SUPPORTING INFORMATION

Transition State Analysis of an Enantioselective Michael Addition by a Bifunctional Thiourea Organocatalyst

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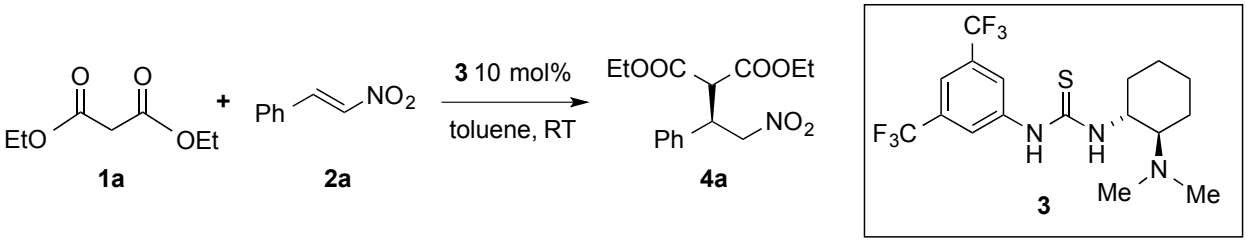
1. Experimental Section

A. General Information

All reagents were measured open to the atmosphere, and reactions were run in sealed flasks. All solvents and commercial reagents were used as provided, unless otherwise noted. Flash column chromatography was performed employing 40-63 μm silica gel (SiliaFlash P60 from Silicycle). Thin-layer chromatography (TLC) was performed on silica gel 60 F_{254} plates (EMD). Organic solutions were concentrated using a Büchi rotary evaporator. ^{1}H and ^{13}C NMR spectra were recorded in $CDCl_3$ (except where noted) on a Bruker Avance III 600, a Bruker Avance III 400, or a Bruker AC 300 instrument. Data for ^{1}H NMR are reported as follows: chemical shift (δ ppm), multiplicity (s = singlet, br s = broad singlet, d = doublet, t = triplet, dd = doublet of doublets, m = multiplet), coupling constant (Hz), integration, and assignment. Data for ^{13}C are reported in terms of chemical shift. Spectra were processed in TopSpin™.

B. ^{13}C KIE experiments

Experimental sample preparation



To a well stirred solution containing 1.2698g (8mmol) of trans-β-nitrostyrene (**2a**), 1.6073g (1.25equiv., 10mmol) of diethyl malonate (**1a**) and dry toluene (16mL) was added 0.0662g (0.16mmol) of thiourea-catalyst (**3**) under nitrogen. The reaction was monitored via ^{1}H NMR analysis until it reached ~80% conversion. After reaching the desired conversion, the reaction mixture was quenched using flash chromatography (5:1 hexanes/ethyl acetate eluent). The fractions were collected and concentrated *in vacuo*. This crude mixture was purified by flash chromatography eluting 5% ethyl acetate in hexanes. By this procedure, two identical reactions were taken to 77 ± 2% and 68 ± 2% conversion based on ^{1}H NMR analysis, comparing the alkene proton of nitrostyrene and the alpha carbons of diethyl malonate to the doublet peak of the product (as shown in the below spectrum).

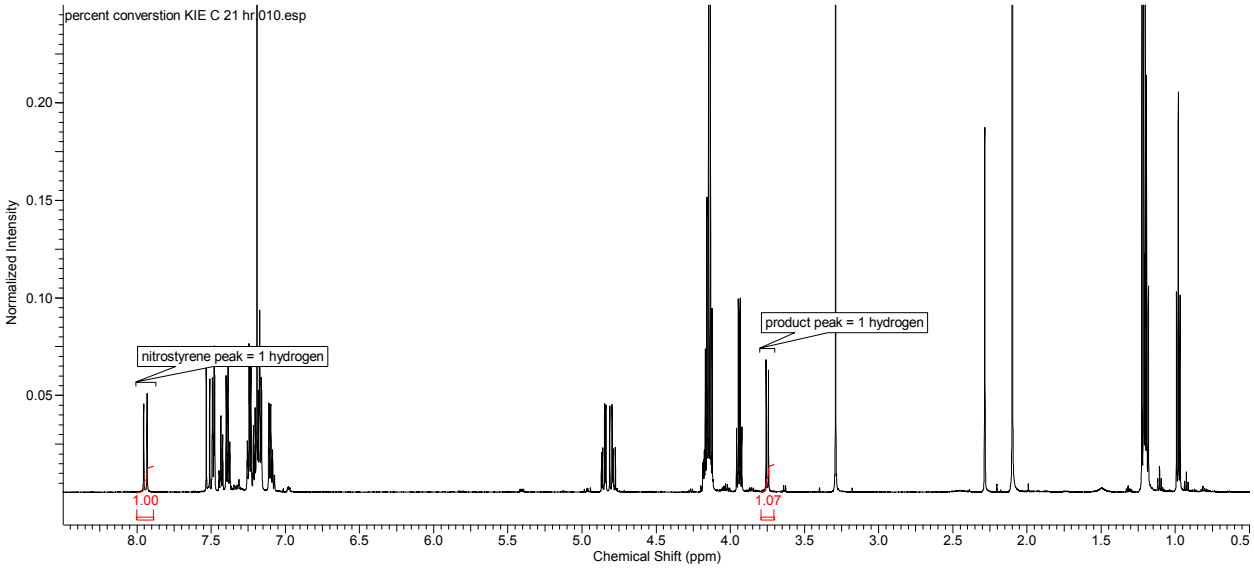
C. ^{13}C Sample preparation for NMR analysis

The recovered starting material (nitrostyrene or diethyl malonate) was carefully weighed and placed into a small dram vial where it was then dissolved in HPLC grade deuterated chloroform ($CDCl_3$). This mixture was then pipetted into a clean NMR tube and filled with $CDCl_3$ to a height of five centimeters.

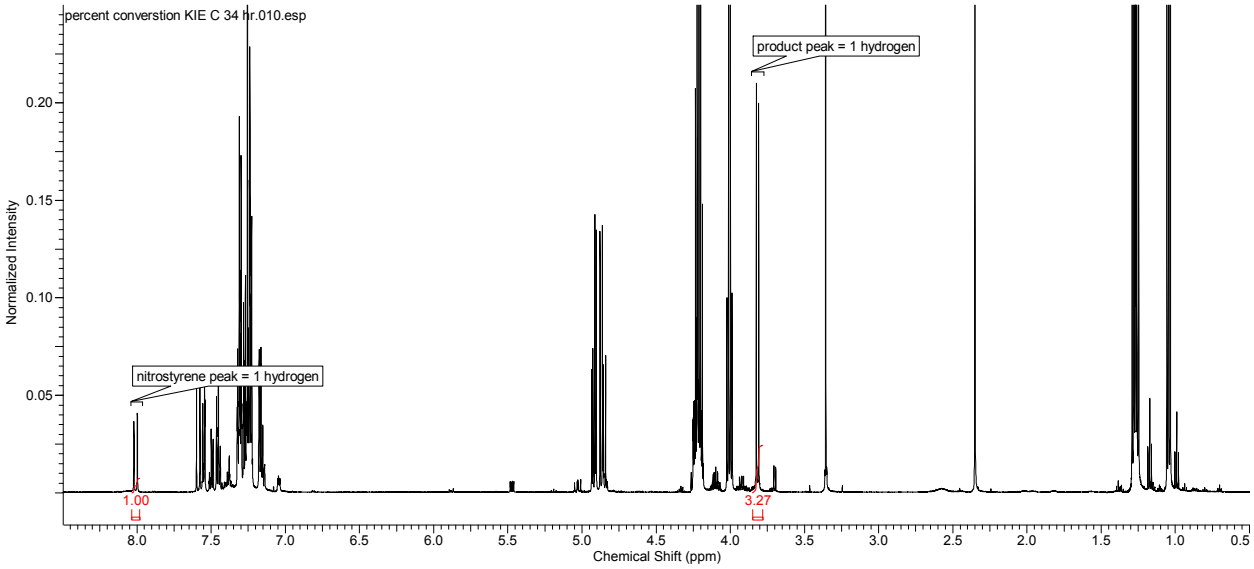
An identical mass of material was withdrawn from the bottle used for the initial experiment and also placed into a clean NMR and filled with $CDCl_3$ to a height of five centimeters.

NMR Spectra of samples analyzed for KIEs

Determination of percent conversion via ^{1}H NMR

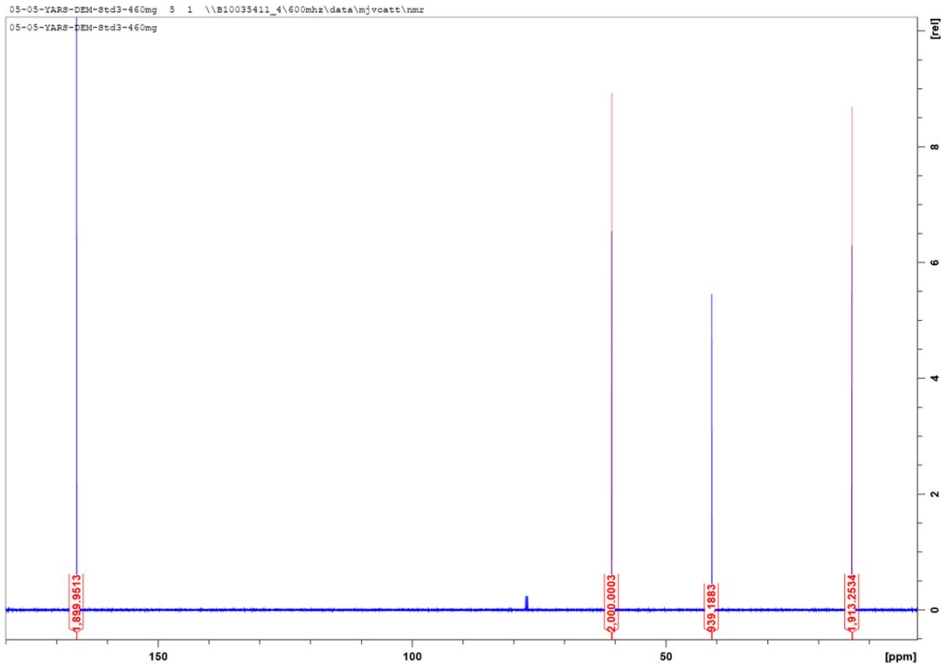


21hrs: 52% conversion

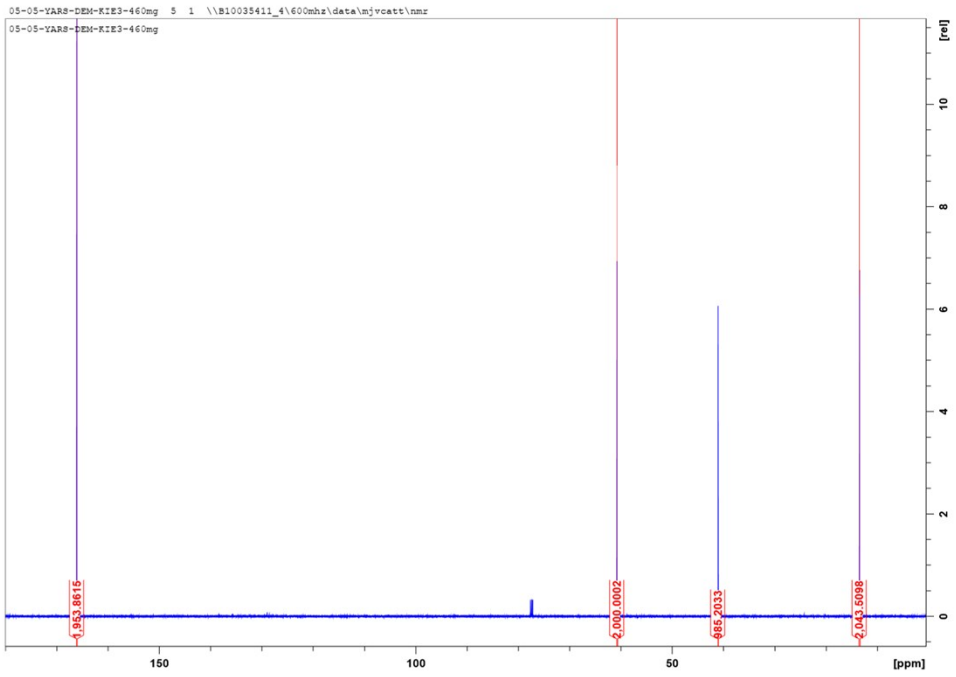


34hrs: 77% conversion

Determination of isotopic enrichment of diethylmalonate

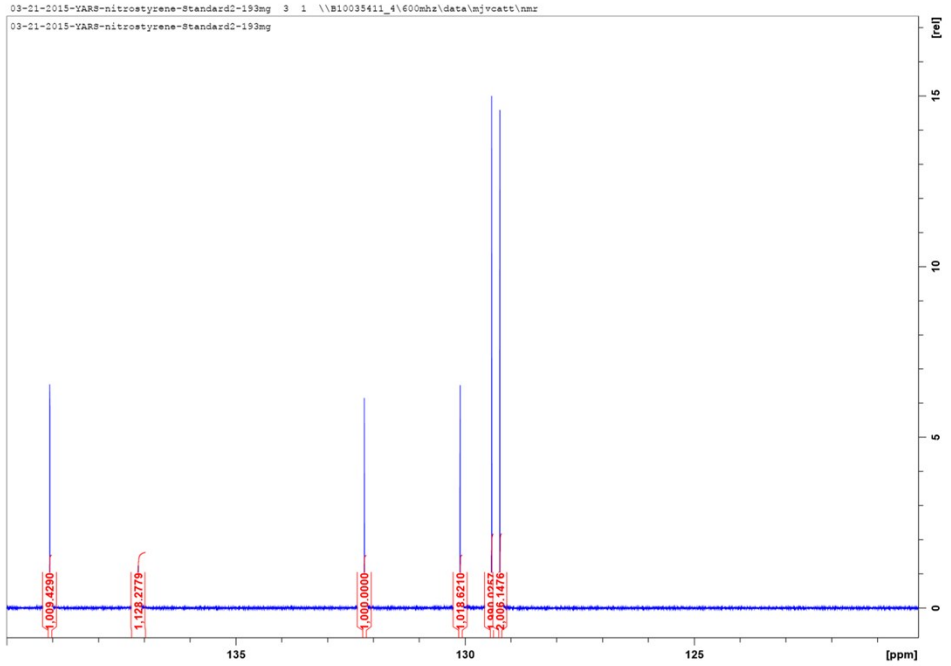


Standard



Experimental

Determination of isotopic enrichment of nitrostyrene



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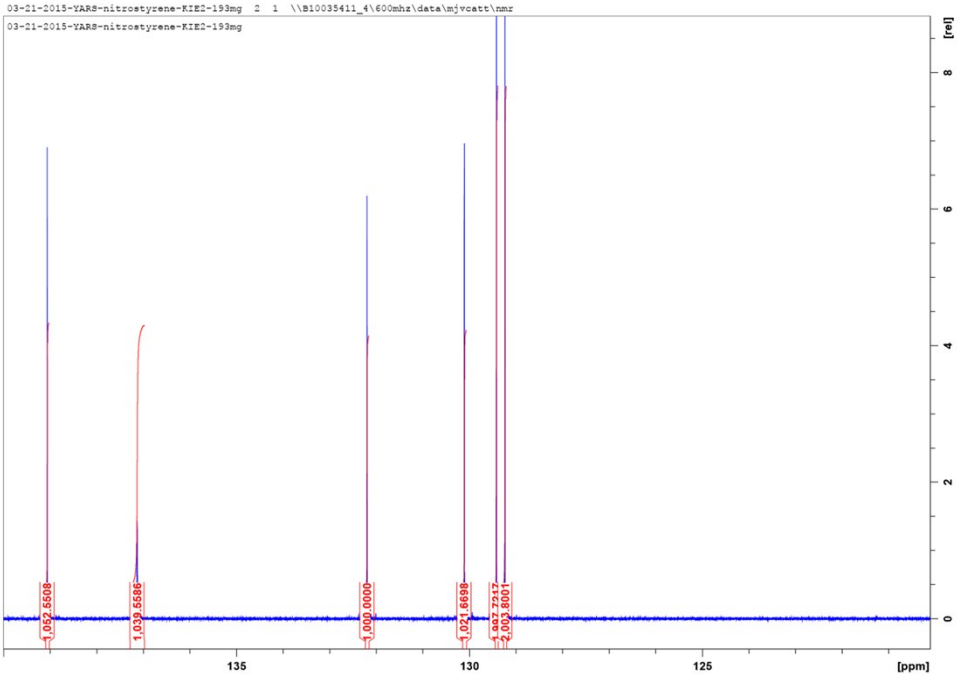


Experimental

Integration data and KIE determination

Diethylmalonate KIE determination

The methylene peak was used as the standard carbon for these samples and integrated to a value of 2000. The relative integrals of all other peaks were then recorded in the tables shown below. The KIE was calculated in the standard way using the average integration of six separate free inductance decay measurements.[1]

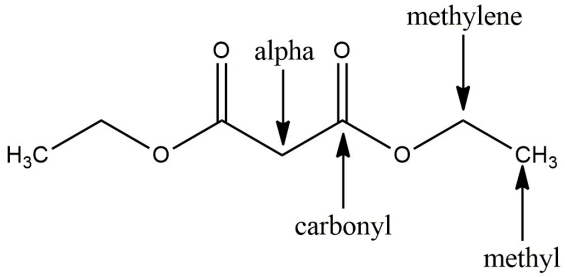


Table S 1. NMR integrations for KIE determination of diethyl malonate

First Standard										
peak	**fid1**	**fid2**	**fid3**	**fid4**	**fid5**	**fid6**	**average**	**stddev**	**cuts**	
carbonyl	1955.72	1957.43	1956.35	1954.83	1955.21	1963.02	1957.09	3.05	6	
methylene	2000.00	2000.00	2000.00	2000.00	2000.00	2000.00	2000.00	0.00	5	
alpha	975.39	969.35	976.79	976.63	980.08	981.27	976.58	4.20	4	
methyl	2042.51	2039.39	2053.60	2041.85	2037.36	2044.75	2043.24	5.68	7	
First Experimental									%Conv:	0.65
peak	**fid1**	**fid2**	**fid3**	**fid4**	**fid5**	**fid6**	**average**	**stddev**	**KIE**	**stdev**
carbonyl	1977.72	1973.59	1972.33	1972.52	1978.64	1968.92	1973.96	3.64	**1.008**	0.002
methylene	2000.00	2000.00	2000.00	2000.00	2000.00	2000.00	2000.00	0.00	**1.000**	0.000
alpha	1009.53	1006.64	1004.95	1003.08	1011.88	1007.97	1007.34	3.17	**1.030**	0.005
methyl	2026.56	2027.53	2034.53	2032.49	2024.33	2032.18	2029.60	4.02	**0.994**	0.003

Second Standard										
peak	**fid1**	**fid2**	**fid3**	**fid4**	**fid5**	**fid6**	**average**	**stddev**	**cuts**	
carbonyl	1983.13	1977.25	1983.91	1984.04	1982.92	1981.79	1982.17	2.54	3	
methylene	2000.00	2000.00	2000.00	2000.00	2000.00	2000.00	2000.00	0.00	5	
alpha	981.78	978.38	980.62	981.38	978.01	978.67	979.81	1.65	4	
methyl	2038.38	2035.10	2044.18	2037.91	2032.89	2040.05	2038.09	3.92	7	
Second Experimental									%Conv:	0.65
peak	**fid1**	**fid2**	**fid3**	**fid4**	**fid5**	**fid6**	**average**	**stddev**	**KIE**	**stdev**
carbonyl	1984.44	1982.42	1986.35	1981.03	1985.91	1985.50	1984.28	2.12	**1.001**	0.002
methylene	2000.00	2000.00	2000.00	2000.00	2000.00	2000.00	2000.00	0.00	**1.000**	0.000
alpha	1012.13	1014.95	1015.49	1014.68	1016.88	1011.52	1014.28	2.05	**1.034**	0.003
methyl	2044.99	2046.16	2052.75	2049.77		2046.38	2048.01	3.19	**1.006**	0.002

Nitrostyrene KIE determination

The *para*-carbon peak of the aromatic ring was used as the standard carbon for these samples and integrated to a value of 1000. The relative integrals of all other peaks were then recorded in the tables shown below. The KIE was calculated in the standard way using the average integration of six separate free inductance decay measurements.[1]

Table S 2. NMR integrations for KIE determination of *β*-nitrostyrene

First Standard										
peak	**fid1**	**fid2**	**fid3**	**fid4**	**fid5**	**fid6**	**average**	**stddev**	**cuts**	
alpha	1023.69	1022.91	1029.27	1026.76	1028.20	1026.60	1026.24	2.49	4	
beta	1068.94	1063.96	1075.94	1062.22	1067.58		1067.73	5.32	22	
para	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	0.00	3	
ipso	1030.87	1031.37	1027.37	1034.06	1034.10	1027.77	1030.92	2.92	4	
First Experimental									%Conv:	80%
peak	**fid1**	**fid2**	**fid3**	**fid4**	**fid5**	**fid6**	**average**	**stddev**	**KIE**	**stdev**
alpha	1075.80	1073.58	1067.41	1074.15	1070.11	1077.49	1073.09	3.72	**1.029**	0.004
beta	1073.16	1060.05	1071.91	1066.47	1061.47	1062.26	1065.89	5.59	**0.999**	0.007
para	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	0.00	**1.000**	0.000
ipso	1022.83	1026.48	1028.23	1029.80	1024.70	1023.71	1025.96	2.71	**0.997**	0.004

Second Standard										
peak	**fid1**	**fid2**	**fid3**	**fid4**	**fid5**	**fid6**	**average**	**stddev**	**cuts**	
alpha	1036.14	1032.84	1033.75	1035.32	1034.99	1033.84	1034.48	1.21	7	
beta	1045.37	1039.98	1041.98	1039.08	1040.97	1041.36	1041.46	2.17	4	
para	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	0.00	5	
ispso	996.05	993.09	995.12	992.31	993.89	993.56	994.00	1.37	3	
Second Experimental									%Conv:	0.71
peak	**fid1**	**fid2**	**fid3**	**fid4**	**fid5**	**fid6**	**average**	**stddev**	**KIE**	**stdev**
alpha	1072.69	1076.17	1073.38	1070.86	1070.95	1072.48	1072.75	1.95	**1.029**	0.002
beta	1043.04	1043.57	1037.80	1039.07	1037.73	1039.70	1040.15	2.56	**0.999**	0.003
para	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	1000.00	0.00	**1.000**	0.000
ipso	985.16	985.61	986.74	985.68	985.39	985.74	985.72	0.55	**0.993**	0.001

2. Theoretical Section

A. Methodology

Given the size of the system (89 atoms), all calculations were first performed using the B3LYP/6-31G* level of theory as implemented in the *Gaussian09*.[2] The default convergence criteria (Maximum force threshold – 4.5×10^{-4}; RMS force threshold – 3×10^{-4}; Maximum displacement threshold – 1.8×10^{-3}; RMS displacement threshold – 1.2×10^{-3}) were used for transition state and ground state optimizations. All transition structures were characterized by a single imaginary frequency and all ground states were confirmed to be minima (no imaginary frequency). Calculations that are discussed but not shown in the manuscript are included. Detailed discussions and predicted KIEs are included wherever relevant.

Almost all calculations performed at B3LYP/6-31G* were recalculated using a B3LYP/6-31+G**/PCM(toluene). The trends in relative energies of the computed transition states were very similar in both these approaches. We have, therefore, included only the geometries and energies of the computations from the B3LYP/6-31+G**/PCM(toluene) calculations in the SI (exceptions are noted). B3LYP/6-31+G**/PCM(toluene) effectively describes the energies and aids in the prediction of KIEs in various bifunctional thiourea-catalyzed reactions. Finally, single point calculations were performed for all transition structures discussed in the manuscript using the B3LYP-D3(BJ)/6-311++G**/PCM(toluene) level of theory. The relative energies in Figure 3 (manuscript) and the absolute free energy barriers discussed in the manuscript are from these high-level single point energy calculations.

The nomenclature for all calculations is retained from the paper. The geometries of all calculations, including those omitted due to their lack of illustrative power can be found below in the geometries section.

B. Transition state analysis

C—C bond formation step

As mentioned in the manuscript, several other binding modes for the C—C bond formation were suggested for similar catalysts and reaction.[3–5] To lend increased credence for the transition state proposed in our manuscript, these binding modes were each explored for they system studied. Binding modes A, B, Zhong, Wong, and Wong′ are all proposed in the literature.

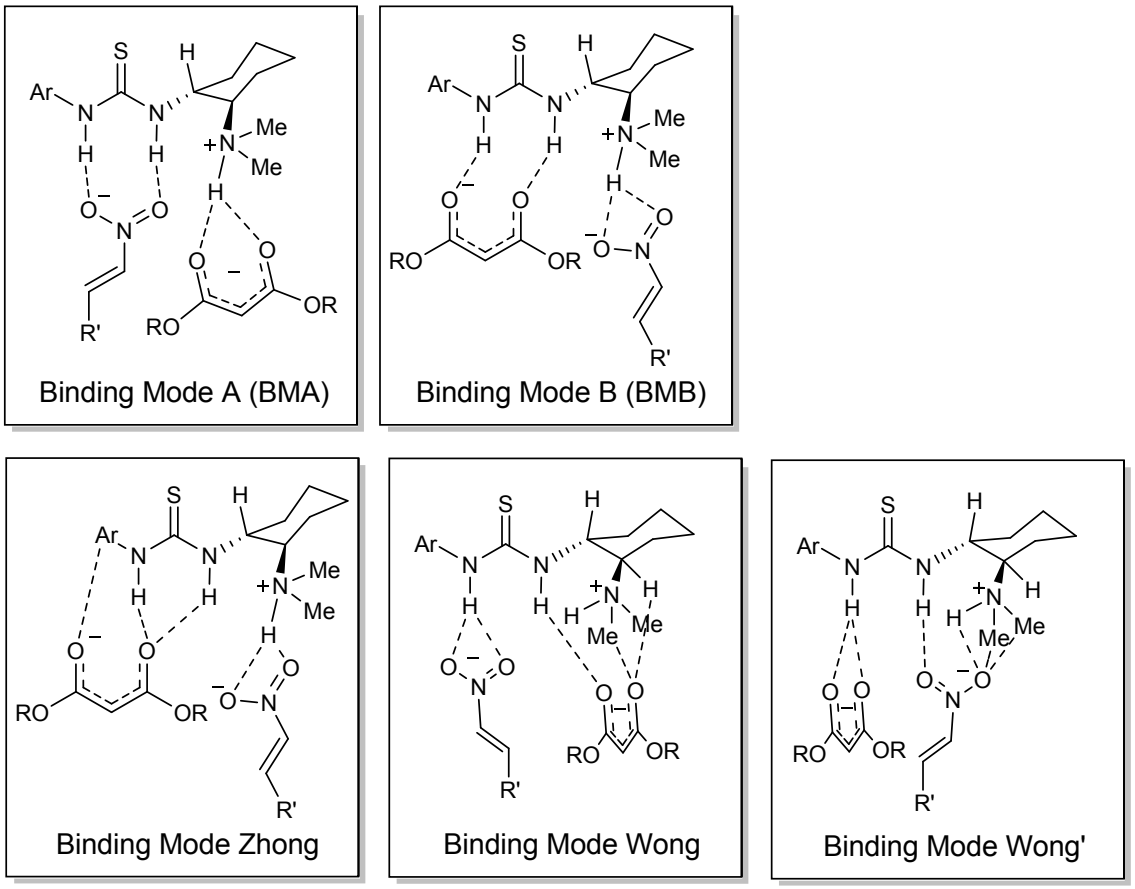


Figure S 1. Explored binding modes

Based on several NMR, crystallographic, and computational studies on similar systems, it has been brought to our attention that the classic orientation of the thiourea moiety ("*anti,anti*") may not, in reality, be the lowest energy conformation.[6–11] Rotating the N—C σ-bond of the thioamide could, in theory, give rise to five complementary binding modes. Upon actual inspection of these coordinates, only BMA and BMB could reasonably support the increased steric bulk of the aryl group in the reactive pocket. These binding modes were designated "BMA′," and "BMB′," respectively.

Optimizations revealed that certain binding modes were not transferrable from the systems which originally reported them to our own system. During optimizations for transition states of the type Binding Mode Zhong, the malonate translates and BMB is found instead. The cases in literature arguing this binding mode as active have the two hydrogen-bond accepting sites on the nucleophile father apart from each other than in the case of the malonate used herein.[3,12] This could account for why, in those cases, Binding Mode Zhong is functional, but is likely not in our case. Binding mode Wong′ also has always led to lowest energy structures of the type BMB instead. Wong′ is proposed with a squareamide catalyst which differs in orientations of its hydrogen-bond donors as compared to the thiourea used herein.[4] This could account for the difference observed.

DFTB+ conformational analysis

Low energy transition structures that emerged from the initial manual search discussed above were used as starting points for a DFTB+ simulations in order to thoroughly explore the conformational space. These simulation were initiated at 300.0K and raised linearly to 600.0K over 100fs. The system was held at 600.0K for 2,000fs then exponentially cooled to 10.0K over 500fs. The final energies for these simulations were compared and the lowest energy structures were either resubmitted to another simulation, or scaled up using DFT calculations.

Several of the low-energy structures from the initial searches at B3LYP/6-31G* were re-calculated at a higher level of theory (B3LYP/6-31+G**/PCM(toluene)) The relative energies of these transition states, along with those of transition states located from geometries obtained from the DFTB+ simulations are recorded in Table S3.

Table S 3. Energies of structures found using B3LYP/6-31+G**/PCM(toluene)

Entry	Binding Mode	Enantiomer formed	Note	ΔFree (kcal mol^{-1})	ΔZPE (kcal mol^{-1})	ΔPE (kcal mol^{-1})
1	A	maj	manuscript	1.7	2.1	1.6
2			1	11.6	13.3	13.3
3		min	Table S4	2.2	2.7	2.4
4			2	3.6	4.0	3.5
5			3	4.1	4.0	3.5
6			1	11.1	12.2	11.8
7	B	maj	manuscript	0.0	0.0	0.0
8			4	0.3	0.1	0.1
9			5	13.3	13.8	12.9
10		min	manuscript	1.5	2.0	2.2
11			6	6.5	6.4	6.2
12			7	7.3	7.6	7.4
13	Wong	maj	Table S4	1.7	2.5	2.4
14			8	1.9	2.7	2.5
15		min	manuscript	0.9	1.1	0.9
16			4	1.2	1.2	1.0
17			5	12.1	13.1	12.9
18	A′	maj	9	11.2	12.6	12.1
19			10	12.0	12.2	11.6
20	B′	maj	9	14.6	13.7	13.7

Notes

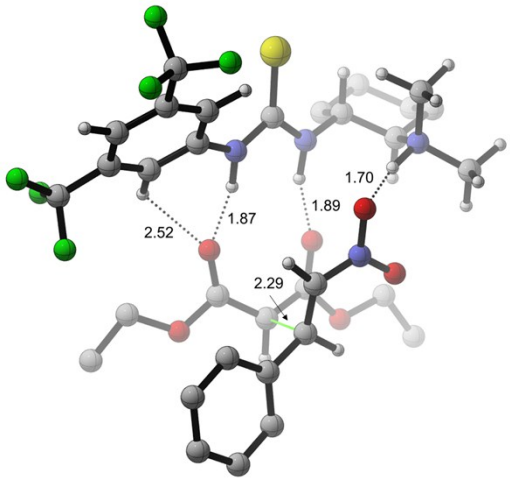
1 methyl groups of the amine used for H-bonding to the malonate
2 Both thioamide protons bonded to the same oxygen
3 Attempting to establish CH-pi interactions with catalyst
4 Aryl group more in-plane with thio-group

5	methyl groups of the amine used for H-bonding to the nitrostyrene
6	Right ester dihedral turned down
7	Carbonyls antiperiplanar
8	methyl groups of the amine moved closer for H-bonding to the malonate
9	Optimization performed using B3LYP/6-31G*
10	Transition state in entry 19 computed at B3LYP/6-31+G** PCM(toluene)
manuscript	Geometry appears in the manuscript
Table S4	Calculation scaled up and geometry included under Table S4

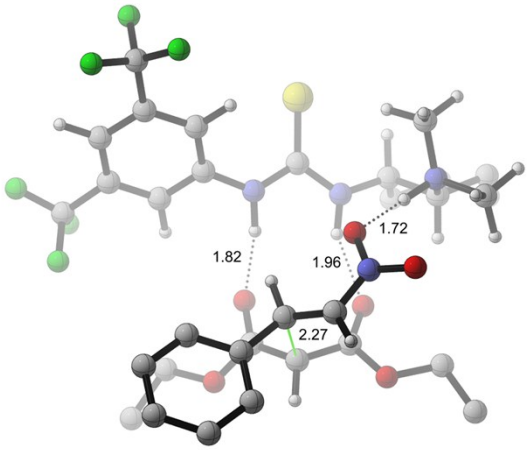
Finally, single point energies for the lowest energy transition structures were computed using the method described in the methodology section. Four of these structures are in the manuscript. The other two are included in the SI along with the coordinates for all calculated structures.

Table S 4. Relative energies for lowest energy transition states representing all major binding modes investigated at the B3LYP-D3(BJ)/6-311++G**/PCM(Toluene) // B3LYP/6-31+G**/PCM(Toluene) level of theory; entries 1-4 along with their relative free energies are discussed in the manuscript

Entry	Binding Mode	Enantiomer formed	ΔFree (kcal mol^{-1})	ΔZPE (kcal mol^{-1})	ΔPE (kcal mol^{-1})
1	B	maj	0.000	0.000	0.000
2	B	min	2.447	2.983	3.133
3	Wong	min	3.282	3.446	3.244
4	A	maj	4.740	5.083	4.618
5	Wong	maj	5.402	6.195	6.034
6	A	min	6.673	7.244	6.895



Entry 1 (also in manuscript)



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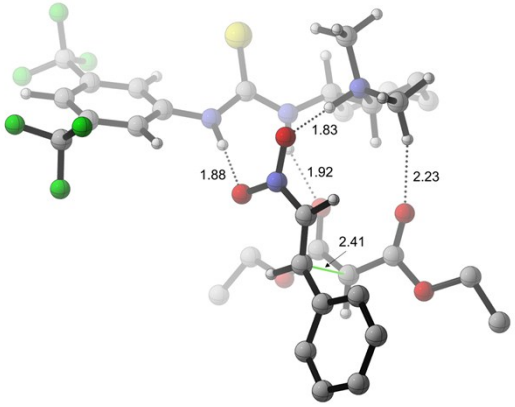

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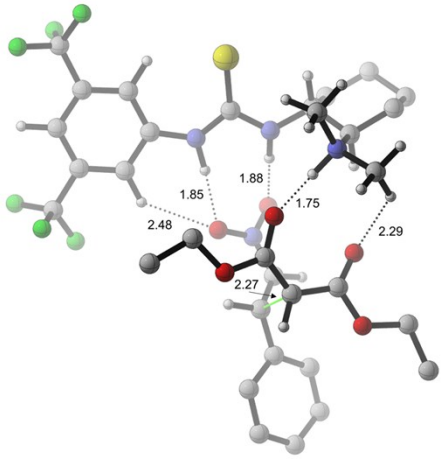

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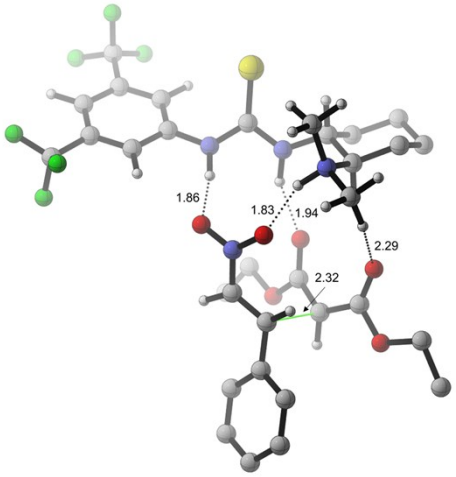

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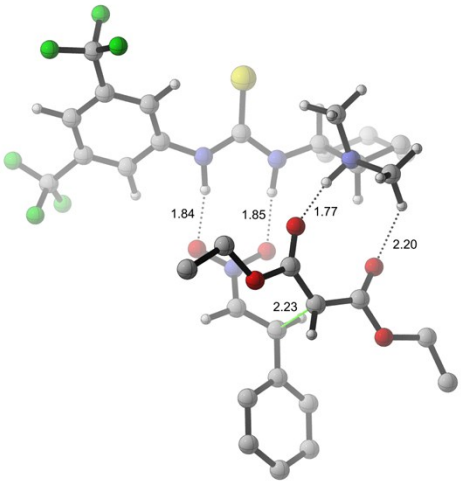
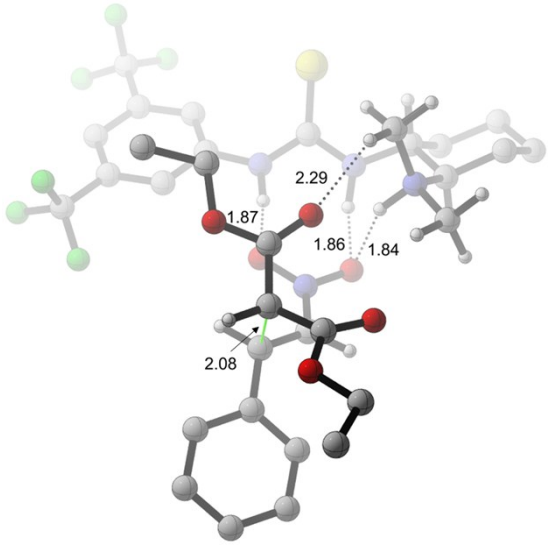


Entry 6

During optimizations, a new binding mode was discovered there the nitroolefin was hydrogen-bonded to both the thiourea and the protonated tertiary amine, and the enolate was hydrogen-bonded to the protons on the methyl-groups adjacent to the amine. This proved to be lowest-energy transition structure when calculated at B3LYP/6-31+G**/PCM(toluene), but it could not be found using any other method. We believe this suggests that the transition state is an artifact on the B3LYP/6-31+G**/PCM(toluene). Nevertheless, it is included here.



Protonation and deprotonation steps

The first and third steps in the catalytic cycle (deprotonation of the malonate and protonation of the nitronate, respectively) were also modeled to better understand the reaction coordinate.

TS1 could occur from a deprotonation of the malonate in its ketone form ($TS1_{C\text{-}dep}$) or a deprotonation of the malonate in its enol form ($TS1_{O\text{-}dep}$) both were located using B3LYP-D3(BJ)/6-311++G**/PCM(toluene) // B3LYP/6-31G* (since we were unable to locate $TS1_{O\text{-}dep}$ at B3LYP/6-311++G**/PCM(toluene), we decided to both these TSs using the lower level of theory).

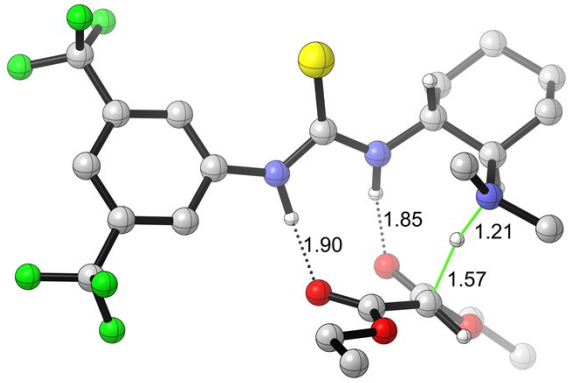


Figure S 2. Lowest energy optimized geometry for $TS1_{C\text{-}dep}$; some atoms omitted for clarity, distance in Å

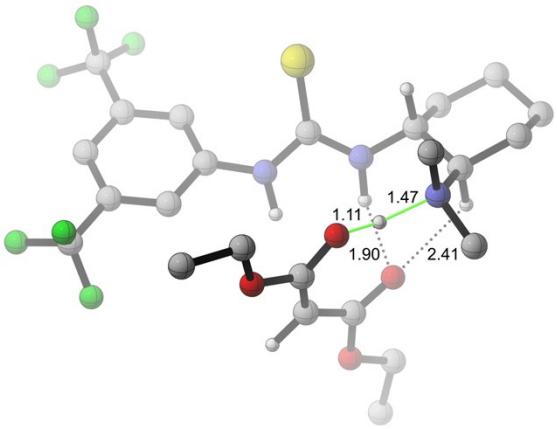


Figure S 3. Lowest energy optimized geometry for $TS1_{O\text{-}dep}$; some atoms omitted for clarity, distance in Å

The protonation of the nitronate could occur at the nitronate-carbon ($TS3_{C\text{-}prot}$) the nitronate-oxygen ($TS3_{O\text{-}prot}$). These transition states were found at the B3LYP-D3(BJ)/6-311++G**/PCM(toluene) // B3LYP/6-31+G**/PCM(toluene) level of theory.

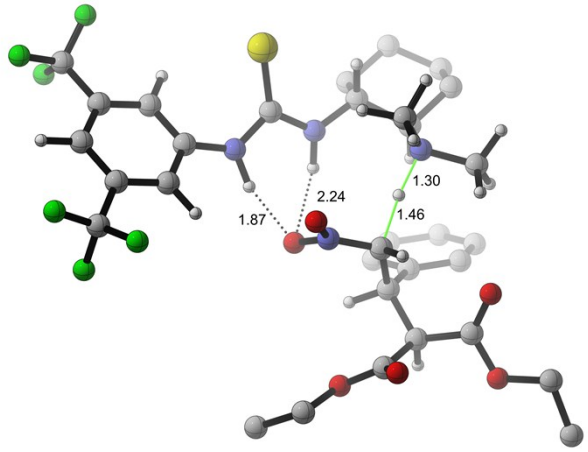


Figure S 4. Lowest energy optimized geometry for $TS3_{C\text{-}prot}$; some atoms omitted for clarity, distance in Å

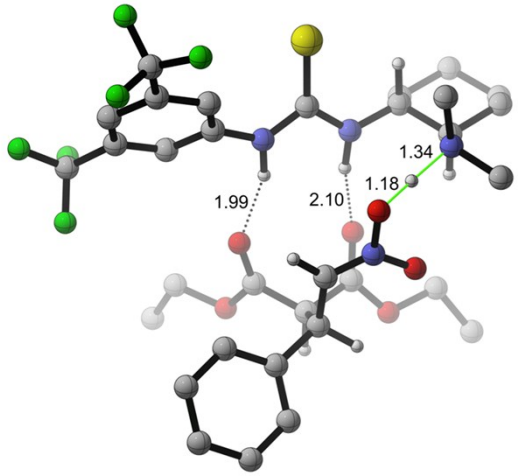


Figure S 5. Lowest energy optimized geometry for $TS3_{O\text{-}prot}$; some atoms omitted for clarity, distance in Å

The free energy profile for the reaction is shown below in Figure S6. $TS3_{O\text{-}prot}$ is lower in energy than $TS3_{C\text{-}prot}$ by 15.7 kcal mol^{-1}. We were unable to locate a tautomerization transition structure with a reasonable energy barrier to support turnover-limiting carbon-carbon bond formation – this does not mean that no transition state exists that can interconvert the O-protonated product to the C-protonated product. As Plata and Singleton noted, computational methods frequently fail at correctly assessing the energy of proton transfers relative to structures not involving proton transfers within the same reaction coordinate.[13]

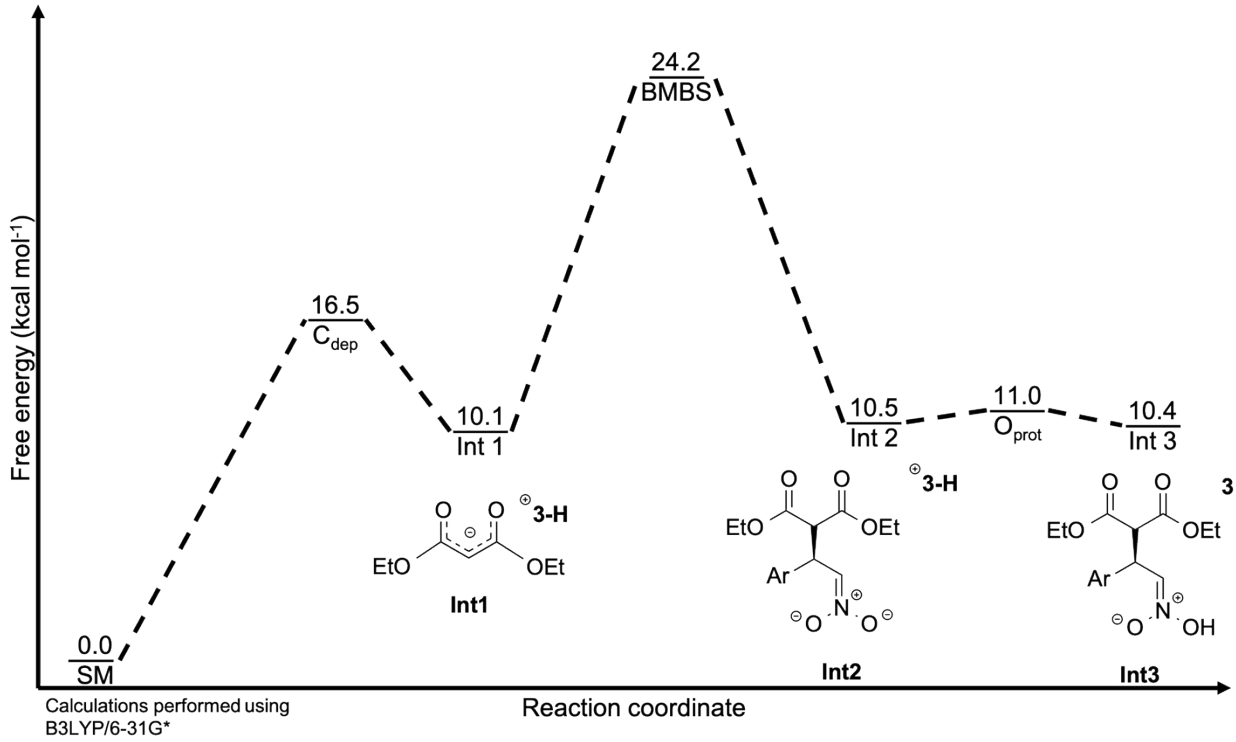


Figure S 6. Free energy profile of the title reaction

We also carried out an extensive investigation to probe if direct C-protonation from Int2 is the operational mechanism. Various confirmations were searched at the B3LYP-D3(BJ)/6-311++G**/PCM(toluene) // B3LYP/6-31G* level of theory and compared to O-protonation and TS2-BMBS at the same level of theory. The most frequently suggested mechanism of protonation involves protonation by the protonated tertiary amine moiety. We also investigated the possibility of thiourea as a Bronsted acid for this protonation step. Table S5 includes the energies of all investigated transition states relative to O-protonation. The results from these investigations suggest that C-protonation is higher in energy than both O-protonation and C-C bond-formation. This would mean that if the reaction proceeds via C-protonation after C-C bond-formation, then C protonation would be the rate-determining step of the reaction. Our experimental KIEs are inconsistent with this computational result. Once again, we attribute this discrepancy to the limitations of DFT calculations to accurately predict relative energies of different steps in a computed reaction coordinate diagram, especially if these steps involve proton transfers.[13] Further exploration of this issue is beyond the scope of the current work.

Table S 5. Conformational analysis of C-protonation

entry	TS	Proton source	Note	ΔFree (kcal mol^{-1})	ΔZPE (kcal mol^{-1})	ΔPE (kcal mol^{-1})
	C--C	NA		11.4	11.6	10.2
	O-prot	3° Amine		0.0	0.0	0.0
1	C-prot	3° Amine	Fig S 4	15.7	16.3	16.3
2	C-prot		1	16.1	18.4	18.4
3	C-prot		2	16.5	18.4	18.5
4	C-prot		3	16.7	18.4	18.4
5	C-prot		4	19.9	20.2	20.0
6	C-prot		5	20.3	20.2	19.9
7	C-prot		6	21.3	21.8	21.7
8	C-prot		7	24.8	26.5	26.3
9	C-prot		3,6	25.6	26.9	27.1
10	C-prot		8	30.1	32.6	35.2
11	C-prot	C-Malonate	9	21.5	7.2	5.6
12	C-prot		5	23.3	9.4	7.9
13	C-prot	O-Malonate	5	20.8	6.9	5.7
14	C-prot		10	24.8	12.1	11.0
15	C-prot	Thiourea NH	11	18.8	19.4	20.1
16	C-prot		1	19.3	20.6	20.9
17	C-prot		12	19.9	20.3	20.8
18	C-prot		3	20.3	20.1	19.6
19	C-prot		3,13	23.5	22.2	21.6
20	C-prot		6	27.1	29.2	30.1
21	C-prot		7	31.5	33.0	33.5
22	C-prot		14	32.3	34.2	34.3
23	C-prot	Thiourea SH		27.7	28.4	29.6

Notes

1 Product's malonate moiety carbonyl antiperiplanar
2 Dual thiourea-nitro H-bond
3 Hydrogen bond between 3° Amine methyl group and product's malonate moiety
4 3° Amine methyl group-product phenyl CH-pi interaction
5 Product's malonate moiety-thiourea H-bond
6 *Anti*-thiourea
7 3° Amine in *anti*-configuration to Cy-group
8 Thiol isomer of catalyst used

9 Malonate bound to thiourea
10 Product's malonate moiety-3° Amine H-bond
11 Product's nitro moiety-3° Amine H-bond
12 Product's malonate moiety-catalyst's Ar-H H-bond
13 Thiourea and 3° Amine H-bonded to product's nitro moiety
14 Proton adjacent to Cy group used as proton source

KIE predictions for all carbon atoms for all TSs discussed in Figure 4 (in manuscript)

B3LYP/6-31+G** PCM KIE predictions @ 298K						
Substrate	Carbon	Imaginary Freq	Scaled Imag. Freq	before tunnlng	w correc.	KIE/wigner
$TS1_{C\text{-}dep}$						
Diethylmalonate	alpha	-1179.2291	-1176.3707	1.008	1.0028	1.011
	carbonyl	-1179.2291	-1178.6807	1.005	1.0005	1.005
	methylene	-1179.2291	-1179.2166	1.000	1.0000	1.000
	methyl	-1179.2291	-1179.2287	1.000	1.0000	1.000
$TS1_{O\text{-}dep}$						
Diethylmalonate	alpha	-395.0017	-394.8853	1.001	1.0001	1.001
	carbonyl	-395.0017	-393.4273	1.009	1.0010	1.010
	methylene	-395.0017	-394.9701	1.001	1.0000	1.001
	methyl	-395.0017	-394.9912	1.000	1.0000	1.000
$TS2_{BMB\text{-}S}$						
Diethylmalonate	alpha	-244.1993	-239.8661	1.029958	1.0019	1.032
	carbonyl	-244.1993	-243.956	1.007181	1.0001	1.007
	methylene	-244.1993	-244.1793	0.999319	1.0000	0.999
	methyl	-244.1993	-244.19	1.00029	1.0000	1.000
Nitrostyrene	para	-244.1993	-244.1822	1.000145	1.0000	1.000
	meta	-244.1993	-244.1917	1.000064	1.0000	1.000
	ortho	-244.1993	-244.1746	1.00008	1.0000	1.000
	ipso	-244.1993	-243.9573	0.990859	1.0001	0.991
	beta	-244.1993	-240.8416	1.029744	1.0015	1.031
	alpha	-244.1993	-243.7932	0.9986	1.0002	0.999
$TS3_{C\text{-}prot}$						
Diethylmalonate	alpha	-1319.1973	-1319.1973	1.000	1.0000	1.000
	carbonyl	-1319.1973	-1319.1971	1.000	1.0000	1.000
	methylene	-1319.1973	-1319.1947	0.999	1.0000	0.999
	methyl	-1319.1973	-1319.1967	0.994	1.0000	0.994
Nitrostyrene	para	-1319.1973	-1319.1969	1.000	1.0000	1.000
	meta	-1319.1973	-1319.1973	1.000	1.0000	1.000
	ortho	-1319.1973	-1319.1973	1.000	1.0000	1.000
	ipso	-1319.1973	-1319.1962	1.001	1.0000	1.001
	beta	-1319.1973	-1319.1825	1.000	1.0000	1.000
	alpha	-1319.1973	-1316.5753	1.013	1.0025	1.015
$TS3_{O\text{-}prot}$						
Diethylmalonate	alpha	-623.4197	-623.4142	0.996208	1.0000	0.996
	carbonyl	-623.4197	-623.4153	0.999699	1.0000	1.000

	methylene	-623.4197	-623.4188	1.000896	1.0000	1.001
	methyl	-623.4197	-623.4196	0.999919	1.0000	1.000
Nitrostyrene	para	-623.4197	-623.4194	0.999699	1.0000	1.000
	meta	-623.4197	-623.4195	0.999899	1.0000	1.000
	ortho	-623.4197	-623.4191	1.000591	1.0000	1.001
	ipso	-623.4197	-623.4134	0.990354	1.0000	0.990
	beta	-623.4197	-623.4063	1.000468	1.0000	1.000
	alpha	-623.4197	-623.4082	0.9925	1.0000	0.993

D. Coordinates and energies of calculated structures

Diethylmalonate 1a (B3LYP/6-31G)*

Free Energy = -574.745481
Zero-point Energy = -574.703272
Potential Energy = -574.894287809
Nimag = 1 (13.1120 cm-1)

Charge = 0 Multiplicity = 1
O 0.74642 -0.22801 -1.28539
C 1.02783 0.23250 -0.20229
C 0.08415 1.02652 0.69161
C -1.33817 0.99844 0.16303
O -1.88627 1.92320 -0.39243
H 0.12929 0.61843 1.70628
C 3.25047 -0.57032 -0.39030
H 3.37430 -0.06321 -1.35236
H 2.89322 -1.58473 -0.59351
C -3.24810 -0.37052 -0.12250
H -3.22089 -0.20090 -1.20321
H -3.90066 0.39017 0.31811
O 2.24025 0.13117 0.37671
O -1.91074 -0.19575 0.40333
C 4.52719 -0.56600 0.42844
H 5.31938 -1.08872 -0.11847
H 4.86245 0.45715 0.62601
H 4.37909 -1.07214 1.38770
C -3.69374 -1.77812 0.22457
H -4.70463 -1.95216 -0.15999
H -3.02285 -2.52000 -0.21990
H -3.70719 -1.92953 1.30885
H 0.42335 2.06589 0.72744
H 3.33716 1.18325 1.85217

*Diethylmalonate 1a (B3LYP-D3(BJ)/6-311++G**/PCM(toluene) // B3LYP/6-31+G**/PCM(toluene))*

Free Energy = -574.792834
Zero-point Energy = -574.750594
Potential Energy = -574.940170888
Single Point Energy = -575.106416475
Nimag = 1 (17.2755 cm-1)

Charge = 0 Multiplicity = 1
C -0.00000 -1.78093 -0.00001
H 0.40672 -2.41648 0.79028
H -0.40688 -2.41626 -0.79039
C -1.12268 -0.95341 0.60565
C 1.12290 -0.95362 -0.60554
O 1.58267 -0.04458 0.27002
O -1.58256 -0.04448 -0.26997
O 1.57099 -1.11426 -1.72365
O -1.57102 -1.11431 1.72362
C -2.67718 0.80638 0.17525
C -3.02235 1.74204 -0.96607
H -2.34978 1.34592 1.06839
H -3.51868 0.16519 0.45239
H -3.84544 2.39678 -0.66210
H -2.16659 2.36840 -1.23496
H -3.33722 1.18300 -1.85221
C 2.67715 0.80643 -0.17526
C 3.02220 1.74220 0.96600
H 2.34965 1.34588 -1.06842
H 3.51873 0.16535 -0.45238
H 3.84518 2.39704 0.66199
H 2.16635 2.36844 1.23488

Nitrostyrene 2a (B3LYP/6-31G)*

Free Energy = -514.050463
Zero-point Energy = -514.014710
Potential Energy = -514.151810275
Nimag = 1 (37.7658 cm-1)

Charge = 0 Multiplicity = 1
C 3.08391 -1.07004 -0.00001
C 1.70484 -1.26525 0.00000
C 0.81979 -0.17135 0.00001
C 1.36065 1.12957 0.00001
C 2.73701 1.32341 0.00001
C 3.60379 0.22506 -0.00001
H 3.75101 -1.92728 -0.00002
H 1.29991 -2.27416 -0.00000
H 0.70091 1.99209 0.00001
H 3.13834 2.33289 -0.00000
H 4.67892 0.38125 -0.00002
C -0.61465 -0.44189 0.00001
H -0.91738 -1.48647 0.00002
C -1.60700 0.45960 -0.00000
H -1.52283 1.53695 -0.00002
N -2.99320 0.03120 -0.00001
O -3.83347 0.93583 -0.00001
O -3.25485 -1.17437 0.00000

*Nitrostyrene 2a (B3LYP-D3(BJ)/6-311++G**/PCM(toluene) // B3LYP/6-31+G**/PCM(toluene))*

Free Energy = -514.090775

Zero-point Energy = -514.055255
Potential Energy = -514.191862736
Single Point Energy = -514.335163604
Nimag = 1 (45.2070 cm-1)

Charge = 0 Multiplicity = 1
C -1.70752 1.26883 0.00003
C -3.08792 1.06973 0.00000
C -3.60442 -0.22854 -0.00001
C -2.73424 -1.32730 -0.00001
C -1.35687 -1.13116 0.00002
C -0.82012 0.17400 0.00003
H -1.30651 2.27848 0.00004
H -3.75739 1.92424 -0.00001
H -4.67855 -0.38715 -0.00003
H -3.13418 -2.33653 -0.00002
H -0.69810 -1.99341 0.00003
C 0.61218 0.44980 0.00006
C 1.60606 -0.45670 0.00009
H 0.90708 1.49611 0.00007
H 1.51544 -1.53287 0.00008
N 2.98636 -0.03345 0.00011
O 3.83507 -0.93800 -0.00013
O 3.26552 1.17217 -0.00014

Catalyst 3 (B3LYP/6-31G)*

Free Energy = -1821.656339
Zero-point Energy = -1821.596687
Potential Energy = -1821.97434781
Nimag = 1 (12.3212 cm-1)

Charge = 0 Multiplicity = 1
N 4.16596 -1.02755 1.66570
C 4.09746 0.08764 2.60995
C 4.67767 -0.68347 0.32480
C 6.07062 -0.02556 0.25263
C 6.52591 0.12832 -1.20905
C 5.49029 0.89433 -2.04611
C 4.08969 0.27288 -1.93059
C 3.65913 0.18245 -0.45631
N 2.33871 -0.41896 -0.27163
C 1.15932 0.24371 -0.45001
N 0.08736 -0.56692 -0.10034
C -1.29329 -0.30411 -0.06856
S 1.03177 1.80732 -1.03961
C 4.82865 -2.18526 2.25831
H 0.31247 -1.55452 -0.06849
H 2.36461 -1.09919 0.49147
H 3.63916 1.20250 -0.04689
H 3.35841 0.86788 -2.48414
H 4.08581 -0.73774 -2.36286
H 6.03820 0.96223 0.73174
H 6.79758 -0.62625 0.81316
H 5.44838 1.93942 -1.70765
H 5.79894 0.92226 -3.09808
H 7.49866 0.63406 -1.24679
H 6.67715 -0.87047 -1.64401
H 4.73996 -1.64576 -0.20541
H 3.55567 -0.23764 3.50467
H 3.54640 0.92442 2.17165
H 5.08778 0.45402 2.93078
H 5.87898 -1.99889 2.54523
H 4.28716 -2.48763 3.16157
H 4.81143 -3.02384 1.55398
C -2.15606 -1.38369 -0.30568
C -3.53675 -1.21652 -0.23105
C -4.08528 0.02983 0.06715
C -3.22336 1.10024 0.30493
C -1.83821 0.94737 0.25148
H -1.74878 -2.35749 -0.56149
C -4.44104 -2.40607 -0.41800
H -5.15898 0.16331 0.11712
C -3.80051 2.46569 0.58231
H -1.18845 1.78669 0.45162
F -3.88393 -3.34092 -1.22074
F -4.71112 -3.01348 0.76120
F -5.62576 -2.05516 -0.96030
F -2.99723 3.19853 1.38226
F -3.97702 3.17011 -0.55703
F -5.00812 2.38234 1.18496

*Catalyst 3 (B3LYP-D3(BJ)/6-311++G**/PCM(toluene) // B3LYP/6-31+G**/PCM(toluene))*

Free Energy = -1821.768991
Zero-point Energy = -1821.707458
Potential Energy = -1822.08140425
Single Point Energy = -1822.53527458
Nimag = 1 (9.5490 cm-1)

Charge = 0 Multiplicity = 1
N 4.22910 -0.54130 1.85779
C 4.19998 0.78809 2.47118
C 4.69173 -0.57517 0.45624
C 6.07944 0.03234 0.16245
C 6.48705 -0.21397 -1.30054
C 5.42295 0.30796 -2.27804
C 4.02897 -0.25259 -1.95493
C 3.64484 0.05344 -0.49644
N 2.33097 -0.47526 -0.12280
C 1.13746 0.07244 -0.46217
N 0.07769 -0.64294 0.07937
C -1.29944 -0.35776 0.04311
S 0.95604 1.42784 -1.44330
C 4.91309 -1.50699 2.71656
H 0.30053 -1.59286 0.35168
H 2.37246 -0.97801 0.76497
H 3.62735 1.14458 -0.36938

H 3.27892 0.17579 -2.62430
H 4.01676 -1.34162 -2.10063
H 6.06075 1.11234 0.35816
H 6.82554 -0.40092 0.83841
H 5.38948 1.40540 -2.22903
H 5.69473 0.05167 -3.30857
H 7.45553 0.25875 -1.50284
H 6.62729 -1.29294 -1.45831
H 4.74133 -1.64439 0.20236
H 3.68335 0.72416 3.43396
H 3.64684 1.48928 1.84128
H 5.20486 1.20491 2.65415
H 5.97152 -1.25619 2.90706
H 4.40353 -1.55258 3.68447
H 4.87329 -2.50244 2.26343
C -2.18956 -1.42798 -0.10728
C -3.56853 -1.20523 -0.08267
C -4.08268 0.07975 0.07824
C -3.18579 1.14156 0.23214
C -1.80680 0.93837 0.22391
H -1.80596 -2.43308 -0.25320
C -4.49643 -2.38632 -0.19631
H -5.15162 0.25049 0.09012
C -3.72545 2.54197 0.37693
H -1.12915 1.76884 0.36057
F -4.09137 -3.26588 -1.14875
F -4.55893 -3.09144 0.96874
F -5.76410 -2.02478 -0.49985
F -2.89187 3.34822 1.07747
F -3.91855 3.13753 -0.83115
F -4.92556 2.56302 1.01060

Int1 (B3LYP/6-31G)*

Free Energy = -2396.383685
Zero-point Energy = -2396.306603
Potential Energy = -2396.87949158
Nimag = 1 (10.4500 cm-1)

Charge = 0 Multiplicity = 1
N 0.33820 -0.54647 -0.29233
C -0.57203 -1.44461 0.21530
S -0.17925 -2.79835 1.14750
N -1.85291 -1.10949 -0.09393
C -3.02820 -1.84570 0.33808
C -3.45182 -2.91927 -0.68660
C -4.70376 -3.67635 -0.22581
C -5.85795 -2.71023 0.06934
C -5.44011 -1.62788 1.08169
C -4.20174 -0.87383 0.57670
N -3.78868 0.27921 1.48339
C -3.39836 -0.11058 2.87243
C -4.78413 1.39298 1.48951
O -1.65774 1.82987 1.42946
C -0.89930 2.44250 0.64322
C -0.97514 2.55238 -0.76647
C -2.06326 2.06701 -1.52803
O -2.96378 1.26734 -1.16623
H -2.76446 -2.36250 1.26664
H -3.63711 -2.43415 -1.65524
H -2.60726 -3.60219 -0.82015
H -5.00486 -4.40432 -0.98813
H -4.46802 -4.25208 0.68035
H -6.18049 -2.22552 -0.86300
H -6.72820 -3.25136 0.45853
H -5.22190 -2.10572 2.04576
H -6.27432 -0.93580 1.24435
H -4.43258 -0.37642 -0.36930
H -0.03662 0.36181 -0.58159
H -2.04604 -0.28377 -0.67098
H -2.99116 0.77704 3.35534
H -4.26939 -0.48046 3.41580
H -2.62036 -0.87294 2.82908
H -4.32238 2.23917 1.99954
H -4.98635 1.66795 0.45442
H -5.69550 1.08757 2.00574
H -2.92423 0.74274 1.08187
H -0.26936 3.21018 -1.25662
C 0.37151 3.05545 2.57697
H 0.45561 2.01156 2.89889
H -0.51038 3.48158 3.06894
C -3.07334 2.03610 -3.68989
H -4.06160 2.28290 -3.28530
H -3.00814 0.94288 -3.74604
O 0.18760 3.10381 1.15113
O -2.05509 2.53505 -2.81100
C 1.62697 3.84629 2.90118
H 1.79225 3.85242 3.98460
H 2.50695 3.40676 2.42289
H 1.53149 4.88264 2.56110
C -2.85090 2.67776 -5.04856
H -3.60852 2.32809 -5.75890
H -2.91874 3.76822 -4.97907
H -1.86236 2.42124 -5.44267
C 1.74625 -0.59124 -0.24442
C 2.43010 0.62031 -0.08548
C 2.47508 -1.77319 -0.43649
C 3.82542 0.64402 -0.10814
H 1.87356 1.54150 0.06013
C 3.86773 -1.73147 -0.44269
H 1.95797 -2.71030 -0.58590
C 4.55750 -0.52856 -0.27918
H 5.63998 -0.50528 -0.30224
C 4.64158 -3.01514 -0.59602
C 4.53158 1.95396 0.11706
F 3.96815 -3.92586 -1.33217
F 4.90037 -3.58834 0.60106
F 5.83552 -2.81047 -1.19813
F 4.57264 2.27553 1.43703
F 5.80930 1.92627 -0.31700
F 3.90895 2.97559 -0.50833

Int2 (B3LYP/6-31G)*

Free Energy = -2910.433498
Zero-point Energy = -2910.343069
Potential Energy = -2911.05741918
Nimag = 1 (9.3597 cm-1)

Charge = 0 Multiplicity = 1
C 4.48389 -0.45906 0.17435
C 3.08293 -0.47657 0.25084
C 2.41113 -1.70844 0.15513
C 3.12518 -2.88811 -0.03447
C 4.51720 -2.87591 -0.12708
C 5.17907 -1.65361 -0.01521
N 2.27846 0.64712 0.47615
C 2.52245 1.98517 0.27852
S 3.81397 2.65214 -0.58269
C 2.38648 -4.19757 -0.08571
C 6.68578 -1.62932 -0.03351
N 1.53511 2.74888 0.83197
C 1.34329 4.16218 0.54633
C -0.15861 4.52762 0.49585
C -0.33502 5.98283 0.04547
C 0.39462 6.92991 1.01763
C 1.87609 6.55975 1.17485
C 2.04865 5.08447 1.56112
N -0.95839 3.51845 -0.31983
C -0.45528 3.25074 -1.70023
C -2.43012 3.78935 -0.33014
O -0.99996 1.72876 1.61098
N -1.31341 0.54517 1.09448
O -0.45996 0.00800 0.27543
C -2.46548 0.00145 1.38372
C -2.88842 -1.28305 0.73933
C -3.75923 -2.15089 1.64197
C -4.86989 -1.64656 2.33513
C -5.64417 -2.48294 3.14077
C -5.32539 -3.83588 3.26720
C -4.22311 -4.34840 2.58223
C -3.44859 -3.51078 1.77889
C -3.57069 -1.07062 -0.66962
C -2.58559 -0.45867 -1.66611
O -2.55038 0.72296 -1.96471
C -4.82112 -0.19883 -0.63808
O -5.02170 0.74140 0.10224
H 1.79897 4.35524 -0.43163
H 1.64019 4.89851 2.56442
H 3.10645 4.80658 1.58106
H 2.34706 7.20441 1.92608
H 2.40221 6.74763 0.22833
H -0.10133 6.88305 1.99768
H 0.28838 7.96201 0.66368
H 0.07136 6.11228 -0.96657
H -1.39682 6.24919 0.00598
H -0.58070 4.41196 1.50223
H 1.27876 0.41491 0.60595
H 0.79014 2.26425 1.34865
H -1.05512 2.44061 -2.11707
H -0.56170 4.15394 -2.30577
H 0.59051 2.94915 -1.65802
H -2.92950 2.89145 -0.69908
H -2.75400 3.98998 0.69206
H -2.65260 4.63993 -0.97647
H -3.84615 -2.05789 -1.04987
H -0.88587 2.63571 0.28896
H -3.09591 0.57319 2.04530
H -1.97578 -1.84243 0.51286
H -2.58586 -3.91622 1.25483
H -3.96011 -5.39868 2.67647
H -5.92875 -4.48410 3.89709
H -6.49868 -2.07306 3.67320
H -5.13683 -0.59884 2.24126
H 1.32763 -1.72686 0.22196
H 5.06962 -3.79257 -0.29272
H 5.01927 0.47691 0.24196
F 1.14526 -4.06114 -0.61895
F 2.21572 -4.73003 1.14622
F 3.04064 -5.11924 -0.82496
F 7.17159 -0.46356 -0.50700
F 7.19846 -1.79423 1.20954
F 7.19389 -2.62282 -0.79868
C -0.68088 -0.93884 -2.99589
C 0.06622 -2.16565 -3.48104
H -0.05670 -0.29209 -2.37291
H -1.08549 -0.34615 -3.82227
H 0.91428 -1.85581 -4.10144
H 0.45012 -2.74934 -2.64015
H -0.58425 -2.80765 -4.08408
C -6.90289 0.17675 -1.71355
C -7.72685 -0.44588 -2.82418
H -6.63134 1.21463 -1.93120
H -7.42695 0.16383 -0.75281
H -8.65897 0.11495 -2.95301
H -7.18101 -0.43009 -3.77284
H -7.97945 -1.48446 -2.58839
O -1.78595 -1.39768 -2.17397
O -5.68715 -0.60072 -1.58653

Int3 (B3LYP/6-31G)*

Free Energy = -2910.433671
Zero-point Energy = -2910.343954
Potential Energy = -2911.05590588
Nimag = 1 (7.7122 cm-1)

Charge = 0 Multiplicity = 1
C 2.23249 -2.81004 0.14567
C 1.71154 -1.71347 -0.56097
C 2.59970 -0.74223 -1.04568
C 3.96761 -0.84164 -0.80142
C 4.49318 -1.92944 -0.10961

C 3.60894 -2.90935 0.34783
N 0.34428 -1.45539 -0.75282
C -0.74450 -2.30011 -0.76429
S -0.64068 -3.98635 -0.81707
C 4.84121 0.28241 -1.28037
C 4.15747 -4.12514 1.05051
N -1.91861 -1.61512 -0.76062
C -3.23898 -2.19619 -0.98045
C -4.25097 -1.78228 0.12021
C -5.63437 -2.39474 -0.20169
C -6.14322 -1.97882 -1.58959
C -5.14117 -2.36656 -2.68172
C -3.75470 -1.78727 -2.37741
N -3.76393 -2.06968 1.50142
C -3.46417 -3.48439 1.78651
C -4.65732 -1.51917 2.53543
O -1.55627 -0.77263 2.24745
N -1.67014 0.55595 1.90408
O -2.81887 1.07833 1.92707
C -0.54968 1.16086 1.60618
C -0.55978 2.63508 1.34755
C 0.74548 3.30546 1.76068
C 1.99775 2.80002 1.38029
C 3.17372 3.45008 1.75609
C 3.11769 4.61558 2.52207
C 1.87793 5.12636 2.90884
C 0.70320 4.47547 2.52930
C -0.94572 3.03394 -0.14541
C -2.30480 2.45342 -0.53249
O -2.48955 1.37068 -1.05644
C 0.12321 2.61793 -1.13749
O 0.42622 1.46524 -1.39479
H -3.10117 -3.27984 -0.96627
H -3.78806 -0.69022 -2.43472
H -3.02265 -2.12437 -3.12025
H -5.48550 -2.01840 -3.66351
H -5.07505 -3.46218 -2.74365
H -6.30076 -0.89019 -1.60824
H -7.12092 -2.43889 -1.77963
H -5.56800 -3.49052 -0.15795
H -6.36139 -2.09318 0.56031
H -4.34167 -0.68788 0.08457
H 0.15048 -0.47292 -0.94495
H -1.88638 -0.59670 -0.80829
H -3.03488 -3.54578 2.79169
H -4.36170 -4.12094 1.76219
H -2.72472 -3.87144 1.08264
H -4.14389 -1.56994 3.50063
H -4.85762 -0.46775 2.32058
H -5.60481 -2.07035 2.62088
H -1.02644 4.12204 -0.16073
H -2.41669 -1.23109 1.87295
H 0.33891 0.54995 1.62692
H -1.37607 3.05597 1.94528
H -0.25898 4.87789 2.83848
H 1.82245 6.02968 3.51043
H 4.03346 5.11972 2.81846
H 4.12926 3.03823 1.44469
H 2.07048 1.89451 0.78531
H 2.20886 0.10535 -1.59579
H 5.55615 -2.00983 0.07896
H 1.56828 -3.56827 0.53389
F 4.50879 1.46013 -0.66903
F 4.69718 0.50781 -2.60635
F 6.14819 0.07093 -1.04146
F 3.29968 -4.60642 1.97457
F 4.40837 -5.13018 0.18138
F 5.32322 -3.85369 1.68237
C -4.63701 2.84928 -0.37870
C -5.55572 3.97049 0.06602
H -4.74790 1.95269 0.23689
H -4.79483 2.57519 -1.42641
H -6.59945 3.65335 -0.03361
H -5.37320 4.23034 1.11325
H -5.40881 4.86631 -0.54580
C 1.82568 3.41696 -2.59501
C 2.29766 4.75594 -3.12581
H 1.47205 2.75447 -3.39030
H 2.60976 2.89640 -2.03733
H 3.13901 4.60190 -3.80968
H 1.49817 5.26680 -3.67165
H 2.63124 5.40366 -2.30932
O -3.27372 3.32077 -0.22498
O 0.71717 3.67883 -1.68783

Below are the coordinates for all transition states appearing in Table S3

Entry 1

Free Energy = -2910.595016
Zero-point Energy = -2910.502702
Potential Energy = -2911.20913576
Nimag = 1 (-244.2815 cm-1)

Charge = 0 Multiplicity = 1
C -4.55525 0.44634 -0.14771
C -3.26422 -0.07438 -0.33273
C -3.10855 -1.46871 -0.46187
C -4.21443 -2.31218 -0.39692
C -5.50079 -1.80390 -0.20118
C -5.64736 -0.42190 -0.08190
N -2.08734 0.67976 -0.44339
C -1.81040 2.00339 -0.22496
S -2.88002 3.13779 0.44692
C -4.00741 -3.80180 -0.47968
C -7.03167 0.15824 0.05707
N -0.52376 2.31285 -0.56908
C -0.00017 3.67263 -0.63904
C 1.42565 3.77952 -0.05085
C 1.92402 5.23246 -0.12896

C 1.89964 5.74623 -1.57971
C 0.50452 5.62265 -2.19967
C -0.00814 4.18229 -2.09675
N 1.50351 3.20980 1.37337
C 0.41338 3.65188 2.30228
C 2.83949 3.43482 2.01765
O 0.79956 0.45617 -2.37496
N 1.09024 -0.52821 -1.61779
O 0.19674 -1.01909 -0.85213
C 2.35484 -1.03178 -1.63348
C 2.74435 -2.00872 -0.70917
C 3.95654 -2.82648 -0.90172
C 4.99831 -2.46225 -1.77496
C 6.10096 -3.29692 -1.95443
C 6.18856 -4.51033 -1.26437
C 5.16187 -4.88462 -0.39153
C 4.05971 -4.05003 -0.21271
C 3.25234 -0.95120 1.23467
C 1.96029 -0.60555 1.79551
O 1.38967 0.49434 1.79994
C 4.15193 0.07389 0.74978
O 3.83970 1.15053 0.23686
H -0.67789 4.30374 -0.05915
H 0.60995 3.51701 -2.71421
H -1.03446 4.10586 -2.46996
H 0.52445 5.93767 -3.24888
H -0.19053 6.29695 -1.68090
H 2.61909 5.16959 -2.17680
H 2.24133 6.78699 -1.59453
H 1.29051 5.87827 0.49357
H 2.94453 5.30820 0.25542
H 2.10597 3.13095 -0.61388
H -1.26930 0.10555 -0.69520
H -0.04720 1.64110 -1.18538
H -0.55866 3.34782 1.91832
H 0.58745 3.17593 3.26746
H 0.45004 4.73612 2.41491
H 2.89566 2.77991 2.88734
H 3.62113 3.15760 1.31393
H 2.92599 4.47475 2.33070
H 3.71799 -1.82332 1.67483
H 1.43155 2.16929 1.29401
H 3.01036 -0.53167 -2.32866
H 1.93785 -2.49549 -0.17372
H 3.26283 -4.34587 0.46450
H 5.21799 -5.82682 0.14550
H 7.04730 -5.15931 -1.40853
H 6.89226 -3.00153 -2.63732
H 4.95037 -1.52685 -2.32260
H -2.11842 -1.88107 -0.62478
H -6.35785 -2.46363 -0.14756
H -4.69499 1.51216 -0.04772
F -5.09167 -4.44681 -0.97712
F -3.76593 -4.34899 0.74700
F -2.95152 -4.13671 -1.26043
F -7.03577 1.35436 0.69120
F -7.61838 0.36262 -1.15692
F -7.86565 -0.66118 0.74816
C 0.05265 -1.51156 2.92430
C -0.39338 -2.84968 3.48285
H -0.60698 -1.16123 2.12522
H 0.08780 -0.73953 3.69937
H 0.28101 -3.19124 4.27432
H -1.39854 -2.75221 3.90567
H -0.42548 -3.61229 2.69896
C 6.45569 0.57100 0.31495
C 7.81113 -0.07456 0.53810
H 6.38045 1.53788 0.82348
H 6.25449 0.73652 -0.74843
H 8.00005 -0.23111 1.60459
H 7.87090 -1.04198 0.03101
H 8.59840 0.57473 0.14069
O 1.38245 -1.68656 2.37867
O 5.45440 -0.32108 0.85134

Entry 2

Free Energy = -2910.579268
Zero-point Energy = -2910.484790
Potential Energy = -2911.19051668
Nimag = 1 (-143.2635 cm-1)

Charge = 0 Multiplicity = 1
C 4.65249 -2.40284 -2.40367
C 3.80320 -2.68906 -1.31770
C 3.92762 -3.94034 -0.68286
C 4.86186 -4.87741 -1.12174
C 5.69745 -4.58020 -2.20302
C 5.58869 -3.33927 -2.83985
C 2.76830 -1.75788 -0.83836
C 2.25118 -0.74321 -1.64652
N 1.06589 -0.13299 -1.35722
O 0.67150 0.82892 -2.09838
O 0.34062 -0.50969 -0.38040
C 4.00111 -0.76646 0.89797
C 4.26104 0.52785 0.31565
O 3.56755 1.54571 0.38658
C 3.14810 -0.92150 2.06127
O 2.44226 -0.07921 2.61339
N 0.79059 3.26775 2.10945
C 0.02289 1.98153 2.31303
C 0.96476 3.73301 0.63976
C -0.39386 3.81994 -0.11396
C -0.25736 4.56959 -1.46135
C 0.41383 5.93682 -1.34102
C 1.79282 5.77128 -0.70410
C 1.68886 5.09608 0.67003
N -0.93911 2.49946 -0.39664
C -2.17942 2.05738 -0.08306
N -2.32499 0.72314 -0.38470
C -3.45346 -0.10606 -0.32529

S -3.34842 3.01706 0.68788
C 2.11208 3.14871 2.83479
H -1.12543 4.34852 0.50723
H 0.32072 3.94050 -2.15089
H -1.26578 4.65359 -1.87884
H 0.49643 6.39722 -2.33174
H -0.20298 6.60970 -0.72905
H 2.43305 5.16781 -1.36084
H 2.29162 6.73868 -0.57918
H 1.15131 5.77208 1.35283
H 2.69716 4.96835 1.06688
H 1.60706 2.97046 0.18832
H -1.43666 0.22410 -0.52098
H -0.36194 1.89680 -1.00117
H 1.90052 2.82282 3.85237
H 2.70582 2.39544 2.31585
H 2.61086 4.11331 2.85909
H 0.13083 1.70474 3.36095
H -1.02537 2.15141 2.08659
H 0.46191 1.20472 1.69006
H 4.79035 -1.49834 0.79805
H 0.25185 4.00436 2.57477
H 2.09811 -2.14940 -0.08299
H 2.74457 -0.32808 -2.51155
H 3.28664 -4.16896 0.16345
H 4.93793 -5.83809 -0.62104
H 6.42627 -5.30811 -2.54704
H 6.23498 -3.10096 -3.67953
H 4.58911 -1.44571 -2.90954
C -3.22143 -1.47777 -0.12725
C -4.28730 -2.37558 -0.10069
C -5.60291 -1.93629 -0.26272
C -5.82266 -0.57379 -0.47004
C -4.76957 0.34246 -0.51060
H -2.20419 -1.83359 0.00183
C -4.00794 -3.83022 0.17189
H -6.42910 -2.63470 -0.23458
C -7.22111 -0.07011 -0.71983
H -4.96361 1.39224 -0.67892
F -2.86898 -4.25742 -0.42951
F -3.85012 -4.07563 1.50405
F -5.00908 -4.63928 -0.25130
F -7.47169 1.09624 -0.07505
F -7.44268 0.16994 -2.04335
F -8.17026 -0.95395 -0.32507
O 3.20184 -2.21349 2.52049
O 5.39814 0.50240 -0.44775
C 2.41034 -2.51728 3.68936
C 2.64229 -3.97653 4.03762
H 1.35676 -2.31592 3.47002
H 2.71429 -1.85448 4.50617
H 2.06027 -4.23950 4.92720
H 2.32945 -4.63221 3.21901
H 3.69910 -4.16654 4.24943
C 5.74840 1.72313 -1.13368
C 7.04849 1.47710 -1.87806
H 5.85227 2.52757 -0.39797
H 4.93644 1.99789 -1.81510
H 7.34691 2.38719 -2.40922
H 7.85082 1.20348 -1.18605
H 6.93699 0.67244 -2.61128

Entry 3

Free Energy = -2910.594311
Zero-point Energy = -2910.501634
Potential Energy = -2911.20788267
Nimag = 1 (-274.8958 cm-1)

Charge = 0 Multiplicity = 1
C 3.90311 -4.11484 0.16714
C 4.13108 -2.94545 -0.58272
C 5.34797 -2.81850 -1.27486
C 6.30299 -3.83604 -1.23616
C 6.06328 -4.99334 -0.49115
C 4.86064 -5.12646 0.21324
C 3.12663 -1.86669 -0.69469
C 1.75991 -2.18805 -0.75792
N 0.85072 -1.28551 -1.21559
O 1.21338 -0.13983 -1.63742
O -0.38712 -1.60328 -1.22284
C 3.54780 -0.75072 1.19075
C 4.39534 0.33463 0.72382
C 2.23607 -0.49947 1.75971
O 1.53940 0.52101 1.69470
O 4.04727 1.43409 0.29180
N 1.36136 3.25338 1.18654
C 0.15205 3.84379 1.84440
C 1.51940 3.55999 -0.31173
C 2.08168 4.96483 -0.57666
C 2.31074 5.17920 -2.08393
C 1.03035 4.94463 -2.89326
C 0.43716 3.56262 -2.59187
C 0.19249 3.36881 -1.08008
N -0.42448 2.07478 -0.80312
C -1.76746 1.89614 -0.64569
N -2.13597 0.57832 -0.67415
C -3.39718 -0.00545 -0.45382
S -2.85575 3.18599 -0.43715
C 2.58670 3.58844 1.98601
H -1.42199 -0.10695 -0.96622
H 0.13267 1.25189 -1.07479
H -0.52411 4.12881 -0.75809
H -0.52066 3.43118 -3.10547
H 1.10979 2.77370 -2.95327
H 1.38557 5.72706 -0.20196
H 3.03130 5.10213 -0.05299
H 0.29154 5.71936 -2.64601
H 1.23596 5.03703 -3.96554
H 2.69149 6.19353 -2.24672
H 3.09359 4.48935 -2.42679

H 2.25054 2.81097 -0.63353
H 0.15152 3.52615 2.88768
H -0.75669 3.49819 1.35610
H 0.21115 4.93171 1.79438
H 2.65273 4.66792 2.11716
H 2.48571 3.10535 2.95852
H 3.45815 3.18897 1.47184
H 1.29745 2.21493 1.24611
H 4.07590 -1.57242 1.65586
H 1.32832 -3.11834 -0.42294
H 3.41780 -1.00675 -1.28723
H 5.53862 -1.92038 -1.85522
H 7.23242 -3.72439 -1.78685
H 6.80596 -5.78491 -0.45681
H 4.67006 -6.02037 0.79988
H 2.98168 -4.22593 0.73021
C -3.68769 -1.17903 -1.16942
C -4.89337 -1.84736 -0.96178
C -5.83390 -1.36902 -0.04638
C -5.53027 -0.21134 0.67037
C -4.32524 0.47013 0.48270
H -2.96566 -1.55951 -1.88325
C -5.16482 -3.13206 -1.69936
H -6.77277 -1.88616 0.10559
C -6.52457 0.34732 1.65474
H -4.10655 1.36050 1.05441
F -4.56027 -3.17355 -2.91117
F -4.71595 -4.21805 -1.00756
F -6.49020 -3.33525 -1.90823
F -5.92603 0.78327 2.79467
F -7.20162 1.41400 1.14899
F -7.45894 -0.56328 2.02403
O 5.70840 -0.03308 0.75341
O 1.77480 -1.60607 2.39322
C 0.44397 -1.54052 2.96508
C 0.16069 -2.87942 3.61951
H -0.27005 -1.31774 2.16694
H 0.41356 -0.72062 3.68924
H -0.83785 -2.86166 4.06806
H 0.19017 -3.69039 2.88571
H 0.88857 -3.09473 4.40778
C 6.66737 0.92047 0.24166
C 8.04816 0.30826 0.38924
H 6.57643 1.85323 0.80731
H 6.42801 1.13916 -0.80416
H 8.80151 1.00639 0.00950
H 8.27332 0.09642 1.43890
H 8.12711 -0.62524 -0.17556

Entry 4

Free Energy = -2910.592061
Zero-point Energy = -2910.499573
Potential Energy = -2911.20607384
Nimag = 1 (-233.8228 cm-1)

Charge = 0 Multiplicity = 1
C -0.28237 -3.62753 0.48011
C 0.86000 -3.75226 -0.33176
C 1.43363 -5.02780 -0.48511
C 0.88364 -6.14384 0.14442
C -0.25370 -6.00570 0.94609
C -0.83292 -4.74329 1.11062
C 1.45724 -2.61460 -1.06382
C 0.72568 -1.45144 -1.33918
N 1.08266 -0.61294 -2.36085
O 0.42009 0.48688 -2.50528
O 2.00551 -0.89135 -3.16175
C 3.15197 -2.09909 0.28016
C 3.81366 -1.09407 -0.53087
O 3.60993 0.12325 -0.50686
C 2.49950 -1.71830 1.51527
O 2.02750 -0.61028 1.80572
N 2.91785 2.05494 1.55895
C 4.27748 1.64460 2.04290
C 2.98714 3.07244 0.41324
C 1.58784 3.56077 -0.01858
C 1.71770 4.47841 -1.25378
C 2.63590 5.67513 -0.97554
C 4.00746 5.20941 -0.47461
C 3.88197 4.27674 0.74401
N 0.67118 2.45429 -0.27575
C -0.64969 2.46432 0.08341
N -1.36594 1.49652 -0.56895
C -2.70565 1.09678 -0.43465
S -1.29690 3.56240 1.20043
C 2.06049 2.44897 2.72346
H 1.14139 4.14583 0.78938
H 2.10440 3.89328 -2.09904
H 0.71313 4.81580 -1.52862
H 2.74702 6.27775 -1.88373
H 2.16976 6.32450 -0.22190
H 4.53178 4.67747 -1.28017
H 4.63301 6.06758 -0.20577
H 3.46078 4.83728 1.58858
H 4.88070 3.94417 1.03826
H 3.43777 2.49363 -0.39831
H -0.85480 1.02849 -1.33238
H 0.91526 1.83383 -1.05255
H 2.07514 1.62278 3.43327
H 2.46861 3.34881 3.18491
H 1.03765 2.62511 2.39480
H 4.15063 0.74134 2.63797
H 4.90645 1.42777 1.18192
H 4.70453 2.43772 2.65512
H 3.60824 -3.08094 0.27638
H 2.51804 1.17678 1.16846
H 2.18187 -2.88944 -1.82296
H -0.10487 -1.10305 -0.74657
H 2.31567 -5.14156 -1.10993
H 1.33891 -7.12008 0.00616

H -0.68745 -6.87345 1.43428
H -1.71981 -4.62772 1.72696
H -0.75192 -2.65941 0.61999
C -3.44034 1.17589 0.75618
C -4.75388 0.69917 0.79065
C -5.35754 0.13258 -0.33086
C -4.61102 0.04204 -1.50917
C -3.30320 0.51730 -1.56859
H -2.99155 1.60680 1.63956
C -5.52305 0.83066 2.08025
H -6.37690 -0.22971 -0.29031
C -5.21760 -0.62414 -2.71678
H -2.74028 0.44940 -2.49354
F -5.87464 2.11953 2.33467
F -6.66884 0.10730 2.08023
F -4.79456 0.41670 3.15116
F -5.05639 -1.97712 -2.68049
F -6.55298 -0.40204 -2.80793
F -4.66240 -0.20092 -3.87707
O 2.40251 -2.76814 2.37150
O 4.69743 -1.65808 -1.39316
C 1.70054 -2.54818 3.61702
C 1.72960 -3.85185 4.39272
H 0.67781 -2.22848 3.39563
H 2.19557 -1.73982 4.16487
H 1.20230 -3.72473 5.34400
H 1.23961 -4.65092 3.82912
H 2.75810 -4.15803 4.60761
C 5.26550 -0.79091 -2.40438
C 6.16456 -1.64003 -3.28341
H 5.82411 0.01077 -1.91023
H 4.44113 -0.34557 -2.96910
H 6.61382 -1.01251 -4.06026
H 6.97117 -2.09722 -2.70140
H 5.59431 -2.43453 -3.77394

Entry 5

Free Energy = -2910.591220
Zero-point Energy = -2910.499551
Potential Energy = -2911.20607672
Nimag = 1 (-232.4418 cm-1)

Charge = 0 Multiplicity = 1
C -0.26336 -3.63045 0.48626
C 0.87779 -3.75128 -0.32792
C 1.45525 -5.02492 -0.48264
C 0.91009 -6.14287 0.14771
C -0.22611 -6.00861 0.95163
C -0.80907 -4.74812 1.11760
C 1.46979 -2.61151 -1.06097
C 0.73347 -1.45109 -1.33523
N 1.08557 -0.61133 -2.35753
O 0.41851 0.48592 -2.50095
O 2.00818 -0.88619 -3.15992
C 3.16473 -2.08976 0.28030
C 3.82151 -1.08235 -0.53175
O 3.61349 0.13424 -0.50730
C 2.51306 -1.71133 1.51656
O 2.03727 -0.60513 1.80776
N 2.91543 2.06425 1.55828
C 4.27741 1.66039 2.04107
C 2.97885 3.08135 0.41174
C 1.57688 3.56440 -0.01725
C 1.70067 4.48195 -1.25310
C 2.61500 5.68224 -0.97738
C 3.98934 5.22181 -0.47920
C 3.87000 4.28909 0.74001
N 0.66395 2.45431 -0.27221
C -0.65687 2.46040 0.08733
N -1.36967 1.48887 -0.56324
C -2.70871 1.08629 -0.43058
S -1.30733 3.55801 1.20296
C 2.05756 2.45546 2.72334
H 1.12997 4.14804 0.79148
H 2.08780 3.89782 -2.09885
H 0.69428 4.81544 -1.52601
H 2.72197 6.28483 -1.88610
H 2.14806 6.33026 -0.22308
H 4.51395 4.69157 -1.28570
H 4.61227 6.08239 -0.21197
H 3.44865 4.84832 1.58538
H 4.87059 3.96029 1.03211
H 3.42988 2.50371 -0.40042
H -0.85698 1.02212 -1.32639
H 0.90958 1.83408 -1.04871
H 2.07665 1.63003 3.43393
H 2.46210 3.35757 3.18350
H 1.03362 2.62667 2.39552
H 4.15520 0.75756 2.63775
H 4.90611 1.44489 1.17955
H 4.70187 2.45632 2.65145
H 3.62457 -3.06994 0.27577
H 2.51909 1.18406 1.16884
H 2.19420 -2.88378 -1.82125
H -0.09755 -1.10589 -0.74140
H 2.33640 -5.13571 -1.10923
H 1.36823 -7.11761 0.00831
H -0.65612 -6.87788 1.44043
H -1.69515 -4.63559 1.73565
H -0.73571 -2.66385 0.62733
C -3.44467 1.16558 0.76089
C -4.75549 0.68474 0.79516
C -5.35684 0.11462 -0.32757
C -4.61028 0.02462 -1.50446
C -3.30295 0.50390 -1.56352
H -2.99743 1.59778 1.64380
C -5.54915 0.82543 2.06893
H -6.37499 -0.25218 -0.28721
C -5.21220 -0.64573 -2.71218
H -2.73904 0.43566 -2.48785

F -6.18612 2.02623 2.14126
F -6.51014 -0.12574 2.18434
F -4.76984 0.73658 3.17571
F -5.02841 -1.99598 -2.68367
F -6.55123 -0.44493 -2.79603
F -4.66932 -0.20757 -3.87291
O 2.42179 -2.76143 2.37311
O 4.70585 -1.64319 -1.39550
C 1.72155 -2.54404 3.62002
C 1.75625 -3.84783 4.39530
H 0.69737 -2.22752 3.40072
H 2.21506 -1.73426 4.16715
H 1.23051 -3.72266 5.34770
H 1.26763 -4.64827 3.83246
H 2.78613 -4.15084 4.60801
C 5.26898 -0.77414 -2.40786
C 6.16971 -1.62011 -3.28821
H 5.82543 0.02972 -1.91483
H 4.44199 -0.33203 -2.97129
H 6.61548 -0.99108 -4.06585
H 6.97888 -2.07431 -2.70743
H 5.60157 -2.41673 -3.77776

Entry 6

Free Energy = -2910.580043
Zero-point Energy = -2910.486501
Potential Energy = -2911.19281088
Nimag = 1 (-112.2684 cm-1)

Charge = 0 Multiplicity = 1
C -4.30200 0.07405 0.51852
C -3.21719 -0.13399 -0.34476
C -3.11503 -1.36524 -1.02319
C -4.07308 -2.35607 -0.84062
C -5.15933 -2.15680 0.01770
C -5.25479 -0.93711 0.68280
N -2.18745 0.78295 -0.60464
C -1.99101 2.09993 -0.26098
S -2.98266 3.02588 0.74128
C -3.90662 -3.68219 -1.53738
C -6.40294 -0.67331 1.62663
N -0.84493 2.59140 -0.82571
C -0.48110 3.99949 -0.83248
C 1.04504 4.17351 -0.70919
C 1.41491 5.66353 -0.66906
C 0.90544 6.38325 -1.93112
C -0.60613 6.19733 -2.11445
C -0.98240 4.71050 -2.10804
N 1.61878 3.39184 0.47160
C 1.01322 3.70333 1.80679
C 3.11801 3.47683 0.53668
O 2.08655 1.22997 -1.65229
N 1.40494 0.17811 -1.77998
O 0.19524 0.24672 -2.19806
C 1.91979 -1.06577 -1.50992
C 3.23090 -1.24056 -1.08846
C 3.88701 -2.55179 -1.12369
C 3.17467 -3.76309 -1.01473
C 3.83593 -4.98505 -1.10304
C 5.22028 -5.02589 -1.30868
C 5.93939 -3.83291 -1.41505
C 5.28012 -2.60831 -1.31554
C 3.32332 -0.96833 1.37342
C 2.00930 -0.42572 1.58911
O 1.62994 0.75089 1.51634
C 4.53078 -0.19456 1.53249
O 4.67234 1.02913 1.54459
H -0.98070 4.45895 0.02491
H -0.55570 4.20914 -2.98786
H -2.06836 4.58305 -2.15769
H -0.93577 6.66269 -3.05009
H -1.14070 6.71163 -1.30385
H 1.43418 5.98847 -2.80973
H 1.15984 7.44691 -1.86546
H 0.97036 6.13568 0.21664
H 2.49903 5.78636 -0.59343
H 1.52371 3.70034 -1.57323
H -1.44680 0.39647 -1.19279
H -0.37005 1.98958 -1.50572
H 1.47097 3.02940 2.52907
H 1.22105 4.74262 2.06307
H -0.06061 3.52177 1.77422
H 3.47948 2.64779 1.14694
H 3.51411 3.36638 -0.47297
H 3.40497 4.43986 0.95933
H 3.42293 -2.02908 1.55843
H 1.42610 2.38820 0.31037
H 1.21220 -1.86420 -1.67121
H 3.86804 -0.36479 -1.12657
H 5.84236 -1.68243 -1.39085
H 7.01372 -3.85598 -1.57244
H 5.73246 -5.98081 -1.38054
H 3.27261 -5.90876 -1.00941
H 2.10403 -3.74952 -0.83725
H -2.28599 -1.53423 -1.70347
H -5.90879 -2.92556 0.15399
H -4.39679 1.01438 1.04316
F -3.18444 -4.55809 -0.78385
F -3.25395 -3.56481 -2.71978
F -5.09432 -4.28048 -1.79196
F -5.97353 -0.51034 2.90618
F -7.07652 0.45775 1.29968
F -7.30556 -1.68309 1.64053
C -0.23105 -1.03573 2.19501
C -0.99521 -2.29520 2.56154
H -0.67751 -0.52322 1.33797
H -0.20326 -0.32460 3.02715
H -2.02605 -2.03782 2.82579
H -1.02124 -2.99956 1.72449
H -0.53395 -2.79562 3.41842

C 6.89467 -0.38724 1.84452
C 7.92760 -1.48106 2.05190
H 6.83890 0.28718 2.70525
H 7.12242 0.22466 0.96412
H 8.91883 -1.03513 2.18799
H 7.69257 -2.07711 2.93900
H 7.96616 -2.15340 1.18934
O 1.11976 -1.42568 1.86983
O 5.61671 -1.02570 1.66184

Entry 7

Free Energy = -2910.597760
Zero-point Energy = -2910.505993
Potential Energy = -2911.21168465
Nimag = 1 (-230.8241 cm-1)

Charge = 0 Multiplicity = 1
C 2.46513 -2.53302 0.43077
C 1.93896 -1.55970 -0.43432
C 2.81333 -0.66995 -1.07376
C 4.19114 -0.76532 -0.86329
C 4.72532 -1.74309 -0.02557
C 3.84423 -2.61757 0.61765
N 0.56022 -1.37558 -0.64349
C -0.43773 -2.31343 -0.69145
S -0.16795 -3.99258 -0.70160
C 5.09398 0.23781 -1.52931
C 4.40601 -3.69759 1.50504
N -1.67502 -1.75842 -0.75495
C -2.90198 -2.49251 -1.03699
C -4.02107 -2.12961 -0.03379
C -5.30652 -2.91029 -0.34728
C -5.77421 -2.64514 -1.78904
C -4.67546 -2.97963 -2.80419
C -3.38322 -2.22147 -2.47918
N -3.57146 -2.30938 1.41932
C -3.07459 -3.67765 1.77538
C -4.61254 -1.86139 2.40018
O -1.55408 -0.68124 2.29111
N -1.81869 0.56442 2.10586
O -3.01032 0.97141 2.16109
C -0.76738 1.40572 1.86673
C -0.97333 2.75798 1.58031
C 0.10028 3.75976 1.71211
C 1.46576 3.41999 1.75342
C 2.43899 4.40473 1.92070
C 2.07080 5.74810 2.04743
C 0.71805 6.10055 2.00571
C -0.25457 5.11620 1.83829
C -1.41200 2.95585 -0.66358
C -2.59470 2.13235 -0.76138
O -2.65823 0.91641 -0.97292
C -0.15548 2.54051 -1.24498
O 0.27018 1.38661 -1.38034
H -2.65990 -3.55478 -0.95213
H -3.53417 -1.14209 -2.60514
H -2.57730 -2.51620 -3.15918
H -5.00682 -2.73207 -3.81888
H -4.48123 -4.06104 -2.79158
H -6.05775 -1.58864 -1.88955
H -6.67738 -3.23310 -1.98599
H -5.12941 -3.98605 -0.22264
H -6.10354 -2.62941 0.34730
H -4.21384 -1.05388 -0.10953
H 0.29751 -0.40983 -0.87097
H -1.75532 -0.73771 -0.82417
H -2.74485 -3.65028 2.81453
H -3.88240 -4.40179 1.66642
H -2.23108 -3.94401 1.13810
H -4.13341 -1.76968 3.37461
H -4.98366 -0.88289 2.09992
H -5.41889 -2.59250 2.44702
H -1.59235 4.02330 -0.66566
H -2.76126 -1.65199 1.59150
H 0.18969 0.90908 1.86755
H -1.97873 3.12625 1.75092
H -1.30449 5.39518 1.80667
H 0.42141 7.14047 2.10533
H 2.83110 6.51221 2.17948
H 3.48709 4.12207 1.95361
H 1.77613 2.38482 1.65800
H 2.40441 0.09477 -1.72480
H 5.79429 -1.81843 0.12892
H 1.80154 -3.20912 0.94931
F 5.02997 1.45888 -0.92078
F 4.76056 0.44957 -2.82887
F 6.39568 -0.13327 -1.50863
F 5.52390 -3.29039 2.16152
F 3.52375 -4.11133 2.44629
F 4.76362 -4.80440 0.79589
C -4.97155 2.16762 -0.47625
C -6.06888 3.19709 -0.27433
H -4.91289 1.46643 0.36290
H -5.11940 1.59557 -1.39794
H -7.03943 2.69390 -0.20824
H -5.91143 3.76154 0.64975
H -6.10411 3.90199 -1.11062
C 1.90742 3.35615 -2.15722
C 2.51454 4.69394 -2.53665
H 1.80814 2.69512 -3.02373
H 2.50834 2.84161 -1.40184
H 3.51652 4.53674 -2.94905
H 1.90641 5.20061 -3.29235
H 2.59897 5.34643 -1.66258
O -3.71823 2.87663 -0.55817
O 0.59139 3.61366 -1.61360

Entry 8

Free Energy = -2910.597259
Zero-point Energy = -2910.505777
Potential Energy = -2911.21153423
Nimag = 1 (-227.9129 cm-1)

Charge = 0 Multiplicity = 1
C -2.46524 -2.56763 -0.39847
C -1.93638 -1.58048 0.44660
C -2.81136 -0.68354 1.07840
C -4.18881 -0.78628 0.87807
C -4.72623 -1.77860 0.05713
C -3.84694 -2.66101 -0.57363
N -0.55795 -1.38871 0.65071
C 0.44764 -2.31863 0.69780
S 0.19212 -3.99978 0.71166
C -5.09196 0.21959 1.53958
C -4.38089 -3.70898 -1.51541
N 1.68067 -1.75351 0.75714
C 2.91378 -2.47752 1.03875
C 4.02898 -2.10731 0.03394
C 5.32098 -2.87700 0.34781
C 5.78764 -2.60559 1.78871
C 4.69264 -2.94781 2.80528
C 3.39394 -2.20080 2.48022
N 3.57962 -2.29339 -1.41851
C 3.09149 -3.66559 -1.77137
C 4.61705 -1.84076 -2.40110
O 1.55134 -0.67892 -2.28931
N 1.81039 0.56820 -2.10579
O 3.00030 0.98033 -2.16181
C 0.75556 1.40517 -1.86749
C 0.95624 2.75849 -1.58180
C -0.12111 3.75620 -1.71439
C -1.48524 3.41130 -1.75690
C -2.46203 4.39245 -1.92468
C -2.09879 5.73723 -2.05070
C -0.74741 6.09475 -2.00785
C 0.22875 5.11400 -1.83997
C 1.39409 2.95899 0.66070
C 2.58129 2.14192 0.75901
O 2.65120 0.92651 0.97125
C 0.14001 2.53649 1.24222
O -0.27891 1.38009 1.37726
H 2.67999 -3.54177 0.95557
H 3.53617 -1.12009 2.60468
H 2.59094 -2.50131 3.16115
H 5.02276 -2.69606 3.81935
H 4.50744 -4.03083 2.79437
H 6.06221 -1.54650 1.88723
H 6.69599 -3.18547 1.98581
H 5.15252 -3.95439 0.22519
H 6.11524 -2.59089 -0.34778
H 4.21298 -1.02992 0.10759
H -0.30069 -0.42050 0.87346
H 1.75340 -0.73219 0.82493
H 2.76127 -3.64262 -2.81048
H 3.90395 -4.38428 -1.66112
H 2.24996 -3.93610 -1.13322
H 4.13666 -1.75457 -3.37542
H 4.98164 -0.85902 -2.10345
H 5.42828 -2.56657 -2.44682
H 1.56857 4.02740 0.66309
H 2.76498 -1.64158 -1.59153
H -0.19943 0.90450 -1.86769
H 1.96016 3.13042 -1.75318
H 1.27759 5.39690 -1.80740
H -0.45459 7.13580 -2.10697
H -2.86186 6.49852 -2.18315
H -3.50902 4.10584 -1.95863
H -1.79177 2.37491 -1.66227
H -2.40113 0.08934 1.71889
H -5.79571 -1.86464 -0.08386
H -1.80320 -3.25617 -0.90390
F -5.05232 1.42925 0.90653
F -4.74014 0.46072 2.82909
F -6.38954 -0.16653 1.54763
F -4.20302 -3.35489 -2.82078
F -3.76181 -4.90529 -1.36010
F -5.70943 -3.92511 -1.35410
C 4.95801 2.18988 0.47465
C 6.05015 3.22533 0.27520
H 4.90418 1.48923 -0.36528
H 5.10764 1.61766 1.39593
H 7.02342 2.72732 0.20991
H 5.89096 3.78987 -0.64852
H 6.08054 3.92955 1.11224
C -1.92745 3.34029 2.15472
C -2.54217 4.67456 2.53432
H -1.82439 2.67977 3.02118
H -2.52553 2.82246 1.39929
H -3.54319 4.51157 2.94677
H -1.93688 5.18460 3.29003
H -2.63038 5.32665 1.66033
O 3.70081 2.89215 0.55559
O -0.61297 3.60529 1.61099

Entry 9

Free Energy = -2910.576630
Zero-point Energy = -2910.484072
Potential Energy = -2911.19115037
Nimag = 1 (-196.5015 cm-1)

Charge = 0 Multiplicity = 1
C 3.10753 -2.19915 0.42729
C 2.35794 -1.25767 -0.29602
C 3.00513 -0.13327 -0.82735
C 4.38037 0.03522 -0.65237
C 5.13786 -0.90544 0.04377

C 4.48143 -2.01605 0.58170
N 0.96327 -1.33395 -0.46080
C 0.16277 -2.43749 -0.60945
S 0.73677 -4.02935 -0.77033
C 5.02828 1.26847 -1.22288
C 5.28197 -3.06181 1.31382
N -1.15778 -2.12630 -0.61267
C -2.22547 -3.04346 -1.00373
C -3.44525 -2.92663 -0.06100
C -4.65438 -3.71500 -0.60667
C -5.02035 -3.34076 -2.04834
C -3.81792 -3.54743 -2.97163
C -2.62636 -2.73102 -2.46769
N -3.19844 -3.47157 1.37183
C -4.15097 -2.84158 2.35972
C -1.80086 -3.41206 1.94066
O -2.07160 -0.42477 3.03375
N -2.43634 0.67025 2.48864
O -3.66769 0.93031 2.34883
C -1.46784 1.55212 2.08694
C -1.79901 2.76978 1.46745
C -0.85726 3.91673 1.50041
C 0.53149 3.76118 1.65964
C 1.37159 4.87397 1.71757
C 0.84303 6.16488 1.61643
C -0.53555 6.33395 1.45639
C -1.37401 5.22058 1.39718
C -2.05465 2.51816 -0.65865
C -3.02932 1.44386 -0.69531
O -2.80834 0.22890 -0.67498
C -0.71034 2.30760 -1.16757
O -0.03251 1.27615 -1.10324
H -1.81458 -4.05650 -0.95994
H -2.85924 -1.66176 -2.53472
H -1.73895 -2.90740 -3.08413
H -4.06260 -3.24783 -3.99667
H -3.55911 -4.61477 -3.00762
H -5.34509 -2.29292 -2.08830
H -5.87344 -3.94977 -2.36660
H -4.41061 -4.78845 -0.58221
H -5.52247 -3.56990 0.04376
H -3.68785 -1.86868 0.07097
H 0.51096 -0.42743 -0.61861
H -1.43661 -1.13887 -0.58964
H -4.11454 -3.42255 3.28204
H -3.81067 -1.82158 2.55013
H -5.16085 -2.85568 1.95527
H -1.83914 -3.91184 2.91013
H -1.11140 -3.93538 1.28060
H -1.52320 -2.36869 2.07736
H -2.46375 3.49582 -0.88432
H -3.43045 -4.46704 1.31771
H -0.46336 1.20663 2.27331
H -2.84574 3.04433 1.54953
H -2.44508 5.35906 1.27419
H -0.95817 7.33168 1.38070
H 1.49873 7.02933 1.66514
H 2.44100 4.73207 1.84468
H 0.96409 2.76954 1.74092
H 2.42134 0.60395 -1.36804
H 6.20447 -0.77416 0.17255
H 2.61905 -3.05838 0.86258
F 4.59018 2.40300 -0.60612
F 4.74800 1.42891 -2.54423
F 6.37585 1.25713 -1.10396
F 6.38158 -2.54008 1.91485
F 4.56151 -3.68557 2.27848
F 5.73023 -4.03779 0.47601
C -5.37342 1.00085 -0.52325
C -6.67112 1.78804 -0.53054
H -5.21005 0.49180 0.43183
H -5.34728 0.26075 -1.33013
H -7.51649 1.10579 -0.39088
H -6.68611 2.52199 0.28054
H -6.80816 2.31459 -1.48022
C 1.15071 3.41829 -2.19649
C 1.43873 4.76873 -2.82522
H 1.25420 2.60381 -2.92013
H 1.81720 3.21749 -1.35250
H 2.46807 4.78592 -3.19782
H 0.76469 4.96164 -3.66545
H 1.32280 5.57306 -2.09296
O -4.29313 1.94007 -0.71401
O -0.21417 3.44420 -1.71544

Entry 10

Free Energy = -2910.595388
Zero-point Energy = -2910.502766
Potential Energy = -2911.20821853
Nimag = 1 (-246.3116 cm-1)

Charge = 0 Multiplicity = 1
C -0.11274 4.71832 -1.97395
C -0.49652 3.42867 -1.56043
C -1.86116 3.17492 -1.33485
C -2.81738 4.17238 -1.53269
C -2.42358 5.44736 -1.94630
C -1.06676 5.71644 -2.16271
C 0.47096 2.32616 -1.38974
C 1.58366 2.22055 -2.23441
N 2.27199 1.04768 -2.37116
O 3.29363 1.00600 -3.11361
O 1.87607 -0.00929 -1.75912
C 1.17063 2.80356 0.71912
C 0.05244 2.36161 1.52679
O -0.24877 1.19802 1.82477
C 2.45367 2.13469 0.78895
O 2.71310 0.99212 1.17934
N 3.80590 -1.92877 -1.21131
C 4.96901 -1.44295 -2.02399

C 4.12475 -1.97577 0.28704
C 2.92596 -2.47599 1.12122
C 3.27006 -2.39820 2.62463
C 4.53172 -3.20204 2.96169
C 5.71499 -2.74817 2.09949
C 5.37768 -2.80888 0.59873
N 1.71268 -1.72656 0.82334
C 0.49042 -2.28850 0.64103
N -0.52483 -1.37002 0.66016
C -1.88600 -1.57314 0.36858
S 0.24811 -3.95944 0.43653
C 3.26338 -3.19761 -1.79613
H 2.71724 -3.51981 0.87298
H 3.40342 -1.34572 2.90607
H 2.40769 -2.77501 3.18395
H 4.77143 -3.09130 4.02509
H 4.34184 -4.27064 2.79106
H 5.98965 -1.71835 2.36599
H 6.59694 -3.36861 2.29280
H 5.21210 -3.85458 0.30938
H 6.23435 -2.44503 0.02468
H 4.30708 -0.92506 0.53885
H -0.30518 -0.44590 1.05319
H 1.77616 -0.71218 0.96206
H 3.05943 -3.01398 -2.85156
H 4.00374 -3.99239 -1.69799
H 2.33952 -3.47571 -1.28956
H 4.58753 -1.10897 -2.98733
H 5.42937 -0.59445 -1.51818
H 5.69276 -2.24781 -2.14803
H 1.23661 3.87557 0.58483
H 3.05494 -1.19881 -1.34722
H 0.06225 1.38434 -1.04200
H 2.00210 3.03449 -2.80630
H -2.17378 2.18475 -1.01498
H -3.86740 3.95268 -1.36343
H -3.16498 6.22635 -2.09747
H -0.75254 6.70715 -2.47794
H 0.93633 4.94760 -2.13502
C -2.83055 -0.90050 1.15301
C -4.19380 -1.01751 0.86530
C -4.63903 -1.80576 -0.19378
C -3.68663 -2.46620 -0.97770
C -2.32286 -2.35322 -0.71406
H -2.49066 -0.29004 1.98257
C -5.17441 -0.24916 1.70991
H -5.69592 -1.89850 -0.40971
C -4.15219 -3.34325 -2.11088
H -1.60127 -2.85553 -1.34217
F -5.11829 1.09166 1.45635
F -6.45680 -0.62766 1.50228
F -4.92752 -0.38889 3.03824
F -4.46791 -4.59828 -1.68670
F -5.26753 -2.85337 -2.71219
F -3.21277 -3.48750 -3.07658
O 3.42930 2.95624 0.30920
O -0.72073 3.40592 1.91399
C 4.77566 2.43985 0.25190
C 5.68886 3.58339 -0.15112
H 4.80685 1.62828 -0.48343
H 5.04316 2.03075 1.23080
H 6.72243 3.22635 -0.21015
H 5.40742 3.98307 -1.12976
H 5.64657 4.39401 0.58259
C -1.92400 3.10538 2.66210
C -2.57381 4.42558 3.03166
H -1.65248 2.52312 3.54764
H -2.58220 2.49178 2.03975
H -3.49241 4.23465 3.59605
H -1.90683 5.03040 3.65365
H -2.83133 4.99996 2.13694

Entry 11

Free Energy = -2910.587464
Zero-point Energy = -2910.495715
Potential Energy = -2911.20181128
Nimag = 1 (-297.4989 cm-1)

Charge = 0 Multiplicity = 1
C -0.41359 4.55734 -1.93852
C -0.68901 3.26248 -1.46187
C -2.01414 2.94261 -1.11856
C -3.03725 3.88197 -1.26045
C -2.75032 5.16367 -1.73648
C -1.43334 5.49821 -2.07260
C 0.35212 2.21630 -1.34408
C 1.34880 2.11899 -2.33097
N 2.07836 0.97535 -2.48881
O 2.94888 0.90341 -3.40071
O 1.86100 -0.02401 -1.71461
C 1.19883 2.73417 0.63808
C 0.09786 2.35039 1.51622
O -0.27333 1.20439 1.78430
C 2.45449 2.00784 0.73440
O 2.62410 0.90358 1.25799
N 3.96703 -1.70016 -1.10212
C 5.07555 -0.97942 -1.81201
C 4.24560 -1.85858 0.39418
C 3.05696 -2.50332 1.13701
C 3.35467 -2.54655 2.65198
C 4.65829 -3.29505 2.95640
C 5.83268 -2.68442 2.18268
C 5.54383 -2.63087 0.67187
N 1.81797 -1.78536 0.86744
C 0.61778 -2.37334 0.64048
N -0.42208 -1.47930 0.68821
C -1.77963 -1.67912 0.38368
S 0.43468 -4.03909 0.35809
C 3.60653 -2.95883 -1.83045
H 2.91021 -3.52917 0.78920

H 3.41234 -1.51847 3.03247
H 2.50427 -3.02733 3.14614
H 4.85856 -3.27039 4.03342
H 4.54682 -4.35297 2.68116
H 6.02492 -1.66711 2.54974
H 6.74972 -3.25937 2.35209
H 5.46114 -3.65537 0.28679
H 6.38676 -2.15786 0.15978
H 4.34620 -0.82462 0.74157
H -0.21447 -0.55420 1.07963
H 1.84961 -0.77429 1.04168
H 3.39827 -2.69198 -2.86694
H 4.44125 -3.65907 -1.79013
H 2.71469 -3.39954 -1.38498
H 4.67775 -0.61343 -2.75849
H 5.38870 -0.13018 -1.20396
H 5.91171 -1.65834 -1.97637
H 1.27240 3.80371 0.49429
H 3.13343 -1.06669 -1.21106
H 0.02192 1.26941 -0.93243
H 1.60023 2.89865 -3.03383
H -2.24431 1.94650 -0.75131
H -4.05595 3.61060 -0.99976
H -3.54402 5.89682 -1.84517
H -1.20179 6.49368 -2.43998
H 0.60306 4.83669 -2.19970
C -2.72045 -0.94725 1.12095
C -4.08242 -1.05557 0.82824
C -4.53495 -1.89314 -0.18964
C -3.58769 -2.61145 -0.92641
C -2.22337 -2.50943 -0.65859
H -2.37789 -0.29427 1.91648
C -5.05258 -0.22453 1.62372
H -5.59155 -1.97902 -0.40937
C -4.05919 -3.54460 -2.01154
H -1.50717 -3.06075 -1.24991
F -4.94048 1.10464 1.32892
F -6.34338 -0.56198 1.39885
F -4.84125 -0.32864 2.96180
F -5.17192 -3.08069 -2.63798
F -3.12176 -3.74690 -2.96817
F -4.38305 -4.77300 -1.52000
O 3.56713 2.56890 0.17760
O -0.56022 3.43502 1.98836
C 3.61132 3.94257 -0.27416
C 5.02172 4.21218 -0.76673
H 3.35541 4.60275 0.56234
H 2.88449 4.08842 -1.07807
H 5.09813 5.24851 -1.11166
H 5.74995 4.06038 0.03544
H 5.27501 3.55159 -1.60103
C -1.73674 3.19841 2.80335
C -2.27082 4.55020 3.23719
H -1.45098 2.57838 3.65811
H -2.46955 2.64475 2.20932
H -3.16310 4.40780 3.85544
H -1.52752 5.09556 3.82675
H -2.54547 5.15977 2.37124

Entry 12

Free Energy = -2910.586167
Zero-point Energy = -2910.493925
Potential Energy = -2911.19992113
Nimag = 1 (-245.9705 cm-1)

Charge = 0 Multiplicity = 1
C 3.82239 0.41947 -0.52700
C 2.69415 0.10009 0.24089
C 2.71546 -1.05779 1.03783
C 3.85006 -1.86461 1.07719
C 4.98656 -1.54363 0.32993
C 4.95256 -0.40102 -0.46847
N 1.49181 0.83119 0.23272
C 1.27913 2.17625 0.11916
S 2.48109 3.32580 -0.21496
C 3.84547 -3.12602 1.90117
C 6.17521 -0.01058 -1.25867
N -0.03722 2.51746 0.29443
C -0.47613 3.89906 0.48038
C -1.86026 4.18013 -0.14051
C -2.18879 5.67599 -0.02136
C -2.18467 6.11231 1.45577
C -0.85463 5.78360 2.14354
C -0.49448 4.30234 1.97059
N -1.96727 3.65157 -1.57556
C -0.82031 3.98679 -2.47579
C -3.26747 4.01224 -2.23109
O -4.07974 1.80917 -0.01954
N -3.55682 0.80133 -0.58922
O -2.57933 0.96501 -1.40476
C -4.06127 -0.44036 -0.33925
C -3.50445 -1.59409 -0.90358
C -4.25448 -2.85828 -0.96513
C -5.27667 -3.18395 -0.05082
C -5.98104 -4.37949 -0.17086
C -5.68303 -5.27469 -1.20582
C -4.66927 -4.96652 -2.11625
C -3.95863 -3.77229 -1.99387
C -1.76059 -2.33544 0.45361
C -1.64329 -1.21857 1.35332
O -0.91763 -0.21344 1.27152
C -0.80561 -2.73502 -0.56835
O -0.75166 -3.88266 -1.00849
H 0.27458 4.51865 -0.01720
H -1.21499 3.67051 2.50810
H 0.49573 4.09352 2.38712
H -0.90575 6.03413 3.20898
H -0.05485 6.40152 1.71322
H -3.00531 5.60336 1.97946
H -2.39434 7.18599 1.51271

H -1.45371 6.27021 -0.58010
H -3.17265 5.88720 -0.44811
H -2.62664 3.59849 0.38281
H 0.66493 0.27179 0.48162
H -0.65063 1.77877 0.63892
H -1.01110 3.52968 -3.44744
H -0.75088 5.06929 -2.58916
H 0.10683 3.59275 -2.06523
H -3.37093 3.39325 -3.12278
H -4.07916 3.78709 -1.54107
H -3.26335 5.06482 -2.51149
H -2.30749 -3.17623 0.85848
H -2.02952 2.60339 -1.47468
H -4.89215 -0.43108 0.34885
H -2.78271 -1.42227 -1.69322
H -3.16385 -3.54352 -2.69636
H -4.42562 -5.65759 -2.91751
H -6.23472 -6.20570 -1.29658
H -6.76258 -4.61676 0.54499
H -5.51263 -2.51021 0.76645
H 1.84301 -1.31504 1.62748
H 5.86972 -2.16950 0.36767
H 3.81482 1.29642 -1.15682
F 3.55987 -4.22214 1.14642
F 2.92910 -3.09254 2.89837
F 5.05204 -3.36334 2.47722
F 6.95694 -1.07778 -1.55951
F 5.86083 0.59346 -2.43198
F 6.96385 0.86394 -0.57501
C -2.56528 -0.27151 3.35673
C -3.54808 -0.67864 4.43909
H -2.87355 0.65301 2.85752
H -1.55856 -0.12286 3.75884
H -3.60163 0.10694 5.20003
H -4.55088 -0.82498 4.02626
H -3.23334 -1.60721 4.92469
C 0.85537 -2.06007 -2.16660
C 0.94768 -0.85854 -3.09125
H 0.46884 -2.94088 -2.68160
H 1.83112 -2.31638 -1.73997
H 1.64372 -1.07990 -3.90769
H -0.03010 -0.62634 -3.52502
H 1.31052 0.02688 -2.56206
O -2.52716 -1.33794 2.38062
O -0.03426 -1.72918 -1.06988

Entry 13

Free Energy = -2910.594984
Zero-point Energy = -2910.501954
Potential Energy = -2911.20790185
Nimag = 1 (-327.6935 cm-1)

Charge = 0 Multiplicity = 1
C 5.37230 3.05816 -0.87393
C 4.09050 3.01500 -0.29492
C 3.70213 4.06906 0.55474
C 4.56725 5.13160 0.80821
C 5.83573 5.16709 0.21712
C 6.23478 4.12624 -0.62583
C 3.20096 1.88814 -0.62425
C 1.80966 2.04367 -0.65150
N 0.99572 1.14096 -1.27077
O 1.47747 0.16305 -1.92862
O -0.26569 1.31251 -1.20670
C 3.73997 0.50239 1.15601
C 2.40616 0.26127 1.65664
O 1.61127 -0.61283 1.29992
C 4.53097 -0.54158 0.53252
O 4.14818 -1.59178 0.01435
N 1.32259 -2.59988 -2.08047
C 2.64004 -2.48246 -2.79198
C 1.45544 -3.31721 -0.72885
C 0.09656 -3.40285 -0.00638
C 0.29535 -4.01178 1.39720
C 0.95131 -5.39676 1.31359
C 2.27366 -5.33507 0.53933
C 2.08781 -4.70878 -0.85524
N -0.54025 -2.09058 0.04856
C -1.86834 -1.86995 -0.14601
N -2.17878 -0.52875 -0.11098
C -3.45040 0.06912 -0.12713
S -2.98401 -3.10212 -0.46752
C 0.26870 -3.13706 -2.99790
H -0.58368 -4.05646 -0.55896
H 0.91606 -3.33322 1.99530
H -0.68574 -4.07374 1.87890
H 1.12064 -5.78922 2.32260
H 0.26528 -6.09593 0.81543
H 3.00236 -4.73793 1.10259
H 2.70264 -6.33712 0.42819
H 1.45183 -5.36470 -1.46439
H 3.06201 -4.64321 -1.34745
H 2.12708 -2.65995 -0.16696
H -1.41438 0.09941 -0.38682
H 0.02002 -1.35327 0.48219
H 0.26304 -2.52447 -3.89998
H 0.50493 -4.16986 -3.25518
H -0.70681 -3.08191 -2.51780
H 2.53013 -1.72832 -3.57109
H 3.39304 -2.16764 -2.06988
H 2.90030 -3.44249 -3.23716
H 4.30889 1.24510 1.69870
H 1.06884 -1.61477 -1.85716
H 3.60050 1.14816 -1.30733
H 1.27292 2.84013 -0.15937
H 2.72864 4.05085 1.03355
H 4.25293 5.93371 1.46940
H 6.50636 5.99803 0.41472
H 7.21717 4.14478 -1.08835
H 5.68805 2.24894 -1.52574

C -3.60278 1.26743 -0.83846
C -4.83109 1.93273 -0.83375
C -5.92295 1.42321 -0.13221
C -5.75607 0.23413 0.58409
C -4.53684 -0.44181 0.59965
H -2.76175 1.66995 -1.39325
C -4.94970 3.24179 -1.56890
H -6.87466 1.93918 -0.13581
C -6.93054 -0.35041 1.32498
H -4.42496 -1.35211 1.17165
F -4.31619 3.21775 -2.76875
F -6.23743 3.58968 -1.80709
F -4.39457 4.26949 -0.86555
F -6.55236 -1.07058 2.40996
F -7.78857 0.60584 1.76381
F -7.66142 -1.18981 0.54032
O 5.85633 -0.20148 0.54343
O 2.05201 1.20488 2.57334
C 6.77680 -1.14100 -0.05324
C 8.18135 -0.60415 0.15414
H 6.53824 -1.24916 -1.11699
H 6.64271 -2.11886 0.41973
H 8.90782 -1.29441 -0.28743
H 8.30421 0.37438 -0.32000
H 8.40762 -0.50184 1.21975
C 0.71305 1.12434 3.11725
C 0.56608 2.23274 4.14316
H 0.57342 0.13648 3.56686
H -0.00843 1.23009 2.30088
H -0.43813 2.19760 4.57801
H 1.29543 2.11924 4.95092
H 0.70600 3.21656 3.68481

Entry 14

Free Energy = -2910.594768
Zero-point Energy = -2910.501754
Potential Energy = -2911.20768947
Nimag = 1 (-253.9874 cm-1)

Charge = 0 Multiplicity = 1
C -3.68377 -4.07803 0.54737
C -4.07901 -3.02207 -0.29672
C -5.36310 -3.06710 -0.87051
C -6.22120 -4.13880 -0.62280
C -5.81534 -5.18152 0.21457
C -4.54450 -5.14424 0.80044
C -3.19444 -1.89117 -0.62558
C -1.80262 -2.04173 -0.65819
N -0.99447 -1.13390 -1.27743
O 0.26791 -1.29959 -1.21748
O -1.48271 -0.15661 -1.93144
C -3.73095 -0.51259 1.16011
C -2.39582 -0.26862 1.65594
O -1.60542 0.60946 1.29907
C -4.52801 0.53081 0.54327
O -4.15067 1.58303 0.02522
N -1.33649 2.60569 -2.07955
C -2.65609 2.48444 -2.78645
C -1.46753 3.31837 -0.72540
C -0.10641 3.40817 -0.00777
C -0.30260 4.01275 1.39811
C -0.96583 5.39464 1.32105
C -2.29084 5.32847 0.55175
C -2.10694 4.70729 -0.84532
N 0.53616 2.09847 0.04251
C 1.86418 1.88325 -0.15898
N 2.18024 0.54334 -0.12243
C 3.45230 -0.05321 -0.13803
S 2.97199 3.12007 -0.48985
C -0.28854 3.15028 -2.99940
H 0.56919 4.06575 -0.56132
H -0.91752 3.32958 1.99694
H 0.68010 4.07830 1.87609
H -1.13315 5.78327 2.33188
H -0.28533 6.09875 0.82225
H -3.01432 4.72591 1.11597
H -2.72534 6.32865 0.44526
H -1.47629 5.36812 -1.45472
H -3.08254 4.63848 -1.33430
H -2.13400 2.65643 -0.16284
H 1.41651 -0.08758 -0.39359
H -0.01900 1.35864 0.47841
H -0.28385 2.54062 -3.90347
H -0.53021 4.18287 -3.25246
H 0.68913 3.09774 -2.52337
H -2.54607 1.73235 -3.56751
H -3.40517 2.16510 -2.06227
H -2.92177 3.44432 -3.22874
H -4.29522 -1.25856 1.70321
H -1.07770 1.62098 -1.86004
H -3.59884 -1.15064 -1.30520
H -1.26113 -2.83736 -0.16994
H -5.68412 -2.25643 -1.51792
H -7.20547 -4.15869 -1.08123
H -6.48250 -6.01533 0.41182
H -4.22486 -5.94786 1.45723
H -2.70830 -4.05864 1.02203
C 3.59990 -1.26469 -0.82540
C 4.82977 -1.92979 -0.81778
C 5.92730 -1.40407 -0.14074
C 5.76568 -0.19826 0.55137
C 4.54611 0.47377 0.56891
H 2.75402 -1.68072 -1.36321
C 4.94699 -3.22327 -1.58038
H 6.88101 -1.91667 -0.14728
C 6.92878 0.34132 1.34236
H 4.44021 1.39749 1.11944
F 4.75431 -3.04743 -2.91597
F 6.15907 -3.80909 -1.43420
F 4.01790 -4.13317 -1.18117

F 7.09431 -0.32899 2.51952
F 8.10322 0.21900 0.67100
F 6.78626 1.64827 1.66046
O -5.85243 0.18740 0.56080
O -2.03458 -1.21449 2.56752
C -6.77850 1.12626 -0.02820
C -8.18041 0.58412 0.18322
H -6.54492 1.23944 -1.09251
H -6.64551 2.10265 0.44811
H -8.91102 1.27401 -0.25207
H -8.30239 -0.39273 -0.29458
H -8.40152 0.47653 1.24939
C -0.69338 -1.13200 3.10556
C -0.53738 -2.24589 4.12418
H -0.55545 -0.14627 3.56039
H 0.02464 -1.23016 2.28523
H 0.46861 -2.20936 4.55476
H -1.26358 -2.14015 4.93581
H -0.67542 -3.22749 3.66052

Entry 15

Free Energy = -2910.596328
Zero-point Energy = -2910.504300
Potential Energy = -2911.21031364
Nimag = 1 (-174.4923 cm-1)

Charge = 0 Multiplicity = 1
C -4.91126 -2.79755 -1.29063
C -3.99192 -2.92957 -0.23168
C -4.23452 -3.91556 0.74518
C -5.35228 -4.74356 0.66702
C -6.25578 -4.60133 -0.39129
C -6.02977 -3.62566 -1.36806
C -2.76912 -2.12486 -0.12422
C -2.24871 -1.38057 -1.17828
N -0.95928 -0.92078 -1.15724
O -0.57927 -0.12511 -2.08295
O -0.14080 -1.28569 -0.26088
C -3.53252 -0.51034 1.49463
C -2.24315 -0.03555 1.92500
O -1.61032 0.93216 1.48437
C -4.39284 0.27990 0.64910
O -4.06370 1.15869 -0.15327
N -1.24395 2.61992 -2.11546
C -2.56453 2.38881 -2.79132
C -1.39882 3.35977 -0.77781
C -0.04251 3.46687 -0.04845
C -0.23898 4.13889 1.32662
C -0.90513 5.51416 1.19119
C -2.23503 5.40739 0.43542
C -2.04998 4.73934 -0.93941
N 0.56728 2.14838 0.08137
C 1.86441 1.85147 -0.19328
N 2.12994 0.51216 -0.03381
C 3.36367 -0.15525 -0.09943
S 2.99265 2.99695 -0.73256
C -0.25073 3.20921 -3.07098
H 0.65129 4.08112 -0.62798
H -0.85160 3.48269 1.95625
H 0.74436 4.22678 1.80017
H -1.06717 5.94710 2.18467
H -0.23200 6.19827 0.65580
H -2.94850 4.81941 1.02737
H -2.68058 6.39831 0.29435
H -1.42427 5.38551 -1.56860
H -3.02429 4.64728 -1.42821
H -2.06065 2.70225 -0.20311
H 1.31282 -0.10831 -0.10982
H 0.00274 1.46851 0.59914
H -0.21682 2.57112 -3.95451
H -0.56939 4.21236 -3.35395
H 0.73582 3.23777 -2.60967
H -2.40809 1.65256 -3.58013
H -3.26929 2.00619 -2.05287
H -2.91940 3.32364 -3.22440
H -4.01641 -1.23333 2.13772
H -0.89310 1.66651 -1.88454
H -2.06203 -2.43761 0.63486
H -2.81020 -1.03975 -2.03366
H -3.53474 -4.02936 1.56865
H -5.51788 -5.50003 1.42822
H -7.12698 -5.24636 -0.45629
H -6.72544 -3.51245 -2.19441
H -4.75445 -2.05007 -2.06140
C 3.37166 -1.45065 -0.63456
C 4.55568 -2.19165 -0.66325
C 5.74669 -1.66212 -0.17028
C 5.72647 -0.37182 0.36968
C 4.55474 0.38141 0.41622
H 2.45043 -1.86980 -1.02606
C 4.51494 -3.59158 -1.21689
H 6.66310 -2.23773 -0.19767
C 7.01289 0.22573 0.87769
H 4.55854 1.37147 0.84904
F 3.86726 -3.65097 -2.40966
F 5.74992 -4.11274 -1.41115
F 3.85702 -4.44739 -0.38534
F 6.80898 1.19349 1.80382
F 7.81912 -0.70643 1.44939
F 7.73982 0.79491 -0.12387
O -5.70034 -0.10114 0.78712
O -1.73978 -0.82050 2.92266
C -6.66949 0.57912 -0.03638
C -8.04073 0.03675 0.32421
H -6.43077 0.40361 -1.09099
H -6.59970 1.65645 0.14622
H -8.80490 0.53062 -0.28547
H -8.09603 -1.04072 0.14237
H -8.26976 0.22152 1.37825
C -0.41127 -0.51082 3.39700

C -0.09705 -1.46143 4.53770
H -0.38213 0.53417 3.72124
H 0.29278 -0.63072 2.56710
H 0.90758 -1.25508 4.92122
H -0.81069 -1.33909 5.35836
H -0.12814 -2.50253 4.20192

Entry 16

Free Energy = -2910.595869
Zero-point Energy = -2910.504055
Potential Energy = -2911.21009635
Nimag = 1 (-143.4868 cm-1)

Charge = 0 Multiplicity = 1
C -4.89962 -2.81153 -1.28260
C -3.97666 -2.93890 -0.22621
C -4.21195 -3.92561 0.75173
C -5.32601 -4.75890 0.67696
C -6.23307 -4.62132 -0.37890
C -6.01440 -3.64494 -1.35664
C -2.75731 -2.12862 -0.12261
C -2.24323 -1.38247 -1.17839
N -0.95635 -0.91553 -1.16008
O -0.58218 -0.11866 -2.08707
O -0.13451 -1.27516 -0.26464
C -3.52346 -0.51529 1.49796
C -2.23508 -0.03506 1.92523
O -1.60713 0.93512 1.48301
C -4.38868 0.27038 0.65331
O -4.06494 1.15037 -0.14995
N -1.25532 2.62509 -2.11667
C -2.57682 2.39024 -2.78946
C -1.40921 3.36329 -0.77800
C -0.05127 3.47495 -0.05226
C -0.24680 4.14480 1.32403
C -0.91856 5.51766 1.19175
C -2.24999 5.40661 0.43929
C -2.06589 4.74059 -0.93664
N 0.56433 2.15886 0.07446
C 1.86216 1.86745 -0.20459
N 2.13223 0.52877 -0.04800
C 3.36390 -0.14198 -0.11099
S 2.98312 3.01871 -0.74632
C -0.26648 3.21857 -3.07416
H 0.63846 4.09263 -0.63302
H -0.85532 3.48563 1.95453
H 0.73739 4.23603 1.79517
H -1.07969 5.94892 2.18611
H -0.24943 6.20491 0.65536
H -2.95971 4.81534 1.03248
H -2.69963 6.39597 0.30033
H -1.44414 5.38970 -1.56674
H -3.04106 4.64536 -1.42311
H -2.06704 2.70292 -0.20199
H 1.31517 -0.09237 -0.11782
H 0.00408 1.47649 0.59354
H -0.23320 2.58182 -3.95866
H -0.58892 4.22115 -3.35484
H 0.72125 3.24954 -2.61555
H -2.41984 1.65548 -3.57956
H -3.27836 2.00425 -2.04969
H -2.93600 3.32436 -3.22052
H -4.00292 -1.24021 2.14219
H -0.90083 1.67270 -1.88733
H -2.04699 -2.43721 0.63514
H -2.80822 -1.04559 -2.03300
H -3.50934 -4.03576 1.57328
H -5.48593 -5.51583 1.43891
H -7.10138 -5.27049 -0.44127
H -6.71292 -3.53534 -2.18106
H -4.74863 -2.06357 -2.05408
C 3.35582 -1.45460 -0.60862
C 4.53298 -2.20245 -0.63549
C 5.73811 -1.66447 -0.18110
C 5.73424 -0.36025 0.31869
C 4.56570 0.40127 0.36700
H 2.42547 -1.88132 -0.96782
C 4.50960 -3.58709 -1.22723
H 6.65185 -2.24454 -0.21064
C 7.00378 0.21700 0.88933
H 4.58458 1.40591 0.76521
F 4.69307 -3.56617 -2.57774
F 5.48559 -4.38195 -0.72155
F 3.32969 -4.22037 -1.01233
F 7.09580 0.00508 2.23443
F 8.11461 -0.33474 0.34034
F 7.09280 1.55629 0.70812
O -5.69413 -0.11707 0.79328
O -1.72628 -0.81764 2.92210
C -6.66784 0.55758 -0.02941
C -8.03546 0.00634 0.33154
H -6.42856 0.38420 -1.08425
H -6.60475 1.63524 0.15376
H -8.80307 0.49564 -0.27750
H -8.08390 -1.07138 0.14918
H -8.26514 0.18908 1.38579
C -0.39817 -0.50211 3.39355
C -0.07743 -1.45093 4.53392
H -0.37277 0.54312 3.71733
H 0.30467 -0.61929 2.56223
H 0.92720 -1.24029 4.91508
H -0.78970 -1.33119 5.35615
H -0.10506 -2.49229 4.19864

Entry 17

Free Energy = -2910.578468
Zero-point Energy = -2910.485167
Potential Energy = -2911.19113410

Nimag = 1 (-254.9545 cm-1)

Charge = 0 Multiplicity = 1
C -4.79881 -3.07803 -1.01742
C -3.92673 -3.02500 0.08563
C -4.19711 -3.85508 1.19000
C -5.29457 -4.71529 1.19112
C -6.15033 -4.75991 0.08612
C -5.89716 -3.93742 -1.01646
C -2.72377 -2.16976 0.12256
C -2.10857 -1.72479 -1.05138
N -0.82589 -1.24927 -1.05093
O -0.32248 -0.82704 -2.13488
O -0.13498 -1.23885 0.02240
C -3.55228 -0.39393 1.28164
C -2.33949 0.16721 1.84028
O -1.70148 1.14523 1.43814
C -4.30198 0.31562 0.26867
O -3.86127 1.07847 -0.59429
N -1.20239 3.22028 -2.40141
C -0.05583 2.34938 -2.85318
C -1.36221 3.51585 -0.88105
C -0.01711 3.56079 -0.11778
C -0.19742 4.14822 1.30455
C -0.92711 5.49284 1.33051
C -2.28990 5.35701 0.64883
C -2.11686 4.85809 -0.79099
N 0.55537 2.22132 -0.00274
C 1.86158 1.90370 -0.18893
N 2.10493 0.56666 -0.00272
C 3.32485 -0.12850 -0.08178
S 3.02556 3.03807 -0.68384
C -2.48609 2.68195 -2.97908
H 0.70552 4.17829 -0.66069
H -0.75434 3.41876 1.90280
H 0.80367 4.23297 1.74001
H -1.04550 5.82654 2.36746
H -0.33076 6.26067 0.81759
H -2.91959 4.65462 1.20941
H -2.81992 6.31567 0.62908
H -1.55517 5.62102 -1.35292
H -3.09902 4.76782 -1.26382
H -1.97532 2.69681 -0.49115
H 1.27811 -0.05094 -0.02784
H -0.05751 1.54512 0.46075
H -2.34990 2.55142 -4.05267
H -2.70743 1.73431 -2.49105
H -3.29568 3.38328 -2.79084
H -0.08361 2.33712 -3.94426
H 0.88692 2.77794 -2.51823
H -0.18741 1.33864 -2.46783
H -4.13468 -1.00124 1.96223
H -1.03785 4.13353 -2.83362
H -2.06437 -2.33407 0.96672
H -2.58058 -1.68109 -2.02026
H -3.53446 -3.82391 2.05077
H -5.48000 -5.35169 2.05140
H -7.00530 -5.42957 0.08314
H -6.55668 -3.96676 -1.87907
H -4.62514 -2.44563 -1.88206
C 3.28890 -1.42667 -0.61479
C 4.45213 -2.19444 -0.66782
C 5.66919 -1.69053 -0.20514
C 5.69233 -0.40120 0.33043
C 4.53720 0.37944 0.40601
H 2.34883 -1.82241 -0.98301
C 4.40372 -3.56101 -1.29882
H 6.57202 -2.28615 -0.25597
C 6.97447 0.13942 0.90760
H 4.57550 1.37194 0.83230
F 4.61229 -3.50723 -2.64507
F 5.35256 -4.39359 -0.79985
F 3.20663 -4.17086 -1.12138
F 7.06284 -0.09005 2.25017
F 8.07309 -0.42937 0.35130
F 7.09329 1.47905 0.74279
O -5.62882 -0.01169 0.31872
O -1.93985 -0.54353 2.93260
C -6.48748 0.57993 -0.67806
C -7.90509 0.11439 -0.39850
H -6.14948 0.27046 -1.67302
H -6.40137 1.67010 -0.62066
H -8.58741 0.54276 -1.14046
H -7.97649 -0.97599 -0.45152
H -8.23347 0.43388 0.59533
C -0.69414 -0.15294 3.55289
C -0.45967 -1.07691 4.73369
H -0.76541 0.89370 3.86568
H 0.10620 -0.23463 2.81114
H 0.47896 -0.80787 5.22928
H -1.27026 -0.99523 5.46451
H -0.38800 -2.11915 4.40808

Entry 18

Free Energy = -2910.578647
Zero-point Energy = -2910.486554
Potential Energy = -2911.19327440
Nimag = 1 (-275.8424 cm-1)

Charge = 0 Multiplicity = 1
C -2.94213 -1.08710 1.08029
C -3.85391 -0.03456 0.97667
C -5.04391 -0.20192 0.25709
C -5.32080 -1.42649 -0.35036
C -4.41736 -2.48804 -0.25138
C -3.23410 -2.30964 0.46411
N -3.63902 1.20256 1.66972
C -2.94930 2.30512 1.21414
S -3.32085 3.82322 1.89591
C -6.58238 -1.60322 -1.15545

C -2.25164 -3.45079 0.57224
N -1.99426 2.09925 0.29322
C -1.31580 3.16387 -0.45654
C 0.22466 3.01307 -0.46982
C 0.87103 3.99114 -1.46913
C 0.31899 3.81152 -2.88863
C -1.19157 4.05538 -2.89103
C -1.87332 3.10577 -1.90431
N 0.93304 3.15306 0.90136
C 0.28513 2.43662 2.05645
C 1.23123 4.55975 1.32514
O -0.50112 -0.16380 -0.86973
N 0.45878 -0.62788 -0.15820
O 0.35302 -0.65347 1.10492
C 1.57885 -1.08487 -0.78891
C 2.67711 -1.57884 -0.06314
C 3.64658 -2.49968 -0.70106
C 3.89461 -2.51530 -2.08547
C 4.78893 -3.43178 -2.63863
C 5.45510 -4.35127 -1.82203
C 5.22039 -4.34530 -0.44367
C 4.32812 -3.42667 0.10933
C 4.05536 0.04215 0.53716
C 3.65938 0.43878 1.88392
O 3.06385 1.46127 2.22269
C 3.92408 1.00152 -0.53721
O 3.08205 1.90240 -0.62495
H -1.60169 4.11063 0.00873
H -1.76169 2.07516 -2.26510
H -2.94803 3.30713 -1.84252
H -1.61277 3.90502 -3.89152
H -1.39548 5.09928 -2.61479
H 0.53599 2.79811 -3.25103
H 0.83026 4.50845 -3.56217
H 0.66897 5.02508 -1.16471
H 1.95284 3.83766 -1.45833
H 0.46655 1.99232 -0.77316
H -4.36507 1.46474 2.32527
H -1.74723 1.14677 0.00138
H 1.00263 2.45037 2.87385
H -0.62671 2.96379 2.33295
H 0.08918 1.40335 1.77749
H 1.70382 4.51601 2.30596
H 1.91316 5.02992 0.62137
H 0.29844 5.12097 1.39214
H 4.93181 -0.59077 0.49467
H 1.84336 2.67188 0.74747
H 1.53172 -1.01075 -1.86423
H 2.47898 -1.78261 0.98291
H 4.15051 -3.42426 1.18123
H 5.72937 -5.05677 0.20005
H 6.14872 -5.06528 -2.25621
H 4.96535 -3.42931 -3.71041
H 3.39212 -1.80899 -2.73773
H -5.74758 0.62034 0.18701
H -4.64121 -3.44294 -0.71161
H -2.01695 -0.95614 1.63066
F -6.36023 -1.42940 -2.48746
F -7.54618 -0.71835 -0.80485
F -7.10840 -2.84549 -1.01422
F -1.27707 -3.37816 -0.36876
F -1.63385 -3.47823 1.77682
F -2.85610 -4.65667 0.40920
C 3.70258 -0.24513 4.17744
C 4.21528 -1.41377 4.99839
H 2.61681 -0.13657 4.25890
H 4.16204 0.69950 4.48543
H 3.97774 -1.25121 6.05489
H 3.74741 -2.35137 4.68296
H 5.30060 -1.51648 4.90216
C 4.73287 1.62300 -2.70379
C 5.85311 1.22033 -3.64498
H 4.83122 2.66384 -2.37999
H 3.74869 1.50697 -3.16910
H 5.82710 1.85309 -4.53835
H 6.82940 1.34114 -3.16595
H 5.74900 0.17732 -3.95820
O 4.04221 -0.49905 2.79375
O 4.80721 0.76379 -1.54258

Entry 19

Free Energy = -2910.393766
Zero-point Energy = -2910.302865
Potential Energy = -2911.01533850
Nimag = 1 (-293.6575 cm-1)

Charge = 0 Multiplicity = 1
C 2.94297 0.89111 0.74931
C 3.92915 -0.09845 0.77956
C 5.20816 0.17662 0.27589
C 5.49521 1.42987 -0.25772
C 4.51054 2.41915 -0.30611
C 3.24112 2.13997 0.19289
N 3.71199 -1.36604 1.39576
C 2.92097 -2.41784 0.98109
S 3.25263 -3.95669 1.62528
C 6.85527 1.70469 -0.84431
C 2.16468 3.19815 0.14647
N 1.91898 -2.15067 0.12423
C 1.15218 -3.17778 -0.58729
C -0.37909 -2.97833 -0.49705
C -1.12293 -3.93901 -1.44368
C -0.66795 -3.76950 -2.89824
C 0.83255 -4.04568 -3.01009
C 1.60539 -3.11766 -2.07073
N -0.99771 -3.07964 0.92044
C -0.23691 -2.39570 2.02600
C -1.33780 -4.46355 1.37513
O 0.39440 0.07912 -0.96660
N -0.49851 0.58961 -0.20927

O -0.32937 0.63561 1.04533
C -1.63150 1.08445 -0.78543
C -2.67200 1.61224 -0.00373
C -3.66800 2.53513 -0.59566
C -3.99403 2.53756 -1.96227
C -4.91358 3.45119 -2.47335
C -5.52984 4.37883 -1.63058
C -5.22133 4.38309 -0.26869
C -4.30292 3.46861 0.24188
C -4.02197 0.04725 0.72577
C -3.50014 -0.34687 2.02825
O -2.92555 -1.39183 2.32532
C -4.00314 -0.91733 -0.34861
O -3.19679 -1.84102 -0.49767
H 1.43834 -4.14009 -0.15482
H 1.48890 -2.08127 -2.41428
H 2.67765 -3.34211 -2.08893
H 1.18274 -3.90119 -4.03923
H 1.03267 -5.09594 -2.75350
H -0.88847 -2.74916 -3.24032
H -1.24220 -4.45139 -3.53685
H -0.92791 -4.97959 -1.15305
H -2.19626 -3.75243 -1.35706
H -0.60647 -1.95366 -0.79458
H 4.47279 -1.70160 1.97386
H 1.69705 -1.18938 -0.15693
H -0.90281 -2.36730 2.88583
H 0.66415 -2.96857 2.24361
H -0.01273 -1.37457 1.72352
H -1.78194 -4.38129 2.36779
H -2.05788 -4.91756 0.69813
H -0.42483 -5.05999 1.42696
H -4.88458 0.69929 0.76033
H -1.89508 -2.55383 0.83182
H -1.64433 0.98999 -1.86005
H -2.39891 1.83509 1.02164
H -4.06982 3.46724 1.30376
H -5.69426 5.10090 0.39616
H -6.24445 5.09202 -2.03235
H -5.14818 3.44084 -3.53457
H -3.52744 1.82334 -2.63312
H 5.97560 -0.58995 0.30776
H 4.73726 3.39837 -0.70973
H 1.95398 0.70833 1.15813
F 6.87355 1.48421 -2.17870
F 7.80687 0.91516 -0.30007
F 7.23056 2.98800 -0.65359
F 1.27498 2.96361 -0.84103
F 1.47390 3.25306 1.30255
F 2.68492 4.42837 -0.07386
C -3.21183 0.39049 4.27335
C -3.56881 1.59554 5.12432
H -2.12855 0.24391 4.21022
H -3.65087 -0.53188 4.66847
H -3.19616 1.45548 6.14499
H -3.11976 2.50727 4.71710
H -4.65381 1.73524 5.16931
C -4.95987 -1.49466 -2.45287
C -6.08912 -1.01515 -3.34703
H -5.10446 -2.53443 -2.13925
H -3.98772 -1.43515 -2.95492
H -6.13370 -1.62617 -4.25532
H -7.05196 -1.09032 -2.83177
H -5.93837 0.02948 -3.63718
O -3.72826 0.62896 2.94899
O -4.94546 -0.64761 -1.28921

Entry 20

Free Energy = -2910.388390
Zero-point Energy = -2910.301119
Potential Energy = -2911.01274317
Nimag = 1 (-295.1158 cm-1)

Charge = 0 Multiplicity = 1
C -1.58200 -3.13271 -1.21693
C -0.31830 -2.73871 -0.75822
C -0.13601 -2.51419 0.61312
C -1.21228 -2.64912 1.48602
C -2.47633 -3.03013 1.03265
C -2.64578 -3.27609 -0.32830
N 0.71649 -2.68715 -1.70826
C 2.02311 -2.25655 -1.63257
S 3.15935 -3.07723 -2.59334
C -1.02384 -2.33475 2.94764
C -4.00001 -3.64362 -0.87317
N 2.30265 -1.20092 -0.83013
C 3.63904 -0.99580 -0.25953
C 4.12415 0.47292 -0.29159
C 5.52517 0.58077 0.33642
C 5.54271 0.05058 1.77824
C 5.05487 -1.39821 1.83729
C 3.66896 -1.52178 1.19690
N 4.10212 1.08868 -1.70066
C 4.67717 0.24721 -2.79481
C 4.70621 2.46237 -1.74476
O 1.81403 2.33055 -2.56117
N 1.30557 2.78090 -1.47968
O 1.98906 2.82217 -0.41934
C 0.00930 3.21571 -1.49458
C -0.62746 3.51122 -0.29150
C -1.94244 4.16261 -0.21412
C -2.81149 4.27381 -1.31425
C -4.03248 4.93293 -1.19232
C -4.41480 5.49041 0.03007
C -3.56490 5.38319 1.13358
C -2.34386 4.72636 1.01125
C -1.15233 1.43330 0.67107
C -0.00900 1.09629 1.48656
O 0.93594 0.34236 1.22914
C -1.39750 0.76011 -0.58036

O -0.56675 0.21745 -1.30530
H 4.31728 -1.61172 -0.85547
H 2.92590 -0.96971 1.78386
H 3.35453 -2.57156 1.17112
H 5.01800 -1.74980 2.87519
H 5.76788 -2.04805 1.30994
H 4.89595 0.68295 2.40214
H 6.55788 0.14068 2.18251
H 6.24835 0.01047 -0.26379
H 5.85832 1.62230 0.34017
H 3.41432 1.09777 0.25788
H 0.57991 -3.28892 -2.51075
H 1.53133 -0.67289 -0.39838
H 4.56105 0.79853 -3.72994
H 5.73798 0.07479 -2.60115
H 4.15073 -0.70609 -2.86401
H 4.38425 2.92160 -2.67934
H 4.30667 3.04277 -0.91541
H 5.79315 2.39125 -1.70956
H -2.01381 1.80945 1.20574
H 3.09811 1.29230 -1.94688
H -0.46858 3.11288 -2.45609
H 0.02187 3.65851 0.56203
H -1.68770 4.63133 1.87297
H -3.85400 5.81215 2.08922
H -5.36819 6.00361 0.12183
H -4.68826 5.01296 -2.05525
H -2.53344 3.84684 -2.27231
H 0.82750 -2.23219 1.00784
H -3.30261 -3.14426 1.72315
H -1.73290 -3.32718 -2.27463
F -1.40286 -1.06746 3.23965
F 0.26518 -2.45711 3.33827
F -1.76304 -3.15047 3.73225
F -4.62541 -2.57022 -1.41935
F -3.90939 -4.57313 -1.85091
F -4.81752 -4.13270 0.08098
C 0.93966 1.41289 3.64995
C 0.61723 2.16929 4.92677
H 1.92225 1.69259 3.25203
H 0.94008 0.33016 3.81216
H 1.36745 1.94911 5.69461
H 0.61112 3.25018 4.75083
H -0.36555 1.87780 5.31077
C -3.05553 0.36457 -2.24909
C -4.53806 0.61885 -2.45596
H -2.83004 -0.70529 -2.27941
H -2.44361 0.85004 -3.01826
H -4.84689 0.25923 -3.44407
H -5.12710 0.09158 -1.69960
H -4.76462 1.68789 -2.38688
O -0.07576 1.74192 2.68923
O -2.70699 0.89034 -0.95767

Below are the coordinates for all transition states appearing in Table S4

Entry 1

Free Energy = -2910.597760
Zero-point Energy = -2910.505993
Potential Energy = -2911.21168465
Single point Energy = -2912.0188256
Nimag = 1 (-230.8241 cm-1)

Charge = 0 Multiplicity = 1
C 2.46513 -2.53302 0.43077
C 1.93896 -1.55970 -0.43432
C 2.81333 -0.66995 -1.07376
C 4.19114 -0.76532 -0.86329
C 4.72532 -1.74309 -0.02557
C 3.84423 -2.61757 0.61765
N 0.56022 -1.37558 -0.64349
C -0.43773 -2.31343 -0.69145
S -0.16795 -3.99258 -0.70160
C 5.09398 0.23781 -1.52931
C 4.40601 -3.69759 1.50504
N -1.67502 -1.75842 -0.75495
C -2.90198 -2.49251 -1.03699
C -4.02107 -2.12961 -0.03379
C -5.30652 -2.91029 -0.34728
C -5.77421 -2.64514 -1.78904
C -4.67546 -2.97963 -2.80419
C -3.38322 -2.22147 -2.47918
N -3.57146 -2.30938 1.41932
C -3.07459 -3.67765 1.77538
C -4.61254 -1.86139 2.40018
O -1.55408 -0.68124 2.29111
N -1.81869 0.56442 2.10586
O -3.01032 0.97141 2.16109
C -0.76738 1.40572 1.86673
C -0.97333 2.75798 1.58031
C 0.10028 3.75976 1.71211
C 1.46576 3.41999 1.75342
C 2.43899 4.40473 1.92070
C 2.07080 5.74810 2.04743
C 0.71805 6.10055 2.00571
C -0.25457 5.11620 1.83829
C -1.41200 2.95585 -0.66358
C -2.59470 2.13235 -0.76138
O -2.65823 0.91641 -0.97292
C -0.15548 2.54051 -1.24498
O 0.27018 1.38661 -1.38034
H -2.65990 -3.55478 -0.95213
H -3.53417 -1.14209 -2.60514
H -2.57730 -2.51620 -3.15918
H -5.00682 -2.73207 -3.81888
H -4.48123 -4.06104 -2.79158
H -6.05775 -1.58864 -1.88955

H -6.67738 -3.23310 -1.98599
H -5.12941 -3.98605 -0.22264
H -6.10354 -2.62941 0.34730
H -4.21384 -1.05388 -0.10953
H 0.29751 -0.40983 -0.87097
H -1.75532 -0.73771 -0.82417
H -2.74485 -3.65028 2.81453
H -3.88240 -4.40179 1.66642
H -2.23108 -3.94401 1.13810
H -4.13341 -1.76968 3.37461
H -4.98366 -0.88289 2.09992
H -5.41889 -2.59250 2.44702
H -1.59235 4.02330 -0.66566
H -2.76126 -1.65199 1.59150
H 0.18969 0.90908 1.86755
H -1.97873 3.12625 1.75092
H -1.30449 5.39518 1.80667
H 0.42141 7.14047 2.10533
H 2.83110 6.51221 2.17948
H 3.48709 4.12207 1.95361
H 1.77613 2.38482 1.65800
H 2.40441 0.09477 -1.72480
H 5.79429 -1.81843 0.12892
H 1.80154 -3.20912 0.94931
F 5.02997 1.45888 -0.92078
F 4.76056 0.44957 -2.82887
F 6.39568 -0.13327 -1.50863
F 5.52390 -3.29039 2.16152
F 3.52375 -4.11133 2.44629
F 4.76362 -4.80440 0.79589
C -4.97155 2.16762 -0.47625
C -6.06888 3.19709 -0.27433
H -4.91289 1.46643 0.36290
H -5.11940 1.59557 -1.39794
H -7.03943 2.69390 -0.20824
H -5.91143 3.76154 0.64975
H -6.10411 3.90199 -1.11062
C 1.90742 3.35615 -2.15722
C 2.51454 4.69394 -2.53665
H 1.80814 2.69512 -3.02373
H 2.50834 2.84161 -1.40184
H 3.51652 4.53674 -2.94905
H 1.90641 5.20061 -3.29235
H 2.59897 5.34643 -1.66258
O -3.71823 2.87663 -0.55817
O 0.59139 3.61366 -1.61360

Entry 2

Free Energy = -2910.595388
Zero-point Energy = -2910.502766
Potential Energy = -2911.20821853
Single point Energy = -2912.01383235
Nimag = 1 (-246.3116 cm-1)

Charge = 0 Multiplicity = 1
C -0.11274 4.71832 -1.97395
C -0.49652 3.42867 -1.56043
C -1.86116 3.17492 -1.33485
C -2.81738 4.17238 -1.53269
C -2.42358 5.44736 -1.94630
C -1.06676 5.71644 -2.16271
C 0.47096 2.32616 -1.38974
C 1.58366 2.22055 -2.23441
N 2.27199 1.04768 -2.37116
O 3.29363 1.00600 -3.11361
O 1.87607 -0.00929 -1.75912
C 1.17063 2.80356 0.71912
C 0.05244 2.36161 1.52679
O -0.24877 1.19802 1.82477
C 2.45367 2.13469 0.78895
O 2.71310 0.99212 1.17934
N 3.80590 -1.92877 -1.21131
C 4.96901 -1.44295 -2.02399
C 4.12475 -1.97577 0.28704
C 2.92596 -2.47599 1.12122
C 3.27006 -2.39820 2.62463
C 4.53172 -3.20204 2.96169
C 5.71499 -2.74817 2.09949
C 5.37768 -2.80888 0.59873
N 1.71268 -1.72656 0.82334
C 0.49042 -2.28850 0.64103
N -0.52483 -1.37002 0.66016
C -1.88600 -1.57314 0.36858
S 0.24811 -3.95944 0.43653
C 3.26338 -3.19761 -1.79613
H 2.71724 -3.51981 0.87298
H 3.40342 -1.34572 2.90607
H 2.40769 -2.77501 3.18395
H 4.77143 -3.09130 4.02509
H 4.34184 -4.27064 2.79106
H 5.98965 -1.71835 2.36599
H 6.59694 -3.36861 2.29280
H 5.21210 -3.85458 0.30938
H 6.23435 -2.44503 0.02468
H 4.30708 -0.92506 0.53885
H -0.30518 -0.44590 1.05319
H 1.77616 -0.71218 0.96206
H 3.05943 -3.01398 -2.85156
H 4.00374 -3.99239 -1.69799
H 2.33952 -3.47571 -1.28956
H 4.58753 -1.10897 -2.98733
H 5.42937 -0.59445 -1.51818
H 5.69276 -2.24781 -2.14803
H 1.23661 3.87557 0.58483
H 3.05494 -1.19881 -1.34722
H 0.06225 1.38434 -1.04200
H 2.00210 3.03449 -2.80630
H -2.17378 2.18475 -1.01498
H -3.86740 3.95268 -1.36343
H -3.16498 6.22635 -2.09747

H -0.75254 6.70715 -2.47794
H 0.93633 4.94760 -2.13502
C -2.83055 -0.90050 1.15301
C -4.19380 -1.01751 0.86530
C -4.63903 -1.80576 -0.19378
C -3.68663 -2.46620 -0.97770
C -2.32286 -2.35322 -0.71406
H -2.49066 -0.29004 1.98257
C -5.17441 -0.24916 1.70991
H -5.69592 -1.89850 -0.40971
C -4.15219 -3.34325 -2.11088
H -1.60127 -2.85553 -1.34217
F -5.11829 1.09166 1.45635
F -6.45680 -0.62766 1.50228
F -4.92752 -0.38889 3.03824
F -4.46791 -4.59828 -1.68670
F -5.26753 -2.85337 -2.71219
F -3.21277 -3.48750 -3.07658
O 3.42930 2.95624 0.30920
O -0.72073 3.40592 1.91399
C 4.77566 2.43985 0.25190
C 5.68886 3.58339 -0.15112
H 4.80685 1.62828 -0.48343
H 5.04316 2.03075 1.23080
H 6.72243 3.22635 -0.21015
H 5.40742 3.98307 -1.12976
H 5.64657 4.39401 0.58259
C -1.92400 3.10538 2.66210
C -2.57381 4.42558 3.03166
H -1.65248 2.52312 3.54764
H -2.58220 2.49178 2.03975
H -3.49241 4.23465 3.59605
H -1.90683 5.03040 3.65365
H -2.83133 4.99996 2.13694

Entry 3

Free Energy = -2910.596328
Zero-point Energy = -2910.504300
Potential Energy = -2911.21031364
Single point Energy = -2912.01365621
Nimag = 1 (-174.4923 cm-1)

Charge = 0 Multiplicity = 1
C -4.91126 -2.79755 -1.29063
C -3.99192 -2.92957 -0.23168
C -4.23452 -3.91556 0.74518
C -5.35228 -4.74356 0.66702
C -6.25578 -4.60133 -0.39129
C -6.02977 -3.62566 -1.36806
C -2.76912 -2.12486 -0.12422
C -2.24871 -1.38057 -1.17828
N -0.95928 -0.92078 -1.15724
O -0.57927 -0.12511 -2.08295
O -0.14080 -1.28569 -0.26088
C -3.53252 -0.51034 1.49463
C -2.24315 -0.03555 1.92500
O -1.61032 0.93216 1.48437
C -4.39284 0.27990 0.64910
O -4.06370 1.15869 -0.15327
N -1.24395 2.61992 -2.11546
C -2.56453 2.38881 -2.79132
C -1.39882 3.35977 -0.77781
C -0.04251 3.46687 -0.04845
C -0.23898 4.13889 1.32662
C -0.90513 5.51416 1.19119
C -2.23503 5.40739 0.43542
C -2.04998 4.73934 -0.93941
N 0.56728 2.14838 0.08137
C 1.86441 1.85147 -0.19328
N 2.12994 0.51216 -0.03381
C 3.36367 -0.15525 -0.09943
S 2.99265 2.99695 -0.73256
C -0.25073 3.20921 -3.07098
H 0.65129 4.08112 -0.62798
H -0.85160 3.48269 1.95625
H 0.74436 4.22678 1.80017
H -1.06717 5.94710 2.18467
H -0.23200 6.19827 0.65580
H -2.94850 4.81941 1.02737
H -2.68058 6.39831 0.29435
H -1.42427 5.38551 -1.56860
H -3.02429 4.64728 -1.42821
H -2.06065 2.70225 -0.20311
H 1.31282 -0.10831 -0.10982
H 0.00274 1.46851 0.59914
H -0.21682 2.57112 -3.95451
H -0.56939 4.21236 -3.35395
H 0.73582 3.23777 -2.60967
H -2.40809 1.65256 -3.58013
H -3.26929 2.00619 -2.05287
H -2.91940 3.32364 -3.22440
H -4.01641 -1.23333 2.13772
H -0.89310 1.66651 -1.88454
H -2.06203 -2.43761 0.63486
H -2.81020 -1.03975 -2.03366
H -3.53474 -4.02936 1.56865
H -5.51788 -5.50003 1.42822
H -7.12698 -5.24636 -0.45629
H -6.72544 -3.51245 -2.19441
H -4.75445 -2.05007 -2.06140
C 3.37166 -1.45065 -0.63456
C 4.55568 -2.19165 -0.66325
C 5.74669 -1.66212 -0.17028
C 5.72647 -0.37182 0.36968
C 4.55474 0.38141 0.41622
H 2.45043 -1.86980 -1.02606
C 4.51494 -3.59158 -1.21689
H 6.66310 -2.23773 -0.19767
C 7.01289 0.22573 0.87769
H 4.55854 1.37147 0.84904

F 3.86726 -3.65097 -2.40966
F 5.74992 -4.11274 -1.41115
F 3.85702 -4.44739 -0.38534
F 6.80898 1.19349 1.80382
F 7.81912 -0.70643 1.44939
F 7.73982 0.79491 -0.12387
O -5.70034 -0.10114 0.78712
O -1.73978 -0.82050 2.92266
C -6.66949 0.57912 -0.03638
C -8.04073 0.03675 0.32421
H -6.43077 0.40361 -1.09099
H -6.59970 1.65645 0.14622
H -8.80490 0.53062 -0.28547
H -8.09603 -1.04072 0.14237
H -8.26976 0.22152 1.37825
C -0.41127 -0.51082 3.39700
C -0.09705 -1.46143 4.53770
H -0.38213 0.53417 3.72124
H 0.29278 -0.63072 2.56710
H 0.90758 -1.25508 4.92122
H -0.81069 -1.33909 5.35836
H -0.12814 -2.50253 4.20192

Entry 4

Free Energy = -2910.595016
Zero-point Energy = -2910.502702
Potential Energy = -2911.20913576
Single point Energy = -2912.01146668
Nimag = 1 (-244.2815 cm-1)

Charge = 0 Multiplicity = 1
C -4.55525 0.44634 -0.14771
C -3.26422 -0.07438 -0.33273
C -3.10855 -1.46871 -0.46187
C -4.21443 -2.31218 -0.39692
C -5.50079 -1.80390 -0.20118
C -5.64736 -0.42190 -0.08190
N -2.08734 0.67976 -0.44339
C -1.81040 2.00339 -0.22496
S -2.88002 3.13779 0.44692
C -4.00741 -3.80180 -0.47968
C -7.03167 0.15824 0.05707
N -0.52376 2.31285 -0.56908
C -0.00017 3.67263 -0.63904
C 1.42565 3.77952 -0.05085
C 1.92402 5.23246 -0.12896
C 1.89964 5.74623 -1.57971
C 0.50452 5.62265 -2.19967
C -0.00814 4.18229 -2.09675
N 1.50351 3.20980 1.37337
C 0.41338 3.65188 2.30228
C 2.83949 3.43482 2.01765
O 0.79956 0.45617 -2.37496
N 1.09024 -0.52821 -1.61779
O 0.19674 -1.01909 -0.85213
C 2.35484 -1.03178 -1.63348
C 2.74435 -2.00872 -0.70917
C 3.95654 -2.82648 -0.90172
C 4.99831 -2.46225 -1.77496
C 6.10096 -3.29692 -1.95443
C 6.18856 -4.51033 -1.26437
C 5.16187 -4.88462 -0.39153
C 4.05971 -4.05003 -0.21271
C 3.25234 -0.95120 1.23467
C 1.96029 -0.60555 1.79551
O 1.38967 0.49434 1.79994
C 4.15193 0.07389 0.74978
O 3.83970 1.15053 0.23686
H -0.67789 4.30374 -0.05915
H 0.60995 3.51701 -2.71421
H -1.03446 4.10586 -2.46996
H 0.52445 5.93767 -3.24888
H -0.19053 6.29695 -1.68090
H 2.61909 5.16959 -2.17680
H 2.24133 6.78699 -1.59453
H 1.29051 5.87827 0.49357
H 2.94453 5.30820 0.25542
H 2.10597 3.13095 -0.61388
H -1.26930 0.10555 -0.69520
H -0.04720 1.64110 -1.18538
H -0.55866 3.34782 1.91832
H 0.58745 3.17593 3.26746
H 0.45004 4.73612 2.41491
H 2.89566 2.77991 2.88734
H 3.62113 3.15760 1.31393
H 2.92599 4.47475 2.33070
H 3.71799 -1.82332 1.67483
H 1.43155 2.16929 1.29401
H 3.01036 -0.53167 -2.32866
H 1.93785 -2.49549 -0.17372
H 3.26283 -4.34587 0.46450
H 5.21799 -5.82682 0.14550
H 7.04730 -5.15931 -1.40853
H 6.89226 -3.00153 -2.63732
H 4.95037 -1.52685 -2.32260
H -2.11842 -1.88107 -0.62478
H -6.35785 -2.46363 -0.14756
H -4.69499 1.51216 -0.04772
F -5.09167 -4.44681 -0.97712
F -3.76593 -4.34899 0.74700
F -2.95152 -4.13671 -1.26043
F -7.03577 1.35436 0.69120
F -7.61838 0.36262 -1.15692
F -7.86565 -0.66118 0.74816
C 0.05265 -1.51156 2.92430
C -0.39338 -2.84968 3.48285
H -0.60698 -1.16123 2.12522
H 0.08780 -0.73953 3.69937
H 0.28101 -3.19124 4.27432
H -1.39854 -2.75221 3.90567

H -0.42548 -3.61229 2.69896
C 6.45569 0.57100 0.31495
C 7.81113 -0.07456 0.53810
H 6.38045 1.53788 0.82348
H 6.25449 0.73652 -0.74843
H 8.00005 -0.23111 1.60459
H 7.87090 -1.04198 0.03101
H 8.59840 0.57473 0.14069
O 1.38245 -1.68656 2.37867
O 5.45440 -0.32108 0.85134

Entry 5

Free Energy = -2910.594984
Zero-point Energy = -2910.501954
Potential Energy = -2911.20790185
Single point Energy = -2912.00921008
Nimag = 1 (-327.6935 cm-1)

Charge = 0 Multiplicity = 1
C 5.37230 3.05816 -0.87393
C 4.09050 3.01500 -0.29492
C 3.70213 4.06906 0.55474
C 4.56725 5.13160 0.80821
C 5.83573 5.16709 0.21712
C 6.23478 4.12624 -0.62583
C 3.20096 1.88814 -0.62425
C 1.80966 2.04367 -0.65150
N 0.99572 1.14096 -1.27077
O 1.47747 0.16305 -1.92862
O -0.26569 1.31251 -1.20670
C 3.73997 0.50239 1.15601
C 2.40616 0.26127 1.65664
O 1.61127 -0.61283 1.29992
C 4.53097 -0.54158 0.53252
O 4.14818 -1.59178 0.01435
N 1.32259 -2.59988 -2.08047
C 2.64004 -2.48246 -2.79198
C 1.45544 -3.31721 -0.72885
C 0.09656 -3.40285 -0.00638
C 0.29535 -4.01178 1.39720
C 0.95131 -5.39676 1.31359
C 2.27366 -5.33507 0.53933
C 2.08781 -4.70878 -0.85524
N -0.54025 -2.09058 0.04856
C -1.86834 -1.86995 -0.14601
N -2.17878 -0.52875 -0.11098
C -3.45040 0.06912 -0.12713
S -2.98401 -3.10212 -0.46752
C 0.26870 -3.13706 -2.99790
H -0.58368 -4.05646 -0.55896
H 0.91606 -3.33322 1.99530
H -0.68574 -4.07374 1.87890
H 1.12064 -5.78922 2.32260
H 0.26528 -6.09593 0.81543
H 3.00236 -4.73793 1.10259
H 2.70264 -6.33712 0.42819
H 1.45183 -5.36470 -1.46439
H 3.06201 -4.64321 -1.34745
H 2.12708 -2.65995 -0.16696
H -1.41438 0.09941 -0.38682
H 0.02002 -1.35327 0.48219
H 0.26304 -2.52447 -3.89998
H 0.50493 -4.16986 -3.25518
H -0.70681 -3.08191 -2.51780
H 2.53013 -1.72832 -3.57109
H 3.39304 -2.16764 -2.06988
H 2.90030 -3.44249 -3.23716
H 4.30889 1.24510 1.69870
H 1.06884 -1.61477 -1.85716
H 3.60050 1.14816 -1.30733
H 1.27292 2.84013 -0.15937
H 2.72864 4.05085 1.03355
H 4.25293 5.93371 1.46940
H 6.50636 5.99803 0.41472
H 7.21717 4.14478 -1.08835
H 5.68805 2.24894 -1.52574
C -3.60278 1.26743 -0.83846
C -4.83109 1.93273 -0.83375
C -5.92295 1.42321 -0.13221
C -5.75607 0.23413 0.58409
C -4.53684 -0.44181 0.59965
H -2.76175 1.66995 -1.39325
C -4.94970 3.24179 -1.56890
H -6.87466 1.93918 -0.13581
C -6.93054 -0.35041 1.32498
H -4.42496 -1.35211 1.17165
F -4.31619 3.21775 -2.76875
F -6.23743 3.58968 -1.80709
F -4.39457 4.26949 -0.86555
F -6.55236 -1.07058 2.40996
F -7.78857 0.60584 1.76381
F -7.66142 -1.18981 0.54032
O 5.85633 -0.20148 0.54343
O 2.05201 1.20488 2.57334
C 6.77680 -1.14100 -0.05324
C 8.18135 -0.60415 0.15414
H 6.53824 -1.24916 -1.11699
H 6.64271 -2.11886 0.41973
H 8.90782 -1.29441 -0.28743
H 8.30421 0.37438 -0.32000
H 8.40762 -0.50184 1.21975
C 0.71305 1.12434 3.11725
C 0.56608 2.23274 4.14316
H 0.57342 0.13648 3.56686
H -0.00843 1.23009 2.30088
H -0.43813 2.19760 4.57801
H 1.29543 2.11924 4.95092
H 0.70600 3.21656 3.68481

Entry 6

Free Energy = -2910.594311
Zero-point Energy = -2910.501634
Potential Energy = -2911.20788267
Single point Energy = -2912.00783821
Nimag = 1 (-274.8958 cm-1)

Charge = 0 Multiplicity = 1
C 3.90311 -4.11484 0.16714
C 4.13108 -2.94545 -0.58272
C 5.34797 -2.81850 -1.27486
C 6.30299 -3.83604 -1.23616
C 6.06328 -4.99334 -0.49115
C 4.86064 -5.12646 0.21324
C 3.12663 -1.86669 -0.69469
C 1.75991 -2.18805 -0.75792
N 0.85072 -1.28551 -1.21559
O 1.21338 -0.13983 -1.63742
O -0.38712 -1.60328 -1.22284
C 3.54780 -0.75072 1.19075
C 4.39534 0.33463 0.72382
C 2.23607 -0.49947 1.75971
O 1.53940 0.52101 1.69470
O 4.04727 1.43409 0.29180
N 1.36136 3.25338 1.18654
C 0.15205 3.84379 1.84440
C 1.51940 3.55999 -0.31173
C 2.08168 4.96483 -0.57666
C 2.31074 5.17920 -2.08393
C 1.03035 4.94463 -2.89326
C 0.43716 3.56262 -2.59187
C 0.19249 3.36881 -1.08008
N -0.42448 2.07478 -0.80312
C -1.76746 1.89614 -0.64569
N -2.13597 0.57832 -0.67415
C -3.39718 -0.00545 -0.45382
S -2.85575 3.18599 -0.43715
C 2.58670 3.58844 1.98601
H -1.42199 -0.10695 -0.96622
H 0.13267 1.25189 -1.07479
H -0.52411 4.12881 -0.75809
H -0.52066 3.43118 -3.10547
H 1.10979 2.77370 -2.95327
H 1.38557 5.72706 -0.20196
H 3.03130 5.10213 -0.05299
H 0.29154 5.71936 -2.64601
H 1.23596 5.03703 -3.96554
H 2.69149 6.19353 -2.24672
H 3.09359 4.48935 -2.42679
H 2.25054 2.81097 -0.63353
H 0.15152 3.52615 2.88768
H -0.75669 3.49819 1.35610
H 0.21115 4.93171 1.79438
H 2.65273 4.66792 2.11716
H 2.48571 3.10535 2.95852
H 3.45815 3.18897 1.47184
H 1.29745 2.21493 1.24611
H 4.07590 -1.57242 1.65586
H 1.32832 -3.11834 -0.42294
H 3.41780 -1.00675 -1.28723
H 5.53862 -1.92038 -1.85522
H 7.23242 -3.72439 -1.78685
H 6.80596 -5.78491 -0.45681
H 4.67006 -6.02037 0.79988
H 2.98168 -4.22593 0.73021
C -3.68769 -1.17903 -1.16942
C -4.89337 -1.84736 -0.96178
C -5.83390 -1.36902 -0.04638
C -5.53027 -0.21134 0.67037
C -4.32524 0.47013 0.48270
H -2.96566 -1.55951 -1.88325
C -5.16482 -3.13206 -1.69936
H -6.77277 -1.88616 0.10559
C -6.52457 0.34732 1.65474
H -4.10655 1.36050 1.05441
F -4.56027 -3.17355 -2.91117
F -4.71595 -4.21805 -1.00756
F -6.49020 -3.33525 -1.90823
F -5.92603 0.78327 2.79467
F -7.20162 1.41400 1.14899
F -7.45894 -0.56328 2.02403
O 5.70840 -0.03308 0.75341
O 1.77480 -1.60607 2.39322
C 0.44397 -1.54052 2.96508
C 0.16069 -2.87942 3.61951
H -0.27005 -1.31774 2.16694
H 0.41356 -0.72062 3.68924
H -0.83785 -2.86166 4.06806
H 0.19017 -3.69039 2.88571
H 0.88857 -3.09473 4.40778
C 6.66737 0.92047 0.24166
C 8.04816 0.30826 0.38924
H 6.57643 1.85323 0.80731
H 6.42801 1.13916 -0.80416
H 8.80151 1.00639 0.00950
H 8.27332 0.09642 1.43890
H 8.12711 -0.62524 -0.17556

Below are the coordinates for the artifact transition state

Free Energy = -2910.599907
Zero-point Energy = -2910.505703
Potential Energy = -2911.21172881
Single Point Energy = -2912.01242709
Nimag = 1 (-315.7834 cm-1)

Charge = 0 Multiplicity = 1
C -4.62634 -0.41438 -0.32762
C -3.22628 -0.52259 -0.32320

C -2.64346 -1.80124 -0.26652
C -3.44622 -2.93913 -0.20310
C -4.83862 -2.84077 -0.18709
C -5.40861 -1.56800 -0.25694
N -2.34813 0.56153 -0.44927
C -2.53141 1.89840 -0.17791
S -3.81049 2.55343 0.71931
C -2.79123 -4.29070 -0.09413
C -6.90864 -1.42980 -0.21290
N -1.51774 2.65435 -0.67421
C -1.34126 4.07975 -0.42601
C 0.15697 4.45163 -0.34952
C 0.32056 5.93094 0.02159
C -0.38112 6.82260 -1.02022
C -1.85898 6.44584 -1.18942
C -2.01990 4.95246 -1.50295
N 0.93412 3.50580 0.56810
C 0.38466 3.37073 1.95497
C 2.40960 3.79194 0.60297
O 0.96955 1.61899 -1.48022
N 1.29235 0.39466 -1.14228
O 0.36789 -0.37556 -0.69429
C 2.55866 0.00866 -1.28006
C 3.01684 -1.26064 -0.78571
C 4.16111 -1.94669 -1.44362
C 5.13315 -1.26277 -2.19476
C 6.17865 -1.95688 -2.80626
C 6.27407 -3.34582 -2.67978
C 5.31276 -4.03820 -1.93673
C 4.26903 -3.34404 -1.32539
C 3.67229 -0.95810 1.16189
C 2.46338 -0.45755 1.84147
O 2.08650 0.70731 1.89382
C 4.82720 -0.04761 1.02459
O 4.78986 1.14762 0.76638
H -1.82613 4.30339 0.52973
H -1.58197 4.71833 -2.48266
H -3.07675 4.67378 -1.54237
H -2.31335 7.04566 -1.98563
H -2.40608 6.68302 -0.26676
H 0.13661 6.72213 -1.98398
H -0.28144 7.87104 -0.71904
H -0.11361 6.11821 1.01168
H 1.38024 6.19748 0.07290
H 0.61496 4.27460 -1.32961
H -1.37913 0.28587 -0.67107
H -0.78135 2.17646 -1.20824
H 0.98311 2.62327 2.47217
H 0.44992 4.33491 2.46003
H -0.65084 3.03826 1.90685
H 2.91055 2.90454 0.99297
H 2.75104 3.98665 -0.41376
H 2.59936 4.65539 1.24001
H 3.94144 -1.97062 1.44262
H 0.87028 2.58716 0.07815
H 3.21222 0.76840 -1.67824
H 2.20851 -1.93253 -0.51208
H 3.52235 -3.88855 -0.75313
H 5.37276 -5.11805 -1.83765
H 7.08596 -3.88395 -3.16010
H 6.91695 -1.41129 -3.38694
H 5.07701 -0.18554 -2.31141
H -1.56291 -1.89534 -0.28978
H -5.45850 -3.72716 -0.13818
H -5.09344 0.55745 -0.38913
F -2.49934 -4.61026 1.19996
F -1.61939 -4.35489 -0.77405
F -3.57950 -5.28835 -0.56430
F -7.37089 -1.32778 1.06510
F -7.34945 -0.32914 -0.86925
F -7.54065 -2.49859 -0.76190
C 0.47986 -1.15813 2.97159
C -0.08917 -2.43209 3.56599
H -0.15590 -0.75296 2.17808
H 0.62060 -0.38257 3.73045
H -1.06715 -2.22121 4.01055
H -0.22176 -3.20169 2.80010
H 0.56606 -2.82731 4.34837
C 7.21647 0.02111 1.00412
C 8.37347 -0.92897 1.24842
H 7.21671 0.85663 1.71071
H 7.23420 0.43450 -0.00887
H 9.31980 -0.39155 1.12706
H 8.33840 -1.33757 2.26293
H 8.35534 -1.76039 0.53766
O 1.76911 -1.48014 2.39138
O 5.98931 -0.73031 1.17587

Below are the coordinates for all transition states appearing in Table S5

Entry 1

Free Energy = -2910.403616
Zero-point Energy = -2910.314343
Potential Energy = -2911.02356879
Single Point Energy = -2912.01113085
Nimag = 1 (-1050.5537 cm-1)

Charge = 0 Multiplicity = 1
C -4.61418 0.72864 -0.81013
C -3.40727 0.16048 -0.38168
C -3.41157 -1.10794 0.20912
C -4.60838 -1.80783 0.36124
C -5.81442 -1.24877 -0.05410
C -5.80313 0.02272 -0.63340
N -2.14732 0.75850 -0.58802
C -1.76103 2.04983 -0.35398
S -2.78933 3.30442 0.10998
C -4.57258 -3.15868 1.02396
C -7.10995 0.65112 -1.04244

N -0.40385 2.21158 -0.49965
C 0.27704 3.48952 -0.36847
C 1.66752 3.37881 0.30730
C 2.23623 4.80017 0.49832
C 2.35746 5.54023 -0.84443
C 1.01667 5.60395 -1.58138
C 0.41052 4.20434 -1.73067
N 1.66875 2.55079 1.58562
C 0.48643 2.72442 2.47587
C 2.91152 2.72469 2.38712
O -0.19503 -0.59277 1.58060
N 0.67371 -0.50692 0.69335
O 0.36463 -0.61349 -0.53739
C 1.98808 -0.15419 1.03074
C 3.07505 -0.48002 0.00619
C 4.35830 0.26238 0.37405
C 5.02700 0.01069 1.58157
C 6.18081 0.71756 1.92543
C 6.69056 1.69091 1.06358
C 6.04484 1.93983 -0.14933
C 4.89336 1.22691 -0.49089
C 3.39909 -2.00687 -0.17060
C 4.39147 -2.20078 -1.31813
O 4.54630 -1.43690 -2.24477
C 2.18891 -2.89709 -0.47976
O 1.89756 -3.30330 -1.58196
H -0.37303 4.10506 0.26106
H 1.02876 3.59184 -2.40327
H -0.59009 4.25910 -2.17094
H 1.14287 6.06837 -2.56641
H 0.31890 6.24120 -1.02061
H 3.09752 5.02187 -1.47100
H 2.75214 6.54740 -0.66572
H 1.58233 5.36850 1.17443
H 3.22421 4.75750 0.96471
H 2.34874 2.82615 -0.35465
H -1.37612 0.08183 -0.60973
H 0.11330 1.42566 -0.88846
H 0.57089 1.99752 3.28663
H 0.47164 3.73575 2.89503
H -0.43544 2.53498 1.93279
H 2.95347 1.91414 3.11779
H 3.78583 2.65685 1.74029
H 2.90294 3.68197 2.91383
H 3.84798 -2.39000 0.75079
H 1.75700 1.36085 1.25785
H 2.17854 -0.48352 2.05155
H 2.74663 -0.12822 -0.97386
H 4.41836 1.39563 -1.45336
H 6.44558 2.67820 -0.83901
H 7.59015 2.23984 1.32851
H 6.68252 0.50557 2.86603
H 4.64569 -0.74374 2.26619
H -2.47539 -1.52834 0.56199
H -6.74310 -1.79478 0.05723
H -4.61935 1.70185 -1.28009
F -4.35972 -3.05933 2.35583
F -3.56748 -3.92687 0.53144
F -5.72223 -3.84360 0.85297
F -7.71108 1.27189 -0.00176
F -6.94855 1.57399 -2.01437
F -7.98444 -0.27360 -1.50196
C 5.96527 -3.70962 -2.24398
C 6.60138 -5.03923 -1.88655
H 6.70771 -2.91321 -2.35749
H 5.38780 -3.76380 -3.17184
H 7.29066 -5.34557 -2.68098
H 7.16529 -4.96548 -0.95097
H 5.84047 -5.81750 -1.77129
C 0.28519 -3.94463 0.47484
C -0.33496 -4.12617 1.84645
H 0.52371 -4.89604 -0.01002
H -0.36291 -3.37526 -0.19726
H -1.30828 -4.61680 1.74629
H 0.30242 -4.73856 2.49296
H -0.48920 -3.15336 2.32261
O 5.06618 -3.35426 -1.16524
O 1.51904 -3.19508 0.64812

Entry 2

Free Energy = -2910.402293
Zero-point Energy = -2910.310243
Potential Energy = -2911.01965392
Single point Energy = -2912.00788565
Nimag = 1 (-1251.5782 cm-1)

Charge = 0 Multiplicity = 1
C 4.81900 -0.44736 -0.57141
C 3.56917 0.13488 -0.32711
C 3.47991 1.51563 -0.10554
C 4.62881 2.30401 -0.13380
C 5.87880 1.73167 -0.36665
C 5.95972 0.35494 -0.57956
N 2.35647 -0.58126 -0.37650
C 2.05941 -1.80809 0.15097
S 3.15320 -2.81873 0.94450
C 4.52612 3.77872 0.15156
C 7.31073 -0.27797 -0.78878
N 0.72972 -2.12364 0.00009
C 0.16153 -3.40540 0.38940
C -1.28639 -3.29629 0.92438
C -1.72946 -4.68461 1.42946
C -1.66554 -5.72917 0.30121
C -0.26669 -5.81191 -0.31822
C 0.21365 -4.42714 -0.76671
N -1.47121 -2.18883 1.95192
C -0.38667 -2.05041 2.96450
C -2.78711 -2.25459 2.64067
O 0.22219 0.99407 1.38168
N -0.59014 0.69004 0.48961

O -0.22670 0.61413 -0.72743
C -1.89713 0.30280 0.83560
C -2.95040 0.50599 -0.27116
C -3.32615 -0.77646 -1.02071
C -4.37381 -1.61961 -0.62194
C -4.66470 -2.79446 -1.32238
C -3.91014 -3.15090 -2.44045
C -2.87011 -2.31533 -2.85606
C -2.58566 -1.14185 -2.15605
C -4.19824 1.24072 0.28997
C -5.12958 1.68508 -0.84238
O -4.83157 1.75746 -2.01175
C -3.80589 2.45875 1.13229
O -3.93727 2.52412 2.33570
H 0.80805 -3.78219 1.18734
H -0.40431 -4.06136 -1.59887
H 1.24867 -4.47170 -1.12029
H -0.26569 -6.50587 -1.16719
H 0.43978 -6.21754 0.41937
H -2.39488 -5.45443 -0.47374
H -1.97545 -6.70470 0.69456
H -1.08462 -4.99863 2.26231
H -2.75376 -4.64555 1.81179
H -1.95217 -3.00042 0.10488
H 1.54057 0.01223 -0.56604
H 0.17758 -1.52015 -0.60462
H -0.59092 -1.15339 3.55321
H -0.36969 -2.92345 3.62485
H 0.57771 -1.93301 2.47648
H -2.95472 -1.29728 3.14096
H -3.57413 -2.41371 1.90234
H -2.80366 -3.05481 3.38384
H -4.76808 0.60996 0.97606
H -1.58914 -1.12382 1.34856
H -2.13064 0.75948 1.79669
H -2.51445 1.17863 -1.01467
H -1.78594 -0.48924 -2.49166
H -2.28860 -2.56774 -3.73911
H -4.14122 -4.05781 -2.99262
H -5.49086 -3.42257 -0.99849
H -4.99446 -1.35937 0.23199
H 2.51068 1.95897 0.09724
H 6.76996 2.34716 -0.39866
H 4.89658 -1.50836 -0.76082
F 4.69589 4.04860 1.46678
F 3.31998 4.27784 -0.19870
F 5.46692 4.48437 -0.51594
F 7.90962 -0.57460 0.38711
F 7.22997 -1.42783 -1.49249
F 8.15033 0.54728 -1.45610
C -7.30666 2.50876 -1.30246
C -8.58222 2.81802 -0.54270
H -7.45750 1.74585 -2.07262
H -6.89010 3.39534 -1.79078
H -9.34092 3.20100 -1.23376
H -8.97867 1.91911 -0.05984
H -8.40521 3.57400 0.22883
C -2.78920 4.60463 1.06733
C -2.21640 5.54477 0.02516
H -2.03902 4.29021 1.79912
H -3.62764 5.04752 1.61357
H -1.84208 6.45092 0.51348
H -1.38648 5.07461 -0.51104
H -2.97997 5.83463 -0.70354
O -6.33901 2.01224 -0.34388
O -3.26842 3.42363 0.37028

Entry 3

Free Energy = -2910.400484
Zero-point Energy = -2910.309059
Potential Energy = -2911.01824239
Single Point Energy = -2912.00766622
Nimag = 1 (-676.7724 cm-1)

Charge = 0 Multiplicity = 1
C -3.98611 1.03572 -0.08034
C -2.73863 0.46409 -0.35802
C -2.61356 -0.92585 -0.41985
C -3.72942 -1.73902 -0.21638
C -4.97256 -1.17942 0.06854
C -5.08734 0.21083 0.14052
N -1.60496 1.25352 -0.66309
C -1.13489 2.35274 0.01100
S -1.75652 2.90831 1.47992
C -3.55889 -3.23580 -0.25346
C -6.41527 0.83046 0.49014
N -0.06653 2.91710 -0.62459
C 0.61986 4.12205 -0.19184
C 2.15901 3.97077 -0.25033
C 2.81972 5.26260 0.27097
C 2.37719 6.48282 -0.55512
C 0.85278 6.63392 -0.56288
C 0.17932 5.33932 -1.03293
N 2.65855 2.71324 0.45461
C 2.16076 2.54357 1.84445
C 4.14419 2.61129 0.41477
O 0.65360 0.99740 -2.63133
N 1.86455 1.16014 -2.29137
O 2.56494 2.02835 -2.85213
C 2.39578 0.48467 -1.17155
C 1.74735 -0.85927 -0.85325
C 2.24463 -2.00223 -1.74605
C 3.60125 -2.34472 -1.85658
C 4.00631 -3.38504 -2.69272
C 3.06676 -4.10354 -3.43558
C 1.71575 -3.77346 -3.33391
C 1.31124 -2.73170 -2.49661
C 1.76353 -1.19364 0.67482
C 3.10171 -1.07308 1.39216
O 4.18873 -0.86928 0.88805

C 1.11687 -2.56786 0.87540
O -0.06831 -2.76639 0.71665
H 0.30410 4.29505 0.84079
H 0.42098 5.15219 -2.08925
H -0.91057 5.41828 -0.96012
H 0.55443 7.46835 -1.20842
H 0.50231 6.87930 0.44961
H 2.74027 6.36819 -1.58614
H 2.85495 7.38413 -0.15317
H 2.55063 5.42183 1.32430
H 3.90997 5.18095 0.22509
H 2.45738 3.81193 -1.29178
H -0.98951 0.89124 -1.39308
H 0.11930 2.58984 -1.57348
H 2.53296 1.59206 2.23136
H 2.52510 3.35129 2.48695
H 1.06981 2.52946 1.85932
H 4.42498 1.59660 0.70410
H 4.47952 2.79275 -0.60849
H 4.60672 3.32804 1.09716
H 1.08734 -0.48583 1.16813
H 2.34526 1.70794 -0.19815
H 3.47574 0.45004 -1.28875
H 0.68471 -0.74869 -1.07395
H 0.25505 -2.48471 -2.42619
H 0.97308 -4.32082 -3.90847
H 3.38630 -4.91086 -4.08942
H 5.06226 -3.63356 -2.76508
H 4.33991 -1.80217 -1.27707
H -1.64486 -1.38081 -0.59164
H -5.83978 -1.81115 0.21708
H -4.09402 2.11153 -0.04774
F -3.11590 -3.72114 0.92576
F -2.66742 -3.61225 -1.19741
F -4.72549 -3.86520 -0.52606
F -6.55434 0.99371 1.82504
F -6.56605 2.04921 -0.07353
F -7.44981 0.06276 0.07892
C 4.10808 -1.16658 3.54678
C 3.66757 -1.35972 4.98502
H 4.63763 -0.21924 3.40147
H 4.76514 -1.97090 3.20245
H 4.54368 -1.36851 5.64238
H 3.00401 -0.55024 5.30551
H 3.13564 -2.30838 5.10564
C 1.50393 -4.87857 1.23517
C 2.69363 -5.79727 1.43115
H 0.96757 -5.08671 0.30541
H 0.78721 -4.94020 2.05991
H 2.35202 -6.83685 1.47981
H 3.39691 -5.70261 0.59799
H 3.22258 -5.56573 2.36145
O 2.91490 -1.16642 2.72385
O 2.01290 -3.51943 1.17010

Entry 4

Free Energy = -2910.404089
Zero-point Energy = -2910.312928
Potential Energy = -2912.00761445
Nimag = 1 (-1048.2376 cm-1)

Charge = 0 Multiplicity = 1
C -4.63990 -0.89692 0.41783
C -3.45896 -0.15810 0.28849
C -3.51812 1.20227 -0.00147
C -4.75755 1.82369 -0.16109
C -5.93678 1.10170 -0.04848
C -5.86100 -0.26330 0.23938
N -2.19330 -0.73544 0.50853
C -1.68530 -1.83084 -0.13601
S -2.57651 -2.79628 -1.19379
C -4.79187 3.30596 -0.40088
C -7.14680 -1.02838 0.37807
N -0.37000 -2.04630 0.13592
C 0.35860 -3.21964 -0.31870
C 1.81153 -2.91980 -0.71866
C 2.40470 -4.20661 -1.32005
C 2.37645 -5.35434 -0.30270
C 0.95843 -5.62248 0.20520
C 0.32179 -4.33705 0.73609
N 1.94300 -1.71557 -1.60971
C 0.97897 -1.63158 -2.72547
C 3.32874 -1.57145 -2.10992
O -0.25208 1.39310 -0.98686
N 0.50887 1.01359 -0.08964
O 0.07357 0.76525 1.06895
C 1.86756 0.73862 -0.38912
C 2.80375 0.91488 0.81922
C 3.35089 -0.39022 1.37425
C 4.57187 -0.97142 1.02046
C 4.96259 -2.19438 1.57186
C 4.14956 -2.85786 2.48576
C 2.93791 -2.28081 2.85960
C 2.55195 -1.06088 2.31288
C 3.86636 2.01998 0.61533
C 3.25679 3.40654 0.36219
O 3.86212 4.30432 -0.17463
C 4.87362 1.78215 -0.50316
O 4.58676 1.42768 -1.62445
H -0.17790 -3.57490 -1.19903
H 0.85329 -3.99730 1.63339
H -0.72092 -4.50498 1.01415
H 0.96980 -6.38647 0.98748
H 0.34395 -6.01581 -0.61270
H 3.02516 -5.09561 0.54262
H 2.79705 -6.25420 -0.76006
H 1.83204 -4.49050 -2.20979
H 3.43309 -4.03732 -1.63925
H 2.38950 -2.66549 0.17545
H -1.49680 -0.08484 0.87888

H 0.05834 -1.47000 0.85011
H 1.16989 -0.70564 -3.26812
H 1.09780 -2.47486 -3.41140
H -0.04021 -1.60963 -2.34994
H 3.47025 -0.53530 -2.41099
H 4.01968 -1.78297 -1.29991
H 3.53226 -2.22982 -2.95504
H 4.43479 2.11548 1.54462
H 1.85129 -0.57690 -0.87146
H 2.14116 1.31315 -1.26726
H 2.16771 1.30734 1.61062
H 1.61240 -0.61043 2.61112
H 2.29793 -2.77388 3.58236
H 4.46147 -3.80534 2.90894
H 5.91189 -2.62841 1.27896
H 5.25006 -0.52425 0.29864
H -2.59674 1.75692 -0.12792
H -6.89400 1.58519 -0.18704
H -4.59373 -1.94769 0.65475
F -3.72469 3.73667 -1.10981
F -4.77288 4.00044 0.77124
F -5.89988 3.70164 -1.06238
F -7.93110 -0.90227 -0.72134
F -6.95508 -2.34676 0.57804
F -7.88859 -0.57500 1.42307
C 1.30761 4.76187 0.59668
C -0.14447 4.54328 0.95882
H 1.43849 5.04055 -0.44938
H 1.78250 5.52267 1.21897
H -0.69289 5.47918 0.82947
H -0.59870 3.78687 0.31676
H -0.24500 4.22576 1.99858
C 7.17225 1.90762 -1.08959
C 8.48375 2.21265 -0.40189
H 6.95234 2.61024 -1.89482
H 7.14515 0.89641 -1.50053
H 9.29962 2.13594 -1.12467
H 8.48182 3.22420 0.00850
H 8.67479 1.50657 0.40911
O 2.00804 3.50077 0.81736
O 6.11984 2.02376 -0.09137

Entry 5

Free Energy = -2910.399754
Zero-point Energy = -2910.310951
Potential Energy = -2911.02061059
Single Point Energy = -2912.00534863
Nimag = 1 (-699.0327 cm-1)

Charge = 0 Multiplicity = 1
C -4.27587 0.33994 -0.44885
C -2.91962 -0.01077 -0.51341
C -2.55395 -1.35567 -0.36688
C -3.52278 -2.33097 -0.13938
C -4.87060 -1.98849 -0.05399
C -5.23047 -0.64912 -0.21441
N -1.87937 0.89648 -0.78127
C -1.71716 2.19694 -0.36616
S -2.81832 3.07174 0.56805
C -3.08913 -3.76595 -0.01981
C -6.69129 -0.27793 -0.20689
N -0.51037 2.69829 -0.76351
C -0.07221 4.06706 -0.54951
C 1.44024 4.14680 -0.21926
C 1.82689 5.62014 0.02493
C 1.48968 6.50257 -1.18932
C 0.00819 6.40607 -1.56392
C -0.39737 4.94465 -1.77777
N 1.85068 3.22355 0.92593
C 0.91877 3.20310 2.08575
C 3.23796 3.48629 1.39361
O 0.73604 -0.37864 -0.92588
N 1.60667 0.51654 -1.08844
O 1.53827 1.29895 -2.07290
C 2.57191 0.75964 -0.10563
C 2.94607 -0.31886 0.91500
C 1.91123 -0.68020 1.98333
C 0.86213 -1.59029 1.78886
C -0.02774 -1.88962 2.82174
C 0.11228 -1.29207 4.07533
C 1.16505 -0.40424 4.29510
C 2.05549 -0.11278 3.25944
C 3.67248 -1.57932 0.31168
C 5.15656 -1.26761 0.08067
O 5.68723 -0.18976 0.25098
C 3.10770 -2.09553 -1.01145
O 3.37600 -1.60265 -2.08663
H -0.65141 4.45045 0.29532
H 0.11827 4.53484 -2.65801
H -1.47293 4.86097 -1.96497
H -0.19717 6.99130 -2.46803
H -0.60432 6.84133 -0.76177
H 2.10516 6.18597 -2.04335
H 1.77066 7.53924 -0.96891
H 1.29457 5.99831 0.90897
H 2.89739 5.70773 0.23300
H 2.00882 3.76313 -1.07565
H -1.01290 0.43222 -1.07386
H 0.02141 2.17918 -1.46888
H 1.27873 2.45878 2.79824
H 0.88714 4.18580 2.56779
H -0.08239 2.92020 1.76507
H 3.54634 2.65086 2.02559
H 3.90942 3.54028 0.53406
H 3.29502 4.41235 1.96938
H 3.62103 -2.39219 1.04293
H 2.00093 2.07253 0.48773
H 3.44491 1.19375 -0.59182
H 3.75639 0.17383 1.46273
H 2.89496 0.55370 3.45492

H 1.30477 0.05008 5.27284
H -0.58487 -1.52567 4.87545
H -0.83457 -2.59262 2.63641
H 0.74655 -2.07429 0.82862
H -1.50504 -1.62805 -0.40963
H -5.62253 -2.74261 0.14202
H -4.57627 1.37121 -0.56547
F -1.94118 -3.88555 0.70289
F -2.82785 -4.31576 -1.22885
F -4.01944 -4.53687 0.57669
F -7.40651 -1.08278 0.61179
F -6.89193 0.99356 0.19380
F -7.23626 -0.39452 -1.44147
C 7.21953 -2.21153 -0.61437
C 7.73886 -3.55754 -1.08157
H 7.73159 -1.86049 0.28727
H 7.32367 -1.43892 -1.38205
H 8.80480 -3.47967 -1.32175
H 7.61558 -4.31731 -0.30316
H 7.20620 -3.89031 -1.97778
C 1.65135 -3.64780 -2.04195
C 0.81378 -4.85055 -1.65211
H 2.42540 -3.90219 -2.77220
H 1.04925 -2.83417 -2.45704
H 0.32853 -5.26244 -2.54382
H 1.43764 -5.63334 -1.20833
H 0.03224 -4.58111 -0.93623
O 5.81094 -2.37167 -0.31314
O 2.29995 -3.15442 -0.83993

Entry 6

Free Energy = -2910.394176
Zero-point Energy = -2910.305806
Potential Energy = -2911.01569624
Single Point Energy = -2912.00543643
Nimag = 1 (-1232.8849 cm-1)

Charge = 0 Multiplicity = 1
C 3.10150 1.21419 -0.76275
C 2.50227 1.06449 0.49521
C 3.23037 0.50167 1.54499
C 4.54364 0.07047 1.34107
C 5.15546 0.23902 0.10331
C 4.42560 0.82128 -0.93842
N 1.14392 1.36045 0.73575
C 0.39106 2.38389 0.23207
S 1.02975 3.79564 -0.43812
C 5.25184 -0.62967 2.46653
C 5.09992 1.04242 -2.26797
N -0.94972 2.14704 0.36754
C -1.97523 3.16069 0.20485
C -3.23319 2.58923 -0.48303
C -4.25963 3.71898 -0.69915
C -4.63589 4.38871 0.63420
C -3.40100 4.91624 1.37266
C -2.35820 3.80719 1.55310
N -2.90254 1.82470 -1.75476
C -2.02069 2.54677 -2.71916
C -4.13245 1.34265 -2.44274
O 0.18181 0.21175 -2.47436
N -0.37243 -0.55061 -1.65728
O 0.28038 -1.10298 -0.73389
C -1.77264 -0.71538 -1.72477
C -2.42796 -1.93060 -1.06113
C -2.06581 -3.28532 -1.68496
C -0.78472 -3.85798 -1.62177
C -0.52809 -5.09063 -2.22327
C -1.53798 -5.78050 -2.89659
C -2.81462 -5.22418 -2.96709
C -3.06997 -3.99068 -2.36585
C -2.47725 -2.00821 0.50892
C -3.63473 -1.19097 1.08602
O -4.31203 -0.37707 0.48685
C -1.22033 -1.62245 1.28561
O -1.00893 -0.49181 1.71437
H -1.53555 3.94143 -0.42192
H -2.74505 3.03198 2.23105
H -1.44265 4.20294 2.00528
H -3.68624 5.33056 2.34708
H -2.95547 5.74130 0.79958
H -5.15696 3.65596 1.26716
H -5.34956 5.19887 0.44272
H -3.84416 4.47385 -1.38067
H -5.16948 3.32895 -1.16542
H -3.68296 1.82714 0.16274
H 0.62407 0.60455 1.17844
H -1.22251 1.28268 0.83528
H -1.78064 1.86068 -3.53235
H -2.53728 3.42770 -3.11138
H -1.08726 2.83379 -2.23719
H -3.83083 0.62089 -3.20416
H -4.77349 0.84727 -1.71229
H -4.65957 2.16705 -2.92659
H -2.68454 -3.05131 0.76829
H -2.03249 -0.68751 -2.78496
H -3.48427 -1.78457 -1.31425
H -4.07106 -3.56688 -2.42821
H -3.61262 -5.74644 -3.48899
H -1.33079 -6.74039 -3.36237
H 0.47189 -5.51330 -2.16578
H 0.01183 -3.33000 -1.11367
H 2.76903 0.40063 2.52261
H 6.17574 -0.08751 -0.05596
H 2.52080 1.59224 -1.59244
F 4.76108 -1.88518 2.65294
F 5.08984 0.01730 3.64328
F 6.57581 -0.75392 2.24763
F 4.22114 1.06342 -3.28867
F 5.76839 2.21911 -2.29279
F 6.00945 0.07432 -2.53169

C -4.88888 -0.80366 3.06925
C -4.95115 -1.35363 4.48086
H -5.82818 -0.94641 2.52616
H -4.65052 0.26480 3.05394
H -5.73443 -0.83586 5.04486
H -5.18156 -2.42354 4.47395
H -3.99852 -1.20782 4.99939
C 0.82996 -2.40693 2.18079
C 1.51638 -3.73465 2.42891
H 0.64835 -1.85448 3.10766
H 1.40902 -1.77800 1.50045
H 2.51147 -3.54599 2.84548
H 0.95076 -4.35305 3.13303
H 1.63597 -4.29033 1.49389
O -3.83852 -1.51786 2.37094
O -0.45104 -2.67224 1.54621
H -2.36103 0.79848 -1.50444

Entry 7

Free Energy = -2910.389449
Zero-point Energy = -2910.300151
Potential Energy = -2911.00965883
Single Point Energy = -2912.00253738
Nimag = 1 (-1211.6929 cm-1)

Charge = 0 Multiplicity = 1
C 3.71124 -1.13779 -1.25758
C 3.32302 0.17664 -0.97067
C 3.35767 0.62488 0.35518
C 3.72015 -0.25219 1.37618
C 4.09936 -1.56418 1.09823
C 4.10123 -1.99219 -0.23055
N 2.98601 1.02429 -2.04139
C 2.13777 2.10702 -2.09858
S 2.35582 3.23660 -3.33794
C 3.64440 0.21779 2.80362
C 4.45051 -3.42324 -0.54373
N 1.16491 2.16874 -1.15274
C 0.43673 3.39978 -0.85193
C -1.06632 3.22024 -0.51939
C -1.68357 4.62054 -0.30996
C -0.98942 5.38262 0.83004
C 0.51342 5.52034 0.57736
C 1.13818 4.14853 0.30622
N -1.84054 2.38388 -1.53333
C -1.46778 2.57590 -2.96437
C -3.32012 2.50545 -1.38408
O -0.12327 -0.49381 -2.66676
N -0.36856 -0.52209 -1.44432
O 0.57043 -0.58547 -0.58834
C -1.68046 -0.33826 -0.98779
C -1.94461 -0.87454 0.42660
C -1.95352 0.17572 1.54366
C -3.07591 0.93545 1.91101
C -3.00009 1.88315 2.93627
C -1.79972 2.09711 3.61640
C -0.67513 1.34693 3.26560
C -0.75623 0.39644 2.24600
C -3.14726 -1.86397 0.46675
C -2.85688 -3.06531 -0.44551
O -3.50559 -3.35782 -1.42728
C -4.51468 -1.32499 0.05592
O -4.72702 -0.33851 -0.62144
H 0.52210 4.01734 -1.75083
H 1.09310 3.52781 1.21249
H 2.19444 4.25525 0.03552
H 1.00682 5.99660 1.43299
H 0.68408 6.17443 -0.28919
H -1.15803 4.84128 1.77132
H -1.45789 6.36758 0.94365
H -1.60629 5.19866 -1.24172
H -2.74642 4.53343 -0.07204
H -1.16792 2.65310 0.41341
H 3.48429 0.87816 -2.90970
H 0.99656 1.32100 -0.60306
H -2.02657 1.84436 -3.55126
H -1.73271 3.58673 -3.28974
H -0.40484 2.40261 -3.11210
H -3.78092 1.66377 -1.90185
H -3.58459 2.43632 -0.32941
H -3.67279 3.44888 -1.80629
H -3.23786 -2.24883 1.48914
H -1.68718 1.24388 -1.25073
H -2.38029 -0.63479 -1.76483
H -1.08525 -1.50910 0.65793
H 0.12393 -0.18194 1.98520
H 0.26686 1.48240 3.78986
H -1.74587 2.82844 4.41871
H -3.88779 2.44971 3.20765
H -4.01961 0.79529 1.39591
H 3.10881 1.65156 0.59171
H 4.40002 -2.23417 1.89448
H 3.68312 -1.49415 -2.28171
F 2.40680 0.00404 3.32854
F 3.88513 1.54240 2.91734
F 4.51844 -0.42772 3.60155
F 3.37125 -4.23562 -0.43266
F 4.92210 -3.56613 -1.80053
F 5.38730 -3.90553 0.30173
C -1.32488 -4.83003 -0.86416
C -0.00347 -5.32202 -0.30682
H -1.23158 -4.46152 -1.88962
H -2.09557 -5.60759 -0.85443
H 0.35249 -6.16865 -0.90414
H 0.75791 -4.53742 -0.33918
H -0.11583 -5.65713 0.72947
C -6.83688 -1.80099 0.12820
C -7.75116 -2.85004 0.73094
H -6.86841 -1.80355 -0.96537
H -7.08602 -0.79082 0.46944

H -8.78747 -2.65040 0.43738
H -7.47952 -3.85039 0.38008
H -7.69442 -2.83897 1.82415
O -1.77322 -3.73424 -0.02297
O -5.48527 -2.11145 0.54657

Entry 8

Free Energy = -2910.391214
Zero-point Energy = -2910.300080
Potential Energy = -2911.00981508
Single Point Energy = -2911.99532910
Nimag = 1 (-1072.2331 cm-1)

Charge = 0 Multiplicity = 1
C 4.73296 0.10714 -0.00521
C 3.41310 -0.35190 -0.11016
C 3.13478 -1.70514 0.13029
C 4.15981 -2.58141 0.48152
C 5.47209 -2.12762 0.60659
C 5.74343 -0.78205 0.35811
N 2.34097 0.46347 -0.51238
C 2.11050 1.80761 -0.28061
S 3.00274 2.77394 0.77327
C 3.85459 -4.04254 0.68493
C 7.16885 -0.29475 0.40827
N 1.00701 2.21194 -0.96098
C 0.29104 3.48784 -0.95064
C -0.38258 3.89396 0.39208
C -1.17908 5.19596 0.15507
C -0.29997 6.32728 -0.40085
C 0.36464 5.92188 -1.71625
C 1.16223 4.63180 -1.52018
N -1.25898 2.78395 1.00691
C -2.36694 3.32118 1.84756
C -0.45266 1.85581 1.85867
O -1.05651 1.08770 -2.42774
N -1.34472 0.45588 -1.37773
O -0.56790 -0.42575 -0.92664
C -2.46966 0.84861 -0.63183
C -3.09123 -0.23230 0.25686
C -4.11363 0.38514 1.20958
C -5.15060 1.20304 0.73475
C -6.07648 1.77105 1.61122
C -5.98659 1.52618 2.98299
C -4.97126 0.69981 3.46745
C -4.04652 0.13210 2.58761
C -3.79023 -1.41350 -0.51524
C -4.17573 -2.52963 0.45716
O -3.63444 -2.75499 1.51656
C -2.94333 -2.07191 -1.61116
O -2.33733 -3.11190 -1.48624
H -0.52510 3.30960 -1.66035
H 2.00787 4.80513 -0.84806
H 1.57793 4.28135 -2.47173
H 1.02425 6.71971 -2.07756
H -0.40615 5.77632 -2.48744
H 0.47187 6.58245 0.33858
H -0.91858 7.22332 -0.53160
H -2.00086 4.99963 -0.54901
H -1.63021 5.54206 1.08763
H 0.40066 4.08609 1.13345
H 1.52494 -0.04710 -0.85434
H 0.63930 1.58080 -1.67141
H -2.88855 2.48091 2.30220
H -1.96966 3.96760 2.63689
H -3.07563 3.87516 1.23422
H -1.13671 1.15438 2.33961
H 0.24366 1.29960 1.24100
H 0.09569 2.41714 2.62007
H -4.69812 -1.03593 -0.99544
H -1.81256 1.98564 0.19208
H -3.15110 1.37202 -1.29952
H -2.29728 -0.69130 0.84938
H -3.27962 -0.53785 2.96457
H -4.90115 0.48753 4.53107
H -6.70795 1.96653 3.66601
H -6.87044 2.40262 1.22104
H -5.24170 1.40099 -0.33059
H 2.11374 -2.06770 0.05725
H 6.26401 -2.80525 0.90140
H 4.96342 1.14617 -0.19243
F 3.98888 -4.74215 -0.46575
F 2.59192 -4.23872 1.12041
F 4.68986 -4.60575 1.58574
F 7.78027 -0.43561 -0.79209
F 7.24810 1.01057 0.73878
F 7.90434 -0.98919 1.30504
C -5.58106 -4.41645 0.73067
C -6.70285 -5.10804 -0.02002
H -5.89164 -4.08748 1.72748
H -4.70402 -5.05989 0.84856
H -7.02523 -5.99701 0.53297
H -7.56506 -4.44349 -0.13695
H -6.37084 -5.42236 -1.01451
C -2.14063 -1.80239 -3.82789
C -2.39169 -0.89130 -5.01328
H -2.37785 -2.84849 -4.04231
H -1.10435 -1.74945 -3.48131
H -1.75654 -1.19500 -5.85279
H -3.43674 -0.94465 -5.33642
H -2.15349 0.14372 -4.75264
O -5.19470 -3.25263 -0.04102
O -2.99485 -1.34850 -2.74489

Entry 9

Free Energy = -2910.388832
Zero-point Energy = -2910.298361
Potential Energy = -2911.00752022

Single Point Energy = -2911.99404147
Nimag = 1 (-607.2734 cm-1)

Charge = 0 Multiplicity = 1
C 2.70403 -1.42264 -1.13868
C 3.51342 -0.29523 -1.28406
C 4.67841 -0.16361 -0.52221
C 5.03012 -1.16108 0.38926
C 4.21601 -2.28240 0.55314
C 3.05370 -2.40223 -0.20791
N 3.19370 0.70581 -2.26080
C 2.49676 1.87359 -2.07002
S 2.78290 3.16004 -3.14029
C 6.32132 -1.04892 1.15576
C 2.12797 -3.56465 0.03606
N 1.60464 1.91027 -1.04508
C 1.13172 3.17953 -0.48521
C -0.35507 3.23415 -0.03275
C -0.64432 4.67223 0.45680
C 0.26325 5.07387 1.62896
C 1.74097 4.96703 1.25108
C 2.04996 3.57414 0.69640
N -1.37105 2.75598 -1.07154
C -1.00720 2.97832 -2.49779
C -2.75680 3.25363 -0.83931
O -0.12839 -0.43217 -2.08548
N -0.54362 -0.33551 -0.91046
O 0.24416 -0.45562 0.07797
C -1.86634 0.07178 -0.68241
C -2.46567 -0.42866 0.64430
C -2.59055 0.59516 1.77845
C -3.72622 1.38311 2.01901
C -3.76596 2.28119 3.08998
C -2.67093 2.41431 3.94412
C -1.53433 1.63459 3.71990
C -1.49941 0.73499 2.65313
C -3.75788 -1.26669 0.39907
C -3.39465 -2.51458 -0.41765
O -3.69025 -2.68763 -1.58032
C -4.90364 -0.56516 -0.32625
O -4.83701 0.48492 -0.93403
H 1.27346 3.91282 -1.28392
H 1.95197 2.82070 1.49139
H 3.08278 3.52669 0.33510
H 2.37967 5.17824 2.11723
H 1.98215 5.72220 0.48996
H 0.04872 4.41767 2.48422
H 0.01336 6.09371 1.94561
H -0.50565 5.37730 -0.37536
H -1.68332 4.75748 0.78203
H -0.50578 2.54834 0.80975
H 3.82117 0.77602 -3.05297
H 1.43691 1.05384 -0.51065
H -1.78199 2.51477 -3.11290
H -0.96473 4.04965 -2.71882
H -0.05059 2.51732 -2.72592
H -3.43409 2.63120 -1.42739
H -3.02017 3.13574 0.21120
H -2.85060 4.29979 -1.14110
H -4.13692 -1.60772 1.36892
H -1.54531 1.56427 -0.87673
H -2.45267 -0.12774 -1.57470
H -1.74898 -1.16244 1.02452
H -0.61373 0.13035 2.48119
H -0.67766 1.71404 4.38469
H -2.70697 3.10819 4.77972
H -4.66153 2.87492 3.25638
H -4.58676 1.31525 1.36335
H 5.30360 0.71533 -0.64173
H 4.48452 -3.05106 1.26870
H 1.79904 -1.50059 -1.72702
F 6.26363 -1.70277 2.33627
F 6.63585 0.23908 1.41742
F 7.35865 -1.57359 0.46382
F 1.27381 -3.31215 1.05680
F 1.37434 -3.85407 -1.04676
F 2.80909 -4.68545 0.36888
C -2.13357 -4.52983 -0.36702
C -1.49769 -5.42331 0.67954
H -1.40123 -4.18394 -1.10268
H -2.95112 -5.02205 -0.90093
H -1.09143 -6.31924 0.19733
H -0.67887 -4.90378 1.18405
H -2.23287 -5.73770 1.42741
C -7.18354 -0.80060 -0.93806
C -8.31098 -1.78953 -0.71374
H -6.90795 -0.71927 -1.99362
H -7.43534 0.20225 -0.57796
H -9.20424 -1.46111 -1.25609
H -8.03346 -2.78429 -1.07569
H -8.56162 -1.86484 0.34927
O -2.66665 -3.36589 0.32175
O -6.03177 -1.28152 -0.20181

Entry 10

Free Energy = -2910.378317
Zero-point Energy = -2910.286022
Potential Energy = -2910.99121442
Single Point Energy = -2911.98112448
Nimag = 1 (-1078.2265 cm-1)

Charge = 0 Multiplicity = 1
C 5.12144 0.93625 0.82817
C 4.33673 -0.05747 0.21715
C 4.94060 -0.88662 -0.74374
C 6.27241 -0.70280 -1.10521
C 7.04336 0.29853 -0.51103
C 6.45572 1.11023 0.45815
N 3.02062 -0.31936 0.59407
C 2.08778 0.56804 0.60916

S 2.29896 2.25059 -0.05569
C 6.90442 -1.64340 -2.09677
C 7.25362 2.22493 1.08376
N 0.83961 0.29320 1.08248
C 0.37532 -1.01413 1.55123
C 0.24889 -2.10289 0.44166
C -0.28910 -3.40886 1.06001
C 0.56850 -3.88758 2.24118
C 0.64888 -2.81986 3.33370
C 1.20368 -1.51710 2.75371
N -0.63231 -1.61477 -0.71904
C -1.37065 -2.69381 -1.43414
C 0.14627 -0.85720 -1.74866
O -1.09599 2.03904 0.00999
N -1.98451 1.38475 -0.62690
O -2.25568 1.66420 -1.80732
C -2.57860 0.27898 0.00639
C -3.95732 -0.14344 -0.49895
C -4.31967 -1.51737 0.06929
C -4.21156 -1.79164 1.44210
C -4.53829 -3.04932 1.95450
C -4.98728 -4.05943 1.10155
C -5.11672 -3.79567 -0.26317
C -4.78909 -2.53699 -0.77149
C -5.12535 0.85824 -0.16285
C -6.41918 0.42993 -0.85535
O -6.48831 -0.20698 -1.88296
C -4.87263 2.31137 -0.58359
O -5.32552 2.82922 -1.57937
H -0.64082 -0.82386 1.91571
H 2.23975 -1.65967 2.43512
H 1.20600 -0.71961 3.50541
H 1.28529 -3.16062 4.15888
H -0.35241 -2.65248 3.75747
H 1.58072 -4.12826 1.88723
H 0.14285 -4.81906 2.63279
H -1.31988 -3.25206 1.40726
H -0.32138 -4.19933 0.30454
H 1.24195 -2.28454 0.01522
H 0.97580 2.49098 -0.22044
H 0.10918 0.98922 0.92333
H -1.94770 -2.22552 -2.23367
H -0.66754 -3.40894 -1.87261
H -2.05990 -3.19995 -0.76420
H -0.55657 -0.45147 -2.47855
H 0.68114 -0.03589 -1.28729
H 0.85386 -1.53092 -2.24182
H -5.28861 0.85957 0.91930
H -1.47975 -0.83818 -0.33040
H -2.49897 0.42287 1.08159
H -3.92517 -0.21451 -1.58854
H -4.92005 -2.32904 -1.82883
H -5.48149 -4.56789 -0.93558
H -5.24473 -5.03764 1.49869
H -4.44948 -3.23567 3.02179
H -3.87826 -1.01542 2.12648
H 4.34915 -1.66909 -1.20615
H 8.08044 0.43595 -0.79092
H 4.69154 1.55621 1.60723
F 6.01542 -2.06861 -3.02370
F 7.39353 -2.75091 -1.49011
F 7.93392 -1.06876 -2.75459
F 7.06752 3.39640 0.43429
F 6.90064 2.43096 2.37244
F 8.58017 1.96862 1.06194
C -8.77786 0.63328 -0.78253
C -9.83155 1.25389 0.11474
H -8.91132 -0.44801 -0.88988
H -8.77793 1.07145 -1.78515
H -10.82666 1.08810 -0.31234
H -9.80732 0.80854 1.11464
H -9.67385 2.33257 0.21284
C -3.68829 4.28762 -0.02018
C -2.90729 4.83482 1.15829
H -4.57818 4.88159 -0.24813
H -3.07616 4.22147 -0.92429
H -2.56140 5.84956 0.93220
H -3.52949 4.87670 2.05868
H -2.03515 4.20615 1.35807
O -7.48774 0.88173 -0.17324
O -4.10907 2.94134 0.32740

Entry 11

Free Energy = -3485.133116
Zero-point Energy = -3485.025390
Potential Energy = -3485.92820983
Single Point Energy = -3487.13432233
Nimag = 1 (-1072.7398 cm-1)

Charge = 0 Multiplicity = 1
C 4.26050 1.44522 0.12895
C 2.98601 0.87636 0.25477
C 2.86596 -0.51096 0.40979
C 4.00173 -1.31830 0.43217
C 5.27203 -0.76222 0.28874
C 5.38533 0.62034 0.13692
N 1.79021 1.62242 0.31655
C 1.42154 2.74791 -0.35634
S 2.41899 3.59277 -1.44111
C 3.84570 -2.81090 0.55323
C 6.75748 1.23793 0.06668
N 0.12740 3.11082 -0.09659
C -0.43414 4.40266 -0.46266
C -1.84644 4.26530 -1.07419
C -2.38295 5.64035 -1.49874
C -2.41722 6.60340 -0.29795
C -1.03893 6.73524 0.35962
C -0.48392 5.35958 0.74786
N -1.87483 3.24020 -2.21564
C -0.81464 3.40287 -3.26002

C -3.21975 3.13970 -2.86560
O -3.74379 1.06285 -0.76828
N -2.74981 0.30012 -0.72704
O -1.65103 0.62144 -1.29193
C -2.81051 -0.85849 0.05349
C -1.72531 -1.90383 -0.15627
C -1.87760 -3.07837 0.81578
C -3.12788 -3.54540 1.24745
C -3.22911 -4.63088 2.12026
C -2.08075 -5.27904 2.57246
C -0.83039 -4.83163 2.14214
C -0.72991 -3.74288 1.27598
C -1.57256 -2.36655 -1.65424
C -2.40314 -3.60088 -1.97965
O -1.97312 -4.72267 -2.12060
C -0.10501 -2.59254 -2.01780
O 0.82729 -2.50867 -1.24492
H 0.24344 4.83285 -1.20542
H -1.09790 4.90410 1.53435
H 0.53481 5.45041 1.14015
H -1.10191 7.37936 1.24470
H -0.34647 7.22770 -0.33793
H -3.14082 6.22881 0.43956
H -2.78580 7.58048 -0.63181
H -1.74280 6.06552 -2.28408
H -3.39181 5.55220 -1.91508
H -2.50895 3.81969 -0.32445
H 1.06773 1.18746 0.89812
H -0.38968 2.61170 0.63541
H -0.92576 2.58352 -3.97313
H -0.95504 4.35619 -3.77346
H 0.17781 3.36121 -2.80821
H -3.24071 2.21512 -3.44380
H -3.98534 3.08372 -2.09545
H -3.37235 3.99642 -3.52270
H -1.91618 -1.55492 -2.30211
H -1.72408 2.29633 -1.76514
H -0.77424 -1.41739 0.06973
H 0.24686 -3.41612 0.93697
H 0.07446 -5.33217 2.47715
H -2.15897 -6.12567 3.24943
H -4.21037 -4.96736 2.44536
H -4.04090 -3.06717 0.90791
H 1.88374 -0.95778 0.49847
H 6.15497 -1.39011 0.29866
H 4.36976 2.51447 0.02049
F 3.67828 -3.40774 -0.64700
F 2.77372 -3.14519 1.31532
F 4.93093 -3.38234 1.12413
F 6.74755 2.43502 -0.55404
F 7.27663 1.43784 1.30233
F 7.62946 0.44250 -0.59529
C -4.63892 -4.36195 -2.28911
C -4.77207 -4.67065 -3.77244
H -5.58283 -4.00788 -1.86709
H -4.29481 -5.23458 -1.72928
H -5.53145 -5.44672 -3.92326
H -5.07656 -3.77895 -4.33044
H -3.82346 -5.03517 -4.17582
C 1.37791 -3.08719 -3.80902
C 2.06829 -1.78690 -4.18987
H 1.23896 -3.74133 -4.67282
H 1.93317 -3.61722 -3.03239
H 3.05366 -2.00348 -4.61818
H 1.48409 -1.23650 -4.93498
H 2.21100 -1.15253 -3.31067
O -3.71355 -3.26913 -2.05812
O 0.02817 -2.84230 -3.32931
H -3.84550 -1.18182 0.10160
O 0.07065 0.44114 2.21755
C -0.89210 -0.03893 2.81611
C -2.30581 0.26748 2.59794
H -2.97574 -0.24159 3.28485
C -2.69743 1.64502 2.31528
O -3.97068 1.87322 2.72972
O -2.04382 2.51245 1.73247
C -4.57534 3.11015 2.32022
H -3.94291 3.94779 2.63293
H -4.63771 3.12077 1.22493
C -5.95180 3.17583 2.95811
H -5.87553 3.15422 4.04993
H -6.45789 4.10273 2.66565
H -6.56876 2.32962 2.63974
O -0.73333 -0.99658 3.75546
C 0.61584 -1.44906 4.00583
H 1.23358 -0.58761 4.27931
H 1.02926 -1.87887 3.08820
C 0.54332 -2.47604 5.12038
H -0.08138 -3.32362 4.82200
H 1.54841 -2.84769 5.34867
H 0.12197 -2.03688 6.03059
H -2.58930 -0.34579 1.30671

Entry 12

Free Energy = -3485.133881
Zero-point Energy = -3485.025484
Potential Energy = -3485.92812379
Single Point Energy = -3487.13066051
Nimag = 1 (-954.4838 cm-1)

Charge = 0 Multiplicity = 1
C -4.83365 -1.16528 -0.76241
C -3.83291 -0.54142 -0.00422
C -4.02295 0.78818 0.40908
C -5.19034 1.46909 0.07607
C -6.19897 0.84795 -0.66049
C -6.00302 -0.46863 -1.07123
N -2.59610 -1.12795 0.33223
C -2.20381 -2.44338 0.39423
S -3.23360 -3.77774 0.23489

C -5.33115 2.91737 0.45620
C -7.09563 -1.18040 -1.82736
N -0.86321 -2.57290 0.61350
C -0.17378 -3.83922 0.83086
C 1.14614 -3.91246 0.03066
C 1.79560 -5.29222 0.18588
C 2.08514 -5.56355 1.67365
C 0.81797 -5.44533 2.53108
C 0.12595 -4.09092 2.32270
N 0.93632 -3.50128 -1.42802
C -0.14557 -4.23182 -2.15649
C 2.21667 -3.50567 -2.21949
O 0.83619 -0.70217 -1.53676
N 1.32202 -0.10129 -0.53927
O 1.18793 -0.56393 0.63438
C 2.16118 1.00012 -0.74276
C 2.30039 1.97735 0.42726
C 3.35865 3.03530 0.11794
C 3.27665 3.88157 -0.99810
C 4.25552 4.84981 -1.22787
C 5.33179 4.98958 -0.35067
C 5.42674 4.14895 0.75872
C 4.44804 3.18124 0.98836
C 0.97490 2.65065 0.93957
C 0.08555 1.68983 1.72886
O -0.97368 1.23466 1.33141
C 0.11027 3.33398 -0.12134
O 0.13411 3.12032 -1.31441
H -0.85758 -4.62339 0.49382
H 0.76200 -3.27956 2.70449
H -0.82172 -4.04940 2.87045
H 1.06232 -5.58197 3.59132
H 0.11856 -6.25070 2.26546
H 2.83817 -4.84154 2.01659
H 2.53020 -6.55961 1.78016
H 1.13356 -6.07539 -0.20903
H 2.73389 -5.33108 -0.37457
H 1.85068 -3.15927 0.39700
H -1.90285 -0.44000 0.62535
H -0.27351 -1.73544 0.66740
H -0.21750 -3.80674 -3.15945
H 0.12140 -5.28757 -2.22878
H -1.09978 -4.11884 -1.64064
H 2.05217 -2.91193 -3.11891
H 3.01996 -3.05369 -1.63556
H 2.46408 -4.53258 -2.49175
H 1.28282 3.42102 1.65413
H 0.67118 -2.49214 -1.37860
H 2.66833 1.40077 1.27991
H 4.53956 2.51663 1.84392
H 6.26498 4.24058 1.44442
H 6.09310 5.74319 -0.53360
H 4.17543 5.49524 -2.09874
H 2.44443 3.78933 -1.68801
H -3.25112 1.28675 0.98372
H -7.10919 1.37779 -0.91272
H -4.70249 -2.18136 -1.10282
F -4.83068 3.73628 -0.50696
F -4.66301 3.21340 1.59618
F -6.61918 3.27461 0.63575
F -6.59822 -2.07435 -2.70887
F -7.91502 -1.86125 -0.99455
F -7.87049 -0.31504 -2.52027
C -0.12283 0.50212 3.77117
C 0.60270 0.42441 5.10012
H -0.14578 -0.46308 3.25612
H -1.15278 0.85396 3.88237
H 0.08804 -0.28210 5.76016
H 1.63358 0.08234 4.96420
H 0.62395 1.40185 5.59206
C -1.65844 4.89786 -0.39394
C -2.47766 5.82990 0.47653
H -2.28323 4.14487 -0.88090
H -1.09980 5.43149 -1.16893
H -3.20277 6.36596 -0.14488
H -3.03114 5.26663 1.23257
H -1.83891 6.56470 0.97702
O 0.59867 1.44398 2.93691
O -0.70748 4.21897 0.47004
H 1.96224 1.42709 -1.71966
O 4.67185 -1.76837 -2.61632
C 4.97426 -0.70684 -2.08797
C 4.70801 -0.26224 -0.72066
H 5.28342 0.60543 -0.41260
C 4.47680 -1.23605 0.33645
O 4.73078 -0.67350 1.56397
O 4.05672 -2.38751 0.24472
C 4.42645 -1.48778 2.70485
H 3.35340 -1.71662 2.70667
H 4.96651 -2.43770 2.63015
C 4.83192 -0.70927 3.94471
H 4.27401 0.23084 4.01696
H 4.62933 -1.30083 4.84489
H 5.90047 -0.47187 3.92310
O 5.60024 0.28837 -2.78910
C 5.85761 0.01016 -4.17493
H 4.91367 -0.22526 -4.67981
H 6.49712 -0.87609 -4.25476
C 6.52272 1.23928 -4.76928
H 7.46489 1.45891 -4.25647
H 6.73729 1.07485 -5.83129
H 5.87273 2.11578 -4.67910
H 3.33230 0.41480 -0.81489

Entry 13

Free Energy = -3485.117449
Zero-point Energy = -3485.011401
Potential Energy = -3485.91372478
Single Point Energy = -3487.12040455
Nimag = 1 (-1165.4472 cm-1)

Charge = 0 Multiplicity = 1
C -3.60518 1.97929 0.23473
C -2.64614 1.52636 -0.68215
C -3.00965 0.55730 -1.62717
C -4.30769 0.05322 -1.65918
C -5.27374 0.51481 -0.76755
C -4.90393 1.47447 0.17553
N -1.29185 1.92050 -0.68898
C -0.69479 3.07771 -0.27941
S -1.51510 4.44656 0.29097
C -4.62782 -1.06015 -2.61755
C -5.91193 1.90046 1.21109
N 0.66954 3.02215 -0.38769
C 1.55409 4.16154 -0.19524
C 2.74118 3.80916 0.73204
C 3.63733 5.03599 0.95566
C 4.15926 5.57673 -0.38729
C 3.00870 5.91086 -1.34312
C 2.08544 4.70144 -1.53999
N 2.26781 3.17252 2.04050
C 1.24861 3.95077 2.81058
C 3.39957 2.76341 2.93061
O 1.32028 0.66104 1.56579
N 2.20256 0.01903 0.91750
O 3.35817 0.48607 0.78622
C 1.85639 -1.25388 0.43901
C 2.74093 -1.78449 -0.67539
C 2.86064 -3.30354 -0.75008
C 1.86363 -4.17774 -0.30058
C 2.04074 -5.55936 -0.41478
C 3.20250 -6.08613 -0.97898
C 4.20167 -5.22023 -1.42804
C 4.02900 -3.84216 -1.31019
C 2.32180 -1.19776 -2.11660
C 2.92136 0.18353 -2.30835
O 2.43740 1.25822 -2.00115
C 0.81453 -1.23856 -2.29825
O 0.04636 -0.31935 -2.06277
H 0.94646 4.94473 0.26608
H 2.61544 3.89525 -2.06331
H 1.21971 4.97048 -2.15466
H 3.40315 6.24305 -2.31071
H 2.42924 6.75169 -0.93666
H 4.81392 4.82290 -0.84751
H 4.78093 6.46050 -0.20285
H 3.06866 5.82625 1.46439
H 4.48791 4.78358 1.59757
H 3.32291 3.00441 0.26930
H -0.67788 1.21531 -1.10001
H 1.08045 2.23118 -0.88695
H 0.95642 3.35069 3.67451
H 1.68714 4.89162 3.14912
H 0.37082 4.14119 2.19097
H 2.98861 2.11474 3.70619
H 4.11687 2.19536 2.34055
H 3.85648 3.64238 3.38594
H 2.77692 -1.85760 -2.85658
H 1.82587 2.24671 1.76662
H 3.74715 -1.39549 -0.50109
H 4.81450 -3.17155 -1.65546
H 5.11732 -5.61609 -1.86016
H 3.33324 -7.16207 -1.06207
H 1.26237 -6.22531 -0.05093
H 0.95692 -3.79035 0.15392
H -2.26349 0.18934 -2.32066
H -6.28787 0.13570 -0.80251
H -3.34196 2.71653 0.97833
F -4.25773 -2.26871 -2.11257
F -3.96956 -0.92430 -3.79310
F -5.94424 -1.13892 -2.89421
F -5.63020 3.11023 1.73439
F -7.16134 1.95688 0.69719
F -5.95605 1.02293 2.24438
C 4.91046 1.27940 -3.02271
C 6.23415 0.89757 -3.65734
H 5.04339 1.73938 -2.03795
H 4.33918 1.97344 -3.64728
H 6.84926 1.79289 -3.79835
H 6.78469 0.19721 -3.02158
H 6.07848 0.42935 -4.63420
C -1.00697 -2.72757 -2.66727
C -1.19344 -4.16515 -3.10682
H -1.51528 -2.02800 -3.33594
H -1.34891 -2.56477 -1.64218
H -2.26059 -4.40928 -3.07471
H -0.83275 -4.31943 -4.12907
H -0.65753 -4.84657 -2.43985
O 4.14224 0.06397 -2.85931
O 0.42659 -2.44473 -2.70110
H 0.77907 -1.30109 0.30089
O 1.87251 -2.68251 2.60791
C 0.90087 -2.61261 3.45490
C -0.46764 -2.49766 3.27406
H -1.06008 -2.43434 4.17725
C -1.19018 -2.56848 2.04339
O -2.54127 -2.50352 2.28115
O -0.76974 -2.68622 0.88271
C -3.39295 -2.62589 1.13628
H -3.14685 -1.84718 0.40788
H -3.21601 -3.59275 0.64958
C -4.83051 -2.50251 1.61225
H -5.01882 -1.51869 2.05337
H -5.51083 -2.63514 0.76303
H -5.06026 -3.26761 2.36128
O 1.26844 -2.68402 4.76950
C 2.66710 -2.77389 5.06762
H 3.19615 -1.91300 4.64146
H 3.08899 -3.67382 4.60679
C 2.79727 -2.81249 6.58128
H 2.26779 -3.67711 6.99423
H 3.85295 -2.88403 6.86710

H 2.37572 -1.90809 7.03274
H 1.84560 -2.02795 1.56293

Entry 14

Free Energy = -3485.101387
Zero-point Energy = -3484.993531
Potential Energy = -3485.89558654
Single Point Energy = -
Nimag = 1 (-1170.7845 cm-1)

Charge = 0 Multiplicity = 1
C 6.60687 1.51984 -0.54407
C 6.86507 2.01040 -1.98213
C 5.82398 3.04526 -2.42691
C 4.39401 2.51914 -2.23835
N 4.87576 0.33030 0.92878
C 4.70869 1.29120 2.06661
C 5.84399 -0.75165 1.29099
O -0.04816 -1.63336 -3.28509
N 0.22454 -1.24120 -2.14766
O 0.93035 -0.18259 -1.99728
C -0.29802 -1.92117 -1.02227
C 0.44893 -1.72200 0.28688
C -0.42052 -1.94234 1.52057
C -1.23205 -3.07699 1.65392
C -1.97576 -3.27805 2.81740
C -1.91647 -2.35567 3.86466
C -1.11626 -1.21896 3.73707
C -0.37420 -1.01625 2.57184
C 1.73139 -2.67752 0.39830
C 2.38734 -2.46698 1.74790
O 2.99381 -1.45823 2.08592
C 2.69624 -2.42401 -0.74628
O 3.61047 -1.60984 -0.74041
H 4.31220 2.91720 -0.13387
H 4.19876 1.68494 -2.92705
H 3.66378 3.30246 -2.46660
H 5.98861 3.32023 -3.47502
H 5.94852 3.96457 -1.83815
H 6.84266 1.14747 -2.66239
H 7.87597 2.42940 -2.04276
H 6.74078 2.35672 0.15458
H 7.34956 0.75733 -0.28770
H 5.06536 0.11752 -1.11805
H 0.47846 1.30257 -1.05149
H 2.44433 0.86631 -1.14832
H 4.39680 0.71241 2.93629
H 5.66206 1.78458 2.26220
H 3.94238 2.02866 1.82398
H 5.42971 -1.28546 2.14485
H 5.93837 -1.43654 0.44868
H 6.80809 -0.31279 1.54717
H 1.37296 -3.70603 0.33137
H 3.97236 -0.16646 0.81488
H 0.83094 -0.70051 0.32398
H 0.24347 -0.12685 2.47457
H -1.07798 -0.48372 4.53686
H -2.50448 -2.51234 4.76528
H -2.61906 -4.15017 2.89504
H -1.31945 -3.78167 0.83181
H -1.21017 2.47245 -2.33260
H -3.98634 4.83944 -0.05741
H -0.37641 3.39271 1.78074
F -4.48393 2.65324 -2.49985
F -2.94509 3.65202 -3.66377
F -4.37022 4.82316 -2.50169
F -1.65186 4.91785 3.16716
F -3.25031 5.96964 2.12245
F -3.59354 3.97466 2.90705
C 2.56302 -3.36678 3.94971
C 1.83742 -4.44896 4.72574
H 2.28924 -2.36375 4.28574
H 3.65239 -3.46975 4.01650
H 2.10871 -4.38778 5.78520
H 0.75496 -4.32029 4.63391
H 2.10478 -5.44438 4.35748
C 3.07311 -2.91661 -3.05093
C 2.48854 -3.86000 -4.08219
H 4.14818 -3.06054 -2.90373
H 2.88480 -1.86891 -3.30033
H 2.96790 -3.68282 -5.05121
H 2.65489 -4.90459 -3.79996
H 1.41483 -3.68296 -4.18583
O 2.17491 -3.50426 2.55733
O 2.39899 -3.19395 -1.78784
H -0.52928 -2.94188 -1.31432
O -2.67900 -0.98922 -0.61876
C -3.79250 -1.56803 -0.32807
C -4.24246 -2.86979 -0.50022
H -5.27324 -3.04774 -0.22341
C -3.51822 -3.98368 -1.01728
O -4.35792 -5.07043 -1.17350
O -2.31838 -4.09299 -1.29341
C -3.74240 -6.26618 -1.65771
H -3.26313 -6.07178 -2.62447
H -2.95061 -6.58401 -0.96749
C -4.83034 -7.32096 -1.77780
H -5.61109 -6.99525 -2.47313
H -4.40766 -8.26235 -2.14821
H -5.29868 -7.51084 -0.80601

Entry 15

Free Energy = -2910.395479
Zero-point Energy = -2910.305989
Potential Energy = -2912.00489608
Single Point Energy = -2912.00520886
Nimag = 1 (-1268.6466 cm-1)

Charge = 0 Multiplicity = 1
C -1.00421 4.58491 -1.68254
C -0.34414 3.90796 -0.65531
C 0.07343 4.63002 0.46681
C -0.15936 6.00097 0.55319
C -0.81442 6.66932 -0.48000
C -1.23870 5.95590 -1.59943
C -0.07117 2.41439 -0.79088
C 1.40083 2.18531 -1.22258
C 2.45602 2.55095 -0.18800
O 3.53488 3.07132 -0.77288
C 4.67728 3.33088 0.09213
C 5.79908 3.84601 -0.78072
C -0.45719 1.61999 0.44865
N -1.80272 1.79081 0.85302
O -2.67712 2.10541 0.02675
O -2.11065 1.47064 2.02834
C 1.70276 0.76977 -1.72527
O 0.71629 0.31463 -2.50973
C 0.85759 -1.03621 -3.03901
C -0.52322 -1.64808 -3.12131
O 2.72984 0.17925 -1.50109
O 2.34600 2.37877 1.00466
N -0.45334 -1.09051 0.19384
C -1.61858 -1.73405 0.28138
N -2.68714 -0.96143 -0.13540
C -4.06340 -1.40815 -0.21436
C -4.99553 -0.38499 0.45753
C -6.44914 -0.85390 0.42473
C -6.89175 -1.07805 -1.02793
C -5.97684 -2.07456 -1.74447
C -4.51169 -1.63760 -1.66451
N -4.50965 -0.05268 1.86026
C -5.28740 1.06320 2.47669
C 0.78615 -1.69383 0.40220
C 1.74256 -1.03580 1.18839
C 3.02681 -1.55440 1.31501
C 3.39986 -2.72560 0.66086
C 2.44655 -3.37740 -0.11530
C 1.15383 -2.88161 -0.24097
C 2.77709 -4.65622 -0.82820
F 2.05283 -5.70558 -0.36310
C 4.04823 -0.81911 2.13448
F 3.49047 -0.08599 3.12185
S -1.86910 -3.30552 0.90837
F 4.07842 -5.00127 -0.72009
F 2.50162 -4.57537 -2.15733
F 4.93063 -1.66569 2.72355
F 4.79441 0.03691 1.38942
C -4.40032 -1.22099 2.78813
H -4.10943 -2.36252 0.31197
H -4.36607 -0.71230 -2.23650
H -3.85565 -2.39416 -2.10100
H -6.27758 -2.17833 -2.79032
H -6.08457 -3.06404 -1.28573
H -6.87811 -0.11876 -1.55842
H -7.92617 -1.43018 -1.03920
H -6.54909 -1.79128 0.98109
H -7.10423 -0.11979 0.89803
H -4.90075 0.56610 -0.07303
H -2.45126 -0.18385 -0.73848
H -4.05273 -0.84991 3.75046
H -5.37764 -1.68380 2.90426
H -3.67847 -1.93392 2.39178
H -4.74860 1.40394 3.35763
H -5.35546 1.87772 1.75869
H -6.27691 0.70981 2.75605
H 1.56814 2.82403 -2.09490
H -3.54773 0.32796 1.75778
H 0.18411 1.74823 1.31233
H -0.66387 2.05791 -1.63311
H -1.34683 4.02999 -2.54977
H -1.75805 6.46416 -2.40393
H -0.99717 7.73542 -0.41079
H 0.17055 6.54653 1.42997
H 0.58031 4.12069 1.27671
H 0.42568 -3.40529 -0.84366
H 4.39925 -3.12284 0.75880
H 1.48193 -0.12061 1.70102
H 1.52168 -1.59971 -2.38841
H 1.32605 -0.95229 -4.02304
H -0.45314 -2.63721 -3.58078
H -0.94849 -1.76266 -2.12399
H -1.19290 -1.03433 -3.72814
H 4.93525 2.39759 0.59385
H 4.37362 4.05687 0.84834
H 6.67632 4.04877 -0.16137
H 6.07511 3.10751 -1.53612
H 5.51190 4.77202 -1.28380
H -0.44880 0.30593 0.28618

Entry 16

Free Energy = -2910.397847
Zero-point Energy = -2910.307478
Potential Energy = -2911.01636759
Single Point Energy = -2912.00392784
Nimag = 1 (-661.7629 cm-1)

Charge = 0 Multiplicity = 1
C -0.60843 4.01205 -2.34165
C -0.49820 2.94142 -1.44527
C -1.56156 2.69415 -0.56569
C -2.70954 3.48728 -0.58780
C -2.80571 4.55236 -1.48488
C -1.75019 4.81457 -2.36005
C 0.76335 2.08085 -1.43370
C 1.75370 2.64273 -0.33400
C 1.25595 2.49253 1.09373
O 0.95677 3.68777 1.62526
C 0.43890 3.67637 2.98046

C 0.11022 5.10929 3.35136
C 0.36078 0.60133 -1.40075
N 1.34052 -0.32339 -1.83676
O 2.55137 -0.01070 -1.84674
O 0.97189 -1.49970 -2.09855
C 3.19648 2.14046 -0.44941
O 3.75354 2.65230 -1.56249
C 5.10781 2.23764 -1.84766
C 5.53374 2.92622 -3.13046
O 3.79660 1.46790 0.36265
O 1.13545 1.44494 1.69737
N -0.64468 -0.85731 0.63067
C 0.17992 -1.82294 1.05198
N 1.50214 -1.39502 1.05201
C 2.62683 -2.15195 1.56187
C 3.66440 -2.39374 0.43694
C 4.87693 -3.18518 0.94096
C 5.54962 -2.42455 2.09767
C 4.55667 -2.15592 3.23599
C 3.31404 -1.41230 2.72714
N 2.99917 -3.02857 -0.78953
C 3.84750 -2.93233 -2.01814
C -2.02121 -1.06366 0.43151
C -2.93839 -0.36205 1.22098
C -4.30731 -0.42621 0.94666
C -4.78366 -1.19989 -0.10900
C -3.86936 -1.91083 -0.89226
C -2.50191 -1.84360 -0.63317
C -4.37767 -2.78955 -2.00344
F -3.46739 -2.93203 -2.99277
C -5.24782 0.40951 1.76832
F -5.16350 1.72906 1.43772
S -0.27662 -3.40228 1.52940
F -5.50560 -2.29086 -2.56299
F -4.67933 -4.03350 -1.56548
F -6.53817 0.05159 1.60464
F -4.96784 0.33459 3.08820
C 2.49376 -4.42687 -0.59396
H 2.23765 -3.10897 1.92523
H 3.59133 -0.40369 2.39199
H 2.57703 -1.29222 3.52846
H 5.04165 -1.57430 4.02903
H 4.25500 -3.11162 3.68802
H 5.94521 -1.47095 1.72153
H 6.40775 -3.00318 2.45936
H 4.55825 -4.17143 1.30285
H 5.60383 -3.35317 0.13695
H 3.98675 -1.41361 0.06851
H 1.59502 -0.38080 1.12371
H 1.98400 -4.72457 -1.51204
H 3.33757 -5.09258 -0.40691
H 1.77379 -4.43660 0.22866
H 3.25094 -3.27330 -2.86522
H 4.11136 -1.88718 -2.17020
H 4.73163 -3.56005 -1.90372
H 1.80519 3.71450 -0.54496
H 2.16605 -2.43752 -1.00510
H -0.54432 0.41190 -1.98056
H 1.30062 2.26497 -2.37250
H 0.20441 4.21550 -3.03591
H -1.81843 5.63789 -3.06639
H -3.70012 5.16913 -1.50720
H -3.52993 3.25411 0.08501
H -1.50358 1.86646 0.13485
H -1.79278 -2.37573 -1.25610
H -5.84399 -1.24279 -0.32569
H -2.56739 0.23276 2.04933
H 5.12082 1.14764 -1.94304
H 5.74583 2.51083 -1.00113
H 6.55961 2.63783 -3.38473
H 4.87948 2.64246 -3.96083
H 5.50027 4.01489 -3.02043
H 1.19698 3.23874 3.63754
H -0.44226 3.02859 3.01004
H -0.28678 5.14433 4.37160
H 1.00291 5.74137 3.30679
H -0.64230 5.52345 2.67324
H -0.07964 0.01047 -0.26479

Entry 17

Free Energy = -2910.395075
Zero-point Energy = -2910.306005
Potential Energy = -2912.00571594
Single Point Energy = -2912.00398396
Nimag = 1 (-1312.1037 cm-1)

Charge = 0 Multiplicity = 1
C 0.49437 5.00581 -0.88319
C -0.16453 3.79457 -1.11044
C -1.07464 3.71503 -2.16964
C -1.32038 4.82376 -2.97677
C -0.65943 6.02787 -2.73970
C 0.25106 6.11613 -1.68866
C 0.10940 2.61771 -0.18405
C -0.98933 2.50908 0.90185
C -2.36197 2.12580 0.35957
O -3.32951 2.83493 0.94179
C -4.69475 2.48073 0.58030
C -5.62097 3.32389 1.42722
C 0.33861 1.30314 -0.90622
N 1.61050 1.15976 -1.48786
O 2.58481 1.83746 -1.10096
O 1.78018 0.20536 -2.29731
C -0.65861 1.56737 2.06036
O 0.66097 1.49362 2.28481
C 1.11347 0.67796 3.40575
C 2.28662 1.37992 4.05374
O -1.49998 1.01059 2.72279
O -2.54965 1.28493 -0.48807
N 0.26733 -0.93943 0.57652

C 1.45026 -1.55663 0.66339
N 2.52168 -0.68434 0.69312
C 3.90518 -1.06853 0.88614
C 4.80961 -0.48318 -0.21244
C 6.26048 -0.92816 -0.02396
C 6.77498 -0.49323 1.35509
C 5.88931 -1.04210 2.47559
C 4.42850 -0.63993 2.26471
N 4.27591 -0.80752 -1.60071
C 5.02762 -0.09446 -2.67778
C -0.90277 -1.64929 0.24416
C -1.99929 -1.63425 1.09727
C -3.20169 -2.22153 0.69669
C -3.31995 -2.84595 -0.53508
C -2.21174 -2.85807 -1.38731
C -1.01848 -2.26267 -1.01170
C -2.37009 -3.50175 -2.73289
F -1.19851 -3.69501 -3.37231
C -4.36587 -2.16999 1.64087
F -4.51925 -0.93726 2.18494
S 1.68227 -3.24882 0.72471
F -3.14737 -2.75169 -3.56235
F -2.98099 -4.71141 -2.64868
F -5.53973 -2.48530 1.04776
F -4.21754 -3.02779 2.68472
C 4.14272 -2.26567 -1.90369
H 3.92502 -2.15871 0.83293
H 4.32612 0.44820 2.36087
H 3.78485 -1.09341 3.02213
H 6.23943 -0.68348 3.44715
H 5.96261 -2.13539 2.49802
H 6.79439 0.60207 1.40428
H 7.80661 -0.83210 1.47798
H 6.32855 -2.01757 -0.10150
H 6.89871 -0.50392 -0.80139
H 4.75251 0.60746 -0.17031
H 2.29737 0.28603 0.87355
H 3.74061 -2.35983 -2.91064
H 5.12049 -2.73881 -1.85273
H 3.45262 -2.72001 -1.19348
H 4.44539 -0.16558 -3.59398
H 5.12866 0.95103 -2.39555
H 6.00205 -0.55574 -2.81852
H -1.09333 3.49516 1.36496
H 3.31481 -0.41063 -1.67348
H -0.42045 0.96544 -1.60214
H 1.02822 2.84300 0.35330
H 1.21101 5.07633 -0.07157
H 0.77632 7.04543 -1.49953
H -0.84936 6.88793 -3.37129
H -2.02797 4.74463 -3.79424
H -1.59873 2.78810 -2.36452
H -0.17120 -2.25510 -1.68198
H -4.25488 -3.29772 -0.83714
H -1.92147 -1.13379 2.05224
H 1.38296 -0.29593 2.99107
H 0.28115 0.54523 4.09368
H 2.71806 0.73351 4.82246
H 3.06546 1.60499 3.32408
H 1.97181 2.31299 4.52585
H -4.82513 1.41328 0.76249
H -4.82322 2.66855 -0.48735
H -6.65802 3.08631 1.17760
H -5.46783 3.12143 2.48912
H -5.45868 4.38862 1.24555
H 0.33983 0.24477 -0.08694

Entry 18

Free Energy = -2910.387315
Zero-point Energy = -2910.299350
Potential Energy = -2912.00825923
Single Point Energy = -2912.00595432
Nimag = 1 (-1205.5121 cm-1)

Charge = 0 Multiplicity = 1
C -1.51687 4.39403 -0.20283
C -1.88869 3.09494 -0.55374
C -3.08486 2.90206 -1.24835
C -3.90135 3.98499 -1.56745
C -3.53028 5.27680 -1.19868
C -2.32961 5.47929 -0.51991
C -1.02324 1.92700 -0.10065
C -1.45692 1.53940 1.36581
C -2.95979 1.32783 1.39364
O -3.57441 2.32484 2.03330
C -5.02283 2.40466 1.92141
C -5.41752 3.83010 2.23792
C -1.07286 0.68176 -0.96128
N -0.91744 0.83745 -2.36043
O -0.32159 1.82059 -2.81652
O -1.27359 -0.12927 -3.07664
C -0.71435 0.33131 1.91328
O 0.48576 0.66486 2.36365
C 1.28483 -0.40865 2.96156
C 2.61504 0.18236 3.36071
O -1.16011 -0.80109 1.95695
O -3.51425 0.40654 0.83878
N 1.03036 -0.98740 -0.72575
C 0.59973 -2.24136 -0.51096
N -0.65500 -2.42940 -1.05718
C -1.39467 -3.67707 -1.06749
C -2.76590 -3.50746 -0.38228
C -3.57778 -4.80227 -0.41059
C -3.77220 -5.27601 -1.85654
C -2.42723 -5.45958 -2.56166
C -1.59913 -4.17454 -2.50733
N -2.60879 -2.94955 1.02612
C -3.91394 -2.53823 1.63128
C 2.28597 -0.42794 -0.54330
C 2.41379 0.93055 -0.89414

C 3.61705 1.60129 -0.73010
C 4.74662 0.95278 -0.23630
C 4.62804 -0.39435 0.08589
C 3.42953 -1.08679 -0.05954
C 5.79871 -1.12712 0.67551
F 5.64782 -1.31393 2.01762
C 3.69667 3.04209 -1.14827
F 2.58377 3.73498 -0.80196
S 1.37318 -3.49002 0.36239
F 6.96701 -0.46684 0.51222
F 5.96206 -2.35855 0.14078
F 4.74720 3.68524 -0.58822
F 3.83055 3.18017 -2.49028
C -1.85691 -3.83245 1.97358
H -0.79630 -4.41127 -0.52642
H -2.09440 -3.38890 -3.09035
H -0.61262 -4.32458 -2.95099
H -2.58182 -5.75651 -3.60201
H -1.87146 -6.27234 -2.07995
H -4.37611 -4.54103 -2.40135
H -4.33835 -6.21066 -1.85476
H -3.05179 -5.58057 0.15129
H -4.55127 -4.65757 0.06234
H -3.31547 -2.72373 -0.91100
H -0.90416 -1.76587 -1.78931
H -1.74802 -3.28627 2.90747
H -2.42309 -4.74613 2.13673
H -0.86922 -4.04070 1.56722
H -3.68975 -1.93983 2.50998
H -4.45891 -1.92994 0.91628
H -4.48153 -3.42098 1.91386
H -1.21438 2.39161 1.99762
H -2.05309 -2.07991 0.94703
H -1.92477 0.04223 -0.77547
H 0.00150 2.29254 -0.01357
H -0.58074 4.55725 0.32051
H -2.02200 6.48154 -0.24470
H -4.16239 6.11981 -1.45236
H -4.82286 3.81954 -2.11402
H -3.38196 1.90434 -1.54661
H 3.36596 -2.13092 0.20253
H 5.67926 1.47980 -0.10472
H 1.56448 1.45362 -1.31241
H 1.38288 -1.21102 2.23248
H 0.72650 -0.79102 3.81815
H 3.24834 -0.61000 3.76661
H 3.12649 0.61214 2.50088
H 2.49347 0.95339 4.12441
H -5.45704 1.68464 2.61854
H -5.30015 2.12008 0.90643
H -6.50339 3.93212 2.16914
H -5.10877 4.11174 3.24670
H -4.95853 4.51736 1.52395
H 0.03610 -0.12924 -0.81076

Entry 19

Free Energy = -2910.389841
Zero-point Energy = -2910.303656
Potential Energy = -2912.00660667
Single Point Energy = -2912.00281914
Nimag = 1 (-1288.4498 cm-1)

Charge = 0 Multiplicity = 1
C 1.32139 4.07045 -0.92141
C 0.15745 3.30384 -1.03840
C -1.00304 3.93184 -1.50012
C -1.00095 5.28610 -1.82214
C 0.16098 6.04369 -1.68489
C 1.32550 5.42844 -1.23315
C 0.21519 1.82001 -0.68300
C 0.05264 1.49034 0.83831
C 1.27541 1.91848 1.65666
O 2.40989 1.61414 1.01623
C 3.66893 2.00015 1.63985
C 4.77405 1.60386 0.68220
C -0.56264 0.90329 -1.61446
N -1.97091 0.92916 -1.63653
O -2.56609 0.43318 -2.61476
O -2.60589 1.30579 -0.62158
C -1.19138 1.99362 1.55418
O -1.31857 3.30973 1.46759
C -2.43326 3.92783 2.15435
C -2.24684 5.42538 2.04408
O -1.94394 1.27038 2.17620
O 1.22333 2.41280 2.75688
N -0.01282 -1.63050 -0.82362
C -1.02298 -2.39378 -0.38003
N -2.24527 -1.95900 -0.85567
C -3.52104 -2.59741 -0.59224
C -4.55582 -1.52689 -0.20938
C -5.91919 -2.14150 0.09763
C -6.40999 -2.95834 -1.10723
C -5.39555 -4.03185 -1.50829
C -4.02442 -3.41329 -1.79002
N -4.01551 -0.65981 0.92391
C -4.92050 0.48262 1.25075
C 1.34129 -1.80027 -0.53723
C 2.24018 -1.37003 -1.52440
C 3.61398 -1.44024 -1.32246
C 4.13795 -1.95752 -0.14224
C 3.24682 -2.38513 0.83783
C 1.86964 -2.29585 0.66586
C 3.76294 -2.90780 2.14904
F 5.09468 -3.14167 2.12892
C 4.51616 -0.98886 -2.43397
F 4.00353 0.07112 -3.10988
S -0.93694 -3.73763 0.66770
F 3.16101 -4.06259 2.51016
F 3.53840 -2.03233 3.16472
F 5.73910 -0.62240 -1.99550

F 4.70976 -1.96402 -3.36059
C -3.61768 -1.40630 2.15949
H -3.36297 -3.28118 0.24218
H -4.08085 -2.76138 -2.67039
H -3.28173 -4.18482 -2.00466
H -5.74874 -4.57586 -2.38814
H -5.30280 -4.76631 -0.69962
H -6.58173 -2.28212 -1.95294
H -7.37505 -3.41030 -0.86480
H -5.84554 -2.79771 0.97067
H -6.64886 -1.36414 0.33268
H -4.64692 -0.82129 -1.04058
H -2.21618 -1.41514 -1.71152
H -3.28943 -0.67402 2.89173
H -4.47584 -1.96205 2.53100
H -2.79680 -2.08140 1.92731
H -4.36212 1.16673 1.88424
H -5.19984 0.97936 0.32461
H -5.79891 0.10979 1.77193
H 0.01163 0.40347 0.93100
H -3.16392 -0.22620 0.53727
H -0.20842 0.92970 -2.64172
H 1.24476 1.51525 -0.88038
H 2.23700 3.59728 -0.59013
H 2.24130 5.99993 -1.13285
H 0.15987 7.09837 -1.93481
H -1.91276 5.75138 -2.17975
H -1.92501 3.37606 -1.59122
H 1.19976 -2.63205 1.44199
H 5.20429 -2.03518 0.00609
H 1.84519 -0.99544 -2.46046
H -2.43640 3.58381 3.19001
H -3.35573 3.59302 1.67395
H -3.06417 5.93701 2.55856
H -1.30412 5.72843 2.50363
H -2.23754 5.73897 0.99874
H 3.74746 1.48722 2.59183
H 3.64014 3.07604 1.82336
H 5.74269 1.86232 1.11735
H 4.76351 0.52773 0.48120
H 4.67750 2.13151 -0.26805
H -0.32961 -0.37401 -1.25495

Entry 20

Free Energy = -2910.376339
Zero-point Energy = -2910.284654
Potential Energy = -2910.99246407
Single Point Energy = -2911.98914973
Nimag = 1 (-778.8415 cm-1)

Charge = 0 Multiplicity = 1
C -2.01747 -2.18533 -1.68686
C -2.38763 -1.53606 -0.49907
C -2.48351 -2.29964 0.67246
C -2.21620 -3.67051 0.65314
C -1.84449 -4.30215 -0.53363
C -1.74384 -3.55259 -1.70725
C -2.66185 -0.03092 -0.54718
C -3.91180 0.39429 0.27806
C -4.36877 1.80841 -0.08801
O -5.38088 2.19139 0.71947
C -5.94195 3.49906 0.46243
C -7.07258 3.70938 1.45182
C -1.43438 0.84049 -0.27141
N -1.03411 1.08030 1.05042
O -1.38405 0.33726 1.98779
O -0.19985 2.02028 1.26299
C -5.09450 -0.55898 0.08821
O -5.44645 -0.62338 -1.21404
C -6.52002 -1.53790 -1.53620
C -6.67303 -1.54527 -3.04529
O -5.64676 -1.17383 0.97102
O -3.91528 2.50416 -0.96970
N 1.00198 0.05899 -1.09334
C 1.63465 1.21175 -1.38870
N 2.83559 1.45564 -0.73617
C 3.57970 2.69402 -0.75830
C 3.42860 3.45393 0.58602
C 4.20138 4.77838 0.58296
C 5.69245 4.51617 0.30752
C 5.88820 3.75578 -1.01101
C 5.07647 2.45308 -1.03341
N 1.96048 3.62103 0.98206
C 1.79051 3.77166 2.46465
C 1.64747 -1.02159 -0.47059
C 1.17067 -1.57433 0.73310
C 1.79747 -2.69133 1.28693
C 2.90902 -3.27545 0.67880
C 3.38651 -2.72743 -0.51165
C 2.76297 -1.62221 -1.08760
C 4.62155 -3.30023 -1.15375
F 4.61791 -3.14365 -2.49519
C 1.32817 -3.23257 2.61354
F 0.02279 -2.99337 2.83772
S 0.95248 2.35934 -2.44459
F 4.76302 -4.61786 -0.89660
F 5.74351 -2.68935 -0.69388
F 1.52219 -4.56813 2.70448
F 2.01511 -2.67052 3.64040
C 1.21437 4.70244 0.25414
H 3.15238 3.29118 -1.57038
H 5.47728 1.75697 -0.28057
H 5.16597 1.95304 -2.00329
H 6.95060 3.53571 -1.16625
H 5.57502 4.39409 -1.84891
H 6.12000 3.93562 1.13734
H 6.22870 5.47154 0.28559
H 3.80461 5.43602 -0.20029
H 4.08280 5.30276 1.53898
H 3.83552 2.80907 1.37528

H 3.19559 0.70862 -0.15324
H 0.16023 4.57546 0.50031
H 1.57729 5.67660 0.58419
H 1.34032 4.55464 -0.81891
H 0.72435 3.74253 2.68283
H 2.27528 2.93025 2.96125
H 2.23735 4.71364 2.78610
H -3.69089 0.38131 1.34722
H 1.45080 2.74301 0.74654
H -1.40850 1.77488 -0.82506
H -2.90093 0.20438 -1.58875
H -1.93891 -1.60776 -2.60520
H -1.45692 -4.03147 -2.64014
H -1.63593 -5.36894 -0.54487
H -2.29205 -4.24116 1.57448
H -2.75960 -1.82476 1.60641
H 3.11701 -1.23089 -2.03545
H 3.38219 -4.14736 1.11380
H 0.31032 -1.14297 1.23320
H -7.43080 -1.20134 -1.02962
H -6.26557 -2.52616 -1.14173
H -7.48176 -2.22590 -3.33348
H -6.91275 -0.54520 -3.42075
H -5.74962 -1.88216 -3.52675
H -6.28821 3.53632 -0.57548
H -5.15146 4.24864 0.57377
H -7.52947 4.69224 1.29162
H -7.84556 2.94427 1.32894
H -6.70458 3.66230 2.48165
H -0.23086 0.29221 -0.78367

Entry 21

Free Energy = -2910.366717
Zero-point Energy = -2910.275973
Potential Energy = -2911.98319026
Single Point Energy = -2911.98385721
Nimag = 1 (-1266.3295 cm-1)

Charge = 0 Multiplicity = 1
C 0.39764 3.47734 0.92238
C 0.79773 2.19356 0.53244
C 0.61816 1.14780 1.44115
C 0.02877 1.37382 2.68009
C -0.37740 2.65581 3.04992
C -0.18124 3.71224 2.16807
C 1.32943 2.02955 -0.89003
C 2.87190 1.83566 -1.00033
C 3.56318 2.94153 -0.20177
O 3.30730 4.14023 -0.73816
C 3.86136 5.29741 -0.05189
C 3.55607 6.51233 -0.89882
C 0.45447 1.11460 -1.78150
N 1.03779 0.24231 -2.74037
O 2.01629 -0.47125 -2.40385
O 0.47636 0.08773 -3.83062
C 3.48743 0.51073 -0.58190
O 4.58468 0.27936 -1.30649
C 5.29095 -0.95589 -1.04100
C 6.43805 -1.04676 -2.02234
O 3.12691 -0.20748 0.32524
O 4.23613 2.76562 0.78517
N -1.11997 -0.76677 -0.67342
C -0.70215 -1.84743 -0.01916
N 0.62667 -2.16104 -0.27150
C 1.27114 -3.47064 -0.13329
C 1.50267 -3.82902 1.34516
C 2.26482 -5.13585 1.52438
C 1.50407 -6.26392 0.81215
C 1.31392 -5.94107 -0.67265
C 0.56601 -4.61898 -0.86601
N 2.15035 -2.61413 2.02387
C 1.43080 -2.24962 3.28153
C -2.41377 -0.25995 -0.48048
C -2.58186 1.00063 0.09584
C -3.85996 1.53933 0.23584
C -4.98341 0.83020 -0.16904
C -4.80570 -0.41961 -0.76657
C -3.53865 -0.95897 -0.93679
C -6.03131 -1.15430 -1.22640
F -5.77266 -2.40426 -1.65665
C -4.03985 2.87989 0.88670
F -2.90345 3.60668 0.90800
S -1.62737 -2.73108 1.12102
F -6.65220 -0.50634 -2.24891
F -6.95867 -1.25801 -0.23839
F -4.97540 3.63318 0.25494
F -4.45168 2.76641 2.17827
C 3.62311 -2.69730 2.24129
H 2.25411 -3.32416 -0.59641
H -0.45450 -4.69876 -0.48559
H 0.49982 -4.36158 -1.92587
H 0.77028 -6.74869 -1.16938
H 2.29760 -5.88252 -1.15610
H 0.52658 -6.40170 1.28678
H 2.05292 -7.20100 0.93403
H 3.27107 -5.06664 1.09960
H 2.37400 -5.36694 2.58775
H 0.52522 -3.91529 1.81501
H 1.05755 -1.60627 -1.00670
H 3.96719 -1.72069 2.57184
H 3.83398 -3.45152 2.99562
H 4.11137 -2.94757 1.30400
H 1.83956 -1.31607 3.66357
H 0.37568 -2.13843 3.03946
H 1.56950 -3.04871 4.00857
H 3.14345 1.98656 -2.04650
H 1.99979 -1.83844 1.35738
H -0.31152 1.69247 -2.29126
H 1.19430 3.01766 -1.33198
H 0.51611 4.30233 0.22834

H -0.49717 4.71351 2.43566
H -0.85010 2.82418 4.01074
H -0.13638 0.54109 3.35210
H 0.92872 0.15613 1.16893
H -3.40494 -1.91912 -1.41196
H -5.97349 1.25252 -0.05508
H -1.72075 1.55135 0.44499
H 4.58442 -1.77955 -1.16484
H 5.63599 -0.94058 -0.00502
H 6.99398 -1.97191 -1.85051
H 6.06899 -1.05115 -3.04955
H 7.12357 -0.20592 -1.89921
H 4.93241 5.13910 0.08049
H 3.39869 5.35661 0.93531
H 3.94997 7.40611 -0.40899
H 4.01792 6.42821 -1.88466
H 2.47895 6.63811 -1.02744
H -0.26385 0.18066 -1.14698

Entry 22

Free Energy = -2910.367546
Zero-point Energy = -2910.275994
Potential Energy = -2910.98522959
Single Point Energy = -2911.98247305
Nimag = 1 (-847.0641 cm-1)

Charge = 0 Multiplicity = 1
C -0.93835 -2.68982 -0.03068
C 0.31250 -2.55288 -0.64189
C 0.70735 -3.51374 -1.58378
C -0.13137 -4.57696 -1.91093
C -1.38393 -4.69682 -1.30315
C -1.78673 -3.74908 -0.36316
C 1.23639 -1.40251 -0.24551
C 2.41850 -2.02589 0.59358
C 3.68273 -1.17451 0.65780
O 4.67668 -1.75071 -0.03362
C 5.94706 -1.05154 -0.06778
C 6.91442 -1.90861 -0.86053
C 1.78360 -0.52144 -1.38816
N 1.14333 -0.56327 -2.65627
O -0.11343 -0.60684 -2.69683
O 1.82977 -0.42734 -3.68140
C 1.94487 -2.28010 2.02685
O 2.30881 -3.50198 2.44569
C 1.89802 -3.86524 3.78958
C 2.36242 -5.28725 4.03663
O 1.33389 -1.47916 2.70262
O 3.80900 -0.11635 1.25150
N -1.20104 1.21490 -0.75369
C -0.36473 2.28709 -0.50767
N 0.92572 1.99973 -0.74442
C 1.94235 3.03144 -0.84931
C 3.04798 2.85639 0.21626
C 4.27568 3.75312 -0.01963
C 4.85381 3.55218 -1.42741
C 3.78138 3.85541 -2.47791
C 2.56090 2.95368 -2.27234
N 2.57607 3.08171 1.68105
C 2.04142 4.45610 1.98133
C -2.54470 0.97719 -0.43497
C -3.18170 -0.05105 -1.15650
C -4.49209 -0.41431 -0.86089
C -5.20948 0.23700 0.14391
C -4.57519 1.25181 0.85709
C -3.25720 1.62257 0.58751
C -5.34037 2.00322 1.91424
F -6.31296 1.24204 2.46831
C -5.12772 -1.57282 -1.58051
F -6.45538 -1.38566 -1.75858
S -0.94476 3.81045 0.03996
F -5.94547 3.10396 1.41192
F -4.53799 2.42271 2.91925
F -4.58109 -1.79016 -2.79266
F -4.99615 -2.72830 -0.87549
C 1.63571 2.03899 2.24455
H 1.47451 4.01565 -0.72920
H 2.83520 1.91461 -2.49263
H 1.76263 3.20944 -2.97671
H 4.18218 3.71047 -3.48778
H 3.49028 4.91324 -2.40356
H 5.20600 2.51723 -1.54242
H 5.72848 4.20095 -1.55295
H 4.00515 4.81143 0.08030
H 5.04070 3.54070 0.74234
H 3.37073 1.81295 0.23158
H 1.37340 0.82028 -1.03773
H 1.62481 2.17540 3.32891
H 0.64270 2.21536 1.83918
H 2.00972 1.04783 1.99867
H 1.88062 4.52157 3.05937
H 2.76219 5.21109 1.67149
H 1.09081 4.56985 1.45071
H 2.70655 -2.97796 0.14846
H 3.44546 2.97499 2.21168
H 2.84949 -0.62189 -1.57955
H 0.68026 -0.76846 0.45347
H -1.25949 -1.95202 0.70039
H -2.76898 -3.81556 0.09467
H -2.04414 -5.51799 -1.56885
H 0.18740 -5.30593 -2.65144
H 1.66896 -3.41669 -2.08359
H -2.78843 2.40955 1.15930
H -6.23181 -0.04335 0.36621
H -2.64080 -0.56694 -1.94274
H 0.81058 -3.76631 3.85670
H 2.34282 -3.15426 4.49324
H 2.06907 -5.60188 5.04398
H 1.91125 -5.97553 3.31531
H 3.45133 -5.36494 3.95490

H 6.28139 -0.88835 0.96146
H 5.79181 -0.07183 -0.53166
H 7.88940 -1.41227 -0.91317
H 7.04973 -2.88552 -0.38628
H 6.55116 -2.06560 -1.88065
H -0.80302 0.51009 -1.38559

Entry 23

Free Energy = -2910.378231
Zero-point Energy = -2910.288655
Potential Energy = -2910.99619861
Single Point Energy = -2911.99005071
Nimag = 1 (-387.2775 cm-1)

Charge = 0 Multiplicity = 1
C -3.02061 0.51710 1.07832
C -3.40200 -0.71392 0.52710
C -4.64938 -0.82395 -0.10365
C -5.47799 0.29107 -0.21708
C -5.08972 1.52783 0.30315
C -3.85982 1.62506 0.95173
N -2.60165 -1.85151 0.68963
C -1.49662 -2.02679 0.07075
S -0.85999 -1.03075 -1.30359
C -6.77918 0.17184 -0.96286
C -3.40318 2.93218 1.54199
N -0.68375 -3.07853 0.50937
C 0.02464 -3.99099 -0.38472
C 1.38263 -4.38149 0.24177
C 2.13293 -5.43354 -0.58783
C 1.26532 -6.68298 -0.80777
C -0.05407 -6.30976 -1.49399
C -0.81203 -5.25619 -0.67735
N 2.22470 -3.14057 0.51646
C 2.92644 -2.56765 -0.67949
C 3.19885 -3.33713 1.63734
O -0.08523 0.15550 2.49475
N 0.74781 0.14505 1.55684
O 1.65048 -0.77902 1.50844
C 0.69075 1.03663 0.53069
C 1.84541 1.16668 -0.43729
C 1.45454 2.12089 -1.56500
C 1.06739 3.44230 -1.29641
C 0.71130 4.30763 -2.33030
C 0.73898 3.86709 -3.65526
C 1.12710 2.55733 -3.93592
C 1.48342 1.69332 -2.89836
C 3.23937 1.62217 0.15079
C 4.31838 1.39008 -0.90315
O 4.36698 0.43330 -1.64977
C 3.68856 0.90348 1.42716
O 4.48424 -0.01784 1.46947
H 0.20278 -3.45235 -1.32015
H -1.12243 -5.69873 0.28153
H -1.73085 -4.94735 -1.18800
H -0.68139 -7.19865 -1.62772
H 0.15514 -5.91971 -2.50005
H 1.05783 -7.16702 0.15717
H 1.82474 -7.40890 -1.40865
H 2.39093 -5.01663 -1.56857
H 3.07465 -5.70648 -0.09660
H 1.17966 -4.79440 1.23794
H -0.25497 0.01608 -0.44226
H -1.15215 -3.55172 1.28026
H 3.40503 -1.63773 -0.37675
H 3.68074 -3.27080 -1.03369
H 2.19261 -2.36123 -1.45887
H 3.71530 -2.39052 1.80233
H 2.64428 -3.61613 2.53461
H 3.91020 -4.12093 1.36995
H 3.19395 2.68797 0.38669
H 1.58897 -2.36766 0.85815
H 0.03111 1.87177 0.72976
H 2.03438 0.18804 -0.88369
H 1.79623 0.67778 -3.12400
H 1.15245 2.20351 -4.96333
H 0.45865 4.54018 -4.46112
H 0.40784 5.32541 -2.09977
H 1.03587 3.79878 -0.26950
H -4.95978 -1.78340 -0.50242
H -5.73776 2.39051 0.21499
H -2.07816 0.58980 1.61552
F -7.69535 1.06680 -0.52937
F -7.32491 -1.05966 -0.83337
F -6.62114 0.38780 -2.29074
F -3.24981 2.85312 2.88202
F -2.20027 3.31291 1.03875
F -4.26906 3.94011 1.29606
C 6.33321 2.23822 -1.81818
C 7.23816 3.44078 -1.63024
H 5.92819 2.18007 -2.83335
H 6.84862 1.29549 -1.60927
H 8.08882 3.37590 -2.31748
H 6.69943 4.37132 -1.83522
H 7.62410 3.48345 -0.60677
C 3.33412 0.83300 3.77671
C 2.39741 1.49756 4.76733
H 4.38808 0.93032 4.05872
H 3.09911 -0.22601 3.64857
H 2.52169 1.04152 5.75608
H 2.60818 2.56863 4.85399
H 1.36002 1.36200 4.44789
O 5.23050 2.37623 -0.88934
O 3.13892 1.48829 2.49824

Below are the coordinates for all transition states appearing in Table S6

Entry 1

Free Energy = -2396.373518
Zero-point Energy = -2396.295042
Potential Energy = -2396.86330935
Nimag = 1 (-798.8826 cm-1)

Charge = 0 Multiplicity = 1
C 3.00426 -1.52270 -0.39419
C 2.14399 -0.41577 -0.37362
C 2.68599 0.87625 -0.37500
C 4.06927 1.05576 -0.38176
C 4.93112 -0.03854 -0.38229
C 4.38356 -1.32288 -0.39024
N 0.74157 -0.52933 -0.43659
C -0.07569 -1.41813 0.21465
S 0.44447 -2.60652 1.29980
C 4.61810 2.45591 -0.32530
C 5.30241 -2.51586 -0.35368
N -1.39396 -1.19574 -0.07637
C -2.46535 -2.05806 0.39397
C -3.76552 -1.28128 0.71000
C -4.79854 -2.24737 1.31876
C -5.10488 -3.40565 0.35224
C -3.83277 -4.15651 -0.05701
C -2.77473 -3.19239 -0.60665
N -3.52433 -0.03740 1.54558
C -2.61874 -0.19650 2.71384
C -4.78357 0.63866 1.95409
C -2.77019 1.99513 -0.16345
C -2.99679 1.42508 -1.48185
O -2.27073 0.63781 -2.09395
C -1.42451 2.39882 0.21482
O -0.35582 2.06486 -0.29298
H -2.09809 -2.52476 1.31301
H -3.11033 -2.75289 -1.55691
H -1.83702 -3.72042 -0.80652
H -4.06857 -4.92481 -0.80276
H -3.42123 -4.68253 0.81562
H -5.59692 -3.00058 -0.54385
H -5.82473 -4.08663 0.82146
H -4.41196 -2.65100 2.26481
H -5.73064 -1.72177 1.54906
H -4.17747 -0.87941 -0.22608
H 0.27326 0.33209 -0.73578
H -1.60410 -0.57898 -0.87243
H -2.42363 0.80026 3.11741
H -3.08841 -0.81614 3.48431
H -1.67581 -0.64470 2.40447
H -4.52623 1.63655 2.31629
H -5.43537 0.73831 1.08322
H -5.29391 0.08527 2.74499
H -3.52886 2.71338 0.13991
H -3.06519 0.78849 0.79744
H 2.01825 1.73170 -0.37025
H 6.00443 0.10422 -0.39406
H 2.59982 -2.52447 -0.41999
F 3.92311 3.30031 -1.12024
F 5.91282 2.51207 -0.70646
F 4.55300 2.96612 0.92887
F 5.59812 -2.87965 0.91530
F 4.75697 -3.59517 -0.95563
F 6.47953 -2.25989 -0.97008
C -4.57067 1.21672 -3.25926
C -5.93783 1.76119 -3.63187
H -4.57350 0.12312 -3.18368
H -3.80862 1.48830 -3.99634
H -6.24924 1.35834 -4.60186
H -6.68952 1.48167 -2.88591
H -5.91586 2.85326 -3.70316
C -0.18232 3.69485 1.78654
C -0.44870 4.55801 3.00651
H 0.31271 4.26142 0.99096
H 0.45586 2.83779 2.02594
H 0.49645 4.94596 3.40139
H -1.09123 5.40735 2.75265
H -0.93884 3.98040 3.79771
O -4.21462 1.78370 -1.98198
O -1.45752 3.22117 1.30548

Entry 2

Free Energy = -2396.376530
Zero-point Energy = -2396.300663
Potential Energy = -2396.86858633
Nimag = 1 (-348.9463 cm-1)

Charge = 0 Multiplicity = 1
N 0.37157 -0.56432 -0.39737
C -0.51986 -1.50392 0.09346
S -0.06927 -2.88196 0.95649
N -1.80504 -1.17708 -0.17617
C -2.97250 -1.93967 0.24621
C -3.35115 -2.99836 -0.81247
C -4.60162 -3.79058 -0.41472
C -5.77895 -2.84959 -0.13504
C -5.40473 -1.80068 0.92470
C -4.16237 -0.98765 0.50518
N -3.81054 0.12072 1.45648
C -3.58488 -0.32795 2.84821
C -4.80779 1.21037 1.42089
O -1.69074 1.45805 1.51257
C -0.99710 2.29017 0.80000
C -1.11738 2.66099 -0.53148
C -2.13108 2.19987 -1.42754
O -2.92000 1.25548 -1.24647
H -2.69712 -2.46675 1.16520
H -3.52158 -2.49023 -1.77249
H -2.49137 -3.66269 -0.94522
H -4.86008 -4.50460 -1.20600

H -4.38721 -4.38529 0.48474
H -6.07134 -2.34053 -1.06491
H -6.65651 -3.41517 0.20127
H -5.20949 -2.31503 1.87497
H -6.25367 -1.12874 1.09608
H -4.38442 -0.47561 -0.43679
H -0.02668 0.34174 -0.63603
H -2.01688 -0.33662 -0.71898
H -3.20554 0.51940 3.42432
H -4.50499 -0.69177 3.32197
H -2.82944 -1.11599 2.86831
H -4.43328 2.04293 2.02413
H -4.91952 1.55035 0.38954
H -5.78259 0.90360 1.82096
H -2.58004 0.87142 1.18943
H -0.45198 3.44118 -0.87644
C 0.24153 2.55957 2.84725
H 0.39649 1.48090 2.94467
H -0.65317 2.82645 3.41925
C -3.09134 2.48984 -3.58647
H -4.10468 2.55522 -3.17585
H -2.90648 1.44012 -3.83950
O 0.02123 2.88313 1.45336
O -2.14592 2.90909 -2.58296
C 1.45499 3.34958 3.30079
H 1.64535 3.14867 4.36080
H 2.34605 3.06796 2.73298
H 1.28864 4.42450 3.17791
C -2.90968 3.40125 -4.78650
H -3.61247 3.12001 -5.57844
H -3.09497 4.44536 -4.51482
H -1.89270 3.32515 -5.18418
C 1.77874 -0.56154 -0.33164
C 2.41901 0.66182 -0.10190
C 2.55256 -1.70736 -0.56738
C 3.81292 0.73614 -0.09584
H 1.83032 1.55606 0.07934
C 3.94250 -1.61687 -0.54513
H 2.07017 -2.65279 -0.77032
C 4.58782 -0.40070 -0.30960
H 5.66910 -0.34000 -0.30953
C 4.76669 -2.86267 -0.74552
C 4.46495 2.05662 0.21211
F 4.12852 -3.77319 -1.51132
F 5.05345 -3.46436 0.43061
F 5.94903 -2.58700 -1.34273
F 4.44878 2.31846 1.54646
F 5.75564 2.09403 -0.17666
F 3.82615 3.08528 -0.38728

Entry 3

Free Energy = -2910.589473
Zero-point Energy = -2910.496294
Potential Energy = -2911.19953704
Nimag = 1 (-1319.1972 cm-1)

Charge = 0 Multiplicity = 1
C 4.78349 0.65666 0.30184
C 3.58505 -0.03051 0.06532
C 3.62244 -1.40521 -0.20930
C 4.84462 -2.07832 -0.24820
C 6.04487 -1.40155 -0.02731
C 5.99597 -0.03222 0.24338
N 2.32037 0.57823 0.16498
C 1.91927 1.80423 -0.30502
S 2.90060 2.85706 -1.19172
C 4.85296 -3.56366 -0.49634
C 7.26702 0.71952 0.54334
N 0.60959 2.06975 -0.01907
C -0.05378 3.33125 -0.33799
C -1.55889 3.16980 -0.66460
C -2.10963 4.55130 -1.08331
C -1.91512 5.60091 0.02389
C -0.44558 5.72617 0.43639
C 0.13090 4.35459 0.80412
N -1.85608 2.07293 -1.67217
C -0.91140 1.98962 -2.81905
C -3.24810 2.13503 -2.19554
O -0.05784 -1.13543 -1.47712
N -0.71389 -0.83956 -0.46023
O -0.14684 -0.77252 0.67731
C -2.06798 -0.44633 -0.58331
C -2.90827 -0.70121 0.68673
C -3.38799 0.53721 1.45054
C -4.52773 1.28265 1.10787
C -4.92040 2.38860 1.86883
C -4.17874 2.77871 2.98703
C -3.04259 2.04685 3.34172
C -2.65839 0.93728 2.58346
C -4.03797 -1.75998 0.46824
C -3.43330 -3.12179 0.09896
O -3.54888 -3.65817 -0.98601
C -5.10286 -1.43433 -0.57661
O -4.96545 -0.67855 -1.52055
H 0.46097 3.72283 -1.21972
H -0.35604 3.97059 1.71137
H 1.20202 4.42896 1.01482
H -0.34108 6.41616 1.28144
H 0.13603 6.15268 -0.39221
H -2.51754 5.31388 0.89672
H -2.30429 6.56508 -0.32266
H -1.60440 4.88520 -1.99941
H -3.17537 4.48036 -1.31190
H -2.08879 2.84912 0.24146
H 1.55698 -0.06965 0.39186
H 0.14584 1.44617 0.63550
H -1.21348 1.14823 -3.44507
H -0.94658 2.90735 -3.41518
H 0.10297 1.81538 -2.46959
H -3.48563 1.17493 -2.65522

H -3.94267 2.30218 -1.37339
H -3.35350 2.92958 -2.93822
H -4.54829 -1.89347 1.42769
H -1.88663 0.92349 -1.05629
H -2.46258 -0.87977 -1.49920
H -2.22754 -1.19709 1.38149
H -1.78151 0.36673 2.87756
H -2.46070 2.32982 4.21438
H -4.48743 3.63565 3.57852
H -5.81130 2.94286 1.58625
H -5.11870 1.00673 0.24223
H 2.69600 -1.93340 -0.40918
H 6.99193 -1.92368 -0.07172
H 4.76518 1.71482 0.52326
F 3.92086 -3.94057 -1.40624
F 4.58183 -4.26741 0.64071
F 6.05162 -4.00835 -0.94579
F 7.28488 1.95006 -0.02501
F 7.43332 0.91631 1.88321
F 8.37227 0.06496 0.11137
C -2.06597 -4.90549 0.90124
C -1.32606 -5.25963 2.17516
H -1.39069 -4.78200 0.05065
H -2.82011 -5.65216 0.63771
H -0.80265 -6.21087 2.03570
H -0.58538 -4.49448 2.42482
H -2.01742 -5.36797 3.01629
C -7.31215 -1.99212 -1.28576
C -8.45323 -2.86586 -0.80490
H -6.93033 -2.30896 -2.26002
H -7.59887 -0.93884 -1.35356
H -9.28390 -2.79956 -1.51483
H -8.14372 -3.91269 -0.73537
H -8.81325 -2.54099 0.17594
O -2.74743 -3.63473 1.12854
O -6.23016 -2.10982 -0.31703

Entry 4

Free Energy = -2910.620532
Zero-point Energy = -2910.528102
Potential Energy = -2911.23093780
Nimag = 1 (-623.4194 cm-1)

Charge = 0 Multiplicity = 1
C 2.74602 -2.25130 0.40637
C 2.13008 -1.33353 -0.46106
C 2.91697 -0.39142 -1.13253
C 4.30292 -0.37168 -0.94620
C 4.92570 -1.28972 -0.10477
C 4.12918 -2.22423 0.56733
N 0.73271 -1.26486 -0.62951
C -0.17081 -2.29742 -0.71228
S 0.28622 -3.92821 -0.83262
C 5.10942 0.68823 -1.64651
C 4.80611 -3.21948 1.47365
N -1.46018 -1.87945 -0.71445
C -2.62141 -2.73470 -0.95103
C -3.73511 -2.51778 0.10519
C -4.93590 -3.43124 -0.22178
C -5.47477 -3.19132 -1.64101
C -4.37596 -3.38221 -2.69132
C -3.16698 -2.49474 -2.37580
N -3.24207 -2.66376 1.52417
C -2.57382 -3.95238 1.82991
C -4.32005 -2.40704 2.51313
O -1.58495 -0.93038 2.28475
N -1.94540 0.31611 1.89348
O -3.19149 0.55434 1.74873
C -0.98667 1.18613 1.69639
C -1.32516 2.60399 1.35146
C -0.32598 3.60541 1.92341
C 1.06283 3.43195 1.81460
C 1.94349 4.38091 2.34126
C 1.45165 5.52007 2.98405
C 0.07106 5.70350 3.09776
C -0.80728 4.75282 2.57143
C -1.55171 2.87376 -0.19630
C -2.69865 2.02356 -0.74083
O -2.57331 0.93414 -1.27618
C -0.30582 2.66065 -1.04002
O 0.38974 1.65749 -1.03140
H -2.25833 -3.76323 -0.89425
H -3.44140 -1.43660 -2.47761
H -2.35190 -2.68475 -3.08245
H -4.75589 -3.15206 -3.69352
H -4.06383 -4.43563 -2.70729
H -5.87397 -2.16942 -1.71028
H -6.31490 -3.86936 -1.83075
H -4.63577 -4.48313 -0.12637
H -5.73956 -3.26271 0.50061
H -4.06162 -1.47181 0.04569
H 0.37896 -0.31621 -0.75729
H -1.64187 -0.87705 -0.75991
H -2.22499 -3.91513 2.86483
H -3.26048 -4.79996 1.72466
H -1.71006 -4.09866 1.18098
H -3.85931 -2.29129 3.49676
H -4.82293 -1.47281 2.26089
H -5.04046 -3.22985 2.55525
H -1.84933 3.91949 -0.28918
H -2.36638 -1.69583 1.84187
H 0.01740 0.82216 1.84697
H -2.30418 2.81044 1.79596
H -1.87985 4.90046 2.67083
H -0.32389 6.58167 3.60038
H 2.13746 6.25453 3.39595
H 3.01468 4.22523 2.25101
H 1.46841 2.55455 1.32070
H 2.44090 0.32525 -1.79166
H 6.00031 -1.27710 0.03090

H 2.14582 -2.96819 0.94699
F 4.95499 1.91164 -1.06065
F 4.73665 0.84606 -2.94410
F 6.43668 0.42486 -1.64387
F 3.93408 -3.91431 2.23840
F 5.52997 -4.13404 0.77084
F 5.68389 -2.61592 2.32096
C -5.07141 1.90523 -0.89834
C -6.25731 2.79384 -0.58106
H -5.06553 0.99106 -0.29946
H -5.02908 1.63583 -1.95741
H -7.18320 2.26133 -0.82139
H -6.27778 3.05640 0.48055
H -6.22948 3.71522 -1.17051
C 1.10365 3.65490 -2.69338
C 1.15188 4.94691 -3.48322
H 0.99302 2.77890 -3.33816
H 1.99131 3.51812 -2.07024
H 2.01786 4.92760 -4.15234
H 0.25078 5.07116 -4.09098
H 1.24972 5.81068 -2.81930
O -3.86416 2.64985 -0.56756
O -0.06068 3.72096 -1.81465

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