70107
H	0.39571	0.90857	2.24489
H	1.58844	-0.67820	-2.40176
H	-1.81307	1.95057	-2.21603
H	0.09470	-2.58596	-2.86011
H	-3.27643	0.07695	-2.85535
H	-3.74712	-2.95580	0.89464
H	-5.00911	-0.92728	1.65397
H	-1.36037	-2.68417	0.17772
N	2.54058	0.25795	-0.33083
C	3.65597	0.51219	-0.50248
C	5.05389	0.83683	-0.71107
H	5.56454	0.92233	0.25209
H	5.53656	0.05180	-1.29956
H	5.14319	1.78614	-1.24621

^{1}**C**$^+$ (t-N,t-O)
SCF (PBE1PBE) Energy = -1166.36897227
Enthalpy 0K = -1165.991888
Enthalpy 298K = -1165.965359
Free Energy 298K = -1166.049825
Lowest Frequency = 22.1906 cm^{-1}
Second Frequency = 30.2200 cm^{-1}

C	-2.17624	0.11099	-1.82261
N	-1.40916	-0.19100	-0.76555
C	-1.81713	-1.14738	0.10819
C	-3.04285	-1.79246	-0.07330
C	-3.83886	-1.46675	-1.16035
C	-3.39573	-0.50079	-2.06117
Ru	0.47457	0.57938	-0.42299
C	-1.32642	3.14018	-0.59770
C	-2.53416	2.83894	-0.00874
C	-2.57671	2.15911	1.22847
C	-1.41136	1.79364	1.86129
C	-0.14857	2.06953	1.26794
C	-0.11059	2.75275	0.02727
H	-3.53550	1.95800	1.69675
C	-0.85737	-1.41547	1.17608
C	-1.06663	-2.34265	2.20214
C	-0.09652	-2.54496	3.17633
C	1.08978	-1.81636	3.12834
C	1.30839	-0.88329	2.11192
C	0.34774	-0.66625	1.11240
H	0.81418	3.21863	-0.30695
O	1.15392	-0.80550	-1.82732

```
C   1.72900 -1.89964 -1.73378
O   1.98279 -2.48767 -0.59501
C   2.17872 -2.65034 -2.93878
H   1.61686 -3.58677 -3.00777
H   2.01934 -2.05567 -3.83639
H   3.23408 -2.91567 -2.83596
H  -1.99051 -2.91255  2.24841
H  -0.26408 -3.26708  3.96870
H   2.23460 -0.31478  2.10434
H   1.85123 -1.96961  3.88817
H  -3.36251 -2.55202  0.63083
H   1.61210 -1.95800  0.14971
H  -1.29115  3.71636 -1.51807
H   0.73963  2.00264  1.88817
H  -3.46120  3.15338 -0.47932
H  -1.44237  1.32004  2.83770
H  -3.97891 -0.22336 -2.93192
H  -4.79111 -1.96607 -1.30997
H  -1.78688  0.87259 -2.49012
N   2.37179  1.17432 -0.11967
C   3.47121  1.52293  0.00030
C   4.84930  1.94964  0.14996
H   5.48296  1.09372  0.39910
H   5.20740  2.39491 -0.78261
H   4.92854  2.69226  0.94875
```

$^{4}G^{+}$ (κ^{1})

SCF (PBE1PBE) Energy = -1332.25088697
Enthalpy 0K = -1331.833478
Enthalpy 298K = -1331.798055
Free Energy 298K = -1331.907619
Lowest Frequency = 5.3048 cm^{-1}
Second Frequency = 21.2623 cm^{-1}

```
N   2.02893 -1.83299  0.44990
C   2.82326 -2.66593  0.54248
N   1.33970  0.43353  2.00819
C   1.73169  0.86867  3.00399
C   2.23159  1.42183  4.24789
H   2.21907  0.65999  5.03189
H   3.25777  1.77395  4.11172
H   1.60722  2.26261  4.56189
C   3.83451 -3.70025  0.64994
H   3.56026 -4.56095  0.03422
H   4.79751 -3.31203  0.30720
H   3.93341 -4.02595  1.68881
O   1.52143  1.31702 -2.54149
C   2.45798  1.19583 -1.75944
C   3.85635  1.66098 -2.12040
H   4.53170  0.80122 -2.16986
H   3.84616  2.17180 -3.08336
H   4.24786  2.32891 -1.34810
O   2.39589  0.68877 -0.55565
N   0.33139 -1.01553 -1.59188
C   0.27459 -1.33945 -2.69703
C   0.23890 -1.61105 -4.11858
H  -0.79041 -1.74866 -4.46009
H   0.67860 -0.74943 -4.63091
H   0.81492 -2.50869 -4.35655
N  -0.42807  1.49419  0.04866
C   0.33144  2.60418  0.15288
C  -1.76941  1.65904 -0.02200
C  -0.17930  3.88933  0.20583
H   1.39874  2.42456  0.19385
C  -2.34668  2.93190  0.04142
C  -1.55543  4.06306  0.15700
H   0.50207  4.72967  0.28035
H  -3.42616  3.00902 -0.02808
H  -2.00222  5.05175  0.19566
C  -2.70624  0.51995 -0.19454
C  -3.68651  0.28540  0.77632
C  -2.73094 -0.22006 -1.37858
C  -4.65472 -0.69572  0.57938
H  -3.69110  0.88049  1.68596
C  -3.69743 -1.20244 -1.57331
H  -2.00755  0.00423 -2.15369
C  -4.65817 -1.44690 -0.59489
H  -5.42023 -0.85783  1.33352
H  -3.71842 -1.76285 -2.50363
H  -5.42234 -2.20131 -0.75765
Ru  0.75579 -0.29740  0.23106
N  -0.67693 -1.39620  1.12240
C  -1.41479 -2.11471  1.64770
C  -2.35857 -3.00559  2.29443
H  -3.37661 -2.69564  2.04446
H  -2.20389 -4.03165  1.94985
H  -2.22745 -2.97345  3.37938
```

^{3}G ($2\kappa^{1}$)

SCF (PBE1PBE) Energy = -1428.05422601
Enthalpy 0K = -1427.633332
Enthalpy 298K = -1427.597391
Free Energy 298K = -1427.704417
Lowest Frequency = 23.0583 cm^{-1}
Second Frequency = 27.5751 cm^{-1}

```
N   0.83427 -0.78146  1.34441
C   1.67114 -1.25099  1.98839
N  -1.53934 -1.97980  0.57506
C  -1.98002 -3.03580  0.71965
C   2.74758 -1.89425  2.71380
H   2.99049 -2.83795  2.21613
H   3.63367 -1.25419  2.70973
H   2.45299 -2.09951  3.74656
C  -2.42274 -4.41116  0.82333
H  -2.60012 -4.68634  1.86625
H  -3.34511 -4.56030  0.25583
H  -1.63813 -5.05218  0.40968
O  -3.70339  1.37756 -0.24867
C  -3.33931  0.58359 -1.12791
O  -2.18899  0.01767 -1.23584
C  -4.29257  0.20730 -2.25257
H  -3.79376  0.31450 -3.21932
H  -4.57439 -0.84594 -2.15324
H  -5.18993  0.82696 -2.21830
O   0.21058 -1.15845 -1.49151
C   0.66446 -2.36976 -1.51999
O   0.79948 -3.14426 -0.57143
C   1.05794 -2.80330 -2.92775
H   1.80825 -2.12196 -3.34281
H   1.45366 -3.82010 -2.91730
H   0.18640 -2.74989 -3.58688
N   0.16153  1.67347 -0.36076
C   1.44297  2.10772 -0.42926
C  -0.81618  2.58777 -0.54433
C   1.74234  3.45179 -0.68283
C  -0.57855  3.92809 -0.80816
H  -1.83522  2.22454 -0.43890
C   0.73157  4.37787 -0.88142
H   2.78609  3.74059 -0.74257
H  -1.42402  4.59329 -0.94741
H   0.96396  5.41823 -1.08998
C   2.60614  1.20355 -0.24484
C   2.83842  0.12405 -1.09946
C   3.55913  1.52043  0.73110
C   3.99492 -0.63809 -0.96242
H   2.09024 -0.12530 -1.84315
C   4.71545  0.75717  0.86548
H   3.38578  2.36634  1.39166
C   4.93575 -0.32594  0.01616
```

```
H   4.16090 -1.48013 -1.62826
H   5.44785  1.01511  1.62607
H   5.84113 -0.91923  0.11230
Ru -0.65882 -0.25538  0.15787
N  -1.63983  0.65361  1.62291
C  -2.34802  1.19809  2.35681
C  -3.36168  1.90444  3.11273
H  -3.78306  1.26501  3.89294
H  -2.94995  2.80418  3.57753
H  -4.15023  2.18446  2.40644
```

^{1}G ($2\kappa^2$) (* single point)
SCF (PBE1PBE) Energy = -1162.83896901
Enthalpy 0K = -1162.514404
Enthalpy 298K = -1162.490651
Free Energy 298K = -1162.564493
Lowest Frequency = 60.7538 cm^{-1}
Second Frequency = 66.9756 cm^{-1}

^{2}G$^+$ (κ^2)
SCF (PBE1PBE) Energy = -1067.02057468
Enthalpy 0K = -1066.698783
Enthalpy 298K = -1066.673445
Free Energy 298K = -1066.756933
Lowest Frequency = 21.4846 cm^{-1}
Second Frequency = 24.9027 cm^{-1}

```
Ru  0.69207 -0.20568  0.10465
N  -0.23172 -1.66149 -0.91466
C  -0.70452 -2.52755 -1.51447
C  -1.29414 -3.61984 -2.26272
H  -2.38343 -3.58680 -2.17667
H  -1.01718 -3.54216 -3.31752
H  -0.93544 -4.57509 -1.86978
O   2.18524 -1.63971  0.64660
C   2.82340 -1.34701 -0.40662
O   2.30496 -0.45362 -1.16702
C   4.12972 -1.97797 -0.75006
H   4.94037 -1.36380 -0.34447
H   4.19678 -2.97045 -0.30276
H   4.25440 -2.03034 -1.83271
N  -0.48510  1.24112 -0.75553
C  -1.78158  1.35939 -0.37932
C   0.02193  2.07557 -1.67580
C  -2.58895  2.35751 -0.92715
C  -0.73444  3.07703 -2.26273
H   1.06161  1.90518 -1.93770
C  -2.06403  3.22345 -1.87541
H  -3.61558  2.45960 -0.59373
H  -0.28417  3.72642 -3.00509
H  -2.68261  4.00506 -2.30497
C  -2.24620  0.37161  0.60321
C  -1.29292 -0.29571  1.39494
C  -3.58642 -0.00701  0.71191
C  -1.66969 -1.30718  2.27502
H  -0.28365  0.17338  1.61316
C  -3.96369 -1.01295  1.59721
H  -4.33819  0.45863  0.08177
C  -3.01055 -1.66789  2.37517
H  -0.91556 -1.79602  2.88389
H  -5.00971 -1.29393  1.67235
H  -3.31281 -2.45199  3.06225
N   1.75375  1.19706  1.06445
C   2.41939  1.97369  1.60343
C   3.25590  2.93864  2.28889
H   3.77024  2.45626  3.12473
H   4.00095  3.34451  1.59918
H   2.64361  3.75854  2.67394
```

^{3}G$^+$ (κ^2)
SCF (PBE1PBE) Energy = -1199.63056724
Enthalpy 0K = -1199.261378
Enthalpy 298K = -1199.230984
Free Energy 298K = -1199.326460
Lowest Frequency = 22.8672 cm^{-1}
Second Frequency = 23.7079 cm^{-1}

```
N  -1.45768  0.77925 -1.49304
C  -2.00518  1.05041 -2.47225
N  -1.78559  1.09404  1.29499
C  -2.57807  1.58568  1.97735
C  -3.58327  2.18465  2.83372
H  -4.13249  2.95620  2.28742
H  -4.28833  1.41677  3.16420
H  -3.11334  2.63746  3.71090
C  -2.69493  1.32124 -3.71673
H  -2.85641  0.37620 -4.24362
H  -3.66223  1.79048 -3.51949
H  -2.09713  1.98525 -4.34637
O  -1.46510 -2.10942 -1.78160
C  -2.10861 -2.19016 -0.73141
C  -3.16122 -3.25870 -0.53241
H  -4.05267 -2.84230 -0.05796
H  -3.41711 -3.71716 -1.48780
H  -2.76899 -4.03185  0.13616
O  -1.94929 -1.41596  0.29823
N   0.92248  1.57337 -0.03628
C   0.66755  2.87992  0.13585
C   2.16018  1.18954 -0.43176
C   1.62007  3.86483 -0.06583
H  -0.34191  3.12414  0.44729
C   3.16062  2.13639 -0.66509
C   2.89403  3.48388 -0.47818
H   1.36075  4.90608  0.09009
H   4.13279  1.80815 -1.01510
H   3.66366  4.22688 -0.66181
C   2.37549 -0.25557 -0.59282
C   3.63418 -0.82784 -0.38517
C   1.29138 -1.10471 -0.88253
C   3.80915 -2.20525 -0.48003
H   4.47830 -0.19992 -0.11606
C   1.46764 -2.48366 -0.97551
H   0.31613 -0.76533 -1.33279
C   2.72968 -3.03547 -0.77481
H   4.79495 -2.63111 -0.31850
H   0.60908 -3.09107 -1.24162
H   2.87374 -4.10829 -0.85843
Ru -0.54130  0.08752  0.15776
N   0.28399 -0.69648  1.80943
C   0.70804 -1.21404  2.74996
C   1.24005 -1.88246  3.92107
H   2.05208 -2.55256  3.62634
H   1.62528 -1.14915  4.63441
H   0.45329 -2.46986  4.40207
```

^{1}G ($\kappa^2\kappa^1$)
SCF (PBE1PBE) Energy = -1162.83828113
Enthalpy 0K = -1162.513981
Enthalpy 298K = -1162.488061
Free Energy 298K = -1162.571908
Lowest Frequency = 24.1761 cm^{-1}
Second Frequency = 27.9289 cm^{-1}

```
Ru -0.67519  0.24271 -0.04359
N   0.15957  1.87930 -0.79177
C   0.60700  2.85267 -1.23097
C   1.16559  4.07775 -1.77077
H   2.21605  4.16960 -1.48118
H   1.09968  4.07761 -2.86242
```

H 0.61904 4.94338 -1.38565
O -2.30679 1.44308 0.69448
C -2.92124 1.22331 -0.38860
O -2.31535 0.57694 -1.30767
C -4.33549 1.67123 -0.58825
H -5.00327 0.86100 -0.27835
H -4.54697 2.54660 0.02766
H -4.52368 1.88372 -1.64210
O -1.78517 -1.37745 0.54605
C -1.52135 -1.99398 1.65178
O -0.57631 -1.73700 2.40374
C -2.50924 -3.08894 1.99588
H -2.77020 -3.66716 1.10655
H -2.09893 -3.73929 2.76901
H -3.42949 -2.62954 2.37084
N 0.55594 -1.02787 -1.03121
C 1.85679 -1.12266 -0.65672
C 0.08160 -1.81864 -2.00584
C 2.71214 -2.02421 -1.29276
C 0.88495 -2.72863 -2.67321
H -0.97205 -1.68912 -2.23106
C 2.22675 -2.83087 -2.31098
H 3.74324 -2.10306 -0.96586
H 0.45994 -3.34667 -3.45642
H 2.88176 -3.53982 -2.80813
C 2.23459 -0.23308 0.44172
C 1.18093 0.30149 1.21549
C 3.55057 0.15996 0.69606
C 1.47319 1.19556 2.24793
H 0.21745 -0.34733 1.42128
C 3.82555 1.06118 1.71889
H 4.36206 -0.21382 0.07719
C 2.78703 1.58071 2.49307
H 0.66014 1.57175 2.86134
H 4.85138 1.36192 1.91121
H 3.00666 2.27930 3.29568

TS(**^{1}G-^{1}H**)
SCF (PBE1PBE) Energy = -1162.83441178
Enthalpy 0K = -1162.513996
Enthalpy 298K = -1162.488488
Free Energy 298K = -1162.571017
Lowest Frequency = -911.3780 cm^{-1}
Second Frequency = 22.6032 cm^{-1}

Ru -0.70124 0.13671 -0.08171
N -0.12756 1.87900 -0.79619
C 0.17744 2.91451 -1.21442
C 0.55507 4.21652 -1.73029
H 1.56430 4.47308 -1.39646
H 0.53555 4.21387 -2.82382
H -0.13828 4.98110 -1.36835
O -2.46556 1.06522 0.72331
C -3.09002 0.80980 -0.35070
O -2.45892 0.27482 -1.31567
C -4.55655 1.09884 -0.46947
H -5.11438 0.20661 -0.16713
H -4.83835 1.92030 0.19108
H -4.81675 1.32743 -1.50445
O -1.55275 -1.66249 0.50882
C -1.14403 -2.15419 1.60627
O -0.22025 -1.64086 2.28879
C -1.81921 -3.39905 2.11223
H -2.43065 -3.85444 1.33312
H -1.07099 -4.10565 2.47738
H -2.45858 -3.13063 2.95887
N 0.71257 -0.90253 -1.10220
C 2.00395 -0.82906 -0.68430
C 0.38931 -1.68512 -2.14287
C 2.99873 -1.55509 -1.34473
C 1.33442 -2.42538 -2.83374
H -0.66418 -1.69102 -2.40490
C 2.66598 -2.35547 -2.42645
H 4.02257 -1.50108 -0.99106
H 1.02751 -3.04369 -3.67012
H 3.43255 -2.92636 -2.94181
C 2.20074 0.03603 0.47568
C 1.01489 0.42595 1.15080
C 3.44945 0.51864 0.87720
C 1.14476 1.29960 2.24090
H 0.16239 -0.55348 1.51008
C 3.54436 1.38687 1.95787
H 4.34899 0.24109 0.33300
C 2.38882 1.77848 2.63726
H 0.25006 1.58958 2.78602
H 4.51531 1.76123 2.26925
H 2.46396 2.45638 3.48378

^{1}H
SCF (PBE1PBE) Energy = -1162.85048309
Enthalpy 0K = -1162.525200
Enthalpy 298K = -1162.498927
Free Energy 298K = -1162.584950
Lowest Frequency = 14.7306 cm^{-1}
Second Frequency = 25.2855 cm^{-1}

Ru 0.63103 0.20681 0.11341
N 0.52663 2.07487 -0.36196
C 0.48783 3.19548 -0.65918
C 0.44957 4.59716 -1.03095
H -0.57320 4.89579 -1.27852
H 0.80634 5.22226 -0.20686
H 1.08390 4.77556 -1.90434
O 2.51194 0.03199 -0.88713
C 3.17845 0.31737 0.16395
O 2.58116 0.57488 1.24242
C 4.68049 0.37297 0.08358
H 5.12063 0.11502 1.04833
H 5.04857 -0.29290 -0.69888
H 4.98628 1.39431 -0.16658
O 0.96046 -1.78766 0.77535
C 0.86408 -2.81492 0.10085
O 0.36813 -2.84529 -1.11053
C 1.31673 -4.14208 0.61547
H 1.65174 -4.04488 1.64677
H 0.50205 -4.86717 0.54352
H 2.13672 -4.50832 -0.00920
N -1.00426 0.28871 1.32807
C -2.22136 0.04761 0.76587
C -0.91238 0.51257 2.64668
C -3.36975 0.03027 1.56267
C -2.01765 0.51008 3.48296
H 0.09374 0.69230 3.01419
C -3.27133 0.26244 2.92601
H -4.33379 -0.16886 1.10705
H -1.89222 0.69610 4.54400
H -4.16069 0.24909 3.54927
C -2.15811 -0.16720 -0.67595
C -0.83664 -0.13118 -1.20746
C -3.27751 -0.35399 -1.49218
C -0.72246 -0.25941 -2.60563
H 0.06688 -1.93058 -1.34118
C -3.11988 -0.50518 -2.86511
H -4.27857 -0.37513 -1.06624
C -1.83995 -0.45113 -3.41850
H 0.26699 -0.20500 -3.05829
H -3.98765 -0.65473 -3.50082
H -1.71374 -0.55406 -4.49407

^{2}G ($\kappa^2\kappa^1$)

SCF (PBE1PBE) Energy = -1295.44689550
Enthalpy 0K = -1295.075102
Enthalpy 298K = -1295.044038
Free Energy 298K = -1295.140259
Lowest Frequency = 28.5847 cm^{-1}
Second Frequency = 30.0193 cm^{-1}

N	-1.91701	0.96029	0.88238
C	-2.84230	1.49729	1.31528
C	-4.04295	2.14055	1.80956
H	-4.36768	1.66748	2.74023
H	-3.86110	3.20175	1.99943
H	-4.83651	2.04220	1.06319
O	-3.15638	0.22037	-1.67819
C	-2.73623	-0.92724	-1.55757
O	-1.66333	-1.30942	-0.93289
C	-3.48790	-2.10368	-2.16490
H	-2.82456	-2.68691	-2.81041
H	-3.83011	-2.77077	-1.36797
H	-4.34485	-1.74833	-2.73860
O	-0.62320	-1.49375	1.58466
C	-0.27549	-1.22405	2.79825
O	0.25645	-0.17371	3.17545
C	-0.56644	-2.34339	3.77874
H	-1.62140	-2.62491	3.72126
H	0.01758	-3.22814	3.50813
H	-0.31381	-2.03511	4.79364
N	1.19367	-1.20641	-0.54103
C	2.43689	-0.67911	-0.43477
C	1.03105	-2.47029	-0.95543
C	3.55850	-1.44245	-0.76495
C	2.10744	-3.27165	-1.30410
H	-0.00249	-2.79903	-1.00297
C	3.39379	-2.74727	-1.20614
H	4.54916	-1.01713	-0.64792
H	1.93436	-4.28955	-1.63607
H	4.25944	-3.35257	-1.45836
C	2.48587	0.70423	0.04960
C	1.35936	1.20238	0.74276
C	3.55572	1.55838	-0.22928
C	1.35051	2.53453	1.16410
H	0.70065	0.52120	1.43176
C	3.52655	2.88552	0.18518
H	4.40416	1.19590	-0.80341
C	2.42125	3.37508	0.88061
H	0.50050	2.89487	1.73517
H	4.36413	3.53937	-0.03958
H	2.40189	4.41021	1.21022
Ru	-0.39606	-0.07853	0.10366
N	-0.36903	1.12924	-1.48439
C	-0.50060	1.77843	-2.43032
C	-0.77531	2.55669	-3.62133
H	-0.61864	3.62153	-3.42996
H	-0.12536	2.24649	-4.44389
H	-1.81857	2.39312	-3.90791

TS(**^{2}G-^{2}H**)
SCF (PBE1PBE) Energy = -1295.44157254
Enthalpy 0K = -1295.073825
Enthalpy 298K = -1295.043273
Free Energy 298K = -1295.137520
Lowest Frequency = -996.8333 cm^{-1}
Second Frequency = 29.0445 cm^{-1}

N	1.85777	-1.18137	0.75614
C	2.79025	-1.80310	1.03522
C	4.02125	-2.51341	1.31696
H	4.32429	-2.35435	2.35532
H	3.89929	-3.58629	1.14570
H	4.80338	-2.13055	0.65432
O	3.36787	0.30948	-1.29538
C	2.89576	1.37121	-0.88912
O	1.75530	1.54725	-0.30178
C	3.67163	2.67322	-1.04976
H	3.07271	3.40392	-1.60201
H	3.87638	3.10475	-0.06529
H	4.61085	2.49474	-1.57528
O	0.41797	0.94765	2.05132
C	-0.25351	0.38658	2.96637
O	-0.94779	-0.65051	2.77816
C	-0.22731	0.99841	4.34018
H	0.47011	1.83499	4.37900
H	-1.23289	1.34232	4.59876
H	0.05281	0.23778	5.07336
N	-1.15480	1.30092	-0.31978
C	-2.38319	0.74862	-0.48694
C	-0.98981	2.62796	-0.40748
C	-3.48589	1.56534	-0.75387
C	-2.04770	3.48259	-0.67537
H	0.03375	2.96334	-0.26620
C	-3.31850	2.93825	-0.85025
H	-4.46844	1.11974	-0.86299
H	-1.87443	4.55134	-0.73886
H	-4.17182	3.57951	-1.05121
C	-2.41751	-0.70845	-0.35391
C	-1.26933	-1.31394	0.22508
C	-3.47630	-1.48527	-0.83296
C	-1.25426	-2.71558	0.30349
H	-0.84191	-0.84013	1.43327
C	-3.42592	-2.87087	-0.74256
H	-4.33329	-1.01312	-1.30707
C	-2.30886	-3.48529	-0.17513
H	-0.39990	-3.20256	0.76714
H	-4.25057	-3.47004	-1.11761
H	-2.26691	-4.56928	-0.10208
Ru	0.38854	0.03966	0.17312
N	0.58239	-0.63323	-1.67885
C	0.83608	-0.96816	-2.75408
C	1.26261	-1.34795	-4.08567
H	1.12834	-2.42158	-4.24165
H	0.68890	-0.80707	-4.84302
H	2.32253	-1.09837	-4.19322

^{2}H
SCF (PBE1PBE) Energy = -1295.45439468
Enthalpy 0K = -1295.081733
Enthalpy 298K = -1295.050622
Free Energy 298K = -1295.146903
Lowest Frequency = 21.7846 cm^{-1}
Second Frequency = 27.2316 cm^{-1}

N	1.66565	-1.55667	-0.09681
C	2.59972	-2.22703	-0.22203
C	3.88160	-2.88032	-0.38926
H	4.15187	-3.44352	0.50796
H	3.86937	-3.56192	-1.24384
H	4.62252	-2.09181	-0.56027
O	3.58167	0.63407	-0.60457
C	3.09573	1.30318	0.31365
O	1.89427	1.24115	0.77579
C	3.95557	2.34573	1.02527
H	3.52001	3.34151	0.89216
H	3.97178	2.14620	2.10103
H	4.97365	2.34010	0.63234
O	0.12572	-0.45542	2.15088
C	-0.45790	-1.41024	2.66618
O	-1.12468	-2.30541	1.98040
C	-0.45712	-1.63094	4.14386
H	0.15733	-0.87491	4.62986
H	-1.48269	-1.58234	4.52075

H	-0.07556	-2.63105	4.36652
N	-1.04804	1.42548	0.27114
C	-2.32113	1.14101	-0.11145
C	-0.74569	2.61948	0.79804
C	-3.32241	2.10551	0.04396
C	-1.70016	3.61000	0.97181
H	0.30057	2.73368	1.07209
C	-3.01234	3.34364	0.58524
H	-4.33955	1.87747	-0.25488
H	-1.41675	4.56425	1.40247
H	-3.78803	4.09420	0.70840
C	-2.49470	-0.20301	-0.66288
C	-1.32516	-1.02172	-0.64165
C	-3.70162	-0.65319	-1.20784
C	-1.46026	-2.29926	-1.22092
H	-1.11261	-2.01505	1.02806
C	-3.79290	-1.92918	-1.75064
H	-4.57781	-0.00861	-1.22311
C	-2.66512	-2.74957	-1.75887
H	-0.59220	-2.95646	-1.25032
H	-4.73178	-2.27825	-2.17048
H	-2.72579	-3.74577	-2.19197
Ru	0.33664	-0.08045	0.06113
N	0.75617	0.43737	-1.76702
C	1.12929	0.76813	-2.80977
C	1.70378	1.20418	-4.06676
H	1.54981	0.45201	-4.84530
H	1.24833	2.14358	-4.39215
H	2.77793	1.35948	-3.92598

$^{-}$OAc (* single point)
SCF (wB97X-D) Energy = -228.424588068
Enthalpy 0K = -228.376170
Enthalpy 298K = -228.371220
Free Energy 298K = -228.402379
Lowest Frequency = 272.7232 cm^{-1}
Second Frequency = 444.2016 cm^{-1}

O	-0.77440	-1.04070	-0.00013
H	-1.71185	-0.80413	-0.00042
C	-0.09310	0.12258	0.00048
O	-0.64494	1.19574	-0.00012
C	1.39325	-0.10776	-0.00002
H	1.67864	-0.68787	0.88126
H	1.67808	-0.68811	-0.88132
H	1.90890	0.85091	-0.00032

AcOH
SCF (wB97X-D) Energy = -229.016577398
Enthalpy 0K = -228.953751
Enthalpy 298K = -228.948276
Free Energy 298K = -228.980902
Lowest Frequency = 74.1530 cm^{-1}
Second Frequency = 426.5462 cm^{-1}

O	-0.77440	-1.04070	-0.00013
H	-1.71185	-0.80413	-0.00042
C	-0.09310	0.12258	0.00048
O	-0.64494	1.19574	-0.00012
C	1.39325	-0.10776	-0.00002
H	1.67864	-0.68787	0.88126
H	1.67808	-0.68811	-0.88132
H	1.90890	0.85091	-0.00032

a-H, 2-phenylpyridine
SCF (wB97X-D) Energy = -479.183810577
Enthalpy 0K = -479.011919
Enthalpy 298K = -479.002292
Free Energy 298K = -479.046538
Lowest Frequency = 52.4988 cm^{-1}
Second Frequency = 95.9802 cm^{-1}

N	-1.36313	-1.14623	-0.25601
C	-2.69399	-1.18890	-0.26374
C	-3.50561	-0.08440	-0.02577
H	-3.13672	-2.16029	-0.47414
H	-4.58558	-0.17779	-0.05037
C	0.72493	0.02409	-0.00643
C	1.46090	1.18733	-0.25366
C	2.80233	-1.19359	0.24947
C	2.85168	1.16192	-0.24308
H	0.95058	2.11763	-0.48380
C	3.52705	-0.02759	0.01335
H	3.32207	-2.12631	0.44568
H	3.40783	2.07221	-0.44434
H	4.61238	-0.04739	0.02269
C	-0.76324	0.02593	-0.00285
C	-2.88543	1.12776	0.25444
H	-3.47291	2.01576	0.46634
C	-1.49866	1.18528	0.27290
H	-0.99346	2.11176	0.52099
C	1.41323	-1.16940	0.23551
H	0.83855	-2.07250	0.40829

Benzene (C_6H_6)
SCF (wB97X-D) Energy = -232.168797265
Enthalpy 0K = -232.068128
Enthalpy 298K = -232.062917
Free Energy 298K = -232.095547
Lowest Frequency = 441.7058 cm^{-1}
Second Frequency = 441.8681 cm^{-1}

C	0.00000	1.40481	0.00000
C	-1.21659	0.70239	0.00000
C	-1.21659	-0.70239	0.00000
C	0.00000	-1.40480	0.00000
C	1.21659	-0.70239	0.00000
C	1.21658	0.70240	0.00000
H	-2.16519	1.25006	0.00000
H	-2.16518	-1.25007	0.00000
H	0.00001	-2.50014	0.00000
H	2.16519	-1.25006	0.00000
H	2.16518	1.25007	0.00000
H	-0.00001	2.50001	0.00000

MeCN
SCF (wB97X-D) Energy = -132.705927825
Enthalpy 0K = -132.660090
Enthalpy 298K = -132.655556
Free Energy 298K = -132.684097
Lowest Frequency = 389.7137 cm^{-1}
Second Frequency = 389.7828 cm^{-1}

C	0.00002	-1.17938	0.00000
H	-1.02596	-1.55381	0.00000
H	0.51299	-1.55382	0.88853
H	0.51299	-1.55382	-0.88853
C	0.00000	0.27994	0.00000
N	-0.00002	1.43687	0.00000

A
SCF (wB97X-D) Energy = -783.983987391
Enthalpy 0K = -783.774675
Enthalpy 298K = -783.758307
Free Energy 298K = -783.819245
Lowest Frequency = 19.2486 cm^{-1}
Second Frequency = 62.2075 cm^{-1}

C	1.85534	-0.71676	1.41715
C	2.47971	0.35451	0.70018
C	2.47746	0.34959	-0.70834
C	1.85225	-0.72698	-1.41677
C	1.25461	-1.78874	-0.71042
C	1.25594	-1.78364	0.71984
Ru	0.42322	0.10689	-0.00076
O	-0.39661	1.75938	-1.08482
C	-0.78798	2.28763	0.00100
C	-1.70938	3.46697	0.00153
H	2.85347	1.20703	-1.25317
H	0.67850	-2.53496	1.24029
O	-1.55626	-0.40450	-0.00577
C	-2.04192	-1.61207	0.00021
O	-1.39722	-2.65696	0.00800
O	-0.40045	1.75534	1.08626
C	-3.56151	-1.62065	-0.00296
H	-3.93432	-1.08800	0.87593
H	-3.93107	-1.09235	-0.88581
H	-3.93161	-2.64578	-0.00089
H	-2.73695	3.09180	-0.00131
H	-1.56099	4.06537	0.90113
H	-1.55737	4.06893	-0.89508
H	1.76363	-0.65712	2.49517
H	0.67552	-2.54353	-1.22406
H	1.75868	-0.67521	-2.49501
H	2.85783	1.21536	1.23807

B^{+}

SCF (wB97X-D) Energy = -1034.58037705
Enthalpy 0K = -1034.248170
Enthalpy 298K = -1034.227198
Free Energy 298K = -1034.297573
Lowest Frequency = 35.3332 cm^{-1}
Second Frequency = 41.5378 cm^{-1}

C	-0.36496	-2.17556	-0.70013
C	-2.76647	-1.28427	1.95380
C	-3.75831	-1.79518	1.11774

```
C  -3.98646 -1.21256 -0.12739
C  -2.20319  0.36858  0.28742
C  -1.28014  3.82930 -0.87570
O   1.07992 -0.08763  1.87050
C   2.10891  0.64037  1.71284
O   2.56883  0.71042  0.52568
C   2.72241  1.40314  2.83761
H  -1.76171  4.78321 -1.06160
H   2.50204  0.91831  3.78865
H   3.79900  1.49201  2.68837
H   2.29448  2.41037  2.85251
H  -4.76737 -1.59676 -0.77501
H  -4.36301 -2.63563  1.44190
H  -2.60193 -1.72147  2.93303
C   0.65261  2.43237 -0.82274
H   1.71396  2.26527 -0.95736
C   0.08534  3.66783 -1.07890
H   0.70988  4.48009 -1.43038
C  -1.39085  1.52215 -0.18015
Ru  0.99889 -0.49531 -0.22509
C   2.24191 -1.57679 -1.64227
H   3.23604 -1.26391 -1.94128
C   2.08448 -2.39078 -0.48493
H   2.95223 -2.71258  0.07690
C   0.78151 -2.66107 -0.00906
H   0.65352 -3.17160  0.93868
C   1.11418 -1.08026 -2.34161
H   1.24395 -0.42245 -3.19181
C  -0.18717 -1.38501 -1.85577
H  -1.05406 -0.93008 -2.32070
H  -1.35763 -2.33884 -0.29853
C  -2.01656  2.74531 -0.42169
H  -3.08046  2.82881 -0.23315
C  -3.21879 -0.12523 -0.53675
H  -3.40316  0.33772 -1.50269
N  -0.06104  1.37324 -0.38762
C  -1.98873 -0.20632  1.54302
H  -1.20811  0.17988  2.18826
```

TS(**B**$^{+}$–**C**$^{+}$)
SCF (wB97X-D) Energy = -1034.55335177
Enthalpy 0K = -1034.222714
Enthalpy 298K = -1034.201908
Free Energy 298K = -1034.272662
Lowest Frequency = -103.7951 cm^{-1}
Second Frequency = 26.1535 cm^{-1}

```
C  -0.65292  2.43225 -0.82215
N   0.06092  1.37318 -0.38712
C   1.39074  1.52221 -0.17989
C   2.01633  2.74539 -0.42164
C   1.27975  3.82928 -0.87565
C  -0.08577  3.66769 -1.07856
Ru -0.99892 -0.49540 -0.22488
C  -2.08344 -2.39154 -0.48612
C  -2.24174 -1.57642 -1.64254
C  -1.11454 -1.07861 -2.34182
C   0.18711 -1.38304 -1.85670
C   0.36577 -2.17464 -0.70190
C  -0.78015 -2.66161 -0.01101
H  -1.24500 -0.41999 -3.19129
C   2.20321  0.36872  0.28769
C   3.21913 -0.12472 -0.53630
C   3.98689 -1.21199 -0.12696
C   3.75848 -1.79495  1.11797
C   2.76631 -1.28441  1.95385
C   1.98848 -0.20652  1.54309
H  -0.65152 -3.17329  0.93602
O  -2.56899  0.70991  0.52599
C  -2.10926  0.63955  1.71323
O  -1.08029 -0.08846  1.87085
C  -2.72302  1.40195  2.83812
H  -2.29507  2.40916  2.85354
H  -3.79957  1.49089  2.68863
H  -2.50291  0.91675  3.78904
H   3.40372  0.33849 -1.50208
H   4.76807 -1.59589 -0.77443
H   2.60154 -1.72186  2.93294
H   4.36323 -2.63538  1.44209
H   3.08024  2.82901 -0.23324
H   1.20760  0.17936  2.18818
H  -2.95081 -2.71467  0.07553
H   1.35868 -2.33785 -0.30086
H  -3.23614 -1.26386 -1.94095
H   1.05356 -0.92699 -2.32133
H  -0.71040  4.47990 -1.43000
H   1.76121  4.78320 -1.06170
H  -1.71429  2.26509 -0.95650
```

C^{+}
SCF (wB97X-D) Energy = -1034.57386448
Enthalpy 0K = -1034.241840
Enthalpy 298K = -1034.220689
Free Energy 298K = -1034.292033
Lowest Frequency = 26.1318 cm^{-1}
Second Frequency = 37.6242 cm^{-1}

```
C   0.38126  2.72724 -0.05443
N   0.57346  1.41770 -0.28160
C   1.81880  0.95294 -0.54287
C   2.89721  1.83640 -0.61206
C   2.69290  3.19065 -0.40260
C   1.41062  3.64892 -0.10887
Ru -0.97891  0.00307 -0.18341
C  -3.05660 -0.69142  0.17390
C  -3.17486  0.72865  0.01528
C  -2.60438  1.33800 -1.10037
C  -1.90756  0.54742 -2.07450
C  -1.88024 -0.86032 -1.96066
C  -2.48053 -1.49195 -0.82955
H  -2.62641  2.41706 -1.20432
C   1.88848 -0.50447 -0.68992
C   3.06864 -1.19639 -0.97066
C   3.06261 -2.58427 -1.04052
C   1.87722 -3.27828 -0.82012
C   0.69569 -2.58627 -0.54607
C   0.66587 -1.18607 -0.48453
H  -2.43047 -2.56652 -0.70858
O  -0.62622  0.15178  1.95258
C   0.08052 -0.44349  2.77388
O   0.88236 -1.43091  2.47015
C   0.07957 -0.07774  4.22274
H   1.08125  0.25279  4.50965
H  -0.64373  0.71286  4.41112
H  -0.15511 -0.96075  4.82185
H   4.00041 -0.66413 -1.13456
H   3.97941 -3.12090 -1.25750
H  -0.21166 -3.15766 -0.37178
H   1.86756 -4.36286 -0.86154
H   3.89087  1.46072 -0.82203
H   0.86328 -1.60397  1.50425
H  -3.41714 -1.15580  1.08453
H  -1.34945 -1.45295 -2.69571
H  -3.62985  1.32376  0.79743
H  -1.40359  1.03025 -2.90305
H   1.20872  4.69680  0.07581
H   3.52592  3.88299 -0.45804
H  -0.63277  3.02528  0.18344
```

B.OAc

SCF (wB97X-D) Energy = -1263.17512334
Enthalpy 0K = -1262.791890
Enthalpy 298K = -1262.765452
Free Energy 298K = -1262.847748
Lowest Frequency = 32.6656 cm^{-1}
Second Frequency = 48.3445 cm^{-1}

C	-0.74398	-1.90540	1.14078
N	-0.40105	-0.63641	0.85519
C	-1.19485	0.36807	1.28623
C	-2.33418	0.10046	2.04078
C	-2.67320	-1.20769	2.34948
C	-1.85852	-2.23256	1.89074
Ru	1.26640	-0.39070	-0.46932
C	2.65232	-0.40287	-2.16784
C	1.62591	-1.37884	-2.35892
C	0.26024	-1.01530	-2.31778
C	-0.09459	0.33661	-2.04953
C	0.90385	1.30694	-1.81782
C	2.27995	0.92742	-1.87158
H	-0.56556	-1.73326	-2.31252
C	-0.87415	1.77674	0.93323
C	-1.76079	2.47230	0.10557
C	-1.48301	3.79181	-0.24227
C	-0.33762	4.42185	0.24076
C	0.53495	3.72992	1.07897
C	0.26825	2.40965	1.42826
H	3.04312	1.64401	-1.58851
O	2.16914	-1.90524	0.75442
C	2.59164	-1.03496	1.57838
O	2.39526	0.18419	1.29444
C	3.25165	-1.44310	2.85924
H	3.91010	-0.65108	3.21676
H	2.47465	-1.61657	3.61008
H	3.80484	-2.37252	2.71895
H	-2.61515	1.93846	-0.30614
H	-2.16238	4.32590	-0.89915
H	1.42427	4.21848	1.46487
H	-0.12695	5.45167	-0.03165
H	-2.94878	0.93295	2.36081
H	0.95759	1.86256	2.06129
H	3.69315	-0.70065	-2.13554
H	0.63087	2.31059	-1.51280
H	1.90162	-2.42459	-2.44176
H	-1.16806	0.51768	-1.87464
H	-2.09150	-3.27428	2.07133
H	-3.56799	-1.42284	2.92374
H	-0.09592	-2.67299	0.74071
O	-2.31812	-2.08285	-1.44248
C	-3.11416	-1.14992	-1.17486
C	-4.48560	-1.54485	-0.60652
H	-4.44595	-2.52938	-0.13447
H	-4.84057	-0.79380	0.10445
H	-5.20954	-1.58915	-1.42731
O	-2.92135	0.08727	-1.34344

TS(**B-C**)1.OAC (* single point)
SCF (wB97X-D) Energy = -1263.13832583
Enthalpy 0K = -1262.760647
Enthalpy 298K = -1262.735961
Free Energy 298K = -1262.812308
Lowest Frequency = -68.5333 cm^{-1}
Second Frequency = 39.5001 cm^{-1}

INT(**B-C**).OAc
SCF (wB97X-D) Energy = -1263.14567531
Enthalpy 0K = -1262.764289
Enthalpy 298K = -1262.737009
Free Energy 298K = -1262.823820
Lowest Frequency = 22.4835 cm^{-1}
Second Frequency = 27.0224 cm^{-1}

C	-1.54362	1.44508	0.40118
N	-0.27534	1.09810	0.16567
C	0.66361	2.03046	-0.09233
C	0.34548	3.37641	-0.13352
C	-0.97302	3.75640	0.11613
C	-1.92196	2.78410	0.38761
Ru	0.40136	-0.89311	0.03620
C	1.24152	-2.81847	-0.64777
C	-0.07137	-3.02239	-0.18526
C	-1.13944	-2.20535	-0.66621
C	-0.88942	-1.22904	-1.67313
C	0.42780	-1.04408	-2.17143
C	1.48960	-1.79537	-1.62114
H	-2.13327	-2.20013	-0.22124
C	2.01649	1.46937	-0.33048
C	2.74917	1.78159	-1.47813
C	3.96896	1.15510	-1.71049
C	4.47202	0.21890	-0.80327
C	3.75281	-0.08270	0.34686
C	2.52147	0.53443	0.59110
H	2.51251	-1.54954	-1.88545
O	-0.11353	-1.12301	2.00506
C	0.00996	-0.26966	2.98264
O	0.69878	0.74733	2.96224
C	-0.80759	-0.65255	4.19985
H	-1.86968	-0.58028	3.94869
H	-0.60867	-1.69040	4.47719
H	-0.57888	0.01224	5.03250
H	2.35067	2.49352	-2.19477
H	4.53326	1.39560	-2.60612
H	4.14737	-0.78562	1.07385
H	5.42930	-0.25654	-0.99149
H	1.11947	4.10728	-0.33802
H	2.00870	0.42822	1.55534
H	2.07057	-3.35431	-0.20183
H	0.63932	-0.23837	-2.86402
H	-0.24640	-3.68892	0.65112
H	-1.71597	-0.53529	-1.92218
H	-2.96004	3.03664	0.56401
H	-1.24957	4.80532	0.09330
H	-2.25582	0.62847	0.54743
O	-3.61303	-0.71327	-0.04097
C	-3.99278	-0.02793	-1.03345
C	-5.50175	0.20631	-1.16055
H	-6.01207	-0.75706	-1.25575
H	-5.87974	0.67526	-0.24675
H	-5.73644	0.83182	-2.02347
O	-3.24779	0.48503	-1.90807

TS(**B-C**)2.OAC
SCF (wB97X-D) Energy = -1263.13733834
Enthalpy 0K = -1262.760181
Enthalpy 298K = -1262.733755
Free Energy 298K = -1262.818052
Lowest Frequency = -977.1404 cm^{-1}
Second Frequency = 15.0560 cm^{-1}

C	-1.50113	1.38195	0.61788
N	-0.26181	1.06856	0.22010
C	0.65649	2.03416	-0.02530
C	0.33116	3.37335	0.14006
C	-0.95491	3.71294	0.55170
C	-1.87906	2.70877	0.79219
Ru	0.31824	-0.91795	-0.09369
C	0.83629	-2.93052	-0.88736
C	-0.42592	-2.98778	-0.25503

```
C  -1.47823 -2.10398 -0.62742
C  -1.24978 -1.13287 -1.62952
C   0.01828 -1.05317 -2.27480
C   1.05104 -1.93916 -1.89061
H  -2.41798 -2.03051 -0.08142
C   1.97635  1.52484 -0.43628
C   2.89152  2.28092 -1.16754
C   4.11034  1.72178 -1.53837
C   4.42384  0.41222 -1.17585
C   3.50685 -0.34130 -0.45159
C   2.26128  0.18663 -0.08598
H   2.04306 -1.81525 -2.30969
O  -0.00947 -1.10607  1.97219
C   0.84338 -0.68573  2.81251
O   1.93704 -0.15640  2.48559
C   0.49438 -0.80775  4.27195
H   0.07847  0.14790  4.60463
H  -0.25475 -1.58408  4.42436
H   1.39220 -1.00832  4.85759
H   2.65032  3.29512 -1.47143
H   4.81997  2.31103 -2.11041
H   3.76083 -1.35259 -0.14443
H   5.38404 -0.01206 -1.45226
H   1.08019  4.13671 -0.03473
H   1.94690 -0.13930  1.13144
H   1.64665 -3.57389 -0.56813
H   0.21700 -0.26927 -2.99547
H  -0.56318 -3.64611  0.59549
H  -2.03680 -0.37209 -1.78100
H  -2.89718  2.92583  1.09010
H  -1.22604  4.75580  0.67982
H  -2.20829  0.55857  0.75291
O  -3.81538 -0.52833  0.31141
C  -4.21891  0.23825 -0.60938
C  -5.71396  0.57813 -0.60275
H  -6.28764 -0.32339 -0.84139
H  -6.02126  0.89455  0.39830
H  -5.94795  1.35484 -1.33302
O  -3.51273  0.74406 -1.51929
```

C.OAc
SCF (wB97X-D) Energy = -1263.15945024
Enthalpy 0K = -1262.777272
Enthalpy 298K = -1262.750133
Free Energy 298K = -1262.837711
Lowest Frequency = 11.9632 cm^{-1}
Second Frequency = 25.7060 cm^{-1}

```
C  -1.42051  1.53422  0.22088
N  -0.20632  1.08088 -0.12273
C   0.75834  1.93413 -0.55222
C   0.49257  3.29306 -0.66339
C  -0.77123  3.77116 -0.32954
C  -1.73539  2.88482  0.12377
Ru  0.25756 -0.96224 -0.07452
C   0.49312 -3.15443 -0.35747
C  -0.66751 -2.92706  0.43549
C  -1.73032 -2.10874 -0.01071
C  -1.58568 -1.41793 -1.23537
C  -0.42254 -1.60231 -2.03937
C   0.60638 -2.47857 -1.59880
H  -2.58873 -1.85111  0.60577
C   2.04871  1.27694 -0.81632
C   3.19391  1.95703 -1.24147
C   4.39123  1.27114 -1.39960
C   4.44714 -0.09305 -1.11972
C   3.30321 -0.77038 -0.70228
C   2.07159 -0.11403 -0.55206
H   1.51886 -2.56853 -2.17781
O   0.50153 -0.66791  2.07540
C   1.25730  0.00550  2.77336
O   2.31976  0.62821  2.31745
C   1.02388  0.18942  4.23999
H   0.75698  1.23380  4.42414
H   0.21251 -0.45682  4.56895
H   1.94013 -0.02208  4.79491
H   3.16044  3.02270 -1.44833
H   5.27987  1.79948 -1.72893
H   3.37039 -1.83381 -0.48431
H   5.38506 -0.63011 -1.22752
H   1.26436  3.97159 -1.00661
H   2.40623  0.46150  1.35328
H   1.29746 -3.78179  0.00598
H  -0.30056 -1.04156 -2.95793
H  -0.70373 -3.34454  1.43630
H  -2.35250 -0.66633 -1.48621
H  -2.73731  3.20405  0.38189
H  -0.99334  4.82915 -0.42583
H  -2.16351  0.80206  0.55568
O  -3.84864 -0.15241  0.78744
C  -4.38880  0.32677 -0.25184
C  -5.88102  0.66604 -0.14625
H  -6.45819 -0.26477 -0.13709
H  -6.08676  1.18017  0.79672
H  -6.20866  1.27457 -0.99126
O  -3.82187  0.54119 -1.35235
```

A.a-H
SCF (wB97X-D) Energy = -1263.19323833
Enthalpy 0K = -1262.810509
Enthalpy 298K = -1262.783594
Free Energy 298K = -1262.869722
Lowest Frequency = 15.2062 cm^{-1}
Second Frequency = 29.0718 cm^{-1}

```
C   1.68429  1.25326 -2.24463
C   0.33253  0.89096 -1.98540
C  -0.02750 -0.46079 -1.81400
C  -1.52135 -1.61387  1.01467
C  -1.10174 -2.94027  1.04454
H  -0.15380 -3.17674  1.51564
C  -2.23791  1.20793  0.38704
H  -1.19783  1.00461  0.61173
O   1.10586  1.28206  1.05309
C   0.47869  3.20853  2.24043
H   1.24085  2.95925  2.98128
H   0.41441  4.28871  2.10821
H  -0.48025  2.83407  2.61390
C   0.78039  2.53496  0.91319
O   0.66490  3.14021 -0.14970
O   3.40301 -0.10170  0.74859
C   2.82117 -0.88532  1.55966
O   1.68100 -1.33243  1.22667
H  -0.88400 -0.86196  1.46908
C   3.43601 -1.23273  2.87905
H   3.09829 -0.49592  3.61379
H   3.10702 -2.22059  3.20375
H   4.52374 -1.18725  2.81631
C  -1.88571 -3.93612  0.46772
H  -1.55882 -4.97143  0.49176
C  -2.72755 -1.26202  0.39646
C  -3.51428 -2.27230 -0.16904
H  -4.45219 -1.99544 -0.63757
C  -3.09644 -3.59764 -0.13388
H  -3.71636 -4.36854 -0.58157
N  -4.44669  0.37839 -0.02633
C  -2.66596  2.51462  0.18940
H  -1.94837  3.32803  0.24370
C  -3.15706  0.15903  0.26836
```

```
C  -4.00584  2.74080 -0.10536
H  -4.39029  3.74146 -0.26905
C  -4.84851  1.63693 -0.19743
H  -5.90356  1.77041 -0.42818
Ru  1.64443  0.00103 -0.46143
C   0.97510 -1.47433 -1.90224
H   0.71419 -2.49465 -1.64450
C   2.31423 -1.14028 -2.20710
H   3.08318 -1.90250 -2.20964
C   2.66500  0.23470 -2.34563
H   3.71064  0.50853 -2.42972
H  -1.03454 -0.72686 -1.51987
H  -0.38639  1.67351 -1.78077
H   1.96257  2.29807 -2.24525
```

B

SCF (wB97X-D) Energy = -1263.19222485
Enthalpy 0K = -1262.809337
Enthalpy 298K = -1262.782552
Free Energy 298K = -1262.867025
Lowest Frequency = 25.7131 cm^{-1}
Second Frequency = 34.9502 cm^{-1}

```
C  -0.54075 -1.95531  2.09411
Ru -0.62430 -0.40858 -0.44303
C  -1.00050 -0.15301 -2.60086
C  -1.87757 -1.13249 -2.07342
C   0.01612 -2.37479 -1.14514
C   0.91832 -1.42161 -1.67802
H  -1.40517  0.73805 -3.06140
H  -2.94323 -0.94834 -2.12742
H   0.37289 -3.15153 -0.48140
H   1.97852 -1.49277 -1.47230
C  -0.37262 -1.91531  3.60571
H  -0.50330 -2.91199  4.02777
H   0.60827 -1.51604  3.87844
H  -1.12620 -1.24204  4.02437
O  -0.16380 -0.84909  1.52499
O  -0.99378 -2.94934  1.53356
C   1.50653  1.76317  0.43269
C  -0.64898  2.56128  0.14754
N   0.21504  1.53056  0.11119
O  -2.33468  0.19716  0.57954
C  -3.35323  0.78334  0.03968
O  -3.38873  1.27176 -1.09399
C  -4.55498  0.85808  0.96688
H  -4.27515  1.36810  1.89248
H  -5.37614  1.38696  0.48273
H  -4.86980 -0.15277  1.23944
C   2.54311  0.70886  0.23431
C   3.42607  0.85707 -0.83924
C   2.68830 -0.37650  1.09946
C   4.41746 -0.09234 -1.07370
H   3.32741  1.71528 -1.49886
C   3.68412 -1.31962  0.86720
H   1.98478 -0.49618  1.91305
C   4.54487 -1.18581 -0.22085
H   5.08987  0.02489 -1.91756
H   3.78466 -2.16634  1.53876
H   5.31682 -1.92771 -0.39937
C  -0.28870  3.83588  0.55698
C   1.92780  3.02131  0.86337
C   1.02241  4.06902  0.94509
H   2.97114  3.15712  1.12372
H   1.34099  5.04915  1.28467
H  -1.03526  4.62111  0.56268
H  -1.65118  2.35143 -0.20367
C  -1.38349 -2.24855 -1.34631
H  -2.05457 -2.92722 -0.83874
C   0.39354 -0.29609 -2.36663
H   1.06935  0.50081 -2.65822
```

TS(**B–C**)
SCF (wB97X-D) Energy = -1263.13562342
Enthalpy 0K = -1262.756177
Enthalpy 298K = -1262.730290
Free Energy 298K = -1262.811032
Lowest Frequency = -296.0086 cm^{-1}
Second Frequency = 37.5105 cm^{-1}

```
C  -2.09775  1.97674 -1.64252
Ru -0.26419 -0.09130  0.75413
C  -0.54884 -1.05022  2.67525
C  -1.79303 -0.53242  2.24615
C  -0.78300  1.67259  1.94435
C   0.47066  1.17331  2.42056
H  -0.44872 -2.11364  2.85540
H  -2.60603 -1.22385  2.06711
H  -0.85839  2.65810  1.50299
H   1.34915  1.80669  2.38764
C  -3.45489  1.78449 -2.31562
H  -3.82569  0.78943 -2.04428
H  -4.17457  2.53029 -1.97210
H  -3.35846  1.81661 -3.40293
O  -1.10279  1.48565 -2.25509
O  -2.06589  2.55885 -0.53083
C   2.19822 -0.84561 -0.74148
C   1.91971 -3.57993 -0.73850
C   0.99634 -2.74726 -0.12646
H   0.09159 -3.11939  0.34478
N   1.14622 -1.41372 -0.11808
O  -1.43735 -0.86602 -0.73894
C  -2.10972 -1.96651 -0.63589
O  -2.06867 -2.75509  0.31497
C  -3.01456 -2.22014 -1.82695
H  -3.01010 -3.28308 -2.07572
H  -4.03791 -1.94830 -1.54904
H  -2.71191 -1.61555 -2.68217
H   1.76480 -4.65198 -0.72312
C   2.24081  0.62454 -0.67449
C   3.45799  1.29309 -0.51426
C   1.02384  1.33353 -0.65837
C   3.47673  2.67178 -0.34104
H   4.38799  0.73190 -0.49039
C   1.07285  2.72775 -0.50662
H   0.00238  1.07301 -1.23207
C   2.28043  3.39110 -0.33655
H   4.42411  3.18533 -0.20943
H   0.12146  3.25393 -0.55288
H   2.29792  4.47026 -0.21822
C   3.15507 -1.63062 -1.38285
C   3.01787 -3.01073 -1.37580
H   3.75045 -3.63543 -1.87623
H   3.97747 -1.14994 -1.89961
C  -1.91371  0.83858  1.87367
H  -2.80064  1.22030  1.38393
C   0.58900 -0.18338  2.77097
H   1.55917 -0.59292  3.02892
```

C

SCF (wB97X-D) Energy = -1263.20755585
Enthalpy 0K = -1262.824443
Enthalpy 298K = -1262.797801
Free Energy 298K = -1262.881432
Lowest Frequency = 24.9426 cm^{-1}
Second Frequency = 38.6740 cm^{-1}

C 3.59756 -0.04531 0.98658
Ru -0.27919 -0.71579 -0.63460
C -1.37616 -2.51638 -1.52579
C -0.33504 -3.01830 -0.74733
C 1.27239 -1.56582 -1.94373
C 0.19893 -1.04244 -2.72900
H -2.39468 -2.83927 -1.34094
H -0.54408 -3.69656 0.06898
H 2.28089 -1.18694 -2.04168
H 0.38624 -0.25258 -3.44661
C 4.88903 0.72238 1.12603
H 5.69095 0.20454 0.60135
H 4.74772 1.71640 0.69015
H 5.14312 0.85967 2.17909
O 2.66085 0.41055 1.79652
O 3.44653 -0.95847 0.19292
C -4.16398 0.47278 0.95245
C -3.08005 -0.24345 0.47643
H -3.06369 -1.32524 0.47770
N -1.96522 0.35327 0.02940
O 0.29592 -0.58796 1.39783
C -0.31860 -1.30067 2.30465
O -1.24469 -2.07268 2.08324
C 0.20550 -1.06459 3.70991
H -0.09113 -0.06351 4.03687
H -0.20826 -1.80530 4.39379
H 1.29760 -1.09994 3.72685
H -5.04559 -0.05159 1.30036
C -0.55432 2.20657 -0.37563
C -0.23436 3.56848 -0.42316
C 0.38040 1.21307 -0.73568
C 1.02905 3.97046 -0.82814
H -0.96630 4.32156 -0.14438
C 1.65268 1.65112 -1.12640
H 1.77178 -0.01712 1.60934
C 1.97349 3.00424 -1.17451
H 1.28030 5.02541 -0.86740
H 2.42028 0.92337 -1.37058
H 2.97010 3.30964 -1.48274
C -1.85152 1.70169 0.07720
C -4.07525 1.86212 0.98585
C -2.91175 2.47688 0.55590
H -4.90224 2.45887 1.35707
H -2.81452 3.55481 0.59683
C 0.98742 -2.49063 -0.92272
H 1.78249 -2.75665 -0.23737
C -1.12257 -1.48617 -2.49456
H -1.94586 -1.04525 -3.04417

B′
SCF (wB97X-D) Energy = -1031.00288311
Enthalpy 0K = -1030.724361
Enthalpy 298K = -1030.703174
Free Energy 298K = -1030.774334
Lowest Frequency = 34.3316 cm^{-1}
Second Frequency = 52.0087 cm^{-1}

C -2.71468 -0.42365 -1.03008
Ru -0.38894 -0.36508 -0.12891
C -4.10072 -0.58949 -1.58351
H -4.83310 -0.15950 -0.89906
H -4.17438 -0.12912 -2.56968
H -4.30986 -1.65858 -1.68525
O -1.71296 -0.34179 -1.81278
O -2.51170 -0.39134 0.21895
C 1.92198 0.96517 -0.28909
C 2.47642 -1.05864 -1.29905
N 1.56900 -0.24865 -0.75315
O -0.37610 -2.45660 0.20443
C 0.11819 -2.28198 1.36306
O 0.40190 -1.09805 1.72188
C 0.32088 -3.44163 2.29248
H 0.53988 -4.34729 1.72516
H 1.12155 -3.22426 3.00034
H -0.60473 -3.60308 2.85303
C 0.70387 1.62781 0.25278
C 0.65964 2.14919 1.57774
C -0.37165 1.88526 -0.64097
C -0.44741 2.82941 2.00953
H 1.49714 1.96420 2.24211
C -1.49182 2.61864 -0.15869
H -0.24281 1.76646 -1.71185
C -1.54068 3.05675 1.13830
H -0.48876 3.19990 3.02871
H -2.30464 2.83429 -0.84441
H -2.40761 3.60111 1.49759
C 3.80856 -0.66885 -1.39500
C 3.23034 1.41432 -0.33290
C 4.18879 0.57442 -0.90010
H 3.48491 2.39189 0.06035
H 5.22503 0.89075 -0.95717
H 4.53343 -1.33856 -1.84265
H 2.11490 -2.02211 -1.64015

TS(**B′-C′**)
SCF (wB97X-D) Energy = -1030.96868327
Enthalpy 0K = -1030.690770
Enthalpy 298K = -1030.670095
Free Energy 298K = -1030.740563
Lowest Frequency = -65.1584 cm^{-1}
Second Frequency = 38.3893 cm^{-1}

C -2.89878 1.09298 -0.57550
Ru -0.48683 -0.27045 0.08700
C -4.35217 1.49001 -0.39129
H -4.63867 2.23597 -1.13324
H -4.98015 0.60312 -0.52002
H -4.52114 1.86897 0.61914
O -2.28987 1.36829 -1.61720
O -2.38881 0.45331 0.42314
C 2.38796 0.03084 -0.18739
C 3.18459 -2.55052 -0.63045
C 1.84930 -2.20933 -0.47480
H 1.05431 -2.94306 -0.53868
N 1.45790 -0.94815 -0.24636
O -1.35364 -2.01347 -0.62984
C -1.48277 -2.44889 0.55986
O -0.95893 -1.74059 1.47324
C -2.23394 -3.70506 0.86177
H -1.83307 -4.17771 1.75934
H -3.27978 -3.44281 1.04603
H -2.19189 -4.38547 0.01035
H 3.45683 -3.58339 -0.81259
C 1.81523 1.37401 0.03974
C 2.42819 2.30846 0.87770
C 0.57698 1.69406 -0.56312
C 1.82437 3.53853 1.10932
H 3.36117 2.05656 1.37258
C -0.01960 2.93772 -0.32545
H 0.15419 1.08687 -1.39737
C 0.60012 3.85106 0.51666
H 2.30370 4.25367 1.77011
H -0.96606 3.14430 -0.81162
H 0.13240 4.80997 0.71317
C 3.74393 -0.23929 -0.33338
C 4.14864 -1.55062 -0.55211
H 5.20045 -1.78694 -0.67241
H 4.46086 0.57290 -0.29264

C′

SCF (wB97X-D) Energy = -1030.97062306
Enthalpy 0K = -1030.691794
Enthalpy 298K = -1030.670253
Free Energy 298K = -1030.743010
Lowest Frequency = 23.9347 cm^{-1}
Second Frequency = 32.3503 cm^{-1}

C	1.58569	1.61544	1.79922
Ru	0.12291	-1.34798	-0.81356
C	1.09777	3.02439	1.99293
H	1.94120	3.71310	1.96856
H	0.41751	3.25982	1.16814
H	0.54391	3.12053	2.92870
O	0.67689	0.71140	2.16790
O	2.67022	1.32462	1.33713
C	-3.76652	-1.59354	1.11873
C	-2.53609	-1.90271	0.56450
H	-2.14421	-2.91456	0.58197
N	-1.75042	-0.98486	-0.01847
O	1.31799	-1.56740	0.83722
C	2.40644	-1.64326	0.13335
O	2.27409	-1.64340	-1.11385
C	3.72563	-1.68788	0.82579
H	3.68322	-2.37665	1.67203
H	4.51128	-1.97686	0.12858
H	3.91079	-0.67945	1.20897
H	-4.36290	-2.37124	1.58027
C	-1.18561	1.20868	-0.70057
C	-1.40522	2.56985	-0.93028
C	0.03978	0.59564	-1.05776
C	-0.40268	3.34514	-1.50002
H	-2.35350	3.03283	-0.67051
C	1.04172	1.40244	-1.61421
H	0.98214	-0.16696	1.85047
C	0.82113	2.75944	-1.83193
H	-0.57018	4.40197	-1.68106
H	2.00018	0.96011	-1.86753
H	1.60946	3.36915	-2.26403
C	-2.15960	0.31201	-0.07123
C	-4.20050	-0.27163	1.06519
C	-3.39111	0.68271	0.46899
H	-5.15792	0.01217	1.48952
H	-3.70452	1.71898	0.42850

C′ (without HOAc)
SCF (wB97X-D) Energy = -801.926072648
Enthalpy 0K = -801.711973
Enthalpy 298K = -801.696094
Free Energy 298K = -801.755940
Lowest Frequency = 38.4939 cm^{-1}
Second Frequency = 42.9476 cm^{-1}

Ru	0.70622	-0.68439	-0.65478
C	-3.21643	-2.35697	0.22577
C	-1.88777	-2.20032	-0.13090
H	-1.26611	-3.05173	-0.38869
N	-1.28158	-1.00424	-0.17493
O	1.72279	-1.15459	1.05890
C	2.85222	-0.79725	0.56739
O	2.87471	-0.40662	-0.63191
C	4.07956	-0.81367	1.42656
H	4.02161	-1.62345	2.15511
H	4.97085	-0.91131	0.80630
H	4.13401	0.13355	1.97169
H	-3.65819	-3.34589	0.24719
C	-1.19359	1.34715	0.07979
C	-1.70327	2.62409	0.33162
C	0.16834	1.15728	-0.25936
C	-0.86734	3.73023	0.25711
H	-2.75074	2.76578	0.58478
C	0.99239	2.28993	-0.32468
C	0.47906	3.55854	-0.07034
H	-1.26081	4.72256	0.45221
H	2.04165	2.16745	-0.57855
H	1.13220	4.42514	-0.12813
C	-1.98610	0.11588	0.14699
C	-3.94987	-1.21919	0.55196
C	-3.32944	0.01970	0.51283
H	-4.99359	-1.29861	0.83775
H	-3.87997	0.91649	0.77080

D⁺ (K^1)
SCF (wB97X-D) Energy = -1281.59786902
Enthalpy 0K = -1281.196122
Enthalpy 298K = -1281.170451
Free Energy 298K = -1281.250936
Lowest Frequency = 32.0699 cm^{-1}
Second Frequency = 37.3154 cm^{-1}

Ru	0.07247	-0.50656	-0.15231
O	-0.12233	-2.57744	-0.66909
C	-0.74467	-2.77497	0.41962
C	-1.33737	-4.10131	0.76471
O	-0.87993	-1.77205	1.20197
H	-2.37521	-4.11505	0.41760
H	-0.79286	-4.90228	0.26443
H	-1.34039	-4.24661	1.84562
C	-2.55848	0.83783	0.30605
C	-3.84416	0.71797	0.83506
C	-2.19888	0.01815	-0.77195
C	-4.74535	-0.18799	0.28374
H	-4.13642	1.29939	1.70320
C	-3.09582	-0.89323	-1.32100
C	-4.37753	-0.99539	-0.79080
H	-5.74037	-0.27379	0.70722
H	-2.78669	-1.51288	-2.15604
H	-5.08800	-1.69894	-1.21089
H	-1.26951	0.22972	-1.35194
C	-1.54466	1.72106	0.92039
C	-0.90146	3.65542	2.20007
H	-1.15687	4.57266	2.71900
C	-1.88610	2.89883	1.58468
H	-2.92128	3.21791	1.60298
C	0.69347	2.05018	1.44587
H	1.70629	1.67205	1.37984
C	0.41616	3.21375	2.14055
H	1.22063	3.75975	2.61828
N	-0.25227	1.31826	0.83397
C	2.00367	0.52969	-1.27897
C	2.06222	1.93309	-1.45395
C	1.26620	-0.25884	-2.19679
C	1.34422	2.53680	-2.46115
H	2.67255	2.52844	-0.78236
C	0.55669	0.39010	-3.23823
C	0.57076	1.76281	-3.34861
H	1.38486	3.61396	-2.58206
H	0.02242	-0.21545	-3.96283
H	0.01948	2.24950	-4.14588
H	1.42018	-1.33192	-2.25029
C	2.77069	-0.14934	-0.19671
C	4.61979	-0.80315	1.15649
H	5.67944	-0.78453	1.38661
C	4.12856	-0.08549	0.06582
H	4.78061	0.49619	-0.57562
C	2.39120	-1.55224	1.63272
H	1.65032	-2.08685	2.21601
C	3.74593	-1.54770	1.94276
H	4.10296	-2.11610	2.79299
N	1.93326	-0.85638	0.58896

TS(**D⁺-E⁺**) (K^1)
SCF (wB97X-D) Energy = -1281.55351714
Enthalpy 0K = -1281.157821
Enthalpy 298K = -1281.132389
Free Energy 298K = -1281.212672
Lowest Frequency = -1177.6862 cm^{-1}
Second Frequency = 34.4799 cm^{-1}

Ru	0.10281	0.01648	-0.34275
O	0.72138	-1.83744	1.84349
C	-0.20556	-1.08350	2.23480
C	-0.84739	-1.30970	3.56971
O	-0.67110	-0.12777	1.52115
H	-1.67671	-2.00956	3.42806
H	-0.13337	-1.75602	4.26115
H	-1.24873	-0.37794	3.96786
C	-2.88435	-0.43020	-0.42937
C	-3.98760	-0.87836	0.29494
C	-1.88449	-1.35221	-0.77717
C	-4.08861	-2.21782	0.66126
H	-4.75203	-0.17639	0.61192
C	-1.98648	-2.69092	-0.41330
C	-3.09115	-3.12517	0.31343
H	-4.94904	-2.55237	1.23099
H	-1.21087	-3.39174	-0.70021
H	-3.17674	-4.16712	0.60139
H	-1.08691	-1.07828	-1.50977
C	-2.69844	0.99969	-0.75210
C	-3.50497	3.17870	-1.36656
H	-4.32105	3.85085	-1.60803
C	-3.75995	1.85180	-1.05208
H	-4.77158	1.46347	-1.06259
C	-1.17931	2.72928	-1.08039
H	-0.13643	3.02866	-1.08583
C	-2.18757	3.62723	-1.38638
H	-1.94057	4.65113	-1.63928
N	-1.42138	1.44767	-0.75938
C	2.93414	-0.44386	-0.56722
C	4.06744	-0.81670	-1.28808
C	1.77661	-1.26652	-0.54719
C	4.08033	-2.02493	-1.97737
H	4.93417	-0.16453	-1.33458
C	1.83088	-2.48561	-1.23828
C	2.96541	-2.86042	-1.95128
H	4.96270	-2.31520	-2.53742
H	0.97905	-3.15812	-1.20053
H	2.98490	-3.80556	-2.48366
H	1.08011	-1.42181	0.64764
C	2.83844	0.81682	0.18607
C	3.66897	2.68902	1.44002
H	4.49660	3.26961	1.83258
C	3.91209	1.55718	0.67513
H	4.92542	1.22795	0.47913
C	1.32724	2.28747	1.20069
H	0.28372	2.51046	1.39149
C	2.35438	3.05644	1.71887
H	2.12510	3.91864	2.33297
N	1.56511	1.21011	0.43530

E⁺ (K^1)
SCF (wB97xD) Energy = -1281.56435281
Enthalpy 0K = -1281.163440
Enthalpy 298K = -1281.137509
Free Energy 298K = -1281.219354
Lowest Frequency = 29.6633 cm^{-1}
Second Frequency = 36.0593 cm^{-1}

Ru	0.13015	0.08973	-0.43279
O	0.71962	-1.98048	1.84423
C	-0.20614	-1.14335	2.20029
C	-0.86015	-1.39994	3.51446
O	-0.56828	-0.19029	1.48367
H	-1.62047	-2.17265	3.36244
H	-0.13444	-1.77389	4.23707
H	-1.34495	-0.49449	3.87554
C	-2.86502	-0.55440	-0.38004
C	-3.88708	-1.11114	0.38818
C	-1.81822	-1.38361	-0.81471
C	-3.86705	-2.46508	0.71263
H	-4.68492	-0.48014	0.76658
C	-1.80317	-2.73866	-0.49708
C	-2.82717	-3.28106	0.27454
H	-4.66675	-2.88300	1.31504
H	-0.99796	-3.37044	-0.85414
H	-2.81837	-4.33645	0.52406
H	-1.08224	-1.02329	-1.57392
C	-2.82095	0.89643	-0.66726
C	-3.85261	2.99994	-1.19766
H	-4.73603	3.59688	-1.39634
C	-3.97037	1.64718	-0.91084
H	-4.94062	1.16426	-0.90221
C	-1.48719	2.76338	-0.99628
H	-0.47796	3.16178	-1.03124
C	-2.58482	3.57110	-1.24666
H	-2.44393	4.61949	-1.48047
N	-1.59327	1.45906	-0.70035
C	2.99920	-0.34293	-0.55083
C	4.21723	-0.81919	-1.03573
C	1.78929	-1.06977	-0.72216
C	4.26787	-2.04591	-1.68883
H	5.12905	-0.24003	-0.92475
C	1.88563	-2.30337	-1.38582
C	3.10277	-2.78802	-1.86249
H	5.21388	-2.41953	-2.06534
H	0.99209	-2.90237	-1.54328
H	3.14215	-3.74428	-2.37462
H	1.05820	-1.70415	0.94434
C	2.85798	0.93373	0.16277
C	3.60924	2.86328	1.38907
H	4.41321	3.47150	1.78909
C	3.89719	1.71379	0.66918
H	4.92425	1.40643	0.51504
C	1.28871	2.41154	1.07629
H	0.23606	2.62555	1.22285
C	2.27964	3.21586	1.60955
H	2.01198	4.09314	2.18555
N	1.56774	1.31306	0.35534

D⁺ (K^2)
SCF (wB97X-D) Energy = -1281.59084445
Enthalpy 0K = -1281.189536
Enthalpy 298K = -1281.163829
Free Energy 298K = -1281.244617
Lowest Frequency = 27.8340 cm^{-1}
Second Frequency = 40.4578 cm^{-1}

Ru	0.27764	0.75780	0.03348
O	1.13925	2.33204	1.18268
C	1.15845	3.10387	0.16818
C	1.66016	4.50892	0.27502
O	0.71177	2.63825	-0.92886
H	2.09330	4.82869	-0.67329
H	0.81682	5.16780	0.50324
H	2.38653	4.59159	1.08381
C	-2.42987	-0.10065	0.93982
C	-3.74080	-0.47799	0.65251
C	-1.95538	1.12642	0.44161
C	-4.56067	0.36513	-0.09448
H	-4.12126	-1.43842	0.98466
C	-2.77594	1.97353	-0.30105

```
C  -4.08588  1.58747 -0.57051
H  -5.57942  0.06212 -0.31169
H  -2.38229  2.91665 -0.66356
H  -4.73606  2.23548 -1.14790
H  -1.05393  1.60578  0.94035
C  -1.48398 -0.94182  1.69674
C  -0.91373 -2.54892  3.38877
H  -1.20596 -3.26897  4.14508
C  -1.87794 -1.87008  2.65763
H  -2.93215 -2.02898  2.85123
C   0.75631 -1.33621  2.18597
H   1.78473 -1.06848  1.97664
C   0.42877 -2.26513  3.15923
H   1.21480 -2.74562  3.72910
N  -0.17108 -0.70634  1.44904
C   1.94688 -1.13211 -1.07180
C   2.62685 -2.14992 -0.39427
C   2.43064  0.19200 -1.01847
C   3.75026 -1.84449  0.36176
H   2.25687 -3.16905 -0.44317
C   3.54387  0.48647 -0.21248
C   4.19252 -0.52218  0.48210
H   4.27825 -2.63752  0.88153
H   3.91069  1.50595 -0.16708
H   5.05821 -0.29347  1.09363
H   2.07335  0.93803 -1.72356
C   0.70233 -1.40537 -1.82646
C  -0.65227 -2.54090 -3.43549
H  -0.78811 -3.30970 -4.18814
C   0.56438 -2.40848 -2.77530
H   1.40602 -3.05321 -3.00126
C  -1.47611 -0.68993 -2.15730
H  -2.25338  0.01421 -1.88978
C  -1.68254 -1.66041 -3.12731
H  -2.64069 -1.71614 -3.62969
N  -0.31014 -0.57050 -1.50625
```

TS(**D⁺-E⁺**) (K^2)
SCF (wB97X-D) Energy = -1281.55634948
Enthalpy 0K = -1281.160437
Enthalpy 298K = -1281.134910
Free Energy 298K = -1281.215529
Lowest Frequency = -1277.5340 cm^{-1}
Second Frequency = 21.4066 cm^{-1}

```
Ru  0.01426  0.68614 -0.01114
O   0.84995  2.44311 -1.20698
C   0.55743  3.23598 -0.19529
C   0.70295  4.70434 -0.39809
O   0.16371  2.71305  0.86309
H   0.07582  5.01673 -1.23721
H   0.42171  5.24325  0.50509
H   1.73823  4.92815 -0.66830
C   2.43330 -0.83153 -0.62529
C   3.69481 -1.38862 -0.42263
C   2.06653  0.36628  0.03309
C   4.60993 -0.75367  0.41271
H   3.97201 -2.32595 -0.89442
C   3.00352  0.98678  0.86988
C   4.26879  0.43358  1.05572
H   5.59075 -1.19110  0.56500
H   2.73422  1.90313  1.38754
H   4.98553  0.92399  1.70623
H   1.47675  1.46625 -0.74359
C   1.39522 -1.44531 -1.46714
C   0.56535 -2.93132 -3.16731
H   0.72655 -3.72970 -3.88332
C   1.61217 -2.47566 -2.38054
H   2.60261 -2.90040 -2.48888
C  -0.84231 -1.31712 -2.11433
H  -1.79147 -0.81205 -1.98294
C  -0.68480 -2.33360 -3.04035
H  -1.52574 -2.64026 -3.65033
N   0.16167 -0.89219 -1.33126
C  -2.59865 -0.28496  0.71078
C  -3.51090 -1.01871 -0.05456
C  -2.51131  1.10801  0.53961
C  -4.28701 -0.37883 -1.01359
H  -3.58467 -2.09323  0.08172
C  -3.27556  1.73547 -0.45062
C  -4.15094  0.99356 -1.23404
H  -4.99216 -0.95375 -1.60486
H  -3.20667  2.81101 -0.57541
H  -4.74913  1.48270 -1.99497
H  -1.95673  1.71500  1.25022
C  -1.69068 -0.96166  1.66580
C  -1.17519 -2.45005  3.47034
H  -1.48307 -3.15863  4.23128
C  -2.11482 -1.87218  2.62516
H  -3.17062 -2.10247  2.71065
C   0.52017 -1.18498  2.34864
H   1.54881 -0.88203  2.19939
C   0.16167 -2.09468  3.33123
H   0.92706 -2.51341  3.97332
N  -0.38660 -0.63258  1.52552
```

E⁺ (K^2)
SCF (wB97X-D) Energy = -1281.57817780
Enthalpy 0K = -1281.176214
Enthalpy 298K = -1281.149986
Free Energy 298K = -1281.232974
Lowest Frequency = 29.0488 cm^{-1}
Second Frequency = 33.0345 cm^{-1}

```
Ru -0.19611 -0.31516 -0.51601
O  -2.37192 -2.37388 -2.07540
C  -1.40148 -3.01450 -1.45580
C  -1.37707 -4.48329 -1.71793
O  -0.58417 -2.45114 -0.72316
H  -0.51236 -4.93507 -1.23625
H  -2.29741 -4.93293 -1.33577
H  -1.35191 -4.66245 -2.79558
C  -2.19656  1.70391  0.02061
C  -3.42499  2.28144  0.34511
C  -2.03267  0.29691 -0.02240
C  -4.51935  1.47788  0.64622
H  -3.54176  3.36046  0.37536
C  -3.14759 -0.48468  0.31927
C  -4.37624  0.09449  0.64157
H  -5.47278  1.93006  0.89580
H  -3.06059 -1.56835  0.37079
H  -5.22044 -0.53902  0.89614
H  -2.42590 -1.45388 -1.75638
C  -0.98579  2.48591 -0.26854
C   0.29424  4.49209 -0.63188
H   0.35825  5.57400 -0.67530
C  -0.90932  3.87668 -0.32190
H  -1.79193  4.47400 -0.12999
C   1.27724  2.32922 -0.82858
H   2.11190  1.67192 -1.03785
C   1.41003  3.70489 -0.89864
H   2.36613  4.14115 -1.16055
N   0.11920  1.72881 -0.50687
C   2.65901 -0.54435  0.43080
C   3.75366  0.31914  0.53492
C   2.39730 -1.17507 -0.79493
C   4.55536  0.57018 -0.57388
H   3.95736  0.81986  1.47629
C   3.19340 -0.90361 -1.90800
C   4.26896 -0.02707 -1.80115
```

H 5.40069 1.24416 -0.48319
H 2.98594 -1.40085 -2.84975
H 4.89282 0.17766 -2.66437
H 1.63283 -1.94705 -0.85800
C 1.77341 -0.76272 1.59842
C 1.41464 -1.21080 3.93295
H 1.79844 -1.41546 4.92624
C 2.28328 -1.01778 2.86805
H 3.35711 -1.08278 3.00016
C -0.40292 -0.88681 2.41295
H -1.45742 -0.81218 2.18469
C 0.04673 -1.14668 3.69651
H -0.67423 -1.29209 4.49181
N 0.43839 -0.69113 1.38058

D⁺ (η^6)
SCF (wB97X-D) Energy = -1281.60720683
Enthalpy 0K = -1281.205053
Enthalpy 298K = -1281.179558
Free Energy 298K = -1281.260352
Lowest Frequency = 15.1794 cm^{-1}
Second Frequency = 39.1796 cm^{-1}

Ru -1.32163 0.16826 -0.62955
O -2.85990 1.33783 0.24579
C -3.30804 0.33715 0.89503
C -4.42106 0.47620 1.87830
O -2.73006 -0.77345 0.68197
H -3.99962 0.77209 2.84402
H -5.11325 1.25448 1.55524
H -4.93833 -0.47521 2.00213
C 0.88677 -1.48208 1.37033
C 2.16911 -1.92276 1.02917
C -0.18257 -2.38149 1.33421
C 2.37242 -3.23233 0.60398
H 3.00224 -1.22751 1.06525
C 0.02566 -3.69197 0.91648
C 1.29823 -4.11698 0.53824
H 3.36890 -3.56266 0.32952
H -0.80789 -4.38652 0.89768
H 1.45582 -5.13963 0.21169
H -1.17524 -2.05545 1.62201
C 0.70394 -0.06415 1.76903
C 1.38440 1.79749 3.14615
H 2.00588 2.21100 3.93320
C 1.50907 0.46689 2.77767
H 2.21539 -0.18701 3.27537
C -0.32927 2.00210 1.50298
H -1.07357 2.57869 0.96974
C 0.44135 2.58152 2.49454
H 0.29771 3.62667 2.74002
N -0.21046 0.71004 1.13782
C 0.52586 0.31496 -1.85505
C 0.12967 -1.05374 -1.77139
C -0.41318 1.28951 -2.27865
C -1.19150 -1.42647 -2.10881
H 0.80339 -1.79533 -1.35959
C -1.73272 0.89233 -2.63626
C -2.12917 -0.46278 -2.57408
H -1.51195 -2.44675 -1.93094
H -2.46958 1.65369 -2.86621
H -3.15395 -0.74590 -2.77793
H -0.12933 2.33429 -2.26205
C 1.87713 0.75226 -1.40558
C 4.23093 0.40839 -1.16626
H 5.12411 -0.18960 -1.31276
C 2.99382 -0.05635 -1.60274
H 2.90518 -1.01873 -2.09427
C 3.12483 2.38687 -0.40739
H 3.13946 3.36695 0.06132
C 4.29920 1.64791 -0.54435
H 5.24051 2.04630 -0.18375
N 1.93849 1.96037 -0.83422

TS(**D⁺–E⁺**) (η^6)
SCF (wB97X-D) Energy = -1281.57865237
Enthalpy 0K = -1281.177677
Enthalpy 298K = -1281.152433
Free Energy 298K = -1281.233627
Lowest Frequency = -98.1259 cm^{-1}
Second Frequency = 15.0295 cm^{-1}

Ru 0.53682 -0.68549 -0.27276
O 0.65941 -1.83984 1.43399
C 1.87019 -2.29249 1.59867
C 2.05505 -3.19248 2.79468
O 2.79304 -1.98970 0.83732
H 3.06920 -3.58917 2.81176
H 1.86822 -2.62440 3.71005
H 1.33066 -4.00967 2.76522
C 1.49303 2.05240 0.33895
C 1.66560 3.08308 -0.58541
C 2.46521 1.04422 0.44964
C 2.79343 3.09276 -1.40263
H 0.91470 3.86210 -0.67792
C 3.58917 1.05680 -0.37814
C 3.75043 2.07957 -1.30721
H 2.92702 3.89478 -2.12128
H 4.32587 0.26780 -0.27340
H 4.62590 2.10192 -1.94745
H 2.40519 0.29781 1.23818
C 0.27204 1.91894 1.16479
C -1.37937 2.64878 2.73635
H -1.81218 3.41974 3.36465
C -0.26590 2.92951 1.95163
H 0.20470 3.90581 1.96487
C -1.33592 0.40451 1.90956
H -1.70804 -0.61141 1.85039
C -1.91394 1.36458 2.72611
H -2.76614 1.10242 3.34108
N -0.28523 0.69093 1.13002
C -1.24254 -0.74324 -1.49998
C -0.35401 0.22484 -2.07501
C -0.75646 -2.06402 -1.25824
C 0.97576 -0.12414 -2.35286
H -0.65722 1.25974 -2.17396
C 0.57800 -2.42839 -1.60995
C 1.44812 -1.45809 -2.12444
H 1.67704 0.64779 -2.64973
H 0.95681 -3.40711 -1.34256
H 2.50024 -1.68475 -2.24285
H -1.40580 -2.76026 -0.74177
C -2.62900 -0.38871 -1.08183
C -4.58725 0.98441 -1.16738
H -5.13344 1.83519 -1.56028
C -3.29225 0.71977 -1.60423
H -2.83246 1.35202 -2.35505
C -4.42834 -0.95514 0.21729
H -4.85054 -1.65084 0.93720
C -5.16851 0.13592 -0.23533
H -6.17597 0.30224 0.12799
N -3.18885 -1.21585 -0.19066

E⁺ (η^6)
SCF (wB97X-D) Energy = -1281.59826073
Enthalpy 0K = -1281.196238
Enthalpy 298K = -1281.170509
Free Energy 298K = -1281.253104
Lowest Frequency = 15.7734 cm^{-1}
Second Frequency = 20.4594 cm^{-1}

```
Ru  0.29096 -0.83875 -0.01359
O   0.98068 -0.61740  2.03214
C   2.07225 -0.39975  2.56805
C   2.21387 -0.30179  4.05258
O   3.19139 -0.23752  1.90970
H   2.58081  0.69424  4.31341
H   1.25575 -0.48637  4.53391
H   2.95900 -1.02323  4.39623
C   2.12096  1.26744 -0.98710
C   3.22062  1.86503 -1.60680
C   2.03906 -0.13588 -0.82495
C   4.27203  1.08122 -2.06630
H   3.26947  2.94214 -1.73375
C   3.12356 -0.89717 -1.28349
C   4.22641 -0.29910 -1.89560
H   5.12623  1.54582 -2.54609
H   3.11819 -1.97691 -1.16075
H   5.05041 -0.91594 -2.24024
H   3.02823 -0.28874  0.94311
C   1.00329  2.02273 -0.41120
C  -0.18316  3.98811  0.30570
H  -0.27053  5.06769  0.36496
C   0.90115  3.41196 -0.33815
H   1.67322  4.03479 -0.77267
C  -0.99527  1.79537  0.78043
H  -1.71088  1.10784  1.21790
C  -1.14510  3.16701  0.88774
H  -1.99757  3.57496  1.41679
N   0.03791  1.24026  0.12830
C  -1.93431 -1.32525 -0.50070
C  -1.08105 -1.22254 -1.65662
C  -1.54498 -2.16376  0.55083
C   0.05415 -2.05409 -1.79263
H  -1.30809 -0.51064 -2.44075
C  -0.33268 -2.91167  0.44977
C   0.42933 -2.93197 -0.73570
H   0.67951 -1.96691 -2.67306
H   0.00470 -3.48297  1.30727
H   1.32049 -3.54193 -0.80865
H  -2.13334 -2.17732  1.45942
C  -3.18185 -0.52097 -0.38795
C  -5.06277  0.60895 -1.34759
H  -5.63646  0.93373 -2.20897
C  -3.88566 -0.11348 -1.52003
H  -3.54526 -0.37469 -2.51559
C  -4.72322  0.43821  1.01017
H  -5.02735  0.63640  2.03439
C  -5.49245  0.89428 -0.05895
H  -6.40449  1.45125  0.12173
N  -3.59446 -0.25115  0.85821
```

D

```
SCF (wB97X-D) Energy = -1510.23153545
Enthalpy 0K = -1509.779421
Enthalpy 298K = -1509.748256
Free Energy 298K = -1509.842455
Lowest Frequency = 18.4317 cm-1
Second Frequency = 24.2832 cm-1

Ru  1.03879  0.14624 -0.28346
O   2.32121  1.39909 -1.50775
C   2.11611  0.62064 -2.48374
C   2.86682  0.77691 -3.77357
O   1.27921 -0.32773 -2.33834
H   2.26667  0.41681 -4.61039
H   3.15342  1.81863 -3.92254
H   3.77631  0.17161 -3.71588
C  -2.27986 -0.22115 -1.22174
C  -3.28007 -0.77257 -0.41877
C  -1.73994 -0.97520 -2.26636
C  -3.72980 -2.06904 -0.64870
H  -3.68951 -0.18865  0.40100
C  -2.20505 -2.26378 -2.50441
C  -3.19928 -2.81312 -1.69862
H  -4.49462 -2.49629 -0.00792
H  -1.78234 -2.84215 -3.31988
H  -3.55592 -3.82155 -1.88435
H  -0.93965 -0.55978 -2.86845
C  -1.86520  1.19274 -1.02787
C  -2.48121  3.52468 -1.04900
H  -3.23135  4.30425 -1.13264
C  -2.83925  2.18854 -1.13383
H  -3.86740  1.89270 -1.30841
C  -0.22744  2.80111 -0.76363
H   0.82889  2.99418 -0.62443
C  -1.13851  3.83694 -0.88181
H  -0.79200  4.86243 -0.83242
N  -0.57017  1.49974 -0.80420
C  -0.55856  0.34464  2.24688
C  -1.49988  0.99801  3.04120
C   0.57396  1.04124  1.79008
C  -1.29846  2.32460  3.41047
H  -2.40313  0.48152  3.35357
C   0.78599  2.35706  2.19733
C  -0.15227  3.00154  2.99721
H  -2.03607  2.83015  4.02563
H   1.69161  2.86572  1.88285
H   0.00959  4.03022  3.30377
H   1.52391  0.45930  1.48032
C  -0.71260 -1.04344  1.78807
C  -1.44672 -3.31978  1.97503
H  -1.97916 -4.10235  2.50531
C  -1.40749 -2.03016  2.48300
H  -1.88327 -1.78615  3.42589
C  -0.10333 -2.57239  0.14434
H   0.43767 -2.72100 -0.78260
C  -0.77868 -3.59674  0.78656
H  -0.77704 -4.59104  0.35637
N  -0.08275 -1.32082  0.62363
O   2.65087 -1.12906 -0.06322
C   3.32879 -1.18292  1.03408
C   4.51845 -2.12607  0.97364
O   3.08490 -0.54024  2.06008
H   4.21213 -3.09614  0.57466
H   5.26758 -1.71348  0.29154
H   4.95819 -2.24641  1.96385
```

TS(**D-E**)

```
SCF (wB97X-D) Energy = -1510.19384855
Enthalpy 0K = -1509.746329
Enthalpy 298K = -1509.715342
Free Energy 298K = -1509.808936
Lowest Frequency = -1250.9548 cm-1
Second Frequency = 25.0805 cm-1

Ru -0.82326 -0.20278  0.64539
O  -2.02400  0.45123  2.31485
C  -1.21600 -0.06983  3.14235
C  -1.54107 -0.08327  4.61058
O  -0.15084 -0.60763  2.71153
H  -2.13757  0.79096  4.87502
H  -2.13203 -0.97828  4.82756
H  -0.62667 -0.12081  5.20399
C   2.43496  1.02833  0.42929
C   3.33669  0.90921 -0.63092
C   2.62198  0.26318  1.58339
C   4.41044  0.02935 -0.54360
H   3.18291  1.49371 -1.53353
C   3.70534 -0.60474  1.67186
```

```
C   4.60122 -0.72351  0.61192
H   5.09671 -0.06819 -1.37878
H   3.84592 -1.19267  2.57345
H   5.44444 -1.40348  0.68476
H   1.90407  0.32983  2.39384
C   1.35450  2.04513  0.37470
C   0.75822  4.37467  0.15195
H   1.03146  5.40565 -0.04698
C   1.71244  3.37150  0.11654
H   2.75415  3.59655 -0.08119
C  -0.84173  2.69546  0.70663
H  -1.84500  2.37680  0.95696
C  -0.54668  4.02726  0.47783
H  -1.33505  4.76710  0.54884
N   0.07131  1.70447  0.62732
C  -0.89334  0.20799 -2.27516
C  -1.11738  0.91171 -3.45715
C  -1.79054  0.31431 -1.18824
C  -2.25785  1.69947 -3.58727
H  -0.40585  0.86453 -4.27678
C  -2.93891  1.09552 -1.35468
C  -3.17484  1.78464 -2.54181
H  -2.43262  2.24468 -4.50965
H  -3.65272  1.15640 -0.53671
H  -4.07006  2.38904 -2.65430
H  -2.09452 -0.84960 -0.47767
C   0.26562 -0.67136 -2.05269
C   2.07280 -2.10242 -2.72990
H   2.70551 -2.52324 -3.50439
C   1.07894 -1.19321 -3.05644
H   0.90361 -0.91552 -4.08907
C   1.39884 -1.91963 -0.45007
H   1.48071 -2.16551  0.60224
C   2.22732 -2.48607 -1.40221
H   2.97809 -3.20612 -1.10078
N   0.46059 -1.01531 -0.75765
O  -2.22796 -1.86201  0.37102
C  -1.76392 -3.02018 -0.09219
C  -1.59291 -4.05290  1.00112
O  -1.50450 -3.23220 -1.25950
H  -1.23388 -4.99332  0.58315
H  -0.88308 -3.67051  1.74112
H  -2.54454 -4.20879  1.51565
```

E
SCF (wB97X-D) Energy = -1510.22502637
Enthalpy 0K = -1509.771997
Enthalpy 298K = -1509.740527
Free Energy 298K = -1509.836658
Lowest Frequency = 14.6062 cm^{-1}
Second Frequency = 17.2370 cm^{-1}

```
Ru  0.73903  0.36678  0.13378
O   1.98168  1.33861  1.59531
C   1.34543  2.44020  1.61883
C   1.79883  3.53369  2.55411
O   0.33760  2.61319  0.88077
H   1.06179  3.64474  3.35489
H   2.77034  3.29735  2.98825
H   1.84608  4.48346  2.01684
C  -2.61164  0.08284  0.89859
C  -3.60950 -0.63294  0.23396
C  -2.55829  1.47398  0.77003
C  -4.53551  0.02950 -0.56588
H  -3.64441 -1.71467  0.32633
C  -3.49520  2.13379 -0.01911
C  -4.48295  1.41515 -0.69031
H  -5.29656 -0.53776 -1.09224
H  -3.44976  3.21464 -0.10981
H  -5.21108  1.93415 -1.30619
H  -1.76911  2.03104  1.26421
C  -1.68934 -0.61452  1.83014
C  -1.43924 -1.96088  3.81912
H  -1.86870 -2.55214  4.62104
C  -2.24904 -1.37539  2.85955
H  -3.32807 -1.46910  2.90439
C   0.42484 -0.99317  2.68705
H   1.48429 -0.80443  2.58521
C  -0.07023 -1.74233  3.73960
H   0.61748 -2.14807  4.47208
N  -0.35028 -0.45967  1.71878
C   1.00158 -2.28344 -1.06273
C   1.50921 -3.56393 -1.30268
C   1.61197 -1.39714 -0.14128
C   2.65396 -3.99097 -0.64247
H   1.02312 -4.23429 -2.00740
C   2.78253 -1.85433  0.48943
C   3.29521 -3.12611  0.24595
H   3.05145 -4.98414 -0.82589
H   3.29947 -1.19636  1.18704
H   4.20146 -3.45010  0.75172
H   3.02243  0.85091 -1.19983
C  -0.14393 -1.70884 -1.77180
C  -1.86436 -1.63511 -3.45919
H  -2.42574 -2.11192 -4.25642
C  -0.86820 -2.32993 -2.79314
H  -0.63153 -3.35000 -3.07210
C  -1.39248  0.23404 -2.05799
H  -1.58386  1.24160 -1.70871
C  -2.12294 -0.31632 -3.09680
H  -2.88843  0.27372 -3.58613
N  -0.43966 -0.43551 -1.39302
O   2.13214  1.18459 -1.38716
C   2.24642  2.43558 -1.93982
C   0.91268  3.04809 -2.22682
O   3.33163  2.90613 -2.14811
H   0.39313  3.20499 -1.27587
H   1.05976  3.99206 -2.74892
H   0.31557  2.36325 -2.83377
```

E (without HOAc)
SCF (wB97X-D) Energy = -1281.18852399
Enthalpy 0K = -1280.800337
Enthalpy 298K = -1280.774667
Free Energy 298K = -1280.856045
Lowest Frequency = 29.6866 cm^{-1}
Second Frequency = 35.7005 cm^{-1}

```
Ru -0.25838 -0.73067 -0.10231
O  -0.75090 -2.73641  0.59580
C  -1.05398 -3.06715 -0.59431
C  -1.63893 -4.42216 -0.88084
O  -0.89026 -2.22547 -1.52727
H  -1.43139 -4.71633 -1.91039
H  -1.24841 -5.16135 -0.17974
H  -2.72408 -4.36547 -0.75052
C   2.68199 -0.09357  0.66347
C   3.78982  0.64818  0.24509
C   2.37402 -1.28645 -0.00387
C   4.56388  0.21401 -0.82667
H   4.02078  1.59130  0.73098
C   3.14230 -1.71341 -1.08276
C   4.23892 -0.96256 -1.49849
H   5.41395  0.80671 -1.14939
H   2.87474 -2.63055 -1.59634
H   4.83686 -1.29105 -2.34226
H   1.56349 -1.92807  0.35998
C   1.80863  0.40324  1.75310
C   1.49687  1.46680  3.88897
H   1.89906  1.93535  4.78084
```

C 2.34241 1.00692 2.89028
H 3.41899 1.09042 2.98771
C -0.34135 0.68432 2.57376
H -1.40011 0.53205 2.40297
C 0.12722 1.29933 3.72312
H -0.58065 1.63503 4.47192
N 0.47145 0.24137 1.59516
C -2.29911 1.26366 -0.51161
C -3.53532 1.91047 -0.40178
C -2.07777 -0.00919 0.06930
C -4.57921 1.30366 0.28149
H -3.69242 2.88963 -0.84738
C -3.15747 -0.60356 0.74642
C -4.38489 0.04236 0.85133
H -5.53855 1.80376 0.36841
H -3.01868 -1.58214 1.19927
H -5.20319 -0.43828 1.38199
C -1.14992 1.81046 -1.23446
C 0.01276 3.39758 -2.62829
H 0.03365 4.33299 -3.17821
C -1.12634 3.01723 -1.93882
H -2.00798 3.64705 -1.94960
C 1.04519 1.37647 -1.89373
H 1.87835 0.68442 -1.85983
C 1.12141 2.55500 -2.61542
H 2.03032 2.79889 -3.15269
N -0.04767 1.01010 -1.20457

$^3D^+$
SCF (wB97X-D) Energy = -1679.81781561
Enthalpy 0K = -1679.272031
Enthalpy 298K = -1679.231939
Free Energy 298K = -1679.345742
Lowest Frequency = 23.4779 cm^{-1}
Second Frequency = 28.4121 cm^{-1}

Ru 0.23298 0.92178 0.45406
C 1.25489 -1.90806 -1.44547
C 0.45070 -3.02740 -1.21368
C 2.60543 -1.95450 -1.10205
C 0.97516 -4.15248 -0.58720
H -0.59049 -3.02391 -1.52188
C 3.12959 -3.08233 -0.47777
C 2.31533 -4.17868 -0.20997
H 0.33777 -5.01098 -0.40246
H 4.18345 -3.11012 -0.21926
H 2.72816 -5.05990 0.27056
H 3.24077 -1.11171 -1.34740
C 0.71397 -0.75435 -2.22481
C 0.12335 0.05921 -4.42630
H 0.05776 -0.08286 -5.49960
C 0.62589 -0.93819 -3.60801
H 0.96726 -1.88049 -4.02003
C -0.17684 1.36179 -2.45538
H -0.49611 2.27162 -1.96576
C -0.28612 1.24328 -3.82838
H -0.68442 2.06848 -4.40687
N 0.30232 0.39703 -1.64444
C -2.71060 -1.07978 0.25375
C -2.64304 -0.91262 -1.13010
C -3.90813 -0.78530 0.91334
C -3.74079 -0.43534 -1.83849
H -1.73174 -1.15340 -1.66018
C -5.00759 -0.30862 0.20626
C -4.92552 -0.12995 -1.17339
H -3.67210 -0.31739 -2.91518
H -5.93278 -0.09007 0.73051
H -5.78713 0.22719 -1.72884
H -3.97430 -0.92785 1.98812
C -1.58762 -1.66181 1.04060
C -0.85441 -3.48514 2.44642
H -1.04830 -4.42523 2.95197
C -1.84169 -2.87080 1.69315
H -2.82169 -3.32077 1.58388
C 0.57952 -1.67418 1.84859
H 1.53934 -1.17004 1.85668
C 0.38686 -2.87079 2.51684
H 1.21051 -3.30711 3.06898
N -0.38013 -1.05727 1.12773
O 2.20881 0.38714 0.84563
C 3.26592 0.73916 0.18210
C 4.55522 0.34476 0.88565
O 3.28750 1.29878 -0.91418
H 4.57786 -0.74194 1.01362
H 5.42071 0.66269 0.30451
H 4.59312 0.78837 1.88426
N 0.98906 2.75550 -0.04126
C 1.67543 3.61322 -0.38601
C 2.64922 4.58222 -0.85943
H 2.93623 5.26293 -0.05583
H 3.51929 4.00801 -1.19100
H 2.24535 5.15642 -1.69528
N 0.20938 1.44112 2.42516
C 0.26865 1.68589 3.54951
C 0.35807 1.99225 4.97071
H 0.06090 3.02795 5.14815
H -0.29967 1.32866 5.53598
H 1.38630 1.85182 5.31098
N -1.65260 1.68385 0.25575
C -2.64521 2.26543 0.16791
C -3.90369 2.98917 0.05833
H -3.73634 4.05839 0.20503
H -4.33793 2.81643 -0.92836
H -4.60124 2.62113 0.81336

INT(**$^3D^+$**)
SCF (wB97X-D) Energy = -1679.79669129
Enthalpy 0K = -1679.251386
Enthalpy 298K = -1679.211136
Free Energy 298K = -1679.325834
Lowest Frequency = 23.5847 cm^{-1}
Second Frequency = 30.1154 cm^{-1}

Ru 0.31147 0.78616 0.28207
C -2.06232 -0.89246 -1.57255
C -1.41715 -2.01496 -2.06587
C -1.43517 0.36898 -1.68368
C -0.15376 -1.90945 -2.66698
H -1.90936 -2.97974 -1.99473
C -0.17612 0.47005 -2.27651
C 0.46625 -0.68132 -2.77549
H 0.32384 -2.79907 -3.06532
H 0.24089 1.45284 -2.46590
H 1.43561 -0.59054 -3.25570
H -1.93744 1.28272 -1.37389
C -3.39754 -1.01310 -0.93555
C -5.61679 -0.19403 -0.51684
H -6.39408 0.55127 -0.65194
C -4.37149 -0.02261 -1.10692
H -4.16084 0.85220 -1.71182
C -4.82205 -2.26586 0.36002
H -4.96675 -3.17467 0.93920
C -5.85289 -1.33977 0.23741
H -6.81167 -1.52013 0.71011
N -3.62229 -2.11834 -0.20734
C 2.94987 -1.56090 0.09935
C 2.75600 -2.79725 -0.51919
C 3.05568 -1.49735 1.48930
C 2.63249 -3.95187 0.24704
H 2.68999 -2.84951 -1.60168

C 2.93588 -2.65123 2.25523
C 2.71697 -3.87988 1.63627
H 2.48407 -4.91045 -0.24051
H 3.02573 -2.59583 3.33532
H 2.63315 -4.78242 2.23320
H 3.23391 -0.53896 1.96451
C 3.15602 -0.34336 -0.72595
C 4.57450 0.80809 -2.30529
H 5.43991 0.82844 -2.95902
C 4.27309 -0.32354 -1.56411
H 4.90709 -1.20185 -1.60039
C 2.65027 1.82885 -1.32940
H 1.97260 2.66369 -1.19195
C 3.75228 1.91726 -2.16296
H 3.94620 2.84341 -2.69087
N 2.31919 0.71688 -0.64017
O 0.34835 2.83418 -0.10065
C -0.67885 3.58590 -0.38068
C -0.32766 5.06188 -0.44766
O -1.82713 3.19698 -0.58265
H -1.20182 5.64562 -0.73398
H 0.03916 5.39968 0.52546
H 0.47659 5.22447 -1.17061
N -1.50669 0.96753 1.17172
C -2.54502 1.10706 1.64597
C -3.87509 1.33261 2.18683
H -3.81323 1.59173 3.24554
H -4.33693 2.15559 1.63636
H -4.47959 0.43134 2.06262
N 1.15675 1.25460 2.00689
C 1.63401 1.63117 2.98541
C 2.24805 2.11200 4.21522
H 3.29447 1.80123 4.25396
H 2.19850 3.20259 4.24641
H 1.72046 1.70349 5.07965
N 0.11118 -1.20545 0.69705
C -0.27503 -2.27728 0.86836
C -0.83084 -3.61196 1.01184
H -0.77218 -3.93818 2.05201
H -1.87443 -3.56325 0.67997
H -0.26667 -4.30668 0.38670

TS(^{3}D$^+$–^{3}E$^+$) (* single point)
SCF (wB97xD) Energy = -1679.75418333
Enthalpy 0K = -1679.217108
Enthalpy 298K = -1679.180823
Free Energy 298K = -1679.279942
Lowest Frequency = -1261.0555 cm^{-1}
Second Frequency = 49.5529 cm^{-1}

^{3}E$^+$
SCF (wB97X-D) Energy = -1679.78218743
Enthalpy 0K = -1679.236663
Enthalpy 298K = -1679.196662
Free Energy 298K = -1679.311253
Lowest Frequency = 18.9951 cm^{-1}
Second Frequency = 25.0306 cm^{-1}

Ru -0.24433 -0.85491 0.38274
C 1.60719 0.80324 -1.61094
C 1.83548 1.41196 -2.85533
C 0.45909 0.00285 -1.38424
C 0.97127 1.23152 -3.92564
H 2.71902 2.03288 -2.97971
C -0.34901 -0.21030 -2.52774
C -0.11758 0.38107 -3.76420
H 1.16358 1.71962 -4.87534
H -1.21616 -0.85979 -2.44132
H -0.78995 0.18451 -4.59417
H 1.40694 -1.74678 -1.62889
C 2.72905 0.98759 -0.63238
C 5.01844 0.49777 -0.04604
H 5.95634 -0.01725 -0.23165
C 3.92565 0.29645 -0.87671
H 3.98689 -0.37719 -1.72527
C 3.67048 2.03150 1.17894
H 3.54085 2.74975 1.98673
C 4.88971 1.38444 1.01941
H 5.71489 1.58974 1.69252
N 2.61347 1.85494 0.37982
C -2.29272 2.06982 -0.13795
C -1.33753 2.63353 -0.98346
C -2.76736 2.81017 0.95018
C -0.83193 3.90231 -0.71653
H -0.99133 2.08976 -1.85202
C -2.27102 4.08382 1.20700
C -1.29504 4.63021 0.37531
H -0.08140 4.32298 -1.37719
H -2.65420 4.65330 2.04835
H -0.90962 5.62625 0.56999
H -3.53095 2.38443 1.59524
C -2.93934 0.75309 -0.41143
C -4.98969 -0.36566 -1.04805
H -6.02337 -0.32903 -1.37489
C -4.27577 0.79877 -0.82403
H -4.73331 1.77048 -0.96831
C -3.02020 -1.55591 -0.43113
H -2.48621 -2.48296 -0.26908
C -4.34182 -1.57589 -0.83763
H -4.84117 -2.52598 -0.98685
N -2.30568 -0.42846 -0.22597
O -0.37037 -2.80243 -0.59566
C 0.46268 -3.33628 -1.33476
C 0.34858 -4.76567 -1.75785
O 1.50528 -2.70979 -1.82106
H 0.09139 -4.79947 -2.82036
H 1.31057 -5.26821 -1.63888
H -0.42167 -5.26989 -1.17734
N 1.59383 -1.38164 1.02595
C 2.62192 -1.69011 1.44878
C 3.92948 -2.06811 1.96484
H 4.37850 -1.21240 2.47301
H 3.83362 -2.90181 2.66368
H 4.57740 -2.36151 1.13597
N -1.11535 -1.79025 2.12580
C -1.61586 -2.27830 3.04394
C -2.25317 -2.89174 4.20214
H -1.77206 -2.54344 5.11849
H -3.31049 -2.61970 4.22898
H -2.16518 -3.97860 4.14288
N -0.04541 0.83200 1.41231
C 0.22255 1.77621 2.01304
C 0.60805 2.98598 2.71893
H 1.31250 2.74302 3.51772
H 1.08215 3.65474 1.99682
H -0.27193 3.47456 3.13981

^{6}F^{2+} (* single point)
SCF (wB97X-D) Energy = -890.854320318
Enthalpy 0K = -890.564279
Enthalpy 298K = -890.539014
Free Energy 298K = -890.616052
Lowest Frequency = 73.4098 cm^{-1}
Second Frequency = 73.4231 cm^{-1}

^{3}A^{2+} (* single point)
SCF (wB97X-D) Energy = -724.782615317
Enthalpy 0K = -724.534247
Enthalpy 298K = -724.516129
Free Energy 298K = -724.577820

Lowest Frequency = 76.7675 cm^{-1}
Second Frequency = 76.8180 cm^{-1}

$^5F^+$ (κ^1) (* single point)
SCF (wB97X-D) Energy = -986.824841951
Enthalpy 0K = -986.530770
Enthalpy 298K = -986.504783
Free Energy 298K = -986.583452
Lowest Frequency = 71.3830 cm^{-1}
Second Frequency = 72.7236 cm^{-1}

$^4F^+$ (κ^2) (* single point)
SCF (wB97X-D) Energy = -854.101039471
Enthalpy 0K = -853.854538
Enthalpy 298K = -853.833075
Free Energy 298K = -853.902123
Lowest Frequency = 72.9526 cm^{-1}
Second Frequency = 74.7472 cm^{-1}

f-**^3F** ($\kappa^2\kappa^1$)
SCF (wB97X-D) Energy = -949.979833956
Enthalpy 0K = -949.731548
Enthalpy 298K = -949.705834
Free Energy 298K = -949.789619
Lowest Frequency = 30.7627 cm^{-1}
Second Frequency = 37.9375 cm^{-1}

Ru	-0.44573	-0.00994	0.00003
N	-2.04821	-1.21305	0.00016
C	-3.00631	-1.85754	0.00023
N	0.58537	-1.04263	1.38154
C	1.44366	-1.43296	2.04354
N	0.58529	-1.04287	-1.38124
C	1.44327	-1.43336	-2.04356
C	-4.22014	-2.66321	0.00053
H	-4.81524	-2.43953	-0.88785
H	-3.96563	-3.72550	-0.00078
H	-4.81364	-2.44133	0.89044
C	2.64315	-1.80466	2.77518
H	2.59535	-1.44136	3.80378
H	2.77858	-2.88800	2.77957
H	3.47764	-1.32806	2.25165
C	2.64232	-1.80541	-2.77572
H	2.59407	-1.44222	-3.80434
H	3.47725	-1.32898	-2.25276
H	2.77749	-2.88878	-2.78010
O	-1.53804	1.46561	-1.09211
C	-1.86396	2.02538	-0.00016
O	-1.53805	1.46570	1.09184
C	-2.58353	3.34321	-0.00020
H	-3.19487	3.44202	0.89790
H	-1.83636	4.14232	-0.00017
H	-3.19482	3.44201	-0.89833
O	1.08979	1.39242	-0.00008
C	2.36198	1.19712	0.00004
O	2.96245	0.11353	0.00013
C	3.15170	2.50347	-0.00008
H	2.88426	3.09583	0.87938
H	4.22408	2.30341	0.00023
H	2.88472	3.09535	-0.88001

m-**^3F** ($\kappa^2\kappa^1$) (* single point)
SCF (wB97X-D) Energy = -949.964521272
Enthalpy 0K = -949.715140
Enthalpy 298K = -949.692687
Free Energy 298K = -949.763990
Lowest Frequency = 68.7412 cm^{-1}
Second Frequency = 73.5359 cm^{-1}

c-**^2F** ($2\kappa^2$)
SCF (wB97X-D) Energy = -817.255814478
Enthalpy 0K = -817.054858
Enthalpy 298K = -817.034030
Free Energy 298K = -817.107876
Lowest Frequency = 12.9419 cm^{-1}
Second Frequency = 37.5746 cm^{-1}

Ru	-0.00006	0.08602	-0.00001
N	1.26578	-1.28192	-0.68445
C	2.03674	-2.02977	-1.10903
N	-1.26569	-1.28221	0.68422
C	-2.03646	-2.03024	1.10885
C	3.00833	-2.96184	-1.66526
H	3.73766	-2.41725	-2.26943
H	3.53253	-3.48347	-0.86125
H	2.50365	-3.69616	-2.29733
C	-3.00769	-2.96273	1.66500
H	-3.77791	-2.41158	2.20949
H	-3.48087	-3.53569	0.86430
H	-2.51335	-3.65227	2.35320
O	1.47678	1.61381	-0.26925
C	1.89659	1.41642	0.91228
C	2.95662	2.29955	1.50613
H	3.49242	1.77224	2.29626
H	3.64471	2.63657	0.72944
H	2.47341	3.17986	1.94046
O	1.37617	0.47981	1.59392
O	-1.37620	0.48003	-1.59390
C	-1.89680	1.41641	-0.91209
O	-1.47708	1.61362	0.26950
C	-2.95679	2.29962	-1.50588
H	-3.64471	2.63685	-0.72914
H	-2.47352	3.17979	-1.94044
H	-3.49278	1.77227	-2.29586

t-**^2F** ($2\kappa^2$)
SCF (wB97X-D) Energy = -817.257141315
Enthalpy 0K = -817.056112
Enthalpy 298K = -817.035201
Free Energy 298K = -817.109430
Lowest Frequency = 20.4590 cm^{-1}
Second Frequency = 20.8161 cm^{-1}

Ru	0.00692	0.00114	0.00001
N	2.01052	-0.00095	0.00005
C	3.16383	-0.00371	0.00006
N	-1.99668	0.00163	-0.00004
C	-3.15013	0.00006	-0.00007
C	4.62003	-0.00848	-0.00004
H	4.99051	-0.52006	0.89110
H	4.99037	-0.52423	-0.88883
H	4.99384	1.01777	-0.00248
C	-4.60639	-0.00294	-0.00003
H	-4.97922	1.02368	0.00071
H	-4.97758	-0.51540	-0.89038
H	-4.97753	-0.51666	0.88962
O	0.00727	-1.85615	1.08787
C	0.00203	-2.50655	-0.00000
C	-0.04487	-4.00971	-0.00001
H	0.43528	-4.40212	-0.89741
H	0.43459	-4.40213	0.89775
H	-1.09045	-4.33240	-0.00044
O	0.00732	-1.85615	-1.08787
O	0.00982	1.85839	1.08788
C	0.00555	2.50877	0.00001
O	0.00987	1.85840	-1.08786
C	-0.03903	4.01202	0.00003
H	0.44088	4.40371	-0.89782
H	-1.08409	4.33640	0.00061
H	0.44181	4.40369	0.89739

c-**^{4}F** ($2\kappa^1$)
SCF (wB97X-D) Energy = -1082.70066035
Enthalpy 0K = -1082.405114
Enthalpy 298K = -1082.374467
Free Energy 298K = -1082.468708
Lowest Frequency = 28.4081 cm^{-1}
Second Frequency = 34.4688 cm^{-1}

N	-1.11210	1.69230	0.17399
C	-1.97001	2.42265	-0.05829
N	1.35695	0.74384	1.59191
C	2.35498	1.11041	2.03567
N	1.11208	-1.69192	0.17450
C	1.96966	-2.42277	-0.05742
C	-3.14693	3.19508	-0.41784
H	-2.92185	3.87342	-1.24312
H	-3.90276	2.46800	-0.72983
H	-3.51255	3.76955	0.43545
C	3.69290	1.53358	2.41452
H	3.71122	2.60127	2.64224
H	4.04841	0.97276	3.28122
H	4.33048	1.32647	1.54943
C	3.14621	-3.19597	-0.41655
H	2.92082	-3.87458	-1.24152
H	3.90247	-2.46948	-0.72887
H	3.51148	-3.77024	0.43703
O	-3.28263	-0.17140	-0.62434
C	-2.46434	-0.70660	-1.38722
O	-1.18966	-0.79133	-1.24551
C	-2.95167	-1.36091	-2.67866
H	-2.51492	-0.84179	-3.53662
H	-2.61059	-2.39877	-2.72331
H	-4.04026	-1.32360	-2.74116
O	1.18970	0.79131	-1.24574
C	2.46435	0.70620	-1.38759
O	3.28263	0.17120	-0.62456
C	2.95163	1.35947	-2.67957
H	2.60889	2.39669	-2.72611
H	4.04032	1.32371	-2.74121
H	2.51641	0.83828	-3.53706
Ru	0.00009	0.00018	0.28210
N	-1.35674	-0.74318	1.59219
C	-2.35476	-1.10965	2.03607
C	-3.69266	-1.53273	2.41508
H	-4.04826	-0.97148	3.28147
H	-4.33021	-1.32611	1.54985
H	-3.71092	-2.60030	2.64336

t-**^{4}F** ($2\kappa^1$) (* single point)
SCF (wB97X-D) Energy = -1082.68973779
Enthalpy 0K = -1082.392272
Enthalpy 298K = -1082.365533
Free Energy 298K = -1082.445936
Lowest Frequency = 70.0770 cm^{-1}

^{1}A
SCF (wB97X-D) Energy = -916.698126403
Enthalpy 0K = -916.442327
Enthalpy 298K = -916.423144
Free Energy 298K = -916.486949
Lowest Frequency = 79.3554 cm^{-1}
Second Frequency = 84.9786 cm^{-1}

Ru	0.25672	0.02914	-0.09363
O	1.40150	0.84278	1.53467
C	1.85571	1.76416	0.75653
C	2.73288	2.87000	1.28088
C	-1.02505	-1.83843	0.15046
C	-0.59810	-1.34082	1.43752
C	-1.57065	-0.69617	2.28559
C	-2.87753	-0.53777	1.86833
O	1.49793	1.72569	-0.48223
H	2.10027	3.72426	1.57869
H	3.29198	2.52909	2.16470
H	3.42336	3.21313	0.49593
C	-3.30747	-1.05730	0.60518
C	-2.41273	-1.70885	-0.22035
H	-2.74949	-2.15628	-1.16126
H	-3.60327	-0.03885	2.51954
H	-0.43094	-2.59871	-0.36734
H	-1.25685	-0.34525	3.27404
C	-1.54777	1.12182	-1.42143
O	-1.36766	1.41656	-0.18261
O	-0.81060	0.18084	-1.91843
C	-2.53269	1.87078	-2.27903
H	-2.83352	1.26043	-3.14286
H	-3.41277	2.15384	-1.68239
H	-2.06018	2.79636	-2.65149
H	0.31420	-1.73008	1.90354
H	-4.35960	-0.96469	0.31441
N	1.71181	-1.18393	-0.45689
C	2.61542	-1.90135	-0.70401
C	3.73741	-2.75110	-1.08696
H	4.32325	-2.27701	-1.89410
H	4.40964	-2.92799	-0.22959
H	3.37953	-3.72966	-1.45106

^{1}A$^+$ (* single point)
SCF (wB97X-D) Energy = -688.071761864
Enthalpy 0K = -687.867219
Enthalpy 298K = -687.852816
Free Energy 298K = -687.906545
Lowest Frequency = 86.6244 cm^{-1}
Second Frequency = 96.6078 cm^{-1}

^{1}B$^+$ (t-O,t-N) (* single point)
SCF (wB97X-D) Energy = -1167.28011091
Enthalpy 0K = -1166.904208
Enthalpy 298K = -1166.880090
Free Energy 298K = -1166.954284
Lowest Frequency = 66.2851 cm^{-1}
Second Frequency = 79.8151 cm^{-1}

TS(**^{1}B$^+$**-**^{1}C$^+$**) (t-O,t-N) (* single point)
SCF (wB97X-D) Energy = -1167.24614610
Enthalpy 0K = -1166.872940
Enthalpy 298K = -1166.847121
Free Energy 298K = -1166.928501
Lowest Frequency = -1108.4338 cm^{-1}
Second Frequency = 37.3798 cm^{-1}

^{1}C$^+$ (t-O,t-N)
SCF (wB97X-D) Energy = -1167.26180468
Enthalpy 0K = -1166.883460
Enthalpy 298K = -1166.856719
Free Energy 298K = -1166.942673
Lowest Frequency = 9.5538 cm^{-1}
Second Frequency = 32.1144 cm^{-1}

Ru	-0.27367	0.16408	-0.17987
O	-1.28062	2.09886	-0.39274
C	-0.90712	3.06699	-1.06048
C	-1.80600	4.21604	-1.37940
C	-0.91892	0.52858	1.94611
C	-2.34345	0.59571	2.10684
C	-3.08059	-0.54734	2.20968
C	-2.44605	-1.82461	2.17396
O	0.30688	3.18556	-1.55598
H	-1.79829	4.40037	-2.45621

H -2.81660 4.00861 -1.03384
H -1.42139 5.11687 -0.89348
C 2.61846 -0.04947 -0.00656
C 3.95795 0.28948 0.19366
C 1.56925 0.86405 0.27400
C 4.29102 1.54187 0.69786
H 4.75345 -0.41543 -0.02801
C 1.94353 2.10381 0.81550
C 3.28216 2.44402 1.01931
H 5.33146 1.80488 0.85327
H 1.17898 2.82621 1.09757
H 3.53570 3.41418 1.43540
H 0.89931 2.50508 -1.17744
C -1.09248 -1.92164 2.03578
C -0.28964 -0.73814 1.90674
H 0.77340 -0.81461 2.11038
H -3.04570 -2.72026 2.30336
H -0.33224 1.41157 2.17539
H -4.15413 -0.49082 2.35998
C 2.18435 -1.38158 -0.45336
C 2.48176 -3.66708 -1.15383
H 3.13225 -4.49454 -1.41588
C 3.02377 -2.44412 -0.79157
H 4.09804 -2.31052 -0.76842
C 0.31103 -2.73591 -0.83916
H -0.77071 -2.79120 -0.83045
C 1.09752 -3.82249 -1.17368
H 0.63463 -4.76371 -1.44361
N 0.83435 -1.54599 -0.49671
H -2.81591 1.56894 2.17726
H -0.59950 -2.88754 2.07324
N -2.17000 -0.63008 -0.90281
C -3.19526 -0.97057 -1.30890
C -4.49929 -1.39911 -1.79442
H -5.05239 -0.53824 -2.17596
H -4.37900 -2.13144 -2.59551
H -5.06225 -1.85143 -0.97489

$^1B^+$ (t-O,t-C6H6)
SCF (wB97X-D) Energy = -1167.28294922
Enthalpy 0K = -1166.904320
Enthalpy 298K = -1166.877854
Free Energy 298K = -1166.961280
Lowest Frequency = 29.9475 cm^{-1}
Second Frequency = 42.3707 cm^{-1}

Ru 0.36062 0.05357 -0.12568
O 1.85679 -1.42010 -0.41869
C 2.05392 -1.02108 -1.60687
C 3.08859 -1.65108 -2.48187
C 1.60544 1.46957 1.33289
C 2.43486 0.71456 2.21060
C 3.66714 0.28124 1.79773
C 4.14487 0.61220 0.50723
O 1.35217 -0.03534 -2.01580
H 4.04746 -1.16057 -2.28714
H 3.19499 -2.70967 -2.24220
H 2.83751 -1.51196 -3.53367
C -2.30781 -0.62027 -0.64907
C -3.11707 -1.39802 0.18124
C -1.31141 -1.23577 -1.43275
C -2.90207 -2.76863 0.26784
H -3.88704 -0.92241 0.78105
C -1.09378 -2.61697 -1.31428
C -1.87341 -3.37723 -0.45506
H -3.53361 -3.37055 0.91388
H -0.32364 -3.08711 -1.91564
H -1.70317 -4.44416 -0.36417
H -0.82533 -0.68284 -2.23202
C 3.37129 1.34867 -0.35208
C 2.07245 1.76816 0.04087
H 1.56378 2.48322 -0.59514
H 5.13982 0.29663 0.21050
H 0.75123 1.99513 1.74774
H 4.29583 -0.29276 2.46971
C -2.39399 0.85871 -0.62088
C -3.53288 2.96198 -0.71927
H -4.43414 3.54654 -0.86726
C -3.56972 1.57504 -0.80188
H -4.48976 1.04459 -1.01957
C -1.18845 2.80269 -0.26934
H -0.23210 3.25844 -0.04308
C -2.32014 3.58454 -0.44725
H -2.24253 4.66242 -0.37145
N -1.21380 1.46476 -0.35580
H 2.08732 0.50626 3.21666
H 3.73757 1.62759 -1.33349
N -0.39778 -0.46338 1.67452
C -0.81103 -0.88411 2.66587
C -1.32751 -1.43965 3.90846
H -0.64173 -2.20303 4.28277
H -1.43220 -0.65187 4.65751
H -2.30395 -1.89426 3.72734

TS(**$^1B^+$**-**$^1C^+$**) (t-O,t-C6H6) (* single point)
SCF (wB97X-D) Energy = -1167.24848144
Enthalpy 0K = -1166.875601
Enthalpy 298K = -1166.849492
Free Energy 298K = -1166.932450
Lowest Frequency = -1288.2245 cm^{-1}
Second Frequency = 25.0436 cm^{-1}

$^1C^+$ (t-O,t-C6H6)

SCF (wB97X-D) Energy = -1167.28867385
Enthalpy 0K = -1166.910046
Enthalpy 298K = -1166.883275
Free Energy 298K = -1166.968966
Lowest Frequency = 17.2162 cm^{-1}
Second Frequency = 28.0733 cm^{-1}

Ru -0.27010 -0.35462 0.37884
O -2.32644 0.28186 0.57107
C -2.80798 1.40717 0.69575
C -4.24155 1.63342 1.04616
C -1.80453 -3.01187 0.30641
C -3.07169 -2.67127 -0.12345
C -3.24544 -1.88569 -1.27764
C -2.14905 -1.43128 -1.98030
O -2.11559 2.51584 0.51904
H -4.72490 0.68237 1.25996
H -4.31253 2.30074 1.90811
H -4.74204 2.12799 0.20920
C 1.85792 0.78727 -1.22330
C 2.49078 1.58015 -2.18514
C 0.45663 0.83457 -1.04556
C 1.74266 2.42336 -2.99588
H 3.56777 1.53722 -2.31769
C -0.27972 1.65974 -1.90523
C 0.35655 2.45045 -2.86217
H 2.23360 3.03924 -3.74102
H -1.36589 1.66802 -1.86254
H -0.23710 3.08384 -3.51436
H -1.21670 2.29493 0.21459
C -0.84159 -1.74962 -1.54784
C -0.66875 -2.55900 -0.40921
H 0.29995 -3.00306 -0.20695
H -2.27750 -0.84461 -2.88391
H -1.67307 -3.66605 1.16218
H -4.24720 -1.65168 -1.62217

C 2.55354 -0.18818 -0.38098
C 4.44997 -1.38585 0.49457
H 5.51869 -1.56862 0.52378
C 3.93137 -0.41581 -0.34704
H 4.58954 0.16841 -0.97843
C 2.23066 -1.84986 1.22869
H 1.51099 -2.38537 1.84017
C 3.58447 -2.12041 1.30365
H 3.94766 -2.88579 1.97843
N 1.72234 -0.91733 0.40606
H -3.94057 -3.03355 0.41606
H 0.00074 -1.52925 -2.19401
N 0.24233 0.99302 1.76764
C 0.60502 1.74062 2.57074
C 1.05524 2.68349 3.58445
H 0.40930 3.56439 3.58294
H 1.01925 2.21343 4.56984
H 2.08106 2.99104 3.36999

$^1B^+$ (t-O,t-O)
SCF (wB97X-D) Energy = -1167.28834726
Enthalpy 0K = -1166.910118
Enthalpy 298K = -1166.883509
Free Energy 298K = -1166.968966
Lowest Frequency = 19.7563 cm^{-1}
Second Frequency = 21.0677 cm^{-1}

Ru -0.47417 0.28228 0.20451
O -2.11865 1.14723 -0.69978
C -2.92645 0.61958 0.14629
C -4.39863 0.84104 0.03701
C -0.86602 -1.30358 -1.82058
C -0.31373 -2.05911 -0.77941
C -1.14078 -2.91178 -0.01469
C -2.48373 -3.01010 -0.30441
O -2.41113 -0.10816 1.04145
H -4.86944 0.73367 1.01429
H -4.60668 1.82270 -0.39010
H -4.81164 0.08101 -0.63287
C 2.51127 -0.62423 0.35090
C 3.46609 -1.63079 0.19043
C 1.55220 -0.76864 1.36446
C 3.46167 -2.74481 1.02593
H 4.19168 -1.57095 -0.61421
C 1.54363 -1.88278 2.19706
C 2.50238 -2.87705 2.02721
H 4.20514 -3.52156 0.88284
H 0.78919 -1.96535 2.97197
H 2.50353 -3.74994 2.67071
H 0.87737 0.06324 1.64495
C -3.03100 -2.27229 -1.37044
C -2.23878 -1.42680 -2.11915
H -2.65915 -0.86267 -2.94389
H -3.11985 -3.66937 0.27598
H -0.22330 -0.73953 -2.48828
H -0.70135 -3.50079 0.78307
C 2.41901 0.49822 -0.60859
C 3.35786 2.05184 -2.18621
H 4.21503 2.47743 -2.69631
C 3.52992 1.03496 -1.25829
H 4.52006 0.66450 -1.02045
C 1.01126 1.95907 -1.75774
H -0.01294 2.28416 -1.90942
C 2.07300 2.51915 -2.44713
H 1.89146 3.30799 -3.16697
N 1.17727 0.97246 -0.86019
H 0.76119 -2.13795 -0.67745
H -4.08359 -2.38332 -1.61190
N -0.41900 1.94066 1.31575
C -0.45106 2.90719 1.94369
C -0.50014 4.12291 2.74266
H -1.01940 4.90649 2.18656
H -1.03540 3.92757 3.67450
H 0.51417 4.45606 2.97246

$^1B^+$ (t-C6H6,t-O)
SCF (wB97X-D) Energy = -1167.29430147
Enthalpy 0K = -1166.915623
Enthalpy 298K = -1166.889045
Free Energy 298K = -1166.973509
Lowest Frequency = 26.6697 cm^{-1}
Second Frequency = 29.0078 cm^{-1}

Ru 0.29919 0.16080 0.20162
O 1.32611 1.83434 0.86918
C 1.79689 2.05276 -0.30256
C 2.74396 3.17635 -0.55839
C 2.30217 -0.97145 1.26656
C 1.87723 -1.77295 0.19653
C 2.64018 -1.79691 -0.99462
C 3.77459 -1.02656 -1.11010
O 1.43132 1.25108 -1.21370
H 2.62416 3.54451 -1.57781
H 2.59332 3.97713 0.16623
H 3.76403 2.79671 -0.44741
C -1.96006 -0.80501 -0.97986
C -2.69133 -1.85063 -0.39293
C -0.87323 -1.09922 -1.82341
C -2.32830 -3.16630 -0.62328
H -3.53719 -1.61492 0.24567
C -0.54025 -2.44008 -2.06945
C -1.24666 -3.46386 -1.46177
H -2.89435 -3.97121 -0.16617
H 0.26001 -2.66682 -2.76484
H -0.98306 -4.49771 -1.65752
H -0.38614 -0.31073 -2.38893
C 4.19802 -0.22371 -0.03345
C 3.48008 -0.20095 1.14185
H 3.81461 0.39585 1.98277
H 4.35810 -1.05219 -2.02404
H 1.83329 -1.05798 2.23972
H 2.33990 -2.44703 -1.80816
C -2.33609 0.61102 -0.73491
C -3.77724 2.51661 -0.71398
H -4.73405 2.98352 -0.92054
C -3.57738 1.16955 -1.00179
H -4.35817 0.55927 -1.44102
C -1.52428 2.63099 0.09182
H -0.68395 3.14226 0.54626
C -2.73624 3.25673 -0.16312
H -2.85664 4.30659 0.07517
N -1.33909 1.33537 -0.19240
H 1.08495 -2.50290 0.33746
H 5.11069 0.35690 -0.12438
N -0.64184 -0.55837 1.84064
C -1.17226 -0.93956 2.79220
C -1.83385 -1.41318 4.00003
H -2.11617 -0.56219 4.62381
H -2.72983 -1.97904 3.73592
H -1.15641 -2.05926 4.56273

TS(**$^1B^+$-$^1C^+$**)1 (t-C6H6,t-O) (*single point)
SCF (wB97xD) Energy = -1167.25015778
Enthalpy 0K = -1166.874375
Enthalpy 298K = -1166.850545
Free Energy 298K = -1166.924671
Lowest Frequency = -64.8529 cm^{-1}
Second Frequency = 68.7960 cm^{-1}

INT(**$^1B^+$-$^1C^+$**) (t-C6H6,t-O)

SCF (wB97X-D) Energy = -1167.25368197
Enthalpy 0K = -1166.876255
Enthalpy 298K = -1166.849444
Free Energy 298K = -1166.934637
Lowest Frequency = 25.9508 cm^{-1}
Second Frequency = 33.3073 cm^{-1}

C	1.66550	-1.28555	-1.62893
N	0.56917	-0.94798	-0.92815
C	-0.56151	-1.68927	-1.04835
C	-0.59813	-2.77587	-1.91968
C	0.52419	-3.11024	-2.66019
C	1.68095	-2.35236	-2.50812
Ru	0.60366	0.55600	0.42164
C	-1.69824	3.02233	0.60311
C	-0.53940	2.75026	-0.14768
C	-0.63027	1.99526	-1.33165
C	-1.88632	1.52145	-1.75146
C	-3.01801	1.79892	-1.00825
C	-2.92363	2.54871	0.17254
H	0.21722	1.91774	-2.00417
C	-1.68952	-1.29859	-0.19003
C	-3.01430	-1.62007	-0.47856
C	-4.02740	-1.22612	0.39094
C	-3.73232	-0.49833	1.54127
C	-2.41330	-0.15862	1.82747
C	-1.39751	-0.54832	0.95988
H	-3.82038	2.76898	0.74183
O	2.00528	-0.35757	1.54268
C	1.83340	-1.55096	2.06840
O	0.81090	-2.21192	1.94290
C	3.03435	-2.03602	2.84566
H	3.87682	-2.18098	2.16392
H	3.33327	-1.28671	3.58209
H	2.79905	-2.97682	3.34107
H	-3.26805	-2.16336	-1.38296
H	-5.05552	-1.49150	0.16842
H	-2.16809	0.38008	2.73638
H	-4.52732	-0.20916	2.22014
H	-1.49882	-3.37379	-1.98387
H	-0.36794	-0.70175	1.41905
H	-1.62715	3.63209	1.49753
H	-3.98580	1.44096	-1.34130
H	0.37879	3.27850	0.09534
H	-1.96405	0.96167	-2.67764
H	2.58953	-2.58703	-3.04889
H	0.50415	-3.96110	-3.33192
H	2.54295	-0.67691	-1.45778
N	2.22503	1.53969	-0.31385
C	3.18727	2.09770	-0.61870
C	4.40992	2.79393	-0.99024
H	4.53956	2.76627	-2.07431
H	4.35482	3.83397	-0.66109
H	5.26269	2.30964	-0.50923

TS(**$^1B^+$–$^1C^+$**)2 (t-C6H6,t-O)
SCF (wB97X-D) Energy = -1167.24954764
Enthalpy 0K = -1166.876530
Enthalpy 298K = -1166.851082
Free Energy 298K = -1166.932487
Lowest Frequency = -862.7425 cm^{-1}
Second Frequency = -38.8324 cm^{-1}

C	1.66595	-1.28584	-1.62841
N	0.56944	-0.94810	-0.92799
C	-0.56123	-1.68937	-1.04836
C	-0.59770	-2.77606	-1.91959
C	0.52480	-3.11057	-2.65978
C	1.68158	-2.35276	-2.50746
Ru	0.60354	0.55612	0.42152
C	-1.69806	3.02222	0.60323
C	-0.53940	2.75028	-0.14788
C	-0.63053	1.99536	-1.33189
C	-1.88665	1.52154	-1.75143
C	-3.01819	1.79894	-1.00792
C	-2.92355	2.54861	0.17291
H	0.21683	1.91783	-2.00456
C	-1.68940	-1.29866	-0.19026
C	-3.01412	-1.62018	-0.47906
C	-4.02740	-1.22645	0.39033
C	-3.73255	-0.49878	1.54081
C	-2.41361	-0.15899	1.82725
C	-1.39764	-0.54847	0.95978
H	-3.82016	2.76877	0.74246
O	2.00507	-0.35703	1.54299
C	1.83332	-1.55040	2.06879
O	0.81098	-2.21160	1.94310
C	3.03418	-2.03516	2.84639
H	3.87712	-2.17921	2.16505
H	3.33221	-1.28606	3.58340
H	2.79917	-2.97634	3.34119
H	-3.26768	-2.16338	-1.38356
H	-5.05545	-1.49187	0.16761
H	-2.16860	0.37963	2.73626
H	-4.52768	-0.20979	2.21961
H	-1.49839	-3.37395	-1.98395
H	-0.36809	-0.70170	1.41897
H	-1.62677	3.63189	1.49770
H	-3.98604	1.44100	-1.34080
H	0.37883	3.27855	0.09497
H	-1.96460	0.96184	-2.67764
H	2.59029	-2.58758	-3.04793
H	0.50487	-3.96149	-3.33142
H	2.54341	-0.67727	-1.45704
N	2.22482	1.53970	-0.31411
C	3.18706	2.09759	-0.61913
C	4.40980	2.79363	-0.99074
H	4.55999	2.73172	-2.07075
H	4.33892	3.84331	-0.69719
H	5.25788	2.33366	-0.47855

$^1C^+$ (t-C6H6,t-O) (* single point)
SCF (wB97X-D) Energy = -1167.26492497
Enthalpy 0K = -1166.889491
Enthalpy 298K = -1166.865012
Free Energy 298K = -1166.940315
Lowest Frequency = 61.0054 cm^{-1}
Second Frequency = 63.9821 cm^{-1}

$^1B^+$ (t-N,t-O) (* single point)
SCF (wB97X-D) Energy = -1167.28504978
Enthalpy 0K = -1166.908484
Enthalpy 298K = -1166.884299
Free Energy 298K = -1166.958688
Lowest Frequency = 65.9415 cm^{-1}
Second Frequency = 70.6084 cm^{-1}

TS(**$^1B^+$–$^1C^+$**) (t-N,t-O)
SCF (wB97X-D) Energy = -1167.25832691
Enthalpy 0K = -1166.881173
Enthalpy 298K = -1166.855108
Free Energy 298K = -1166.939042
Lowest Frequency = -64.3622 cm^{-1}
Second Frequency = 20.3265 cm^{-1}

C	-1.96052	-1.83057	0.51189
N	-1.32578	-0.65386	0.57388
C	-1.98448	0.44345	1.00336
C	-3.32365	0.38894	1.36397
C	-3.98719	-0.83207	1.29790

```
C  -3.29463 -1.95910  0.86965
Ru  0.63713 -0.25934  0.03579
C   0.47668 -0.51007 -2.31914
C  -0.39637 -1.57745 -2.66611
C  -1.74760 -1.36312 -2.76360
C  -2.27987 -0.06741 -2.56408
C  -1.45004  0.97794 -2.24842
C  -0.05299  0.77167 -2.07614
H  -2.40991 -2.17818 -3.03720
C  -1.16182  1.67918  0.98701
C  -1.62160  2.83127  0.33767
C  -0.79447  3.93638  0.20458
C   0.50622  3.91391  0.71727
C   0.94881  2.80440  1.41995
C   0.11877  1.68270  1.57658
H   0.60005  1.63736 -2.01115
O   1.13166 -2.28306 -0.01801
C   1.42405 -2.27763  1.22531
O   1.27993 -1.17094  1.83335
C   1.93211 -3.49993  1.91360
H   1.62849 -3.49315  2.96097
H   1.57035 -4.39657  1.40956
H   3.02552 -3.49895  1.87354
H  -2.62140  2.84302 -0.08439
H  -1.15820  4.82116 -0.30748
H   1.92731  2.80415  1.88840
H   1.14929  4.77949  0.60031
H  -3.82520  1.28733  1.70522
H   0.39804  0.91054  2.28552
H   1.54148 -0.65000 -2.46495
H  -1.84552  1.98246 -2.16245
H   0.02666 -2.55519 -2.86680
H  -3.34253  0.10330 -2.70203
H  -3.77655 -2.92730  0.80733
H  -5.03128 -0.90273  1.58270
H  -1.37094 -2.66513  0.15033
N   2.59276  0.25146 -0.34925
C   3.70216  0.51121 -0.52727
C   5.10360  0.84079 -0.74623
H   5.62971  0.86202  0.21065
H   5.56271  0.08883 -1.39161
H   5.18375  1.82011 -1.22288
```

$^{1}C^{+}$ (t-N,t-O)
SCF (wB97X-D) Energy = -1167.29579274
Enthalpy 0K = -1166.917291
Enthalpy 298K = -1166.890667
Free Energy 298K = -1166.975646
Lowest Frequency = 27.5072 cm^{-1}
Second Frequency = 29.1104 cm^{-1}

```
C  -2.17482  0.06538 -1.83743
N  -1.39923 -0.21749 -0.78081
C  -1.81784 -1.12237  0.13740
C  -3.06455 -1.73526  0.00587
C  -3.87010 -1.42822 -1.07926
C  -3.41584 -0.51553 -2.02808
Ru  0.49452  0.57171 -0.46044
C  -1.39437  3.09903 -0.65999
C  -2.58435  2.74962 -0.06544
C  -2.59309  2.09175  1.18485
C  -1.41212  1.80087  1.82430
C  -0.16765  2.12639  1.22062
C  -0.16162  2.77944 -0.03003
H  -3.53984  1.84453  1.65331
C  -0.84781 -1.36707  1.21111
C  -1.06499 -2.25359  2.26822
C  -0.09328 -2.43126  3.24596
C   1.09962 -1.71803  3.16773
C   1.32302 -0.82638  2.11706
C   0.36085 -0.63330  1.11590
H   0.74583  3.25838 -0.38884
O   1.19796 -0.87249 -1.81785
C   1.72290 -1.98609 -1.70105
O   1.94204 -2.56896 -0.55008
C   2.15264 -2.78080 -2.89002
H   1.53768 -3.68260 -2.95534
H   2.04101 -2.19022 -3.79705
H   3.18905 -3.10158 -2.76456
H  -1.99270 -2.81321  2.33894
H  -0.26531 -3.12269  4.06321
H   2.25482 -0.26920  2.08329
H   1.86154 -1.85233  3.92937
H  -3.39715 -2.45178  0.74682
H   1.59644 -2.02099  0.18751
H  -1.38633  3.64979 -1.59515
H   0.73001  2.08674  1.82764
H  -3.52507  3.00181 -0.54396
H  -1.41559  1.33308  2.80281
H  -4.00781 -0.25599 -2.89718
H  -4.84023 -1.90070 -1.18960
H  -1.77522  0.78887 -2.53931
N   2.42320  1.20477 -0.15071
C   3.51424  1.55937 -0.01313
C   4.89191  1.99838  0.16233
H   5.50125  1.16801  0.52614
H   5.29335  2.34612 -0.79214
H   4.93102  2.81543  0.88608
```

$^{4}G^{+}$ (κ^{1})
SCF (wB97X-D) Energy = -1333.32250716
Enthalpy 0K = -1332.903488
Enthalpy 298K = -1332.868300
Free Energy 298K = -1332.975486
Lowest Frequency = 17.5718 cm^{-1}
Second Frequency = 19.3905 cm^{-1}

```
N   1.91551 -2.02703  0.19800
C   2.67339 -2.89351  0.16462
N   1.17531 -0.01471  2.15432
C   1.49793  0.24315  3.22982
C   1.91491  0.57797  4.58439
H   1.82391 -0.29807  5.22990
H   2.95507  0.91076  4.57529
H   1.28556  1.37927  4.97740
C   3.64702 -3.97571  0.11567
H   3.40892 -4.65281 -0.70730
H   4.64510 -3.56032 -0.03943
H   3.63287 -4.53371  1.05417
O   1.83419  1.72773 -2.14115
C   2.67632  1.37221 -1.32029
C   4.13129  1.79384 -1.45317
H   4.77054  0.90978 -1.52827
H   4.26421  2.42198 -2.33375
H   4.44408  2.34098 -0.55953
O   2.45901  0.64591 -0.26013
N   0.39396 -0.67707 -1.78632
C   0.45084 -0.62947 -2.93429
C   0.57621 -0.41995 -4.36625
H  -0.40919 -0.32223 -4.82647
H   1.13759  0.51011 -4.49443
H   1.11385 -1.24735 -4.83271
N  -0.39525  1.49672  0.26945
C   0.39797  2.54461  0.57280
C  -1.71867  1.73516  0.13041
C  -0.06453  3.83684  0.74511
H   1.44918  2.31114  0.67632
C  -2.24939  3.01638  0.29631
C  -1.42241  4.08447  0.60373
H   0.63927  4.62666  0.97870
```

```
H  -3.31625  3.15385  0.16420
H  -1.82845  5.08302  0.72469
C  -2.67728  0.64548 -0.19791
C  -3.66258  0.30186  0.73172
C  -2.67908  0.03795 -1.45262
C  -4.61515 -0.66373  0.42129
H  -3.67952  0.79381  1.70003
C  -3.62631 -0.93320 -1.76086
H  -1.94330  0.34201 -2.18627
C  -4.59344 -1.28939 -0.82400
H  -5.38326 -0.91761  1.14541
H  -3.62429 -1.39730 -2.74193
H  -5.34374 -2.03362 -1.07214
Ru  0.70517 -0.38144  0.20476
N  -0.85734 -1.58445  0.75854
C  -1.66440 -2.35220  1.05508
C  -2.68960 -3.31757  1.42435
H  -3.20958 -3.65455  0.52554
H  -2.23515 -4.17317  1.92834
H  -3.41408 -2.84371  2.08956
```

^{3}G ($2\kappa^{1}$)
SCF (wB97X-D) Energy = -1429.19314937
Enthalpy 0K = -1428.770819
Enthalpy 298K = -1428.735115
Free Energy 298K = -1428.839768
Lowest Frequency = 21.1322 cm^{-1}
Second Frequency = 35.7936 cm^{-1}

```
N   0.99452 -0.58120  1.38714
C   1.94711 -1.01204  1.87059
N  -1.05951 -2.27557  0.61370
C  -1.05814 -3.42498  0.66086
C   3.16139 -1.65302  2.34489
H   3.49186 -2.32381  1.54676
H   3.93320 -0.90743  2.54200
H   2.96200 -2.22986  3.25052
C  -0.89864 -4.86894  0.62022
H  -0.93312 -5.29366  1.62536
H  -1.68053 -5.32287  0.00816
H   0.08032 -5.05827  0.17020
O  -3.95991  0.65750 -0.27993
C  -3.43325 -0.09535 -1.11453
O  -2.19554 -0.42463 -1.18972
C  -4.28666 -0.71673 -2.21497
H  -3.81159 -0.56396 -3.18703
H  -4.35165 -1.79716 -2.05322
H  -5.28993 -0.28855 -2.21213
O   0.45837 -1.08285 -1.43139
C   1.23806 -2.10586 -1.46444
O   1.59135 -2.82626 -0.52158
C   1.76420 -2.39231 -2.87051
H   2.38114 -1.55510 -3.21491
H   2.36098 -3.30559 -2.87868
H   0.92944 -2.48068 -3.57051
N  -0.23419  1.73025 -0.33115
C   0.93662  2.40271 -0.40220
C  -1.37113  2.43268 -0.52457
C   0.97725  3.77590 -0.65733
C  -1.39398  3.79274 -0.79192
H  -2.30039  1.87801 -0.43078
C  -0.19498  4.48645 -0.85917
H   1.94495  4.26169 -0.70971
H  -2.34926  4.28316 -0.93881
H  -0.16936  5.55154 -1.06635
C   2.24126  1.71292 -0.21315
C   2.68723  0.76064 -1.12816
C   3.07207  2.09565  0.84288
C   3.93464  0.16764 -0.96510
H   2.03230  0.46342 -1.93723
C   4.32494  1.51026  0.99888
H   2.72823  2.84619  1.54907
C   4.75634  0.54094  0.09541
H   4.26410 -0.58847 -1.67072
H   4.96444  1.81341  1.82277
H   5.73319  0.08170  0.21520
Ru -0.62443 -0.34829  0.20773
N  -1.82028  0.35126  1.66907
C  -2.69108  0.75544  2.30655
C  -3.90211  1.25995  2.93201
H  -4.25946  0.56777  3.69713
H  -3.72780  2.23852  3.38393
H  -4.64279  1.34332  2.13096
```

^{1}G ($2\kappa^{2}$) (* single point)
SCF (wB97xD) Energy = -1163.74040586
Enthalpy 0K = -1163.414453
Enthalpy 298K = -1163.390903
Free Energy 298K = -1163.464438
Lowest Frequency = 59.8125 cm^{-1}
Second Frequency = 65.3033 cm^{-1}

2G^{+} (κ^{2})
SCF (wB97X-D) Energy = -1067.85310277
Enthalpy 0K = -1067.530473
Enthalpy 298K = -1067.504877
Free Energy 298K = -1067.589833
Lowest Frequency = 15.7779 cm^{-1}
Second Frequency = 17.0123 cm^{-1}

```
Ru  0.70426 -0.24419  0.09260
N  -0.37559 -1.64400 -0.91070
C  -0.96607 -2.46180 -1.46620
C  -1.71180 -3.50068 -2.16096
H  -2.77147 -3.42241 -1.90914
H  -1.58711 -3.38693 -3.23984
H  -1.34168 -4.48224 -1.85719
O   2.12950 -1.78092  0.58362
C   2.75452 -1.51238 -0.48247
O   2.27329 -0.57891 -1.21765
C   4.01403 -2.21716 -0.87178
H   4.86973 -1.62810 -0.52854
H   4.05630 -3.19847 -0.39932
H   4.07746 -2.30555 -1.95705
N  -0.42022  1.29759 -0.73066
C  -1.70143  1.47181 -0.33301
C   0.11709  2.13220 -1.63423
C  -2.46522  2.52368 -0.83596
C  -0.59516  3.18703 -2.17985
H   1.14257  1.91867 -1.91603
C  -1.90898  3.38899 -1.76726
H  -3.47930  2.66812 -0.48241
H  -0.12431  3.83435 -2.90968
H  -2.49174  4.21312 -2.16391
C  -2.21396  0.47551  0.63000
C  -1.31147 -0.19667  1.46922
C  -3.55696  0.09777  0.65551
C  -1.73487 -1.21744  2.31390
H  -0.28695  0.21297  1.66423
C  -3.98430 -0.91746  1.50738
H  -4.26981  0.57013 -0.01276
C  -3.07858 -1.57941  2.33312
H  -1.01445 -1.71734  2.95209
H  -5.03184 -1.19968  1.51794
H  -3.41939 -2.37108  2.99140
N   1.88327  1.10811  1.05564
C   2.60128  1.84060  1.58180
C   3.51211  2.75620  2.25355
H   4.02177  2.23435  3.06649
H   4.25388  3.12583  1.54232
```

H 2.95321 3.60053 2.66264

$^3G^+$ (κ^2) (* single point)
SCF (wB97X-D) Energy = -1200.57033475
Enthalpy 0K = -1200.200328
Enthalpy 298K = -1200.173341
Free Energy 298K = -1200.253717
Lowest Frequency = 63.8071 cm^{-1}
Second Frequency = 68.6312 cm^{-1}

^1G ($\kappa^2\kappa^1$)
SCF (wB97X-D) Energy = -1163.73549072
Enthalpy 0K = -1163.409611
Enthalpy 298K = -1163.383532
Free Energy 298K = -1163.468031
Lowest Frequency = 21.1779 cm^{-1}
Second Frequency = 29.3721 cm^{-1}

Ru	-0.68947	0.35222	-0.02281
N	0.40322	1.85187	-0.80824
C	1.04949	2.71402	-1.22172
C	1.88046	3.80149	-1.71916
H	2.88043	3.72215	-1.28653
H	1.95599	3.75140	-2.80763
H	1.44520	4.76238	-1.43565
O	-2.15673	1.78972	0.67178
C	-2.79643	1.60329	-0.40117
O	-2.27850	0.84965	-1.29149
C	-4.14987	2.21168	-0.62299
H	-4.90609	1.50381	-0.27108
H	-4.24720	3.13563	-0.05176
H	-4.31646	2.39333	-1.68572
O	-1.99345	-1.10850	0.62785
C	-1.69915	-1.90814	1.59820
O	-0.63788	-1.90993	2.22908
C	-2.80880	-2.88801	1.93991
H	-3.15819	-3.39220	1.03547
H	-2.45902	-3.61920	2.66884
H	-3.65767	-2.33710	2.35511
N	0.38322	-1.12708	-0.96648
C	1.66682	-1.35410	-0.60473
C	-0.20629	-1.92393	-1.87001
C	2.39406	-2.39770	-1.17413
C	0.46560	-2.97414	-2.47359
H	-1.24077	-1.68545	-2.09030
C	1.79043	-3.21363	-2.11963
H	3.41251	-2.57905	-0.85050
H	-0.04720	-3.59315	-3.20011
H	2.34145	-4.03497	-2.56557
C	2.19131	-0.43552	0.42070
C	1.25952	0.18194	1.27245
C	3.53957	-0.08973	0.50922
C	1.68591	1.11137	2.21719
H	0.25439	-0.33018	1.46940
C	3.95728	0.84941	1.44777
H	4.26232	-0.52804	-0.17300
C	3.03276	1.45121	2.30037
H	0.95493	1.56085	2.88061
H	5.00794	1.11497	1.51147
H	3.36544	2.17914	3.03371

TS(**^1G-^1H**)
SCF (wB97X-D) Energy = -1163.72779076
Enthalpy 0K = -1163.406255
Enthalpy 298K = -1163.380669
Free Energy 298K = -1163.463653
Lowest Frequency = -1103.1881 cm^{-1}
Second Frequency = 25.9767 cm^{-1}

Ru	-0.71945	0.15335	-0.09564
N	-0.05616	1.88452	-0.83932
C	0.32870	2.89536	-1.24072
C	0.81747	4.17655	-1.73092
H	1.79833	4.38484	-1.29774
H	0.90409	4.15517	-2.81955
H	0.12601	4.97198	-1.44394
O	-2.47214	1.16041	0.67400
C	-3.09496	0.89913	-0.39870
O	-2.47713	0.32319	-1.34695
C	-4.55570	1.22929	-0.53362
H	-5.13830	0.36084	-0.21184
H	-4.81525	2.07516	0.10421
H	-4.80245	1.43985	-1.57527
O	-1.61561	-1.63181	0.54133
C	-1.20019	-2.11716	1.63361
O	-0.25203	-1.61194	2.29525
C	-1.88871	-3.34227	2.17626
H	-2.49865	-3.81458	1.40656
H	-1.14916	-4.04315	2.56738
H	-2.53245	-3.03950	3.00715
N	0.69603	-0.96562	-1.08268
C	1.97873	-0.90968	-0.64749
C	0.36577	-1.78148	-2.09494
C	2.96392	-1.69022	-1.25534
C	1.30044	-2.57566	-2.73727
H	-0.68264	-1.77124	-2.37294
C	2.62504	-2.52573	-2.30799
H	3.98160	-1.65292	-0.88444
H	0.99178	-3.22012	-3.55176
H	3.38241	-3.14025	-2.78369
C	2.18724	0.00307	0.48411
C	1.01521	0.41393	1.16177
C	3.43977	0.50826	0.83795
C	1.15890	1.32639	2.21523
H	0.14577	-0.55768	1.54298
C	3.54936	1.41976	1.88138
H	4.32998	0.21622	0.28716
C	2.40625	1.82905	2.56914
H	0.27109	1.63362	2.76061
H	4.52304	1.81275	2.15707
H	2.49356	2.53919	3.38653

^1H
SCF (wB97X-D) Energy = -1163.74556828
Enthalpy 0K = -1163.418972
Enthalpy 298K = -1163.392687
Free Energy 298K = -1163.478344
Lowest Frequency = 26.4787 cm^{-1}
Second Frequency = 26.9764 cm^{-1}

Ru	0.63280	0.22340	0.12803
N	0.53398	2.11888	-0.35622
C	0.48901	3.23212	-0.66334
C	0.44015	4.63434	-1.05506
H	-0.57306	4.89989	-1.36549
H	0.73297	5.27060	-0.21646
H	1.12253	4.81192	-1.88968
O	2.53891	0.03305	-0.85531
C	3.19441	0.30841	0.20395
O	2.59003	0.57174	1.27610
C	4.70199	0.34551	0.13911
H	5.12868	0.16343	1.12619
H	5.06993	-0.38722	-0.58108
H	5.01768	1.33816	-0.19691
O	0.91430	-1.80644	0.78583
C	0.86957	-2.82652	0.10125
O	0.45104	-2.85664	-1.14206
C	1.30385	-4.15824	0.63106
H	1.55255	-4.07103	1.68703
H	0.51150	-4.89502	0.48188

H 2.17973 -4.49507 0.07005
N -1.04252 0.30280 1.33138
C -2.24030 0.03834 0.74718
C -0.97736 0.53056 2.65071
C -3.40339 0.00086 1.52034
C -2.09738 0.51047 3.46551
H 0.01783 0.72660 3.03654
C -3.33378 0.23835 2.88409
H -4.35512 -0.21726 1.04986
H -1.99736 0.70024 4.52765
H -4.23392 0.20982 3.48986
C -2.14872 -0.17888 -0.70080
C -0.82479 -0.11922 -1.21398
C -3.25375 -0.38871 -1.52874
C -0.68985 -0.24942 -2.60910
H 0.15569 -1.95393 -1.39833
C -3.07631 -0.54153 -2.89914
H -4.25962 -0.42890 -1.11746
C -1.79163 -0.46486 -3.43621
H 0.30442 -0.17740 -3.04713
H -3.93271 -0.70970 -3.54434
H -1.64978 -0.56938 -4.50890

^{2}G ($\kappa^2\kappa^1$)
SCF (wB97X-D) Energy = -1296.46028843
Enthalpy 0K = -1296.087441
Enthalpy 298K = -1296.056013
Free Energy 298K = -1296.154312
Lowest Frequency = 17.8377 cm^{-1}
Second Frequency = 22.1201 cm^{-1}

N -1.94625 0.85923 0.99687
C -2.89640 1.32517 1.44862
C -4.13475 1.88502 1.96724
H -4.46481 1.31405 2.83768
H -3.98782 2.92700 2.25912
H -4.89932 1.83194 1.18864
O -3.13519 0.37296 -1.69212
C -2.71121 -0.78131 -1.66414
O -1.65633 -1.21569 -1.04900
C -3.44429 -1.89952 -2.39904
H -2.75990 -2.41729 -3.07698
H -3.80350 -2.63667 -1.67539
H -4.28732 -1.49522 -2.96045
O -0.58626 -1.65954 1.45929
C -0.28923 -1.49273 2.70297
O 0.18454 -0.46287 3.19642
C -0.56466 -2.71348 3.56654
H -1.61103 -3.01209 3.46249
H 0.04715 -3.55132 3.22039
H -0.33743 -2.50022 4.61129
N 1.22693 -1.14499 -0.65064
C 2.46449 -0.62409 -0.49890
C 1.07035 -2.36800 -1.17554
C 3.59143 -1.34597 -0.88966
C 2.15181 -3.12874 -1.59160
H 0.03977 -2.69835 -1.25139
C 3.43371 -2.60835 -1.44397
H 4.57860 -0.92707 -0.73258
H 1.98618 -4.11348 -2.01237
H 4.30236 -3.18454 -1.74564
C 2.51625 0.72377 0.10158
C 1.45647 1.13701 0.92937
C 3.53394 1.62819 -0.20508
C 1.44646 2.42636 1.45594
H 0.79242 0.40437 1.50284
C 3.51069 2.91806 0.31621
H 4.33295 1.33821 -0.88110
C 2.46649 3.31991 1.14623
H 0.63721 2.70996 2.12015
H 4.30713 3.61238 0.06767
H 2.45369 4.32517 1.55564
Ru -0.38695 -0.09386 0.11411
N -0.36703 1.29885 -1.35763
C -0.58199 2.01378 -2.23443
C -0.99176 2.85797 -3.34521
H -0.92290 3.91243 -3.07030
H -0.36443 2.67304 -4.21962
H -2.02974 2.60858 -3.58087

TS(**^{2}G-^{2}H**)
SCF (wB97X-D) Energy = -1296.45136620
Enthalpy 0K = -1296.082425
Enthalpy 298K = -1296.051913
Free Energy 298K = -1296.145370
Lowest Frequency = -1131.2062 cm^{-1}
Second Frequency = 23.1575 cm^{-1}

N 1.79581 -1.07128 1.12076
C 2.82618 -1.51621 1.37795
C 4.19471 -1.96668 1.56787
H 4.57029 -1.65106 2.54325
H 4.26183 -3.05348 1.48864
H 4.78456 -1.49790 0.77448
O 3.49643 0.09647 -1.05099
C 2.96992 1.19734 -0.84475
O 1.79594 1.42948 -0.36949
C 3.73934 2.47809 -1.16407
H 3.16874 3.08987 -1.86901
H 3.86333 3.06823 -0.25161
H 4.71717 2.24414 -1.58713
O 0.19183 1.24943 1.95152
C -0.60133 0.86920 2.85772
O -1.31648 -0.16871 2.75813
C -0.70813 1.69715 4.11206
H 0.00681 2.51903 4.09363
H -1.72460 2.09066 4.19520
H -0.53129 1.06175 4.98298
N -1.15785 1.20053 -0.60573
C -2.37038 0.62726 -0.79506
C -0.96481 2.49600 -0.89113
C -3.43366 1.38677 -1.28735
C -1.98176 3.29370 -1.38931
H 0.04490 2.85177 -0.71109
C -3.23819 2.72614 -1.58749
H -4.40834 0.92972 -1.41169
H -1.79031 4.33737 -1.60914
H -4.06043 3.32547 -1.96518
C -2.43519 -0.79787 -0.43553
C -1.37503 -1.29319 0.36367
C -3.43341 -1.64814 -0.91499
C -1.38365 -2.66084 0.67007
H -1.07200 -0.60458 1.51549
C -3.40789 -3.00137 -0.59958
H -4.21968 -1.26683 -1.56091
C -2.37879 -3.50722 0.19367
H -0.59549 -3.05594 1.30504
H -4.18462 -3.66017 -0.97501
H -2.35838 -4.56447 0.44276
Ru 0.31983 0.03296 0.24088
N 0.71844 -0.94575 -1.47473
C 1.24103 -1.37476 -2.40644
C 2.04734 -1.82983 -3.52690
H 2.08620 -2.92050 -3.55660
H 1.64215 -1.45756 -4.46995
H 3.05217 -1.42660 -3.37096

^{2}H
SCF (wB97X-D) Energy = -1296.46629370
Enthalpy 0K = -1296.092260

Enthalpy 298K = -1296.061235
Free Energy 298K = -1296.156190
Lowest Frequency = 27.8128 cm^{-1}
Second Frequency = 28.2984 cm^{-1}

N	1.56706	-1.71712	-0.07290
C	2.56900	-2.27813	-0.17822
C	3.92714	-2.77940	-0.30498
H	4.21017	-3.35899	0.57603
H	4.03412	-3.40041	-1.19656
H	4.55843	-1.88792	-0.38718
O	3.67974	0.45485	-0.43090
C	3.15586	1.09201	0.49896
O	1.94161	1.02964	0.90160
C	4.00820	2.09109	1.28580
H	3.61351	3.10220	1.14274
H	3.94836	1.87127	2.35534
H	5.04814	2.05930	0.95699
O	-0.13760	-0.57501	2.12151
C	-0.82443	-1.48209	2.58485
O	-1.51848	-2.32158	1.85112
C	-0.93825	-1.71738	4.05985
H	-0.29848	-1.01738	4.59389
H	-1.97873	-1.58838	4.36877
H	-0.65127	-2.74620	4.29004
N	-1.00762	1.47169	0.22145
C	-2.27437	1.29221	-0.23066
C	-0.64100	2.62998	0.78729
C	-3.20593	2.32685	-0.10827
C	-1.52406	3.68777	0.93071
H	0.39331	2.65899	1.11924
C	-2.82971	3.52821	0.47227
H	-4.21985	2.18596	-0.46361
H	-1.19315	4.61025	1.39319
H	-3.55040	4.33415	0.56971
C	-2.51867	-0.03251	-0.82027
C	-1.41114	-0.92772	-0.77075
C	-3.73115	-0.38864	-1.41558
C	-1.61085	-2.18567	-1.37193
H	-1.43496	-2.05020	0.90566
C	-3.88932	-1.64825	-1.98173
H	-4.56149	0.31232	-1.45080
C	-2.82231	-2.54432	-1.96094
H	-0.78822	-2.89848	-1.37840
H	-4.83309	-1.92553	-2.44051
H	-2.93520	-3.52767	-2.41059
Ru	0.27081	-0.14201	0.05336
N	0.93425	0.42015	-1.72536
C	1.60436	0.75981	-2.59909
C	2.61108	1.19183	-3.55483
H	2.67308	0.49850	-4.39604
H	2.38488	2.19225	-3.92952
H	3.56050	1.20453	-3.01025