

# Decreasing Distortion Energies without Strain: Diazo-Selective 1,3-Dipolar Cycloadditions

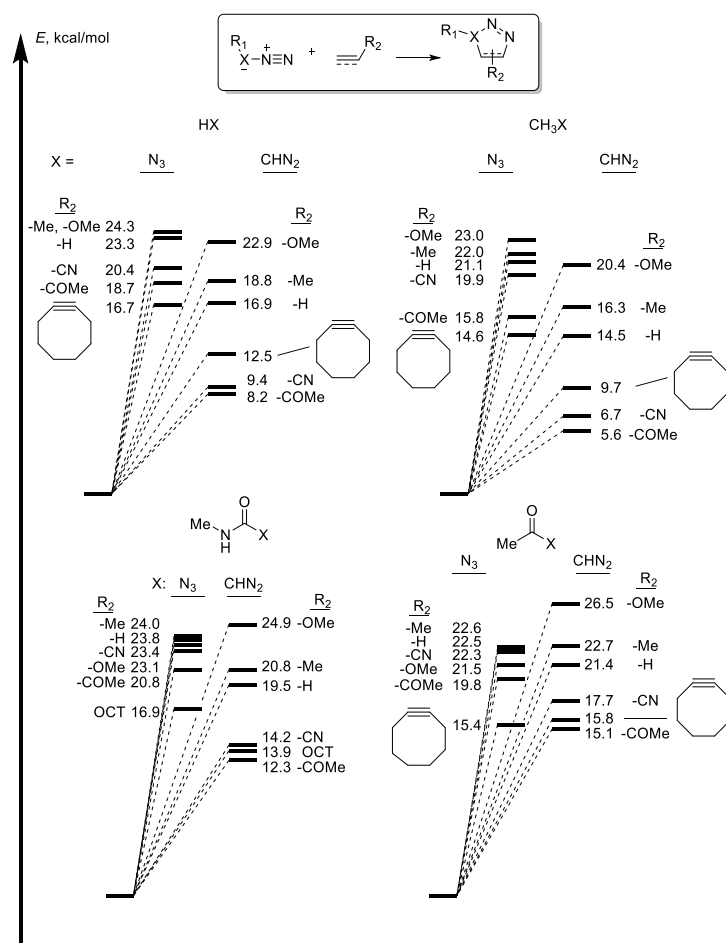
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









**Figure S1.** Substituent effects on activation energies of azido- and diazo-cycloadditions calculated at the M06-2X/6-31+G(2d,p) level of theory. Energies (kcal/mol) include solvation corrections (water) on gas phase geometries using IEFPCM model (radii=UFF).











**Table S1.** Gas-phase activation energies (kcal/mol) of azido- and diazo-cycloadditions calculated at the M06-2X/6-31+G(2d,p) level of theory.

		$\Delta E^\ddagger$	$\Delta G^\ddagger$	$\Delta E^\ddagger$	$\Delta G^\ddagger$	$\Delta E^\ddagger$	$\Delta G^\ddagger$	$\Delta E^\ddagger$	$\Delta G^\ddagger$	$\Delta E^\ddagger$	$\Delta G^\ddagger$	$\Delta E^\ddagger$	$\Delta G^\ddagger$
	1 CH	16.5	27.7	18.1	29.6	22.1	33.5	11.6	23.0	8.5	20.6	11.0	22.6
	2 N	22.1	33.0	23.1	34.3	22.9	34.0	21.0	32.4	18.4	30.0	14.8	26.0
	3 CH	14.2	26.3	15.7	28.2	19.5	32.3	8.8	21.3	6.0	18.7	8.3	20.6
	4 N	20.3	31.9	21.2	33.2	21.7	33.8	17.8	30.3	15.9	28.1	13.1	24.8
	5 CH	19.2	30.9	20.2	32.8	23.0	35.9	15.0	27.2	11.4	23.7	12.8	25.3
	6 N	24.1	34.9	24.4	35.9	23.5	34.6	24.1	35.7	20.6	32.3	16.4	28.4
	7 CH	20.7	31.9	21.9	33.5	24.7	36.9	17.6	29.2	13.8	25.8	14.5	26.7
	8 N	23.2	34.9	23.6	36.3	22.6	35.0	23.7	36.9	19.6	32.7	15.3	27.8











**Table S2.** Gas-phase reaction energies (kcal/mol) of azido- and diazo-cycloadditions calculated at the M06-2X/6-31+G(2d,p) level of theory.

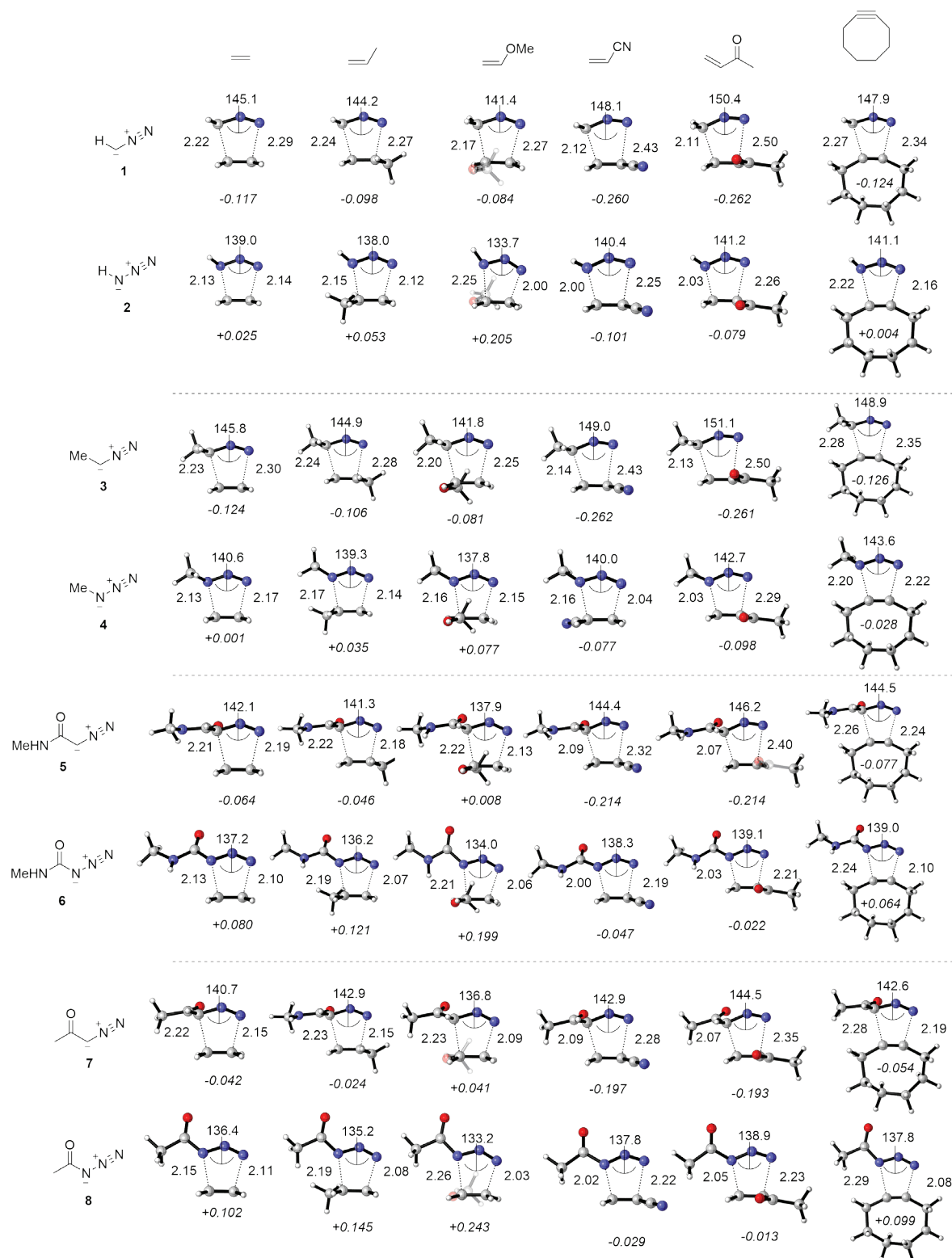
													
<b>X</b>		$\Delta E^\ddagger$	$\Delta G^\ddagger$	$\Delta E^\ddagger$	$\Delta G^\ddagger$	$\Delta E^\ddagger$	$\Delta G^\ddagger$	$\Delta E^\ddagger$	$\Delta G^\ddagger$	$\Delta E^\ddagger$	$\Delta G^\ddagger$	$\Delta E^\ddagger$	$\Delta G^\ddagger$
	<b>1</b> CH	-35.8	-23.7	-35.5	-23.5	-30.0	-17.3	-31.0	-19.0	-34.8	-22.5	-61.2	-48.3
	<b>2</b> N	-25.5	-13.7	-25.7	-13.6	-25.8	-13.4	-19.5	-7.5	-24.1	-12.0	-75.4	-62.6
	<b>3</b> CH	-38.6	-25.9	-38.1	-24.8	-37.1	-18.1	-34.1	-20.9	-37.6	-24.1	-63.5	-49.3
	<b>4</b> N	-29.3	-16.9	-28.7	-15.6	-29.3	-16.0	-25.3	-12.5	-28.4	-15.2	-81.1	-67.3
	<b>5</b> CH	-33.8	-21.5	-33.8	-20.5	-22.1	-9.2	-28.3	-15.6	-32.3	-19.1	-59.2	-45.5
	<b>6</b> N	-21.4	-9.8	-21.2	-8.6	-23.8	-11.0	-14.5	-2.3	-20.9	-8.2	-66.3	-53.0
	<b>7</b> CH	-28.3	-16.8	-28.2	-16.0	-19.2	-6.5	-23.1	-10.9	-27.2	-16.2	-52.9	-39.8
	<b>8</b> N	-23.7	-11.1	-23.2	-9.7	-24.2	-10.1	-16.8	-4.2	-23.3	-9.9	-64.8	-49.9

**Table S3.** Activation energies of azido- and diazo-cycloadditions calculated at the M06-2X/6-31+G(2d,p) level of theory. Energies (kcal/mol) include solvation corrections (water) on gas phase geometries using IEFPCM model (radii=UFF).

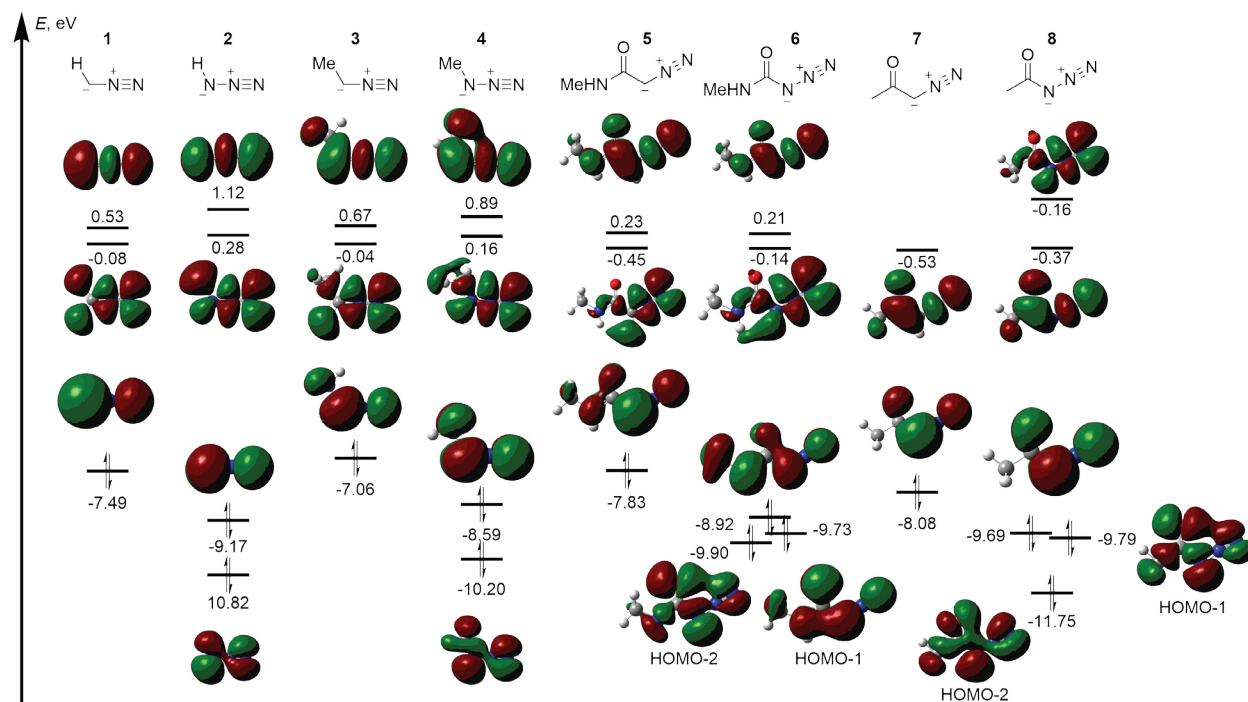
													
<b>X</b>		$\Delta E^\ddagger$	$\Delta G^\ddagger$	$\Delta E^\ddagger$	$\Delta G^\ddagger$	$\Delta E^\ddagger$	$\Delta G^\ddagger$	$\Delta E^\ddagger$	$\Delta G^\ddagger$	$\Delta E^\ddagger$	$\Delta G^\ddagger$	$\Delta E^\ddagger$	$\Delta G^\ddagger$
	<b>1</b> CH	16.9	28.0	18.8	30.2	22.9	34.2	9.4	20.9	8.2	20.3	12.5	24.1
	<b>2</b> N	23.3	34.2	24.3	35.6	24.3	35.2	20.4	31.6	18.7	30.1	16.7	27.8
	<b>3</b> CH	14.5	26.4	16.3	28.6	20.4	33.1	6.7	19.1	5.6	18.3	9.7	21.9
	<b>4</b> N	21.1	32.7	22.0	34.1	23.0	35.0	19.9	32.3	15.8	27.9	14.6	26.3
	<b>5</b> CH	19.5	31.1	20.8	32.4	24.9	37.6	14.2	25.9	12.3	26.0	13.9	26.1
	<b>6</b> N	23.8	35.6	24.0	34.5	23.1	35.3	23.4	34.4	20.8	33.5	16.9	29.2
	<b>7</b> CH	21.4	32.5	22.7	34.1	26.5	38.7	17.1	28.5	15.1	26.7	15.8	27.9
	<b>8</b> N	22.5	33.0	22.6	36.1	21.5	34.6	22.3	34.2	19.8	32.2	15.4	28.6

**Table S4.** Reaction energies of azido- and diazo-cycloadditions calculated at the M06-2X/6-31+G(2d,p) level of theory. Energies (kcal/mol) include solvation corrections (water) on gas phase geometries using IEFPCM model (radii=UFF).

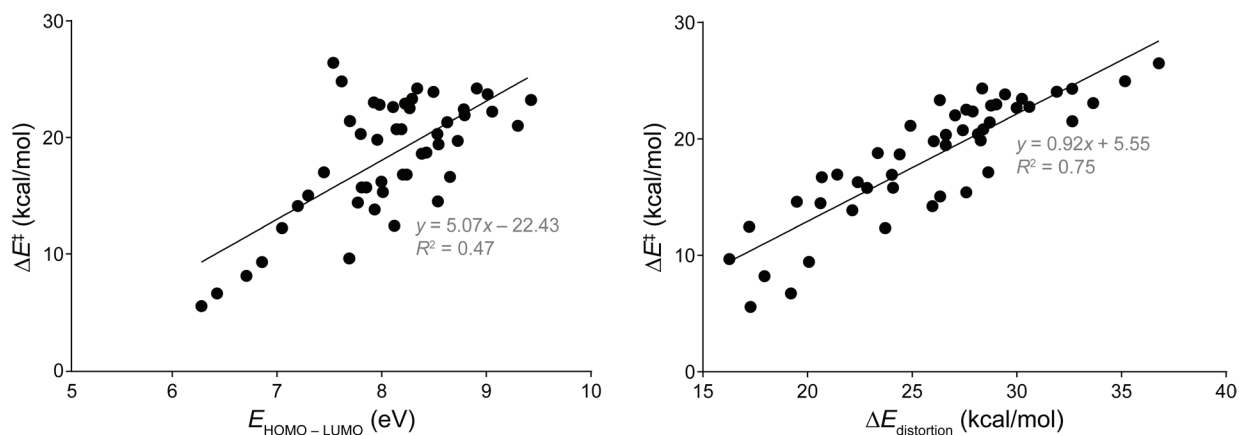
													
	<b>X</b>	$\Delta E^\ddagger$	$\Delta G^\ddagger$	$\Delta E^\ddagger$	$\Delta G^\ddagger$	$\Delta E^\ddagger$	$\Delta G^\ddagger$	$\Delta E^\ddagger$	$\Delta G^\ddagger$	$\Delta E^\ddagger$	$\Delta G^\ddagger$	$\Delta E^\ddagger$	$\Delta G^\ddagger$
	<b>1</b> CH	-37.4	-25.4	-37.1	-25.1	-31.5	-18.8	-31.9	-19.8	-34.5	-22.3	-62.5	-49.5
	<b>2</b> N	-26.8	-15.3	-27.1	-15.0	-26.2	-13.8	-20.7	-8.8	-23.9	-12.0	-77.8	-64.9
	<b>3</b> CH	-40.1	-27.3	-39.6	-26.5	-33.0	-19.5	-34.7	-21.7	-37.1	-23.7	-64.5	-50.4
	<b>4</b> N	-30.9	-18.5	-30.4	-17.2	-30.1	-16.7	-25.5	-12.6	-28.1	-15.1	-83.5	-69.7
	<b>5</b> CH	-32.9	-20.6	-32.3	-20.5	-23.9	-10.8	-26.0	-12.3	-29.6	-17.2	-56.3	-42.6
	<b>6</b> N	-26.7	-15.0	-26.1	-13.5	-26.5	-13.6	-18.3	-6.3	-23.4	-11.1	-70.3	-57.0
	<b>7</b> CH	-27.7	-16.5	-27.5	-15.4	-20.7	-8.0	-21.6	-9.7	-25.0	-12.4	-51.4	-38.3
	<b>8</b> N	-29.4	-17.1	-28.7	-15.4	-27.6	-13.8	-21.0	-8.2	-26.3	-11.9	-68.7	-54.3



**Figure S2.** Transition state geometries of azido- and diazo-cycloadditions calculated at the M06-2X/6-31+G(2d,p) level of theory. NBO charges on dipolarophiles (*italics*) include solvation corrections (water) on gas phase geometries using IEFPCM model (radii=UFF). All activation energies (kcal/mol) are listed in Tables S1 and S3.



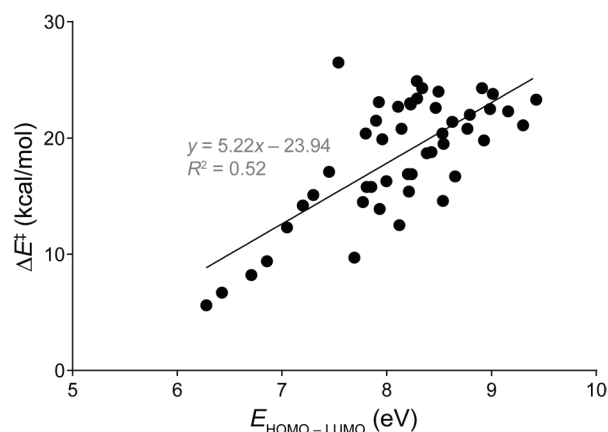
**Figure S3.** Orbitals calculated at the HF/6-31G(d) level of theory. Orbital energies (eV) obtained at the M06-2X/6-31+G(2d,p) level of theory, including single point solvation corrections (water) using IEFPCM (radii = UFF).



**Figure S4.** Plots of activation energies versus FMO gap (left) and distortion energies (right) for cycloadditions from Table S3. FMO gap is defined by the smaller of the NED/IED HOMO-LUMO energy difference.









Upon examination of calculated TS geometries (Figure S2) and FMO energies (Figure S3), we realized that the dominant interactions in the TS might not necessarily be between the HOMO of the dipole and the LUMO of the dipolarophile, or *vice versa*. In nearly every dipole examined (1–6), the HOMO and LUMO orbitals reside within orthogonal  $\pi$ -systems. The azide can rotate to allow interactions of both  $\pi$ -systems with dipolarophile FMOs. Calculated diazo compound transition states, however, display a geometry in which the HOMO can interact directly with unoccupied orbitals of the dipolarophile, but leaving the LUMO orthogonal to the nascent bonds. Accordingly, we reexamined the correlation of activation energies with FMO gaps, but used

instead diazo LUMO+1 energies for IED gaps in relevant cases (Figure S9). The  $R^2$  increased only slightly to 0.52, confirming that distortion energies are a much better descriptor of reactivity.



**Figure S5.** Plot of activation energies versus FMO gap for cycloadditions from Figures S5 and S6 and Tables S1–S4. FMO gap is defined by the smaller of the NED/IED HOMO-LUMO energy difference using LUMO+1 for IED diazo cycloadditions when relevant.

**Table S5.** Distortion/interaction analysis for cycloadditions calculated at the M06-2X/6-31+G(2d,p) level of theory. Energies include solvation corrections (water) on gas phase geometries using IEFPCM model (radii=UFF). All energies in kcal/mol.

	$\Delta E_{distortion}$		$\Delta E_{int}$	$\Delta E_{act}^{\ddagger}$		$\Delta E_{distortion}$		$\Delta E_{int}$	$\Delta E_{act}^{\ddagger}$		
	Diazo	Dipolarophile				Azide	Dipolarophile				
	ethylene, <b>a</b>	16.9	4.5	-4.5	16.9		ethylene, <b>a</b>	21.5	4.8	-3.0	23.3
	propene, <b>b</b>	17.9	5.5	-4.6	18.8		propene, <b>b</b>	22.2	6.2	-4.0	24.3
	methyl vinyl ether, <b>c</b>	20.9	7.9	-5.9	22.9		methyl vinyl ether, <b>c</b>	25.9	6.7	-8.3	24.3
	acrylonitrile, <b>d</b>	14.0	6.1	-10.6	9.4		acrylonitrile, <b>d</b>	19.8	6.8	-6.3	20.4
	methyl vinyl ketone, <b>e</b>	12.0	6.0	-9.7	8.2		methyl vinyl ketone, <b>e</b>	18.7	5.7	-5.7	18.7
	cyclooctyne, <b>f</b>	14.2	3.0	-4.8	12.5		cyclooctyne, <b>f</b>	18.2	2.5	-4.0	16.7
	ethylene, <b>a</b>	16.3	4.3	-6.1	14.5		ethylene, <b>a</b>	20.4	4.5	-3.8	21.1
	propene, <b>b</b>	17.2	5.2	-6.1	16.3		propene, <b>b</b>	21.1	6.0	-5.0	22.0
	methyl vinyl ether, <b>c</b>	20.7	7.5	-7.7	20.4		methyl vinyl ether, <b>c</b>	23.0	6.0	-6.1	23.0
	acrylonitrile, <b>d</b>	13.5	5.7	-12.5	6.7		acrylonitrile, <b>d</b>	21.7	6.6	-8.4	19.9
	methyl vinyl ketone, <b>e</b>	11.8	5.5	-11.7	5.6		methyl vinyl ketone, <b>e</b>	17.5	5.4	-7.1	15.8
	cyclooctyne, <b>f</b>	13.4	2.9	-6.6	9.7		cyclooctyne, <b>f</b>	17.1	2.4	-4.9	14.6
	ethylene, <b>a</b>	21.3	5.3	-7.1	19.5		ethylene, <b>a</b>	24.3	5.1	-5.6	23.8
	propene, <b>b</b>	21.9	6.5	-7.6	20.8		propene, <b>b</b>	25.3	6.6	-7.9	24.0
	methyl vinyl ether, <b>c</b>	26.7	8.4	-10.2	24.9		methyl vinyl ether, <b>c</b>	27.2	6.4	-10.6	23.1
	acrylonitrile, <b>d</b>	18.8	7.2	-11.8	14.2		acrylonitrile, <b>d</b>	22.9	7.3	-6.8	23.4
	methyl vinyl ketone, <b>e</b>	16.8	7.0	-11.4	12.3		methyl vinyl ketone, <b>e</b>	21.5	5.9	-6.7	20.8
	cyclooctyne, <b>f</b>	18.5	3.6	-8.3	13.9		cyclooctyne, <b>f</b>	21.3	2.8	-7.1	16.9
	ethylene, <b>a</b>	22.7	6.0	-7.3	21.4		ethylene, <b>a</b>	23.0	4.6	-5.1	22.5
	propene, <b>b</b>	23.5	7.1	-7.9	22.7		propene, <b>b</b>	23.9	6.1	-7.3	22.6
	methyl vinyl ether, <b>c</b>	28.1	8.7	-10.3	26.5		methyl vinyl ether, <b>c</b>	26.5	6.2	-11.1	21.5
	acrylonitrile, <b>d</b>	20.7	8.0	-11.5	17.1		acrylonitrile, <b>d</b>	21.3	6.6	-5.5	22.3
	methyl vinyl ketone, <b>e</b>	19.0	7.3	-11.3	15.1		methyl vinyl ketone, <b>e</b>	20.5	5.5	-6.2	19.8
	cyclooctyne, <b>f</b>	20.1	4.0	-8.3	15.8		cyclooctyne, <b>f</b>	20.4	2.4	-7.4	15.4

Although distortion/interaction analysis is a better descriptor of reactivity than are ground state FMO gaps, distortion/interaction analysis does not provide the “back of the envelope” predicting power provided by the well-established FMO approach.<sup>2</sup> Moreover, the two approaches are linked intricately, and one cannot be evaluated without the other. For simplicity,

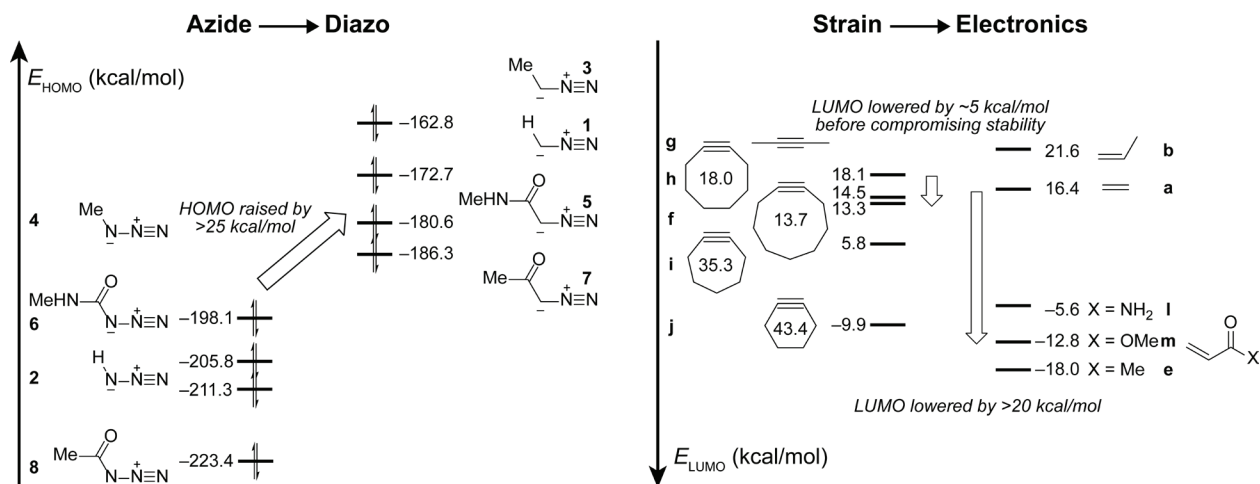
our subsequent discussion will focus on the differences of ground state FMO energies of the diazo and azides dipoles, as well as the two approaches of strain and electronic activation.

The decreased distortion energies result from the higher HOMO of diazo compounds relative to analogous azides.<sup>3</sup> This leads to an earlier transition state, where less bending is required to allow for sufficient interactions towards bond formation. Despite an earlier, less synchronous TS, larger interaction energies are also observed relative to azide dipoles.

As the diazoacetamide **5** has been shown to endure cellular metabolism, this alternative approach can provide increased reaction rates without compromising selectivity. This approach is in stark contrast to the high amount of strain (~20 kcal/mol for **c**) associated with pre-distortion towards the TS geometry—a strategy that lowers the energy of the dipolarophile LUMO by only ~5 kcal/mol before compromising reactant stability.

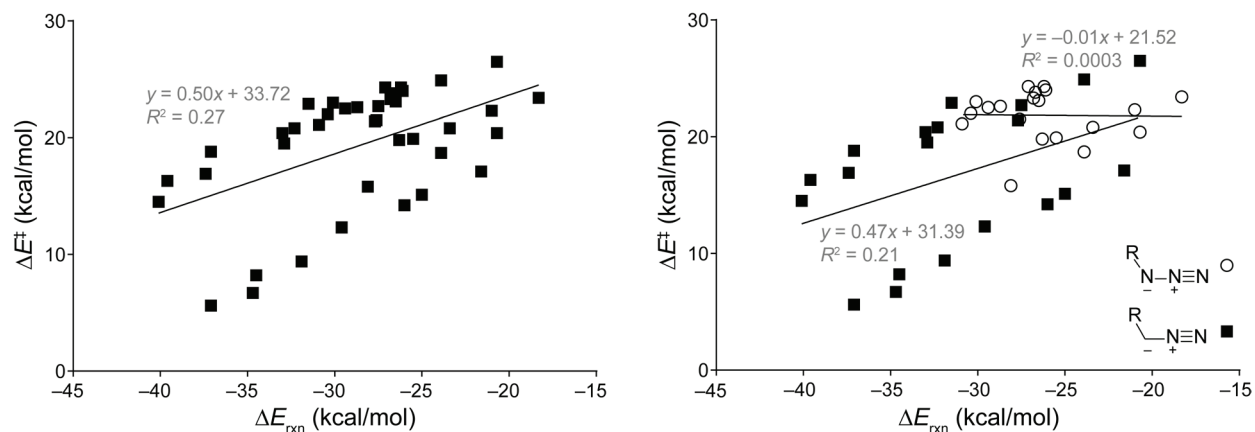
In all cases, the HOMO is raised substantially upon diazotization (Figure S6). For the transformation from the carbamoyl azide **6** to the diazoacetamide **5**, an increase of ~25 kcal/mol is observed. Even from the nonconjugated methyl azide **4** to diazoacetamide **3**, an increase of almost 20 kcal/mol is observed.

In contrast, increasing strain by almost 20 kcal/mol from 2-butyne (**g**) to cyclooctyne (**f**) leads to only ~5 kcal/mol decrease in the LUMO energy of the alkyne. The strategy of electronic activation provides much larger effects, where the LUMO of methyl vinyl ketone **e** is ~35 kcal/mol lower than that of propene **b**.



**Figure S6.** Comparison of the strategies of distortion-acceleration and electronic tuning. All orbital energies calculated at the M06-2X/6-31+G(2d,p) level of theory, including solvation corrections (water) on gas-phase geometries using IEFPCM model (radii=UFF). Contained within cycloalkynes are strain energies (kcal/mol) calculated utilizing isodesmic equation as in ref. 1.

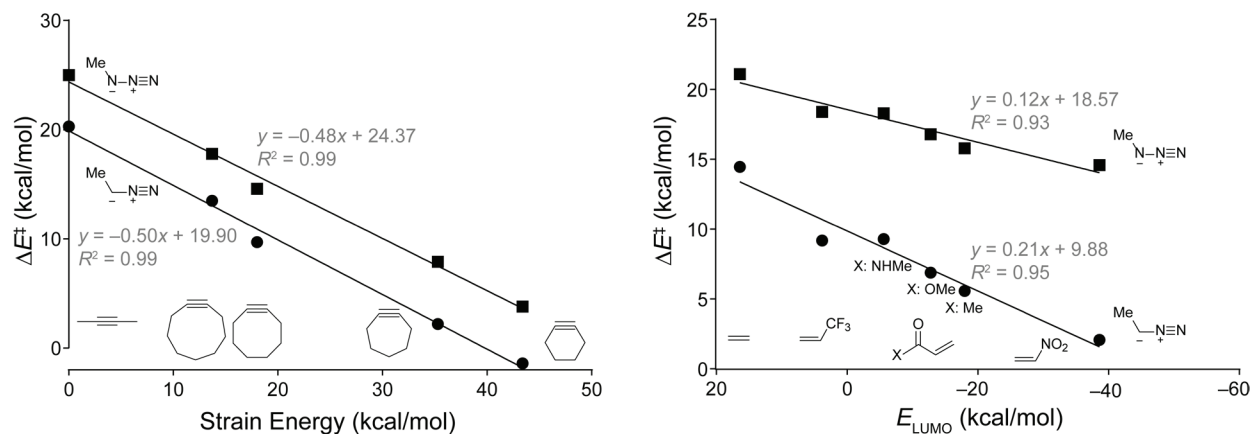




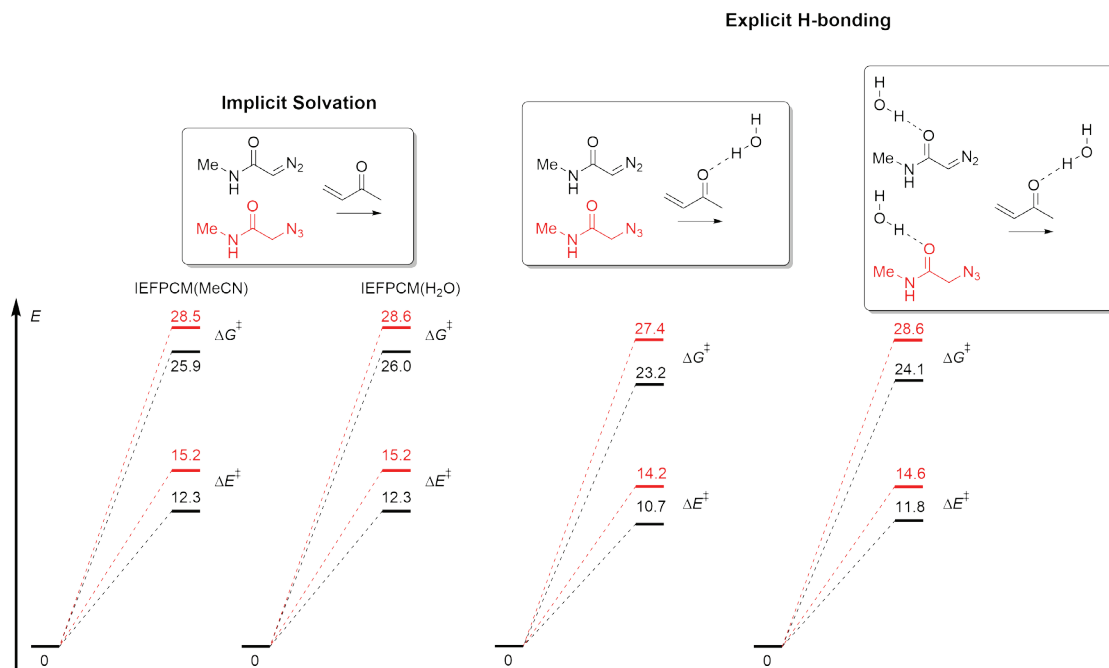
**Figure S7.** Plots of activation energies versus reaction energies (left) and separated by dipoles (right) for cycloadditions from Tables S1 and S3.

**Table S6.** Intrinsic reaction barriers of azido- and diazo-cycloadditions calculated at the M06-2X/6-31+G(2d,p) level of theory. Energies (kcal/mol) include solvation corrections (water) on gas phase geometries using IEFPCM model (radii=UFF).

		$\Delta E_0^\ddagger$ , kcal/mol						
		X	a	b	c	d	e	f
$\begin{array}{c} \text{H} \\   \\ \text{X}-\text{N}^+\equiv\text{N} \end{array}$	<b>1</b>	CH	32.9	34.9	37.0	22.5	22.1	37.2
	<b>2</b>	N	35.4	36.6	36.2	29.9	29.4	47.7
$\begin{array}{c} \text{Me} \\   \\ \text{X}-\text{N}^+\equiv\text{N} \end{array}$	<b>3</b>	CH	31.3	33.1	35.0	20.4	19.8	34.4
	<b>4</b>	N	34.8	35.6	36.5	31.4	28.1	47.1
$\begin{array}{c} \text{O} \\    \\ \text{MeHN}-\text{X}-\text{N}^+\equiv\text{N} \end{array}$	<b>5</b>	CH	34.0	35.1	35.9	25.5	24.9	36.6
	<b>6</b>	N	35.9	35.9	35.1	31.9	31.4	45.2
$\begin{array}{c} \text{O} \\    \\ \text{X}-\text{N}^+\equiv\text{N} \end{array}$	<b>7</b>	CH	33.8	35.1	36.1	26.8	26.1	37.0
	<b>8</b>	N	35.7	35.5	33.9	31.9	31.6	42.9



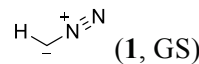
**Figure S8.** Plots comparing activation by strain (left) or electron-withdrawing substituents (right) for 1,3-dipolar cycloadditions of methyl azide (squares) and diazo ethane (circles). Strain energy calculated from the isodesmic equation found in ref. 1. Activation energies calculated at the M06-2X/6-31+G(2d,p) level of theory. Energies (kcal/mol) include solvation corrections (water) on gas phase geometries using IEFPCM model (radii=UFF).



**Figure S9.** Implicit and explicit solvation for azido- and diazo-cycloadditions with methyl vinyl ketone calculated at the M06-2X/6-31+G(2d,p) level of theory. Implicit solvation includes solvation corrections (acetonitrile or water) on gas phase geometries using IEFPCM model (radii=UFF). All energies in kcal/mol.

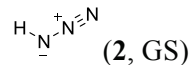
### Cartesian coordinates, total energies, and imaginary frequencies (for TSs)

All energies include IEFPCM single point corrections. TS frequencies are from gas phase optimized structures.



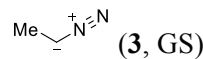
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C	0.00039300	1.13852100	0.00000000
H	0.95562000	1.63464300	0.00000000
H	-0.95453000	1.63522600	0.00000000

HF: -148.6872913  
Sum of electronic and zero-point Energies: -148.655401  
Sum of electronic and thermal Energies: -148.651784  
Sum of electronic and thermal Enthalpies: -148.650840  
Sum of electronic and thermal Free Energies: -148.678988



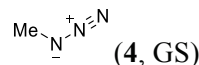
N	-0.11051000	0.01535000	0.00002200
N	-1.23253400	0.01323200	-0.00001200
N	1.11873600	-0.13930400	-0.00000800
H	1.57015400	0.77505400	-0.00001200

HF: -164.7338402  
Sum of electronic and zero-point Energies: -164.712079  
Sum of electronic and thermal Energies: -164.708892  
Sum of electronic and thermal Enthalpies: -164.707948  
Sum of electronic and thermal Free Energies: -164.735043



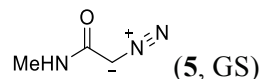
N	-0.78379800	0.11415700	-0.00006400
N	-1.83312200	-0.32074200	0.00003200
C	0.41771000	0.58896200	0.00003900
H	0.48836000	1.66606500	-0.00000700
C	1.60075600	-0.33547600	-0.00000100
H	1.26763100	-1.37540100	-0.00024700
H	2.22597300	-0.18257700	-0.88515500
H	2.22568100	-0.18291200	0.88540200

HF: -187.9847358  
Sum of electronic and zero-point Energies: -187.923633  
Sum of electronic and thermal Energies: -187.918780  
Sum of electronic and thermal Enthalpies: -187.917836  
Sum of electronic and thermal Free Energies: -187.950716



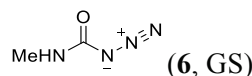
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N	-0.71122300	-0.11313200	-0.00000400
N	-1.76425600	0.28699900	0.00000100
N	0.39482300	-0.65083800	0.00000100
H	2.42800900	-0.30139300	0.00056600
H	1.50928500	0.92898100	-0.89387800
H	1.50866600	0.92973700	0.89333200

HF: -204.0206358  
Sum of electronic and zero-point Energies: -203.969536  
Sum of electronic and thermal Energies: -203.965200  
Sum of electronic and thermal Enthalpies: -203.964255  
Sum of electronic and thermal Free Energies: -203.995885



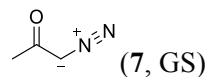
C	0.30852100	0.03905300	-0.02920200
N	-2.02771400	-0.22212300	0.01247700
N	-2.99960900	0.33676500	0.04001300
O	0.22780700	1.25507100	-0.03578400
N	1.50346700	-0.61999200	-0.05770900
H	1.51615300	-1.60579700	0.14568500
C	2.73859300	0.13170600	0.05051200
H	2.86639000	0.56630800	1.04724000
H	3.57565100	-0.53248600	-0.16735100
H	2.72785900	0.94470800	-0.67669500
C	-0.87166200	-0.83196100	-0.01577300
H	-0.89422800	-1.90863500	-0.05928700

HF: -356.6537399  
Sum of electronic and zero-point Energies: -356.564577  
Sum of electronic and thermal Energies: -356.556859  
Sum of electronic and thermal Enthalpies: -356.555915  
Sum of electronic and thermal Free Energies: -356.596660



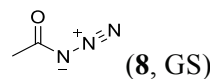
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N	-1.91935900	-0.24006900	0.00597900
N	-2.93184200	0.22914000	0.01530700
O	0.16838200	1.27155300	-0.01331900
N	1.43866600	-0.61549000	-0.03405100
H	1.39919700	-1.61792500	0.04883400
C	2.70338700	0.08784700	0.02575600
H	2.90633300	0.46968400	1.03108300
H	3.50047100	-0.59496900	-0.26894700
H	2.68008500	0.93129700	-0.66596500
N	-0.83172400	-0.84368000	-0.00354200

HF: -372.6951283  
Sum of electronic and zero-point Energies: -372.616742  
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Sum of electronic and thermal Enthalpies: -372.609293  
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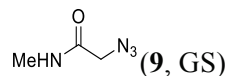
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N	-1.51026600	-0.31408700	-0.00001400
N	-2.51783800	0.17278900	0.00008800
O	0.58814200	1.36600500	-0.00004100
C	-0.29153700	-0.80538500	-0.00010800
H	-0.19976600	-1.87892700	-0.00006400
C	2.18499100	-0.42187300	0.00007000
H	2.32784800	-1.05073100	0.88383300
H	2.32797200	-1.05073500	-0.88367100
H	2.91395500	0.38739300	0.00011900

HF: -301.3032478  
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Sum of electronic and thermal Enthalpies: -301.225732  
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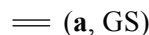
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N	1.40906400	-0.30703000	0.00049600
N	2.45301900	0.08275600	-0.00006500
O	-0.53526500	1.35497600	-0.00004300
N	0.26782800	-0.81744800	-0.00048400
C	-2.12162800	-0.45600700	-0.00001400
H	-2.22482800	-1.10235600	-0.87487900
H	-2.23131600	-1.08393300	0.88755500
H	-2.87917900	0.32506600	-0.01024100

HF: -317.3438519  
Sum of electronic and zero-point Energies: -317.283581  
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
C	0.65675200	0.06180100	0.04343900
N	-2.24704800	-0.12009700	-0.06844100
N	-2.91424700	-0.97514600	0.21976000
O	0.33894400	-1.10332200	-0.07454100
N	-1.62893800	0.87174100	-0.47593200
C	-0.39286000	1.15534100	0.24197900
H	-0.56489900	1.25580900	1.32263900
H	-0.04110500	2.11733000	-0.13372500
N	1.94517100	0.47622300	0.07109500
H	2.14998600	1.46121300	0.06595900
C	3.02736000	-0.48229900	-0.05705700
H	3.03789100	-0.93263300	-1.05359100
H	3.97443500	0.02660800	0.12218300
H	2.90005900	-1.27985100	0.67733000

HF: -411.9771915  
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C	0.66435800	-0.00008500	0.00004100
C	-0.66415000	-0.00005700	0.00023700
H	-1.23307300	-0.92416800	-0.00038000
H	-1.23215500	0.92463800	-0.00077200
H	1.23233300	-0.92467700	-0.00045600
H	1.23164900	0.92506100	-0.00006300

HF: -78.5496162  
Sum of electronic and zero-point Energies: -78.498367  
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Sum of electronic and thermal Enthalpies: -78.494384  
Sum of electronic and thermal Free Energies: -78.520545

 (b, GS)

C	0.13374800	0.45840000	-0.00006200
C	1.27609900	-0.22222200	0.00000500
H	2.23732000	0.28002500	0.00019600
H	1.28512400	-1.30894600	-0.00010200
C	-1.23002700	-0.16309500	0.00002400
H	0.16844800	1.54673300	-0.00002500
H	-1.16553700	-1.25410200	-0.00004000
H	-1.80205900	0.14888100	0.87995600
H	-1.80221500	0.14890800	-0.87978900


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 (c, GS)

C	-1.43208000	0.56882900	0.00000600
C	-0.73461900	-0.56695400	0.00011400
H	-1.21751000	-1.53892800	0.00010000
H	-0.97692400	1.54998200	-0.00018600
H	-2.51183300	0.51190800	-0.00017500
O	0.60585500	-0.71540200	-0.00012300
C	1.36088600	0.47718100	0.00004500
H	2.40881900	0.18028000	-0.00030400
H	1.14253200	1.07308900	-0.89384900
H	1.14295200	1.07254700	0.89441300


HF: -193.0440017

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Sum of electronic and thermal Enthalpies: -192.952444

Sum of electronic and thermal Free Energies: -192.984651

 (d, GS)

C	-0.59209500	0.51064500	0.00000000
C	-1.59645800	-0.36333800	0.00000000
H	-1.41677300	-1.43220900	0.00000000
H	-0.76195300	1.58141100	0.00000000
C	0.78288600	0.09451500	0.00000000
N	1.89100500	-0.22569500	0.00000000
H	-2.62430800	-0.02027000	0.00000100


HF: -170.7768791

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Sum of electronic and thermal Energies: -170.721532

Sum of electronic and thermal Enthalpies: -170.720588

Sum of electronic and thermal Free Energies: -170.751504

 (e, GS)

C	-0.80108200	-0.66801300	-0.00027900
C	-2.00425100	-0.10036100	0.00015000
H	-2.91451300	-0.68948500	0.00016300
H	-2.08837200	0.98245800	0.00079000
O	0.44251000	0.16561200	-0.00004600
C	0.39810600	1.37338800	-0.00012500
C	-0.68142700	-1.74810900	-0.00043300
H	1.74873100	-0.59044700	0.00019000
H	1.79885900	-1.23998700	0.88038400
H	1.79939000	-1.23900500	-0.88073500
H	2.58577200	0.10627400	0.00074400


HF: -231.1542877

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Sum of electronic and thermal Energies: -231.058701

Sum of electronic and thermal Enthalpies: -231.057757

Sum of electronic and thermal Free Energies: -231.093857

 (f, GS)

C	-0.60193400	-1.45435800	0.03121100
C	0.60223300	-1.45448400	-0.03118600
C	1.95545600	-0.90990900	-0.12215800
H	2.66833200	-1.43561600	0.51939000
H	2.32135800	-0.99684100	-1.15152000
C	-1.95528300	-0.91015700	0.12213900
H	-2.66797400	-1.43602200	-0.51948500
C	-2.32122700	-0.99721100	1.15147400
C	1.85505800	0.58026800	0.28114400
H	2.80071400	1.06766200	0.01943200
H	1.75991000	0.64211400	1.37136000
H	-1.85521100	0.58006800	-0.28110600
C	-1.76016700	0.64199200	-1.37132600
H	-2.80092800	1.06727900	-0.01928000
C	0.68342700	1.34478600	-0.37273400
H	1.00165200	2.38716400	-0.47471800
H	0.54436000	0.97321100	-1.39596400
C	-0.68365900	1.34476200	0.37270400
H	-1.00199300	2.38711700	0.47458000
H	-0.54456000	0.97329900	1.39597000


HF: -311.8801675

Sum of electronic and zero-point Energies: -311.699679

Sum of electronic and thermal Energies: -311.691905

Sum of electronic and thermal Enthalpies: -311.690960

Sum of electronic and thermal Free Energies: -311.731416

 (g, GS)

C	-0.60257500	0.00039100	-0.00036600
C	0.60257900	0.00052100	-0.00009900
C	2.06539300	-0.00021600	0.00008200
H	2.45370900	-0.45221900	-0.91609400
H	2.45439000	1.01893800	0.06721000
C	-2.06539500	-0.00019600	0.00011600
H	-2.45392800	-0.45561800	-0.91427200
H	-2.45295400	-0.56504300	0.85175400
H	-2.45433000	1.01921800	0.06349900
H	2.45310700	-0.56828000	0.84950600


HF: -155.9143825

Sum of electronic and zero-point Energies: -155.829768

Sum of electronic and thermal Energies: -155.824123

Sum of electronic and thermal Enthalpies: -155.823179

Sum of electronic and thermal Free Energies: -155.857557

 (h, GS)

C	-1.64427900	1.26615400	-0.08671300
C	-2.06998200	-0.04898700	0.58718000
C	-0.20338800	1.37006000	-0.60806000
C	0.86562700	-1.47745200	-0.08732700
C	-0.33110500	-1.58216600	-0.19433000
C	-1.77482200	-1.33385700	-0.21724500
C	2.20980200	-0.93739000	0.13274700
C	0.91241100	1.27759100	0.45420000
H	-2.32269900	-2.17652700	0.21580200
H	-2.12438500	-1.22421600	-1.25134400
H	2.95180800	-1.40246200	-0.52243200
H	2.51096600	-1.16230700	1.16228700
H	1.15413300	2.28687600	0.80337000
H	0.55735200	0.72717200	1.33331100
H	-0.04725600	0.60260800	-1.37047800
H	-0.10779300	2.33041800	-1.12950300
C	2.19229600	0.59992200	-0.07259300
C	3.07819200	1.01129000	0.42126600
H	2.29793400	0.82156000	-1.14088500
H	-1.59090700	-0.15043400	1.56692600
H	-3.14870900	0.00491300	0.77326000
H	-2.31713500	1.44769300	-0.93482700
H	-1.83085900	2.08016800	0.62609300


HF: -351.1844134

Sum of electronic and zero-point Energies: -350.974413

Sum of electronic and thermal Energies: -350.965723

Sum of electronic and thermal Enthalpies: -350.964779

Sum of electronic and thermal Free Energies: -351.007215

 (i, GS)

C	0.58999100	-1.42059600	-0.13159600
C	-0.59013500	-1.42003500	0.13235900
C	-1.74892200	-0.52882600	0.30549400
H	-2.68062000	-0.91482800	-0.11627100
H	-1.92579600	-0.33037100	1.36823700
C	1.74849000	-0.52909100	-0.30591100
H	2.68083000	-0.91491500	0.11455100
H	1.92384100	-0.33087300	-1.36898600
C	-1.29902600	0.74357300	-0.45402600
H	-2.10321400	1.48912900	-0.42563200
C	-1.18700700	0.44508100	-1.50122200
C	1.29951500	0.74347100	0.45377800
H	1.18853800	0.44526500	1.50116000
H	2.10379200	1.48887100	0.42443200
C	0.00005800	1.46992500	0.00033600
H	-0.25967200	2.13570200	0.83221500
H	0.25948900	2.13641600	-0.83108800


HF: -272.5552824

Sum of electronic and zero-point Energies: -272.403786

Sum of electronic and thermal Energies: -272.397057

Sum of electronic and thermal Enthalpies: -272.396113

Sum of electronic and thermal Free Energies: -272.434117

 (j, GS)

C	-0.60785600	-1.29316400	0.02883400
C	0.60527400	-1.29198800	-0.02937800
C	1.58955700	-0.19252100	-0.11711300
H	2.44748700	-0.28828300	0.55244100
H	1.97278300	-0.09358800	-1.13726200
C	-1.58931200	-0.19027100	0.11760400
H	-2.44875300	-0.28440000	-0.55024900
H	-1.97068300	-0.09102500	1.13845300
C	0.71441500	1.04282400	0.29033500
H	1.22809000	1.95828100	-0.02408100
H	0.65360200	1.06462200	1.38462700
C	-0.71294000	1.04343300	-0.29065200
H	-0.65207400	1.06468900	-1.38496900
H	-1.22527600	1.95982900	0.02326200

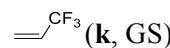
HF: -233.2450163

Sum of electronic and zero-point Energies: -233.123169

Sum of electronic and thermal Energies: -233.117512

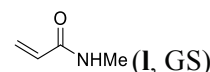
Sum of electronic and thermal Enthalpies: -233.116568

Sum of electronic and thermal Free Energies: -233.151732

 (**k**, GS)

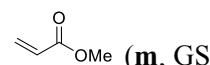
C	0.98019400	0.65583600	0.00000700
C	2.10092100	-0.04934600	-0.00000800
H	3.06666300	0.44224700	-0.00000400
H	2.08394600	-1.13344800	-0.00002700
H	0.95992100	1.74025500	0.00006500
C	-0.37142400	0.01956700	0.00001300
C	-0.31853200	-1.31642600	-0.00037800
F	-1.08357200	0.39155300	-1.07640100
F	-1.08330500	0.39094000	1.07676700

HF: -415.5203675  
 Sum of electronic and zero-point Energies: -415.462799  
 Sum of electronic and thermal Energies: -415.457193  
 Sum of electronic and thermal Enthalpies: -415.456249  
 Sum of electronic and thermal Free Energies: -415.492344

 (**l**, GS)

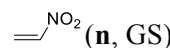
C	-1.34505300	-0.65301600	-0.00007500
C	-2.50493200	-0.00617000	0.00004800
H	-3.45190200	-0.53372000	-0.00004600
H	-2.51113400	1.07953800	0.00023500
C	-0.05962900	0.10929400	0.00008700
O	-0.00670100	1.32568600	0.00000800
C	2.37174700	-0.03750300	0.00003400
H	2.49719100	0.59175800	0.88521400
H	3.13330600	-0.81771100	-0.00114200
H	2.49635000	0.59358100	-0.88394500
H	-1.30094700	-1.73937100	-0.00027900
N	1.06241400	-0.65662300	-0.00011800
H	0.98104800	-1.65882500	0.00015600

HF: -286.512298  
 Sum of electronic and zero-point Energies: -286.404496  
 Sum of electronic and thermal Energies: -286.397281  
 Sum of electronic and thermal Enthalpies: -286.396337  
 Sum of electronic and thermal Free Energies: -286.436133

 (**m**, GS)

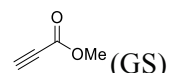
C	-0.03943800	0.10894500	-0.00045300
C	-1.31631500	-0.64908900	0.00001900
H	-1.24516000	-1.73078400	0.00023500
O	0.06165800	1.30836100	-0.00002800
C	-2.47544300	-0.00003800	0.00018800
H	-2.48947600	1.08560000	-0.00002100
H	-3.42123200	-0.52963600	0.00055100
O	1.01362000	-0.72245000	-0.00029400
C	2.28779800	-0.07991200	0.00031900
H	3.02378500	-0.88171200	0.00045600
H	2.39545500	0.54505300	-0.88867200
H	2.39478700	0.54476300	0.88959100

HF: -306.3696751  
 Sum of electronic and zero-point Energies: -306.273754  
 Sum of electronic and thermal Energies: -306.267156  
 Sum of electronic and thermal Enthalpies: -306.266212  
 Sum of electronic and thermal Free Energies: -306.304261

 (**n**, GS)

C	-0.73868500	-0.64813400	-0.00014500
C	-1.85767000	0.05283700	-0.00000400
H	-2.81431200	-0.45481800	0.00065800
H	-1.82764700	1.13597300	-0.00114800
O	0.58474600	1.24283200	0.00019900
H	-0.62606700	-1.72232800	0.00084700
O	0.55919100	0.03173800	-0.00004300
N	1.53173100	-0.69398400	-0.00009500


HF: -283.0031858  
 Sum of electronic and zero-point Energies: -282.947544  
 Sum of electronic and thermal Energies: -282.942866  
 Sum of electronic and thermal Enthalpies: -282.941922  
 Sum of electronic and thermal Free Energies: -282.975392

 (GS)

C	-1.46463900	-0.10757700	0.00000500
C	-2.62924200	-0.40058500	0.00019500
H	-3.66319800	-0.66207800	0.00065800
C	-0.06767300	0.30444100	-0.00044200
O	0.29701900	1.44761800	0.00065000
O	0.74638100	-0.75257100	-0.00043500
C	2.14020700	-0.43097400	0.00035500
H	2.39205200	0.14763500	0.89096500
H	2.65937400	-1.38707800	-0.00033500
H	2.39265300	0.14931500	-0.88901500

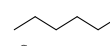
HF: -305.1136683  
 Sum of electronic and zero-point Energies: -305.041527  
 Sum of electronic and thermal Energies: -305.035219  
 Sum of electronic and thermal Enthalpies: -305.034274  
 Sum of electronic and thermal Free Energies: -305.071432

Structures for strain energy calculations:<sup>1</sup>

 (GS)

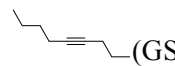
C	0.85665500	1.17935200	-0.23292100
C	-0.59334000	1.33141500	0.23287500
C	-1.44963900	0.15197200	-0.23307100
C	-0.85665600	-1.17934300	0.23293900
C	0.59333100	-1.33142000	-0.23287500
C	1.44964500	-0.15197800	0.23305300
H	-2.47666500	0.25994800	0.13148700
H	-0.61402400	1.37812000	1.33071000
H	-1.01348400	2.27475000	-0.13163500
H	0.88687100	1.22003900	-1.33077200
H	1.46411400	2.01446500	0.13148200
H	-0.88684900	-1.21998500	1.33079400
H	-1.46412000	-2.01447400	-0.13141100
H	1.01348400	-2.27475000	0.13164100
H	0.61400000	-1.37813700	-1.33070900
H	1.49998600	-0.15736700	1.33088900
H	2.47665400	-0.25994500	-0.13155500
H	-1.49993800	0.15734700	-1.33091200

HF: -235.7742892  
 Sum of electronic and zero-point Energies: -235.603840  
 Sum of electronic and thermal Energies: -235.598139  
 Sum of electronic and thermal Enthalpies: -235.597195  
 Sum of electronic and thermal Free Energies: -235.632582

 (GS)

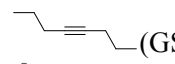
C	-1.87852800	-0.55283800	0.00000200
H	-1.83049500	-1.20933200	0.87786400
H	-1.83045900	-1.20931900	-0.87786600
H	-0.66527900	0.37336800	0.00003200
H	-0.71244200	1.03195700	0.87845300
H	-0.71242900	1.03199000	-0.87836500
C	0.66527900	-0.37336800	0.00002400
H	0.71242500	-1.03198200	-0.87837900
H	0.71244600	-1.03196400	0.87843900
C	1.87852800	0.55283800	-0.00000300
H	1.83049200	1.20933000	0.87786000
H	1.83046300	1.20932100	-0.87787000
C	3.20088900	-0.20925600	-0.00002200
C	3.28041800	-0.85105600	-0.88355700
H	4.05809700	0.46938600	-0.00004600
H	3.28045400	-0.85103700	0.88352300
C	-3.20088900	0.20925600	-0.00002500
H	-3.28041000	0.85106300	-0.88355600
H	-4.05809700	-0.46938600	-0.00006400
H	-3.28046200	0.85103000	0.88352400

HF: -236.9677202  
 Sum of electronic and zero-point Energies: -236.778572  
 Sum of electronic and thermal Energies: -236.770102  
 Sum of electronic and thermal Enthalpies: -236.769158  
 Sum of electronic and thermal Free Energies: -236.811305

 (GS)

C	3.73213700	0.29634400	-0.17726300
C	2.30048300	-0.17999300	0.04697700
C	4.73962000	-0.84945000	-0.14515500
C	-1.21040100	0.13553500	0.42432300
C	-0.08680600	0.53168500	0.23374000
C	1.29223100	0.97544000	0.01637900
C	-2.58959500	-0.31592400	0.62404000
C	-4.95174000	-0.37525200	-0.28774600
H	1.55969500	1.71373700	0.78194100
H	1.35860900	1.49165000	-0.94882900
H	-2.97007300	0.08746800	1.57012500
H	-2.60363800	-1.40787700	0.72507500
H	-5.60936500	-0.07368400	-1.10700600
H	-4.99302800	-1.46651600	-0.20877300
H	4.51630300	-1.58726200	-0.92243300
H	5.76001100	-0.49125700	-0.30551900
C	-3.52231200	0.10240300	-0.52008500
H	-3.49667100	1.19276500	-0.61579200
H	-3.13346500	-0.30381800	-1.45945400
H	2.02664000	-0.91401000	-0.72023800
H	2.22527000	-0.69441600	1.01229900
H	3.79398800	0.81588900	-1.14185900
H	3.99077600	1.03749300	0.58967200
H	4.71191600	-1.36559000	0.81982400
H	-5.35867200	0.04069000	0.63971400

HF: -352.3955342  
 Sum of electronic and zero-point Energies: -352.167518  
 Sum of electronic and thermal Energies: -352.155594  
 Sum of electronic and thermal Enthalpies: -352.154650  
 Sum of electronic and thermal Free Energies: -352.207784

 (GS)

C	-4.39850500	0.00449100	-0.10228200
C	-2.95504700	0.49632300	-0.11217100
C	0.56841500	0.20205900	0.12946200
C	-0.56841900	-0.20207800	0.12945100
C	-1.96325900	-0.64919300	0.12906700
C	1.96325400	0.64917900	0.12906800
C	4.39850400	-0.00446800	-0.10227900
H	-2.18946400	-1.13113400	1.08794500

H	-2.09846900	-1.41648200	-0.64258700
H	2.18946300	1.13111700	1.08794600
H	2.09845200	1.41647200	-0.64258400
H	5.09937400	-0.82473800	-0.27675100
H	4.56191600	0.74776600	-0.88077600
C	2.95505500	-0.49632600	-0.11217800
H	2.80821500	-1.25957100	0.65874600
H	2.72170900	-0.97032600	-1.07122000
H	-2.72168900	0.97033800	-1.07120300
H	-2.80820100	1.25955400	0.65876800
H	-4.56192800	-0.74773400	-0.88078600
H	-4.65037300	-0.45276800	0.86021500
H	4.65035500	0.45279400	0.86022300
H	-5.09935300	0.82478000	-0.27675700

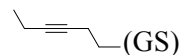
HF: -313.0991436

Sum of electronic and zero-point Energies: -312.899545

Sum of electronic and thermal Energies: -312.889838

Sum of electronic and thermal Enthalpies: -312.888894

Sum of electronic and thermal Free Energies: -312.934732



C	3.62535400	-0.47469900	0.15987400
C	0.11476300	-0.18688700	-0.11069300
C	1.24900900	0.22412700	-0.09554600
C	2.64260900	0.67770300	-0.07641400
C	-1.27650800	-0.64480500	-0.12976400
C	-3.71990200	-0.01300200	0.07087800
H	2.76285100	1.43516200	0.70520700
H	2.87088300	1.17205200	-1.02668300
H	-1.41508900	-1.41641000	0.63694500
H	-1.48624900	-1.12443300	-1.09349500
H	-4.43040100	0.80031200	0.23868500
H	-3.95383800	-0.46838800	-0.89701000
C	-2.28103000	0.49126900	0.10326100
H	-2.06508300	0.96255000	1.06767300
H	-2.13016300	1.25936000	-0.66205400
H	3.52817700	-1.22822000	-0.62509900
H	3.42642500	-0.95820600	1.11918000
H	-3.88767500	-0.76992800	0.84388300
H	4.65439000	-0.10609600	0.16320100

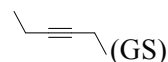
HF: -273.8023806

Sum of electronic and zero-point Energies: -273.631195

Sum of electronic and thermal Energies: -273.621923

Sum of electronic and thermal Enthalpies: -273.620979

Sum of electronic and thermal Free Energies: -273.666503



C	2.96103800	0.45508400	-0.00019800
C	-0.56324500	0.21260800	0.00011200
C	0.56324200	-0.21602900	0.00014900
C	1.94833900	-0.69567200	0.00012100
C	-1.94835900	0.69568100	0.00012900
H	2.10781300	-1.33130300	-0.87744600
H	2.10797700	-1.33095500	0.87791400
H	-2.10788300	1.33132100	-0.87742300
H	-2.10800400	1.33093100	0.87793900
C	-2.96101500	-0.45512400	-0.00019800
H	-2.82796300	-1.08287100	-0.88446700
H	-2.82808600	-1.08327400	0.88380400
H	2.82813500	1.08321500	0.88382000
H	2.82800800	1.08285800	-0.88445200
H	3.98255500	0.06604400	-0.00019600
H	-3.98254900	-0.06612700	-0.00017900

HF: -234.5054778

Sum of electronic and zero-point Energies: -234.363521

Sum of electronic and thermal Energies: -234.356367

Sum of electronic and thermal Enthalpies: -234.355422

Sum of electronic and thermal Free Energies: -234.394533

## Transition States

### ≡ (+diazomethane, 1-a TS)

C	1.42904700	-0.57630800	-0.00010100
C	1.23887600	0.78274300	0.00008400
H	1.36312100	1.35002000	0.91651000
H	1.36308700	1.35024300	-0.91621100
N	-1.21091500	-0.27072500	-0.00007300
N	-0.73718100	-1.31127000	0.00011700
H	1.62743800	-1.11377000	0.91982100
C	-0.96926300	1.04742000	-0.00002400
H	-1.26797100	1.53900000	-0.92124100
H	-1.26810300	1.53895800	0.92120500
H	1.62714300	-1.11361800	-0.92015700

HF: -227.2138468

Sum of electronic and zero-point Energies: -227.126798

Sum of electronic and thermal Energies: -227.121384

Sum of electronic and thermal Enthalpies: -227.120440

Sum of electronic and thermal Free Energies: -227.154873

Frequencies: -496.5105

### ≡ (+diazomethane, 1-b TS)

C	-1.03590100	0.26689900	-0.51854300
C	-0.26649800	1.36224800	-0.21005500
C	0.14332000	1.98314000	-0.99927300
H	-0.38419900	1.84950400	0.75410100
N	1.37100300	-0.72933700	0.05075400

N	0.51389400	-1.38147200	-0.33806500
H	-1.17396500	0.00298200	-1.56315800
C	1.73123800	0.52465900	0.35432600
H	1.90323200	0.68070200	1.41511800
H	2.47958300	0.93417500	-0.31773700
C	-1.99705300	-0.34759800	0.46480900
H	-3.00267200	0.07356900	0.35129000
H	-2.07640300	-1.43054300	0.33397000
H	-1.67388800	-0.15512500	1.49363900

HF: -266.5118707

Sum of electronic and zero-point Energies: -266.396619

Sum of electronic and thermal Energies: -266.389713

Sum of electronic and thermal Enthalpies: -266.388769

Sum of electronic and thermal Free Energies: -266.426939

Frequencies: -506.8782

### ≡<sup>OMe</sup> (+diazomethane, 1-c TS)

C	0.01347800	1.35110900	0.57445800
C	-0.49917700	0.12754400	0.95155900
H	-0.40842100	-0.21309900	1.97628700
N	1.74425400	-0.36747400	-0.44349200
N	1.78426600	0.74726400	-0.70679600
H	0.64165800	1.88498100	1.27503200
C	1.03910600	-1.25442100	0.29273500
H	0.51023600	-1.99121400	-0.30860400
H	-0.39619300	1.92418400	-0.24520400
O	-1.58900700	-0.47396300	0.36052700
C	-1.88921600	-0.05049300	-0.94716200
H	-1.00239400	-0.09920800	-1.59474500
H	-2.65377700	-0.72895000	-1.32675700
H	-2.27940900	0.97412100	-0.95907300
H	1.61557200	-1.66007300	1.12132000

HF: -341.6973118

Sum of electronic and zero-point Energies: -341.577024

Sum of electronic and thermal Energies: -341.569265

Sum of electronic and thermal Enthalpies: -341.568320

Sum of electronic and thermal Free Energies: -341.609066

Frequencies: -534.9596

### ≡<sup>CN</sup> (+diazomethane, 1-d TS)

C	0.65882600	0.57447600	0.73038700
C	-0.22474900	1.44614700	0.12407700
H	-0.82345300	2.09552100	0.75322900
H	0.01202900	1.83636600	-0.85959600
N	-1.46742500	-0.85893000	-0.07242700
N	-0.68797200	-1.43176200	0.51749500
C	1.73100700	-0.00305800	-0.01455700
H	0.67816600	0.43287300	1.80236700
C	-1.87039400	0.31388700	-0.59319400
H	-1.84428600	0.31754100	-1.67912100
N	2.58312100	-0.47451700	-0.63901500
H	-2.78467500	0.68544300	-0.13953200

HF: -319.4527798

Sum of electronic and zero-point Energies: -319.366002

Sum of electronic and thermal Energies: -319.359034

Sum of electronic and thermal Enthalpies: -319.358090

Sum of electronic and thermal Free Energies: -319.397169

Frequencies: -470.6683

### ≡<sup>Me</sup> (+diazomethane, 1-e TS)

C	0.30728400	-0.61300700	-0.86558500
C	-0.76220700	-1.41104800	-0.51855900
H	-1.38050800	-1.84946200	-1.29534200
H	-0.68877000	-1.96585400	0.41162700
N	-1.61992600	1.00383500	0.10904600
N	-0.74002000	1.58754000	-0.29612000
C	1.26606700	-0.23040500	0.17370700
O	1.04269000	-0.44393100	1.35595600
H	0.49028600	-0.31096900	-1.89052500
C	-2.23267500	-0.16443600	0.34927200
H	-2.25075900	-0.40967200	1.40678900
C	2.53098000	0.46956800	-0.27154900
H	3.10929000	-0.18693800	-0.92918400
H	2.27638600	1.36668600	-0.84466400
H	3.12843600	0.74139500	0.59813900
H	-3.16295300	-0.27739900	-0.19868800

HF: -379.832299

Sum of electronic and zero-point Energies: -379.706902

Sum of electronic and thermal Energies: -379.698157

Sum of electronic and thermal Enthalpies: -379.697213

Sum of electronic and thermal Free Energies: -379.740491

Frequencies: -446.3588

### ≡ (+diazomethane, 1-f TS)

C	-0.46118100	-0.64416800	-0.10136200
C	-0.55807200	0.58209600	-0.01939900
N	-3.07347300	-0.22582300	0.03175800
N	-2.70778200	-1.29872400	-0.07609700
C	-2.76798600	1.06281700	0.12541200
H	-3.04485100	1.65025300	-0.74355000
H	0.08162600	1.91071400	0.06863600
C	-0.44123700	2.64815400	-0.55078600

H	0.01272500	2.27384600	1.10309400
C	0.26076300	-1.92098000	-0.19023200
H	-0.26726400	-2.71400200	0.34915000
H	0.29412500	-2.23499000	-1.24147900
C	1.55597600	1.83288400	-0.35282100
H	2.00296200	2.82039000	-0.18991900
H	1.60380300	1.64228100	-1.43177600
C	1.69211500	-1.77727400	0.34936600
H	1.64988100	-1.64109500	1.43686700
H	2.21314600	-2.72557900	0.17323900
C	2.38707300	0.76821700	0.38795600
H	3.40097300	1.16691400	0.49374000
C	2.00132200	0.65893400	1.41017800
C	2.50518400	-0.62947900	-0.27269400
H	3.55905100	-0.92368000	-0.23328000
H	2.25686900	-0.55159100	-1.33965700
H	-2.94571300	1.49302200	1.10537900

HF: -460.5507177  
Sum of electronic and zero-point Energies: -460.335234  
Sum of electronic and thermal Energies: -460.324066  
Sum of electronic and thermal Enthalpies: -460.323122  
Sum of electronic and thermal Free Energies: -460.372050  
Frequencies: -441.1093

### ≡(+hydrozoic acid, 2-a TS)

C	-1.22243100	-0.76553000	-0.01326800
C	-1.33185000	0.60753200	-0.00561000
H	-1.53377900	1.14882300	-0.92169900
H	-1.54540400	1.13221400	0.91858800
N	1.21003600	0.19878300	-0.01837500
N	0.88904400	-1.01700400	0.11518500
H	-1.32606000	-1.31820800	-0.93971600
H	0.70968300	1.23770800	-0.00283500
H	-1.35907400	-1.33434600	0.89780800
H	1.43866000	-1.61690100	-0.49954500

HF: -243.2496876  
Sum of electronic and zero-point Energies: -243.173290  
Sum of electronic and thermal Energies: -243.168123  
Sum of electronic and thermal Enthalpies: -243.167179  
Sum of electronic and thermal Free Energies: -243.201157  
Frequencies: -524.0068

### ≡(+hydrozoic acid, 2-b TS)

C	0.96618200	0.21475200	0.51609100
C	0.27532800	1.36788300	0.20635200
H	-0.14111100	1.98443800	0.99459000
H	0.43016200	1.85028900	-0.75280500
N	-1.49171900	-0.46083300	-0.17633700
N	-0.65100500	-1.20233100	0.40742900
H	1.09231700	-0.04816500	1.56091700
N	-1.62717100	0.66195300	-0.41363800
C	1.93413500	-0.40875800	-0.45536100
H	2.92228300	0.05360200	-0.35391200
H	2.05432900	-1.48132600	-0.28278600
H	1.59788000	-0.25891300	-1.48533400
H	-0.62046600	-2.13471200	-0.00533300

HF: -282.5489732  
Sum of electronic and zero-point Energies: -282.444468  
Sum of electronic and thermal Energies: -282.437855  
Sum of electronic and thermal Enthalpies: -282.436911  
Sum of electronic and thermal Free Energies: -282.474466  
Frequencies: -527.0742

### ≡<sup>OMe</sup>(+hydrozoic acid, 2-c TS)

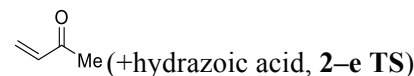
C	-0.05961000	1.33495500	0.44021700
C	0.55872600	0.21323800	0.96885400
H	0.40728300	-0.09292600	1.99530100
N	-1.71959700	-0.38986800	-0.42023500
N	-1.56735700	0.72960700	-0.73101500
H	0.40582800	1.88164200	-0.36863800
N	-1.14230400	-1.15359100	0.40402200
H	-0.68188600	1.90649900	1.11641100
O	1.59786700	-0.42545700	0.42060200
C	1.82183100	-0.21125000	-0.96162800
H	2.58241600	-0.93091700	-1.26148600
H	0.89758700	-0.38384500	-1.52500300
H	2.18757700	0.80353800	-1.15011300
H	-1.50262700	-2.10502200	0.37465200

HF: -357.740921  
Sum of electronic and zero-point Energies: -357.631398  
Sum of electronic and thermal Energies: -357.623572  
Sum of electronic and thermal Enthalpies: -357.622627  
Sum of electronic and thermal Free Energies: -357.663641  
Frequencies: -491.3743

### ≡<sup>CN</sup>(+hydrozoic acid, 2-d TS)

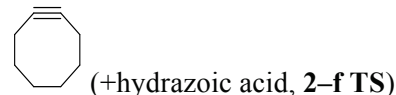
C	0.57871800	0.46976200	0.71489400
C	-0.26266400	1.40690800	0.13241100
H	0.00128600	1.83632600	-0.82591500
N	-1.51466400	-0.81508300	-0.11267300
H	-0.68721400	-1.36764200	0.45463100
N	0.58732900	0.31360500	1.78506300
C	-1.74772400	0.31019300	-0.64840000
N	1.71895800	-0.01544500	-0.00500400
H	2.63492800	-0.40433000	-0.59117800
N	-0.88066400	2.02028800	0.77864500
H	-2.71530900	0.60046300	-0.50826300

HF: -335.481162  
Sum of electronic and zero-point Energies: -335.405287  
Sum of electronic and thermal Energies: -335.398591  
Sum of electronic and thermal Enthalpies: -335.397646  
Sum of electronic and thermal Free Energies: -335.436169  
Frequencies: -538.7689



C	0.21054100	-0.35609900	-0.85541800
C	-0.79002800	-1.28653100	-0.64172200
H	-1.42345400	-1.59661400	-1.46573500
H	-0.66493600	-1.98615300	0.17738200
N	-1.73399600	0.92849200	0.28720000
N	-0.77456400	1.48812200	0.00714400
C	1.32247400	-0.24629900	0.11996700
O	1.29212200	-0.82065100	1.18784600
H	0.32475900	0.13025600	-1.81774800
C	2.47958800	0.63811400	-0.28120500
H	2.92997800	0.26518400	-1.20657800
H	2.11314300	1.65051100	-0.47972400
H	3.22395700	0.65896100	0.51388700
N	-2.20424500	-0.24187300	0.36716200
H	-3.18623500	-0.27522600	0.09548000

HF: -395.8613121  
Sum of electronic and zero-point Energies: -395.746918  
Sum of electronic and thermal Energies: -395.738311  
Sum of electronic and thermal Enthalpies: -395.737367  
Sum of electronic and thermal Free Energies: -395.780917  
Frequencies: -516.7753



C	-0.51569400	-0.64048000	-0.07257800
C	-0.52715800	0.58898500	0.01624100
N	-3.03615800	-0.16309000	0.03642800
N	-2.59831300	-1.21720800	-0.08307200
C	0.09248700	1.91911700	0.09041900
H	-0.44541500	2.63461200	-0.53832500
H	0.02863200	2.28984300	1.12133200
C	0.19362900	-1.92767700	-0.16508300
H	-0.33770000	-2.70500300	0.39242100
C	0.20207700	-2.24969600	-1.21387900
H	1.56533100	1.83376000	-0.34170000
H	2.02226100	2.81268900	-0.15888500
H	1.60600000	1.66663900	-1.42452800
C	1.63390500	-1.78832900	0.34768100
H	1.61175500	-1.64191200	1.43427200
C	2.14298800	-2.74269000	0.17166200
H	2.38811300	0.74382100	0.37059300
H	3.41513000	1.11422400	0.44679200
H	2.03094800	0.64065800	1.40381600
C	2.44676000	-0.65343500	-0.30085500
H	3.49445200	-0.97040700	-0.30438600
H	2.15956400	-0.56405800	-1.35692500
N	-2.69757300	1.04412900	0.00785700
H	-3.27062500	1.61371400	0.62984100

HF: -476.5892411  
Sum of electronic and zero-point Energies: -476.385132  
Sum of electronic and thermal Energies: -476.374013  
Sum of electronic and thermal Enthalpies: -476.373069  
Sum of electronic and thermal Free Energies: -476.422099  
Frequencies: -479.5296

### ≡(+diazaoethane, 3-a TS)

C	1.84434700	-0.47270200	-0.25059700
C	0.84363300	-1.30155500	0.18609000
H	0.28769600	-1.90685300	-0.52416200
H	0.84795400	-1.67104300	1.20664600
C	-2.01411500	-0.42087000	-0.39934100
N	-0.23917100	1.12728800	0.19167200
N	0.75928200	1.55080300	-0.17806300
H	2.04437600	-0.34207500	-1.30776600
C	-0.91612500	0.02212600	0.53190500
H	-1.11315900	-0.01946100	1.60053300
H	-2.93340700	0.16270300	-0.29071200
H	-1.67838000	-0.35993500	-1.43789100
H	-2.24905700	-1.46498100	-0.17752400
H	2.60676400	-0.10699100	0.42726400


HF: -266.5144982  
Sum of electronic and zero-point Energies: -266.398942  
Sum of electronic and thermal Energies: -266.392087  
Sum of electronic and thermal Enthalpies: -266.391143  
Sum of electronic and thermal Free Energies: -266.429190  
Frequencies: -482.7115

### ≡(+diazaoethane, 3-b TS)

C	1.35930400	-0.46226700	-0.52115800
C	0.38549600	-1.30392500	-0.04543900
H	-0.24573000	-1.85666900	-0.73472400
H	0.48273900	-1.73504300	0.94785100
C	-2.53292900	-0.41878200	-0.19174100
N	-0.68671600	1.12407400	0.14921000
N	0.25803300	1.52991700	-0.36025900


H	1.44242300	-0.30925600	-1.59334900
C	-1.31344100	0.01977200	0.57504400
H	-1.35304800	-0.03312500	1.66047500
H	-3.43004500	0.15437400	0.06156500
H	-2.35453000	-0.33797300	-1.26730100
H	-2.72528300	-1.46862100	0.04433400
C	2.54004000	-0.03573400	0.31044900
H	3.40995600	-0.67500900	0.11964300
H	2.83624100	0.99550600	0.09761700
H	2.30724000	-0.10649300	1.37830300

HF: -305.8126031  
Sum of electronic and zero-point Energies: -305.668829  
Sum of electronic and thermal Energies: -305.660481  
Sum of electronic and thermal Enthalpies: -305.659537  
Sum of electronic and thermal Free Energies: -305.701269  
Frequencies: -495.2963

 (+diazioethane, 3-c TS)


C	0.53388600	-1.64324500	0.40970700
C	0.67276200	-0.37601300	0.93397600
H	0.51286300	-0.19512100	1.99067500
N	-1.67282100	-0.42351900	-0.37703000
N	-1.36469900	-1.45177800	-0.78739100
C	0.10670300	-2.41329500	1.03882200
C	-1.26876500	0.54475400	0.47903000
H	1.07782200	-1.97861500	-0.46140700
O	1.51069200	0.59006200	0.42180100
C	2.00427800	0.35855700	-0.87558900
H	1.19226000	0.14321900	-1.58348900
H	2.51820300	1.27142400	-1.17943300
H	2.71342700	-0.47797100	-0.88795700
C	-1.00155200	1.91129000	-0.09072700
H	-1.91008500	2.50988700	-0.20678000
H	-0.32281900	2.43231600	0.58883500
H	-0.50273700	1.83490400	-1.05988600
H	-1.85217700	0.50778100	1.39877900

HF: -380.9984547  
Sum of electronic and zero-point Energies: -380.849165  
Sum of electronic and thermal Energies: -380.840174  
Sum of electronic and thermal Enthalpies: -380.839230  
Sum of electronic and thermal Free Energies: -380.882603  
Frequencies: -538.5164

 (+diazioethane, 3-d TS)


C	-1.03780000	-0.59663200	0.72256300
C	-0.03981100	-1.31967000	0.10400300
H	0.66271100	-1.86819200	0.72393200
C	-0.22085100	-1.73573400	-0.88137600
H	2.77500800	-0.36407000	-0.01879100
N	0.85999300	1.13165400	-0.09439000
N	0.00797200	1.58798500	0.50089900
C	-2.19545500	-0.18708900	-0.00592700
H	-1.06320600	-0.45546400	1.79451300
H	1.44872400	0.03875000	-0.61159100
C	1.35673700	0.02201700	-1.69521600
N	-3.11885300	0.14749400	-0.61720600
H	3.60512500	0.25225900	-0.37413500
H	2.73715700	-0.31327600	1.07236400
H	2.97454700	-1.39927600	-0.30674700

HF: -358.7536989  
Sum of electronic and zero-point Energies: -358.638564  
Sum of electronic and thermal Energies: -358.630122  
Sum of electronic and thermal Enthalpies: -358.629178  
Sum of electronic and thermal Free Energies: -358.671820  
Frequencies: -444.2037

 (+diazioethane, 3-e TS)


C	0.66406700	-0.61680200	-0.82139000
C	-0.42189900	-1.34149100	-0.38631400
H	-1.11570300	-1.75947300	-1.11011500
C	-0.32437900	-1.87143000	0.55657500
C	-3.14433200	-0.17383600	-0.18185200
N	-1.12728900	1.11779800	0.22234900
N	-0.23298900	1.64337800	-0.23464300
O	1.71823000	-0.27166200	0.13693700
C	1.58081400	-0.46342100	1.33528600
H	0.79075700	-0.34056900	-1.86209900
C	-1.81452300	0.00186500	0.50644200
C	-1.74748200	-0.23381400	1.56571100
C	2.97597700	0.36113400	-0.41691600
H	3.46128100	-0.32491100	-1.11824600
H	2.71993800	1.26997600	-0.97055000
H	3.65826500	0.60217900	0.39776200
H	-3.93765000	0.43269300	0.26388300
H	-3.06153200	0.07345600	-1.24336200
H	-3.43318800	-1.22421400	-0.09723000

HF: -419.132974  
Sum of electronic and zero-point Energies: -418.979355  
Sum of electronic and thermal Energies: -418.969015  
Sum of electronic and thermal Enthalpies: -418.968071  
Sum of electronic and thermal Free Energies: -419.015407  
Frequencies: -421.9262

 (+diazioethane, 3-f TS)


C	0.01806600	0.84473500	-0.13132700
C	0.34303200	-0.34183400	-0.19392900
C	3.09579000	-1.11315600	0.90752200
N	2.66104200	0.91931100	-0.34603600
N	2.10187900	1.91377500	-0.29791500
C	2.62261400	-0.40574400	-0.33261500
H	2.82587400	-0.84302200	-1.30624500
C	-0.03467000	-1.76934900	-0.18837800
H	0.57323800	-2.35206400	-0.89092800
H	0.15754500	-2.18980000	0.80840900
C	-0.92183600	1.96674700	-0.01328900
H	-0.50084900	2.77314000	0.59617700
H	-1.09071600	2.39311200	-1.01045700
C	-1.52229700	-1.93764900	-0.53018600
H	-1.76570000	-3.00325600	-0.44527200
H	-1.67604500	-1.66413700	-1.58103500
C	-2.25804900	1.49454600	0.58036400
H	-2.10865100	1.24784500	1.63865300
C	-2.95602600	2.33942100	0.55218100
H	-2.48840000	-1.12590100	0.35295400
H	-3.40792300	-1.71331900	0.44354800
H	-2.07686800	-1.05943500	1.36892100
C	-2.89228700	0.28915500	-0.13546300
H	-3.97691500	0.37876900	-0.01587700
H	-2.70285700	0.37178400	-1.21403100
H	4.18553600	-1.19682800	0.96913700
H	2.72622200	-0.59820200	1.79785900
H	2.68191100	-2.12491400	0.90269700

HF: -499.8514837  
Sum of electronic and zero-point Energies: -499.607896  
Sum of electronic and thermal Energies: -499.595117  
Sum of electronic and thermal Enthalpies: -499.594173  
Sum of electronic and thermal Free Energies: -499.647169  
Frequencies: -422.4877

 (+diazioethane, 3-g TS)

C	1.35465900	0.32029100	0.06162900
C	0.34296000	0.99001000	-0.10996800
C	-2.36650900	-0.24358100	0.66462100
N	-0.54099700	-1.48824000	-0.34074600
N	0.53842200	-1.81980300	-0.15186300
C	-1.36165300	-0.44124000	-0.43873900
H	-1.67987900	-0.26164800	-1.46362400
C	-0.39168700	2.27083300	-0.20567600
H	-0.98780000	2.32871700	-1.12175200
C	-1.07610500	2.39558700	0.63959900
C	2.75006600	-0.09282400	0.30401500
H	2.82562400	-0.70974400	1.20384300
H	3.13181200	-0.69196300	-0.52741100
H	-3.20322300	-0.94752400	0.61493200
H	-1.88089000	-0.33619200	1.63969800
H	-2.77771400	0.76500100	0.57844400
H	3.39683800	0.78166600	0.42755700
H	0.30234200	3.11580600	-0.19831300

HF: -343.8689837  
Sum of electronic and zero-point Energies: -343.720981  
Sum of electronic and thermal Energies: -343.710914  
Sum of electronic and thermal Enthalpies: -343.709970  
Sum of electronic and thermal Free Energies: -343.755853  
Frequencies: -488.7146

 (+diazioethane, 3-h TS)

C	-2.40047700	1.76473600	0.32901500
C	-1.22602500	2.07245900	-0.60719200
C	-2.47407400	0.32400700	0.83986900
C	0.25521100	-0.89171700	-0.26882000
C	0.51361200	0.30384600	-0.08502700
C	0.16451700	1.74567000	-0.03701300
C	-0.55486400	-2.08371700	-0.59767400
C	-2.70548000	-0.72599000	-0.26182000
H	0.91111200	2.31708900	-0.59989600
H	0.23257100	2.10344800	1.00069900
H	-0.04648800	-3.00017000	-0.28436800
H	-0.63975700	-2.13544500	-1.69130400
H	-3.78102500	-0.90548300	-0.36335300
H	-2.37075100	-0.33530800	-1.23041700
N	2.24057700	-1.89655000	0.25216800
N	2.77800200	-0.91951900	0.50347100
H	3.46828800	1.18549300	-0.47428800
H	4.54436200	1.19532000	-0.27402100
H	3.29569200	0.77227100	-1.47165300
H	3.12309800	2.22163900	-0.46556300
H	-1.55257100	0.09122800	1.38131900
H	-3.28294800	0.25244400	1.57660000
H	-1.97511900	-2.04981700	-0.00240200
H	-2.53071000	-2.88792000	-0.43688100
H	-1.92473400	-2.23397400	1.07763900
H	-1.33920900	1.54457800	-1.56023900
H	-1.25575100	3.14276900	-0.84319500
H	-2.33985200	2.44007600	1.19244700
H	-3.33400100	2.01594600	-0.19176500
H	2.68543900	0.40995000	0.55231400
C	2.65473800	0.78526800	1.57269700



HF: -539.1495333  
 Sum of electronic and zero-point Energies: -538.876481  
 Sum of electronic and thermal Energies: -538.862893  
 Sum of electronic and thermal Enthalpies: -538.861949  
 Sum of electronic and thermal Free Energies: -538.916462  
 Frequencies: -454.8830



## (+diazaoethane, 3-i TS)

C	0.20622200	-0.92362300	-0.21002500
C	-0.09780000	0.26530600	-0.23271900
N	-2.55124100	-0.78247000	-0.33227500
N	-2.24061900	-1.87138500	-0.30862000
C	0.53974000	1.59965300	-0.22283900
H	0.04741300	2.32316700	-0.88285300
H	0.52765500	2.02810000	0.78814400
C	1.41297400	-1.75381600	-0.01015300
H	1.21301500	-2.69528900	0.51036300
C	1.85267500	-2.01508200	-0.98078700
C	1.98369700	1.34105100	-0.70204400
H	2.50883500	2.29656600	-0.82436300
H	1.90178200	0.89905100	-1.70082000
C	2.36992900	-0.87447400	0.82147700
H	1.83856600	-0.63295700	1.74838400
C	3.25263300	-1.45738900	1.11313400
C	2.88475700	0.43845600	0.17743500
H	3.27711400	1.04742100	1.00147300
H	3.75539500	0.19482400	-0.44390900
C	-2.76526400	1.25637200	0.96098200
H	-2.23568100	2.21253800	0.94824600
H	-3.83239700	1.46145200	1.09411900
H	-2.40328300	0.68241900	1.81656600
C	-2.45779600	0.52578000	-0.31720200
H	-2.61945400	0.98392900	-1.28550400

HF: -460.5384036  
 Sum of electronic and zero-point Energies: -460.323877  
 Sum of electronic and thermal Energies: -460.312028  
 Sum of electronic and thermal Enthalpies: -460.311084  
 Sum of electronic and thermal Free Energies: -460.362147  
 Frequencies: -260.2937



## (+diazaoethane, 3-j TS)

C	-0.56702800	0.98289400	-0.04488600
C	-0.22781200	-0.17346400	-0.26408700
N	2.37078500	0.80373500	-0.24929100
N	2.22261100	1.90987100	-0.07239000
C	-0.94449600	-1.46200400	-0.30790300
H	-0.69888700	-2.09381700	-1.16674700
C	-0.75762200	-2.04919800	0.59875000
C	-1.94752400	1.48542700	0.19472400
H	-2.02598200	2.20965900	1.00986000
H	-2.32771800	1.97593800	-0.70787600
C	-2.43800200	-1.00130500	-0.38017400
H	-3.08515100	-1.84487900	-0.11605900
H	-2.65765500	-0.73612400	-1.42116400
C	-2.76902700	0.20138100	0.52217600
H	-2.57097200	-0.07321400	1.56558400
C	-3.83967900	0.42365400	0.44532500
H	2.52276400	-1.39644200	0.75510500
H	1.95807500	-2.31800100	0.59028800
C	3.57205000	-1.66686500	0.91606100
H	2.13751900	-0.92769000	1.66400300
C	2.32445400	-0.48475400	-0.42122200
H	2.42226900	-0.80510800	-1.44865400

HF: -421.2333036  
 Sum of electronic and zero-point Energies: -421.048964  
 Sum of electronic and thermal Energies: -421.037797  
 Sum of electronic and thermal Enthalpies: -421.036853  
 Sum of electronic and thermal Free Energies: -421.087178  
 Frequencies: -107.5314



## (+diazaoethane, 3-k TS)

C	-0.40722900	0.46494400	-0.82026800
C	0.53232800	1.30955500	-0.29207100
H	1.20357500	1.84171000	-0.95801600
H	0.35044600	1.78031500	0.66887400
N	1.52778400	-1.08046600	0.15569100
N	0.66512700	-1.59116400	-0.36883500
H	-0.47381100	0.24101900	-1.87636900
C	3.41157400	0.43904700	-0.14108000
H	3.33619400	0.27242700	-1.21865400
C	3.58709700	1.50409500	0.02977200
H	4.27492200	-0.11161400	0.24310400
C	2.12262400	0.06122100	0.54095700
C	2.05593900	0.19802000	1.61782900
H	-1.59521000	0.08221000	-0.01473800
F	-1.27190000	-0.14211400	1.27884200
F	-2.19365600	-1.02539200	-0.47426200
F	-2.54991700	1.03790400	0.01193800

HF: -603.4926572  
 Sum of electronic and zero-point Energies: -603.371722  
 Sum of electronic and thermal Energies: -603.361538  
 Sum of electronic and thermal Enthalpies: -603.360594  
 Sum of electronic and thermal Free Energies: -603.408124  
 Frequencies: -439.7732



## NHMe (+diazaoethane, 3-l TS)

C	-0.15715700	-0.71456100	0.87692800
C	0.93797200	-1.35939800	0.35661100
H	1.69511200	-1.75584700	1.02663900
H	0.82172800	-1.85631800	-0.60129200
N	1.47911700	1.16612900	-0.13464700
N	0.58187100	1.56691900	0.43742400
C	-1.29334400	-0.43545900	-0.02003500
O	-1.21489400	-0.56599600	-1.23689000
H	-0.24967400	-0.50553700	1.93665700
C	3.59100700	-0.03542000	-0.01851900
H	3.60444000	0.14718100	1.05905700
H	3.91360400	-1.06456900	-0.19495100
H	4.31162400	0.63205400	-0.49970900
C	-3.56228600	0.43923000	-0.22893000
H	-3.76180700	-0.29675200	-1.00912800
H	-4.44399700	0.53596300	0.40647100
C	-3.35712300	1.40068500	-0.71308500
C	2.19420600	-0.11565100	-0.56264200
H	2.03325400	-0.05385100	-1.62469800
N	-2.44610800	-0.01184400	0.57429600
H	-2.41455600	0.23626300	1.54915800

HF: -474.4850692  
 Sum of electronic and zero-point Energies: -474.313357  
 Sum of electronic and thermal Energies: -474.301718  
 Sum of electronic and thermal Enthalpies: -474.300774  
 Sum of electronic and thermal Free Energies: -474.351740  
 Frequencies: -450.9068



## OMe (+diazaoethane, 3-m TS)

C	-0.17071300	-0.74066500	0.81122300
C	0.91082300	-1.37389700	0.24582100
H	1.65759200	-1.82725300	0.89091700
H	0.78206700	-1.82114200	-0.73502600
N	1.48632100	1.15454400	-0.15352500
N	0.57386900	1.56454500	0.38233000
C	-1.31002300	-0.40525400	-0.03862200
O	-1.31703900	-0.46604700	-1.25050000
H	-0.26107300	-0.56307800	1.87444600
C	3.57633400	-0.05666800	0.09455800
H	3.49860000	0.07775000	1.17654300
C	3.92382100	-1.07427100	-0.09957400
H	4.32470400	0.63771300	-0.29721000
O	-2.37554700	0.01435300	0.67224900
C	-3.49948500	0.40979600	-0.10623900
H	-3.85754700	-0.42436500	-0.71364100
H	-4.26167200	0.71901300	0.60772500
H	-3.23368800	1.23886900	-0.76612500
C	2.22519700	0.10774000	-0.55398700
H	2.15376000	-0.02961900	-1.63020900

HF: -494.3464422  
 Sum of electronic and zero-point Energies: -494.186462  
 Sum of electronic and thermal Energies: -494.175460  
 Sum of electronic and thermal Enthalpies: -494.174515  
 Sum of electronic and thermal Free Energies: -494.223594  
 Frequencies: -433.5855

NO<sub>2</sub> (+diazaoethane, 3-n TS)

C	0.75216700	-0.58038600	-0.81712300
C	-0.28875100	-1.31641100	-0.31666800
H	-0.95016600	-1.80062200	-1.02806700
H	-0.16014200	-1.79778900	0.64552000
N	-1.10887700	1.11439600	0.14292700
N	-0.26595900	1.66306400	-0.37111400
O	1.58164900	-0.25366800	1.28157100
H	0.96164500	-0.35866400	-1.85053700
C	-3.07136400	-0.29492700	-0.12254200
H	-3.02428000	-0.11215500	-1.19894500
H	-3.30312400	-1.35088700	0.03624000
H	-3.88492500	0.29787600	0.30397600
N	1.79894600	-0.16496000	0.07541800
O	2.81516100	0.27854500	-0.40973600
C	-1.73903900	-0.00825700	0.52192100
H	-1.63663600	-0.16438200	1.59297800


HF: -470.9874157  
 Sum of electronic and zero-point Energies: -470.867819  
 Sum of electronic and thermal Energies: -470.858621  
 Sum of electronic and thermal Enthalpies: -470.857677  
 Sum of electronic and thermal Free Energies: -470.902738  
 Frequencies: -397.1941



## (+methyl azide, 4-a TS)


C	0.84609700	-1.29755000	-0.08928700
C	1.85075000	-0.39409800	0.16631200
H	2.17522900	-0.19818600	1.18084400
H	2.53187900	-0.09238800	-0.62114300
N	-0.27453400	1.05219700	-0.12651000
N	-0.82791200	-0.03463300	-0.44403600
H	0.37235600	-1.83337800	0.72822400
N	0.76883800	1.48915100	0.09964400
H	0.73891500	-1.74334000	-1.07063800
C	-2.07839600	-0.35765700	0.23789600
H	-2.89106200	0.29106900	-0.09902300

H -2.31976900 -1.38411900 -0.03927200  
 H -1.98299700 -0.29083100 1.32779700  
 HF: -282.5392961  
 Sum of electronic and zero-point Energies: -282.434238  
 Sum of electronic and thermal Energies: -282.427655  
 Sum of electronic and thermal Enthalpies: -282.426711  
 Sum of electronic and thermal Free Energies: -282.464367  
 Frequencies: -497.2071

 (+methyl azide, 4-b TS)


C	1.11019400	-0.51071200	0.51928400
C	1.66564000	0.69172400	0.17223300
H	1.99093300	1.39547700	0.93813500
H	2.14320200	0.81381500	-0.80366500
N	-0.83227000	1.15157900	-0.13694600
N	-0.98707400	0.05968000	0.47208100
H	0.99017300	-0.74649200	1.57150400
N	0.01689100	1.88076100	-0.42883000
C	1.08517400	-1.67180800	-0.44024700
H	2.02125600	-2.23732700	-0.37746500
H	0.27010500	-2.36857800	-0.22827800
H	0.97792400	-1.31896500	-1.47095500
C	-2.02965000	-0.83421600	-0.01851700
H	-1.98511100	-1.73240400	0.59822600
H	-3.02056600	-0.38804800	0.10082000
H	-1.87889400	-1.11154600	-1.06897500

HF: -321.8386057  
 Sum of electronic and zero-point Energies: -321.705588  
 Sum of electronic and thermal Energies: -321.697546  
 Sum of electronic and thermal Enthalpies: -321.696602  
 Sum of electronic and thermal Free Energies: -321.737745  
 Frequencies: -492.4136

 (+methyl azide, 4-c TS)


C	-0.85229800	-1.48586700	0.48377400
C	-0.79117300	-0.19149500	0.95842200
H	-0.53551900	0.02007500	1.98844100
N	1.42738400	-0.68875800	-0.41960000
N	0.90887000	-1.67776600	-0.73042900
H	-1.47785400	-1.75705000	-0.35441300
N	1.25850900	0.23037700	0.43090400
H	-0.57338300	-2.28050700	1.16323800
O	-1.40036800	0.88114600	0.39030900
C	-1.78083200	0.74216900	-0.96282800
H	-2.09416700	1.73096700	-1.29747100
H	-0.93738900	0.39332000	-1.57198200
C	-2.61678900	0.04218700	-1.07083700
H	1.61989700	1.58789100	0.04471400
H	1.18251400	2.24235400	0.79986300
H	2.70438000	1.73088200	0.04511900
H	1.21424000	1.86544100	-0.93504300

HF: -397.029433  
 Sum of electronic and zero-point Energies: -396.891003  
 Sum of electronic and thermal Energies: -396.882060  
 Sum of electronic and thermal Enthalpies: -396.881116  
 Sum of electronic and thermal Free Energies: -396.924750  
 Frequencies: -513.5967

 (+methyl azide, 4-d TS)

C	0.36962000	-1.81191100	0.07357900
C	-0.48583600	-0.91242200	0.69090200
H	-0.51240500	-0.81360300	1.76798100
N	1.54003400	0.40200900	-0.22195200
N	1.89586800	-0.63433600	-0.59879100
H	0.13270500	-2.19185000	-0.91195400
N	0.66278100	0.90665200	0.52096100
H	1.01263600	-2.42960200	0.68878600
N	-2.56662100	-0.02063200	-0.56934800
C	-1.65017800	-0.43758900	-0.00363100
C	-0.02361800	2.10356300	0.02995800
H	-0.83391400	2.30066300	0.73097100
H	0.65987300	2.95542900	0.03276200
H	-0.44325500	1.95326500	-0.96948500


HF: -374.7681786  
 Sum of electronic and zero-point Energies: -374.663515  
 Sum of electronic and thermal Energies: -374.655595  
 Sum of electronic and thermal Enthalpies: -374.654651  
 Sum of electronic and thermal Free Energies: -374.695892  
 Frequencies: -490.8896

 (+methyl azide, 4-e TS)

C	0.63789900	-0.34555900	-0.85568100
C	-0.42196200	-1.20029600	-0.62645500
H	-1.09129500	-1.46096800	-1.44115200
H	-0.33489900	-1.91058000	0.18899200
N	-1.22830600	1.05205000	0.30916600
N	-0.25177400	1.57876300	0.01988900
O	1.75822500	-0.29869900	0.11208900
C	1.70673900	-0.87742600	1.17776100
H	0.77001100	0.14066700	-1.81556300
C	2.95796300	0.52775300	-0.28931200
H	3.38089900	0.14280000	-1.22263500
H	2.64492200	1.56069900	-0.47246800
H	3.70843700	0.49838000	0.49986000


N	-1.76745200	-0.08140500	0.39373300
C	-3.17019600	-0.19314600	0.00075100
H	-3.34524600	0.18789500	-1.01153600
H	-3.41020200	-1.25591900	0.03459900
H	-3.81539100	0.33026100	0.70994100

HF: -435.1517036  
 Sum of electronic and zero-point Energies: -435.008975  
 Sum of electronic and thermal Energies: -434.998817  
 Sum of electronic and thermal Enthalpies: -434.997873  
 Sum of electronic and thermal Free Energies: -435.045201  
 Frequencies: -481.5145

 (+methyl azide, 4-f TS)


C	0.01177600	0.86592300	-0.11840500
C	0.31720200	-0.32748900	-0.13103700
N	2.58625400	0.93734400	-0.22700800
N	1.96779000	1.90324500	-0.23453200
C	0.00931300	-1.76539400	-0.11763300
H	0.64639400	-2.30970500	-0.82254300
H	0.21869500	-2.17290300	0.88056900
C	-0.96363300	1.96464100	-0.05262700
H	-0.57581500	2.79547300	0.54515100
H	-1.12056000	2.35926700	-1.06432200
H	-1.47115500	-1.99120400	-0.46404100
C	-1.68409400	-3.05823000	-0.33352300
H	-1.62193100	-1.76929400	-1.52709600
C	-2.29663900	1.46578700	0.52428900
H	-2.16299700	1.25033900	1.59133100
H	-3.01795500	2.28841500	0.45979600
C	-2.46865400	-1.16758100	0.37201400
H	-3.38103300	-1.76597300	0.46096500
H	-2.08165900	-1.06187200	1.39425000
C	-2.88048000	0.22458100	-0.17501900
H	-3.97016400	0.29576700	-0.09837300
H	-2.65310700	0.27730900	-1.24804800
N	2.51000200	-0.30691000	-0.32046700
C	3.31428100	-1.09045300	0.61458100
C	2.95503400	-2.11718600	0.53670900
H	4.37259800	-1.07539400	0.33923300
H	3.19620800	-0.74463200	1.64722800

HF: -515.8786431  
 Sum of electronic and zero-point Energies: -515.645948  
 Sum of electronic and thermal Energies: -515.633372  
 Sum of electronic and thermal Enthalpies: -515.632427  
 Sum of electronic and thermal Free Energies: -515.685468  
 Frequencies: -454.4883

 (+methyl azide, 4-g TS)

C	-1.37514900	0.25088700	-0.04034700
C	-0.39766100	1.00107700	0.04333200
C	2.52916200	-0.28801800	-0.35149900
N	0.56908200	-1.40973900	0.18491900
N	-0.53515400	-1.72305000	0.08322100
C	0.37597200	2.25266500	0.10197800
H	0.95168300	2.31043400	1.02943400
H	1.07709700	2.32343800	-0.73510200
C	-2.78516700	-0.15481900	-0.17931600
H	-2.91551400	-0.78350600	-1.06390700
H	-3.10241100	-0.74301200	0.68546500
H	3.25619800	-1.00800300	0.03447000
H	2.40624500	-0.43296200	-1.43074300
H	2.91508400	0.71509000	-0.16616000
H	-3.43730300	0.71779300	-0.26833700
H	-0.29357800	3.11577800	0.05511100
N	1.26029500	-0.37946400	0.36255700

Frequencies: -504.7893  
 Sum of electronic and zero-point Energies: -359.759472  
 Sum of electronic and thermal Energies: -359.749760  
 Sum of electronic and thermal Enthalpies: -359.748816  
 Sum of electronic and thermal Free Energies: -359.793974  
 Frequencies: -525.0290

 (+methyl azide, 4-h TS)

C	-2.33683500	1.83268000	0.30350800
C	-1.18630900	2.08260200	-0.67914200
C	-2.43119400	0.41021200	0.86096000
C	0.23828700	-0.94569300	-0.27256500
C	0.47598900	0.26300700	-0.16891100
C	0.21195000	1.71656100	-0.15238900
C	-0.61742300	-2.12950000	-0.51681100
C	-2.70879700	-0.67290000	-0.19746700
H	0.96356800	2.22458700	-0.76707400
H	0.34371700	2.09551600	0.86982800
H	-0.12712800	-3.03970900	-0.16181400
H	-0.72633900	-2.23832600	-1.60351000
H	-3.79062900	-0.82139600	-0.27949200
H	-2.37603800	-0.33154800	-1.18536500
N	2.57697400	0.30437600	0.46378600
N	2.14109200	-1.88950700	0.11759800
C	2.74213400	-0.92672800	0.30754800
C	3.59216700	1.19781900	-0.08386600
H	4.54886100	1.07745700	0.43209100
H	3.73501300	1.04736100	-1.16000000
H	3.23770400	2.21374100	0.09261400

H	-1.50518000	0.17496600	1.39306200
H	-3.22571900	0.38124200	1.61587900
C	-2.01908600	-2.00959900	0.10840700
H	-2.61567700	-2.84638400	-0.27013700
H	-1.94757700	-2.14283600	1.19451800
H	-1.35409900	1.54420700	-1.61830400
H	-1.18455500	3.14856300	-0.93385000
H	-2.23056400	2.53029300	1.14410300
H	-3.27925100	2.09415400	-0.19543300

HF: -555.1776955

Sum of electronic and zero-point Energies: -554.915557  
 Sum of electronic and thermal Energies: -554.902144  
 Sum of electronic and thermal Enthalpies: -554.901200  
 Sum of electronic and thermal Free Energies: -554.955615  
 Frequencies: -470.3559



(+methyl azide, 4-i TS)

C	0.16479700	-0.90344200	-0.19448800
C	-0.11583100	0.29362000	-0.16318500
N	-2.47385400	-0.77975300	-0.27673100
N	-2.07464000	-1.84264500	-0.31970000
C	0.51097300	1.62823900	-0.15277800
H	-0.00383700	2.34570100	-0.80046000
O	0.51952500	2.05012900	0.86055300
C	1.37994300	-1.73353300	-0.04138400
H	1.18847900	-2.68752500	0.45936800
H	1.79515300	-1.97133500	-1.02858300
C	1.94440500	1.37631500	-0.66893400
H	2.46817500	2.33348600	-0.77977200
C	1.83874600	0.95899400	-1.67588800
H	2.35791200	-0.87787800	0.78941900
H	1.84870200	-0.65930700	1.73441100
H	3.24513100	-1.47003600	1.04544200
C	2.86190100	0.45086800	0.16830200
C	3.27250000	1.03750500	0.99959800
C	3.71852900	0.22208900	-0.47734900
N	-2.31401900	0.45404600	-0.33374100
C	-2.89712400	1.21924800	0.77221400
H	-2.45999800	2.21603500	0.71152200
H	-3.98161700	1.30701700	0.66403900
H	-2.65374800	0.77508300	1.74333900

HF: -476.5646465

Sum of electronic and zero-point Energies: -476.360666  
 Sum of electronic and thermal Energies: -476.349252  
 Sum of electronic and thermal Enthalpies: -476.348308  
 Sum of electronic and thermal Free Energies: -476.398461  
 Frequencies: -379.1130



(+methyl azide, 4-j TS)

C	-0.44617300	1.01224300	-0.01295900
C	-0.14080800	-0.17513100	-0.17693100
N	2.26607100	0.75353100	-0.21563000
N	2.11097300	1.86621100	-0.12448800
C	-0.84831800	-1.46249200	-0.25748500
H	-0.55825400	-2.07700100	-1.11500200
C	-0.70162800	-2.06231000	0.64905700
H	-1.86122700	1.46560800	0.17272500
H	-1.97585400	2.21083300	0.96498800
H	-2.21243600	1.93637500	-0.75257500
C	-2.33768800	-1.01077000	-0.38951300
H	-2.99079500	-1.85542300	-0.14718000
C	-2.51847700	-0.74854900	-1.43859700
H	-2.69475700	0.19576300	0.49525000
H	-2.52398400	-0.07203700	1.54565400
H	-3.76324200	0.41672300	0.38951300
N	1.97665600	-0.44255000	-0.40743500
C	2.48861900	-1.37617300	0.60349400
H	1.99996300	-2.33015700	0.40703500
H	3.56901400	-1.50905400	0.50518600
H	2.24190200	1.04402900	1.61730200

HF: -437.2610693

Sum of electronic and zero-point Energies: -437.086616  
 Sum of electronic and thermal Energies: -437.076250  
 Sum of electronic and thermal Enthalpies: -437.075306  
 Sum of electronic and thermal Free Energies: -437.123009  
 Frequencies: -263.8522



(+methyl azide, 4-k TS)

C	-0.39862300	0.35389800	-0.83066300
C	0.54058300	1.26484000	-0.40777100
H	1.18717000	1.74026700	-1.13811300
H	0.39741400	1.79757900	0.52514700
N	1.58731700	-1.03173600	0.07925800
N	0.65516300	-1.54456200	-0.35435300
C	-0.51084200	0.08164400	-1.87178300
C	3.40164200	0.41910800	0.06424500
H	3.59212700	0.26686500	-1.00396200
H	3.54263800	1.47144200	0.31164400
H	4.10671900	-0.17201000	0.65312400
C	-1.58901700	0.06991700	0.02081700
F	-1.26915200	0.00937500	1.32523600
F	-2.18217300	-1.08557400	-0.30439600
F	-2.53774200	1.02359600	-0.09058300
N	2.02307300	0.09644800	0.42821700

HF: -619.5133601

Sum of electronic and zero-point Energies: -619.403006  
 Sum of electronic and thermal Energies: -619.393140  
 Sum of electronic and thermal Enthalpies: -619.392196  
 Sum of electronic and thermal Free Energies: -619.439199  
 Frequencies: -475.2042



(+methyl azide, 4-l TS)

C	-0.13426100	-0.44976400	0.93245500
C	0.93961900	-1.24176600	0.59097600
H	1.68329600	-1.49610800	1.34022700
H	0.82865100	-1.91406400	-0.25258800
N	1.57938900	1.10275800	-0.26388300
N	0.59827400	1.53725200	0.14710600
C	-1.33239900	-0.45417200	0.05189100
O	-1.36689300	-1.04558600	-1.01456000
H	-0.22545600	-0.02976400	1.92777000
C	3.59819700	-0.05181900	-0.19707800
C	3.83397500	0.25938300	0.82694600
H	3.88758000	-1.09390200	-0.33391100
H	4.16020000	0.55927800	-0.90708800
C	-3.56433600	0.44212000	-0.32320600
H	-3.91027200	-0.52533000	-0.69021400
H	-4.35771700	0.90730300	0.26323900
H	-3.33355200	1.07085000	-1.18992200
N	-2.40438400	0.24584200	0.52207500
H	-2.24600000	0.88886300	1.28075700
N	2.16579600	0.00994600	-0.47372100

HF: -490.5056535

Sum of electronic and zero-point Energies: -490.344943  
 Sum of electronic and thermal Energies: -490.333468  
 Sum of electronic and thermal Enthalpies: -490.332524  
 Sum of electronic and thermal Free Energies: -490.383550  
 Frequencies: -489.1564

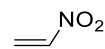


(+methyl azide, 4-m TS)

C	-0.15746800	-0.47534100	0.88646800
C	0.90887100	-1.26216300	0.50161300
H	1.63008800	-1.58566700	1.24626700
H	0.79686100	-1.88594700	-0.37843300
N	1.59068400	1.09884400	-0.22408800
N	0.60926800	1.54284500	0.17023500
C	-1.33226800	-0.39356600	0.00298000
O	-1.38268200	-0.80757500	-1.13073300
H	-0.26746900	-0.10173500	1.89555500
N	2.16576200	0.00195500	-0.45541000
C	3.58574100	-0.09527100	-0.12566800
H	3.78429200	0.16315600	0.92055800
H	3.86627700	-1.13383200	-0.30192500
H	4.18255600	0.54056500	-0.78313900
O	-2.36448300	0.22249700	0.60565400
C	-3.52546100	0.37832900	-0.20525000
H	-3.90210100	-0.59583100	-0.52412200
H	-4.25752200	0.88755800	0.41944700
H	-3.29215400	0.97492300	-1.08959800

HF: -510.3655206

Sum of electronic and zero-point Energies: -510.216467  
 Sum of electronic and thermal Energies: -510.205677  
 Sum of electronic and thermal Enthalpies: -510.204733  
 Sum of electronic and thermal Free Energies: -510.253537  
 Frequencies: -485.7886

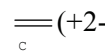


(+methyl azide, 4-n TS)

C	-0.71157900	-0.30613900	0.84468700
C	0.30289100	-1.18377200	0.54145600
H	0.93773600	-1.52064400	1.35474200
H	0.18029400	-1.84713500	-0.30577700
N	1.20799800	1.06027200	-0.22936700
N	0.26932300	1.61812100	0.11195200
O	-1.67225000	-0.58588500	-1.21604900
H	-0.93390000	0.10294100	1.81691300
C	3.07801900	-0.31618800	-0.02229600
H	3.26882600	-0.04439500	1.02155500
H	3.26292600	-1.38125500	-0.16190800
H	3.74804500	0.24097500	-0.67991900
H	1.68325300	-0.09371300	-0.40106600
N	-1.81431900	-0.16656300	-0.08078200
O	-2.81571300	0.38079700	0.33681800

HF: -487.0024494

Sum of electronic and zero-point Energies: -486.893829  
 Sum of electronic and thermal Energies: -486.884900  
 Sum of electronic and thermal Enthalpies: -486.883955  
 Sum of electronic and thermal Free Energies: -486.928573  
 Frequencies: -485.9644



(+2-diazo-N-methylacetamide, 5-a TS)

C	-2.48667300	0.98596500	-0.54129600
C	-1.35023600	1.51274000	0.03159600
H	-0.50105500	1.77306400	-0.59201700
H	-1.41364900	2.03806100	0.97944200
C	0.89502800	-0.34298900	0.01613900
N	-1.30338900	-1.10448900	0.50485900
N	-2.29830000	-1.14514400	-0.05906000
O	0.88172800	-0.82750900	-1.09854200
H	-2.51775700	0.76915000	-1.60271000

N	1.99044000	0.26528000	0.54221600
H	1.98277900	0.56142000	1.50368600
C	3.22211600	0.33302700	-0.21959500
H	3.01722100	0.73552600	-1.21354600
H	3.92174600	0.98949200	0.29822800
H	3.67138400	-0.65714400	-0.33843000
C	-0.32433600	-0.25753900	0.86833700
H	-0.22722600	-0.13625900	1.94300100
H	-3.44392100	1.05000800	-0.03651100

HF: -435.1756004

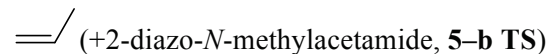
Sum of electronic and zero-point Energies: -435.031934

Sum of electronic and thermal Energies: -435.021908

Sum of electronic and thermal Enthalpies: -435.020964

Sum of electronic and thermal Free Energies: -435.067688

Frequencies: -523.2692



C	2.15945300	-0.61850700	-0.63053700
C	1.04051200	-1.26285500	-0.14562400
H	0.22739400	-1.51507900	-0.81861000
H	1.11751900	-1.87192200	0.75187500
C	-1.37474700	0.36298600	0.05828500
N	0.76577900	1.30234400	0.50961600
N	1.73198800	1.45099400	-0.08750200
O	-1.48226800	0.96182300	-0.99382500
H	2.17425200	-0.33722400	-1.67958000
N	-2.36597500	-0.41773200	0.56776200
C	-2.17600300	-0.98691100	1.37614200
H	-3.56009600	-0.67181600	-0.21493000
H	-3.33896100	-1.27588500	-1.10048700
H	-4.28694200	-1.19273300	0.40874100
C	-3.98442800	0.27704000	-0.54679100
H	-0.11741000	0.35018600	0.85517000
C	-0.15843200	0.15609900	1.92261600
C	3.49213100	-0.68760600	0.06872000
H	4.09138700	-1.52453000	-0.30676900
H	4.07314500	0.22732200	-0.07802000
H	3.35761200	-0.83433400	1.14585500

HF: -474.4739542

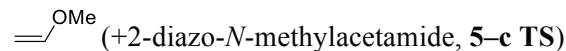
Sum of electronic and zero-point Energies: -474.302560

Sum of electronic and thermal Energies: -474.290849

Sum of electronic and thermal Enthalpies: -474.289905

Sum of electronic and thermal Free Energies: -474.341148

Frequencies: -528.5415



C	-2.42287600	0.46716000	0.47052500
C	-1.15681100	0.72019400	0.97783300
C	1.02717600	-0.76682200	-0.16297300
N	-1.18131800	-1.69457900	-0.24686300
N	-2.22070900	-1.35640900	-0.60285300
O	1.05335200	-0.57483000	-1.36387300
C	-2.80556000	0.99817000	-0.38972300
H	-0.18808400	-1.22726500	0.55485300
H	-0.06714100	-1.81484200	1.46180000
H	-3.16083400	0.05592700	1.14785100
O	-0.25847600	1.58999400	0.42419100
C	-0.54638800	2.05241800	-0.88351000
H	-1.41218100	2.72487700	-0.87239400
H	0.33700100	2.59995400	-1.21161800
H	-0.72106700	1.21273800	-1.56920900
N	-0.96053300	0.60757300	2.03803500
N	2.08413900	-0.49765200	0.65534600
C	1.89869600	-0.45290100	1.64546900
C	3.18096700	0.30230300	0.14342100
H	2.87201700	1.33822300	-0.03609800
H	4.00070200	0.28307700	0.86246100
H	3.52120300	-0.12605900	-0.79943100

HF: -549.6603137

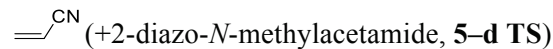
Sum of electronic and zero-point Energies: -549.482873

Sum of electronic and thermal Energies: -549.470792

Sum of electronic and thermal Enthalpies: -549.469848

Sum of electronic and thermal Free Energies: -549.521378

Frequencies: -560.1123



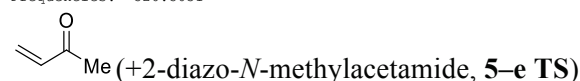
C	-1.94161200	-0.44995200	0.84303400
C	-0.82669100	-1.13427900	0.38207800
H	-0.02741400	-1.33752300	1.08744900
C	-0.95128700	-1.86297700	-0.41200800
H	1.60040800	0.28304700	-0.06652900
N	-0.50659400	1.28371600	-0.55157500
N	-1.43065100	1.65017300	-0.00489900
O	1.75609900	0.96406200	0.92614900
C	-3.17917700	-0.53584200	0.13382800
H	-1.97665500	-0.03581400	1.84151100
N	2.54129900	-0.56343600	-0.55222800
H	2.40122900	-0.99740000	-1.44985500
C	3.84166900	-0.65602200	0.08650300
H	3.70374500	-0.71065900	1.16712700
H	4.34366800	-1.55902100	-0.26101800
H	4.46095500	0.21706700	-0.13862600
C	0.28291600	0.21030100	-0.77660000
H	0.24971600	-0.12099100	-1.81110200
N	-4.16374300	-0.60026600	-0.46937800

HF: -527.4106274

Sum of electronic and zero-point Energies: -527.267575

Sum of electronic and thermal Energies: -527.255899

Sum of electronic and thermal Enthalpies: -527.254955  
 Sum of electronic and thermal Free Energies: -527.306871  
 Frequencies: -520.5031



C	-1.56270700	-0.29564200	0.94866800
C	-0.40189200	-1.00442700	0.68825800
H	0.37228900	-1.04942400	1.44859800
H	-0.48609500	-1.86601800	0.03177700
N	1.99322400	0.30871600	-0.10351700
C	-0.13282700	1.15343900	0.76742800
N	-1.06272600	1.65327200	-0.36033000
O	2.19335700	1.24704800	0.64128700
C	-2.70852400	-0.47089300	0.05049900
O	-2.59357800	-1.05136300	-1.01808700
N	-1.67791100	0.29527900	1.84973400
H	2.90912200	-0.66117700	-0.34573600
H	2.72039600	-1.36133200	-1.04383800
C	4.22100600	-0.59892100	0.27061200
H	4.10963700	-0.37701200	1.33319700
C	4.71322000	-1.56412600	0.15145300
H	4.83737400	0.18360800	-0.18145600
C	0.65991900	0.06135400	-0.73526500
H	0.58913900	-0.51874100	-1.65135900
C	-4.02499600	0.13460300	0.48071200
H	-4.35275900	-0.31478000	1.42329700
H	-3.89679200	1.20738100	0.65749200
H	-4.77789400	-0.02779100	-0.28985200

HF: -587.7908713

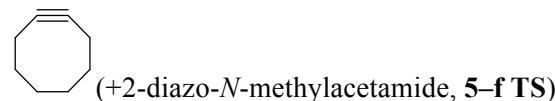
Sum of electronic and zero-point Energies: -587.609498

Sum of electronic and thermal Energies: -587.596813

Sum of electronic and thermal Enthalpies: -587.595868

Sum of electronic and thermal Free Energies: -587.649153

Frequencies: -503.8735



C	-1.05988500	1.01369600	-0.17732800
C	-0.37390700	0.04177800	-0.51042500
C	2.50939900	0.26172600	0.14583100
N	1.25886600	2.10759200	-0.68256900
N	0.36684100	2.73326800	-0.35283900
O	2.62642800	0.75187100	1.25115300
N	3.08679900	-0.92421000	-0.20337100
H	2.81190100	-1.35587500	-1.07109400
C	3.70916500	-1.74462800	0.81726100
H	2.97116700	-2.15355300	1.51606200
H	4.24695200	-2.56177300	0.33551100
H	4.41340200	-1.13546700	1.38553300
C	1.68384000	0.86822100	-0.93026300
H	1.89512600	0.66641600	-1.97515300
C	-0.24760400	-1.41312400	-0.72581700
H	0.34408800	-1.63596400	-1.62298000
H	0.29218100	-1.85751100	0.12201500
H	-2.29297800	1.66021200	0.29588400
H	-2.06132800	2.50149700	0.95699600
H	-2.82382400	2.08314200	-0.56688200
C	-1.62845800	-2.06895300	-0.85833900
H	-1.47269200	-3.14832200	-0.97017500
H	-2.09473700	-1.72184900	-1.78815000
C	-3.19945200	0.65525200	1.02072800
H	-2.72056700	0.36332400	1.96311100
H	-4.12482700	1.17758100	1.28941800
C	-2.58798300	-1.81711600	0.31912200
H	-3.20655000	-2.71467600	0.42102400
H	-2.00951900	-1.74806900	1.25002300
C	-3.55145700	-0.60803700	0.21748100
H	-4.53116000	-0.94602700	0.57023400
H	-3.69265500	-0.33855200	-0.83807700

HF: -668.5138707

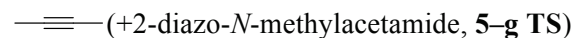
Sum of electronic and zero-point Energies: -668.242174

Sum of electronic and thermal Energies: -668.226322

Sum of electronic and thermal Enthalpies: -668.225378

Sum of electronic and thermal Free Energies: -668.286510

Frequencies: -464.2204



C	-2.16778700	0.49092500	-0.18757100
C	-1.12252200	1.05597800	0.15974200
N	-0.74148600	-1.50029200	0.69555100
N	-1.79289300	-1.62192000	0.26753700
C	0.19598100	-0.57363600	0.93128700
H	0.36063100	-0.37403700	1.98624700
C	-0.24728500	2.23795400	0.31121300
H	0.11390700	2.34553200	1.33950500
H	0.62723400	2.16239000	-0.34306400
C	-3.52573900	0.32342500	-0.73009000
H	-3.50926600	-0.33880100	-1.59998900
H	-4.18577100	-0.13445600	0.01175800
H	-3.95317600	1.28417900	-1.03126600
H	-0.78822700	3.15092000	0.04790700
C	1.34721200	-0.59731000	-0.01022700
N	2.41369700	0.14784600	0.39666500
C	2.33178300	0.70527800	1.23109300
C	3.50341200	0.40857400	-0.52303600
H	4.30810300	0.90996300	0.01503400

H	3.87310800	-0.53587700	-0.92510800
H	3.18100500	1.03292700	-1.36312700
O	1.32322700	-1.18286500	-1.07439600

HF: -512.5308233

Sum of electronic and zero-point Energies: -512.354593

Sum of electronic and thermal Energies: -512.341525

Sum of electronic and thermal Enthalpies: -512.340581

Sum of electronic and thermal Free Energies: -512.394550

Frequencies: -518.7177

(+2-diazo-*N*-methylacetamide, 5-h TS)

C	-2.42336400	2.34763700	0.31859200
C	-1.15136400	2.21596400	-0.52618200
C	-3.05847800	1.02673400	0.75816100
C	-0.85327400	-1.07797700	-0.22046200
C	-0.20854000	-0.05828000	0.06637200
C	-0.01539000	1.41149700	0.12673100
C	-2.01480100	-1.84896200	-0.71838200
C	-3.58177000	0.16266500	-0.40473800
H	0.92457000	1.66268400	-0.37872300
H	0.10629700	1.72765300	1.17395700
H	-1.90447300	-2.91092900	-0.48023200
H	-2.01302000	-1.77581500	-1.81377700
H	-4.64704400	0.37001200	-0.54996500
H	-3.09074900	0.45140500	-1.34259300
N	0.50595600	-2.71133200	0.33306000
N	1.35245200	-2.07055800	0.74880500
N	-2.32961400	0.45756000	1.34239800
H	-3.88698500	1.24629500	1.44152700
C	-3.37124700	-1.34227400	-0.19690300
H	-4.14942700	-1.91086300	-0.71716800
H	-3.46836100	-1.58240400	0.86897100
H	-1.37320400	1.76458300	-1.49882400
H	-0.77716700	3.22536900	-0.73360900
H	-2.18544200	2.93925600	1.21217500
H	-3.15750200	2.93317100	-0.25038300
C	1.71824900	-0.79627200	0.93986300
H	1.71587600	-0.49551400	1.98373900
C	2.78793200	-0.30954900	0.02901300
N	3.36511700	0.86048000	0.42231100
C	3.00934600	1.33613300	1.23505100
C	4.25546200	1.56359600	-0.48024000
H	3.73094700	1.88752400	-1.38513000
H	4.66512300	2.43317800	0.03411600
H	5.07251900	0.90461700	-0.77952100
O	3.08664500	-0.87283900	-1.00526700

HF: -707.8118115

Sum of electronic and zero-point Energies: -707.511254

Sum of electronic and thermal Energies: -707.495160

Sum of electronic and thermal Enthalpies: -707.494216

Sum of electronic and thermal Free Energies: -707.555312

Frequencies: -490.3344

(+2-diazo-*N*-methylacetamide, 5-i TS)

C	-1.32180900	1.04256400	-0.16715000
C	-0.60692700	0.11329200	-0.54327400
N	1.10628100	2.13519200	-0.52873200
N	0.32837700	2.86203500	-0.15430800
C	-0.67883700	-1.34753800	-0.76181700
H	-0.14664400	-1.67860100	-1.66241600
H	-0.23640100	-1.88427400	0.08830400
H	-2.66370200	1.23473100	0.42432300
H	-2.70908500	2.07826800	1.11957200
H	-3.39943900	1.43086200	-0.36528400
C	-2.18358900	-1.65501100	-0.90525100
H	-2.31989600	-2.71067700	-1.17042700
C	-2.53689100	-1.07033600	-1.76159000
C	-2.97021300	-0.08426200	1.16377200
H	-2.17097400	-0.21754300	1.90035000
H	-3.90260500	0.01886000	1.73234400
C	-3.09696400	-1.37224600	0.31221400
C	-3.00183800	-2.21088200	1.01299700
H	-4.12321100	-1.42907400	-0.07115000
C	1.52502200	0.93539700	-0.89717400
C	1.70432800	0.81794900	-1.95829700
C	2.27242800	0.17693000	0.13304500
N	2.75599500	-1.02004600	-0.31030900
O	2.41321600	0.56765400	1.27434300
C	2.42215700	-1.36817400	-1.19516400
C	3.29799200	-1.96736600	0.64457600
H	3.78968500	-2.77586900	0.10252500
H	4.03035400	-1.45895600	1.27272700
H	2.51974900	-2.38218100	1.29463200

HF: -629.2015034

Sum of electronic and zero-point Energies: -628.959367

Sum of electronic and thermal Energies: -628.945287

Sum of electronic and thermal Enthalpies: -628.944343

Sum of electronic and thermal Free Energies: -629.000849

Frequencies: -260.2937

(+2-diazo-*N*-methylacetamide, 5-j TS)

C	-1.69542700	0.92581300	-0.00915500
C	-0.89441000	0.09502200	-0.44837800
N	0.77232300	2.16718700	-0.39072300
N	0.11157900	2.95887100	0.04761800
C	-0.91247900	-1.37422000	-0.59844500
H	-0.56356500	-1.73738500	-1.57190800
H	-0.29647500	-1.85336600	0.17304300
C	-3.07721300	0.61990000	0.46683600
H	-3.35292400	1.15625100	1.37880400
H	-3.80315000	0.90765800	-0.30208200
C	-2.42128700	-1.72326700	-0.40783600
H	-2.51761700	-2.79428500	-0.20004100
H	-2.93686200	-1.52799100	-1.35590700
C	-3.10380200	-0.91496800	0.70792700
C	-2.59670400	-1.12261600	1.65814800
H	-4.14077000	-1.25337500	0.81551200
C	1.19167700	1.00003300	-0.84711000
C	1.27984200	0.93679200	-1.92316600
C	2.01487700	0.20737400	0.09225100
N	2.50056900	-0.94944800	-0.44316200
H	2.12436200	-1.26263100	-1.32396100
C	3.13888900	-1.92166600	0.42358600
C	3.57827200	-2.70757400	-0.19137600
H	3.92725200	-1.42978600	0.99462100
H	2.42891600	-2.36288900	1.13133400
O	2.21664700	0.54136500	1.24285000

HF: -589.8983058

Sum of electronic and zero-point Energies: -589.685386

Sum of electronic and thermal Energies: -589.671561

Sum of electronic and thermal Enthalpies: -589.670616

Sum of electronic and thermal Free Energies: -589.728447

Frequencies: -235.4844

(+2-diazo-*N*-methylacetamide, 5-k TS)

C	1.24033700	-0.27647000	-0.81234900
C	0.20340400	-1.04758800	-0.33689100
H	-0.58466500	-1.34716000	-1.01882100
H	0.37840200	-1.70878700	0.50630900
N	-0.27485800	1.37971800	0.54912700
N	0.64857100	1.74855000	-0.00418100
H	1.27276400	0.08799400	-1.83047000
C	-1.03527100	0.29674700	0.79194000
C	-1.01524700	-0.01450900	1.83245500
H	2.54171500	-0.28030300	-0.09258600
F	2.36694000	-0.25574200	1.24816900
F	3.31113200	0.76782100	-0.41293000
C	3.28116500	-1.38089200	-0.34457000
F	-2.32134700	0.28192800	0.02964500
N	-3.23604500	-0.60406400	0.49844300
H	-3.10502000	-1.01787100	1.40664500
O	-2.47873700	0.93267200	-0.98341400
C	-4.50299300	-0.77875900	-0.18702500
H	-4.97357000	-1.69624700	0.16681600
H	-5.17399800	0.06744700	-0.01193600
H	-4.32065100	-0.85569600	-1.25982200

HF: -772.151062

Sum of electronic and zero-point Energies: -772.002186

Sum of electronic and thermal Energies: -771.989713

Sum of electronic and thermal Enthalpies: -771.988769

Sum of electronic and thermal Free Energies: -772.042090

Frequencies: -501.0964

(+2-diazo-*N*-methylacetamide, 5-l TS)

C	-1.12405200	-0.20521300	1.01318000
H	0.01058700	-0.95222800	0.76596600
C	0.80397300	-0.97042700	1.50670800
H	-0.09891700	-1.83449500	0.14278000
C	2.42302900	0.30302100	-0.14208500
N	0.28654400	1.15720700	-0.76547800
N	-0.63646300	1.64407200	-0.31806300
O	2.66064500	1.25624300	0.57352300
C	-2.31182900	-0.45157800	0.17176500
O	-2.25002300	-1.08961400	-0.87395700
C	-4.67334800	0.01134300	-0.21979900
H	-4.90647200	-1.03200700	-0.44280800
H	-5.50795600	0.45659200	0.32288900
H	-4.53627300	0.53797600	-1.16956900
H	-1.20879400	0.41744900	1.89639000
N	3.31770200	-0.68893300	-0.37944300
C	3.09811400	-1.40826300	-1.04813700
H	4.64318100	-0.63355200	0.20645300
H	4.56037100	-0.40607000	1.27063400
H	5.12605300	-1.60252500	0.07974800
C	5.25417500	0.14259600	-0.26358100
H	1.07378100	0.06304400	-0.73508700
H	0.96869700	-0.54503500	-1.62937300
N	-3.48387000	0.08889600	0.60156300
H	-3.47344200	0.69346500	1.40538100

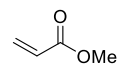
HF: -643.14415

Sum of electronic and zero-point Energies: -642.944730

Sum of electronic and thermal Energies: -642.930692

Sum of electronic and thermal Enthalpies: -642.929748

Sum of electronic and thermal Free Energies: -642.986586  
Frequencies: -523.2053

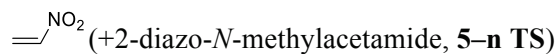


**(+2-diazo-*N*-methylacetamide, 5-m TS)**

C	-1.11363000	-0.29192500	0.94871500
C	0.00811400	-1.02448700	0.60594500
H	0.80472000	-1.13049600	1.33572500
H	-0.12466300	-1.84654300	-0.09119500
C	2.41406300	0.32184000	-0.12295500
N	0.28593100	1.19921400	-0.74069500
N	-0.64180300	1.65735400	-0.27764800
O	2.61332000	1.22005900	0.66961600
C	-2.31689100	-0.44910600	0.13202500
O	-2.35069200	-0.99585400	-0.95064800
O	-3.40027700	0.11283600	0.69726800
C	-4.59467600	0.02812400	-0.07387700
H	-4.86394800	-1.01605000	-0.24740200
H	-5.36285700	0.52993600	0.51230100
H	-4.46187800	0.52385300	-1.03803500
H	-1.18878900	0.26022000	1.87552800
N	3.33552500	-0.62536900	-0.42952400
H	3.08120400	-1.38412800	-1.04045700
C	4.60668800	-0.66716100	0.26856400
H	4.49388900	-1.05432500	1.28577700
H	5.29496600	-1.30375100	-0.28762000
H	5.01501100	0.34250200	0.32766000
H	1.08466800	0.11210400	-0.77540200
C	1.02595400	-0.41227100	-1.72518200

HF: -663.0040822

Sum of electronic and zero-point Energies: -662.816847  
Sum of electronic and thermal Energies: -662.803260  
Sum of electronic and thermal Enthalpies: -662.802316  
Sum of electronic and thermal Free Energies: -662.858483  
Frequencies: -511.6685

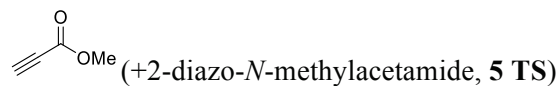


**(+2-diazo-*N*-methylacetamide, 5-n TS)**

C	1.62416900	-0.24706100	-0.95256500
C	0.48421600	-0.96752500	-0.66538800
H	-0.26876800	-1.02798900	-1.44464100
H	0.58238400	-1.82579000	-0.01009100
N	0.16790000	1.19211900	0.73110100
N	1.06928500	1.72009400	0.30565100
O	2.57158800	-0.91593700	1.00881700
H	1.83653500	0.30070900	-1.85571400
N	2.75625700	-0.40392900	-0.09221300
O	3.83301700	0.00734000	-0.48243100
C	-0.60130100	0.08102000	0.72903000
H	-0.52058800	-0.47013900	1.66201500
C	-1.93919000	0.28873700	0.08422500
C	-2.85469500	-0.66128200	0.39032400
H	-2.67934300	-1.28837400	1.15873800
C	-4.17271300	-0.63271200	-0.21795900
H	-4.63947100	-1.61052400	-0.09952300
H	-4.80706200	0.13352900	0.23708600
H	-4.06673500	-0.40639300	-1.27959100
O	-2.12701400	1.17499800	-0.72343400

HF: -639.6434214

Sum of electronic and zero-point Energies: -639.496145  
Sum of electronic and thermal Energies: -639.483741  
Sum of electronic and thermal Enthalpies: -639.482796  
Sum of electronic and thermal Free Energies: -639.536970  
Frequencies: -496.3669



**(+2-diazo-*N*-methylacetamide, 5 TS)**

C	1.11022500	-0.22204800	-0.78768600
C	-0.01308300	-0.27621400	-1.29674100
H	-0.68384100	-0.09103700	-2.11269600
C	-2.36657800	-0.00863100	0.32253300
N	-0.46821200	-1.26285800	1.03383500
N	0.61086900	-1.11233700	1.33952300
O	-2.20559100	0.82250900	1.19028100
C	2.51978200	-0.09061800	-0.50914100
O	3.34713100	-0.93236800	-0.75242300
O	2.79550700	1.08262900	0.07949900
H	4.16794500	1.26430800	0.42671200
C	4.79425500	1.23327000	-0.46710600
H	4.22215200	2.24271300	0.90067800
H	4.49086800	0.48236400	1.11706100
N	-3.39403500	0.02450600	-0.56763600
H	-3.56999000	-0.77974900	-1.14741000
C	-4.41596000	1.04887300	-0.45268300
H	-3.93509900	2.02148800	-0.34078800
H	-5.02187100	1.04731600	-1.35876000
H	-5.05745600	0.88012300	0.41763600
C	-1.38076700	-1.10281100	0.06221400
H	-1.70512200	-2.04097600	-0.37877500

HF: -661.7459307

Sum of electronic and zero-point Energies: -661.582624  
Sum of electronic and thermal Energies: -661.568356  
Sum of electronic and thermal Enthalpies: -661.567411  
Sum of electronic and thermal Free Energies: -661.625735  
Frequencies: -499.7057

**(+methyl carbamoyl azide, 6-a TS)**

C	2.69710700	0.88585900	0.36359500
C	1.47529000	1.48946300	0.15111900
H	0.81256700	1.70315600	0.98346800
H	1.29245800	2.04874500	-0.75874900
C	-0.98610900	-0.42741900	-0.03729900
N	1.18810700	-1.07104900	-0.34863500
N	2.30724900	-1.12691600	-0.08322700
O	-1.32110100	-1.43588200	0.53774900
H	3.01486900	0.63652500	1.36864100
N	-1.79105600	0.64520800	-0.25585400
H	-1.48034900	1.32610900	-0.93043400
C	-3.19526700	0.57501200	0.09509500
H	-3.28875900	0.12336000	1.08313800
H	-3.60573500	1.58494200	0.12280900
H	-3.76597200	-0.03151800	-0.61579300
N	0.31898100	-0.16317400	-0.54219200
H	3.48063900	0.96977100	-0.38079900

HF: -451.209474

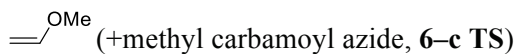
Sum of electronic and zero-point Energies: -451.077157  
Sum of electronic and thermal Energies: -451.068264  
Sum of electronic and thermal Enthalpies: -451.067320  
Sum of electronic and thermal Free Energies: -451.111446  
Frequencies: -489.1682

**(+methyl carbamoyl azide, 6-b TS)**

C	1.52095900	1.16138600	-0.36237100
C	2.70990300	0.46790100	-0.23524100
H	3.30770900	0.24796500	-1.11277400
H	3.23519500	0.47981600	0.71372700
N	0.98978200	-1.43065400	-0.12523900
N	0.17828500	-0.55236700	-0.56770900
H	1.21124700	1.48728600	-1.35005300
N	2.12420400	-1.48884600	0.07795600
C	0.89058700	1.85459100	0.81402600
H	1.31162600	2.86026900	0.92260800
H	-0.19079600	1.95915000	0.69723000
H	1.08906100	1.30439300	1.73837200
C	-1.10640900	-0.54174300	0.03835800
O	-1.42848200	-1.18031600	1.01383300
N	-1.91061000	0.35303400	-0.59678400
H	-1.63980600	0.63230700	-1.52626500
C	-3.28928700	0.50171000	-0.17678700
H	-3.69893900	1.41197900	-0.61606900
H	-3.90285900	-0.35519300	-0.47344200
H	-3.32072500	0.58331600	0.91053700

HF: -490.5101253

Sum of electronic and zero-point Energies: -490.349586  
Sum of electronic and thermal Energies: -490.338368  
Sum of electronic and thermal Enthalpies: -490.337424  
Sum of electronic and thermal Free Energies: -490.388747  
Frequencies: -486.1959

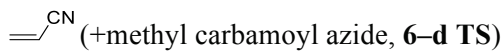


**(+methyl carbamoyl azide, 6-c TS)**

C	-2.56849300	0.26668300	-0.59563800
C	-1.54790600	-0.61789400	-0.89511500
H	-1.13961200	-0.68324100	-1.89601500
C	1.46783800	0.60932700	-0.00551300
N	-0.57562600	1.66831600	0.23166800
N	-1.71041600	1.88912600	0.33698800
O	2.15730400	1.45106000	0.52180500
H	-3.23781300	0.08075600	0.23310200
N	1.91290700	-0.60806500	-0.42379000
H	1.21222000	-1.31459100	-0.59692700
C	3.27319600	-1.00768100	-0.12694800
H	3.41572300	-1.23362600	0.93537800
H	3.52201200	-1.88769400	-0.72103700
H	3.94794900	-0.19375200	-0.39483400
N	0.09417700	0.74046700	-0.31551000
H	-2.95808400	0.85755400	-1.41382800
O	-1.19159200	-1.69165000	-0.16204200
C	-1.55951200	-1.66815100	1.20665000
H	-1.06356300	-2.51866400	1.67222600
H	-1.21971200	-0.73527100	1.67246200
H	-2.64284500	-1.76935900	1.32526000

HF: -565.7037892

Sum of electronic and zero-point Energies: -565.538031  
Sum of electronic and thermal Energies: -565.526714  
Sum of electronic and thermal Enthalpies: -565.525770  
Sum of electronic and thermal Free Energies: -565.575963  
Frequencies: -451.4284

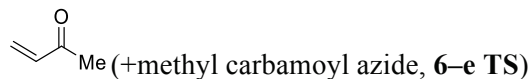


**(+methyl carbamoyl azide, 6-d TS)**

C	-2.03048700	-0.31667200	0.83313500
C	-0.85501500	-1.02421400	0.60757700
H	-0.84410200	-1.80181200	-0.14675000
C	1.65281400	0.35357200	-0.11075900
N	-0.41627800	1.31188200	-0.35424000
N	-1.45592600	1.62830000	0.00677300
O	2.16123000	1.34748500	0.34391900
H	-2.22644800	0.14000700	1.79408900
N	2.27562900	-0.83334300	-0.30297100
H	1.82907700	-1.49988200	-0.91320000
C	3.70013800	-0.94354100	-0.04605400
H	3.92098200	-0.48648000	0.91904000
H	3.97230000	-1.99850300	-0.01442600
H	4.29078600	-0.43474900	-0.81378800

N	0.26676200	0.24132200	-0.46705700
C	-3.17026500	-0.54633400	-0.00607500
N	-4.08017700	-0.73389100	-0.69164900
H	-0.14562400	-1.13522000	1.42075100

HF: -543.4368959  
Sum of electronic and zero-point Energies: -543.305051  
Sum of electronic and thermal Energies: -543.293745  
Sum of electronic and thermal Enthalpies: -543.292800  
Sum of electronic and thermal Free Energies: -543.344246  
Frequencies: -512.5936



C	-1.64536900	-0.27662700	0.87276200
C	-0.48127700	-1.00785000	0.70947000
H	0.21823200	-1.11533000	1.53180200
H	-0.48358700	-1.78399900	-0.04939300
C	2.08366900	0.38776100	-0.11367100
N	-0.01218400	1.28574200	-0.39454800
N	-1.06698100	1.62321600	-0.10363400
O	2.62302100	1.44260100	0.11506800
C	-2.76539300	-0.48579100	-0.08052300
O	-2.61740300	-1.12667600	-1.09921500
H	-1.85014100	0.24317200	1.80189200
N	2.69184100	-0.82347200	-0.10097100
H	2.20513500	-1.59305200	-0.53360400
C	4.12821500	-0.90131100	0.08609200
H	4.41098600	-0.25833900	0.92011500
H	4.39821300	-1.93131500	0.31997600
H	4.67317500	-0.57291100	-0.80439600
C	-4.07931200	0.16509900	0.27625300
H	-4.44303100	-0.23111500	1.22971600
H	-3.93103600	1.24214100	0.40520000
H	-4.81203200	-0.02117100	-0.50784300
N	0.69103000	0.22977500	-0.39264500

HF: -603.8183969  
Sum of electronic and zero-point Energies: -603.648261  
Sum of electronic and thermal Energies: -603.635887  
Sum of electronic and thermal Enthalpies: -603.634942  
Sum of electronic and thermal Free Energies: -603.688142  
Frequencies: -478.7419



C	1.18350800	-0.98260200	-0.23966700
C	0.53764400	0.06369500	-0.34665300
C	-2.73995500	-0.32466700	0.11190400
N	-1.19458900	-1.92255900	-0.38752800
O	-0.22828700	-2.53453100	-0.31419200
O	-3.38467000	-1.01624500	0.86551500
N	-3.02565400	0.97247700	-0.17683800
H	-2.57704500	1.37392300	-0.98424100
C	-4.23954000	1.57083300	0.33977200
H	-4.32215700	1.34336000	1.40323000
H	-4.18531900	2.65208300	0.20856500
C	-5.13292200	1.18661200	-0.16353600
H	0.35599800	1.51946900	-0.39202700
H	-0.26313200	1.80731800	-1.24817700
H	-0.17428900	1.84689500	0.51064100
C	2.45956600	-1.69357500	-0.03436500
H	2.29500500	-2.62861500	0.50914400
H	2.86706500	-1.96958500	-1.01488900
C	1.72441000	2.21658200	-0.48886900
H	1.55536900	3.29139400	-0.36170300
H	2.12044400	2.07923800	-1.50167300
C	3.46356000	-0.80677800	0.71511600
C	3.12533300	-0.68277000	1.75078100
H	4.41356000	-1.35074300	0.76047900
C	2.76932000	1.73350600	0.53357200
H	3.40103900	2.59172500	0.78133700
H	2.26032800	1.45760000	1.46611800
C	3.70262100	0.57741100	0.08757800
H	4.72834300	0.86907300	0.33342700
H	3.67426400	0.48393600	-1.00622900
N	-1.55308800	-0.72463300	-0.56223700

HF: -668.5138707  
Sum of electronic and zero-point Energies: -668.242174  
Sum of electronic and thermal Energies: -668.226322  
Sum of electronic and thermal Enthalpies: -668.225378  
Sum of electronic and thermal Free Energies: -668.286510  
Frequencies: -434.2154



C	2.12070200	0.85035200	0.49915800
C	0.96825200	1.47736200	0.07157400
H	0.19987300	1.73260700	0.79475200
H	0.97601000	2.07734200	-0.83259700
C	-1.33015500	-0.24451000	0.10892900
N	0.78470800	-1.09293400	-0.61122600
N	1.80747300	-1.19354300	-0.10482700
O	-1.30566200	-0.91542000	1.11390400
C	2.23728100	0.56726000	1.53876300
C	-0.18569400	-0.18420600	-0.83159700
C	-0.36040600	0.04575500	-1.87713300
C	-2.48519600	0.66167900	-0.24816500
H	-2.12613200	1.63734800	-0.58899200

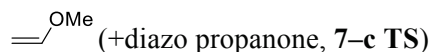
H	-3.05193700	0.21025700	-1.06919200
H	-3.13548600	0.77690700	0.61812200
H	3.03337300	0.91715700	-0.08198100

HF: -379.8220215  
Sum of electronic and zero-point Energies: -379.696547  
Sum of electronic and thermal Energies: -379.687827  
Sum of electronic and thermal Enthalpies: -379.686882  
Sum of electronic and thermal Free Energies: -379.730335  
Frequencies: -526.9691



C	-1.79623600	-0.45286700	0.63346500
C	-0.72181400	-1.24199400	0.26993400
H	0.02198200	-1.51137100	1.01305700
H	-0.81092500	-1.92020000	-0.57494300
C	1.79994600	0.12378500	0.05946900
N	-0.21380200	1.22733200	-0.60612400
N	-1.18102100	1.48748500	-0.04771700
O	1.93528100	0.85239800	1.01429600
H	-1.84043800	-0.09164500	1.65689400
C	0.60733900	0.18038800	-0.81729200
H	0.68207500	-0.13563500	-1.85221300
C	2.78170900	-0.97129000	-0.28714100
H	2.25787300	-1.90464600	-0.51450800
H	3.34548900	-0.68007300	-1.17934700
H	3.47048400	-1.11601500	0.54427900
C	-3.09482700	-0.47343100	-0.13086300
H	-3.77363700	-1.23472300	0.26817700
H	-3.60928500	0.49017300	-0.07778000
H	-2.91881600	-0.70631600	-1.18652000

HF: -419.120636  
Sum of electronic and zero-point Energies: -418.967219  
Sum of electronic and thermal Energies: -418.956965  
Sum of electronic and thermal Enthalpies: -418.956020  
Sum of electronic and thermal Free Energies: -419.003365  
Frequencies: -530.6380



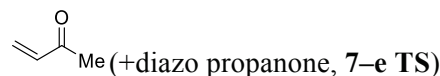
C	2.12306100	-0.03627700	-0.50815800
C	0.94883900	0.52428100	-0.99429200
C	-1.49542600	-0.37062700	0.18013100
N	0.43008200	-1.81389900	0.28697000
N	1.52732900	-1.69137000	0.61290800
O	-1.45928200	-0.15654800	1.37136600
H	2.66126200	0.41338500	0.31482000
C	-0.44964000	-1.14794900	-0.51445000
H	-0.71648700	-1.69989700	-1.41124600
C	-2.54182400	0.22931300	-0.72676400
H	-2.06229500	0.73655200	-1.56911200
H	-3.18569200	-0.56151500	-1.12488500
H	-3.14061200	0.94065500	-0.15919600
H	2.71336300	-0.62919500	-1.19591600
O	0.31650700	1.59488700	-0.43182900
C	0.74379200	1.98331100	0.86264200
H	1.73936600	2.43972700	0.81730300
H	0.01914700	2.71804500	1.21170700
H	0.74882500	1.13241600	1.55132100
H	0.69339600	0.44768200	-2.04490000

HF: -494.3075685  
Sum of electronic and zero-point Energies: -494.148136  
Sum of electronic and thermal Energies: -494.137352  
Sum of electronic and thermal Enthalpies: -494.136408  
Sum of electronic and thermal Free Energies: -494.184567  
Frequencies: -552.5338



C	-1.53665600	-0.35741900	0.84917100
C	-0.46881800	-1.14385500	0.43342000
H	0.28738500	-1.39375500	1.17115800
H	-0.63472600	-1.88869200	-0.33783900
C	2.03872600	0.07581900	-0.01191700
N	0.01231300	1.21478300	-0.58923200
N	-0.88995300	1.64086100	-0.04685300
O	2.28084200	0.86862900	0.84663000
C	-2.76659900	-0.38190300	0.12113200
H	-1.56438300	0.07446100	1.84048400
C	0.74077200	0.08486800	-0.75263100
H	0.71267400	-0.30124000	-1.76731300
C	2.95298600	-1.07022200	-0.36370800
H	2.39155300	-2.00736000	-0.43233400
H	3.40177600	-0.88287200	-1.34466200
H	3.73831900	-1.15292100	0.38632800
N	-3.74261700	-0.39649900	-0.49837000

HF: -472.0554712  
Sum of electronic and zero-point Energies: -471.930648  
Sum of electronic and thermal Energies: -471.920255  
Sum of electronic and thermal Enthalpies: -471.919311  
Sum of electronic and thermal Free Energies: -471.967629  
Frequencies: -524.3700



C	-1.16353400	-0.23912500	0.92999700
C	-0.04515200	-1.03091400	0.71671100
H	0.69277000	-1.11704000	1.50923100

H	-0.16992000	-1.89989100	0.07649100
C	2.41400500	0.13944200	0.01287600
N	0.36156100	1.07390400	-0.79017600
N	-0.55578600	1.60641000	-0.39161000
O	2.66057600	1.14107900	0.63860200
C	-2.31166300	-0.38806900	0.02525000
H	-2.21820000	-1.01649400	-1.01614100
O	-1.26487400	0.37078100	1.82017800
C	1.11374500	-0.04752100	-0.69338500
H	1.07222700	-0.66145400	-1.58793200
C	-3.59513100	0.30514000	0.41859100
H	-3.95666700	-0.09199800	1.37217300
H	-3.40835000	1.37452600	0.56005900
H	-4.34839500	0.15752400	-0.35445800
C	3.33858000	-1.05055000	-0.05246100
H	2.78675200	-1.98235600	0.10440400
C	3.78984600	-1.09824300	-1.04896400
H	4.12207600	-0.94114600	0.69616100

HF: -532.4361266  
Sum of electronic and zero-point Energies: -532.272904  
Sum of electronic and thermal Energies: -532.260622  
Sum of electronic and thermal Enthalpies: -532.259677  
Sum of electronic and thermal Free Energies: -532.312802  
Frequencies: -514.9140



(+diazopropane, 7-f TS)

C	-0.56105200	0.96781400	-0.28434100
C	-0.06211200	-0.14865700	-0.47035500
C	2.69991300	-0.30779500	0.46124200
N	1.92028300	1.58688600	-0.74705600
N	1.10730700	2.35722300	-0.53668500
O	2.75541500	0.31742600	1.49460700
C	2.15282800	0.26893300	-0.78634800
H	2.43543900	-0.12409400	-1.75610700
C	-0.21713800	-1.61449500	-0.54643700
H	0.34781600	-2.03106100	-1.38877200
C	0.19747700	-2.06879800	0.36404000
H	-1.67724500	1.87171400	0.03739700
H	-1.32100500	2.73960600	0.60158700
H	-2.09594000	2.26288600	-0.89878100
H	-1.69598100	-2.00028100	-0.68365400
H	-1.75049300	-3.09489600	-0.69550400
C	-2.06014700	-1.65819800	-1.65969300
H	-2.77081200	1.14537500	0.83156700
H	-2.37570400	0.88488800	1.82090300
H	-3.58471900	1.86016100	0.99870600
C	-2.61752000	-1.45973200	0.42508800
H	-3.39048200	-2.21608400	0.59329200
C	-2.05400600	-1.39535100	1.36542100
H	-3.34306500	-0.11624000	0.16511100
H	-4.36960100	-0.22816100	0.52882100
C	-3.42802400	0.05181400	-0.91721000
C	3.15150900	-1.74806000	0.35994300
H	2.62182800	-2.29487100	-0.42320100
H	4.21896100	-1.75175900	0.11491500
H	3.01616300	-2.23571600	1.32564300

HF: -613.1605228  
Sum of electronic and zero-point Energies: -612.906812  
Sum of electronic and thermal Energies: -612.892355  
Sum of electronic and thermal Enthalpies: -612.891411  
Sum of electronic and thermal Free Energies: -612.948573  
Frequencies: -468.0343

= (+azido propanone, 8-a TS)

C	1.39886900	1.37506000	0.03619400
C	2.49575900	0.55119600	0.15322100
H	3.15080600	0.39352700	-0.69569400
H	2.91035600	0.33071900	1.12959300
N	0.55270400	-1.13811700	-0.14616700
N	-0.15210300	-0.08550500	-0.27101600
H	1.17109700	1.86400200	-0.90339300
N	1.66944700	-1.38293800	-0.01208400
O	-1.53206000	-0.13252700	-0.00615800
C	-2.14683100	-1.14320200	0.21481300
H	0.93047600	1.79583300	0.91934000
C	-2.13634100	1.24774100	-0.03059500
H	-1.80897500	1.79710800	-0.91611600
H	-3.22094200	1.15729100	-0.01500100
H	-1.80587200	1.80423000	0.85166100

HF: -395.8601176  
Sum of electronic and zero-point Energies: -395.746086  
Sum of electronic and thermal Energies: -395.737421  
Sum of electronic and thermal Enthalpies: -395.736477  
Sum of electronic and thermal Free Energies: -395.782015  
Frequencies: -443.0213

= (+azido propanone, 8-b TS)

C	-1.51849600	0.75611600	0.47538000
C	-2.33986500	-0.35241100	0.48104500
H	-2.56259400	-0.86054400	1.41164600
H	-3.04531800	-0.49836000	-0.33071900
N	-0.09849700	-1.41820700	-0.24545100
N	0.35922400	-0.24424500	-0.04602800
H	-1.09064500	1.08650200	1.41768900
H	-1.14178500	-1.90834800	-0.19823700
C	-1.54443300	1.75843300	-0.64439100
H	-2.31769600	2.50991600	-0.45033700

H	-0.59065500	2.27936200	-0.74870300
H	-1.77724500	1.27028300	-1.59445000
C	1.74469900	-0.04167100	0.02391800
C	2.07532300	1.40645900	0.28651800
H	1.37391900	1.85344200	0.99462400
H	3.09448400	1.47194200	0.66408600
H	2.00893200	1.95967600	-0.65520500
O	2.57135700	-0.90477200	-0.12693100

HF: -435.1609381  
Sum of electronic and zero-point Energies: -435.018635  
Sum of electronic and thermal Energies: -435.009569  
Sum of electronic and thermal Enthalpies: -435.008625  
Sum of electronic and thermal Free Energies: -435.052780  
Frequencies: -431.5090

= OMe (+azido propanone, 8-c TS)

C	-1.99400400	0.80730400	-0.75719300
C	-1.34779000	-0.41009400	-0.89180100
H	-0.89868500	-0.71305900	-1.82915100
C	1.94634000	-0.07379200	0.04667500
N	0.28247800	1.52272100	0.21048500
N	-0.74203300	2.06616000	0.23343800
O	2.74014200	0.49774000	0.75152200
H	-2.77585000	0.93789700	-0.02152100
N	0.67388300	0.40802500	-0.28724700
H	-2.05485100	1.42370300	-1.64474200
O	-1.44546000	-1.44226800	-0.04876400
C	-1.92619900	-1.16583200	1.25628500
H	-1.79101700	-2.08185400	1.82920900
H	-1.34761600	-0.35261000	1.70902700
H	-2.98810800	-0.90136200	1.23650800
C	2.19489800	-1.41298400	-0.60201600
H	1.34567100	-2.08073800	-0.43324000
H	2.30484400	-1.27581800	-1.68182800
H	3.10839300	-1.84256400	-0.19467300

HF: -510.3550945  
Sum of electronic and zero-point Energies: -510.207349  
Sum of electronic and thermal Energies: -510.197242  
Sum of electronic and thermal Enthalpies: -510.196298  
Sum of electronic and thermal Free Energies: -510.243674  
Frequencies: -427.0488

= CN (+azido propanone, 8-d TS)

C	-1.75822700	-0.35033200	0.79086500
C	-0.65544200	-1.16390800	0.57656000
H	-0.62640400	-1.80802800	-0.29384900
C	2.13643900	0.03995700	-0.17907000
N	0.15077800	1.24382400	0.01288800
O	-0.87471800	1.63098300	0.34201300
N	2.85180300	1.00300700	-0.17221800
H	-2.01383300	-0.01352400	1.78670800
O	0.72412500	0.12023800	-0.15742000
C	-2.79961000	-0.28298900	-0.19220100
N	-3.63144200	-0.22702200	-0.99084500
H	-0.06835100	-1.47874200	1.43186600
C	2.60387800	-1.38975400	-0.21844000
H	2.39780200	-1.87250900	0.74160200
H	2.07675100	-1.94499600	-0.99757300
H	3.67619100	-1.40025600	-0.40373500

HF: -488.0871666  
Sum of electronic and zero-point Energies: -487.973614  
Sum of electronic and thermal Energies: -487.963359  
Sum of electronic and thermal Enthalpies: -487.962414  
Sum of electronic and thermal Free Energies: -488.011141  
Frequencies: -459.7028

= Me (+azido propanone, 8-e TS)

C	1.41330800	-0.36312700	-0.92832000
C	0.24285000	-1.09278000	-1.01027300
H	-0.19061700	-1.32844400	-1.97474100
H	0.00317400	-1.74914400	-0.17902700
C	-2.38582700	0.11008600	0.20772600
N	-0.47785600	1.31999700	-0.30172700
N	0.61313100	1.65176400	-0.38824100
O	-2.89279400	0.97547000	0.86637100
C	2.18497000	-0.39497300	0.34011700
O	1.71115900	-0.86864100	1.35122400
H	1.89070400	0.02774000	-1.82018900
C	3.56330400	0.21673000	0.30741600
H	4.17899200	-0.29026400	-0.44221700
H	3.48720800	1.26822200	0.01165300
H	4.02799700	0.13748300	1.28939300
N	-1.18651000	0.28852000	-0.52496800
C	-2.92504200	-1.28523100	0.05013700
H	-2.81594100	-1.63751900	-0.97744800
H	-2.36014300	-1.95681900	0.70405600
H	-3.97102200	-1.29208400	0.35149300

HF: -548.4687555  
Sum of electronic and zero-point Energies: -548.316622  
Sum of electronic and thermal Energies: -548.304645  
Sum of electronic and thermal Enthalpies: -548.303701  
Sum of electronic and thermal Free Energies: -548.356697  
Frequencies: -441.9892





(+azido propanone, 8-f TS)

C	0.74077100	-0.96231600	-0.12182500
C	0.28743200	0.18357300	-0.09934600
C	-3.26333000	0.22964300	0.07835900
N	-1.77718800	-1.52152000	-0.09271000
N	-0.89496600	-2.25260800	-0.14502100
O	-4.25150800	-0.45634300	0.14024400
C	0.33721500	1.64791000	-0.05896700
H	-0.37827100	2.08597900	-0.76051300
C	0.05648400	1.99081400	0.94453800
C	1.89123900	-1.88543300	-0.12965100
H	1.65665100	-2.79615700	0.42892500
H	2.08213900	-2.19427200	-1.16476700
C	1.76398000	2.11678700	-0.39589200
C	1.80221800	3.19794600	-0.22469900
H	1.94270200	1.96199500	-1.46617300
C	3.13582200	-1.20140000	0.45211500
H	2.99125700	-1.05717600	1.52946200
H	3.97499000	-1.89686000	0.34078500
C	2.88015000	1.42827700	0.41134400
C	3.68495200	2.15917100	0.53398300
H	2.51368200	1.21557000	1.42424700
C	3.50445000	0.14469000	-0.19710900
H	4.59182900	0.24643700	-0.12760400
C	3.27902100	0.09954500	-1.27094100
N	-1.95544000	-0.26826100	-0.05094100
C	-3.27398800	1.73603700	0.11902000
H	-2.57539500	2.10230900	0.87525700
H	-2.95513600	2.12930700	-0.85059900
H	-4.28435100	2.07625300	0.33856700

HF: -629.2004689

Sum of electronic and zero-point Energies: -628.958749

Sum of electronic and thermal Energies: -628.945032

Sum of electronic and thermal Enthalpies: -628.944088

Sum of electronic and thermal Free Energies: -628.999975

Frequencies: -378.4290



(+2-azido-N-methylacetamide, 9-a TS)

C	2.74030400	-1.11708300	0.26633600
C	2.02613000	-0.53309800	1.28484300
H	2.50524700	0.15492100	1.97157200
C	-1.24677300	0.09940700	0.06087000
N	1.40341200	0.76114700	-0.90960500
N	2.15799900	0.07478500	-1.44237800
O	-0.77284000	-0.95400900	-0.31123800
N	-2.58202800	0.30563600	0.16723600
H	-2.92585700	1.21597600	0.42410500
C	-3.51971900	-0.74424700	-0.18518600
H	-3.29884200	-1.64914400	0.38501000
H	-4.53018400	-0.40862800	0.04790700
H	-3.45318200	-0.98593400	-1.24940000
N	1.03829800	1.07573200	0.26148100
C	-0.37753200	1.29380100	0.46689200
H	-0.72157100	2.19845400	-0.04992300
H	-0.49916900	1.46985500	1.53970100
H	2.36550600	-2.00921400	-0.22001400
H	1.09008600	-0.97530000	1.60991400
H	3.79245500	-0.89269300	0.13136200

HF: -490.4961994

Sum of electronic and zero-point Energies: -490.335358

Sum of electronic and thermal Energies: -490.324198

Sum of electronic and thermal Enthalpies: -490.323253

Sum of electronic and thermal Free Energies: -490.374030

Frequencies: -490.1220



(+2-azido-N-methylacetamide, 9-e TS)

C	-1.76218700	-0.53003100	-0.67015900
C	-0.93111800	0.39041200	-1.27457000
H	-0.05259100	0.04377200	-1.80860400
H	-1.35419000	1.34948500	-1.55523900
C	2.31059600	0.05154600	-0.03173300
N	-0.26424300	0.45018800	1.22138400
N	-1.06374300	-0.32116100	1.49327400
O	1.73643500	-1.01386800	-0.12786700
C	-3.13909400	-0.13931000	-0.29215200
H	-3.52295500	1.01117200	-0.35372500
O	-1.49662000	-1.58073700	-0.64378500
N	0.12262600	1.19568100	0.27606600
H	1.55062100	1.37392100	0.11283900
C	1.96947900	1.96745200	0.93371500
N	1.67134100	1.95813400	-0.80411000
H	3.65826400	0.16610300	-0.05664800
C	4.08457300	1.07153000	0.05196600
C	4.49449500	-1.01018700	-0.21462500
H	4.27810400	-1.50805700	-1.16297000
H	5.54028400	-0.70411000	-0.19777000
H	4.31042600	-1.72040400	0.59494900
C	-4.03786500	-1.25172700	0.19730000
H	-4.16376600	-2.00113600	-0.59072300
H	-3.57002800	-1.75111200	1.05162300
H	-5.00786800	-0.84668100	0.48375600

HF: -643.1087358

Sum of electronic and zero-point Energies: -642.910155  
 Sum of electronic and thermal Energies: -642.896323  
 Sum of electronic and thermal Enthalpies: -642.895378  
 Sum of electronic and thermal Free Energies: -642.952625  
 Frequencies: -477.4251



(+2-azido-N-methylacetamide, 9-f TS)

C	-1.14805900	1.08081400	0.07925700
C	-0.64713800	0.25849300	-0.68950900
C	2.64952000	-0.15355500	0.18172300
N	1.10377700	2.17355400	-0.52691100
N	0.34202100	2.70259300	0.14324000
O	2.66415500	0.57025000	1.15653900
C	2.81313700	-1.49621100	0.26276500
H	2.71068000	-2.05950500	-0.56419800
H	2.96968500	-2.13701500	1.55464600
H	2.05445600	-2.05004300	2.14734400
H	3.20735600	-3.18983200	1.40211300
C	3.78055100	-1.65809400	2.10683300
H	-0.63732200	-1.01052600	-1.43251400
H	-0.27637900	-0.86364700	-2.45639600
C	0.05667800	-1.71021900	-0.94491100
C	-2.20038600	1.53922100	0.99845300
H	-1.76668500	2.08617100	1.84123100
H	-2.84814500	2.24830800	0.46775300
C	-2.04710400	-1.62198500	-1.45359300
C	-1.97486700	-2.61408800	-1.91367300
H	-2.68186100	-1.01659500	-2.11099200
C	-3.03209700	0.35095300	1.50257200
H	-2.41633600	-0.24881000	2.18360400
H	-3.85902000	0.75129500	2.10015200
C	-2.71795300	-1.74535500	-0.07243900
H	-3.35366000	-2.63585500	-0.10215300
H	-1.94958200	-1.95177200	0.68449200
C	-3.60058500	-0.55983900	0.39925200
H	-4.53627700	-0.98078500	0.78056200
H	-3.88153600	0.05553700	-0.46574000
N	1.23347700	1.20414400	-1.31517000
N	2.45739500	0.41972000	-1.22001500
H	3.33563000	1.02560700	-1.46704200
H	2.36313100	-0.36378600	-1.97575500

HF: -723.8356564

Sum of electronic and zero-point Energies: -723.546507

Sum of electronic and thermal Energies: -723.530386

Sum of electronic and thermal Enthalpies: -723.529442

Sum of electronic and thermal Free Energies: -723.591089

Frequencies: -452.4287



(+2-azido-N-methylacetamide, 9-g TS)

C	2.44405000	0.29379800	0.48311700
C	1.62781000	1.08331800	-0.00081700
C	-1.01712100	-0.12507300	-1.41245900
N	0.93613300	-1.27167700	-0.88267600
N	1.84775600	-1.61156400	-0.26899200
C	0.93009200	2.34698400	-0.28804300
H	0.91509900	2.55019500	-1.36232100
H	-0.10540000	2.31139700	0.06721500
C	3.58153400	-0.17534500	1.29381900
H	3.23671200	-0.89077700	2.04470500
H	4.31511400	-0.68956400	0.66781400
H	-1.39754800	-0.87378300	-2.11838500
H	-1.23658100	0.85977400	-1.83450100
H	4.07379400	0.65874300	1.80002000
H	1.42881700	3.18064900	0.21390600
N	0.42229200	-0.19771900	-1.29223300
C	-1.73932800	-0.31611100	-0.07732000
N	-2.94089000	0.30525800	0.02646300
O	-1.27464100	-0.99824700	0.81051900
C	-3.76917700	0.10787300	1.20126100
H	-4.66850100	0.71669700	1.10715700
H	-4.05088200	-0.94343600	1.30650700
H	-3.22288600	0.40565900	2.09888800
H	-3.29480200	0.83767400	-0.75044300

HF: -567.8542365

Sum of electronic and zero-point Energies: -567.660841

Sum of electronic and thermal Energies: -567.647515

Sum of electronic and thermal Enthalpies: -567.646571

Sum of electronic and thermal Free Energies: -567.701199

Frequencies: -500.9363



(+2-azido-N-methylacetamide, 9-h TS)

C	2.76615400	2.33015500	-0.45091100
C	1.33854100	2.30037600	0.10874300
C	3.46184400	0.97073400	-0.55793000

C	1.11627000	-1.06303100	0.20676800
C	0.57603800	-0.06410900	-0.27935500
C	0.37012600	1.35662400	-0.62518600
C	2.16220800	-1.79264500	0.95819700
C	3.69280800	0.26486900	0.79108000
H	-0.65712900	1.64223300	-0.36658400
H	0.46540900	1.48547800	-1.71201400
H	2.11620800	-2.86285300	0.74007700
H	1.93105100	-1.68422900	2.02550800
H	4.67840500	0.54783000	1.17547800
H	2.96695900	0.61811800	1.53363200
N	-1.15191100	-0.90797300	-1.33560000
N	-0.23915900	-2.66869000	-0.25551800
N	-1.01644800	-2.05347000	-0.83534700
C	-2.47392000	-0.32092200	-1.36677300
H	-3.18504300	-0.96539800	-1.89793400
H	-2.38294800	0.60640100	-1.93912700
H	2.87632900	0.32262400	-1.21616500
H	4.42855200	1.11049000	-1.05595500
C	3.58512200	-1.26365000	0.70093400
H	4.24597200	-1.73936800	1.43325400
H	3.92539900	-1.59426300	-0.28776100
H	1.34240100	2.03044500	1.17007600
O	0.93128000	3.31652200	0.05178600
H	2.73671700	2.78630700	-1.44894400
H	3.36821700	3.00099100	0.17585900
C	-3.02999500	-0.04850200	0.03197700
O	-2.76195900	-0.76128500	0.97537700
N	-3.85993100	1.01958900	0.13088000
H	-4.04885000	1.58257500	-0.68121200
C	-4.51760300	1.32273900	1.38804100
H	-3.77583400	1.50905300	2.16824200
H	-5.13722400	2.21018600	1.25833300
H	-5.14360300	0.48511200	1.70601900

HF: -763.1351778  
Sum of electronic and zero-point Energies: -762.817050  
Sum of electronic and thermal Energies: -762.799971  
Sum of electronic and thermal Enthalpies: -762.799027  
Sum of electronic and thermal Free Energies: -762.862543  
Frequencies: -467.5035

(+2-azido-*N*-methylacetamide, 9-i TS)

C	-1.07413700	-0.98138400	-0.46648600
C	-0.68294900	-0.35501500	0.51675800
N	1.23552200	-2.07598700	0.07188600
N	0.66378800	-2.51044700	-0.80827800
C	-1.17100000	0.63006300	1.50127500
H	-0.80467400	0.44386300	2.51667100
H	-0.86248300	1.64680000	1.21921000
C	-2.22237400	-0.97625100	-1.39527100
H	-1.93189300	-1.17079300	-2.43188300
H	-2.93611700	-1.75935400	-1.11176800
C	-2.70862600	0.49528600	1.45356100
H	-3.15838000	1.12673400	2.22941000
H	-2.93228300	-0.54140100	1.72500800
C	-2.84334200	0.42960100	-1.26129200
H	-2.06018100	1.14170400	-1.54546300
C	-3.65119800	0.55015000	-1.99330200
C	-3.41988800	0.83588300	0.11878700
H	-3.56209700	1.92287000	0.07595100
H	-4.42892200	0.41464800	0.20503900
N	1.26521900	-1.36074300	1.09559200
C	2.39967600	-0.43626300	1.20591200
H	2.23014200	0.12232900	2.12847000
H	3.34405000	-0.98083100	1.28845100
C	2.45783800	0.46276800	-0.02364400
N	1.99696200	1.72753500	0.14280100
O	2.86594400	0.03483900	-1.08461300
C	1.77004300	2.57026900	-1.01595800
H	1.58781800	3.59325400	-0.68520100
H	2.65736800	2.54823600	-1.64944800
H	0.91773300	2.21313500	-1.60458300
H	1.50168200	1.93768100	0.99449300

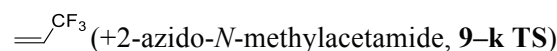
HF: -629.2015034  
Sum of electronic and zero-point Energies: -628.959367  
Sum of electronic and thermal Energies: -628.945287  
Sum of electronic and thermal Enthalpies: -628.944343  
Sum of electronic and thermal Free Energies: -629.000849  
Frequencies: -377.3401

(+2-azido-*N*-methylacetamide, 9-j TS)

C	-1.34297000	-0.76326100	-0.78378200
C	-0.99162800	-0.44763000	0.35995800
N	0.95538600	-2.07946000	-0.11594900
N	0.67816300	-2.50927300	-1.11720100
C	-1.55063600	0.35706200	1.45871300
H	-1.55507900	-0.15511500	2.42593000
H	-1.01561600	1.30768900	1.59086100
C	-2.59790000	-0.25806100	-1.42176300

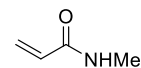
H	-2.44996800	0.07946200	-2.45144400
H	-3.33323100	-1.06965500	-1.46283200
C	-3.01059900	0.62071200	0.97231100
C	-3.43477000	1.45519900	1.54044800
H	-3.60636400	-0.26958300	1.20527400
C	-3.11087200	0.90925700	-0.53517300
H	-2.51793400	1.80431100	-0.76510400
H	-4.15148900	1.14076000	-0.78934900
N	0.78675700	-1.46830500	0.96325700
C	1.84226600	-0.51390200	1.33150700
H	1.44715200	0.02550900	2.19501700
H	2.75209700	-1.04174700	1.63029500
C	2.17529100	0.40255400	0.15900600
O	2.75683100	-0.03721900	-0.81284300
N	1.77340100	1.69125700	0.26567100
C	1.86015700	2.57103700	-0.88535500
H	1.13524000	2.28486300	-1.65458600
H	1.67507200	3.59691600	-0.56603500
H	2.86110100	2.49952500	-1.31237100
H	1.14454700	1.93348800	1.01365300

HF: -589.8983058  
Sum of electronic and zero-point Energies: -589.685386  
Sum of electronic and thermal Energies: -589.671561  
Sum of electronic and thermal Enthalpies: -589.670616  
Sum of electronic and thermal Free Energies: -589.728447  
Frequencies: -250.0064



C	-1.43084100	-0.70389400	-0.25747500
C	-0.67856200	-0.10299000	-1.23760400
O	0.18841500	-0.62371600	-1.62631700
H	-1.12282100	0.66226600	-1.86411700
N	0.10935800	0.95973500	0.98597500
N	-0.67601100	0.33829500	1.54293000
H	-1.16145200	-1.66777300	0.15433200
C	1.88386000	1.32926100	-0.45442800
H	1.97546200	1.50587700	-1.53002700
H	2.35436200	2.17884200	0.05392300
N	0.45979300	1.28742000	-0.18514400
C	2.60665200	0.02518500	-0.10177200
O	2.00219400	-0.98522800	0.19584900
N	3.95613600	0.08236100	-0.17221000
H	4.40751100	0.96251800	-0.35899100
C	4.76109500	-1.08787300	0.12947100
H	5.80606000	-0.86081800	-0.08048700
H	4.65416200	-1.37444000	1.17905200
H	4.44215300	-1.92877500	-0.48960800
C	-2.85359200	-0.30381000	-0.06589500
F	-3.67400900	-0.87489100	-0.97439400
F	-3.02556300	1.02487300	-0.19224100
F	-3.32687400	-0.65910500	1.13561300

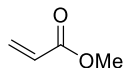
HF: -827.4703639  
Sum of electronic and zero-point Energies: -827.304056  
Sum of electronic and thermal Energies: -827.290576  
Sum of electronic and thermal Enthalpies: -827.289632  
Sum of electronic and thermal Free Energies: -827.345811  
Frequencies: -475.2350

(+2-azido-*N*-methylacetamide, 9-l TS)

C	-1.35600100	-0.37283500	-0.78558200
C	-0.47182400	0.56275400	-1.27264100
H	0.41725900	0.23251600	-1.79882800
H	-0.84706500	1.56144000	-1.46834900
C	2.72995800	0.01506700	0.02570000
N	0.11297400	0.33408700	1.24225400
N	-0.72661500	-0.43501500	1.37179100
O	2.13759900	-1.02679400	-0.16769300
C	-2.73948700	0.05388500	-0.45027900
O	-3.09834100	1.22049700	-0.46847400
H	-1.13965100	-1.43167400	-0.87094700
N	0.56074300	1.17300000	0.40912000
C	1.99706600	1.32671200	0.32419900
H	2.39994900	1.78284900	1.23617900
H	2.17138600	2.03135500	-0.49406300
N	4.07930900	0.11212300	-0.01470900
H	4.52160300	0.99413900	0.18443400
C	4.89504300	-1.05634200	-0.29090500
H	4.62003900	-1.49022700	-1.25502400
H	5.94273600	-0.75730600	-0.31519100
H	4.75239400	-1.81730500	0.48034300
N	-3.59614300	-0.95626400	-0.12229300
C	-3.19538400	-1.85463700	0.09447800
H	-4.91815000	-0.64633800	0.38096500
H	-5.40631300	0.05040200	-0.30207100
H	-5.50403400	-1.56491600	0.43523500
H	-4.87849300	-0.17919100	1.37126400

HF: -698.46284  
Sum of electronic and zero-point Energies: -698.245843  
Sum of electronic and thermal Energies: -698.230905

Sum of electronic and thermal Enthalpies: -698.229961  
 Sum of electronic and thermal Free Energies: -698.289691  
 Frequencies: -484.9341



**(+2-azido-*N*-methylacetamide, 9-m TS)**

C	-1.36407200	-0.41681000	-0.72134700
C	-0.50370400	0.49639000	-1.29291300
H	0.36987400	0.13425400	-1.82405200
H	-0.89370800	1.47324800	-1.55775400
C	2.70917500	0.01549600	-0.02742500
N	0.13724200	0.47640000	1.20491700
N	-0.69253400	-0.27683300	1.43688400
O	2.09823700	-1.01970700	-0.19734500
O	-2.72960600	0.01146600	-0.37741700
C	-3.12466100	1.15364300	-0.36634500
O	-3.51042000	-1.03497000	-0.05249900
C	-4.83898700	-0.69616100	0.33187300
H	-5.35048700	-0.17493900	-0.48009600
H	-5.33367100	-1.64066400	0.55323800
H	-4.82689100	-0.05229000	1.21402300
H	-1.15292400	-1.47756200	-0.72303600
N	0.56077200	1.23407000	0.28331300
C	1.99658600	1.36127800	0.14002900
H	2.42721500	1.92202700	0.97769900
H	2.15066700	1.95951200	-0.76287800
N	4.06035600	0.07530000	0.00845000
H	4.51558500	0.95168300	0.20289600
C	4.85541700	-1.12855500	-0.15443700
H	4.60938600	-1.61644700	-1.10021100
H	5.91088200	-0.85712800	-0.15193400
H	4.65911700	-1.83459600	0.65649100

HF: -718.3224768

Sum of electronic and zero-point Energies: -718.117403

Sum of electronic and thermal Energies: -718.102992

Sum of electronic and thermal Enthalpies: -718.102047

Sum of electronic and thermal Free Energies: -718.160413

Frequencies: -483.2897

**(+2-azido-*N*-methylacetamide, 9-n TS)**

C	-1.78347400	-0.71889000	-0.48959300
C	-0.96644700	0.09872700	-1.23340500
H	-0.09358600	-0.35484000	-1.68872900
H	-1.39826200	0.97740400	-1.69634100
N	-0.30721200	0.58887400	1.18436200
N	-1.07333200	-0.15490800	1.58853500
O	-3.41915200	0.88439700	-0.38083500
H	-1.62856000	-1.76860500	-0.30102600
C	1.46511300	1.37758200	-0.09263900
H	1.55423200	1.82433900	-1.08690900
H	1.87039200	2.09934800	0.62483900
N	0.04495600	1.18196000	0.12289900
N	-3.13764100	-0.29053300	-0.21537300
O	-3.91219300	-1.13787100	0.18418200
C	2.26178100	0.06904100	-0.05036600
N	1.71138400	-1.00987900	0.04230800
O	3.60235000	0.20921500	-0.14171100
H	4.00723400	1.13076200	-0.16072300
C	4.46871800	-0.95669200	-0.11562900
H	5.49526700	-0.63688300	-0.29284200
H	4.40616600	-1.46498200	0.84995100
H	4.16882000	-1.66057600	-0.89465100

HF: -694.9596288

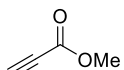
Sum of electronic and zero-point Energies: -694.794766

Sum of electronic and thermal Energies: -694.781405

Sum of electronic and thermal Enthalpies: -694.780461

Sum of electronic and thermal Free Energies: -694.837077

Frequencies: -491.0360



**(+2-azido-*N*-methylacetamide, 9 TS)**

C	-1.86861600	0.75346700	-0.14780200
C	-0.91645300	1.44587100	-0.51841400
C	-0.45525200	2.33459000	-0.89594200
C	3.10694800	-0.10873800	0.06597500
N	0.19653100	-0.73755300	0.02535000
N	-0.81850700	-1.18873300	0.28817700
O	2.99317100	-1.31448200	0.08660700
O	-3.19298100	0.34170200	0.26787800
C	-3.63993600	0.49422600	1.37449000
O	-3.85507900	-0.25119500	-0.73476300
C	-5.15884800	-0.72040400	-0.38939800
H	-5.78642400	0.10971100	-0.05915300
H	-5.55803700	-1.16758800	-1.29779900
H	-5.09323400	-1.46088500	0.41020100
N	4.30436300	0.51831800	-0.00249400
H	4.34212800	1.52016100	-0.08390800

C	5.53271500	-0.25409000	-0.04581900
H	5.58517500	-0.84810700	-0.96178200
H	6.38075300	0.42908900	-0.00613800
H	5.57435900	-0.93501000	0.80677900
N	0.72335600	0.28692400	-0.48728400
C	1.89518000	0.81967100	0.18972500
H	1.70421400	0.98641000	1.25835300
H	2.09320600	1.78567400	-0.28039100

HF: -717.0628467

Sum of electronic and zero-point Energies: -716.882230

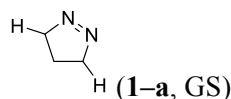
Sum of electronic and thermal Energies: -716.867608

Sum of electronic and thermal Enthalpies: -716.866664

Sum of electronic and thermal Free Energies: -716.926094

Frequencies: -469.5824

**PRODUCTS**



C	-1.19247000	0.25894900	0.00011300
C	0.00069000	1.22476500	-0.00005100
H	0.00106900	1.86528200	-0.88209600
H	0.00119800	1.86543100	0.88188600
N	0.61333300	-1.10893500	-0.00004600
N	-0.61444100	-1.10846400	0.00004100
C	-1.83416000	0.33667700	-0.88114700
H	1.19256000	0.25764800	-0.00006500
H	1.83444800	0.33477900	0.88114300
H	1.83442400	0.33477200	-0.88129000
H	-1.83390700	0.33667600	0.88155900

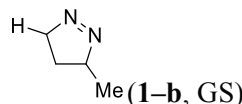
HF: -227.3072274

Sum of electronic and zero-point Energies: -227.213414

Sum of electronic and thermal Energies: -227.209694

Sum of electronic and thermal Enthalpies: -227.208749

Sum of electronic and thermal Free Energies: -227.239972



C	-0.72914600	0.04893500	-0.53004400
C	0.27404800	1.18900900	-0.31611200
H	0.60941400	1.60272800	-1.26917900
H	-0.14624000	2.00007800	0.28101700
N	1.17728300	-0.98227600	0.15174700
N	0.07348600	-1.19571600	-0.34275500
H	-1.13190000	0.01564400	-1.54549600
C	1.41850600	0.46445200	0.39511500
H	1.42643900	0.60125900	1.48153000
H	2.41524200	0.70995700	0.02435600
C	-1.87303800	0.01419700	0.47843700
H	-2.54075900	0.86559300	0.32679700
H	-2.44929600	-0.90790300	0.37371400
H	-1.48050400	0.05867200	1.49993800

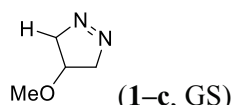
HF: -266.6075875

Sum of electronic and zero-point Energies: -266.485692

Sum of electronic and thermal Energies: -266.479912

Sum of electronic and thermal Enthalpies: -266.478968

Sum of electronic and thermal Free Energies: -266.515098



C	-0.62257600	-1.17011900	0.41980300
C	0.20751400	-0.00463000	0.95703400
H	0.27564700	-0.00976000	2.04466400
N	-1.37177000	0.61985600	-0.72958400
N	-1.37232000	-0.61249500	-0.73515900
C	-1.36815700	-1.51332500	1.14492400
H	-0.62187500	1.16627000	0.43064000
H	-0.03139400	2.03053200	0.12055000
H	-0.03251400	-2.03167400	0.10128300
O	1.54226600	-0.00320200	0.50366800
C	1.71338400	0.00449600	-0.89738500
H	1.27530700	0.89805900	-1.36041900
H	2.78886800	0.00334000	-1.07608000
H	1.27161400	-0.88195200	-1.37047000
H	-1.36755000	1.50276800	1.15885200

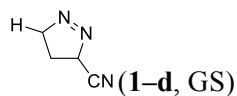
HF: -341.7909883

Sum of electronic and zero-point Energies: -341.663579

Sum of electronic and thermal Energies: -341.657228

Sum of electronic and thermal Enthalpies: -341.656284

Sum of electronic and thermal Free Energies: -341.693602



C	-0.34509300	-0.01553700	0.75751400
C	0.57240500	-1.18321200	0.37484600
H	1.11698200	-1.52576500	1.25616100
H	0.02687600	-2.02232200	-0.05389500
N	1.40041200	0.94577100	-0.32848200
N	0.43918000	1.22356700	0.37848500
C	-1.60410600	0.00206100	0.00459500
H	-0.57439800	0.04995600	1.82206800
C	1.51339400	-0.50265800	-0.61989100
H	1.21177600	-0.63038600	-1.66487900
N	-2.57687400	-0.00939100	-0.61158600
H	2.56014200	-0.79504300	-0.53075900

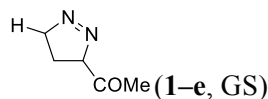
HF: -319.5245682

Sum of electronic and zero-point Energies: -319.431865

Sum of electronic and thermal Energies: -319.425895

Sum of electronic and thermal Enthalpies: -319.424951

Sum of electronic and thermal Free Energies: -319.462115



C	-0.00799500	0.10060000	0.74471100
C	1.10993200	-0.93124900	0.71101100
H	1.62552400	-0.97641300	1.67141100
H	0.72660100	-1.91911500	0.45771600
N	1.58973700	1.04622700	-0.55955200
N	0.54206700	1.30310700	0.02581000
C	-1.27251100	-0.30172000	-0.02783400
O	-1.31735500	-1.33525800	-0.64476300
C	-0.30046600	0.43641100	1.74375900
C	2.02046000	-0.36176100	-0.37998600
H	1.89409400	-0.84867000	-1.35201500
C	-2.41129300	0.68151400	0.01605000
H	-2.79257700	0.74731500	1.04046000
H	-2.04590900	1.67551800	-0.25793700
H	-3.20717400	0.36041100	-0.65470900
H	3.08455900	-0.36303800	-0.13810100

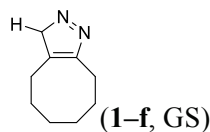
HF: -379.9060842

Sum of electronic and zero-point Energies: -379.774892

Sum of electronic and thermal Energies: -379.767094

Sum of electronic and thermal Enthalpies: -379.766149

Sum of electronic and thermal Free Energies: -379.808350



C	-0.77854000	-0.59021500	-0.35141300
C	-0.94996900	0.72617500	-0.14082900
N	-2.86846600	-0.50310000	0.40947800
N	-1.98838000	-1.28970600	0.01044900
C	-2.34322000	0.86148600	0.37392800
H	-2.99874400	1.47201500	-0.25911200
C	-0.03853900	1.89718000	-0.32374200
H	-0.38687800	2.48614000	-1.18273500
H	-0.14842900	2.55751400	0.54791800
C	0.35574200	-1.44639700	-0.82650800
H	-0.09174600	-2.40259200	-1.11247400
H	0.81199200	-1.03082900	-1.72999900
C	1.44033100	1.55512400	-0.50263900
H	1.97930100	2.49580700	-0.65134100
H	1.57424600	0.98896800	-1.42970300
C	1.43412800	-1.70429800	0.24287900
H	0.93940900	-1.83585500	1.21311600
H	1.92297400	-2.65734100	0.01391100
C	2.05709400	0.78580900	0.68589000
H	2.92122200	1.34534600	1.05696800
C	1.34056300	0.74909500	1.51732700
H	2.52425200	-0.63802200	0.36171300
H	3.21953400	-0.96411300	1.14356800
H	3.10511200	-0.61228900	-0.57066500
H	-2.39829500	1.27672700	1.38804100

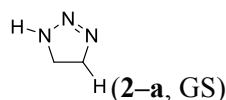
HF: -460.6761426

Sum of electronic and zero-point Energies: -460.454703

Sum of electronic and thermal Energies: -460.445125

Sum of electronic and thermal Enthalpies: -460.444181

Sum of electronic and thermal Free Energies: -460.489359



C	-0.44717700	1.09453300	0.12359900
C	-1.16694000	-0.23424200	-0.09579000
H	-1.98305000	-0.43449800	0.59701300
H	-1.53648000	-0.34188200	-1.12140400
N	1.01029800	-0.69124000	0.04059400
N	0.91508400	0.66729300	-0.20396900
H	-0.52961400	1.43711000	1.16267100
N	-0.09298300	-1.24141900	0.09431500
H	-0.78184200	1.88164200	-0.55116400
H	1.68889900	1.15343600	0.22945100

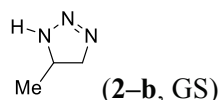
HF: -243.3359379

Sum of electronic and zero-point Energies: -243.253097

Sum of electronic and thermal Energies: -243.248926

Sum of electronic and thermal Enthalpies: -243.247981

Sum of electronic and thermal Free Energies: -243.279952



C	-0.70850600	-0.05941400	0.54943600
C	0.30568100	-1.17707400	0.29559400
H	0.74778000	-1.55934800	1.22184800
H	-0.08505500	-2.01565200	-0.28364600
N	1.27468200	0.72069000	-0.34604300
N	0.21833800	1.07708700	0.47065400
H	-1.13071000	-0.11807700	1.55403500
N	1.38421300	-0.50384900	-0.46658800
C	-1.80769400	0.00442000	-0.50583500
H	-2.44897400	-0.87977600	-0.44571100
H	-2.43736100	0.88823900	-0.36580100
H	-1.36753500	0.04505600	-1.50752600
H	-0.15566500	1.97447200	0.18547200

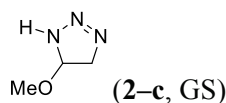
HF: -282.6372294

Sum of electronic and zero-point Energies: -282.526489

Sum of electronic and thermal Energies: -282.521017

Sum of electronic and thermal Enthalpies: -282.520073

Sum of electronic and thermal Free Energies: -282.555163



C	0.68709000	-1.21330900	-0.01279000
C	-0.18794900	-0.34047400	0.88613700
H	-0.25171900	-0.70099300	1.91151400
N	1.30534500	0.88596300	-0.38002700
N	1.39699000	-0.24511100	-0.87460300
H	0.13112800	-1.93295500	-0.61450500
N	0.60761900	0.87465600	0.81088800
H	1.43904900	-1.74478200	0.57873600
O	-1.51718300	-0.18173400	0.46973700
C	-1.70111200	0.26934100	-0.85940600
H	-2.77757000	0.35407900	-1.00778700
H	-1.23780700	1.24971300	-1.02241400
H	-1.29106000	-0.43767500	-1.59013600
H	0.16758700	1.76457700	1.00924400

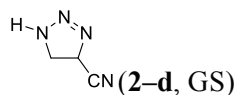
HF: -357.828287

Sum of electronic and zero-point Energies: -357.711940

Sum of electronic and thermal Energies: -357.705773

Sum of electronic and thermal Enthalpies: -357.704829

Sum of electronic and thermal Free Energies: -357.741729



C	-0.32517500	-0.01013400	0.74805100
C	0.58823800	-1.16885100	0.33241900
H	0.04801100	-2.00002000	-0.11750200
N	1.40523600	0.86915100	-0.35942800
N	0.48042700	1.20583900	0.38809500
H	-0.54952600	0.01789700	1.81394400
N	1.40260500	-0.46416500	-0.65597200
C	-1.58991800	0.01252800	-0.00100900
N	-2.58173700	0.00302500	-0.58513900
H	1.18499700	-1.51631200	1.18293500
H	2.33193800	-0.79971000	-0.86904000

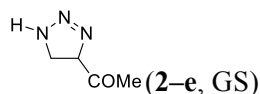
HF: -335.5523131

Sum of electronic and zero-point Energies: -335.470683

Sum of electronic and thermal Energies: -335.464920

Sum of electronic and thermal Enthalpies: -335.463976

Sum of electronic and thermal Free Energies: -335.500529



C	0.03771300	-0.04351500	0.74366600
C	1.10109100	-1.08201200	0.40605100
H	1.71868000	-1.34071100	1.27265500
H	0.65707900	-1.97748900	-0.02890000
N	1.63446300	1.01907900	-0.39400700
N	0.64701300	1.24643800	0.31809300
C	-1.29467300	-0.26469400	0.00673400
O	-1.59952000	-1.36133100	-0.38571500
H	-0.19889800	0.02583800	1.80937800
C	-2.17885400	0.94184500	-0.15283100
H	-2.26038800	1.48103000	0.79543800
H	-1.71223800	1.63213200	-0.86192000
H	-3.15928200	0.63238600	-0.51249500
N	1.85162700	-0.31636000	-0.58916700
H	2.82782600	-0.51638400	-0.75459300

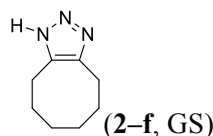
HF: -395.9347165

Sum of electronic and zero-point Energies: -395.814750

Sum of electronic and thermal Energies: -395.807132

Sum of electronic and thermal Enthalpies: -395.806188

Sum of electronic and thermal Free Energies: -395.847966



C	-0.79769000	-0.65380900	-0.34665200
C	-0.96758900	0.69988200	-0.14051200
N	-2.81175300	-0.41325500	0.44487300
N	-1.95350600	-1.28268100	0.02882200
C	-0.10942500	1.90791800	-0.33802700
H	-0.45789800	2.46706800	-1.21468600
H	-0.23161600	2.57337700	0.52683600
C	0.36076700	-1.47853900	-0.82054900
H	-0.06473100	-2.45132700	-1.08215400
H	0.79188300	-1.06883000	-1.73989000
C	1.37305400	1.57205500	-0.50455400
H	1.90770500	2.51237000	-0.66745600
H	1.50572700	0.99252500	-1.42355400
C	1.45958900	-1.69136300	0.23666900
H	0.97532400	-1.84813500	1.20823400
H	1.98574000	-2.62256000	-0.00058300
C	1.98827000	0.81682300	0.69320200
H	2.82061000	1.40520000	1.09120000
H	1.25309000	0.74308900	1.50562900
C	2.51099600	-0.58614600	0.36101000
H	3.21729400	-0.89086400	1.14149900
C	3.09180100	-0.53240600	-0.57025700
N	-2.22905000	0.78109600	0.34838900
H	-2.74259600	1.60345200	0.62707000

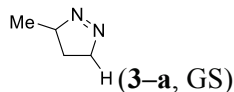
HF: -476.7477573

Sum of electronic and zero-point Energies: -476.535713

Sum of electronic and thermal Energies: -476.526532

Sum of electronic and thermal Enthalpies: -476.525588

Sum of electronic and thermal Free Energies: -476.569956



C	-1.19247000	0.25894900	0.00011300
C	0.00069000	1.22476500	-0.00005100
H	0.00106900	1.86528200	-0.88209600
H	0.00119800	1.86543100	0.88188600
N	0.61333300	-1.10893500	-0.00004600
N	-0.61444100	-1.10846400	0.00004100
H	-1.83416000	0.33667700	-0.88114700
C	1.19256000	0.25764800	-0.00006500
H	1.83444800	0.33477900	0.88114300
H	1.83442400	0.33477200	-0.88129000
H	-1.83390700	0.33667600	0.88155900

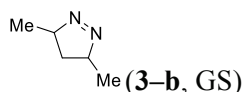
HF: -227.3072274

Sum of electronic and zero-point Energies: -227.213414

Sum of electronic and thermal Energies: -227.209694

Sum of electronic and thermal Enthalpies: -227.208749

Sum of electronic and thermal Free Energies: -227.239972



C	-0.72914600	0.04893500	-0.53004400
C	0.27404800	1.18900900	-0.31611200
H	0.60941400	1.60272800	-1.26917900
H	-0.14624000	2.00007800	0.28101700

N	1.17728300	-0.98227600	0.15174700
N	0.07348600	-1.19571600	-0.34275500
H	-1.13190000	0.01564400	-1.54549600
C	1.41850600	0.46445200	0.39511500
H	1.42643900	0.60125900	1.48153000
H	2.41524200	0.70995700	0.02435600
C	-1.87303800	0.01419700	0.47843700
H	-2.54075900	0.86595300	0.32679700
H	-2.44929600	-0.90790300	0.37371400
H	-1.48050400	0.05867200	1.49993800

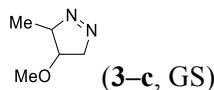
HF: -266.6075875

Sum of electronic and zero-point Energies: -266.485692

Sum of electronic and thermal Energies: -266.479912

Sum of electronic and thermal Enthalpies: -266.478968

Sum of electronic and thermal Free Energies: -266.515098



C	-0.62257600	-1.17011900	0.41980300
C	0.20751400	-0.00463000	0.95703400
H	0.27564700	-0.00976000	2.04466400
N	-1.37177000	0.61985600	-0.72958400
N	-1.37232000	-0.61249500	-0.73515900
H	-1.36815700	-1.51332500	1.14492400
C	-0.62187500	1.16627000	0.43064000
H	-0.03139400	2.03053200	0.12055000
H	-0.03251400	-2.03167400	0.10128300
O	1.54226600	-0.00320200	0.50366800
C	1.71338400	0.00449600	-0.89738500
H	1.27530700	0.89805900	-1.36041900
H	2.78886800	0.00334000	-1.07608000
H	1.27161400	-0.88195200	-1.37047000
H	-1.36755000	1.50276800	1.15885200

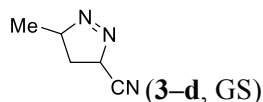
HF: -341.7909883

Sum of electronic and zero-point Energies: -341.663579

Sum of electronic and thermal Energies: -341.657228

Sum of electronic and thermal Enthalpies: -341.656284

Sum of electronic and thermal Free Energies: -341.693602



C	-0.34509300	-0.01553700	0.75751400
C	0.57240500	-1.18321200	0.37484600
H	1.11698200	-1.52576500	1.25616100
H	0.02687600	-2.02232200	-0.05389500
N	1.40041200	0.94577100	-0.32848200
N	0.43918000	1.22356700	0.37848500
C	-1.60410600	0.00206100	0.00459500
H	-0.57439800	0.04995600	1.82206800
C	1.51339400	-0.50265800	-0.61989100
H	1.21177600	-0.63038600	-1.66487900
N	-2.57687400	-0.00939100	-0.61158600
H	2.56014200	-0.79504300	-0.53075900

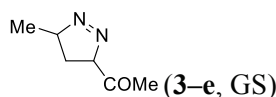
HF: -319.5245682

Sum of electronic and zero-point Energies: -319.431865

Sum of electronic and thermal Energies: -319.425895

Sum of electronic and thermal Enthalpies: -319.424951

Sum of electronic and thermal Free Energies: -319.462115



C	-0.00799500	0.10060000	0.74471100
C	1.10993200	-0.93124900	0.71101100
H	1.62552400	-0.97641300	1.67141100
H	0.72660100	-1.91911500	0.45771600
N	1.58973700	1.04622700	-0.55955200
N	0.54206700	1.30310700	0.02581000
C	-1.27251100	-0.30172000	-0.02783400
O	-1.31735500	-1.33525800	-0.64476300
H	-0.30046600	0.43641100	1.74375900
C	2.02046000	-0.36176100	-0.37998600
H	1.89409400	-0.84867000	-1.35201500
C	-2.41129300	0.68151400	0.01605000
H	-2.79257700	0.74731500	1.04046000
H	-2.04590900	1.67551800	-0.25793700
H	-3.20717400	0.36041100	-0.65470900
H	3.08455900	-0.36303800	-0.13810100

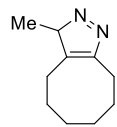
HF: -379.9060842

Sum of electronic and zero-point Energies: -379.774892

Sum of electronic and thermal Energies: -379.767094

Sum of electronic and thermal Enthalpies: -379.766149

Sum of electronic and thermal Free Energies: -379.808350

**(3-f, GS)**

C	-0.77854000	-0.59021500	-0.35141300
C	-0.94996900	0.72617500	-0.14082900
N	-2.86846600	-0.50310000	0.40947800
N	-1.98838000	-1.28970600	0.01044900
C	-2.34322000	0.86148600	0.37392800
H	-2.99874400	1.47201500	-0.25911200
C	-0.03853900	1.89718000	-0.32374200
H	-0.38687800	2.48614000	-1.18273500
H	-0.14842900	2.55751400	0.54791800
C	0.35574200	-1.44639700	-0.82650800
H	-0.09174600	-2.40259200	-1.11247400
H	0.81199200	-1.03082900	-1.72999000
C	1.44033100	1.55512400	-0.50263900
H	1.97930100	2.49580700	-0.65134100
H	1.57424600	0.98896800	-1.42970300
C	1.43412800	-1.70429800	0.24287900
H	0.93940900	-1.83585500	1.21311600
H	1.92297400	-2.65734100	0.01391100
C	2.05709400	0.78580900	0.68589000
H	2.92122200	1.34534600	1.05696800
H	1.34056300	0.74909500	1.51732700
C	2.52425200	-0.63802200	0.36171300
H	3.21953400	-0.96411300	1.14356800
H	3.10511200	-0.61228900	-0.57066500
H	-2.39829500	1.27672700	1.38804100

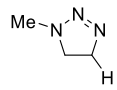
HF: -460.6761426

Sum of electronic and zero-point Energies: -460.454703

Sum of electronic and thermal Energies: -460.445125

Sum of electronic and thermal Enthalpies: -460.444181

Sum of electronic and thermal Free Energies: -460.489359

**(4-a, GS)**

C	-0.19504000	1.14286700	0.06875900
C	-1.56325500	0.47889500	-0.02932300
H	-2.28429400	0.79023000	0.72531700
H	-2.01205900	0.59997000	-1.02144700
N	-0.03715100	-1.14320400	-0.02785100
N	0.64473600	0.01683000	-0.32913300
H	0.04088200	1.45532300	1.09858300
H	-1.24829900	-0.96176800	0.13958000
C	-0.06530900	1.98835400	-0.60696600
H	2.03105300	0.00738600	0.08862400
H	2.47399500	-0.94702500	-0.19765000
H	2.56352500	0.81338200	-0.42024400
H	2.13170600	0.14186800	1.17587700

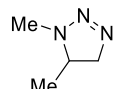
HF: -282.6279067

Sum of electronic and zero-point Energies: -282.517175

Sum of electronic and thermal Energies: -282.511632

Sum of electronic and thermal Enthalpies: -282.510688

Sum of electronic and thermal Free Energies: -282.545966

**(4-b, GS)**

C	-0.19289600	0.75009900	0.53765600
C	-1.57460200	0.12075700	0.36333000
H	-2.00969100	-0.20436600	1.31498800
H	-2.29481800	0.75443700	-0.15713100
N	-0.09735800	-1.36053100	-0.38712000
N	0.61075300	-0.47008500	0.38080500
H	-0.04907300	1.14956800	1.54420700
N	-1.30631900	-1.09891500	-0.43646000
C	0.11057500	1.81609300	-0.51328600
H	-0.58415400	2.65249800	-0.39686300
H	1.12649800	2.20732200	-0.41444400
H	-0.01011000	1.40676400	-1.52169900
C	2.02310400	-0.40015800	0.06705300
H	2.53269500	0.15397200	0.85873000
H	2.41692000	-1.41676300	0.04093600
H	2.22511900	0.08253600	-0.89781400

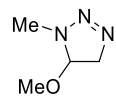
HF: -321.927889

Sum of electronic and zero-point Energies: -321.789084

Sum of electronic and thermal Energies: -321.782239

Sum of electronic and thermal Enthalpies: -321.781295

Sum of electronic and thermal Free Energies: -321.819515

**(4-c, GS)**

C	-1.06452700	-1.14601300	0.58057300
C	-0.26283000	0.10421200	0.93256200
H	-0.10271800	0.23889700	2.00227400
N	0.70395700	-1.12868300	-0.75618700
N	-0.40950200	-1.66281500	-0.63942200
H	-2.12559600	-0.96372200	0.40826100
H	0.97668800	-0.25489300	0.26536500
H	-0.95401900	-1.90542500	1.36132700
O	-0.80755300	1.32022800	0.48979400
C	-1.12611500	1.37998100	-0.88816000
H	-1.51169000	2.38305600	-1.07158000
H	-0.24409700	1.20889100	-1.51707700
H	-1.89048200	0.64250400	-1.16116800
C	2.02956400	0.71273900	0.04088600
H	2.41600500	1.04570500	1.00663000
H	2.82964600	0.21741000	-0.50980000
H	1.68882200	1.59009200	-0.52068000

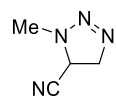
HF: -397.1199368

Sum of electronic and zero-point Energies: -396.975511

Sum of electronic and thermal Energies: -396.967827

Sum of electronic and thermal Enthalpies: -396.966883

Sum of electronic and thermal Free Energies: -397.007199

**(4-d, GS)**

C	0.75303100	-1.46318600	0.37532700
C	-0.26401600	-0.37607900	0.74788400
H	-0.49949300	-0.35686300	1.81252400
N	1.42351600	0.42490700	-0.59483700
N	1.61131200	-0.79346700	-0.62759700
H	0.31690500	-2.36783300	-0.04435800
H	0.50036200	0.80558900	0.35967800
H	1.38238000	-1.72270000	1.23187000
N	-2.51633000	-0.58288300	-0.60017200
C	-1.53050300	-0.50140000	-0.01035800
C	-0.17803300	2.05985700	0.08274000
H	-0.65616100	2.41261100	0.99862100
H	0.57540700	2.78410100	-0.22627400
H	-0.93393800	1.95649700	-0.70543700

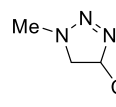
HF: -374.8451071

Sum of electronic and zero-point Energies: -374.735767

Sum of electronic and thermal Energies: -374.728512

Sum of electronic and thermal Enthalpies: -374.727568

Sum of electronic and thermal Free Energies: -374.767479

**(4-e, GS)**

C	-0.45976600	0.06231300	0.80878900
C	0.74176000	-0.85938600	0.66598600
H	1.30157300	-0.97218100	1.60548000
H	0.45968800	-1.83721900	0.27323200
N	1.12747800	1.21188100	-0.25178100
N	0.04891800	1.38026000	0.33882000
O	-1.66647500	-0.36634900	-0.04382800
O	-1.79250800	-1.51154100	-0.39408800
H	-0.82215000	0.17805000	1.83440400
C	-2.66573400	0.70899900	-0.37361400
H	-2.91428300	1.28558300	0.52200900
H	-2.20920900	1.41178300	-1.07683100
H	-3.55762000	0.26059800	-0.80941000
N	1.51590000	-0.09174900	-0.30344300
C	2.93861100	-0.31542100	-0.43285800
H	3.45405100	-0.22286900	0.53387100
H	3.10962000	-1.31624900	-0.83401600
H	3.34194200	0.42114600	-1.12805700

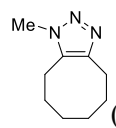
HF: -435.2268823

Sum of electronic and zero-point Energies: -435.078895

Sum of electronic and thermal Energies: -435.069876

Sum of electronic and thermal Enthalpies: -435.068932

Sum of electronic and thermal Free Energies: -435.113882

**(4-f, GS)**

C	-0.25568600	-0.98034100	-0.36438500
C	-0.79506600	0.28852900	-0.26048200
N	-2.31677600	-1.24002000	0.27504200
N	-1.22960500	-1.87244100	-0.02357400

C	-0.27632700	1.67156500	-0.48859200
H	-0.73152400	2.08964200	-1.39586200
H	-0.59932900	2.31427100	0.34183100
C	1.10852100	-1.49099100	-0.72039000
H	0.97113400	-2.55815700	-0.91556600
H	1.46937800	-1.04773100	-1.65475100
C	1.24649900	1.73682400	-0.60077100
H	1.51786700	2.77483300	-0.81415100
H	1.56811400	1.16056700	-1.47393000
C	2.16577900	-1.32785000	0.38664500
H	1.68874400	-1.53647400	1.35221000
C	2.92973300	-2.10008500	0.24497100
H	1.98632100	1.25012900	0.66402300
H	2.60928900	2.06580200	1.04345400
H	1.25909000	1.02899900	1.45650200
C	2.88025100	0.02327400	0.45064500
H	3.60859700	-0.02647100	1.26791800
H	3.46397400	0.16908500	-0.46898700
N	-2.07148100	0.06333000	0.13816100
C	-3.10986500	1.03152800	0.40867000
H	-3.29639100	1.64824700	-0.47374500
H	-4.00909100	0.47243100	0.66349700
H	-2.82709900	1.67295200	1.24703000

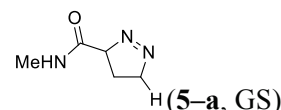
HF: -516.042437

Sum of electronic and zero-point Energies: -515.802267

Sum of electronic and thermal Energies: -515.791550

Sum of electronic and thermal Enthalpies: -515.790605

Sum of electronic and thermal Free Energies: -515.838304



C	2.66292300	0.12539200	0.33966600
C	1.51816400	1.10772400	0.08760000
H	1.10677200	1.50344200	1.01813700
H	1.80585200	1.95020000	-0.53868700
C	-0.94852900	0.44213200	-0.16544600
N	0.93351600	-1.18848000	-0.27401200
N	2.05763600	-1.22622700	0.21962400
O	-1.35315000	1.56869500	0.05216400
H	3.13243400	0.20327000	1.32143100
N	-1.72607300	-0.65760700	-0.08675100
H	-1.28563100	-1.55969400	-0.18605400
C	-3.11690200	-0.54683000	0.30455800
H	-3.63064100	0.16648400	-0.34348000
H	-3.58833500	-1.52503200	0.21010000
H	-3.20980000	-0.19650300	1.33667400
C	0.49506400	0.19852700	-0.59101800
H	0.51883800	0.27943500	-1.68510300
H	3.45584100	0.17337300	-0.41452800

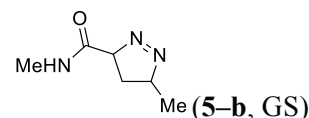
HF: -435.2652997

Sum of electronic and zero-point Energies: -435.115333

Sum of electronic and thermal Energies: -435.106428

Sum of electronic and thermal Enthalpies: -435.105484

Sum of electronic and thermal Free Energies: -435.150058



C	1.97437500	-0.05465000	-0.54142400
C	1.19395800	-1.03758100	0.33663500
H	0.81385900	-1.90188600	-0.20798600
H	1.81673000	-1.38634400	1.16414100
C	-1.30158400	-0.45848300	0.17877500
N	0.45889000	1.23524000	0.55243000
N	1.44704300	1.29029500	-0.17447400
O	-1.59744500	-1.57451500	-0.20264100
H	1.72336500	-0.16932100	-1.60326600
N	-2.13589600	0.59847200	0.09076500
H	-1.78356200	1.50873800	0.34490100
C	-3.44919900	0.45026800	-0.50421100
H	-4.05737700	-0.24517200	0.07964500
H	-3.93746900	1.42449800	-0.52630200
C	-3.36905900	0.05978000	-1.52208500
H	0.04954600	-0.16953300	0.84683900
C	-0.11498100	-0.24164000	1.92583600
C	3.48455500	-0.07542000	-0.37249200
H	3.88411600	-1.04799500	-0.67083000
H	3.95359600	0.69913800	-0.98321100
H	3.75017100	0.10066900	0.67450200

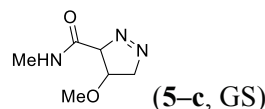
HF: -474.5646225

Sum of electronic and zero-point Energies: -474.387252

Sum of electronic and thermal Energies: -474.376654

Sum of electronic and thermal Enthalpies: -474.375710

Sum of electronic and thermal Free Energies: -474.425434



C	2.38658300	-0.25836800	-0.72897200
C	0.97393100	0.25549600	-1.00660700
C	-1.17233300	-0.43330600	0.26403300
N	1.09672700	-1.37673300	0.74565600
N	2.26507100	-1.06455600	0.51171400
O	-1.34855300	-0.17550400	1.43501200
H	3.13974000	0.52040300	-0.60325400
C	0.17645700	-0.86016100	-0.30146600
H	0.02784100	-1.69596900	-0.99825400
H	2.72394600	-0.94114900	-1.51666800
O	0.71175700	1.54712400	-0.53144200
C	1.07392500	1.81374500	0.81785400
H	2.15351700	1.69942900	0.97312200
H	0.80270200	2.85435000	0.99700300
H	0.53399900	1.17053000	1.51854400
H	0.75506000	0.29067800	-2.07543500
N	-2.16507700	-0.35925200	-0.65944200
C	-1.93135200	-0.45209900	-1.63449200
H	-3.45787100	0.18706800	-0.29280600
H	-3.39312200	1.25910100	-0.08255900
H	-4.16018000	0.01618600	-1.10890100
H	-3.81897700	-0.31748700	0.60461000

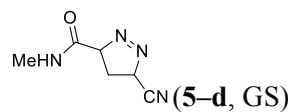
HF: -549.7437069

Sum of electronic and zero-point Energies: -549.560705

Sum of electronic and thermal Energies: -549.549485

Sum of electronic and thermal Enthalpies: -549.548541

Sum of electronic and thermal Free Energies: -549.598524



C	-1.70688300	-0.06631900	0.49026000
C	-0.96114200	-0.96953800	-0.49832900
H	-0.61405000	-1.89623900	-0.04315000
H	-1.58675600	-1.19519300	-1.36183200
N	1.52786000	-0.44508200	-0.17295000
C	-0.18081800	1.29887700	-0.47145600
N	-1.17780800	1.32258200	0.24014100
O	1.71932300	-1.56301500	0.26183400
C	-3.16287400	-0.07780000	0.35172900
H	-1.46032300	-0.28709400	1.53438400
N	2.43817100	0.54764800	-0.11556600
H	2.14766600	1.47803100	-0.37625700
C	3.71998400	0.33683200	0.53102300
H	4.17355300	-0.57877500	0.14799300
H	4.36957100	1.18325600	0.30931600
C	3.60751700	0.23724000	1.61463100
H	0.21268000	-0.07596700	-0.88290300
H	0.41581000	-0.05132700	-1.95663300
N	-4.30601900	-0.11175600	0.22172400

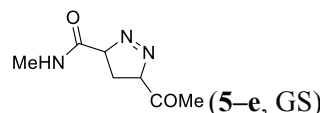
HF: -527.4800388

Sum of electronic and zero-point Energies: -527.331665

Sum of electronic and thermal Energies: -527.321917

Sum of electronic and thermal Enthalpies: -527.320973

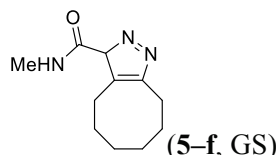
Sum of electronic and thermal Free Energies: -527.367764



C	1.53998500	0.02812500	0.76353500
C	0.42976400	1.04261500	0.53179600
H	-0.07941100	1.31200100	1.45808200
H	0.80357700	1.94547900	0.05227900
C	-1.99457700	0.42520900	-0.05532600
N	-0.09425300	-1.16059300	-0.25637800
N	0.95997500	-1.29715000	0.35703200
O	-2.42457200	1.47451400	0.38311900
C	2.76683200	0.21020200	-0.14552000
O	2.73387800	0.97902100	-1.07094200
H	1.87306800	-0.07484600	1.79979700
N	-2.77160300	-0.64501400	-0.32394200
H	-2.32089200	-1.51037600	-0.57848600
C	-4.19631300	-0.60156600	-0.06071800
H	-4.64659000	0.24645500	-0.58097400
H	-4.64841900	-1.52637500	-0.41896800
C	-4.39579200	-0.48936900	1.00893500
C	3.95667600	-0.65355100	0.17312500
H	4.37851500	-0.34308200	1.13484700
H	3.63453400	-1.69389300	0.27898100
H	4.70925900	-0.55758700	-0.60842300
C	-0.51215700	0.25943300	-0.38062800
H	-0.38238800	0.51979700	-1.43805300

HF: -587.8630569

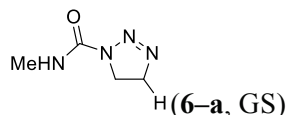
Sum of electronic and zero-point Energies: -587.676338  
 Sum of electronic and thermal Energies: -587.663773  
 Sum of electronic and thermal Enthalpies: -587.662829  
 Sum of electronic and thermal Free Energies: -587.717971



C	-0.80983100	1.15459500	-0.48570800
C	-0.16360000	0.05588100	-0.92044900
C	2.24494500	-0.40934100	-0.20423100
N	1.29390000	1.86065000	-0.58180900
N	0.13602500	2.21794400	-0.28616500
O	2.29992200	-1.61103700	-0.38144700
N	3.01376300	0.24744200	0.68318800
H	2.93601300	1.25230400	0.73076500
C	3.99446000	-0.46988600	1.47351400
H	4.67463900	-1.02674100	0.82402600
H	4.56228400	0.24894700	2.06380700
H	3.50421100	-1.18127100	2.14299700
C	1.27578800	0.46528400	-1.01722100
C	1.64263200	0.43098900	-2.05223800
C	-0.65010200	-1.30822600	-1.28337400
H	-0.58942100	-1.41764500	-2.37465900
H	0.06667000	-2.03299700	-0.88041200
C	-2.23483600	1.47430900	-0.14991800
H	-2.30014400	2.56598300	-0.13651300
H	-2.91118500	1.12925800	-0.93711800
C	-2.06060500	-1.64762900	-0.80320500
H	-2.28704100	-2.65931100	-1.15280600
H	-2.79130300	-0.99619000	-1.29322900
C	-2.69325200	0.93375400	1.21863400
H	-1.86353700	1.03380100	1.92961900
C	-3.49718300	1.57889300	1.58898900
H	-2.22941400	-1.58023300	0.73108600
H	-2.58638500	-2.55003500	1.09011700
H	-1.25036600	-1.42565600	1.20363800
C	-3.20559500	-0.50734500	1.22678200
H	-3.49818700	-0.74693300	2.25542100
H	-4.12646800	-0.56432800	0.62721600

HF: -668.6315593

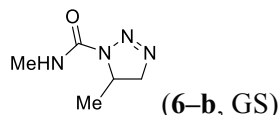
Sum of electronic and zero-point Energies: -668.353940  
 Sum of electronic and thermal Energies: -668.339680  
 Sum of electronic and thermal Enthalpies: -668.338736  
 Sum of electronic and thermal Free Energies: -668.395916



C	-2.53326200	-0.78123400	0.03722100
C	-1.05781100	-1.19613800	0.06329200
H	-0.73985500	-1.59526800	1.03213600
H	-0.81961100	-1.91679700	-0.72239200
C	0.92264600	0.41437200	-0.02605000
N	-1.35313100	1.12207700	-0.06703600
N	-2.50250500	0.69911500	0.06237300
O	1.33841400	1.54119500	0.08068100
H	-3.11206400	-1.13788100	0.88935900
N	1.72595300	-0.69753000	0.02383000
H	1.38239000	-1.54808700	-0.39291300
C	3.16445800	-0.48891200	0.01881400
C	3.42888500	0.18234100	0.83607800
H	3.65606800	-1.45001800	0.17269000
H	3.51204400	-0.04171800	-0.91797900
N	-0.43406800	0.10108000	-0.19374000
H	-3.04509900	-1.08384800	-0.88007400

HF: -451.2955779

Sum of electronic and zero-point Energies: -451.157637  
 Sum of electronic and thermal Energies: -451.148716  
 Sum of electronic and thermal Enthalpies: -451.147772  
 Sum of electronic and thermal Free Energies: -451.192089

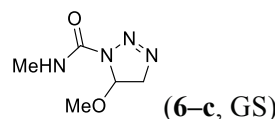


C	1.05636300	0.89493500	-0.33576000
C	2.45431500	0.30347700	-0.53558300
H	2.74068000	0.22053000	-1.58899500
H	3.23686300	0.84310000	0.00020800
N	1.16251800	-1.39282700	0.13499700
H	0.31134700	-0.36653200	-0.21901600
N	0.73530800	1.44891200	-1.22157400
N	2.34621200	-1.07409300	-0.00410500

C	0.94843600	1.74695800	0.92541500
H	1.55478100	2.65083900	0.81740100
H	-0.08522400	2.03869100	1.12168300
H	1.31971300	1.18073800	1.78537200
C	-1.05636700	-0.52276400	0.05673500
O	-1.52373100	-1.50170500	0.58230500
N	-1.80660600	0.56213800	-0.32968600
C	-1.43368500	1.13743100	-1.06903300
H	-3.25319700	0.43734600	-0.25948200
H	-3.69826000	1.41090900	-0.46847500
H	-3.63945600	-0.30464200	-0.96569600
H	-3.53246200	0.12661200	0.74738100

HF: -490.5954681

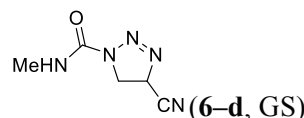
Sum of electronic and zero-point Energies: -490.429423  
 Sum of electronic and thermal Energies: -490.419283  
 Sum of electronic and thermal Enthalpies: -490.418339  
 Sum of electronic and thermal Free Energies: -490.465215



C	2.32052600	-0.18270100	-0.77646100
C	0.93392000	0.45234100	-0.84105100
H	0.58536300	0.64473400	-1.85557300
C	-1.20998100	-0.65010000	0.02677900
N	1.00714800	-1.46499500	0.48722700
N	2.19814400	-1.24932000	0.23675600
O	-1.75479600	-1.60703600	0.52672700
H	3.10675800	0.52265500	-0.50389700
N	-1.85527600	0.46641900	-0.41113300
C	-1.31946000	1.32217200	-0.45892000
H	-3.28508200	0.56206400	-0.17559900
H	-3.52083600	0.65666700	0.88937400
H	-3.66973600	1.42880700	-0.71403600
H	-3.77067600	-0.33849400	-0.55270800
N	0.17843300	-0.62124400	-0.22375800
H	2.58782500	-0.65945900	-1.72387700
O	0.80712500	1.68315800	-0.16849900
C	1.12140800	1.64608100	1.21601200
H	0.98593100	2.66063100	1.58908000
H	0.45371000	0.96609500	1.75815000
H	2.15859700	1.33455300	1.38486300

HF: -565.7883828

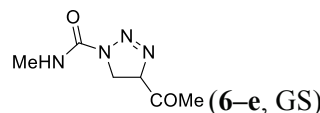
Sum of electronic and zero-point Energies: -565.617072  
 Sum of electronic and thermal Energies: -565.606111  
 Sum of electronic and thermal Enthalpies: -565.605167  
 Sum of electronic and thermal Free Energies: -565.654007



C	-1.99132300	0.01233000	0.69509500
C	-0.61992800	-0.68386100	0.70770100
H	-0.65043900	-1.64583300	0.19375800
C	1.56818500	0.34192100	-0.13951900
N	-0.52228800	1.48055100	-0.15701500
N	-1.69598800	1.40007500	0.21230500
O	2.18019200	1.34205300	-0.40813100
H	-2.45031500	0.08491700	1.68193300
N	2.14734300	-0.87088100	0.12352100
C	1.58927300	-1.69895400	-0.01569800
H	3.57930500	-0.99622600	-0.10283500
H	4.09075600	-0.19200400	0.42549900
H	3.91260600	-1.95490100	0.29513600
H	3.83336700	-0.92720900	-1.16500000
N	0.16116400	0.30657600	-0.03121900
C	-2.94558800	-0.62506100	-0.21970500
N	-3.67326500	-1.15683300	-0.93558400
H	-0.22945000	-0.81346500	1.72094500

HF: -543.508229

Sum of electronic and zero-point Energies: -543.371512  
 Sum of electronic and thermal Energies: -543.360967  
 Sum of electronic and thermal Enthalpies: -543.360023  
 Sum of electronic and thermal Free Energies: -543.409196



C	-1.56504900	0.06278900	0.77492100
C	-0.20576700	-0.63099900	0.77015700
H	0.19960500	-0.80036700	1.77131600
H	-0.26646100	-1.57406200	0.22009000
C	1.96894300	0.38979400	-0.13365800
N	-0.12116000	1.53367400	-0.10746800
N	-1.29275100	1.43637800	0.27511200



O	2.58038300	1.37123600	-0.47449700
C	-2.61051100	-0.60554500	-0.13453000
O	-2.43031900	-1.71741900	-0.55970800
H	-2.01269200	0.15320900	1.76930100
N	2.55285800	-0.81894600	0.14006500
H	1.97707700	-1.64492800	0.09281700
C	3.96583200	-0.97105300	-0.16452200
H	4.52040900	-0.16540300	0.31673500
H	4.30751300	-1.92732600	0.23256700
H	4.16090600	-0.92712200	-1.24069700
C	-3.84002100	0.20581000	-0.43391500
H	-4.26196200	0.61165800	0.49011700
H	-3.55442900	1.06382500	-1.04959800
H	-4.57058400	-0.41163700	-0.95458300
N	0.57813100	0.37558600	0.05727100

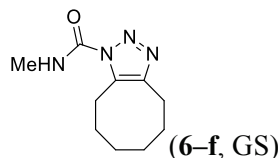
HF: -603.8940748

Sum of electronic and zero-point Energies: -603.718652

Sum of electronic and thermal Energies: -603.706355

Sum of electronic and thermal Enthalpies: -603.705410

Sum of electronic and thermal Free Energies: -603.759099



C	0.94539600	-1.05620200	-0.52884700
C	0.00570700	-0.06352700	-0.36292000
C	-2.42258800	-0.27129800	0.39412200
N	-0.86929500	-2.06743300	0.12246200
N	0.35123300	-2.25431300	-0.22685300
O	-2.98052300	-0.63728000	1.39096600
H	-2.91325400	0.62035800	-0.49809100
H	-2.49900400	0.64736700	-1.41619100
C	-4.25211400	1.14872400	-0.30612600
H	-4.34136600	1.53380000	0.71052500
H	-4.41335300	1.96135100	-1.01440000
C	-5.01354500	0.37691700	-0.45058300
H	0.06644700	1.42993000	-0.45565800
H	-0.41280200	1.77657100	-1.37962500
H	-0.51679500	1.85610900	0.36948600
C	2.40157700	-1.04728500	-0.88616700
H	2.62096000	-2.06330000	-1.22598000
H	2.60357000	-0.38388500	-1.73256100
C	1.49337900	1.97885800	-0.40376000
H	1.42354700	3.06794300	-0.48034200
C	2.03665500	1.65529500	-1.29665700
C	3.33324400	-0.71539800	0.29441500
H	2.94347800	-1.21916400	1.18734900
H	4.31386000	-1.15941700	0.09179000
C	2.27973300	1.59052900	0.86689800
H	2.57000900	2.50386200	1.39451800
H	1.63090100	1.03556700	1.55695800
C	3.54583100	0.76979600	0.59527000
H	4.20568900	0.83843200	1.46726600
H	4.09197500	1.23506400	-0.23692100
N	-1.10857800	-0.74847500	0.04309400

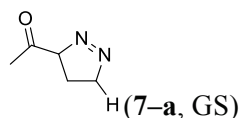
HF: -684.6954104

Sum of electronic and zero-point Energies: -684.428455

Sum of electronic and thermal Energies: -684.414437

Sum of electronic and thermal Enthalpies: -684.413493

Sum of electronic and thermal Free Energies: -684.469863



C	-2.02068500	0.36165000	-0.37989900
C	-1.10980800	0.93156900	0.71063300
H	-0.72632500	1.91922900	0.45679600
H	-1.62523300	0.97727000	1.67109600
C	1.27262200	0.30165200	-0.02790600
N	-0.54217500	-1.30304900	0.02594500
N	-1.58991600	-1.04626400	-0.55936200
O	1.31779500	1.33529600	-0.64460500
H	-1.89488800	0.84840600	-1.35208000
C	0.00795900	-0.10047400	0.74463100
H	0.30044300	-0.43600400	1.74376900
C	2.41119700	-0.68183200	0.01603100
H	2.79269000	-0.74736900	1.04037200
H	2.04554400	-1.67583200	-0.25761100
H	3.20701700	-0.36109900	-0.65498900
H	-3.08467900	0.36283100	-0.13753700

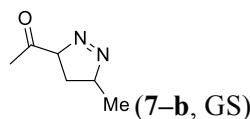
HF: -379.9060841

Sum of electronic and zero-point Energies: -379.774892

Sum of electronic and thermal Energies: -379.767093

Sum of electronic and thermal Enthalpies: -379.766149

Sum of electronic and thermal Free Energies: -379.808351



C	1.59681700	-0.23296800	-0.35640500
C	0.71968100	-0.80733000	0.76056500
H	0.40999600	-1.83246300	0.55836600
H	1.24578500	-0.76722800	1.71813100
C	-1.68104700	-0.35298000	-0.03532800
N	0.02559700	1.36667000	0.02008000
N	1.08567600	1.15104300	-0.55889400
O	-1.63841100	-1.38805400	-0.65008800
H	1.41224300	-0.74237000	-1.31004900
C	-0.46394300	0.14545600	0.75508900
H	-0.79908600	0.48201200	1.74030400
C	-2.89154700	0.54143100	-0.01123300
H	-3.30261100	0.56290100	1.00363300
H	-2.59631000	1.56408000	-0.26327900
H	-3.64366100	0.17017100	-0.70614800
C	3.08895000	-0.19403400	-0.07413600
H	3.47633200	-1.20829300	0.05124300
H	3.62504000	0.28672800	-0.89520300
H	3.28718600	0.36746200	0.84408600

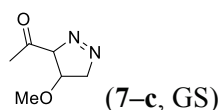
HF: -419.2066328

Sum of electronic and zero-point Energies: -419.047318

Sum of electronic and thermal Energies: -419.038165

Sum of electronic and thermal Enthalpies: -419.037220

Sum of electronic and thermal Free Energies: -419.082311



C	2.03994100	-0.17901400	-0.69458600
C	0.64735700	0.39618800	-0.94034100
C	-1.56491300	-0.40336200	0.10793800
N	0.67827400	-1.48123500	0.54826500
N	1.86003200	-1.16351100	0.40359200
O	-1.86466700	-0.56347000	1.26069700
H	2.79547100	0.55890400	-0.42012600
C	-0.19405300	-0.79092500	-0.43441500
H	-0.34651200	-1.50569600	-1.25530900
C	-2.49534400	0.22185900	-0.90277700
H	-2.09137800	1.20024100	-1.18453000
H	-2.55627300	-0.38934600	-1.80817900
H	-3.48403100	0.34485200	-0.46201800
H	2.40190300	-0.73728700	-1.56495100
O	0.38451000	1.60052700	-0.26362000
C	0.67506500	1.62041500	1.12709600
H	1.74295500	1.46078700	1.31798600
H	0.39894200	2.61548500	1.47572300
H	0.09981400	0.86932600	1.67855400
H	0.46391000	0.60854600	-1.99425200

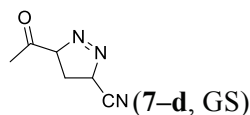
HF: -494.3877786

Sum of electronic and zero-point Energies: -494.223314

Sum of electronic and thermal Energies: -494.213317

Sum of electronic and thermal Enthalpies: -494.212372

Sum of electronic and thermal Free Energies: -494.258951



C	-1.30594300	-0.20462000	0.36192100
C	-0.48717800	-0.71740000	-0.82801900
H	-0.21048200	-1.76317400	-0.70479800
H	-1.03580600	-0.58192100	-1.76068900
C	1.90313400	-0.37384100	0.03500900
N	0.26353900	1.39229800	0.02811800
N	-0.79018400	1.18582100	0.61756300
O	1.75587100	-1.37445000	0.68763000
C	-2.75152600	-0.17143000	0.14194800
H	-1.10231900	-0.76900800	1.27810900
C	0.72192200	0.20451400	-0.76407700
H	1.07577700	0.57470700	-1.72912800
C	3.18801500	0.40239400	-0.02715400
H	3.59675800	0.33822000	-1.04117100
H	2.98829300	1.45857800	0.17732600
H	3.90480900	-0.00181500	0.68612500
N	-3.88400300	-0.16349700	-0.06347900

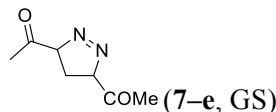
HF: -472.1223214

Sum of electronic and zero-point Energies: -471.992326

Sum of electronic and thermal Energies: -471.982901

Sum of electronic and thermal Enthalpies: -471.981957

Sum of electronic and thermal Free Energies: -472.028460



C	-0.94486800	-0.11725400	0.37523000
C	-0.02379000	-1.07743800	-0.36749800
H	0.30339700	-1.90261100	0.26310900
H	-0.53249400	-1.47270000	-1.24807400
C	2.34690600	-0.26043600	0.20160800
N	0.61664000	1.23147100	-0.55945600
N	-0.45290300	1.25059100	0.04194600
O	2.28154800	-0.89594000	1.22199300
C	-2.43299000	-0.22457600	0.03419600
O	-2.84624900	-1.15986000	-0.60151800
H	-0.86147200	-0.19704300	1.46752000
C	1.13546500	-0.16579600	-0.74036100
H	1.48057800	-0.24641700	-1.77478400
C	-3.32042200	0.88169800	0.54005100
H	-3.13497500	1.06644300	1.60196600
H	-3.06904100	1.80658200	0.01242200
H	-4.36416100	0.62018000	0.37070500
C	3.56802000	0.51293400	-0.21514400
H	3.98031000	0.07172700	-1.12861100
H	3.28455200	1.54296300	-0.45140000
H	4.31483600	0.48805400	0.57742100

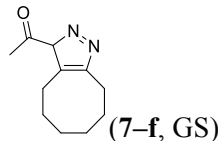
HF: -532.5046344

Sum of electronic and zero-point Energies: -532.336732

Sum of electronic and thermal Energies: -532.326063

Sum of electronic and thermal Enthalpies: -532.325119

Sum of electronic and thermal Free Energies: -532.375126



C	0.36002700	-1.13741900	-0.45012500
C	-0.24527300	0.01136700	-0.80027700
C	-2.42785900	0.62159700	0.41669400
N	-1.78913600	-1.64454600	-0.16903500
N	-0.63696700	-2.10481000	-0.07078100
O	-1.83325400	1.43731200	1.07021000
C	-1.70238000	-0.24339600	-0.63107500
H	-2.26937300	-0.17947000	-1.57068200
C	0.29655800	1.32804700	-1.25153200
H	0.10028700	1.44200300	-2.32637900
C	-0.28279500	2.11240100	-0.74905400
H	1.78445300	-1.58361200	-0.33064700
H	1.75859900	-2.67697400	-0.32459500
C	2.36580600	-1.28616900	-1.20778400
H	1.78247700	1.55130900	-0.96913200
C	2.04031900	2.54466900	-1.34876700
H	2.38301100	0.84822900	-1.55524600
C	2.47422400	-1.09414800	0.95785800
H	1.74719200	-1.13349900	1.77840300
C	3.26837600	-1.80406000	1.21275300
C	2.15029500	1.45500700	0.52849800
H	2.63443600	2.38855000	0.83092100
H	1.23459700	1.38090500	1.12937400
C	3.09505000	0.30201000	0.88746600
H	3.54573100	0.50999800	1.86451300
H	3.92451200	0.28901600	0.16638400
C	-3.90356500	0.36072400	0.55755400
H	-4.41392000	0.67670100	-0.35841600
H	-4.07641400	-0.71211400	0.67628800
H	-4.29564200	0.91789100	1.40762400

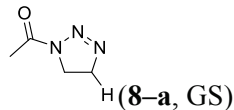
HF: -613.2727407

Sum of electronic and zero-point Energies: -613.013904

Sum of electronic and thermal Energies: -613.000760

Sum of electronic and thermal Enthalpies: -612.999816

Sum of electronic and thermal Free Energies: -613.054056



C	0.75519700	1.17318700	-0.00010400
C	2.17938100	0.60216000	0.00011100
H	2.75961200	0.87220900	-0.88386500
H	2.75917700	0.87183800	0.88449500
N	0.80925800	-1.17719600	-0.00003500
N	-0.01418100	-0.07009400	0.00031000
H	0.53988200	1.76925100	-0.88993600
C	2.00077300	-0.86850700	-0.00020900
N	-1.39562900	-0.22603100	0.00004000
O	-1.92707500	-1.30555500	-0.00000800
H	0.53980700	1.76985200	0.88929300
C	-2.15748300	1.07990200	-0.00007000

H	-1.91022100	1.67441900	-0.88425400
H	-3.22069500	0.84790200	-0.00036800
H	-1.91070800	1.67424100	0.88437200

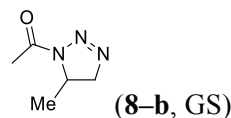
HF: -395.9489776

Sum of electronic and zero-point Energies: -395.828780

Sum of electronic and thermal Energies: -395.821069

Sum of electronic and thermal Enthalpies: -395.820125

Sum of electronic and thermal Free Energies: -395.861822



C	-0.80814500	0.79488500	0.38220200
C	-2.09438000	-0.02851600	0.50820000
H	-2.38640700	-0.22792200	1.54368000
H	-2.94417300	0.41530500	-0.01376500
N	-0.55086600	-1.44137400	-0.28611100
N	0.12959000	-0.29985300	0.10180100
H	-0.55161800	1.27772200	1.32679500
N	-1.76535400	-1.33198200	-0.10918200
C	-0.87227200	1.80691800	-0.75686700
H	-1.64164700	2.55591700	-0.54860300
H	0.07965200	2.32460000	-0.89160100
H	-1.12621100	1.29785200	-1.69180100
C	1.51896300	-0.28555500	0.02741000
C	2.18098600	1.02349600	0.40026400
H	1.62386200	1.60013000	1.14022200
H	3.17428800	0.78861900	0.78092100
H	2.29739400	1.63182600	-0.50112500
O	2.15379400	-1.25236900	-0.30719300

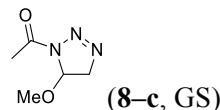
HF: -435.2483825

Sum of electronic and zero-point Energies: -435.100454

Sum of electronic and thermal Energies: -435.091482

Sum of electronic and thermal Enthalpies: -435.090537

Sum of electronic and thermal Free Energies: -435.134744



C	-1.88030100	0.48738300	-0.82648800
C	-0.65943300	-0.42984100	-0.81668000
H	-0.35113700	-0.75242700	-1.81029500
C	1.65494000	0.25835400	0.03140200
N	-0.35690700	1.52476200	0.42956500
N	-1.55942000	1.54475000	0.15197900
O	2.29743800	0.97131900	0.75393300
H	-2.80505500	-0.02285300	-0.55450900
N	0.30056900	0.50020600	-0.23652500
H	-2.01520200	0.97168700	-1.79785900
O	-0.81012700	-1.60561000	-0.07105600
C	-1.14140100	-1.42164000	1.29637100
H	-1.22422300	-2.41889100	1.72677800
H	-0.36144000	-0.86170900	1.82522100
H	-2.09765400	-0.89823700	1.41469000
C	2.22232800	-0.93785700	-0.69422700
H	1.66105000	-1.84254800	-0.44944300
H	2.16427500	-0.78243900	-1.77582100
H	3.26440100	-1.04467000	-0.39918400

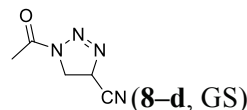
HF: -510.4391094

Sum of electronic and zero-point Energies: -510.285655

Sum of electronic and thermal Energies: -510.276023

Sum of electronic and thermal Enthalpies: -510.275079

Sum of electronic and thermal Free Energies: -510.320694



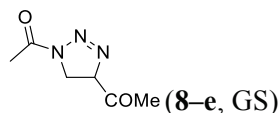
C	-1.57996200	0.08536400	0.68721500
C	-0.30736500	-0.78057300	0.66560500
H	-0.41093300	-1.66054900	0.03009500
C	1.99157500	-0.01266600	-0.19566900
N	0.08122600	1.42411600	-0.02172600
N	-1.11288800	1.45156300	0.28134400
O	2.69155300	0.87884200	-0.58789900
H	-2.02632900	0.16552800	1.67969200
N	0.63698000	0.18352800	0.10422200
C	-2.60925600	-0.37588300	-0.25015200
N	-3.39845800	-0.77534000	-0.98642700
H	-0.01085900	-1.08489800	1.67213500
C	2.46040000	-1.43237300	0.01064200
H	2.29614500	-1.75401000	1.04306200
H	1.91639300	-2.11564300	-0.64809100
H	3.52280000	-1.47144400	-0.22143100

HF: -488.1612448

Sum of electronic and zero-point Energies: -488.042679

Sum of electronic and thermal Energies: -488.033317

Sum of electronic and thermal Enthalpies: -488.032373  
 Sum of electronic and thermal Free Energies: -488.078613



C	-1.15330700	0.05845200	0.77031300
C	0.13146600	-0.76402700	0.71598900
H	0.47016300	-1.08627200	1.70306800
H	0.01072200	-1.63090800	0.06250400
C	2.37921100	0.06971200	-0.21028600
N	0.43180200	1.44746100	-0.00253800
N	-0.75451800	1.42454600	0.33938300
O	3.04084900	0.97130400	-0.65074800
C	-2.27282600	-0.45597400	-0.15059100
O	-2.20597200	-1.55666900	-0.63270400
H	-1.57934700	0.14318700	1.77514800
C	-3.42227500	0.48416900	-0.38398300
H	-3.78309900	0.88830200	0.56624600
H	-3.06716300	1.33626200	-0.97131100
H	-4.22072300	-0.03520800	-0.91190400
N	1.04022100	0.23106200	0.14691400
C	2.90067700	-1.33098100	0.00607300
H	2.80294300	-1.62547400	1.05492100
H	2.33804800	-2.04860500	-0.59793400
H	3.94922500	-1.34794600	-0.28453100

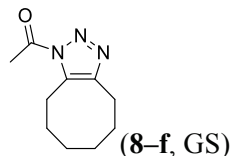
HF: -548.5470119

Sum of electronic and zero-point Energies: -548.390005

Sum of electronic and thermal Energies: -548.379707

Sum of electronic and thermal Enthalpies: -548.378763

Sum of electronic and thermal Free Energies: -548.426960



C	0.47605900	-1.03004300	-0.49220100
C	-0.32042000	0.08044900	-0.35476600
C	-2.81466900	0.17101600	0.27450600
N	-1.46893400	-1.78554400	0.13073500
N	-0.28455500	-2.13612600	-0.19005900
O	-3.60671300	-0.37815200	0.97749500
C	-0.01839700	1.54545800	-0.44750100
H	-0.46082500	1.97073700	-1.35531900
H	-0.48950900	2.05580000	0.40090500
C	1.91778500	-1.24332300	-0.84558400
H	1.97628000	-2.28396900	-1.17640100
H	2.21706500	-0.62886000	-1.69938200
H	1.47822700	1.86330900	-0.42318500
C	1.57557300	2.94811800	-0.52611400
H	1.95467000	1.44096300	-1.31227000
C	2.89416000	-1.05061000	0.32894600
H	2.43412700	-1.47430900	1.22997300
H	3.79141600	-1.64601300	0.12944100
C	2.20526800	1.39235100	0.85494400
H	2.62679400	2.26501400	1.36254800
H	1.48256300	0.95341700	1.55504600
C	3.33478200	0.38736800	0.60486000
H	3.99546500	0.37262000	1.47853300
H	3.94622100	0.74764600	-0.23400400
N	-1.53510000	-0.43793100	0.03731900
C	-3.09476400	1.46313600	-0.44696500
H	-2.64584100	2.30501700	0.08474300
H	-2.70266100	1.44570900	-1.46499600
H	-4.17568900	1.59585900	-0.45695400

HF: -629.3420891

Sum of electronic and zero-point Energies: -629.092803

Sum of electronic and thermal Energies: -629.080253

Sum of electronic and thermal Enthalpies: -629.079309

Sum of electronic and thermal Free Energies: -629.132086

## References

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