Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Aromaticity-Promoted CS_2 Activation by Heterocycle-Bridged P/N-FLPs: A Comparative DFT Study with CO_2 Capture

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Table S1. Activation barriers and reaction energies (kcal mol^{-1}) of **4**, **10** and **16** capture CS_2 and CO_2 in the gas phase and THF solvent, respectively.

Entry	gas phase	THF solvent
4.closed	-1.6	0.8
4	0.0	0.0
TS4	14.8	13.7
4p	-29.1	-31.5
TS4-CO_2	6.3	6.9
4-CO_2p	-38.1	-37.5
10.closed	6.4	8.9
10	0.0	0.0
TS10	14.6	15.7
10p	-16.3	-19.4
TS10-CO_2	5.4	8.3
10-CO_2p	-24.8	-25.1
16	0.0	0.0
16.open	12.4	7.4
TS16	22.1	18.2
16p	-24.9	-31.2
TS16-CO_2	17.3	15.2
16-CO_2p	-33.2	-36.0

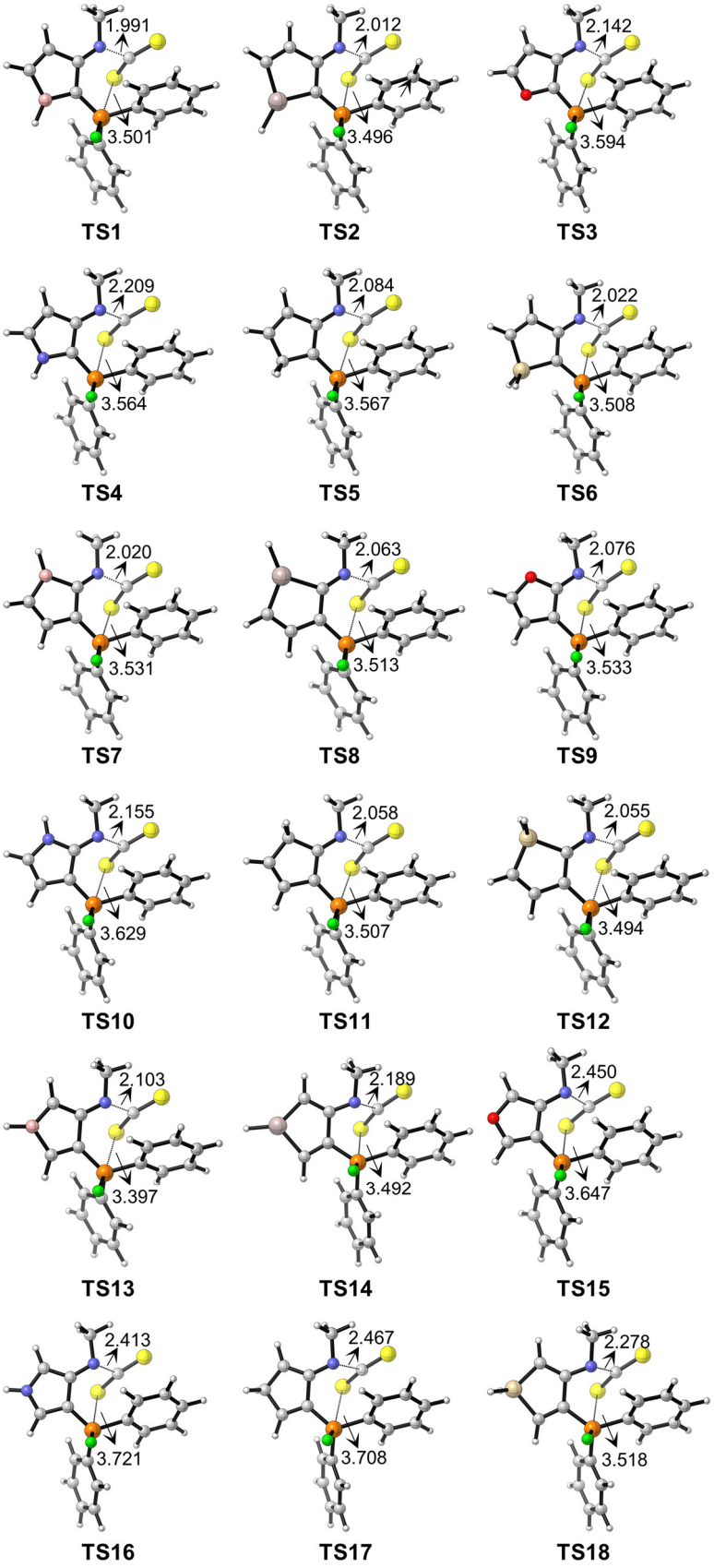

Figure S1. Selected bond distances (Å) in the transition states of FLPs activate CS_2.

Table S2. The NICS(1)$_{zz}$ values (ppm) of bridged ring in the process of reactions.

Entry	NICS(1)$_{zz}$	Entry	NICS(1)$_{zz}$
1	0.8	**10**	-9.3
TS1	9.2	**TS10**	-17.0
1p	24.7	**10p**	-25.5
2	0.8	**11**	-2.5
TS2	4.5	**TS11**	-4.9
2p	9.4	**11p**	-7.3
3	-9.1	**12**	1.8
TS3	-15.7	**TS12**	2.4
3p	-23.6	**12p**	3.3
4	-9.4	**13**	13.5
TS4	-17.1	**TS13**	19.5
4p	-27.3	**13p**	26.2
5	-5.1	**14**	5.7
TS5	-7.0	**TS14**	8.7
5p	-9.9	**14p**	11.2
6	-1.4	**15**	-20.0
TS6	-0.3	**TS15**	-17.1
6p	0.6	**15p**	-22.9
7	2.8	**16**	-24.2
TS7	13.7	**TS16**	-18.0
7p	36.5	**16p**	-26.7
8	3.4	**17**	-8.0
TS8	8.2	**TS17**	-8.9
8p	15.0	**17p**	-10.0
9	-7.1	**18**	0.5
TS9	-13.8	**TS18**	0.2
9p	-20.9	**18p**	0.7

Table S3. Energy decomposition analysis of FLPs capture CS_2 and CO_2 (in parentheses). The energies are given in kcal mol^{-1}.

Entry		$\Delta E^{\neq}$	$\Delta E^{\neq}_{int}$	$\Delta E^{\neq}_{deform}$ (FLP)	$\Delta E^{\neq}_{deform}$ (CE_2)
I	**TS1**	12.3 (1.1)	-13.4 (-21.4)	8.1 (7.7)	17.6 (14.8)
	TS2	11.6 (0.1)	-15.1 (-20.4)	8.7 (7.7)	18.0 (12.8)
	TS3	4.1 (-4.2)	-15.2 (-17.8)	5.8 (5.4)	13.6 (8.2)
	TS4	2.8 (-5.1)	-15.2 (-16.9)	6.2 (5.4)	11.9 (6.4)
	TS5	7.1 (-2.8)	-14.6 (-18.5)	6.7 (6.1)	15.1 (9.5)
	TS6	10.7 (-0.5)	-15.2 (-19.7)	8.3 (7.5)	17.6 (11.7)
II	**TS7**	12.5 (2.0)	-12.8 (-20.8)	9.1 (8.3)	16.2 (14.5)
	TS8	10.7 (0.6)	-13.1 (-18.9)	8.7 (7.7)	15.1 (11.8)
	TS9	5.3 (-4.0)	-15.6 (-18.8)	5.4 (5.3)	15.5 (9.5)
	TS10	2.0 (-5.8)	-15.8 (-17.3)	4.5 (4.6)	13.4 (6.9)
	TS11	8.4 (-1.4)	-14.7 (-19.0)	7.3 (6.9)	15.8 (10.6)
	TS12	10.2 (0.2)	-13.4 (-18.6)	8.3 (7.7)	15.3 (11.1)
III	**TS13**	18.6 (12.7)	-12.0 (-21.6)	15.9 (14.1)	14.8 (20.2)
	TS14	32.4 (17.4)	-15.4 (-11.7)	33.2 (16.1)	14.6 (13.0)
	TS15	14.3 (8.7)	-14.3 (-16.3)	22.5 (18.1)	6.1 (6.9)
	TS16	11.9 (7.6)	-14.8 (-16.2)	19.5 (17.2)	7.2 (6.5)
	TS17	22.8 (7.1)	-15.2 (-25.4)	31.5 (13.6)	6.6 (18.9)
	TS18	30.2 (13.2)	-15.6 (-31.2)	34.0 (19.1)	11.8 (25.3)

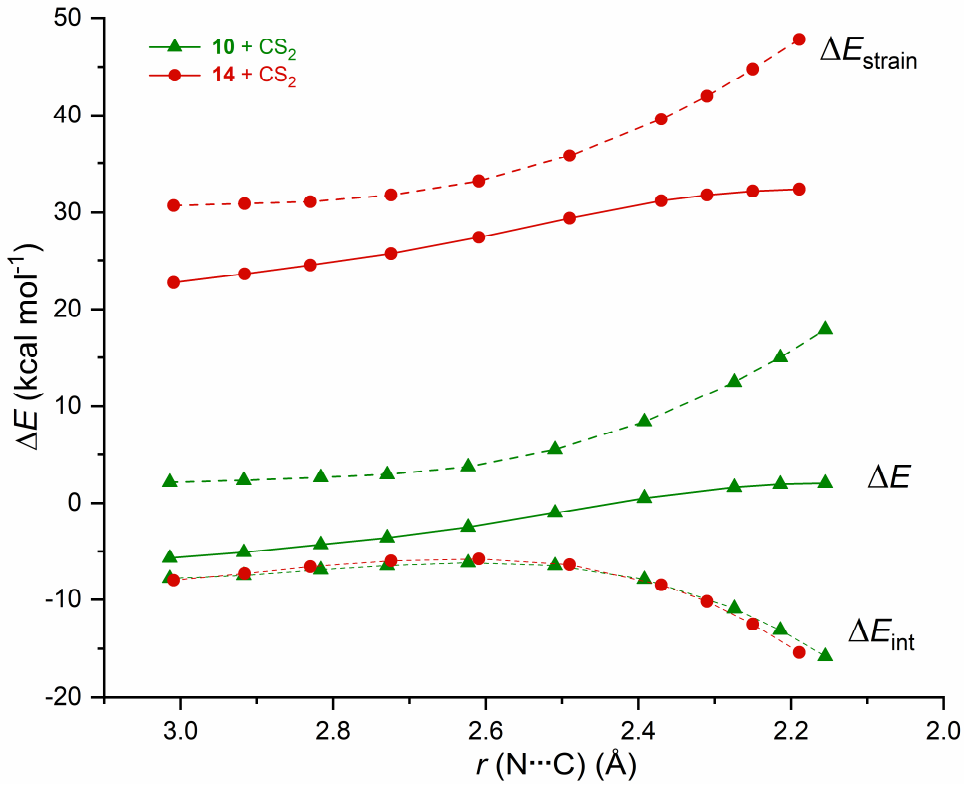

Figure S2. The distortion-interaction analysis (DIA) for CS_2 activation by FLPs **10** (green) and **14** (red) along the reaction coordinates projected onto the forming N…C bond distance.

Cartesian coordinates of all molecules and transition states:

CS_2

Sum of electronic and thermal Free Energies = -834.412313 a.u.

C	0.00000000	0.00000000	0.00000000
S	0.00000000	0.00000000	1.55446200
S	0.00000000	0.00000000	-1.55446200

1

Sum of electronic and thermal Free Energies = -1177.620328 a.u.

P	0.16105600	-0.20030400	0.56224900
C	-0.79811300	-1.46767900	0.03720300
C	-2.28010800	-1.43094100	0.08285400
C	-0.32288900	1.46071800	0.04912700
C	0.09920800	2.57857100	0.77397500
C	-1.05610700	1.62142000	-1.12895700
C	-0.21840200	3.85664000	0.32082900
H	0.66472800	2.45031100	1.69262200
C	-1.36867600	2.90119700	-1.57902100
H	-1.39448700	0.74420500	-1.67400800
C	-0.95039800	4.01748200	-0.85501900
H	0.10393100	4.72576500	0.88626500
H	-1.94526300	3.02707800	-2.49045900
H	-1.19777900	5.01498000	-1.20651400
C	1.90158800	-0.44004000	0.15084300
C	2.26213300	-0.68379800	-1.17911100
C	2.88719900	-0.34559100	1.13682300
C	3.60263400	-0.83810600	-1.51720900
H	1.49345500	-0.76198500	-1.94343300
C	4.22897500	-0.50278200	0.79186500
H	2.60807000	-0.16042200	2.16910100
C	4.58643000	-0.74839300	-0.53172400
H	3.87948800	-1.03245600	-2.54884200
H	4.99308900	-0.43620200	1.56039900
H	5.63226700	-0.87157000	-0.79740800
N	-2.94132400	-0.42953300	0.52262000
C	-4.38718900	-0.44210000	0.56185200
H	-4.75862200	0.42854800	0.01023000
H	-4.86151200	-1.34274000	0.15423500
H	-4.70910800	-0.31861800	1.60162600
F	0.26798800	0.02594900	2.15651400
C	-1.73877100	-3.57084600	-0.74687500
H	-1.90467800	-4.57383900	-1.13291400
B	-0.37221000	-2.82855100	-0.44831700
H	0.73213700	-3.25560700	-0.59386000

C	-2.76357900	-2.75248600	-0.43634900
H	-3.81674600	-2.99654200	-0.53279700

TS1

Sum of electronic and thermal Free Energies = -2011.992049 a.u.

P	0.78064900	0.24236200	-0.95579100
F	1.32309100	0.18754600	-2.47169300
C	-0.00043400	1.72426200	-0.73283700
C	-1.35888300	2.03066600	-0.30254600
C	-0.53289200	4.08281800	-1.13417600
H	-0.51675100	5.14201200	-1.37562100
C	-0.20088300	-1.26155600	-0.90984200
C	0.12089100	-2.33996800	-0.08191500
C	-1.28440900	-1.34211000	-1.79183800
C	-0.64103700	-3.50343900	-0.14608000
H	0.94278500	-2.26296400	0.62468300
C	-2.03572800	-2.51088100	-1.85531900
H	-1.53535500	-0.49364800	-2.42424100
C	-1.71135900	-3.59065400	-1.03504400
H	-0.40450400	-4.33735600	0.50721500
H	-2.87862900	-2.57497700	-2.53627200
H	-2.30446800	-4.49937900	-1.07838800
C	2.34350600	0.01727400	-0.09027100
C	3.21283400	-1.00555400	-0.49049200
C	2.69914700	0.87976800	0.94850700
C	4.43198900	-1.16822200	0.15937900
H	2.93853900	-1.66533000	-1.31011000
C	3.92422100	0.71527100	1.59146100
H	2.01400200	1.66908500	1.24558300
C	4.78550800	-0.30799800	1.20039800
H	5.10789300	-1.96001600	-0.14856900
H	4.20319400	1.38493800	2.39895600
H	5.73841400	-0.43582600	1.70567700
N	-2.19874400	1.26746400	0.31147600
C	-3.56128800	1.68937200	0.57995000
H	-3.63700200	2.10866200	1.59046900
H	-3.92489900	2.41427400	-0.15064400
H	-4.19936500	0.80313400	0.53708300
C	-1.74825600	-0.18096300	1.60109200
S	-2.91639600	-1.27283700	1.52830700
S	-0.39201400	0.27061400	2.34284500
C	-1.61710800	3.48412700	-0.61810500
H	-2.55674500	3.96469400	-0.36762300
B	0.61207100	2.99412400	-1.27615500

H	1.70582600	3.13877000	-1.72800900

1p

Sum of electronic and thermal Free Energies = -2012.012348 a.u.

P	-0.66523500	-0.17451000	-0.55584200
F	-1.22155500	-0.11390700	-2.14250800
C	0.35432300	-1.57327600	-0.89724300
C	1.65314100	-1.68400200	-0.45928300
C	1.52086300	-3.48824100	-1.96708400
H	1.79570600	-4.39552900	-2.49471700
C	0.07520100	1.48766400	-0.71758600
C	-0.15639900	2.51132000	0.20385200
C	0.90099000	1.71479400	-1.82238300
C	0.43032500	3.75979200	0.01309600
H	-0.78020200	2.33140900	1.07471000
C	1.51261500	2.95558200	-1.98983600
H	1.05896600	0.92432200	-2.55128700
C	1.27324300	3.97991500	-1.07575400
H	0.24098900	4.55545500	0.72701900
H	2.16642900	3.12354400	-2.84051600
H	1.74398200	4.94932800	-1.21042000
C	-2.37192700	-0.29413300	0.06571600
C	-3.28325100	0.68764800	-0.33386800
C	-2.78488600	-1.34556700	0.88631700
C	-4.60089300	0.62980200	0.11325100
H	-2.96436400	1.48837700	-0.99574500
C	-4.11150400	-1.41208400	1.30666100
H	-2.07500700	-2.10796600	1.19518600
C	-5.01643700	-0.42119400	0.92969700
H	-5.30477600	1.40054300	-0.18591200
H	-4.43431500	-2.23612800	1.93556300
H	-6.04665500	-0.46964300	1.26979900
N	2.34247000	-0.90930900	0.43604900
C	3.80617600	-0.83922900	0.30651200
H	4.29796200	-1.46862900	1.05272900
H	4.08306600	-1.13823900	-0.70269700
H	4.11471300	0.19273900	0.47051200
C	1.75378000	-0.28016100	1.55091700
S	2.70010800	0.37159000	2.74000400
S	0.02446000	-0.30169400	1.70664400
C	2.34264500	-2.86917000	-1.11203000
H	3.34371900	-3.17648100	-0.82598900
B	0.15189000	-2.66977800	-1.97095500
H	-0.80555300	-2.85133200	-2.64768800

2

Sum of electronic and thermal Free Energies = -1395.174053 a.u.

P	0.16194500	-0.00819000	0.60409600
C	-0.76017000	-1.28078100	0.05697800
C	-2.23169900	-1.23089100	0.14600000
C	-0.25762500	1.66888500	0.08063300
C	0.22627700	2.77349000	0.78732600
C	-1.00837800	1.85252100	-1.08277800
C	-0.04268500	4.06092000	0.32797300
H	0.80436600	2.62621800	1.69537800
C	-1.27538800	3.14118900	-1.53806300
H	-1.39095900	0.98413200	-1.61300900
C	-0.79158300	4.24397200	-0.83411200
H	0.32985600	4.91981600	0.87810800
H	-1.86570200	3.28513200	-2.43801800
H	-1.00166000	5.24846700	-1.19013300
C	1.90907900	-0.28239800	0.23634600
C	2.54341400	0.39819100	-0.80676500
C	2.61224300	-1.23967900	0.97632600
C	3.87196500	0.11253300	-1.11489800
H	2.00107100	1.14936100	-1.37602500
C	3.94031900	-1.52031700	0.66563400
H	2.12080900	-1.75843500	1.79553200
C	4.56875800	-0.84656500	-0.38111000
H	4.36262700	0.64016000	-1.92720200
H	4.48395000	-2.26391800	1.24046700
H	5.60430200	-1.06711800	-0.62309000
N	-2.83129200	-0.25016300	0.72208600
C	-4.28362600	-0.22174500	0.79226500
H	-4.58782300	0.70902400	1.27594100
H	-4.75690800	-0.25522700	-0.19855700
H	-4.68302700	-1.05320500	1.38854300
F	0.22837800	0.20746300	2.20469600
C	-2.18496500	-3.40674800	-1.03674700
H	-2.71544400	-4.25017400	-1.47482400
C	-2.91445000	-2.41652100	-0.48021400
H	-4.00381500	-2.43527200	-0.45282300
Al	-0.30406200	-2.90155600	-0.80734200
H	1.05672500	-3.58823100	-1.21192600

TS2

Sum of electronic and thermal Free Energies = -2229.546440 a.u.

P	0.75177100	0.14440200	-0.85481100

F	1.29179500	0.19756000	-2.38415400
C	0.10627200	1.64387400	-0.47091900
C	-1.25976900	1.97104400	-0.14319600
C	-0.64069000	4.33605600	-0.61654600
H	-0.90755300	5.38983200	-0.63887800
C	-0.29166000	-1.31821300	-0.95179400
C	-0.02470800	-2.46344400	-0.19858800
C	-1.36904400	-1.29137700	-1.84438200
C	-0.83336200	-3.58763200	-0.34912400
H	0.79406500	-2.47191200	0.51588600
C	-2.16811500	-2.41927900	-1.99318500
H	-1.58026600	-0.38994700	-2.41469400
C	-1.89775200	-3.56715000	-1.24787600
H	-0.63669000	-4.47440200	0.24519900
H	-3.00693600	-2.40012500	-2.68202900
H	-2.52847000	-4.44430700	-1.35866900
C	2.31287500	-0.26463300	-0.04718900
C	3.13540700	-1.25401100	-0.60140500
C	2.70809300	0.40921500	1.11014400
C	4.34668100	-1.56727700	0.00668400
H	2.82928100	-1.77098800	-1.50745600
C	3.92559900	0.09611100	1.71185200
H	2.05473500	1.16584200	1.53624400
C	4.74074800	-0.89152600	1.16297400
H	4.98522100	-2.33326100	-0.42252200
H	4.23276000	0.61980500	2.61178700
H	5.68738600	-1.13671800	1.63561200
N	-2.16027200	1.12706900	0.27967900
C	-3.55569900	1.51186600	0.39997000
H	-3.75941400	2.01601200	1.35393000
H	-3.87686700	2.14957500	-0.42758700
H	-4.15394600	0.59816800	0.37226300
C	-1.80852200	-0.33465800	1.61735200
S	-3.00703300	-1.38804000	1.49342600
S	-0.47018800	0.05862800	2.41968100
C	-1.58541200	3.44654700	-0.25935200
H	-2.59241400	3.74937900	0.01846400
Al	0.98436100	3.29220600	-0.88955900
H	2.47148400	3.63831800	-1.27373200

2p

Sum of electronic and thermal Free Energies = -2229.582876 a.u.

P	0.65805300	0.16394500	-0.35872600
F	1.15412900	0.50941600	-1.96600800

C	-0.31186700	1.63422500	-0.36198400
C	-1.61518100	1.63303900	0.02915100
C	-1.89762300	3.84874300	-1.02523400
H	-2.46612900	4.76410800	-1.16501800
C	-0.08816600	-1.40796000	-0.91623100
C	0.16144100	-2.61955500	-0.26837300
C	-0.94964400	-1.36754000	-2.01597700
C	-0.43759900	-3.78835900	-0.73149300
H	0.80756300	-2.64827900	0.60452100
C	-1.57320200	-2.53391700	-2.45393600
H	-1.12845100	-0.42658000	-2.52923500
C	-1.31268100	-3.74546300	-1.81603300
H	-0.23447700	-4.72961000	-0.23017500
H	-2.25489800	-2.49636900	-3.29849900
H	-1.79385900	-4.65574700	-2.16146200
C	2.39831100	0.12971300	0.17257600
C	3.28297100	-0.69850600	-0.52471100
C	2.85934400	0.91803800	1.22913800
C	4.62160600	-0.75483400	-0.14572000
H	2.92533100	-1.29020300	-1.36292900
C	4.20615900	0.87769100	1.58473400
H	2.17127000	1.55938500	1.77317100
C	5.08476000	0.03587900	0.90541300
H	5.30458000	-1.40915300	-0.67900200
H	4.56489300	1.49918600	2.39953600
H	6.13113200	-0.00291300	1.19351500
N	-2.28989300	0.58526000	0.66540100
C	-3.72274100	0.42522400	0.38688700
H	-4.33534700	0.80681100	1.20887900
H	-3.95734700	0.94267500	-0.54294900
H	-3.93290700	-0.63857200	0.27056500
C	-1.71944100	-0.24186600	1.62525100
S	-2.65426900	-1.21150900	2.59052400
S	0.01640000	-0.20833100	1.84436100
C	-2.41898400	2.88359200	-0.24676200
H	-3.38787500	2.96578300	0.24508700
Al	-0.07442700	3.23874500	-1.43100900
H	1.12651000	3.86362400	-2.22407700

3

Sum of electronic and thermal Free Energies = -1227.349135 a.u.

P	0.22732500	-0.05613700	0.62295900
C	-0.66498500	-1.38245900	0.13137400
C	-2.11115000	-1.58402400	0.05108900

C	-0.50749600	1.49731500	0.10089000
C	-0.32499800	2.65181500	0.86764200
C	-1.19348100	1.55644700	-1.11574400
C	-0.82914000	3.86813800	0.41204000
H	0.19639400	2.59922500	1.81806400
C	-1.69527000	2.77386500	-1.56248000
H	-1.35537600	0.64717400	-1.68636800
C	-1.51156900	3.92865800	-0.80125900
H	-0.69198400	4.76529000	1.00787600
H	-2.23925500	2.81979600	-2.50079400
H	-1.90651000	4.87736300	-1.15319800
C	1.94695900	-0.23152700	0.11152700
C	2.23066900	-0.81514200	-1.12805800
C	2.98418600	0.26414500	0.90845900
C	3.54943800	-0.90696600	-1.56339300
H	1.42014700	-1.20438600	-1.73750400
C	4.30122400	0.17319800	0.46390300
H	2.76323200	0.70918300	1.87328700
C	4.58364500	-0.41159600	-0.76944700
H	3.76961800	-1.36673200	-2.52195700
H	5.10641400	0.55573800	1.08373600
H	5.61175000	-0.48319100	-1.11225000
N	-3.01061400	-0.66983600	0.14862300
C	-4.38463500	-1.11519100	0.01810400
H	-5.05073600	-0.25113800	0.07962500
H	-4.57512800	-1.61799900	-0.94357200
H	-4.67057700	-1.81404200	0.81986100
F	0.46399000	0.26872900	2.20291000
C	-0.98296300	-3.54705900	-0.13981600
H	-0.62702900	-4.56364800	-0.24812900
C	-2.22873600	-3.03830500	-0.16130900
H	-3.14283900	-3.59924900	-0.29015600
O	-0.01122300	-2.63111600	0.04492500

TS3

Sum of electronic and thermal Free Energies = -2061.735139 a.u.

P	0.85938000	0.08381600	-0.99341800
F	1.39407000	-0.06410500	-2.50630100
C	0.13796300	1.60247600	-0.75787300
C	-1.19214400	2.01926700	-0.46380900
C	0.17148700	3.79180500	-0.82562000
H	0.66840800	4.74287900	-0.95985600
C	-0.26557700	-1.29522400	-0.85384200
C	-0.02954900	-2.32284500	0.06341500

C	-1.35019600	-1.35353100	-1.73574100
C	-0.88350400	-3.42234000	0.08794900
H	0.79918000	-2.25614900	0.76318200
C	-2.19153800	-2.45913800	-1.70752200
H	-1.54110200	-0.53267400	-2.42131700
C	-1.95511200	-3.49204900	-0.80041000
H	-0.71575200	-4.21764100	0.80703800
H	-3.04070600	-2.50687000	-2.38156400
H	-2.62155700	-4.34916100	-0.77404500
C	2.39576300	-0.16205600	-0.10005900
C	3.27740900	-1.17422600	-0.50064500
C	2.69276500	0.64717900	0.99975800
C	4.45599000	-1.37742800	0.20942800
H	3.04361700	-1.79284000	-1.36326200
C	3.88025800	0.44266200	1.69883000
H	1.99699000	1.42635200	1.29821400
C	4.75570200	-0.56838300	1.30706900
H	5.14240300	-2.16130500	-0.09516100
H	4.11817600	1.07118600	2.55112600
H	5.67812100	-0.72769500	1.85779500
N	-2.21404000	1.25323200	-0.15060800
C	-3.47226300	1.94632500	0.05157500
H	-3.44650200	2.62678800	0.91846300
H	-3.75235800	2.52899800	-0.83663300
H	-4.25725600	1.20696400	0.22614100
C	-1.97058400	-0.01035300	1.56227500
S	-3.26262800	-0.93772700	1.52977300
S	-0.60424800	0.43085600	2.27024800
C	-1.11014900	3.47601300	-0.53798900
H	-1.91974000	4.17221000	-0.37643700
O	0.96234100	2.71213500	-0.96031700

3p

Sum of electronic and thermal Free Energies = -2061.792101 a.u.

P	0.64764300	0.07449600	-0.52421800
F	1.27935900	-0.07287200	-2.07367900
C	-0.51956400	1.28995900	-1.10947400
C	-1.81527200	1.50676000	-0.70200300
C	-1.36797700	2.73882300	-2.50145600
H	-1.30104400	3.40962100	-3.34479200
C	0.08403000	-1.66370500	-0.54179000
C	0.20824600	-2.50194800	0.56926700
C	-0.48460000	-2.14976500	-1.72437900
C	-0.22344000	-3.82385400	0.49054600

H	0.62962000	-2.12474100	1.49571700
C	-0.94646600	-3.46229900	-1.78424300
H	-0.56013400	-1.50483100	-2.59441200
C	-0.81016000	-4.30185500	-0.68002200
H	-0.11485200	-4.47390000	1.35315100
H	-1.40288600	-3.83031200	-2.69819800
H	-1.16252900	-5.32794000	-0.73082200
C	2.31234100	0.43450000	0.12732800
C	3.30874000	-0.52045600	-0.09675200
C	2.61129100	1.62248900	0.79678000
C	4.59833300	-0.29571800	0.37703500
H	3.07693400	-1.43148100	-0.64204900
C	3.91165300	1.85213700	1.24208600
H	1.83693800	2.36388400	0.97012400
C	4.90118200	0.89165600	1.04264100
H	5.36825900	-1.04429100	0.21668200
H	4.14664300	2.78105400	1.75251300
H	5.90999900	1.06918200	1.40335400
N	-2.50456800	0.90920000	0.35449000
C	-3.96630100	0.90967300	0.26994300
H	-4.38825600	1.75932100	0.81706800
H	-4.25291400	0.94945100	-0.78070100
H	-4.34441700	-0.00748600	0.71965900
C	-1.90468600	0.48228000	1.51474900
S	-2.77827900	0.04675500	2.85740100
S	-0.15211000	0.49135500	1.61015000
C	-2.36684400	2.45830400	-1.62304700
H	-3.35695500	2.88884200	-1.61309300
O	-0.25976400	2.03575200	-2.22041600

4

Sum of electronic and thermal Free Energies = -1207.480765 a.u.

P	0.19006800	-0.05559500	0.61694000
C	-0.62120200	-1.40403200	0.05386900
C	-2.07515900	-1.63642800	0.02587900
C	-0.54100000	1.50554800	0.11350000
C	-0.27065500	2.66440400	0.84723200
C	-1.30663800	1.56957100	-1.05430800
C	-0.76676300	3.89012700	0.40823900
H	0.31446200	2.60790600	1.75997100
C	-1.80102700	2.79643300	-1.48388600
H	-1.53696200	0.65698300	-1.59493500
C	-1.52980200	3.95552100	-0.75582600
H	-0.56071500	4.79053700	0.97883400

H	-2.40808400	2.84653800	-2.38253800
H	-1.91928100	4.91123100	-1.09473600
C	1.92658100	-0.17668600	0.12144600
C	2.22015200	-0.39459300	-1.23105500
C	2.96551600	-0.05074500	1.04828700
C	3.54408700	-0.49193700	-1.65021700
H	1.40818300	-0.48345300	-1.94985700
C	4.28966300	-0.14878600	0.62251500
H	2.73824200	0.11667000	2.09582000
C	4.57914600	-0.36952900	-0.72238900
H	3.76780900	-0.65935300	-2.69944400
H	5.09486300	-0.05445000	1.34480400
H	5.61192200	-0.44515900	-1.04974500
N	-2.96969800	-0.73864100	0.26451800
C	-4.34571400	-1.18665800	0.19196400
H	-5.01179500	-0.34266900	0.38905100
H	-4.60576700	-1.59503100	-0.79844500
H	-4.56685400	-1.96785700	0.93722400
F	0.41285600	0.23991600	2.20829400
C	-0.95822600	-3.59528700	-0.37465100
H	-0.67115200	-4.61317000	-0.61167700
C	-2.20519800	-3.06468200	-0.29243600
H	-3.13255900	-3.60860400	-0.39975300
N	0.02123800	-2.67766000	-0.08332500
H	0.92761300	-2.74478000	-0.53065400

TS4

Sum of electronic and thermal Free Energies = -2041.869419 a.u.

P	0.82815400	0.06507100	-0.99145400
F	1.38748600	-0.12688600	-2.50223800
C	0.17452600	1.61623900	-0.81348900
C	-1.16148900	2.04844700	-0.49258000
C	0.19494300	3.86511400	-0.79641700
H	0.62004300	4.85421300	-0.90851000
C	-0.31054400	-1.30193500	-0.84857100
C	-0.06849400	-2.33826700	0.05688400
C	-1.40690200	-1.34636100	-1.71646800
C	-0.92773700	-3.43406000	0.08330200
H	0.76861700	-2.28192100	0.74756500
C	-2.25296400	-2.44799500	-1.68660500
H	-1.60545100	-0.51532400	-2.38681000
C	-2.01066900	-3.49055500	-0.79162900
H	-0.75504200	-4.23586400	0.79400300
H	-3.11180200	-2.48464500	-2.34905100

H	-2.68149600	-4.34425400	-0.76416400
C	2.37069400	-0.19867800	-0.10219100
C	3.24050900	-1.22244400	-0.50041500
C	2.68395100	0.61218600	0.99309400
C	4.42005200	-1.43603400	0.20555600
H	2.99515200	-1.84328400	-1.35812200
C	3.87287900	0.39822100	1.68756500
H	1.99657200	1.39876100	1.29284700
C	4.73501900	-0.62493600	1.29735400
H	5.09499700	-2.23055200	-0.09729300
H	4.12064800	1.02710100	2.53688900
H	5.65757200	-0.79292400	1.84530400
N	-2.18255000	1.26266000	-0.20633700
C	-3.43011600	1.95960200	0.03653600
H	-3.38594900	2.62036800	0.91928600
H	-3.72106200	2.57043400	-0.83037700
H	-4.22069700	1.22454300	0.20556700
C	-1.93803700	0.00525800	1.59312000
S	-3.23914800	-0.90221800	1.56352700
S	-0.56523900	0.46907300	2.26399500
C	-1.08758000	3.49858000	-0.50004600
H	-1.90374400	4.17271900	-0.28686500
H	1.87092700	2.78046100	-1.42721200
N	0.98726200	2.76621200	-0.93815700

4p

Sum of electronic and thermal Free Energies = -2041.939458 a.u.

P	0.60484700	0.06556900	-0.48533500
F	1.32394600	-0.07568100	-2.04711100
C	-0.63673100	1.10797300	-1.20906100
C	-1.94711900	1.34412700	-0.80116700
C	-1.59503900	2.41712200	-2.75095600
H	-1.65022200	3.01122300	-3.65148100
C	0.27591900	-1.72910400	-0.45370000
C	0.51593000	-2.50335400	0.68407000
C	-0.23670900	-2.32451600	-1.61049600
C	0.25872300	-3.87197700	0.65639000
H	0.89095600	-2.04075900	1.59202000
C	-0.52309800	-3.68743200	-1.62071800
H	-0.40859600	-1.72293200	-2.49793300
C	-0.26900800	-4.46289100	-0.49058500
H	0.45600600	-4.47188400	1.53941100
H	-0.93729800	-4.14353800	-2.51487200
H	-0.48543000	-5.52713300	-0.50223300

C	2.22773900	0.62231600	0.14557100
C	3.31773000	-0.23957100	-0.01079100
C	2.40009400	1.87499900	0.73727200
C	4.57331700	0.14399500	0.45216500
H	3.18389300	-1.20298100	-0.49555900
C	3.66659700	2.26370400	1.17094600
H	1.55185400	2.54157200	0.86296900
C	4.74935900	1.39697200	1.03899500
H	5.41572100	-0.53272100	0.34536800
H	3.80140000	3.24199900	1.62208700
H	5.73143000	1.69775400	1.39180000
N	-2.61134900	0.81153700	0.31507300
C	-4.07343700	0.78322100	0.24547400
H	-4.50206700	1.68376800	0.69839700
H	-4.36749200	0.70537300	-0.80078600
H	-4.43567400	-0.08246100	0.79773700
C	-2.00274900	0.46357500	1.48691100
S	-2.84614300	0.10119700	2.87338000
S	-0.24592500	0.49809200	1.58586500
C	-2.54863900	2.17886400	-1.78120600
H	-3.55366800	2.57342800	-1.77240300
H	0.39063800	1.68763900	-2.94575100
N	-0.46206100	1.76310400	-2.40755100

5

Sum of electronic and thermal Free Energies = -1191.435202 a.u.

P	0.18788000	-0.11310800	0.60870000
C	-0.62116200	-1.47075800	0.10039500
C	-2.08411000	-1.59624600	0.06187300
C	-0.51628000	1.46780700	0.10228300
C	-0.30208900	2.61885000	0.86408200
C	-1.20774800	1.54508100	-1.11009100
C	-0.78132700	3.84707700	0.41126700
H	0.22651100	2.55411300	1.81002100
C	-1.68349800	2.77322600	-1.55712600
H	-1.39064600	0.63766000	-1.67884600
C	-1.46949800	3.92441800	-0.79762300
H	-0.61882300	4.74125200	1.00552900
H	-2.22948700	2.83202600	-2.49390500
H	-1.84384200	4.88207000	-1.14797100
C	1.93216200	-0.19837000	0.13510900
C	2.25024700	-0.37824200	-1.21636100
C	2.95437100	-0.07511500	1.08005200
C	3.58116400	-0.43713300	-1.61796900

H	1.45163600	-0.47200600	-1.94896700
C	4.28689000	-0.13803700	0.67321200
H	2.70856500	0.06568500	2.12748300
C	4.60036700	-0.31843800	-0.67200200
H	3.82366100	-0.57549400	-2.66728800
H	5.07921300	-0.04602600	1.41003800
H	5.63912100	-0.36571500	-0.98568100
N	-2.90174600	-0.66495900	0.38899400
C	-4.32796400	-0.87191100	0.28418200
H	-4.77297800	-0.02571200	-0.25193300
H	-4.63075500	-1.79471800	-0.22958500
H	-4.77144400	-0.87820800	1.28758500
F	0.37737700	0.18648800	2.20280400
C	-1.18951900	-3.66289600	-0.52117600
H	-1.09919900	-4.70326700	-0.81944500
C	-2.34168700	-2.99423100	-0.39557000
H	-3.32484100	-3.41325200	-0.57144500
C	0.01496500	-2.81991900	-0.18639800
H	0.55209300	-3.25250100	0.66997400
H	0.72714900	-2.80394500	-1.02308100

TS5

Sum of electronic and thermal Free Energies = -2025.815751 a.u.

P	0.81166200	0.21643700	-0.93298200
F	1.36083600	0.17072600	-2.45871400
C	0.10339800	1.71426900	-0.63547700
C	0.85323600	2.99876400	-0.94020000
C	-1.26278500	2.01104200	-0.32876700
C	-0.23079800	4.03301800	-0.82588400
H	1.30591700	3.00846800	-1.94161200
H	-0.04618300	5.09152600	-0.97773200
C	-0.23978500	-1.23403300	-0.89888000
C	0.04525300	-2.31742000	-0.06450300
C	-1.31805900	-1.28308600	-1.78898100
C	-0.75122700	-3.45829300	-0.12876800
H	0.86859100	-2.26415600	0.64277600
C	-2.10248600	-2.42871100	-1.85188800
H	-1.54375900	-0.42510000	-2.41675800
C	-1.81648600	-3.51538600	-1.02497900
H	-0.54322700	-4.29692000	0.52813900
H	-2.94425200	-2.46927200	-2.53595500
H	-2.43744200	-4.40532600	-1.06909700
C	2.37476100	-0.09565300	-0.09017600
C	3.26684500	-1.04621200	-0.60296300

C	2.68543300	0.60413000	1.07851300
C	4.46530300	-1.29492400	0.05801300
H	3.02354100	-1.58334700	-1.51594800
C	3.89173200	0.35649200	1.73128000
H	1.97785600	1.32976200	1.47099600
C	4.77679900	-0.59263700	1.22376400
H	5.15779600	-2.03215200	-0.33650200
H	4.13555100	0.90067000	2.63840000
H	5.71395500	-0.78739800	1.73704200
N	-2.19935400	1.18885300	0.06000900
C	-3.54643100	1.70801200	0.20805600
H	-3.65647300	2.32681400	1.11093600
H	-3.84909400	2.29814300	-0.66483200
H	-4.23441700	0.86376100	0.29444400
C	-1.88835300	-0.17963600	1.60081900
S	-3.11482400	-1.19380400	1.50964100
S	-0.55332700	0.27665100	2.36194900
C	-1.40535400	3.48350300	-0.49417900
H	-2.33326700	4.01722800	-0.32804600
H	1.66238500	3.21725700	-0.22740300

5p

Sum of electronic and thermal Free Energies = -2025.863656 a.u.

P	0.64492000	0.11137500	-0.49697900
F	1.24392100	0.05121600	-2.08738800
C	-0.37316600	1.50331900	-0.92008800
C	-0.05866200	2.54286400	-1.96121000
C	-1.65293300	1.67874700	-0.48851300
C	-1.31686600	3.35383600	-2.01728300
H	0.17752200	2.06906600	-2.92229800
H	-1.43539300	4.23964300	-2.63034000
C	-0.07873100	-1.55557500	-0.68827700
C	0.07430900	-2.55210900	0.27844200
C	-0.81009400	-1.81567300	-1.85131800
C	-0.49119000	-3.80828900	0.07290200
H	0.61969500	-2.34585900	1.19449800
C	-1.40335000	-3.06254000	-2.03455500
H	-0.91146300	-1.04538500	-2.61046200
C	-1.23851800	-4.06134200	-1.07630800
H	-0.36188900	-4.58268100	0.82266100
H	-1.98583500	-3.25521300	-2.93056800
H	-1.69478900	-5.03587900	-1.22350200
C	2.35229800	0.25690200	0.12625600
C	3.27165200	-0.72779000	-0.24805600

C	2.75471700	1.32611400	0.92929000
C	4.58572400	-0.65428400	0.20607500
H	2.96047000	-1.54328100	-0.89531400
C	4.07924300	1.40856600	1.35514900
H	2.03897400	2.08899200	1.22309500
C	4.99131900	0.41541500	1.00356500
H	5.29509000	-1.42781500	-0.07223700
H	4.39348200	2.24618400	1.97034300
H	6.01911700	0.47570600	1.34906700
N	-2.37426700	0.92174000	0.43532400
C	-3.83298100	0.90258000	0.29025000
H	-4.30631000	1.61031000	0.97821100
H	-4.08280300	1.14348000	-0.74262000
H	-4.19494200	-0.09744100	0.52822200
C	-1.81698400	0.33353100	1.55315000
S	-2.75127600	-0.27076000	2.78359100
S	-0.07180800	0.30319100	1.70023900
C	-2.23456700	2.84323400	-1.17856700
H	-3.22902800	3.23107100	-0.99358800
H	0.81091500	3.16143400	-1.69795700

6

Sum of electronic and thermal Free Energies = -1442.822456 a.u.

P	0.17057100	0.03712700	0.59324800
C	-0.76784700	-1.23679100	0.08313500
C	-2.23933500	-1.18244100	0.15259200
C	-0.29043500	1.69275300	0.04124800
C	0.12924800	2.82173900	0.74915800
C	-1.00127600	1.83438500	-1.15292200
C	-0.16583100	4.09287500	0.26085100
H	0.67477000	2.70808300	1.68146300
C	-1.29295100	3.10623000	-1.63668900
H	-1.34047500	0.94689100	-1.68067300
C	-0.87455600	4.23474800	-0.93109800
H	0.15584800	4.97112800	0.81248500
H	-1.85375900	3.21747400	-2.55984900
H	-1.10488600	5.22651000	-1.30950800
C	1.90931900	-0.24878400	0.18943100
C	2.26871200	-0.45426900	-1.14796800
C	2.88977100	-0.26071700	1.18562900
C	3.60058600	-0.67760600	-1.48377600
H	1.50510800	-0.44221000	-1.92206100
C	4.22225700	-0.48653800	0.84329500
H	2.61117400	-0.10179100	2.22241100

C	4.57730500	-0.69520100	-0.48772200
H	3.87552300	-0.83921400	-2.52158300
H	4.98174400	-0.50183500	1.61913500
H	5.61613600	-0.87183500	-0.75071600
N	-2.86813600	-0.15331100	0.59074500
C	-4.32128900	-0.16492100	0.62306700
H	-4.67034500	0.81494700	0.95618300
H	-4.76791900	-0.36206000	-0.36160700
H	-4.70907300	-0.91309300	1.32824400
F	0.29738500	0.31269700	2.18404600
C	-2.02777200	-3.47380000	-0.63430000
H	-2.41521400	-4.43470000	-0.96323800
C	-2.85708900	-2.46651100	-0.31325800
H	-3.94087300	-2.54920800	-0.35729900
Si	-0.24006600	-2.93004300	-0.41724800
H	0.49415000	-3.73281500	0.59471200
H	0.53801800	-3.02459300	-1.68100500

TS6

Sum of electronic and thermal Free Energies = -2277.196418 a.u.

P	0.75451100	0.06026600	-0.86168500
F	1.28561200	0.06821400	-2.39051100
C	0.21839300	1.60587400	-0.46300100
C	-1.12731400	2.00817100	-0.14906800
C	-0.23387600	4.24039600	-0.56140600
H	-0.29326300	5.32401100	-0.60413400
C	-0.41569900	-1.29927300	-0.94213200
C	-0.23580800	-2.46235800	-0.19076400
C	-1.48598600	-1.18759000	-1.83649300
C	-1.12856900	-3.52091900	-0.34342900
H	0.58044600	-2.53418800	0.52306400
C	-2.36901300	-2.25042600	-1.98641900
H	-1.62615100	-0.27179100	-2.40543200
C	-2.18751100	-3.41683400	-1.24249600
H	-1.00060800	-4.42128800	0.24909400
H	-3.20352800	-2.16614200	-2.67548700
H	-2.88386800	-4.24262600	-1.35477200
C	2.27914600	-0.45818000	-0.05345100
C	3.03993800	-1.49465700	-0.61066400
C	2.70534300	0.17973100	1.11395400
C	4.22184400	-1.89154200	0.00584900
H	2.70899700	-1.98236500	-1.52413700
C	3.89462200	-0.21760000	1.72242400
H	2.10179700	0.97653200	1.53972200

C	4.64800500	-1.25203800	1.17163200
H	4.81276500	-2.69463500	-0.42368400
H	4.22781300	0.27856100	2.62856100
H	5.57233800	-1.56248400	1.65008200
N	-2.09408300	1.22037900	0.23574700
C	-3.45175500	1.72684200	0.33489300
H	-3.62036200	2.27198300	1.27365800
H	-3.70631300	2.37227100	-0.51103800
H	-4.13075000	0.87136600	0.31974700
C	-1.86607700	-0.23255600	1.62282400
S	-3.14968500	-1.18060000	1.51179200
S	-0.49825000	0.06339800	2.41447500
C	-1.30832000	3.49763900	-0.25616100
H	-2.28110700	3.92592000	-0.03255300
H	1.88651000	3.17900900	-2.11098500
Si	1.25020800	3.11786400	-0.77315200
H	2.30556500	3.39235200	0.23524100

6p

Sum of electronic and thermal Free Energies = -2277.236543 a.u.

P	0.65365400	0.07384700	-0.38647200
F	1.21413900	0.34574900	-1.97176200
C	-0.30977700	1.55930100	-0.47493500
C	-1.58794300	1.64570400	-0.01552500
C	-1.59708400	3.85173900	-1.00588200
H	-2.00505700	4.83863700	-1.19889200
C	-0.13562600	-1.48884500	-0.90898300
C	-0.01042100	-2.67410000	-0.18074000
C	-0.90064700	-1.46379100	-2.07959900
C	-0.63764800	-3.83289800	-0.63224100
H	0.56060800	-2.69058100	0.74279300
C	-1.55412000	-2.61748600	-2.50650600
H	-0.97905900	-0.54582200	-2.65526400
C	-1.41787200	-3.80367600	-1.78694800
H	-0.53061100	-4.75399800	-0.06776400
H	-2.16110000	-2.59061100	-3.40658300
H	-1.92170200	-4.70469600	-2.12443800
C	2.37892500	0.03719700	0.19947000
C	3.25652700	-0.86882400	-0.40351000
C	2.83393600	0.89860500	1.19980800
C	4.58206300	-0.93049300	0.01807100
H	2.90451300	-1.51753600	-1.20106700
C	4.16952600	0.85155800	1.59508500
H	2.15119100	1.60235200	1.66818100

C	5.04023500	-0.06799600	1.01345600
H	5.25929200	-1.64532400	-0.43950600
H	4.52505000	1.52982300	2.36470900
H	6.07698500	-0.11118100	1.33382400
N	-2.29987500	0.66058600	0.67713300
C	-3.74957700	0.59343100	0.45674500
H	-4.29987000	1.05294500	1.28329500
H	-3.98299300	1.08749400	-0.48606000
H	-4.04035900	-0.45558500	0.39568000
C	-1.74810500	-0.16516900	1.64348000
S	-2.69791100	-1.06780800	2.65797400
S	-0.00785900	-0.18913800	1.82244600
C	-2.27939300	2.94435400	-0.28810000
H	-3.26367600	3.12117400	0.13873300
H	0.21563100	2.85892100	-2.90788200
Si	0.06677000	3.10657500	-1.45919800
H	1.21777100	3.88786100	-0.95358900

7

Sum of electronic and thermal Free Energies = -1177.600104 a.u.

P	-0.16616700	-0.14379700	-0.58986000
C	0.66094500	-1.50553700	-0.07273400
C	0.06722000	-2.77289800	0.24277600
C	2.14105800	-1.67724900	-0.04192000
H	-1.01456700	-2.91087300	0.24056500
C	0.53665900	1.43159500	-0.07324700
C	0.33158900	2.58415700	-0.83631600
C	1.21631400	1.50493000	1.14580200
C	0.81235500	3.80930800	-0.37913500
H	-0.18954800	2.52266700	-1.78681400
C	1.69314800	2.73149800	1.59743900
H	1.38825700	0.59896000	1.72032400
C	1.49101100	3.88292100	0.83599500
H	0.65934800	4.70443700	-0.97428800
H	2.22977500	2.78785700	2.53960500
H	1.86657900	4.83880200	1.18949900
C	-1.91474700	-0.22176400	-0.14280300
C	-2.26327300	-0.47563800	1.18940900
C	-2.91269000	-0.00174600	-1.09671100
C	-3.60359100	-0.51453800	1.56136600
H	-1.48516900	-0.64906200	1.92874300
C	-4.25366600	-0.04262100	-0.71759400
H	-2.64320900	0.19185800	-2.12984900
C	-4.59890600	-0.29845300	0.60768200

H	-3.87092100	-0.71529400	2.59427700
H	-5.02776000	0.12263900	-1.46076200
H	-5.64456800	-0.33061000	0.89918800
N	2.92169600	-0.72790000	-0.39956300
C	4.35411000	-0.93947900	-0.37143500
H	4.80743000	-0.16606300	0.25876100
H	4.65482700	-1.92866300	-0.00734400
H	4.74699800	-0.79115400	-1.38326400
F	-0.30270800	0.12945600	-2.18286000
C	0.97268300	-3.77013100	0.55675300
H	0.63240500	-4.76212000	0.83547500
B	2.37099900	-3.20667400	0.43262300
H	3.41882400	-3.73899200	0.63137900

TS7

Sum of electronic and thermal Free Energies = -2011.972396 a.u.

P	0.78371900	0.19357900	-0.95031400
F	1.36149600	0.12119400	-2.45810500
C	0.07214400	1.71512300	-0.73335100
C	0.76538200	2.88651600	-1.20442000
C	-1.26539500	2.13400800	-0.30833200
C	0.04467700	4.06472900	-1.16721600
H	1.78827900	2.81526500	-1.57965700
H	0.47173900	4.99791100	-1.51608400
C	-0.30701100	-1.22583900	-0.91992000
C	-0.05040500	-2.33792300	-0.11301200
C	-1.39052200	-1.22212100	-1.80572300
C	-0.88199700	-3.45030800	-0.19934700
H	0.77435500	-2.32430600	0.59424200
C	-2.21143700	-2.34174900	-1.89066600
H	-1.58638700	-0.34831000	-2.42242400
C	-1.95473300	-3.45401200	-1.09035000
H	-0.69826900	-4.30958700	0.43773700
H	-3.05570600	-2.34159500	-2.57279900
H	-2.60234500	-4.32367800	-1.15087400
C	2.32268100	-0.12463200	-0.06845700
C	3.15263400	-1.17955800	-0.47012500
C	2.69532700	0.70398200	0.99254600
C	4.34921400	-1.40824100	0.20102500
H	2.86545800	-1.81182600	-1.30676500
C	3.89980300	0.47446900	1.65466700
H	2.03910100	1.51681500	1.29303300
C	4.72083300	-0.58098600	1.26264900
H	4.99431700	-2.22564300	-0.10604200

H	4.19283400	1.11762800	2.47851000
H	5.65669500	-0.76034900	1.78376200
N	-2.12352500	1.43376700	0.34671800
C	-3.44359200	1.95016200	0.65743800
H	-3.53135800	2.08781200	1.74077100
H	-3.64812100	2.89096500	0.14526600
H	-4.18183000	1.19892200	0.36182200
C	-1.80864100	-0.12156000	1.59682400
S	-3.06289200	-1.10142000	1.45576900
S	-0.43516400	0.21175600	2.36377500
B	-1.32826300	3.73763900	-0.65019800
H	-2.26690900	4.44323700	-0.45695400

7p

Sum of electronic and thermal Free Energies = -2012.003565 a.u.

P	0.62975400	-0.13094600	0.48526600
F	1.23199900	-0.08305000	2.07440200
C	-0.38427900	-1.53193200	0.91811000
C	-0.02798800	-2.52659700	1.98433800
C	-1.67094300	-1.71977300	0.51913600
C	-1.02715200	-3.38974400	2.27511300
H	0.96031300	-2.50817400	2.43663300
H	-0.92915100	-4.17935600	3.01022500
C	-0.10694500	1.52838800	0.69721400
C	0.00632700	2.52503200	-0.27504500
C	-0.80527100	1.78265700	1.88197700
C	-0.56550200	3.77560400	-0.05403500
H	0.52672700	2.32408000	-1.20665600
C	-1.40554800	3.02381700	2.08101500
H	-0.87359600	1.01363700	2.64583600
C	-1.28032700	4.02272300	1.11694500
H	-0.46612300	4.55030400	-0.80803100
H	-1.96184400	3.21201500	2.99439400
H	-1.74155800	4.99291300	1.27680100
C	2.33442800	-0.24858700	-0.15087600
C	3.24353400	0.74308900	0.23031100
C	2.74517400	-1.30375800	-0.96803400
C	4.55555600	0.69128300	-0.23247400
H	2.92591600	1.54735900	0.88841100
C	4.06793600	-1.36426700	-1.40300800
H	2.03874700	-2.07427200	-1.26413600
C	4.96942300	-0.36385500	-1.04512200
H	5.25694800	1.47020600	0.05084200
H	4.38915100	-2.19123400	-2.02883500

H	5.99582100	-0.40729200	-1.39716500
N	-2.39628900	-1.02742000	-0.42973700
C	-3.86174200	-1.09392100	-0.34304200
H	-4.26946500	-1.67101300	-1.17651600
H	-4.13381000	-1.54945100	0.60638800
H	-4.26710100	-0.08229800	-0.39422100
C	-1.85147700	-0.36874300	-1.52448700
S	-2.80544700	0.26866100	-2.71885500
S	-0.10976700	-0.32400600	-1.69516700
B	-2.19227700	-3.02976600	1.33344500
H	-3.21765300	-3.59798200	1.13449600

8

Sum of electronic and thermal Free Energies = -1395.155049 a.u.

P	0.25494300	-0.05411400	0.61478100
C	-0.91720000	-1.16147900	0.13906600
C	-0.60658100	-2.54502900	-0.20708700
C	-2.35354400	-0.81089500	0.17572500
H	0.44509700	-2.84144500	-0.17916600
C	0.02175100	1.63877700	0.03672400
C	0.52461300	2.71649400	0.76893000
C	-0.58856500	1.85409100	-1.20193100
C	0.41076300	4.00977100	0.26192900
H	0.99101700	2.54797800	1.73466700
C	-0.69889200	3.14683500	-1.70366900
H	-0.99493600	1.00972200	-1.75262700
C	-0.19891800	4.22510200	-0.97226700
H	0.79620800	4.84836300	0.83401800
H	-1.18154900	3.31481500	-2.66176900
H	-0.28802100	5.23401000	-1.36449000
C	1.92246800	-0.59597500	0.17401500
C	2.20972100	-0.88654000	-1.16523100
C	2.92513600	-0.70083900	1.14175000
C	3.49196100	-1.28335700	-1.53104000
H	1.42639800	-0.80984400	-1.91569300
C	4.20832000	-1.10037900	0.76933500
H	2.70246400	-0.47694100	2.17994400
C	4.49170100	-1.39082900	-0.56313200
H	3.71072000	-1.51103900	-2.56982200
H	4.98488700	-1.18591300	1.52338500
H	5.49187300	-1.70221600	-0.84981300
N	-2.73712000	0.31948200	0.64291300
C	-4.14856000	0.62902600	0.64662500
H	-4.32136600	1.53747700	0.05761900

H	-4.77513600	-0.18142600	0.23924700
H	-4.47030400	0.84690100	1.67113200
F	0.46683900	0.22772500	2.19847000
C	-1.57613500	-3.44179900	-0.56918900
H	-1.25808600	-4.44583000	-0.83360200
Al	-3.23722800	-2.50806800	-0.46731700
H	-4.74938500	-2.87174900	-0.74957400

TS8

Sum of electronic and thermal Free Energies = -2229.529942 a.u.

P	0.78437700	0.20255000	-0.90624700
F	1.33746600	0.28436100	-2.42551200
C	-0.07280300	1.63662000	-0.57793700
C	0.62649500	2.87950800	-0.94135100
C	-1.45195300	1.78451800	-0.16760700
C	0.04206000	4.11284000	-0.89586900
H	1.66484400	2.77392500	-1.27282500
H	0.63167400	4.96823100	-1.20837900
C	-0.14130900	-1.33093300	-0.97003600
C	0.26539500	-2.46550300	-0.26360700
C	-1.24093700	-1.38629100	-1.83382900
C	-0.43034500	-3.66025800	-0.42919700
H	1.10134500	-2.41111100	0.42839600
C	-1.92684800	-2.58469500	-1.99658900
H	-1.55611400	-0.49427100	-2.36956100
C	-1.51873200	-3.72052900	-1.29759000
H	-0.12770400	-4.54010500	0.12968500
H	-2.78398000	-2.63016400	-2.66104400
H	-2.06066900	-4.65369700	-1.41986400
C	2.36947600	-0.00960900	-0.07226900
C	3.30043300	-0.93378200	-0.56358900
C	2.67352500	0.77342000	1.04379600
C	4.52824200	-1.08084200	0.07381700
H	3.06601300	-1.52897700	-1.44275500
C	3.90877900	0.62810300	1.67176300
H	1.94125200	1.48781500	1.41122600
C	4.83040900	-0.30010600	1.19098500
H	5.25085600	-1.79832600	-0.30265100
H	4.14798700	1.23705200	2.53794200
H	5.79040900	-0.41517300	1.68574900
N	-2.20445300	0.88151800	0.37303800
C	-3.59610200	1.17500700	0.65781100
H	-3.76453800	1.19260700	1.74090200
H	-3.90570500	2.13428000	0.22678900

H	-4.22551800	0.38153700	0.24288400
C	-1.67838900	-0.64794000	1.65371200
S	-2.80684500	-1.76535500	1.50445300
S	-0.35184300	-0.14015800	2.40046600
Al	-1.75914200	3.78193000	-0.38307400
H	-3.05836500	4.63420900	-0.10766200

8p

Sum of electronic and thermal Free Energies = -2229.572942 a.u.

P	0.68719500	0.12357500	-0.41539600
F	1.19635300	0.35243700	-2.02348600
C	-0.41634200	1.54098600	-0.56496000
C	0.03983600	2.75508800	-1.32277000
C	-1.70883400	1.48819200	-0.14866400
C	-0.78525700	3.80506800	-1.52439600
H	1.06386400	2.72747100	-1.69419400
H	-0.42304000	4.65951900	-2.08619100
C	-0.00895700	-1.50680400	-0.86766700
C	0.17934900	-2.64468900	-0.08003600
C	-0.75825500	-1.58867100	-2.04618900
C	-0.36848500	-3.86177800	-0.47910300
H	0.73740200	-2.58046600	0.84917200
C	-1.33502900	-2.79999400	-2.41956600
H	-0.88493200	-0.70799300	-2.66865800
C	-1.13494500	-3.93862200	-1.64038800
H	-0.21115200	-4.74487400	0.13232200
H	-1.93140000	-2.85541300	-3.32542900
H	-1.57830100	-4.88474900	-1.93683900
C	2.42039300	0.24446400	0.13686000
C	3.36174200	-0.60286700	-0.45562900
C	2.81722200	1.16984200	1.10473700
C	4.69362500	-0.54231200	-0.05466000
H	3.05280100	-1.30150800	-1.22829000
C	4.15778300	1.24531700	1.47850200
H	2.08633000	1.82983900	1.56421400
C	5.09310200	0.38410400	0.90835100
H	5.42112800	-1.21218100	-0.50301900
H	4.46699100	1.97367400	2.22191100
H	6.13449300	0.43638300	1.21188200
N	-2.30293500	0.48102700	0.61134200
C	-3.76286300	0.36591400	0.51380600
H	-4.24492200	0.75876300	1.41410000
H	-4.09277100	0.91558600	-0.36752900
H	-4.03773700	-0.68498900	0.41098000

C	-1.67890100	-0.24428700	1.60855300
S	-2.53024000	-1.18157100	2.68117400
S	0.05805200	-0.08727600	1.78727800
Al	-2.45241500	3.24239600	-0.74207400
H	-3.90800400	3.81487800	-0.56045900

9

Sum of electronic and thermal Free Energies = -1227.371250 a.u.

P	-0.19953600	-0.10978300	-0.62168300
C	0.67882700	-1.43974000	-0.11690000
C	0.20087100	-2.79745800	0.12734000
C	2.12308600	-1.48655500	0.07247600
H	-0.81437800	-3.15762500	0.03370600
C	0.39918600	1.50598000	-0.10120600
C	1.54913200	2.05549900	-0.67892100
C	-0.29688800	2.20651700	0.88955700
C	1.99581600	3.30481700	-0.25872300
H	2.10076300	1.49769300	-1.42715200
C	0.15992700	3.45463400	1.30586600
H	-1.19547600	1.78558200	1.33295800
C	1.30513100	4.00302100	0.73148500
H	2.89089900	3.73012000	-0.70209300
H	-0.38142400	3.99777900	2.07440700
H	1.66045500	4.97681800	1.05593300
C	-1.94364500	-0.29893300	-0.21404500
C	-2.30934300	-0.84642400	1.02187700
C	-2.92707900	0.15406300	-1.09989600
C	-3.65565200	-0.94656500	1.36327900
H	-1.53996500	-1.19277000	1.70742000
C	-4.27196500	0.05191000	-0.75071300
H	-2.63987700	0.57775300	-2.05712800
C	-4.63558100	-0.49788000	0.47767100
H	-3.93864700	-1.37470400	2.32001100
H	-5.03525700	0.39947100	-1.44008800
H	-5.68496100	-0.57722000	0.74609900
N	3.00714500	-0.59208000	-0.11805800
C	4.37877700	-0.94935100	0.19864000
H	4.49724000	-1.23751400	1.25212100
H	4.73187100	-1.79250800	-0.41083200
H	5.02270200	-0.08870300	0.00296300
F	-0.29314900	0.13493200	-2.22504600
C	1.26751200	-3.51684600	0.50380300
H	1.38074900	-4.54971800	0.79661800
O	2.42725000	-2.76970900	0.50782300

TS9

Sum of electronic and thermal Free Energies = -2061.754553 a.u.

P	0.83985200	0.12292000	-0.98974600
F	1.38476800	0.00984900	-2.50237200
C	0.12374500	1.64752000	-0.78194400
C	0.77856400	2.91695600	-1.05238000
C	-1.21850500	1.95411700	-0.41667600
C	-0.15557400	3.86604100	-0.87513200
H	1.80268400	3.06717200	-1.36590400
H	-0.14899600	4.93858800	-0.99095900
C	-0.23687000	-1.29908800	-0.87664500
C	0.02590600	-2.33873200	0.01946100
C	-1.32164400	-1.36852800	-1.75774000
C	-0.79952400	-3.45997600	0.02269000
H	0.85097200	-2.26370600	0.72255700
C	-2.13524200	-2.49534100	-1.75089600
H	-1.53313400	-0.54121800	-2.42988000
C	-1.87117300	-3.53962800	-0.86482700
H	-0.61080900	-4.26424800	0.72646900
H	-2.98357900	-2.55142600	-2.42536500
H	-2.51578400	-4.41357100	-0.85416100
C	2.38382500	-0.10790400	-0.10099800
C	3.25652700	-1.13387300	-0.48669300
C	2.70787100	0.73767300	0.96339600
C	4.45202700	-1.31352400	0.20107300
H	3.00257000	-1.78205100	-1.32175100
C	3.91167700	0.55613300	1.64110400
H	2.01689500	1.52418500	1.25529300
C	4.77780700	-0.46809800	1.26334800
H	5.13085400	-2.10801800	-0.09282600
H	4.16815400	1.21162600	2.46731900
H	5.71273500	-0.60979700	1.79752600
N	-2.20291600	1.19717800	-0.03046800
C	-3.47852300	1.85869000	0.18747300
H	-3.45248900	2.53057200	1.05680700
H	-3.76874100	2.44796700	-0.68955300
H	-4.23616300	1.09149100	0.35923500
C	-1.87841400	-0.06871000	1.58204700
S	-3.14030700	-1.04232700	1.58815000
S	-0.49493000	0.36767400	2.27274900
O	-1.35581800	3.31772900	-0.48854500

9p

Sum of electronic and thermal Free Energies = -2061.801432 a.u.

P	0.65539400	0.07611200	-0.53758100
F	1.30429400	-0.08244500	-2.09289200
C	-0.49097100	1.29052500	-1.14197300
C	-0.38520400	2.12713200	-2.31128500
C	-1.76503000	1.47677900	-0.66420300
C	-1.57323300	2.75599900	-2.43407200
H	0.47869800	2.21587200	-2.95274000
H	-1.97937400	3.47367000	-3.12851600
C	0.11092000	-1.66630600	-0.55374900
C	0.30781700	-2.52378100	0.53140400
C	-0.52052700	-2.13425200	-1.71082500
C	-0.11431300	-3.84861200	0.45104800
H	0.77713900	-2.15846000	1.43967600
C	-0.97230400	-3.45045000	-1.77058200
H	-0.65320200	-1.47174100	-2.56118800
C	-0.76332900	-4.30983100	-0.69326300
H	0.04999400	-4.51450300	1.29254300
H	-1.47808300	-3.80548900	-2.66345100
H	-1.10804400	-5.33848100	-0.74419900
C	2.31668300	0.45974700	0.10718900
C	3.32671200	-0.48406000	-0.10160300
C	2.59840600	1.66269700	0.75734600
C	4.61313100	-0.23272500	0.36796900
H	3.10817900	-1.40678400	-0.63260100
C	3.89543800	1.91901800	1.19780200
H	1.81197700	2.39408300	0.91989200
C	4.89890900	0.96974600	1.01366100
H	5.39389900	-0.97255300	0.21979500
H	4.11692700	2.85926000	1.69335200
H	5.90503400	1.16771700	1.37122500
N	-2.47872500	0.92070700	0.37887100
C	-3.94521700	0.94790500	0.29708800
H	-4.34621600	1.71256100	0.96705400
H	-4.23364600	1.15809900	-0.73031600
H	-4.32692000	-0.02361100	0.61062500
C	-1.87579500	0.44423000	1.52857300
S	-2.76775600	-0.04094600	2.83641500
S	-0.12606000	0.45129500	1.62608300
O	-2.42579300	2.35969900	-1.43457700

10

Sum of electronic and thermal Free Energies = -1207.499282 a.u.

P	-0.18464100	-0.12167300	-0.61471800

C	0.68512500	-1.45860200	-0.10828300
C	0.18266300	-2.80271200	0.16374700
C	2.13643000	-1.49228400	0.06672700
H	-0.84350800	-3.13407000	0.08521900
C	0.39644900	1.50037200	-0.08601400
C	1.53207100	2.07407300	-0.66878000
C	-0.30222900	2.18244700	0.91570400
C	1.96051700	3.32816200	-0.24325600
H	2.08696200	1.52854300	-1.42328300
C	0.13709600	3.43482400	1.33849100
H	-1.19031000	1.74405800	1.36329800
C	1.26748600	4.00734100	0.75843800
H	2.84409500	3.77224800	-0.69154500
H	-0.40686600	3.96251500	2.11598400
H	1.60897200	4.98473100	1.08716500
C	-1.93418700	-0.30526400	-0.22314000
C	-2.31612000	-0.84313500	1.01209300
C	-2.90645800	0.14451700	-1.12261100
C	-3.66650900	-0.93630800	1.33901800
H	-1.55562400	-1.18870000	1.70779500
C	-4.25575500	0.04869500	-0.78849600
H	-2.60698700	0.56132800	-2.07911700
C	-4.63524300	-0.49119300	0.43932800
H	-3.96162100	-1.35695300	2.29547600
H	-5.00992300	0.39374000	-1.48916400
H	-5.68786700	-0.56555500	0.69638600
N	2.98951200	-0.56008700	-0.19412300
C	4.36622500	-0.86485200	0.12362100
H	4.50969900	-1.12946900	1.18584500
H	4.76510600	-1.69889500	-0.48190200
H	4.99047800	0.00822500	-0.08344400
F	-0.26148000	0.12979100	-2.21799700
C	1.23371100	-3.55275700	0.55708300
H	1.26778100	-4.58740300	0.86751900
N	2.39577000	-2.77233800	0.55894700
H	3.32793700	-3.15032500	0.63071400

TS10

Sum of electronic and thermal Free Energies = -2041.888364 a.u.

P	0.84762300	0.10504500	-1.00556700
F	1.37536700	-0.07561700	-2.51923100
C	0.15308000	1.63963800	-0.80972400
C	0.88084700	2.88542400	-0.95830500
C	-1.21356300	1.95804700	-0.50921200

C	-0.00747700	3.89103900	-0.76785700
H	1.92897200	2.99222400	-1.20319000
H	0.12374400	4.96188300	-0.81796200
C	-0.21187100	-1.32571400	-0.82845400
C	0.06298200	-2.30443000	0.13010800
C	-1.28115500	-1.47523400	-1.71837700
C	-0.73392500	-3.44514000	0.18927000
H	0.87883700	-2.17016300	0.83526600
C	-2.06420500	-2.62135100	-1.65722400
H	-1.50654000	-0.69225700	-2.43665100
C	-1.78800300	-3.60534400	-0.70748300
H	-0.53483700	-4.20171400	0.94149600
H	-2.89994100	-2.73954000	-2.33949400
H	-2.40964300	-4.49441600	-0.65563800
C	2.39489700	-0.10457400	-0.11530900
C	3.29754600	-1.09688300	-0.51982400
C	2.67661800	0.70213600	0.99089500
C	4.48196100	-1.27857800	0.18645200
H	3.07410600	-1.71772100	-1.38355100
C	3.86870400	0.51742100	1.68886700
H	1.96423900	1.46374800	1.29633000
C	4.76598700	-0.47102600	1.28944600
H	5.18426800	-2.04600700	-0.12394800
H	4.09216200	1.14363700	2.54686500
H	5.69209100	-0.61445900	1.83842900
N	-2.22111100	1.14779200	-0.24731100
C	-3.49893400	1.80086900	-0.05819900
H	-3.51624500	2.47372000	0.81915300
H	-3.78881100	2.38266900	-0.94684000
H	-4.26509600	1.03877100	0.09992900
C	-1.96500300	-0.02051500	1.54522700
S	-3.20082800	-1.02158500	1.51156900
S	-0.65012300	0.53315600	2.27187000
H	-2.08430200	3.86581900	-0.27507700
N	-1.25337000	3.33775500	-0.49487800

10p

Sum of electronic and thermal Free Energies = -2041.937527 a.u.

P	0.65885100	0.07713100	-0.55224900
F	1.30243300	-0.07316800	-2.10755400
C	-0.42571900	1.36935000	-1.09876800
C	-0.23466000	2.29682000	-2.17143100
C	-1.70116800	1.57653300	-0.59694600
C	-1.37586700	3.04209700	-2.27151400

H	0.65133500	2.37633100	-2.78372600
H	-1.64464900	3.84922800	-2.93584700
C	0.01892700	-1.63170700	-0.61386700
C	0.17690500	-2.53646000	0.43857400
C	-0.64849500	-2.02286100	-1.77942400
C	-0.32091600	-3.83177600	0.31742300
H	0.67393400	-2.22957800	1.35370400
C	-1.17386400	-3.30886100	-1.88008500
H	-0.75088900	-1.32318400	-2.60395800
C	-1.00465200	-4.21579300	-0.83508000
H	-0.18778400	-4.53466300	1.13400600
H	-1.70574400	-3.60407300	-2.77966400
H	-1.40698500	-5.22125700	-0.91770900
C	2.33503000	0.35891900	0.10555000
C	3.29774500	-0.63068400	-0.11240100
C	2.67253000	1.53653000	0.77523300
C	4.59240000	-0.45102400	0.36787400
H	3.03660700	-1.53306600	-0.65900100
C	3.97774800	1.72104300	1.22712600
H	1.92140900	2.30319600	0.94337300
C	4.93381100	0.72560700	1.03381600
H	5.33639000	-1.22644900	0.21226300
H	4.24298200	2.64131800	1.73856200
H	5.94638700	0.86750000	1.39984600
N	-2.42107900	0.91168600	0.39589400
C	-3.87738100	0.87549800	0.25641300
H	-4.35146800	1.68420000	0.82441300
H	-4.12676900	0.94579700	-0.80389100
H	-4.24451700	-0.07013200	0.65389600
C	-1.83814200	0.42523700	1.54755000
S	-2.74876400	-0.08091700	2.83972700
S	-0.09108600	0.41211400	1.64758000
H	-3.17646700	2.98527700	-1.13584800
N	-2.26552100	2.58847700	-1.31673300

11

Sum of electronic and thermal Free Energies = -1191.439322 a.u.

P	-0.21032600	-0.10622800	-0.61341900
C	0.72440100	-1.40297900	-0.13320900
C	0.26055100	-2.77217400	0.10682500
C	2.19279600	-1.42498100	-0.08097500
H	-0.78438300	-3.06629200	0.08157900
C	0.38075300	1.51159600	-0.08578500
C	0.12407200	2.65062300	-0.85296900

C	1.02940700	1.62466100	1.14716000
C	0.51835600	3.90256500	-0.38425200
H	-0.36978900	2.55905300	-1.81519900
C	1.42036100	2.87650200	1.60975300
H	1.24610200	0.72884500	1.72226500
C	1.16397500	4.01541100	0.84524400
H	0.32378900	4.78762000	-0.98242600
H	1.93373500	2.96349800	2.56251500
H	1.47242600	4.99185200	1.20756300
C	-1.93725100	-0.34109900	-0.13509000
C	-2.22693000	-0.78908800	1.15932200
C	-2.97863600	-0.03732300	-1.01754900
C	-3.55043800	-0.93910900	1.56335300
H	-1.41446100	-1.02640100	1.84155400
C	-4.30193000	-0.18791900	-0.60661300
H	-2.75468100	0.30576400	-2.02239400
C	-4.58800700	-0.63822500	0.68072100
H	-3.77144000	-1.29151200	2.56627100
H	-5.10887500	0.04390000	-1.29514200
H	-5.62023200	-0.75579000	0.99739500
N	2.96207700	-0.43769100	-0.33940800
C	4.38905100	-0.67288800	-0.22363800
H	4.67151700	-1.08054900	0.75915100
H	4.74364600	-1.38196300	-0.98700700
H	4.92407000	0.26838900	-0.36780000
F	-0.41970300	0.19772100	-2.20041000
C	1.29072500	-3.59392600	0.37179400
H	1.20867000	-4.64956400	0.60263400
C	2.59927700	-2.84983400	0.31280000
H	3.13441300	-2.84528900	1.27430900
H	3.29997200	-3.26467200	-0.42579200

TS11

Sum of electronic and thermal Free Energies = -2025.818419 a.u.

P	0.80934400	0.15577900	-0.96048800
F	1.36361000	0.07246700	-2.47688800
C	0.09468800	1.67488100	-0.72896500
C	0.80354100	2.91726900	-1.06326000
C	-1.24562000	2.00811500	-0.35806500
C	-0.01374800	3.97697000	-0.94892000
H	1.84014200	2.94789200	-1.38663200
H	0.24000500	5.00541500	-1.17414300
C	-0.25855100	-1.27952900	-0.89484800
C	0.01592000	-2.35749300	-0.04931400

C	-1.34551900	-1.32067000	-1.77484200
C	-0.79956500	-3.48524100	-0.09403800
H	0.84320800	-2.30769300	0.65345300
C	-2.15021900	-2.45347900	-1.81664200
H	-1.56212900	-0.46701500	-2.41191900
C	-1.87416000	-3.53487800	-0.98017700
H	-0.60048200	-4.31917500	0.57149000
H	-2.99924500	-2.48733900	-2.49195000
H	-2.51031200	-4.41466300	-1.00774200
C	2.36196400	-0.11582400	-0.09040600
C	3.21903800	-1.14543000	-0.50006100
C	2.71158900	0.71299800	0.97858300
C	4.42154600	-1.34750100	0.16926100
H	2.94720400	-1.77934300	-1.34049000
C	3.92246500	0.51078000	1.63784000
H	2.03405700	1.50531900	1.28652200
C	4.77162900	-0.51884000	1.23696200
H	5.08748100	-2.14573700	-0.14371500
H	4.19832300	1.15462700	2.46706400
H	5.71217300	-0.67725400	1.75647400
N	-2.18245900	1.22733900	0.09756800
C	-3.47989500	1.81986200	0.35574200
H	-3.46496500	2.46459300	1.24811600
H	-3.82509300	2.41736400	-0.49645800
H	-4.20307900	1.01961300	0.52665000
C	-1.83731000	-0.14661200	1.59055900
S	-3.07914800	-1.14770800	1.55378800
S	-0.46329900	0.28002300	2.30484100
C	-1.37595900	3.52552800	-0.50608300
H	-1.68011100	3.94543600	0.46400900
H	-2.16447300	3.79523700	-1.22240600

11p

Sum of electronic and thermal Free Energies = -2025.861257 a.u.

P	-0.65224000	0.09963500	0.50200500
F	-1.25656500	0.01892100	2.08545700
C	0.41887500	1.44283900	0.98090900
C	0.12805800	2.45813800	2.00307400
C	1.70981300	1.58020500	0.57056500
C	1.21423800	3.22498300	2.19305800
H	-0.82664300	2.53314500	2.50909600
H	1.31562700	4.04544000	2.89241900
C	0.02412700	-1.59171500	0.65176900
C	-0.10448800	-2.54302100	-0.36307100

C	0.68742500	-1.92103100	1.83883000
C	0.41762300	-3.82194000	-0.18366000
H	-0.59853600	-2.28564600	-1.29495700
C	1.23858300	-3.19027900	1.99709400
H	0.76626700	-1.18753500	2.63567100
C	1.09808200	-4.14337500	0.98959500
H	0.30595600	-4.56070200	-0.97124700
H	1.76759400	-3.43668200	2.91289200
H	1.52009400	-5.13588800	1.11788700
C	-2.35108500	0.31534400	-0.12302000
C	-3.29484200	-0.66311700	0.20380300
C	-2.72344800	1.42903900	-0.87845000
C	-4.60435800	-0.53834300	-0.25204200
H	-3.00633500	-1.51381800	0.81536500
C	-4.04357300	1.56130600	-1.30560800
H	-1.98952500	2.18884300	-1.13216000
C	-4.98031100	0.57517800	-1.00276500
H	-5.33317000	-1.30634800	-0.01127500
H	-4.33512900	2.43339300	-1.88284300
H	-6.00466400	0.67524200	-1.34927600
N	2.40514300	0.86719000	-0.40041500
C	3.86897100	0.86546400	-0.31671100
H	4.29825100	1.63712100	-0.96397100
H	4.16292700	1.02951600	0.71824000
H	4.23903100	-0.10284200	-0.65098300
C	1.82230400	0.34803100	-1.54394400
S	2.72948300	-0.19027300	-2.82514600
S	0.07765100	0.35216000	-1.67922900
C	2.33523500	2.73499400	1.32183300
H	2.69638000	3.49100500	0.61081300
H	3.19703600	2.43422300	1.93051800

12

Sum of electronic and thermal Free Energies = -1442.811546 a.u.

P	0.32815200	-0.03656300	0.63849800
C	-0.89980800	-1.09160400	0.19867300
C	-0.69617800	-2.50707500	-0.10327200
C	-2.31654400	-0.68411200	0.20566900
H	0.31225100	-2.91921800	-0.05789700
C	0.14656900	1.65680100	0.04675000
C	0.67411200	2.72655300	0.77305900
C	-0.45530900	1.87777700	-1.19534300
C	0.59473700	4.01848000	0.25586900
H	1.13223200	2.55365700	1.74183700

C	-0.53174000	3.16905800	-1.70635200
H	-0.88171600	1.04039300	-1.74154800
C	-0.00608200	4.23962100	-0.98146900
H	0.99952200	4.85131800	0.82291700
H	-1.00788700	3.34205800	-2.66674800
H	-0.06855600	5.24750500	-1.38140500
C	1.95357500	-0.67078100	0.16814100
C	2.16221500	-1.08850300	-1.15197400
C	3.00580500	-0.70924200	1.08746700
C	3.41537400	-1.54725600	-1.54584900
H	1.34073200	-1.06210400	-1.86391800
C	4.25910400	-1.17039200	0.68676600
H	2.84405400	-0.38742600	2.11109000
C	4.46405400	-1.58844800	-0.62624600
H	3.57287800	-1.87443200	-2.56901200
H	5.07393100	-1.20435200	1.40355300
H	5.44137800	-1.94768100	-0.93489600
N	-2.70025400	0.46390900	0.61631600
C	-4.10606700	0.79185200	0.56176900
H	-4.73644500	-0.01334900	0.15056000
H	-4.46234300	1.03520000	1.56891100
H	-4.24451900	1.68786900	-0.05430500
F	0.59271400	0.25491100	2.21314400
C	-1.76246700	-3.27164600	-0.44739000
H	-1.63523800	-4.31972200	-0.69497700
Si	-3.29580700	-2.23312900	-0.41475000
H	-3.94813300	-2.00800900	-1.73197000
H	-4.35387900	-2.65751900	0.53671700

TS12

Sum of electronic and thermal Free Energies = -2277.187202 a.u.

P	-0.80443500	-0.22331700	-0.91544400
F	-1.34477200	-0.34731500	-2.43416700
C	0.18110900	-1.57600600	-0.60215500
C	-0.36743300	-2.89360700	-0.95673400
C	1.55832900	-1.60335200	-0.18664400
C	0.41840600	-3.99441200	-0.88890400
H	-1.40483400	-2.95313200	-1.29243000
H	0.04612000	-4.96808200	-1.18488800
C	-0.02224900	1.38706900	-0.95755800
C	-0.52240500	2.46475900	-0.22232300
C	1.06272600	1.55700400	-1.82480000
C	0.06429200	3.71939500	-0.36405900
H	-1.34528200	2.32110000	0.47258900

C	1.63848400	2.81484500	-1.96370500
H	1.45416200	0.70777600	-2.37934400
C	1.13643600	3.89440000	-1.23720800
H	-0.31029700	4.55637200	0.21660800
H	2.48430200	2.95037900	-2.63026800
H	1.59344600	4.87407100	-1.34105300
C	-2.39758700	-0.17689500	-0.07513500
C	-3.41181600	0.66230100	-0.55425900
C	-2.62404100	-0.99929800	1.03122700
C	-4.64693400	0.68479800	0.08524600
H	-3.23565700	1.28881400	-1.42524100
C	-3.86680700	-0.97877300	1.66089300
H	-1.82716300	-1.64514800	1.39130700
C	-4.87244100	-0.13538100	1.19220900
H	-5.43432800	1.33603400	-0.28149800
H	-4.04621600	-1.61813200	2.51954400
H	-5.83821000	-0.11752100	1.68873000
N	2.26167200	-0.63631400	0.31191600
C	3.65567300	-0.87689500	0.63489000
H	3.76293900	-1.14605600	1.69429900
H	4.08627500	-1.67330900	0.01639000
H	4.22704500	0.03912000	0.46329300
C	1.60885700	0.78830800	1.64080300
S	2.63520600	2.00406600	1.52917500
S	0.32664200	0.15338600	2.36860900
Si	2.10068900	-3.45547600	-0.35265000
H	2.57787200	-3.93627200	0.96755000
H	3.19277700	-3.65836300	-1.33800300

12p

Sum of electronic and thermal Free Energies = -2277.230015 a.u.

P	-0.71643100	-0.13971200	-0.42853200
F	-1.21103900	-0.39092800	-2.03589300
C	0.50139900	-1.45037300	-0.60693800
C	0.20812900	-2.67475200	-1.39540900
C	1.78320000	-1.31686500	-0.17071000
C	1.20261000	-3.56719700	-1.56915100
H	-0.79128100	-2.79561400	-1.80663700
H	1.06436900	-4.47079100	-2.15170400
C	-0.16007800	1.54911300	-0.85418000
C	-0.43206400	2.65293000	-0.04251900
C	0.56699400	1.71335600	-2.03816300
C	0.00958100	3.91791100	-0.42356800
H	-0.97349600	2.52668900	0.89009100

C	1.03814200	2.97478400	-2.39358700
H	0.75921600	0.85782200	-2.67864900
C	0.75373100	4.07857400	-1.59091800
H	-0.21302700	4.77401700	0.20570600
H	1.61806800	3.09530300	-3.30373200
H	1.11393400	5.06334300	-1.87389100
C	-2.43092100	-0.41359900	0.12707500
C	-3.43772400	0.37368800	-0.44007600
C	-2.74934500	-1.39171400	1.07164200
C	-4.75874100	0.19988600	-0.03648700
H	-3.18772300	1.11419000	-1.19494000
C	-4.07821800	-1.58037900	1.44722500
H	-1.96710900	-2.00419800	1.51177400
C	-5.08019000	-0.77942500	0.90306700
H	-5.53823400	0.82297100	-0.46440100
H	-4.32631400	-2.34935200	2.17236300
H	-6.11272900	-0.91969600	1.20885300
N	2.30882700	-0.31035200	0.63369100
C	3.76298100	-0.11881800	0.58004700
H	4.24557300	-0.58192900	1.44648200
H	4.13528500	-0.55203400	-0.34786600
H	3.98670100	0.94821200	0.59573100
C	1.61899900	0.33682500	1.64480100
S	2.39098000	1.27239500	2.77524600
S	-0.10742200	0.07480200	1.77992000
Si	2.72338800	-2.86858700	-0.76683900
H	3.27168300	-3.60495000	0.39452400
H	3.82383900	-2.55608600	-1.70834100

13

Sum of electronic and thermal Free Energies = -1177.590875 a.u.

P	0.04691700	-0.26497700	-0.55029100
C	0.44026700	-2.01604000	-0.76158000
C	0.46048600	-2.32260100	0.69143100
C	0.76536200	-3.64217000	0.97076200
H	0.84102900	-4.06491400	1.96549900
C	1.32394300	0.96387400	-0.15271400
C	2.50820700	0.99062000	-0.89230700
C	1.13548000	1.86181400	0.90088800
C	3.50926400	1.90218300	-0.56337100
H	2.64242300	0.30265200	-1.72247900
C	2.13123000	2.78453900	1.21404100
H	0.20438800	1.85560100	1.46373300
C	3.32116300	2.79944900	0.48714900

H	4.43325300	1.91654500	-1.13352700
H	1.97715900	3.49119600	2.02409500
H	4.09967600	3.51448000	0.73622200
C	-1.63469800	0.38753600	-0.30164100
C	-2.56687000	-0.27768200	0.49823200
C	-1.98837200	1.58447300	-0.93533900
C	-3.84620700	0.25135100	0.66323200
H	-2.29738700	-1.21289200	0.98111700
C	-3.25870600	2.12171000	-0.74775600
H	-1.26920800	2.08935000	-1.57381200
C	-4.18923800	1.45392000	0.04876500
H	-4.57257400	-0.27708200	1.27325200
H	-3.52550600	3.05652400	-1.23147300
H	-5.18348200	1.86909900	0.18574800
N	0.14825300	-1.12161100	1.18036500
C	0.06195600	-0.76419500	2.57564000
H	-0.07710100	-1.66573300	3.18091300
H	0.97608100	-0.25426900	2.90416400
H	-0.78881900	-0.09319000	2.73990300
F	0.06899400	0.11973000	-2.17417700
H	0.76222600	-3.08771500	-2.60365900
B	0.96228600	-4.26085900	-0.40197500
H	1.24769100	-5.38665800	-0.68184000
C	0.71944400	-3.07883900	-1.51852800

TS13

Sum of electronic and thermal Free Energies = -2011.955896 a.u.

P	0.76802400	0.16753700	-0.93758600
F	1.25017000	0.11675600	-2.46651300
C	0.08894700	1.76190300	-0.71517700
C	-1.32398800	2.18963100	-0.32637600
C	-0.29680100	-1.26700700	-0.86709600
C	-0.00684600	-2.35171500	-0.03428200
C	-1.40086500	-1.29820200	-1.72723500
C	-0.82253500	-3.47851900	-0.07511800
H	0.82894700	-2.30616300	0.65847500
C	-2.20510800	-2.43200700	-1.76426600
H	-1.63345700	-0.44106700	-2.35345400
C	-1.91315400	-3.52017800	-0.94260900
H	-0.61255900	-4.31754200	0.58038900
H	-3.06595800	-2.45977800	-2.42444600
H	-2.54933400	-4.39992400	-0.96658500
C	2.32875900	-0.08892800	-0.09138800
C	3.13134200	-1.16568500	-0.49182500

C	2.76253900	0.78979000	0.90518500
C	4.36449200	-1.36735300	0.11892400
H	2.79662700	-1.83630300	-1.27959900
C	4.00078600	0.58216900	1.50741000
H	2.13321200	1.62302700	1.20530900
C	4.79621900	-0.49445000	1.11846100
H	4.98910500	-2.20045800	-0.18746300
H	4.34124100	1.26140200	2.28233900
H	5.75959400	-0.65348800	1.59374000
N	-2.18187300	1.31390100	0.10966600
C	-3.54823600	1.75454000	0.29280900
H	-3.65425900	2.34623200	1.21296100
H	-3.87913800	2.36313400	-0.55548900
H	-4.19339300	0.87599800	0.37520900
C	-1.74209600	-0.07940300	1.62243600
S	-2.96595000	-1.09104300	1.64279900
S	-0.34603500	0.39439300	2.26304800
C	-1.45090400	3.59060300	-0.56019400
H	-2.37737500	4.09439900	-0.30940100
C	0.79801800	2.83497000	-1.13956100
H	1.81177100	2.74556000	-1.53200000
B	-0.15407400	4.13559100	-1.00887900
H	0.20490500	5.25130500	-1.23500000

13p

Sum of electronic and thermal Free Energies = -2012.007870 a.u.

P	0.67552800	0.11487800	-0.57076100
F	1.22086700	-0.01008500	-2.15180100
C	-0.15747900	1.67209300	-0.90589300
C	-1.53359800	2.03364100	-0.34764500
C	-0.29314000	-1.41896100	-0.71914700
C	-0.28908200	-2.40725100	0.26781300
C	-1.06145300	-1.58228300	-1.87728400
C	-1.04187400	-3.56470600	0.08584400
H	0.28146000	-2.26507000	1.18091600
C	-1.84134400	-2.72533300	-2.03342200
H	-1.04416400	-0.82213800	-2.65303400
C	-1.82534700	-3.71965800	-1.05626600
H	-1.03226800	-4.33416000	0.85137200
H	-2.45146000	-2.84270300	-2.92388800
H	-2.42739800	-4.61459400	-1.18332500
C	2.38351200	0.04114200	0.05046000
C	3.16413500	-1.06011300	-0.31262400
C	2.92060500	1.05922800	0.84073100

C	4.47613300	-1.15417800	0.14413000
H	2.74887400	-1.83607300	-0.95011400
C	4.24303400	0.97055700	1.27010900
H	2.31274100	1.91676500	1.11741700
C	5.01673000	-0.13823700	0.93147400
H	5.07844100	-2.01677700	-0.12412600
H	4.66456400	1.76691500	1.87569600
H	6.04315000	-0.20953000	1.27880800
N	-2.28843900	1.13248100	0.40100600
C	-3.74433000	1.19699500	0.25325900
H	-4.18846800	1.79794900	1.05331500
H	-3.96925100	1.63097000	-0.71983100
H	-4.14508700	0.18541100	0.31859800
C	-1.75640700	0.37122000	1.42320800
S	-2.69064300	-0.53922400	2.43284900
S	-0.01111200	0.46050000	1.65792800
C	-1.93820800	3.24772200	-0.79803400
H	-2.89365900	3.68444300	-0.53267500
C	0.33710600	2.67455100	-1.64626900
H	1.28746300	2.60623600	-2.16526500
B	-0.76310400	3.83284700	-1.61332000
H	-0.67695500	4.90936600	-2.11178200

14

Sum of electronic and thermal Free Energies = -1395.164383 a.u.

P	0.04821600	-0.06454700	-0.47527500
C	1.78650300	-0.59851200	-0.67677200
C	2.01720600	-0.72922100	0.79774000
C	3.23950700	-1.07172300	1.30036000
H	3.41811000	-1.14661200	2.36818500
C	-0.35264900	1.67690400	-0.13535800
C	0.26838200	2.68425100	-0.87757200
C	-1.25029100	2.01326800	0.88117400
C	0.00729800	4.02197700	-0.58831400
H	0.94833000	2.41895200	-1.68241200
C	-1.52420800	3.35184500	1.15455600
H	-1.75360000	1.23171300	1.44601100
C	-0.88931100	4.35670300	0.42562700
H	0.49762700	4.80299800	-1.16182500
H	-2.23369000	3.60895300	1.93555300
H	-1.09842200	5.39991000	0.64362200
C	-1.40790900	-1.14811800	-0.29793000
C	-1.38076200	-2.27274300	0.53043600
C	-2.57527900	-0.83459500	-1.00452100

C	-2.51146400	-3.08020100	0.64916300
H	-0.47250400	-2.51980200	1.07309300
C	-3.70975800	-1.62845900	-0.86363500
H	-2.58910900	0.02857300	-1.66330800
C	-3.67765000	-2.75419200	-0.03982300
H	-2.47969900	-3.96163200	1.28266200
H	-4.61642500	-1.37398100	-1.40440400
H	-4.56076500	-3.37851500	0.06098700
N	0.76010100	-0.42276900	1.21484300
C	0.35712700	-0.29092200	2.59077600
H	0.94382400	-0.97539700	3.21437500
H	0.50647000	0.73339200	2.95906000
H	-0.70190000	-0.54935400	2.69898400
F	-0.21175600	0.13867400	-2.12664600
H	2.54089700	-0.70819200	-2.64944000
C	2.73685300	-0.81705600	-1.58614900
Al	4.22984600	-1.27367900	-0.32539800
H	5.72316000	-1.64887600	-0.68447800

TS14

Sum of electronic and thermal Free Energies = -2229.506799 a.u.

P	0.69776700	0.10201900	-0.84911100
F	0.99408400	0.13356300	-2.42117400
C	0.03694700	1.73250700	-0.49544700
C	-1.46564700	1.93925600	-0.40431000
C	-0.12059800	-1.49003900	-0.70128000
C	0.30751800	-2.40163000	0.26730000
C	-1.12467700	-1.83451100	-1.61402900
C	-0.27786000	-3.66438900	0.32416900
H	1.07608300	-2.12632900	0.98430000
C	-1.68424800	-3.10499300	-1.56292600
H	-1.47392000	-1.10651200	-2.33878400
C	-1.26456400	-4.01695700	-0.59307300
H	0.03709100	-4.36751300	1.08847700
H	-2.46389200	-3.37671300	-2.26747500
H	-1.71823500	-5.00253100	-0.54626500
C	2.34313900	-0.06412100	-0.14248200
C	3.26593300	-0.87351900	-0.81710000
C	2.68519600	0.53843600	1.07249600
C	4.53471600	-1.06736400	-0.28011200
H	2.99393600	-1.34507300	-1.75773100
C	3.95591300	0.33348200	1.60532400
H	1.96302300	1.15868900	1.59501000
C	4.87777400	-0.46529200	0.93079100

H	5.25361100	-1.68806200	-0.80552900
H	4.22338400	0.79968100	2.54827000
H	5.86764400	-0.62016100	1.34969000
N	-2.14302100	0.78657400	-0.41336100
C	-3.57212000	0.90879500	-0.59038900
H	-4.06732100	1.40960500	0.25692200
H	-3.79486200	1.48401300	-1.49969800
H	-4.00873100	-0.08854400	-0.69242800
C	-1.92076200	-0.26523600	1.49337700
S	-3.01296600	-1.41399900	1.43404600
S	-0.74757700	0.47108300	2.30874200
C	-1.89646600	3.25901600	-0.37673600
H	-2.96246600	3.44602900	-0.30571000
C	0.89145700	2.77292000	-0.52392500
H	1.96111700	2.62022900	-0.65487600
Al	-0.35508300	4.33663900	-0.36174700
H	0.05629600	5.85697600	-0.26519800

14p

Sum of electronic and thermal Free Energies = -2229.573271 a.u.

P	0.66824600	0.03697600	-0.49019400
F	1.16331800	0.09482600	-2.09893000
C	-0.13002500	1.66408200	-0.61346400
C	-1.52905000	1.86800600	-0.05173200
H	-0.64677300	5.72512000	-1.35456600
C	-0.28037400	-1.48797600	-0.80467900
C	-0.23081500	-2.58695700	0.05513000
C	-1.07626500	-1.53035500	-1.95500700
C	-0.96483700	-3.73218000	-0.24649800
H	0.36027300	-2.54199700	0.96516500
C	-1.83718800	-2.66353900	-2.22856200
H	-1.09569000	-0.68242500	-2.63358500
C	-1.77541600	-3.76779400	-1.37882500
H	-0.91976400	-4.58653500	0.42153000
H	-2.46881300	-2.68731100	-3.11156700
H	-2.36313500	-4.65445200	-1.59780700
C	2.39874100	-0.09404900	0.05664900
C	3.18256600	-1.11700300	-0.48486000
C	2.94939300	0.80662300	0.97078300
C	4.51028300	-1.25299200	-0.08730800
H	2.75644600	-1.79947600	-1.21515300
C	4.28607600	0.68086400	1.34251800
H	2.33938500	1.60382600	1.38796500
C	5.06342400	-0.35269000	0.82230100

H	5.11452000	-2.05697400	-0.49650200
H	4.71651800	1.38785700	2.04511200
H	6.10167200	-0.45491300	1.12386600
N	-2.22065000	0.74523300	0.48299600
C	-3.64425100	0.63122300	0.16645200
H	-4.26344800	1.07653000	0.95262400
H	-3.82132800	1.13203100	-0.78512000
H	-3.89857300	-0.42711700	0.09128600
C	-1.70768000	-0.02662600	1.49361600
S	-2.63462400	-1.04328700	2.41065600
S	0.02952200	0.10401100	1.76938600
C	-2.10110300	3.08327600	-0.19399200
H	-3.10605700	3.24031000	0.18519200
H	1.51289100	2.54740000	-1.58431100
Al	-0.72816300	4.19942700	-0.97910100
C	0.53329400	2.70963400	-1.14322000

15

Sum of electronic and thermal Free Energies = -1227.344256 a.u.

P	-0.00432500	-0.25683400	-0.46569000
C	-1.07319100	-1.66609500	-0.81339700
C	-1.36480600	-1.88171900	0.56637500
C	-2.32480400	-2.83917600	0.62995900
H	-2.88760300	-3.34104600	1.39864100
C	1.80051600	-0.28220400	-0.13622600
C	2.68645200	0.31429300	-1.04739300
C	2.31789100	-0.85853400	1.03044700
C	4.05272100	0.35120500	-0.78150600
H	2.30705500	0.73848800	-1.96915700
C	3.68791400	-0.83047300	1.28543700
H	1.64472500	-1.34509700	1.72606400
C	4.55754000	-0.22002100	0.38536500
H	4.72414900	0.82043700	-1.49459800
H	4.07316300	-1.29076900	2.19045200
H	5.62458500	-0.19573200	0.58751800
C	-0.80171200	1.35697100	-0.17532600
C	-2.14112800	1.40944600	0.21886000
C	-0.08221400	2.53973300	-0.35342800
C	-2.75741400	2.64051000	0.42847300
H	-2.70348300	0.48761900	0.35389100
C	-0.69597200	3.76991500	-0.12251400
H	0.95728100	2.50273800	-0.66842900
C	-2.03366300	3.82159500	0.26445500
H	-3.80206600	2.67701600	0.72313800

H	-0.12927000	4.68732900	-0.25128600
H	-2.51307000	4.78086200	0.43625000
N	-0.51265000	-0.97942800	1.18484100
C	-0.74201400	-0.38641800	2.47875500
H	-0.55407500	-1.11165900	3.28188900
H	-0.04901000	0.45114500	2.61137100
H	-1.76489600	0.00346000	2.59497300
F	0.24927300	0.11644100	-2.09168100
H	-1.99821500	-2.71306300	-2.57862800
C	-1.85570300	-2.51037700	-1.52801700
O	-2.61272100	-3.23288700	-0.67592600

TS15

Sum of electronic and thermal Free Energies = -2061.718566 a.u.

P	0.84031000	0.08908600	-1.00122600
F	1.32831200	-0.06871500	-2.51984300
C	0.15861100	1.65792200	-0.80480300
C	-1.24315700	2.03979800	-0.55866200
C	-0.23083200	-1.32368900	-0.80580200
C	0.08748100	-2.32854600	0.11323300
C	-1.34258600	-1.44166800	-1.64837800
C	-0.70638700	-3.47045000	0.17533500
H	0.93515700	-2.21575300	0.78365800
C	-2.11680800	-2.59417300	-1.58777200
H	-1.61485300	-0.62853700	-2.31327700
C	-1.79715100	-3.60544800	-0.68166700
H	-0.47517000	-4.24836200	0.89578100
H	-2.98488100	-2.69097300	-2.23168100
H	-2.41499200	-4.49721600	-0.62981200
C	2.38498800	-0.12102900	-0.11334500
C	3.29183300	-1.08844100	-0.56807000
C	2.66891400	0.63866400	1.02596400
C	4.48467400	-1.28824300	0.11830100
H	3.06660600	-1.67460600	-1.45511800
C	3.86745600	0.43164200	1.70572300
H	1.95583700	1.37891200	1.37703100
C	4.77070500	-0.52845100	1.25387200
H	5.19114200	-2.03367300	-0.23295000
H	4.09146000	1.01988600	2.58984300
H	5.70290000	-0.68692300	1.78790100
N	-2.25174100	1.18437500	-0.44241600
C	-3.50378800	1.85201700	-0.17153400
H	-3.46455600	2.47960300	0.74091400
H	-3.80810300	2.51115900	-1.00388200

H	-4.29514300	1.10887500	-0.03349700
C	-1.99155600	-0.07605700	1.64209600
S	-3.23231700	-1.03037800	1.50247200
S	-0.69842100	0.59349500	2.26637400
C	-1.16542100	3.42893300	-0.45326300
H	-1.89876900	4.20404600	-0.31235900
C	0.90423100	2.82094500	-0.85010800
H	1.95688900	3.01037500	-1.01068300
O	0.12797300	3.86530900	-0.65077800

15p

Sum of electronic and thermal Free Energies = -2061.794985 a.u.

P	0.66154700	0.07663500	-0.52155000
F	1.31103300	-0.04067900	-2.08608700
C	-0.41324400	1.38895400	-1.07649900
C	-1.72327100	1.69159800	-0.55784200
C	-0.03948000	-1.60501100	-0.63374800
C	-0.03355400	-2.49633300	0.44285600
C	-0.60448000	-1.98872300	-1.85590400
C	-0.57828100	-3.76917600	0.29032800
H	0.37921700	-2.19508900	1.40033200
C	-1.17777800	-3.25061500	-1.98994200
H	-0.59171000	-1.30337000	-2.69746000
C	-1.15864800	-4.14392200	-0.91998800
H	-0.56370600	-4.45988200	1.12761300
H	-1.63068100	-3.53748600	-2.93420700
H	-1.59897300	-5.13082600	-1.02849300
C	2.35282400	0.29806800	0.12695000
C	3.27906000	-0.71991200	-0.11817100
C	2.73262300	1.44590400	0.82477900
C	4.57993800	-0.59789000	0.36234600
H	2.98443000	-1.59963200	-0.68416200
C	4.04509600	1.57282600	1.27650700
H	2.01081500	2.23482700	1.01647700
C	4.96458500	0.54948400	1.05552600
H	5.29530300	-1.39547100	0.18619800
H	4.34357500	2.47016900	1.80981200
H	5.98238700	0.64634900	1.42158100
N	-2.43481300	0.97494900	0.41442500
C	-3.89442300	1.02662100	0.32987500
H	-4.29317500	1.81110900	0.98240300
H	-4.17000500	1.21607000	-0.70795900
H	-4.30419100	0.07131500	0.65679600
C	-1.84569100	0.41544100	1.51722000

S	-2.72184900	-0.21846300	2.77364800
S	-0.08480700	0.45028100	1.63349000
C	-2.17453300	2.75092600	-1.28641700
H	-3.09181500	3.31769200	-1.28691300
C	-0.19017000	2.28780000	-2.07518000
H	0.64362100	2.43665300	-2.74385300
O	-1.23635400	3.12052400	-2.20143600

16

Sum of electronic and thermal Free Energies = -1207.485256 a.u.

P	-0.00552800	-0.33724900	-0.47133000
C	-1.19657600	-1.65345200	-0.65915700
C	-1.45995900	-1.71769300	0.72820200
C	-2.54871800	-2.52994600	0.92657200
H	-3.10286000	-2.84517900	1.79687400
C	1.80630900	-0.40738800	-0.20927100
C	2.66354400	0.18029400	-1.15175400
C	2.35273500	-0.99032500	0.93996400
C	4.03913500	0.19479800	-0.93702700
H	2.25027900	0.62370000	-2.05009600
C	3.73283500	-0.98913000	1.14063700
H	1.68658600	-1.44806700	1.66269300
C	4.57734800	-0.39266500	0.20758600
H	4.69171500	0.65986300	-1.67017300
H	4.14549300	-1.45537600	2.03059800
H	5.65178600	-0.38731200	0.36873900
C	-0.68063300	1.33558300	-0.24530800
C	-2.02405800	1.57815700	-0.54499300
C	0.10874600	2.35914700	0.28377000
C	-2.57192600	2.83856100	-0.31586100
H	-2.63851600	0.78068600	-0.95575500
C	-0.44320400	3.62027000	0.50726800
H	1.15381900	2.17567400	0.52255800
C	-1.78305600	3.86133700	0.20998300
H	-3.61637700	3.02223300	-0.55080100
H	0.17634300	4.41363000	0.91539000
H	-2.21147300	4.84376500	0.38588700
N	-0.47126500	-0.90119000	1.28294000
C	-0.75275900	-0.07767400	2.43879100
H	-0.97125100	-0.71430400	3.30521000
H	0.13213500	0.52143200	2.67949100
H	-1.60156400	0.61047000	2.28861100
F	0.18966100	-0.10968800	-2.13813800
H	-2.26146200	-2.66874200	-2.36725100

C	-2.10945000	-2.44185000	-1.32224100
N	-2.91490500	-2.96723400	-0.35407100
H	-3.66736000	-3.61571600	-0.53384100

TS16

Sum of electronic and thermal Free Energies = -2041.862299 a.u.

P	0.85418100	0.10405600	-0.98770700
F	1.33193900	-0.08602300	-2.51294000
C	0.16994400	1.65124800	-0.76465800
C	-1.24368300	2.00698500	-0.59527300
C	-0.18023500	-1.33756300	-0.76480900
C	0.13896400	-2.28228700	0.21448500
C	-1.25567500	-1.54146600	-1.63687000
C	-0.61901700	-3.44653600	0.31355100
H	0.96223900	-2.10779700	0.90208100
C	-1.99257400	-2.71551200	-1.54078600
H	-1.52957100	-0.77502300	-2.35446200
C	-1.67359500	-3.66562500	-0.56997500
H	-0.38624200	-4.17667800	1.08201500
H	-2.83262000	-2.87743500	-2.20860600
H	-2.26336800	-4.57424800	-0.49046700
C	2.41722800	-0.09102200	-0.12165200
C	3.38296600	-0.96335400	-0.64012600
C	2.64081300	0.57541600	1.08772700
C	4.57506400	-1.15904600	0.05015900
H	3.20255400	-1.47939700	-1.57892500
C	3.83768700	0.37270800	1.77215500
H	1.87932500	1.23950100	1.48696900
C	4.80117900	-0.49128600	1.25461900
H	5.32729100	-1.83076800	-0.35152200
H	4.01358500	0.88784900	2.71128200
H	5.73214400	-0.64714700	1.79175300
N	-2.24214200	1.13190800	-0.54521800
C	-3.52864100	1.76414400	-0.36804500
H	-3.58007600	2.38609700	0.54758000
H	-3.78417800	2.41863600	-1.21981200
H	-4.30645200	0.99837600	-0.29462300
C	-2.10051600	-0.04883000	1.55393000
S	-3.31270000	-1.04134800	1.38357400
S	-0.86889700	0.65405600	2.26464800
C	-1.22768600	3.40859600	-0.45141700
H	-2.03495500	4.10962300	-0.31520500
C	0.93634200	2.83180900	-0.73335700
H	2.00163200	2.98563400	-0.83129900

H	0.35889600	4.81377500	-0.50023100
N	0.08125500	3.84363300	-0.55106200

16p

Sum of electronic and thermal Free Energies = -2041.937298 a.u.

P	0.65011800	0.08850700	-0.52298000
F	1.30969800	-0.01740300	-2.08890100
C	-0.43105000	1.39427600	-1.06202800
C	-1.73497900	1.67198300	-0.54243100
C	-0.01730900	-1.60669500	-0.65026400
C	0.04859500	-2.52406800	0.40153500
C	-0.61885600	-1.97259700	-1.85971100
C	-0.47266900	-3.80533800	0.23640800
H	0.48956400	-2.23644100	1.35075000
C	-1.16815400	-3.24386000	-2.00604100
H	-0.65309600	-1.26418700	-2.68172600
C	-1.08905200	-4.16326500	-0.96121100
H	-0.41183700	-4.51644600	1.05438700
H	-1.64964200	-3.51761000	-2.94013300
H	-1.51082900	-5.15724200	-1.07895700
C	2.34020500	0.32072800	0.12817100
C	3.27896500	-0.68517000	-0.11833400
C	2.70684500	1.47001400	0.83070500
C	4.57809000	-0.55003500	0.36404100
H	2.99495500	-1.56629200	-0.68760700
C	4.01706600	1.61081700	1.28485900
H	1.97414600	2.24827300	1.02504700
C	4.94899200	0.59912900	1.06164300
H	5.30268100	-1.33899900	0.18628000
H	4.30424100	2.50917200	1.82286300
H	5.96506300	0.70626000	1.42985100
N	-2.43733500	0.93730000	0.43053900
C	-3.89638400	0.95996500	0.33845800
H	-4.31495400	1.74784500	0.97499100
H	-4.17049000	1.12542500	-0.70386100
H	-4.29010300	0.00351300	0.68122300
C	-1.84871700	0.38521000	1.53376600
S	-2.72369700	-0.23842600	2.80144500
S	-0.08984200	0.40829500	1.64391700
C	-2.23355900	2.74286800	-1.25126200
H	-3.17986000	3.25733700	-1.18460100
C	-0.19031400	2.30427800	-2.07242500
H	0.67314800	2.41102900	-2.71147800
H	-1.36758400	3.88475900	-2.81124600

N	-1.27468200	3.11488400	-2.16511500

17

Sum of electronic and thermal Free Energies = -1191.418646 a.u.

P	-0.02763500	-0.19558300	-0.46796200
C	-0.96423100	-1.70542200	-0.86585500
C	-1.23599500	-2.00503100	0.53110800
C	-2.04427300	-3.08275900	0.64102900
H	-2.44218300	-3.55892600	1.52744500
C	1.77479100	-0.15050100	-0.12360500
C	2.63400600	0.57085500	-0.96608900
C	2.31635400	-0.81942700	0.97986200
C	3.99608600	0.64616300	-0.68773000
H	2.23929200	1.05675800	-1.85037700
C	3.68321500	-0.75589600	1.24573400
H	1.66954100	-1.40806600	1.61971400
C	4.52455200	-0.01525500	0.41961500
H	4.64672700	1.21406600	-1.34623500
H	4.08804200	-1.29021300	2.10010900
H	5.58874900	0.03819500	0.63074000
C	-0.90285800	1.37837300	-0.14923900
C	-2.15217100	1.37033400	0.47607000
C	-0.33625800	2.59242200	-0.54631200
C	-2.82865600	2.56770300	0.70170900
H	-2.60122400	0.42681200	0.77621000
C	-1.00034300	3.79013400	-0.29304800
H	0.62477900	2.60298600	-1.05165200
C	-2.24897700	3.77872200	0.32755500
H	-3.80644400	2.55321800	1.17407000
H	-0.54655900	4.73136000	-0.58890800
H	-2.77092200	4.71253300	0.51540200
N	-0.53222100	-0.98532300	1.13028400
C	-0.61146300	-0.57889000	2.50688500
H	-1.65239200	-0.42452000	2.82750800
H	-0.15587600	-1.32350400	3.17536300
H	-0.07473000	0.36690300	2.63393300
F	0.22432300	0.24400300	-2.07949700
H	-1.57976800	-2.60899200	-2.76021200
C	-1.57400400	-2.57662500	-1.67694000
C	-2.32030200	-3.55783400	-0.78173900
H	-3.39187400	-3.55083600	-1.03098900
H	-1.97083600	-4.58518500	-0.96326400

TS17

Sum of electronic and thermal Free Energies = -2025.779403 a.u.

P	0.80112000	0.11950800	-0.94575700
F	1.17100500	0.02764500	-2.49501000
C	0.13797100	1.72520900	-0.68224300
C	-1.31136700	2.05800600	-0.59467500
C	-0.16648500	-1.36273700	-0.70429400
C	0.20152200	-2.27082900	0.29391600
C	-1.22196000	-1.64438700	-1.58135900
C	-0.48983000	-3.47379900	0.41073500
H	1.01034900	-2.04008300	0.98176200
C	-1.88538100	-2.86012900	-1.46999700
H	-1.53561900	-0.90543200	-2.31033900
C	-1.52135100	-3.77079900	-0.47720200
H	-0.22143600	-4.17424900	1.19489600
H	-2.70637400	-3.08503600	-2.14314800
H	-2.05640700	-4.71156200	-0.38595200
C	2.39263000	-0.06213200	-0.13899400
C	3.35085000	-0.88975900	-0.73828500
C	2.65274000	0.55382800	1.09016900
C	4.57619600	-1.08777400	-0.11043400
H	3.14058300	-1.36927600	-1.69037600
C	3.88101100	0.34334300	1.71326500
H	1.89976000	1.18375700	1.55503200
C	4.83936500	-0.47226300	1.11401100
H	5.32435200	-1.72168300	-0.57571200
H	4.08644300	0.81805100	2.66742300
H	5.79592400	-0.63061100	1.60306500
N	-2.20456300	1.06897300	-0.64698500
C	-3.56451700	1.54751000	-0.58159300
H	-3.76054900	2.15092300	0.32598900
H	-3.81537800	2.18291400	-1.44881600
H	-4.25651000	0.69908400	-0.57656000
C	-2.08184900	-0.04536000	1.55020100
S	-3.22384900	-1.10918700	1.35791000
S	-0.92543700	0.76652600	2.27147400
C	-1.36348300	3.42925300	-0.43641200
H	-2.26442100	4.02196000	-0.35118700
C	0.91495300	2.82783500	-0.60153500
H	1.99910400	2.87293700	-0.64211200
C	0.01604100	4.01858500	-0.44254000
H	0.20428400	4.72938900	-1.26401900
H	0.27825100	4.55563900	0.48383800

17p

Sum of electronic and thermal Free Energies = -2025.860398 a.u.

P	0.67540100	0.08998600	-0.52632900
F	1.26756400	0.01315800	-2.10908600
C	-0.25286800	1.57672700	-0.91540900
C	-1.57934200	1.89573000	-0.34417700
C	-0.22365500	-1.48438700	-0.73705700
C	-0.28757600	-2.45857800	0.26272200
C	-0.87739600	-1.69059900	-1.95808900
C	-0.99102800	-3.63889600	0.03385400
H	0.19158400	-2.28986000	1.22203300
C	-1.60772500	-2.85767300	-2.16566300
H	-0.81048800	-0.94219500	-2.74155400
C	-1.65879000	-3.83548400	-1.17313500
H	-1.03290400	-4.39419800	0.81232800
H	-2.12828300	-3.00568300	-3.10707700
H	-2.22285500	-4.74873800	-1.33898400
C	2.39037600	0.08837600	0.09305500
C	3.21297700	-0.98414600	-0.26302000
C	2.88754900	1.12841300	0.88068800
C	4.52675100	-1.02683200	0.19597000
H	2.82795200	-1.77779100	-0.89769400
C	4.21248200	1.09234600	1.31136300
H	2.24611500	1.96098200	1.15674900
C	5.02819700	0.01253500	0.97899900
H	5.16118500	-1.86790800	-0.06681800
H	4.60231600	1.90635800	1.91488200
H	6.05601800	-0.01862900	1.32820200
N	-2.31862900	1.01754600	0.47152600
C	-3.77433200	1.05189000	0.33330900
H	-4.22268600	1.69651100	1.09719500
H	-4.01257100	1.42116500	-0.66391900
H	-4.16662300	0.04343500	0.46663300
C	-1.76497900	0.32108200	1.51182000
S	-2.67283200	-0.50454700	2.62524800
S	-0.00591300	0.36625200	1.67820600
C	-1.98717900	3.08710100	-0.82846400
H	-2.92530400	3.58280700	-0.61201700
C	0.13349900	2.58074200	-1.72397400
H	1.05357200	2.61589400	-2.29486100
C	-0.92602400	3.64370900	-1.73152500
H	-1.29051400	3.82013400	-2.75338900
H	-0.54092100	4.60706100	-1.36855200

Sum of electronic and thermal Free Energies = -1442.811342 a.u.

P	0.04775900	-0.04966400	-0.43562500
C	-1.69113700	-0.52931800	-0.75611900
C	-2.04123500	-0.54739600	0.68018900
C	-3.32932900	-0.79523300	1.02961000
H	-3.69908200	-0.82114200	2.04811100
C	1.38792200	-1.26094100	-0.12054600
C	2.48621600	-1.33136800	-0.99039300
C	1.34056000	-2.12505600	0.97886600
C	3.52765500	-2.22080800	-0.74111800
H	2.51546100	-0.70535900	-1.87438900
C	2.37680800	-3.02681300	1.21576800
H	0.48194200	-2.11045900	1.63983100
C	3.47728600	-3.06933000	0.36367800
H	4.37419800	-2.25857900	-1.42030000
H	2.31842800	-3.69822200	2.06723500
H	4.28687100	-3.76847800	0.55220100
C	0.52442700	1.69363600	-0.15372500
C	-0.33164400	2.55672300	0.53518300
C	1.74015200	2.17655600	-0.64716800
C	0.02614400	3.88986100	0.72924200
H	-1.28453700	2.19163800	0.90920900
C	2.10890400	3.50079300	-0.42641600
H	2.39985000	1.51826200	-1.20372700
C	1.25051700	4.36011700	0.25880400
H	-0.65191900	4.55852300	1.25110700
H	3.06224900	3.86413400	-0.79841100
H	1.53411100	5.39591400	0.42107100
N	-0.81478700	-0.24175800	1.19590200
C	-0.53500000	0.05825900	2.57490700
H	-1.17988900	0.86769300	2.94543300
H	-0.69078100	-0.82089300	3.21565900
H	0.50720300	0.37712600	2.67206900
F	0.46034100	0.06592100	-2.06520400
H	-2.47304500	-0.74688200	-2.73927800
C	-2.63658400	-0.76463500	-1.66656400
Si	-4.19439100	-1.06288200	-0.59736900
H	-5.26689100	-0.09005200	-0.93377600
H	-4.75861500	-2.41919100	-0.82417100

TS18

Sum of electronic and thermal Free Energies = -2277.158480 a.u.

P	0.71850600	0.01680000	-0.86945400
F	1.03149800	0.03618400	-2.43538400

C	0.09733800	1.65773800	-0.52484000
C	0.95834000	2.69237200	-0.52476200
C	-1.37776200	1.93255900	-0.41377800
H	2.03281100	2.57935800	-0.64456200
C	-0.17971700	-1.52625000	-0.71506600
C	0.21927200	-2.46215000	0.24360200
C	-1.20985400	-1.81771200	-1.61758400
C	-0.42023800	-3.69807500	0.29922000
H	1.00749000	-2.22590800	0.95305500
C	-1.82312000	-3.06323200	-1.56745300
H	-1.53946200	-1.06658300	-2.32722500
C	-1.43158300	-3.99987300	-0.60949200
H	-0.12809200	-4.41982200	1.05511300
H	-2.62377700	-3.29466900	-2.26262500
H	-1.92735900	-4.96504600	-0.56419100
C	2.34430100	-0.19638200	-0.13670000
C	3.24772300	-1.04702400	-0.78723700
C	2.69042800	0.41475300	1.07310100
C	4.50214900	-1.27403200	-0.23061400
H	2.97202900	-1.52435300	-1.72391900
C	3.94719600	0.17635700	1.62498100
H	1.98348000	1.06674100	1.57748300
C	4.84972900	-0.66367100	0.97508800
H	5.20648800	-1.92678000	-0.73646200
H	4.21836800	0.64873200	2.56372500
H	5.82854000	-0.84453000	1.40923700
N	-2.14620500	0.84034300	-0.45706700
C	-3.56264900	1.11117100	-0.53498800
H	-3.94427500	1.65070800	0.34894900
H	-3.79366300	1.72120400	-1.42148300
H	-4.11075000	0.16809000	-0.61510900
C	-1.95523700	-0.27307800	1.52054700
S	-3.10002900	-1.35839000	1.41795000
S	-0.74951000	0.43391100	2.30079800
Si	-0.12218000	4.25094900	-0.33681100
H	0.27005600	4.99433400	0.89039300
H	0.13567500	5.16302500	-1.48357100
C	-1.66808600	3.28128300	-0.31074600
H	-2.69145000	3.62530500	-0.22336500

18p

Sum of electronic and thermal Free Energies = -2277.230667 a.u.

P	0.68691700	0.02790400	-0.47256600
F	1.19447100	0.16598400	-2.07467800

C	-0.23085500	1.58685400	-0.58263100
C	0.29453500	2.68770700	-1.14990900
C	-1.60235100	1.72658900	0.01678300
H	1.26111100	2.66452100	-1.64269300
C	-0.19050500	-1.52579300	-0.84822400
C	-0.12911300	-2.64161200	-0.01053200
C	-0.94934900	-1.57015200	-2.02367900
C	-0.81299300	-3.80426500	-0.35924100
H	0.43198900	-2.59779600	0.91813600
C	-1.66127900	-2.72264800	-2.34462700
H	-0.97790500	-0.70885400	-2.68449400
C	-1.58685700	-3.84260200	-1.51698700
H	-0.75781300	-4.67128000	0.29147000
H	-2.26449300	-2.74831500	-3.24716400
H	-2.13575000	-4.74405000	-1.77328000
C	2.42240200	-0.01509200	0.07674400
C	3.26197500	-0.98299100	-0.48238700
C	2.92045700	0.89825700	1.00817200
C	4.59416700	-1.05317800	-0.08354600
H	2.87551300	-1.67392900	-1.22662500
C	4.26205200	0.83960300	1.37992200
H	2.26759200	1.65278300	1.43923900
C	5.09553200	-0.14016600	0.84340200
H	5.24240900	-1.81513400	-0.50551800
H	4.65184200	1.55686900	2.09565700
H	6.13736700	-0.19074700	1.14560900
N	-2.25806700	0.60201000	0.57761500
C	-3.69427800	0.47772800	0.32778800
H	-4.27701100	0.90840800	1.14939500
H	-3.92174500	0.98783500	-0.60796300
H	-3.94434500	-0.58120000	0.25204500
C	-1.68482900	-0.18245200	1.54543400
S	-2.54993500	-1.24450700	2.47207200
S	0.05614300	-0.00764900	1.77595500
Si	-0.97025300	4.06533300	-0.97870700
H	-0.51989100	5.20100200	-0.14187800
H	-1.41888400	4.57872400	-2.29387400
C	-2.18171100	2.93674500	-0.12576900
H	-3.17531100	3.13931900	0.25843500

2.closed

Sum of electronic and thermal Free Energies = -1395.164841 a.u.

P	0.07676700	0.03065800	-0.63534500
C	1.80196000	0.11565300	-0.64186200

C	1.97206900	0.08021600	0.77727600
C	3.34532500	0.13411900	1.35519300
H	3.47450300	0.11836800	2.43711100
C	-0.96897400	1.45114500	-0.18480000
C	-0.87989700	2.61721200	-0.94687400
C	-1.85224700	1.39014500	0.89529500
C	-1.66028500	3.72476400	-0.61746400
H	-0.20138600	2.65582400	-1.79472600
C	-2.64429600	2.49062800	1.21155100
H	-1.92457500	0.47674300	1.48196100
C	-2.54325500	3.66147000	0.45878700
H	-1.58274300	4.63394300	-1.20632400
H	-3.33689300	2.43687800	2.04646500
H	-3.15571800	4.52250600	0.71028500
C	-0.82072800	-1.52651100	-0.34660900
C	-0.20241900	-2.61005500	0.28122200
C	-2.13331000	-1.64508100	-0.80876900
C	-0.89725800	-3.80481500	0.45041600
H	0.82329300	-2.51462300	0.62899300
C	-2.83188800	-2.83781500	-0.62525300
H	-2.60800300	-0.80675300	-1.31287800
C	-2.21442100	-3.91728700	0.00331300
H	-0.41165500	-4.64829300	0.93237900
H	-3.85454800	-2.92446600	-0.98026900
H	-2.75679300	-4.84817500	0.14141700
N	0.80598200	-0.00839400	1.36820200
C	0.53799400	-0.10987800	2.78010500
H	1.45534100	-0.22737900	3.36791600
H	0.01131800	0.78426100	3.13651100
H	-0.10465400	-0.97935800	2.97025800
F	-0.26146900	0.11702500	-2.24057100
C	4.35776900	0.20559900	0.46629700
H	5.37646100	0.24853100	0.84863500
Al	3.53404400	0.21620100	-1.35141200
H	4.21650200	0.28999200	-2.76842600

4.closed

Sum of electronic and thermal Free Energies = -1207.483285 a.u.

P	-0.04730600	0.30721500	-0.43892300
C	-1.17710000	1.66056100	-0.60194700
C	-1.40021700	1.79187800	0.74246100
C	-2.35451400	2.82437300	0.93672700
H	-2.78806200	3.20451900	1.85058900
C	-0.71932300	-1.36822500	-0.23236200

C	-2.01998000	-1.64337100	-0.66146000
C	0.03282300	-2.36518700	0.39243700
C	-2.56657000	-2.90906000	-0.46043200
H	-2.60262200	-0.86677100	-1.15031300
C	-0.51592800	-3.63217700	0.58690900
H	1.04600900	-2.15528300	0.72793000
C	-1.81577500	-3.90448000	0.16412500
H	-3.57869900	-3.11832700	-0.79426500
H	0.07374800	-4.40559200	1.07041100
H	-2.24219600	-4.89142600	0.31819800
C	1.76733800	0.34677700	-0.18883100
C	2.33202200	0.87474800	0.97905700
C	2.60892100	-0.20715200	-1.16535300
C	3.71458700	0.85595300	1.16098400
H	1.67689700	1.30059800	1.73029400
C	3.98707900	-0.23918900	-0.96903500
H	2.18236800	-0.61192000	-2.07554800
C	4.54364100	0.29559000	0.19230300
H	4.14115100	1.27864000	2.06602700
H	4.62695300	-0.67767300	-1.72926000
H	5.61986900	0.27564700	0.33987100
N	-0.50257100	0.88853800	1.33508100
C	-0.98076600	0.04078100	2.41313000
H	-1.26815900	0.66969100	3.26438100
H	-1.84479300	-0.58682800	2.13857300
H	-0.17149800	-0.61877300	2.74326900
F	0.12075400	0.10601800	-2.11681000
C	-2.62811800	3.29837900	-0.34439000
H	-3.29674600	4.09141100	-0.65080200
N	-1.90636400	2.60787600	-1.27851200
H	-1.93760000	2.75360500	-2.27613300

5.closed

Sum of electronic and thermal Free Energies = -1191.419873 a.u.

P	-0.01796900	0.32179600	-0.52273500
C	-1.13522800	1.67084900	-0.62864200
C	-1.39879600	1.68108800	0.71035100
C	-2.50836700	2.60069900	0.99524000
H	-2.94712100	2.81412500	1.96276600
C	-0.68691400	-1.34851900	-0.26397900
C	-1.97108700	-1.64886000	-0.72357800
C	0.04969600	-2.31601100	0.42330200
C	-2.51951400	-2.90811400	-0.48715600
H	-2.53879700	-0.89624100	-1.26498700

C	-0.49884100	-3.57735600	0.65072600
H	1.04983700	-2.08542800	0.78354900
C	-1.78431600	-3.87351800	0.19982300
H	-3.51936600	-3.13668300	-0.84460600
H	0.07859700	-4.32760200	1.18314600
H	-2.21105900	-4.85585900	0.38024200
C	1.78706500	0.36879000	-0.21104900
C	2.32052500	0.96901000	0.93589700
C	2.65471700	-0.23169200	-1.13458300
C	3.69845700	0.97623100	1.14888500
H	1.64782300	1.42914100	1.65101200
C	4.02863100	-0.24033600	-0.90599300
H	2.25232100	-0.69006000	-2.03082300
C	4.55403400	0.36699000	0.23364400
H	4.10126100	1.45575600	2.03635300
H	4.68935300	-0.71651500	-1.62459400
H	5.62664400	0.36591400	0.40630800
N	-0.52609600	0.83820200	1.32582300
C	-0.90224600	0.05205500	2.48252400
H	-1.29255700	0.71042300	3.26897000
H	-1.66148100	-0.71515700	2.26304400
H	-0.01600200	-0.45404500	2.87929100
F	0.18344300	0.10076100	-2.17433000
C	-2.85818100	3.15482100	-0.18682300
H	-3.63009300	3.90664600	-0.31966000
C	-2.02371800	2.63248800	-1.34707000
H	-1.50201400	3.46203200	-1.84361700
H	-2.66161400	2.16066700	-2.10629300

8.closed

Sum of electronic and thermal Free Energies = -1395.146593 a.u.

P	0.05725300	-0.02752600	-0.56836500
C	1.77543200	-0.34613400	-0.64649300
C	1.99437000	-0.39792000	0.74477800
C	-0.61135700	1.61478000	-0.15904600
C	-0.17736900	2.72545400	-0.88484300
C	-1.54223100	1.77391800	0.87023300
C	-0.65974600	3.99439100	-0.56757300
H	0.53395900	2.59399400	-1.69581700
C	-2.03601300	3.04026700	1.17385900
H	-1.88989300	0.90516800	1.42600800
C	-1.58928400	4.15215400	0.45911800
H	-0.31518200	4.85826500	-1.12827200
H	-2.76742300	3.15959000	1.96787300

H	-1.97004400	5.14046600	0.69981700
C	-1.20302500	-1.31647600	-0.29996800
C	-0.93131000	-2.45796000	0.45790200
C	-2.45751500	-1.16191800	-0.89711300
C	-1.90869600	-3.43753800	0.61870300
H	0.04778000	-2.58002600	0.91355200
C	-3.44011700	-2.13374300	-0.71808000
H	-2.66207000	-0.28311800	-1.50288400
C	-3.16596100	-3.27228700	0.03800000
H	-1.68926700	-4.32836500	1.19984100
H	-4.41598800	-2.00484100	-1.17676800
H	-3.92988600	-4.03282300	0.17136600
N	0.80635800	-0.21494600	1.29252200
C	0.48373800	-0.16541400	2.69247300
H	1.36492000	-0.42851300	3.28935900
H	0.14923600	0.83810800	2.98566100
H	-0.32363700	-0.87304700	2.92544000
F	-0.25343100	0.12349700	-2.19283800
C	4.13742700	-0.67351100	-1.10862200
H	4.95240300	-0.78466200	-1.81615700
C	2.86352100	-0.48487800	-1.58527500
H	2.63676300	-0.43698200	-2.65209000
Al	3.99381700	-0.67871900	0.80210300
H	4.94510000	-0.83293000	2.05077000

10.closed

Sum of electronic and thermal Free Energies = -1207.489013 a.u.

P	0.00216200	-0.31687800	-0.53338600
C	1.10313800	-1.68537000	-0.69688400
C	1.35511700	-1.74283500	0.65292500
C	0.72222400	1.32778500	-0.26184400
C	2.03143500	1.57416100	-0.68274900
C	0.00101000	2.32712100	0.39489400
C	2.61812400	2.81443900	-0.43876800
H	2.58749600	0.79501700	-1.19851800
C	0.59018700	3.56842300	0.63165100
H	-1.01845000	2.13797200	0.72364400
C	1.89907300	3.81219600	0.21872500
H	3.63634200	3.00256100	-0.76666900
H	0.02540200	4.34414500	1.14059500
H	2.35691200	4.77923300	0.40551700
C	-1.80056200	-0.33538100	-0.20560300
C	-2.33929000	-0.91814300	0.94790900
C	-2.66136400	0.28326000	-1.12442400

C	-3.71521700	-0.88969600	1.17199400
H	-1.67111100	-1.39132700	1.65798600
C	-4.03257900	0.32624100	-0.88460600
H	-2.25675000	0.72898700	-2.02562200
C	-4.56338600	-0.26335400	0.26170200
H	-4.12201500	-1.35599700	2.06465000
H	-4.68688900	0.81557200	-1.60017300
H	-5.63421700	-0.23550400	0.44299200
N	0.50010000	-0.89692600	1.31568700
C	0.98924400	-0.08097800	2.41221000
H	1.28893200	-0.71904100	3.25419400
H	1.84295400	0.56126100	2.14007000
H	0.17877700	0.56469300	2.76397300
F	-0.21254000	-0.06202500	-2.17643800
C	2.70978800	-3.19675100	-0.35117400
H	3.48470600	-3.94762700	-0.39855900
C	1.96013600	-2.62802600	-1.34955000
H	2.03295800	-2.85968600	-2.40230700
N	2.34236600	-2.64137100	0.88822800
H	2.73566200	-2.89933100	1.78110100

11.closed

Sum of electronic and thermal Free Energies = -1191.420438 a.u.

P	0.00016200	-0.30249900	-0.56395700
C	1.10094700	-1.66828700	-0.67535000
C	1.37043600	-1.69331400	0.66733200
C	2.50866600	-2.63788500	0.95073100
H	2.21566500	-3.42309600	1.65859600
C	0.70539400	1.34349800	-0.26152500
C	1.98008900	1.63834100	-0.75060000
C	0.00525900	2.29655100	0.48189800
C	2.55582700	2.87977200	-0.48595000
H	2.51783700	0.89683400	-1.33612700
C	0.58107500	3.54035000	0.73589500
H	-0.98715000	2.06807000	0.86439300
C	1.85737600	3.83155200	0.25616200
H	3.54807100	3.10538300	-0.86564300
H	0.03252800	4.28050300	1.31117400
H	2.30560600	4.80020300	0.45718200
C	-1.79753500	-0.33839100	-0.22865500
C	-2.32981300	-1.01753700	0.87311600
C	-2.66070200	0.34450400	-1.09652700
C	-3.70576900	-1.02002500	1.09711200
H	-1.65985300	-1.54129800	1.54608900

C	-4.03224000	0.35883100	-0.85437200
H	-2.25747800	0.86206500	-1.96009200
C	-4.55776600	-0.32684600	0.23979000
H	-4.10996000	-1.56142600	1.94747300
H	-4.69089200	0.89955100	-1.52762800
H	-5.62868600	-0.32197400	0.42215500
N	0.52243700	-0.85404700	1.29305700
C	0.85091500	-0.15080800	2.51192300
H	1.24148600	-0.85511000	3.25757900
H	1.59777200	0.64475900	2.36040800
H	-0.05371100	0.30898800	2.92324500
F	-0.20949800	-0.05046000	-2.20114900
C	2.79402200	-3.17298100	-0.44988500
H	3.56319300	-3.90852000	-0.65259600
C	1.97912700	-2.60183700	-1.36740000
H	1.98520900	-2.79982200	-2.43258100
H	3.37450800	-2.11808100	1.38251900

13.open

Sum of electronic and thermal Free Energies = -1177.582181 a.u.

P	0.13769200	-0.18448300	0.52219900
C	-0.67325500	-1.53088500	-0.18333600
C	-0.13413400	-2.52396200	-0.94741900
C	-2.16330600	-1.70909100	-0.04662000
H	0.93261100	-2.56954000	-1.16862200
C	-0.47425500	1.44211600	0.09140800
C	-0.00412200	2.55762100	0.79349800
C	-1.35497100	1.59285600	-0.98292100
C	-0.42720100	3.82999500	0.42179800
H	0.68073900	2.43088400	1.62827000
C	-1.76722900	2.87093300	-1.35220000
H	-1.72512000	0.71690800	-1.50837000
C	-1.30611300	3.98447600	-0.65112600
H	-0.07373400	4.69858500	0.96859100
H	-2.45575800	2.99493800	-2.18206100
H	-1.63482100	4.97851700	-0.93981200
C	1.90068800	-0.25881500	0.18513900
C	2.49203800	0.59482300	-0.75096300
C	2.66746500	-1.22880300	0.84302500
C	3.85199600	0.47515100	-1.02869000
H	1.89534700	1.34761500	-1.25956700
C	4.02579500	-1.33944400	0.56240700
H	2.20257500	-1.89083000	1.56905000
C	4.61592900	-0.48899900	-0.37325700

H	4.31352900	1.13565000	-1.75599800
H	4.62245500	-2.08950500	1.07193200
H	5.67589400	-0.57876500	-0.59151300
N	-2.76275700	-0.80615500	0.65361800
C	-4.19412200	-0.90305800	0.84395700
H	-4.66582800	0.01160600	0.46505100
H	-4.65604100	-1.76881300	0.35616200
H	-4.40523100	-0.94794700	1.91835800
F	0.10020400	-0.19607000	2.11635900
H	-3.57172800	-3.22682900	-0.81012100
B	-1.33358200	-3.48504100	-1.39775300
H	-1.19336000	-4.45211400	-2.08794200
C	-2.53879300	-2.89661300	-0.78139400

16.open

Sum of electronic and thermal Free Energies = -1207.465534 a.u.

P	0.13295600	-0.08317700	-0.85036200
C	-1.14413100	-1.21605600	-0.76892900
C	-1.77017200	-1.45171300	0.52674700
C	-2.85563400	-2.30400700	0.23037600
H	-3.59444400	-2.76358100	0.86683300
C	1.73654100	-0.51376700	-0.15916700
C	2.86176800	-0.57987200	-0.98956800
C	1.83790500	-0.76906900	1.21542500
C	4.10002400	-0.90095000	-0.43865700
H	2.77396200	-0.38443200	-2.05375600
C	3.08377300	-1.09243400	1.74800700
H	0.93286700	-0.73348600	1.82317000
C	4.21014500	-1.15564600	0.92786500
H	4.97644700	-0.95216700	-1.07757600
H	3.17238000	-1.29854500	2.81034300
H	5.17738500	-1.40670200	1.35382400
C	-0.31256000	1.57066100	-0.32060400
C	-1.65205900	1.87458800	-0.06120600
C	0.67987000	2.54925200	-0.21213800
C	-1.99593200	3.17471000	0.29431400
H	-2.40150700	1.08933700	-0.11361200
C	0.32503500	3.84973000	0.13697100
H	1.72253400	2.29659700	-0.39110700
C	-1.01100200	4.15891200	0.38928800
H	-3.03165700	3.41784100	0.50973500
H	1.08934800	4.61618200	0.21945400
H	-1.28562200	5.17164700	0.67014900
N	-1.29358700	-0.88703100	1.63105700

C	-2.09259300	-1.16071200	2.79757600
H	-2.14909200	-2.24212900	3.03350600
H	-1.66786100	-0.65696600	3.67259400
H	-3.14008800	-0.81181900	2.69110400
F	0.48539100	0.07280100	-2.40175300
H	-1.65880100	-2.00477800	-2.82389100
C	-1.82391600	-1.93208200	-1.75921200
N	-2.82821900	-2.56797400	-1.13849900
H	-3.48844800	-3.16878400	-1.61000600

17.open

Sum of electronic and thermal Free Energies = -1191.382279 a.u.

P	0.10972900	-0.11629700	0.54440300
C	-0.78129300	-1.41479200	-0.21681800
C	-0.29104900	-2.39011900	-1.00862700
C	-2.24746800	-1.51689300	-0.01285700
H	0.74278100	-2.53976900	-1.30608000
C	-0.34797200	1.54799500	0.09213600
C	0.49588300	2.59679800	0.48421100
C	-1.49590200	1.79340900	-0.66970100
C	0.18224000	3.90123000	0.12005200
H	1.38959600	2.39627900	1.07067000
C	-1.78751300	3.10362700	-1.04299400
H	-2.16434500	0.97209300	-0.91015300
C	-0.95710600	4.15066000	-0.64751500
H	0.82442600	4.71922400	0.43079100
H	-2.67662800	3.30540300	-1.63174900
H	-1.19879100	5.16986100	-0.93515100
C	1.86832200	-0.32622600	0.22522200
C	2.45149600	0.24153200	-0.91308100
C	2.62385200	-1.14064200	1.07570900
C	3.79265300	-0.00433000	-1.19502600
H	1.86241700	0.87389000	-1.57290800
C	3.96657700	-1.37600400	0.79016000
H	2.16580000	-1.58296000	1.95586700
C	4.54851700	-0.81003800	-0.34349700
H	4.24732200	0.43575800	-2.07701200
H	4.55631400	-2.00233800	1.45210100
H	5.59520800	-0.99681000	-0.56431900
N	-2.78954700	-0.58962400	0.76590400
C	-4.20928500	-0.75928000	0.93685900
H	-4.60944200	0.02848300	1.58380100
H	-4.75952100	-0.72082100	-0.02521300
H	-4.46450900	-1.73437900	1.39484200

F	0.04747200	-0.23546900	2.11828800
H	-3.64289700	-3.02884700	-0.81442100
C	-2.64122600	-2.62476000	-0.75307100
C	-1.44952300	-3.25832200	-1.42270800
H	-1.49835500	-3.29061200	-2.52476400
H	-1.24294600	-4.29645700	-1.10898800

TS2'

Sum of electronic and thermal Free Energies = -1395.163828 a.u.

P	-0.05632900	-0.03336500	-0.69035100
C	-1.75974700	-0.19828500	-0.62512100
C	-1.95490400	-0.18742900	0.79969900
C	-3.34689600	-0.32986500	1.32343300
H	-3.51392300	-0.33068500	2.40002000
C	1.06112500	-1.38442700	-0.20430700
C	1.09533100	-2.53338800	-0.99687700
C	1.87555900	-1.29194500	0.92650500
C	1.93369400	-3.59240400	-0.65045400
H	0.46758000	-2.59860500	-1.88141200
C	2.72343900	-2.34375400	1.26144400
H	1.84369200	-0.39388200	1.53897600
C	2.74826500	-3.49733000	0.47591900
H	1.95309800	-4.48818000	-1.26401900
H	3.36055600	-2.26679900	2.13765100
H	3.40447400	-4.32081600	0.74246200
C	0.74720600	1.56211600	-0.35847700
C	0.02102000	2.61925600	0.19353300
C	2.08414200	1.74305400	-0.71827300
C	0.63466500	3.85281600	0.39145300
H	-1.02160400	2.46815400	0.46253700
C	2.69834000	2.97793400	-0.51188800
H	2.64489900	0.92236700	-1.15972200
C	1.97449500	4.03131100	0.04292700
H	0.06869300	4.67562000	0.81817600
H	3.73900600	3.11650500	-0.78957300
H	2.45243100	4.99377000	0.20117000
N	-0.83286600	-0.03911800	1.44759900
C	-0.67392800	0.03223100	2.87880000
H	-1.62796600	0.03972700	3.41851500
H	-0.08494400	-0.82240600	3.23519200
H	-0.12591100	0.94653800	3.13971700
F	0.26495900	-0.10225000	-2.28532500
C	-4.32986800	-0.45410600	0.40752400
H	-5.35342300	-0.56088800	0.76336400

Al	-3.46325400	-0.40115100	-1.38180300
H	-4.08561300	-0.50561000	-2.82466700

TS4'

Sum of electronic and thermal Free Energies = -1207.467099 a.u.

P	-0.11897300	-0.30638400	-0.73486700
C	0.84022800	-1.71063900	-0.56056300
C	1.36194100	-1.68165100	0.76178700
C	2.61069100	-2.42081600	0.70972300
H	3.29703300	-2.61813400	1.52133000
C	0.64477100	1.29592400	-0.38541400
C	2.02551300	1.37019100	-0.17943700
C	-0.12691800	2.45871700	-0.43035900
C	2.62850400	2.61089900	-0.00650000
H	2.61485800	0.45594700	-0.13878800
C	0.48517900	3.70058500	-0.26104700
H	-1.20092800	2.39820200	-0.58967800
C	1.85929800	3.77609300	-0.04743900
H	3.69917600	2.67050300	0.16436300
H	-0.11360100	4.60584000	-0.29384700
H	2.33410000	4.74341900	0.08857000
C	-1.82950000	-0.29055200	-0.14638700
C	-2.13452600	0.07429400	1.16881800
C	-2.85117900	-0.63842100	-1.03673400
C	-3.46298200	0.09862100	1.58390700
H	-1.32377900	0.30872400	1.85058900
C	-4.17702400	-0.62365800	-0.60838000
H	-2.61590900	-0.91514900	-2.05959200
C	-4.48300900	-0.25288400	0.69960600
H	-3.70099000	0.38279900	2.60448400
H	-4.96870700	-0.89773200	-1.29910500
H	-5.51723200	-0.24016000	1.03147900
N	0.72402400	-0.91696800	1.62733000
C	1.40599700	-0.59736400	2.85776000
H	1.69840400	-1.49837400	3.42175600
H	2.32291000	-0.00131500	2.69409100
H	0.74655600	-0.00977000	3.50577200
F	-0.39130700	-0.20460500	-2.32242600
C	2.77328300	-2.82138900	-0.59423400
H	3.54817700	-3.44847300	-1.01861900
N	1.78199800	-2.33680700	-1.40566400
H	1.52254200	-2.81040600	-2.26027000

TS5'

Sum of electronic and thermal Free Energies = -1191.418844 a.u.

P	-0.01244000	0.19647900	-0.71413700
C	-0.57239200	1.80674400	-0.68387000
C	-0.77143100	2.01190600	0.68830900
C	-1.44041000	3.32110700	0.86086000
H	-1.73053700	3.77684400	1.80052000
C	-1.08483900	-1.18835400	-0.22692300
C	-2.15978500	-1.51534600	-1.05562200
C	-0.84929900	-1.92331200	0.93703600
C	-3.00604500	-2.56935200	-0.71273400
H	-2.33394000	-0.94782900	-1.96586200
C	-1.68723100	-2.98362400	1.26979100
H	-0.01311100	-1.65535000	1.57858100
C	-2.76915400	-3.30352500	0.44741100
H	-3.84605200	-2.81821300	-1.35438200
H	-1.50138100	-3.55612500	2.17383300
H	-3.42676000	-4.12635800	0.71264800
C	1.70880800	-0.21111600	-0.30574000
C	2.52748600	0.74257600	0.30111700
C	2.22346800	-1.45975100	-0.65924600
C	3.86300000	0.44408000	0.55560300
H	2.10578900	1.70642400	0.57465100
C	3.56023800	-1.75772900	-0.39665200
H	1.58400400	-2.19679500	-1.13978800
C	4.37833500	-0.80630600	0.20959600
H	4.50236000	1.18461600	1.02700800
H	3.96152900	-2.72906500	-0.67015300
H	5.42012000	-1.03785100	0.41219300
N	-0.34061600	1.02402000	1.43501500
C	-0.60360200	0.90649600	2.84578300
H	-0.98013400	1.84687500	3.27278300
H	-1.35218400	0.12602700	3.04751000
H	0.31204800	0.63464400	3.38538300
F	0.05563400	-0.14851700	-2.30587900
C	-1.61212400	3.85341500	-0.36404400
H	-2.06264300	4.82131200	-0.56408400
C	-1.09274800	2.96318500	-1.48191500
H	-0.33499200	3.49890700	-2.07057000
H	-1.90755800	2.70670900	-2.17297100

TS8’

Sum of electronic and thermal Free Energies = -1395.144439 a.u.

P	0.01720100	-0.01076400	-0.73496300
C	-1.69537100	-0.05590700	-0.65051500

C	-2.01459400	-0.06527500	0.74794600
C	1.02826000	-1.42333600	-0.20575600
C	1.08519700	-2.54383800	-1.03810800
C	1.72789100	-1.41184100	1.00351200
C	1.83805700	-3.65359400	-0.65660000
H	0.54296900	-2.54960900	-1.97965200
C	2.48780500	-2.51685300	1.37495600
H	1.66924800	-0.53820100	1.64764800
C	2.53944500	-3.63973300	0.54713800
H	1.87738800	-4.52599200	-1.30186600
H	3.03465500	-2.50552800	2.31314400
H	3.12684800	-4.50423000	0.84259800
C	0.90291500	1.51843000	-0.33483200
C	0.19356600	2.63384600	0.11414300
C	2.28176900	1.59637000	-0.54263200
C	0.86664100	3.82650400	0.36162200
H	-0.87974200	2.55510200	0.26891400
C	2.95236700	2.79293700	-0.29327100
H	2.83098900	0.72762500	-0.89844600
C	2.24551600	3.90533200	0.15969900
H	0.31706000	4.69486900	0.71232800
H	4.02423800	2.85548600	-0.45534200
H	2.76891700	4.83695100	0.35420300
N	-0.94302800	0.00876100	1.47725400
C	-0.98518500	0.01588200	2.91853400
H	-2.01785200	-0.03557200	3.29318900
H	-0.42510400	-0.83898800	3.31848800
H	-0.51439200	0.92851900	3.30533700
F	0.32288900	-0.09123600	-2.32272100
C	-4.05987700	-0.24545100	-1.21806100
H	-4.83224400	-0.31296400	-1.97752500
C	-2.74873800	-0.15485600	-1.62804800
H	-2.47145400	-0.15278100	-2.68470600
Al	-4.03132000	-0.22286700	0.69236500
H	-5.08116700	-0.28785200	1.87072900

TS10’

Sum of electronic and thermal Free Energies = -1207.485503 a.u.

P	-0.08462300	0.25447400	-0.74716000
C	0.87908400	1.66842800	-0.68130000
C	1.25774300	1.72727500	0.67254600
C	-1.79824800	0.20612800	-0.15513300
C	-2.81717700	0.63343200	-1.01245800
C	-2.10758500	-0.24729500	1.13039600

C	-4.14196200	0.61143700	-0.58025300
H	-2.57860600	0.97961100	-2.01337500
C	-3.43436100	-0.28327500	1.54943600
H	-1.30446100	-0.55593900	1.79112700
C	-4.45086000	0.15064600	0.69794700
H	-4.93083800	0.94971700	-1.24527500
H	-3.67422300	-0.64040000	2.54646400
H	-5.48415600	0.13060900	1.03234000
C	0.73518100	-1.32108800	-0.40167500
C	2.10959800	-1.35808300	-0.15105000
C	-0.00013400	-2.50566100	-0.46976400
C	2.74176600	-2.58075000	0.04496600
H	2.67223700	-0.42794600	-0.10640800
C	0.63996900	-3.72976400	-0.27403200
H	-1.06844700	-2.47613100	-0.67076000
C	2.00755900	-3.76753100	-0.01498900
H	3.80879200	-2.60997900	0.24473200
H	0.06761800	-4.65115200	-0.32525800
H	2.50466500	-4.72096200	0.13810600
N	0.64293800	0.90296900	1.50491900
C	1.28005600	0.56637400	2.75327600
H	2.25680100	0.06607100	2.61873100
H	1.44545000	1.44982000	3.39317100
H	0.63961400	-0.11711800	3.32046400
F	-0.40045600	0.08234100	-2.32657000
C	2.50379300	3.19990900	-0.51125100
H	3.24972800	3.96964600	-0.64411000
C	1.67249500	2.61484400	-1.41988600
H	1.63365500	2.83233200	-2.47745900
N	2.27705000	2.64245600	0.76235200
H	2.73421300	2.93552500	1.61248400

TS11'

Sum of electronic and thermal Free Energies = -1191.420294 a.u.

P	0.01377100	0.20077400	-0.70416000
C	0.76825600	1.74586000	-0.71966800
C	0.96639600	1.93590800	0.65172000
C	1.68218200	3.25465900	0.87284100
H	2.65370100	3.11124600	1.36438400
C	-1.70913900	-0.04845400	-0.17681900
C	-2.73770400	0.40444000	-1.00562100
C	-2.01191900	-0.68419900	1.02937100
C	-4.06666500	0.23324200	-0.61936600
H	-2.50052100	0.88949500	-1.94815200

C	-3.33937600	-0.87078900	1.40320500
H	-1.20510100	-1.03432300	1.66827700
C	-4.36750600	-0.40559400	0.58169700
H	-4.86515300	0.59451400	-1.26051600
H	-3.57255200	-1.37196900	2.33803500
H	-5.40318500	-0.54266900	0.87898900
C	0.99075900	-1.29017500	-0.35711400
C	2.29954200	-1.19223400	0.11976000
C	0.43617100	-2.54118600	-0.63231300
C	3.04838000	-2.34628900	0.32792800
H	2.72314900	-0.21142900	0.32220900
C	1.18771400	-3.69641600	-0.41626300
H	-0.57936200	-2.61487300	-1.01454800
C	2.49155600	-3.59926300	0.06375900
H	4.06702200	-2.26977100	0.69656900
H	0.75430300	-4.66931100	-0.62816700
H	3.07729700	-4.49875900	0.22952800
N	0.49050000	0.94159600	1.35844300
C	0.68376500	0.76712000	2.77313400
H	1.20371100	1.62755500	3.21662800
H	-0.27779800	0.65070000	3.28930700
H	1.28308800	-0.13267000	2.97508100
F	-0.25139500	-0.07940000	-2.29167800
C	1.81939800	3.76571200	-0.55783200
H	2.29081300	4.70938700	-0.80375100
C	1.29276500	2.88982500	-1.44456600
H	1.27231700	3.01719900	-2.52071300
H	1.09332400	3.92448300	1.51212800

TS13'

Sum of electronic and thermal Free Energies = -1177.581447 a.u.

P	0.03373600	-0.10761900	-0.80501100
C	-0.81166400	-1.64553900	-0.77468100
C	-1.11690700	-2.06956400	0.62228700
C	-1.86283600	-3.28008900	0.60648400
H	-2.18926000	-3.76284900	1.52164300
C	1.72637300	0.02480500	-0.20306800
C	2.77516200	-0.25466200	-1.08418000
C	1.98805000	0.41191000	1.11518100
C	4.09192200	-0.15187600	-0.63865700
H	2.56871600	-0.54945500	-2.10844000
C	3.30528800	0.52605300	1.54548300
H	1.16002900	0.60287300	1.79071600
C	4.35589700	0.23992700	0.67153900

H	4.90827200	-0.37618800	-1.31803700
H	3.51309200	0.82961700	2.56681500
H	5.38279100	0.32132900	1.01545800
C	-0.93280300	1.32724000	-0.32718700
C	-2.28184700	1.17479600	0.00581300
C	-0.34020500	2.59325500	-0.35552700
C	-3.03896400	2.30184400	0.31036200
H	-2.72551500	0.18281400	0.03925300
C	-1.10541000	3.71480700	-0.04584300
H	0.71059600	2.70266200	-0.61350700
C	-2.45177200	3.56735300	0.28559600
H	-4.08655100	2.19146900	0.57216400
H	-0.65103100	4.70052800	-0.06295600
H	-3.04642700	4.44316400	0.52809700
N	-0.64100900	-1.20699900	1.47418400
C	-0.86513100	-1.45230400	2.88475500
H	-1.93852300	-1.45629600	3.12090900
H	-0.45272600	-2.42325400	3.19108100
H	-0.38574700	-0.66933800	3.47984400
F	0.27785100	0.14772900	-2.36951300
H	-1.20173000	-2.34685500	-2.76832600
B	-2.04828100	-3.65793700	-0.81941100
H	-2.61027600	-4.58952600	-1.31651600
C	-1.30747400	-2.49084000	-1.69496400

TS16'

Sum of electronic and thermal Free Energies = -1207.463988 a.u.

P	0.07762600	-0.12513700	-0.80349100
C	-0.99514300	-1.46195700	-0.73187200
C	-1.41884700	-1.71403700	0.62724500
C	-2.40405100	-2.71047000	0.51866400
H	-2.99583400	-3.22744000	1.25694100
C	1.75904100	-0.25908200	-0.16694000
C	2.79002800	-0.59793300	-1.05053700
C	2.03068700	-0.01400700	1.18378000
C	4.09718800	-0.69457700	-0.57855300
H	2.57756900	-0.78142800	-2.09913300
C	3.34245600	-0.10392200	1.64115500
H	1.20572900	0.21088400	1.85185200
C	4.37253900	-0.44609100	0.76497700
H	4.89787900	-0.96050300	-1.26187300
H	3.55830400	0.08431400	2.68839700
H	5.39259500	-0.52123800	1.13081700
C	-0.63269600	1.46193400	-0.34859500

C	-1.97899800	1.55246500	0.01512700
C	0.16493700	2.60501300	-0.43162900
C	-2.52504900	2.80054400	0.29242400
H	-2.57379500	0.64646700	0.10100100
C	-0.39126400	3.85280500	-0.15312100
H	1.21443000	2.52392700	-0.70586700
C	-1.73327600	3.94823300	0.20770400
H	-3.56754600	2.87891000	0.58514300
H	0.22397900	4.74507800	-0.21592500
H	-2.16522100	4.92001600	0.42881100
N	-0.84162600	-0.97856100	1.57805300
C	-1.39093600	-1.14839200	2.89631400
H	-1.30324800	-2.18935000	3.26248200
H	-0.86233400	-0.50792100	3.61203300
H	-2.46663100	-0.88473400	2.95120100
F	0.38559400	0.06566800	-2.36887100
H	-1.64149000	-2.41026800	-2.67944500
C	-1.68146000	-2.30200700	-1.60582600
N	-2.50596500	-3.03668800	-0.83742900
H	-3.12693100	-3.74503100	-1.20050500

TS17'

Sum of electronic and thermal Free Energies = -1191.380835 a.u.

P	0.04533000	-0.17864200	0.57686400
C	-0.74446300	-1.51703400	-0.25075600
C	-0.34586900	-2.46222800	-1.11929600
C	-2.18527900	-1.54608900	0.02461500
H	0.65718300	-2.65181300	-1.48872400
C	-0.39549200	1.48596500	0.07595200
C	0.45473300	2.52931800	0.45989400
C	-1.51330500	1.73315900	-0.72841000
C	0.16974200	3.83216500	0.06008900
H	1.33243900	2.32859700	1.06980300
C	-1.77001200	3.03505200	-1.14821400
H	-2.17986400	0.91551400	-0.98453700
C	-0.93861900	4.08171000	-0.74805700
H	0.81545700	4.64656500	0.37324100
H	-2.63289700	3.23400800	-1.77593900
H	-1.15619600	5.09705400	-1.06664300
C	1.81955000	-0.33156300	0.24413100
C	2.32759200	0.09779900	-0.98782700
C	2.66235700	-0.95478300	1.16910000
C	3.67277800	-0.09509100	-1.28939000
H	1.67503500	0.58849100	-1.70686500

C	4.01019600	-1.13872200	0.86439400
H	2.26920100	-1.29081700	2.12387700
C	4.51398800	-0.71156100	-0.36253200
H	4.06485800	0.24022000	-2.24463200
H	4.66469900	-1.61716500	1.58645800
H	5.56416300	-0.85702600	-0.59761400
N	-2.51489200	-0.59088600	0.89513700
C	-3.91508900	-0.48216300	1.20443600
H	-4.08303100	0.33575800	1.91275200
H	-4.53056700	-0.28246400	0.30454400
H	-4.31750400	-1.40664100	1.65735300
F	0.05552500	-0.29307200	2.15160600
H	-3.73834100	-2.89464400	-0.78855200
C	-2.70931000	-2.56244400	-0.75017200
C	-1.58689300	-3.23273200	-1.51462300
H	-1.69747700	-3.19878000	-2.61139200
H	-1.44221800	-4.29793100	-1.26651900

CS_2 (in THF solvent)

Sum of electronic and thermal Free Energies = -834.414169 a.u.

C	0.00000000	0.00000000	0.00000000
S	0.00000000	0.00000000	1.55446200
S	0.00000000	0.00000000	-1.55446200

4.closed (in THF solvent)

Sum of electronic and thermal Free Energies = -1207.508685 a.u.

P	0.00506800	-0.25590100	-0.40209400
C	0.63181800	-1.89754600	-0.62515000
C	0.76288600	-2.14827400	0.71674400
C	1.21501300	-3.48386400	0.87875700
H	1.44731000	-4.03382500	1.78061200
C	1.13123500	1.15328300	-0.19027700
C	2.39576200	1.11909300	-0.78496000
C	0.75860600	2.24679800	0.59612100
C	3.28681400	2.17287600	-0.58590500
H	2.68478300	0.27131200	-1.40135900
C	1.64892500	3.30382800	0.78353000
H	-0.22234100	2.27785000	1.06524600
C	2.91394400	3.26596100	0.19679800
H	4.27032400	2.14106000	-1.04611200
H	1.35343500	4.15497200	1.39049400
H	3.60766900	4.08837900	0.34727600
C	-1.74912700	0.19901900	-0.16525700
C	-2.56837800	-0.50311600	0.72465200

C	-2.28253800	1.26381000	-0.90324100
C	-3.91052800	-0.15015100	0.86504400
H	-2.15043500	-1.31770900	1.30632800
C	-3.61607500	1.63222000	-0.73724400
H	-1.65550300	1.80930100	-1.60227800
C	-4.43364400	0.92131900	0.14207100
H	-4.54404900	-0.70914500	1.54792600
H	-4.01740900	2.46905700	-1.30182300
H	-5.47628800	1.20240800	0.26279800
N	0.25607700	-0.99222000	1.34436200
C	1.05424400	-0.40281200	2.40859800
H	1.15078900	-1.12916400	3.22458200
H	2.06872600	-0.10835200	2.09091700
H	0.54660700	0.48044700	2.80726600
F	-0.11081900	0.04496000	-2.09535400
C	1.28950900	-3.98903600	-0.42034800
H	1.59574500	-4.97097900	-0.75689200
N	0.91288000	-3.04296400	-1.32882100
H	0.90849500	-3.16587600	-2.33377900

4.open (in THF solvent)

Sum of electronic and thermal Free Energies = -1207.510028 a.u.

P	0.19994100	-0.05997600	0.59605600
C	-0.65225400	-1.40407900	0.07022300
C	-2.10406500	-1.60896100	0.05277600
C	-0.51270300	1.50872800	0.08740300
C	-0.32976400	2.65078400	0.87409500
C	-1.17209000	1.59361200	-1.14378200
C	-0.81556200	3.87857700	0.42702500
H	0.18133900	2.58530800	1.82979700
C	-1.65534900	2.82290400	-1.58152500
H	-1.32075400	0.69913400	-1.74225800
C	-1.47691100	3.96428100	-0.79743700
H	-0.67845600	4.76575800	1.03808100
H	-2.17683300	2.88891700	-2.53173500
H	-1.85655800	4.92207600	-1.14198400
C	1.93708600	-0.20489000	0.13640500
C	2.25562100	-0.45103000	-1.20608700
C	2.95390000	-0.05187900	1.08505800
C	3.58929800	-0.55111500	-1.59359900
H	1.46398500	-0.56256900	-1.94418300
C	4.28670600	-0.15283900	0.68802400
H	2.71088500	0.14066500	2.12505700
C	4.60396900	-0.40245100	-0.64652700

H	3.83521700	-0.74253400	-2.63383200
H	5.07615600	-0.03718600	1.42471800
H	5.64387800	-0.48022000	-0.95076200
N	-2.99312600	-0.71315900	0.37202600
C	-4.37083700	-1.15437600	0.26509700
H	-5.03952500	-0.33310100	0.54036500
H	-4.63934000	-1.47170300	-0.75672800
H	-4.59470100	-2.00211800	0.93475800
F	0.35504400	0.20506200	2.19775300
C	-1.02151800	-3.55893700	-0.47507100
H	-0.75105300	-4.56642100	-0.76904600
C	-2.26638800	-3.00435500	-0.35038200
H	-3.20389400	-3.52654800	-0.48067400
N	-0.04295300	-2.67107400	-0.16242100
H	0.91286500	-2.77957600	-0.47962300

TS4 (in THF solvent)

Sum of electronic and thermal Free Energies = -2041.902327 a.u.

P	0.87501900	0.05570900	-0.98099000
F	1.37607800	-0.17524900	-2.50780700
C	0.17323700	1.58659200	-0.77993900
C	-1.20430100	1.99700300	-0.63403700
C	0.16524300	3.83046000	-0.65459600
H	0.59422500	4.82460900	-0.64702500
C	-0.17662400	-1.37382500	-0.75304900
C	0.04525800	-2.23053400	0.32942800
C	-1.14890400	-1.66992200	-1.71528100
C	-0.71748800	-3.39066200	0.44974800
H	0.80522400	-1.99984500	1.07183300
C	-1.89935900	-2.83367500	-1.58931200
H	-1.31936600	-0.99546700	-2.54950700
C	-1.68284900	-3.69238800	-0.50962000
H	-0.55255600	-4.05769500	1.29048000
H	-2.65631200	-3.06815700	-2.33164300
H	-2.27312000	-4.59961200	-0.41532400
C	2.43300200	-0.10789700	-0.10414500
C	3.38968300	-1.02840900	-0.55334000
C	2.65318400	0.63464700	1.06192600
C	4.56879400	-1.19786800	0.16650100
H	3.21315900	-1.60832500	-1.45525000
C	3.83938000	0.46127100	1.77272300
H	1.90386400	1.34100800	1.40982500
C	4.79281700	-0.45338000	1.32644800
H	5.31261000	-1.90984400	-0.17809100

H	4.01505900	1.03803300	2.67571000
H	5.71463600	-0.58896300	1.88490100
N	-2.24330500	1.18285300	-0.53054200
C	-3.51427800	1.86796500	-0.39957100
H	-3.57450100	2.49978900	0.50519500
H	-3.72157900	2.51537500	-1.26593900
H	-4.31923300	1.12922000	-0.34351200
C	-2.17928100	0.04769400	1.50498000
S	-3.42755500	-0.91587600	1.35594700
S	-0.94739900	0.69531700	2.26746800
C	-1.15027300	3.43983000	-0.55036600
H	-1.99422400	4.10406700	-0.43016300
H	1.96328400	2.78717300	-0.94705800
N	0.96540000	2.75111400	-0.78016300

4p (in THF solvent)

Sum of electronic and thermal Free Energies = -2041.974457 a.u.

P	0.63584600	0.05100800	-0.51150000
F	1.31018400	-0.07289600	-2.08505800
C	-0.51648100	1.25599800	-1.11405000
C	-1.81452400	1.52191500	-0.68386000
C	-1.39069300	2.77390300	-2.50434200
H	-1.40060300	3.46516700	-3.33523300
C	0.11831700	-1.69367400	-0.55884600
C	0.45672600	-2.59228300	0.45652400
C	-0.63926900	-2.11853700	-1.65431600
C	0.04902900	-3.92113500	0.36424100
H	1.03386200	-2.26220400	1.31619500
C	-1.06875300	-3.44296000	-1.72487300
H	-0.89720700	-1.42061300	-2.44705200
C	-0.71994800	-4.34501100	-0.72043100
H	0.32328700	-4.62145700	1.14754200
H	-1.67038300	-3.76847400	-2.56849900
H	-1.04917500	-5.37844300	-0.78071600
C	2.28868200	0.45227300	0.14389200
C	3.31182700	-0.48751800	-0.01934400
C	2.54875100	1.68419000	0.74951600
C	4.59115200	-0.20070100	0.45210600
H	3.11448400	-1.43732100	-0.51047000
C	3.83823000	1.97286500	1.19402000
H	1.75583500	2.41772700	0.86946000
C	4.85555600	1.02919200	1.05529900
H	5.38205400	-0.93645300	0.33948400
H	4.04302800	2.93477300	1.65469900

H	5.85593800	1.25314900	1.41448100
N	-2.51490500	0.91261100	0.37645400
C	-3.97823800	0.93798700	0.27303500
H	-4.38724100	1.80964500	0.79429100
H	-4.24917000	0.96939800	-0.78123700
H	-4.38233800	0.03408600	0.72612800
C	-1.93452000	0.45777400	1.51308600
S	-2.82147700	0.01779200	2.87197400
S	-0.18408700	0.40369600	1.62681800
C	-2.36546600	2.48557300	-1.56791100
H	-3.35274800	2.92227400	-1.52219300
H	0.56087000	2.00904900	-2.77088000
N	-0.29982100	2.02134900	-2.23518700

10.closed (in THF solvent)

Sum of electronic and thermal Free Energies = -1207.516306 a.u.

P	-0.00155100	-0.27241500	-0.48842500
C	0.90721400	-1.76817600	-0.71684500
C	1.13414300	-1.90966100	0.63380000
C	0.88179700	1.29027000	-0.21409400
C	2.14559000	1.46902900	-0.78421200
C	0.32823600	2.29398200	0.58569800
C	2.85654700	2.64465100	-0.54543600
H	2.57418200	0.69193100	-1.41276700
C	1.03829100	3.47256900	0.81284900
H	-0.65314200	2.16022300	1.03531900
C	2.30363800	3.64706900	0.25194100
H	3.84001400	2.77831500	-0.98710200
H	0.60274200	4.25218900	1.43147100
H	2.85667200	4.56436100	0.43370500
C	-1.79961000	-0.12447400	-0.19762400
C	-2.46667800	-0.97140000	0.69305200
C	-2.52298100	0.84992200	-0.89776300
C	-3.84457400	-0.85113900	0.87278700
H	-1.90503500	-1.71727100	1.24517100
C	-3.89481600	0.98543100	-0.69391200
H	-2.01532300	1.50703900	-1.59774000
C	-4.55850300	0.13100200	0.18703400
H	-4.35738300	-1.52204100	1.55622500
H	-4.44507600	1.75329800	-1.23029700
H	-5.62996500	0.23056900	0.33777400
N	0.40274700	-0.95791400	1.31142000
C	1.00151600	-0.25266300	2.43329900
H	1.23718800	-0.96492400	3.23369200

H	1.92454200	0.28974700	2.17143800
H	0.28081400	0.46621100	2.83328800
F	-0.19326700	0.05406100	-2.15372800
C	2.23952300	-3.53330300	-0.40380100
H	2.88590400	-4.39745800	-0.46544000
C	1.60322400	-2.82308500	-1.39353100
H	1.65096000	-3.03645800	-2.45273000
N	1.95380200	-2.96359600	0.84646600
H	2.30439300	-3.30564200	1.73325400

10.open (in THF solvent)

Sum of electronic and thermal Free Energies = -1207.530515 a.u.

P	0.21068300	-0.10678400	0.60036800
C	-0.73404200	-1.40869300	0.12717300
C	-0.27231700	-2.76218600	-0.17530900
C	-2.19718400	-1.42535100	0.07885100
H	0.75607800	-3.09751400	-0.19888300
C	-0.36815300	1.51610700	0.07976100
C	-0.25398500	2.62598300	0.92221800
C	-0.85769700	1.66320000	-1.22276200
C	-0.64001100	3.88315600	0.45905400
H	0.12409300	2.51334200	1.93346700
C	-1.23761900	2.92190000	-1.67869100
H	-0.95439200	0.79494500	-1.86978500
C	-1.12914100	4.03128700	-0.83809800
H	-0.55932700	4.74528200	1.11452300
H	-1.62443000	3.03568600	-2.68701600
H	-1.42989000	5.01233100	-1.19492200
C	1.93737200	-0.35143300	0.14875400
C	2.24536000	-0.75279000	-1.15763400
C	2.96117700	-0.09050700	1.06569300
C	3.57615200	-0.90145700	-1.53902500
H	1.44924300	-0.95138700	-1.87094400
C	4.29102000	-0.24307800	0.67566400
H	2.72619700	0.22398900	2.07770200
C	4.59812000	-0.64794000	-0.62270500
H	3.81425400	-1.21560800	-2.55089300
H	5.08582100	-0.04606700	1.38891000
H	5.63561300	-0.76549400	-0.92251700
N	-3.02470100	-0.46611100	0.35805400
C	-4.42777500	-0.79232300	0.19627600
H	-4.68097400	-1.09127200	-0.83588100
H	-4.75259200	-1.61274600	0.86026100
H	-5.03588900	0.08287600	0.44097600

F	0.35476100	0.14738800	2.19822000
C	-1.36560700	-3.50825200	-0.44684500
H	-1.44864100	-4.54737000	-0.73432200
N	-2.51203300	-2.71617000	-0.32764600
H	-3.45515100	-3.07550300	-0.38728700

TS10 (in THF solvent)

Sum of electronic and thermal Free Energies = -2041.919645 a.u.

P	0.86696100	0.11189600	-0.99805800
F	1.38604400	-0.06856900	-2.52136900
C	0.12341500	1.62633600	-0.81235300
C	0.84070100	2.88539600	-0.91135700
C	-1.26714400	1.92701800	-0.59068100
C	-0.07180300	3.87727300	-0.75624700
H	1.90078400	3.00723500	-1.09284500
H	0.04455400	4.95155300	-0.78136100
C	-0.13144300	-1.36293100	-0.80391800
C	0.12957400	-2.25872500	0.23736900
C	-1.11670600	-1.64306100	-1.75838900
C	-0.60359300	-3.44097300	0.32316700
H	0.89632800	-2.04035300	0.97640200
C	-1.83815000	-2.82844400	-1.66766400
H	-1.31784900	-0.94079200	-2.56271800
C	-1.58067500	-3.72589800	-0.62922000
H	-0.40758400	-4.13740400	1.13285500
H	-2.60346400	-3.05029900	-2.40531900
H	-2.14816600	-4.64989200	-0.56168200
C	2.41680600	-0.03806800	-0.10491100
C	3.34750200	-1.00867300	-0.50125100
C	2.66491500	0.76947100	1.00988800
C	4.52789900	-1.16295700	0.21914900
H	3.14993600	-1.63918700	-1.36447800
C	3.85183300	0.61009700	1.72342100
H	1.93778600	1.51735100	1.31391900
C	4.77871400	-0.35425700	1.32995600
H	5.25154300	-1.91283700	-0.08575600
H	4.04900600	1.23804800	2.58699900
H	5.70117800	-0.47799100	1.89017100
N	-2.27748100	1.10240900	-0.39399500
C	-3.56112100	1.75099500	-0.21297800
H	-3.59626600	2.40154200	0.68014700
H	-3.83833800	2.36415200	-1.08487800
H	-4.33468600	0.98757100	-0.09525400
C	-2.06419600	-0.03843400	1.56053500

S	-3.27891500	-1.05533000	1.47745800
S	-0.81360000	0.62561000	2.28550200
H	-2.17311600	3.83430900	-0.41478000
N	-1.32100100	3.30561700	-0.54924400

10p (in THF solvent)

Sum of electronic and thermal Free Energies = -2041.975570 a.u.

P	-0.67104700	-0.07021500	-0.57161000
F	-1.29968800	0.05584800	-2.14254200
C	0.37366000	-1.41865700	-1.04414100
C	0.15188200	-2.39919000	-2.06240100
C	1.64693200	-1.63814900	-0.53480200
C	1.27701100	-3.17808800	-2.12130900
H	-0.74139100	-2.50400400	-2.66181600
H	1.52262900	-4.03239900	-2.73489800
C	0.02166100	1.61154000	-0.66601400
C	-0.25892600	2.58964000	0.29182300
C	0.85117300	1.90657200	-1.75228700
C	0.28164900	3.86586100	0.15285400
H	-0.89309400	2.35989800	1.14363600
C	1.41404300	3.17697500	-1.86794500
H	1.05976800	1.14964400	-2.50429700
C	1.12513600	4.15767900	-0.92007400
H	0.05240500	4.62824900	0.89144900
H	2.07092600	3.39967300	-2.70375500
H	1.55724700	5.14973400	-1.01574700
C	-2.34545100	-0.30333400	0.09840900
C	-3.28651300	0.71369400	-0.09033700
C	-2.70269600	-1.48938600	0.74467700
C	-4.58267400	0.54940100	0.39472600
H	-3.01280900	1.62694400	-0.61309500
C	-4.00813000	-1.65475700	1.20426000
H	-1.97189800	-2.28198400	0.88336000
C	-4.94427700	-0.63400600	1.03878000
H	-5.31066000	1.34419900	0.26107200
H	-4.28956400	-2.58084300	1.69685900
H	-5.95746900	-0.76218400	1.40888200
N	2.39230700	-0.93810800	0.42095700
C	3.85050100	-0.94365500	0.25280700
H	4.30860000	-1.74693400	0.83894000
H	4.07841900	-1.06747800	-0.80631000
H	4.24804800	0.01084700	0.59511000
C	1.83293700	-0.39244500	1.54126600
S	2.77070400	0.16257200	2.81582400

S	0.08993400	-0.33125300	1.66390500
H	3.09201800	-3.10172600	-1.02151800
N	2.17798100	-2.69908200	-1.19785300

16.closed (in THF solvent)

Sum of electronic and thermal Free Energies = -1207.511651 a.u.

P	-0.00638700	-0.31449100	-0.43949500
C	-1.13123100	-1.67940500	-0.66828700
C	-1.38621600	-1.78932000	0.71814000
C	-2.42835700	-2.66660000	0.90104200
H	-2.96162300	-3.03459900	1.76467300
C	1.80987300	-0.33266000	-0.21408200
C	2.62332800	0.42500400	-1.06999900
C	2.40156000	-1.06457700	0.82174700
C	4.00303300	0.45641800	-0.88203700
H	2.17871600	0.99592600	-1.87799300
C	3.78657500	-1.04975000	0.99065100
H	1.77202700	-1.64263000	1.48943700
C	4.58826800	-0.28589400	0.14473500
H	4.62147500	1.05687600	-1.54318500
H	4.23566300	-1.63307700	1.78953800
H	5.66578900	-0.26773900	0.28378500
C	-0.73335500	1.33556000	-0.20839000
C	-2.04441200	1.57354500	-0.63290500
C	-0.01704500	2.34600200	0.43964000
C	-2.63499600	2.81616500	-0.40647200
H	-2.60344900	0.79101200	-1.14085000
C	-0.60990100	3.58998100	0.65705600
H	1.00171600	2.16900500	0.77716000
C	-1.91892600	3.82561300	0.23756300
H	-3.65417100	2.99549600	-0.73725500
H	-0.04724900	4.37336000	1.15706800
H	-2.37967800	4.79425200	0.41007800
N	-0.43439500	-0.93448600	1.29002900
C	-0.75320200	-0.15288900	2.46622900
H	-0.96087800	-0.82300800	3.30950500
H	0.10826100	0.46639300	2.73752100
H	-1.62566800	0.50845300	2.32902100
F	0.17365600	-0.04474400	-2.13338800
H	-2.15742500	-2.72149900	-2.39379800
C	-2.00723500	-2.50506800	-1.34552700
N	-2.77248400	-3.09254200	-0.38660200
H	-3.49901600	-3.77171900	-0.58038800

16.open (in THF solvent)

Sum of electronic and thermal Free Energies = -1207.499821 a.u.

P	0.16193700	-0.09972800	0.54682000
C	-0.77727200	-1.36822000	-0.08646800
C	-0.28965000	-2.45761700	-0.84013900
C	-2.23845700	-1.48497700	0.02424300
H	0.71805400	-2.71381400	-1.13769800
C	-0.34716400	1.56086100	0.11720800
C	0.18424100	2.64681900	0.82365700
C	-1.20760900	1.76237200	-0.96573300
C	-0.15529800	3.94184300	0.44225600
H	0.85707100	2.48460300	1.66217000
C	-1.53969300	3.06204800	-1.34077500
H	-1.62097300	0.91023900	-1.49874500
C	-1.01484300	4.14724600	-0.63849800
H	0.25025200	4.78871400	0.98749100
H	-2.21351800	3.22582500	-2.17619100
H	-1.27824400	5.15926800	-0.93285600
C	1.90318200	-0.33601600	0.18785100
C	2.53896900	0.43593600	-0.79043000
C	2.60201900	-1.34010100	0.87105200
C	3.87989600	0.19790700	-1.08579200
H	1.99516400	1.21644200	-1.31685300
C	3.94275600	-1.56634900	0.57203000
H	2.10428000	-1.93744800	1.63088600
C	4.57889800	-0.79934100	-0.40556200
H	4.37794900	0.79418200	-1.84425100
H	4.48972800	-2.34015900	1.10216500
H	5.62518700	-0.97869900	-0.63597500
N	-2.99794200	-0.63283500	0.70502000
C	-4.39847400	-0.97247100	0.63726900
H	-4.99195900	-0.24591400	1.20355700
H	-4.79344200	-0.98308700	-0.39965900
H	-4.62118500	-1.97548000	1.05562100
F	0.12459800	-0.07560700	2.14937400
H	-3.47773900	-3.15167700	-0.90801600
H	-1.28533800	-4.02812200	-1.75288300
C	-2.54154000	-2.65168100	-0.71521000
N	-1.34570000	-3.18402900	-1.19461900

TS16 (in THF solvent)

Sum of electronic and thermal Free Energies = -2041.896779 a.u.

P	0.88853800	0.10489900	-0.97555800
F	1.34283000	-0.08965700	-2.50906000

C	0.15661000	1.63506700	-0.76376500
C	-1.26665500	1.98818400	-0.66772000
C	-0.09738900	-1.36979200	-0.72794200
C	0.15919200	-2.20209800	0.36619200
C	-1.05318000	-1.72194900	-1.68753700
C	-0.55103700	-3.39379500	0.50023700
H	0.90655900	-1.92981200	1.10733200
C	-1.74714200	-2.91932300	-1.55095800
H	-1.25617200	-1.06518000	-2.52810300
C	-1.49606000	-3.75320200	-0.45951800
H	-0.35959200	-4.04069100	1.35106600
H	-2.48958300	-3.19766200	-2.29281300
H	-2.04406800	-4.68555700	-0.35519600
C	2.45184500	-0.03856000	-0.10837000
C	3.43479200	-0.89607000	-0.62083200
C	2.65450900	0.63017200	1.10427200
C	4.62593200	-1.06967300	0.07778100
H	3.27156600	-1.42237800	-1.55745800
C	3.85001300	0.44783200	1.79701500
H	1.88662300	1.28614400	1.50485000
C	4.83255300	-0.39857100	1.28441400
H	5.39167800	-1.72907300	-0.31936100
H	4.01073000	0.96672000	2.73713900
H	5.76286600	-0.53829700	1.82749600
N	-2.27740000	1.11830600	-0.69846500
C	-3.55784400	1.76238300	-0.52648600
H	-3.63103500	2.33797500	0.41974100
H	-3.78812700	2.47379800	-1.34157700
H	-4.35465300	1.01069800	-0.51733900
C	-2.24574400	-0.06797800	1.53228400
S	-3.41383400	-1.09118200	1.27612000
S	-1.10094800	0.73382000	2.26284600
C	-1.25973300	3.38489900	-0.48000800
H	-2.07062400	4.08913400	-0.37802700
C	0.91462500	2.81976600	-0.66318700
H	1.98383300	2.97830900	-0.69965700
H	0.33119500	4.79581800	-0.41233400
N	0.05455300	3.82419900	-0.50003700

16p (in THF solvent)

Sum of electronic and thermal Free Energies = -2041.975554 a.u.

P	0.67330000	0.08070300	-0.55807600
F	1.29854600	0.00209900	-2.14117800
C	-0.33134200	1.48027100	-0.97113800

C	-1.62022900	1.77561500	-0.42526100
C	-0.10801500	-1.55243600	-0.73324900
C	0.15647100	-2.60364100	0.14860200
C	-1.00415200	-1.72710200	-1.79177800
C	-0.46745100	-3.83439000	-0.04071400
H	0.83918800	-2.46386300	0.98239200
C	-1.64818500	-2.95300900	-1.95658400
H	-1.20419400	-0.91071800	-2.48176700
C	-1.37587500	-4.00734000	-1.08619000
H	-0.25330700	-4.65407600	0.63872200
H	-2.35760400	-3.08246000	-2.76878600
H	-1.87344800	-4.96376200	-1.21944000
C	2.36494000	0.20758100	0.10228400
C	3.26008900	-0.83631000	-0.15183300
C	2.77739500	1.33758500	0.81297900
C	4.56471400	-0.75674200	0.33167800
H	2.94475200	-1.70622000	-0.72248900
C	4.09163100	1.41974100	1.27038500
H	2.08274800	2.15142200	1.00427600
C	4.98154000	0.37086000	1.03922600
H	5.25619200	-1.57368400	0.14724100
H	4.41573400	2.30281700	1.81316300
H	6.00131900	0.43351300	1.40809000
N	-2.36758100	0.99115700	0.48169000
C	-3.82560700	1.05993000	0.34738400
H	-4.24312200	1.79649300	1.04201000
H	-4.06238500	1.33610200	-0.67948300
H	-4.25400100	0.08360400	0.57297500
C	-1.81784100	0.33839300	1.53376200
S	-2.74736000	-0.36033800	2.74764200
S	-0.06561900	0.27784100	1.66854400
C	-2.06174600	2.93301500	-1.02897900
H	-2.98524600	3.48258700	-0.92057300
C	-0.04101800	2.47434800	-1.88972300
H	0.83120300	2.61871800	-2.51051300
H	-1.13459300	4.17515800	-2.46864600
N	-1.08297800	3.33836600	-1.89876200

CO_2 (in THF solvent)

Sum of electronic and thermal Free Energies = -188.526583 a.u.

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.16280200
O	0.00000000	0.00000000	-1.16280200

TS4-CO_2 (in THF solvent)

Sum of electronic and thermal Free Energies = -1396.025651 a.u.

P	-0.57536100	-0.11237700	-0.91799700
C	0.25486700	-1.56602500	-0.69755800
C	1.59360600	-1.84989200	-0.21395500
C	0.38728300	1.37481000	-0.67876100
C	1.51299400	1.57954700	-1.48521500
C	-0.00742800	2.33660200	0.25625800
C	2.24973800	2.75046300	-1.34522300
H	1.81642500	0.82315600	-2.20405600
C	0.74013200	3.50553400	0.39179500
H	-0.88345500	2.17577500	0.87918500
C	1.86458800	3.71046500	-0.40661100
H	3.12754600	2.91180400	-1.96350900
H	0.44164400	4.25341400	1.12016200
H	2.44526200	4.62215400	-0.29791100
C	-2.18318500	-0.03322400	-0.11919000
C	-2.40425200	-0.80530500	1.02615400
C	-3.18026500	0.82309000	-0.60603900
C	-3.63211400	-0.72485500	1.68119700
H	-1.61979500	-1.45888300	1.39888700
C	-4.40068800	0.90131000	0.05824500
H	-3.00304700	1.42259100	-1.49511300
C	-4.62532900	0.12707700	1.19897600
H	-3.81054200	-1.32532400	2.56809500
H	-5.17659000	1.56344200	-0.31426800
H	-5.57990700	0.18987500	1.71372600
N	2.47063700	-0.96516600	0.20970200
C	3.73588900	-1.52082700	0.64665000
H	3.62985600	-2.21081100	1.50339800
H	4.25171800	-2.07669500	-0.15340700
H	4.39497600	-0.70595800	0.96092900
C	1.74072500	0.30798100	2.02237900
O	0.63859000	-0.09095900	2.10709700
O	2.74492400	0.87670800	2.22886200
F	-1.04840000	0.04414500	-2.46757500
C	0.48925800	-3.80484700	-0.68651900
H	0.19391200	-4.83378800	-0.85164900
C	1.68836600	-3.30152600	-0.24902700
H	2.54762700	-3.88807100	0.04403500
N	-0.39499600	-2.80617400	-0.91522600
H	-1.25232600	-2.92321800	-1.44070500

4-CO_2p (in THF solvent)

Sum of electronic and thermal Free Energies = -1396.096407 a.u.

P	-0.29422900	-0.04417900	-0.43858200
C	1.12581300	-0.92259600	-0.99664100
C	2.26337900	-1.19995600	-0.24471700
C	-0.21492700	1.76471100	-0.21793000
C	0.21502900	2.57341700	-1.27587100
C	-0.56430600	2.34618700	1.00589500
C	0.30223500	3.95396300	-1.10608500
H	0.48843900	2.12743400	-2.22724900
C	-0.50305800	3.73007500	1.16040200
H	-0.88286400	1.72128800	1.83442800
C	-0.06393200	4.53397900	0.10851600
H	0.65107200	4.57557100	-1.92573300
H	-0.78900700	4.17732000	2.10799800
H	-0.00463900	5.61129100	0.23612300
C	-1.88461000	-0.84041200	-0.04731400
C	-1.92669500	-2.06068400	0.63062800
C	-3.06989300	-0.22401500	-0.45785700
C	-3.15457200	-2.66804000	0.88777000
H	-1.00572500	-2.53520700	0.95699400
C	-4.29679500	-0.82119400	-0.17295300
H	-3.03718900	0.72243900	-0.99116000
C	-4.33944100	-2.04591900	0.49340600
H	-3.18452500	-3.62288200	1.40460500
H	-5.21729700	-0.33154500	-0.47749800
H	-5.29584400	-2.51538500	0.70622000
N	2.43477600	-0.88427000	1.09894800
C	3.74523000	-1.08780200	1.69782300
H	3.99998700	-2.15280000	1.70230400
H	4.50294900	-0.53744600	1.13199300
H	3.71595500	-0.71927900	2.72092400
C	1.38651600	-0.41769900	1.86274200
O	0.20727000	-0.34130900	1.24803100
O	1.50335500	-0.14181100	3.04491500
F	-0.79655000	0.14229700	-2.06515600
C	2.62967000	-1.85529500	-2.36012300
H	3.01448300	-2.24894700	-3.29052600
C	3.21833400	-1.79418000	-1.10564200
H	4.21260900	-2.13159100	-0.84948400
N	1.39211100	-1.32158400	-2.28980800
H	0.73291300	-1.23953900	-3.05464400

TS10-CO_2 (in THF solvent)

Sum of electronic and thermal Free Energies = -1396.043916 a.u.

P	-0.57988800	-0.18132700	-0.89560300
C	0.31639000	-1.59057900	-0.63997500
C	-0.19416900	-2.92604800	-0.92014900
C	1.68649300	-1.72813300	-0.19441700
H	-1.18691800	-3.16903900	-1.27703900
C	0.25874200	1.38727500	-0.67262300
C	1.33959500	1.69156700	-1.50899800
C	-0.18556700	2.30855900	0.28060100
C	1.97986700	2.91975800	-1.38151000
H	1.68234700	0.97026200	-2.24635700
C	0.46646600	3.53449400	0.40567500
H	-1.02623300	2.07170800	0.92727100
C	1.54551800	3.83822000	-0.42333000
H	2.82112600	3.15816200	-2.02524200
H	0.12846200	4.24980400	1.14941600
H	2.05146200	4.79434500	-0.32330500
C	-2.19713100	-0.17221600	-0.11386900
C	-2.40767100	-0.94889100	1.02957700
C	-3.21919200	0.64232900	-0.62047300
C	-3.64984800	-0.91727200	1.66203000
H	-1.60547300	-1.57083500	1.41776900
C	-4.45469200	0.67014300	0.01900400
H	-3.04985200	1.24786800	-1.50717600
C	-4.66875900	-0.10988100	1.15799600
H	-3.81942800	-1.52243200	2.54749400
H	-5.25070600	1.29745800	-0.37098600
H	-5.63519600	-0.08679400	1.65357300
N	2.51393900	-0.80780300	0.23772400
C	3.83678100	-1.27437900	0.59935600
H	3.82656600	-1.99772700	1.43517200
H	4.35946900	-1.75526300	-0.24412000
H	4.44046300	-0.41998600	0.91683000
C	1.75720700	0.41724300	2.00151700
O	0.67195200	-0.02203800	2.11986300
O	2.73075500	1.04413900	2.19617300
F	-1.02861600	-0.08255300	-2.45181700
C	0.81684100	-3.79790100	-0.69267000
H	0.85904100	-4.87212900	-0.80548100
N	1.93865200	-3.08649200	-0.26873600
H	2.80971500	-3.51499100	0.01493200

10-CO_2p (in THF solvent)

Sum of electronic and thermal Free Energies = -1396.097131 a.u.

P	-0.32296500	-0.04912000	-0.48489900

C	1.04928900	-1.00825500	-1.03019400
C	1.36718200	-1.53107500	-2.32931600
C	2.15101400	-1.25971500	-0.21809200
H	0.72829700	-1.50167800	-3.20027000
C	-0.12701800	1.75166000	-0.25820300
C	0.39612600	2.51597400	-1.30727000
C	-0.47954900	2.37070700	0.94576400
C	0.57448700	3.88897300	-1.14740500
H	0.66930600	2.04006400	-2.24454500
C	-0.32647400	3.74885700	1.08968500
H	-0.87221400	1.77920100	1.76708800
C	0.20670200	4.50750900	0.04768300
H	0.99465600	4.47505700	-1.95974900
H	-0.61512500	4.22653900	2.02155300
H	0.33704400	5.57952700	0.16732600
C	-1.94757200	-0.75732200	-0.06363900
C	-2.04682700	-1.97981400	0.60416400
C	-3.10338400	-0.07193300	-0.44733900
C	-3.30201400	-2.51988000	0.87839900
H	-1.14824000	-2.50871100	0.90872900
C	-4.35700600	-0.60206800	-0.14540800
H	-3.02767600	0.87529200	-0.97481100
C	-4.45703700	-1.82861900	0.51099200
H	-3.37663300	-3.47689700	1.38674300
H	-5.25372200	-0.05926000	-0.43031500
H	-5.43449900	-2.24606800	0.73621000
N	2.36620500	-0.90168400	1.09830500
C	3.67784400	-1.10803600	1.69677700
H	3.90652600	-2.17706200	1.76866000
H	4.44563400	-0.60460600	1.10149000
H	3.66130500	-0.68013200	2.69668700
C	1.31149500	-0.41803600	1.86409800
O	0.14479400	-0.34524000	1.25064200
O	1.45375100	-0.13068500	3.03998700
F	-0.83594600	0.17535400	-2.08794400
C	2.61379400	-2.08304600	-2.25129400
H	3.21997000	-2.59203200	-2.98603900
N	3.08337500	-1.90511400	-0.95911800
H	3.99163900	-2.21092100	-0.62951900

TS16-CO_2 (in THF solvent)

Sum of electronic and thermal Free Energies = -1396.014073 a.u.

P	0.51131800	-0.01921400	-1.11531500
C	-0.19566900	1.54693200	-1.05043400

C	-0.60454100	2.15238900	0.20949100
C	-0.63478900	-1.36445400	-0.85122900
C	-2.00538600	-1.11331700	-0.98150300
C	-0.16704000	-2.65302800	-0.55728200
C	-2.91210600	-2.15576400	-0.80506700
H	-2.35683800	-0.10822000	-1.20123400
C	-1.08034800	-3.68828800	-0.39044000
H	0.89794800	-2.84634000	-0.45747800
C	-2.44945200	-3.43764600	-0.50873400
H	-3.97729100	-1.96380400	-0.89148400
H	-0.72623200	-4.68859600	-0.16086200
H	-3.15933200	-4.24760200	-0.36675900
C	1.99715800	-0.27933700	-0.15070600
C	1.89506100	-0.66999700	1.19037700
C	3.24469900	-0.05136900	-0.74265900
C	3.05911300	-0.84206400	1.93509500
H	0.91836000	-0.81555500	1.64427000
C	4.40062800	-0.22806100	0.01417400
H	3.31782400	0.25870000	-1.78127400
C	4.30662800	-0.62338000	1.34885600
H	2.98984100	-1.14295900	2.97609600
H	5.37214700	-0.05729200	-0.43964300
H	5.21047500	-0.75962100	1.93599400
N	-0.48484100	1.52589100	1.39504200
C	-0.85392500	2.38566200	2.49615600
H	-0.73946000	1.84964500	3.44713000
H	-0.22656200	3.29633200	2.55650900
H	-1.90416600	2.73857900	2.44109400
C	-2.11491700	-0.15692000	1.91394100
O	-1.38836800	-0.96391700	2.35857300
O	-3.06913200	0.43703100	1.57993100
C	-1.07830000	3.42338400	-0.15886200
H	-1.46746300	4.23810800	0.43225900
C	-0.43297700	2.44581000	-2.09378200
H	-0.25910200	2.35834100	-3.15705100
N	-0.95277900	3.54904400	-1.53983700
H	-1.22333700	4.37171000	-2.06539300
F	1.01597100	-0.18288800	-2.62014000

16-CO_2p (in THF solvent)

Sum of electronic and thermal Free Energies = -1396.095601 a.u.

P	-0.32297500	0.04951900	-0.45657400
C	1.01367200	1.07347500	-0.99086900
C	2.15024600	1.37354600	-0.17937800

C	-1.97564500	0.68491900	-0.02761600
C	-2.12261700	1.88409400	0.67325800
C	-3.10368400	-0.03251500	-0.43503900
C	-3.39822300	2.36990400	0.95496900
H	-1.24537300	2.43616300	0.99790200
C	-4.37715300	0.44210300	-0.12426600
H	-2.99040200	-0.96157000	-0.98744600
C	-4.52523500	1.64637900	0.56370900
H	-3.51028800	3.30952700	1.48832200
H	-5.25208500	-0.12596900	-0.42704000
H	-5.51844400	2.02092900	0.79534900
C	-0.04312400	-1.74552800	-0.29290900
C	-0.34972100	-2.41083500	0.89903500
C	0.49112400	-2.45873500	-1.37175700
C	-0.14029100	-3.78520900	1.00140700
H	-0.74909500	-1.85713200	1.74316900
C	0.72672800	-3.82717900	-1.25326100
H	0.72863700	-1.94634700	-2.29932500
C	0.40409800	-4.49262500	-0.07027200
H	-0.39340600	-4.29944800	1.92408300
H	1.15641900	-4.37343400	-2.08803800
H	0.57901400	-5.56142000	0.01675300
N	2.35695200	0.90423700	1.11739600
C	3.66134300	1.11690700	1.72107000
H	3.69548400	0.58915900	2.67189600
H	4.43888700	0.72805000	1.05654700
H	3.83632900	2.18558300	1.89298700
C	1.32310500	0.38083800	1.86234400
O	1.46444700	0.02825800	3.02249800
O	0.13667500	0.32986800	1.25986200
C	3.01449700	2.13305300	-0.93641600
H	3.98460000	2.55129100	-0.71428400
C	1.23294900	1.66453300	-2.22748800
H	0.61838300	1.67673600	-3.11538500
N	2.42298000	2.29768500	-2.17143300
H	2.82906000	2.82869300	-2.93296200
F	-0.83600200	-0.14720100	-2.07262900

17NMe$_2$.closed

Sum of electronic and thermal Free Energies = -1225.991451 a.u.

P	-0.00276600	-0.17637900	0.31205900
C	0.87040000	-1.80885700	0.52762200
C	1.06367300	-2.01400000	-0.90152800
C	1.80725100	-3.12451500	-1.12962300

H	2.13389100	-3.54836600	-2.07015200
C	-1.79678600	0.00568600	-0.11036300
C	-2.58311400	0.97469600	0.52982300
C	-2.39336600	-0.81389500	-1.07429400
C	-3.92094400	1.14406600	0.18325100
H	-2.14769400	1.57299200	1.32314100
C	-3.74131100	-0.66210400	-1.39906900
H	-1.79885000	-1.57544500	-1.56696000
C	-4.50500700	0.32523100	-0.78253200
H	-4.51060200	1.90951300	0.67953000
H	-4.19003400	-1.31698100	-2.14026000
H	-5.55144900	0.45149500	-1.04538500
C	1.00340200	1.31197100	-0.08657600
C	2.27237000	1.15476300	-0.65234900
C	0.52226900	2.59695300	0.17448600
C	3.05518200	2.27084400	-0.93998000
H	2.64990300	0.15701100	-0.86512300
C	1.29397000	3.71373700	-0.14346500
H	-0.45167900	2.72818900	0.63435200
C	2.56398300	3.55270400	-0.69425500
H	4.04605500	2.13780700	-1.36437900
H	0.90397900	4.70931700	0.04760400
H	3.16914000	4.42289800	-0.93156300
N	0.40005500	-0.93472300	-1.40299200
C	0.42483000	-0.47030100	-2.75950700
H	-0.05168100	-1.18848100	-3.44354300
H	-0.12680100	0.47414600	-2.82420400
H	1.45142000	-0.28861600	-3.11553200
H	1.52435500	-2.91564300	2.30716700
C	1.46819800	-2.78112500	1.23243900
N	-0.23621900	0.27559600	2.02734900
C	-1.04578200	-0.68001400	2.77911900
H	-0.50075200	-1.61573900	2.99092500
H	-1.33553500	-0.23480900	3.73863600
H	-1.95961500	-0.93908800	2.23943800
C	0.98823000	0.53669500	2.77850500
H	1.57959100	1.32729100	2.31366600
H	0.71921800	0.86733900	3.78851600
H	1.62553900	-0.35987000	2.87693000
C	2.11899000	-3.72765700	0.23257800
H	1.71893200	-4.74583100	0.35532100
H	3.19868300	-3.79883200	0.43479900

TS17NMe$_2$'

Sum of electronic and thermal Free Energies = -1225.984789 a.u.

P	-0.11256400	-0.05546300	0.48813400
C	0.80456000	-1.59449300	0.58269200
C	1.23338500	-1.95893400	-0.77023000
C	2.12192700	-3.00451800	-0.65727200
H	2.63863300	-3.52418600	-1.45362500
C	-1.81608600	-0.06683100	-0.17149100
C	-2.73513800	0.84834000	0.36212300
C	-2.22495400	-0.96107000	-1.16517800
C	-4.04367300	0.88206000	-0.11254500
H	-2.43000200	1.51852500	1.16053400
C	-3.54327100	-0.93550100	-1.61708700
H	-1.49000300	-1.63862700	-1.58777400
C	-4.45049700	-0.01234900	-1.10150900
H	-4.74543500	1.60201600	0.29800400
H	-3.85634300	-1.63693300	-2.38461800
H	-5.47335900	0.00964100	-1.46669000
C	0.89791200	1.32791700	-0.10753500
C	2.24441600	1.13803000	-0.43298100
C	0.32749900	2.59892100	-0.17576800
C	3.01577800	2.23002800	-0.81644200
H	2.67723300	0.14072200	-0.40478300
C	1.10351500	3.68640200	-0.57907800
H	-0.71824800	2.74670000	0.07938000
C	2.44719100	3.50352100	-0.89366400
H	4.06156000	2.08386700	-1.06935600
H	0.65458600	4.67296300	-0.64460000
H	3.05214100	4.35020200	-1.20469400
N	0.66123400	-1.12541700	-1.64650900
C	1.12191000	-1.17959500	-3.00658300
H	0.95974300	-2.17078300	-3.46850700
H	0.59040600	-0.43835600	-3.61355500
H	2.20595200	-0.96809700	-3.08942600
H	1.24647400	-2.32783900	2.60219600
C	1.35584200	-2.37858600	1.52421400
N	-0.42796000	0.44417500	2.10093900
C	-1.26875600	-0.44532400	2.90494200
H	-0.68420200	-1.24614200	3.37991900
H	-1.75256700	0.14154900	3.69421600
H	-2.04894900	-0.90547400	2.29532300
C	0.68607800	0.96362300	2.89419100
H	1.23794700	1.72358400	2.33970200
H	0.27394000	1.42915300	3.79583500
H	1.38624400	0.17237000	3.20296600

C	2.23923600	-3.37919000	0.80532900
H	1.90519200	-4.40484400	1.03352500
H	3.26334800	-3.30408000	1.20624000

17NMe$_2$.open

Sum of electronic and thermal Free Energies = -1225.994766 a.u.

P	0.12727400	-0.09101100	0.32857500
C	-0.02428000	1.63915400	-0.16686300
C	-1.25311500	2.13346700	-0.62222300
C	1.09362600	2.47879300	-0.07353100
C	-1.34740300	3.47402400	-0.99100100
H	-2.11672600	1.46637100	-0.63268900
C	0.98149500	3.81801100	-0.43698200
H	2.04677500	2.09176100	0.27724300
C	-0.23785300	4.31328200	-0.89931900
H	-2.29666200	3.86321300	-1.34655400
H	1.84581300	4.47094500	-0.36328000
H	-0.32184700	5.35727800	-1.18778600
C	1.86960600	-0.53319900	0.08387500
C	2.42074300	-0.46830500	-1.20273900
C	2.66301600	-0.92237500	1.16432000
C	3.75575400	-0.80429000	-1.40349900
H	1.80939700	-0.14351700	-2.04202700
C	4.00018200	-1.26240800	0.95704100
H	2.23376900	-0.94410000	2.16210500
C	4.54452300	-1.20598600	-0.32366300
H	4.18180900	-0.75035100	-2.40070100
H	4.61551700	-1.56665200	1.79828000
H	5.58615400	-1.46884700	-0.48277100
N	-2.87750900	-0.35341100	0.34657700
C	-4.30786300	-0.50008200	0.43958000
H	-4.81680500	-0.35534700	-0.53422800
H	-4.60778800	-1.50819800	0.79000800
H	-4.72017400	0.23327700	1.14271600
N	-0.17575900	-0.23677600	1.96671400
C	-0.98277900	0.78962000	2.64368600
H	-2.03928600	0.67573700	2.37372400
H	-0.83558000	0.65878100	3.72021100
H	-0.63419800	1.78682000	2.36935100
C	-0.55002500	-1.59341500	2.39640000
H	0.06494400	-2.34161900	1.88747900
H	-0.36802400	-1.67100100	3.47286700
H	-1.60833700	-1.78343800	2.17382100
C	-2.32926000	-1.23465800	-0.49121700

C	-0.84653100	-1.21062600	-0.65420000
C	-0.41852900	-2.17508300	-1.49219400
H	0.60745100	-2.40841900	-1.75854100
H	-3.80764700	-2.57008300	-1.43380700
C	-2.77802900	-2.26356000	-1.30457900
C	-1.62034700	-2.92701700	-1.99761600
H	-1.65245000	-2.87077300	-3.09892400
H	-1.49995000	-3.99743200	-1.75982800

TS17NMe$_2$

Sum of electronic and thermal Free Energies = -2060.385057 a.u.

P	0.86434000	-0.09643600	0.52290100
C	0.12982500	-1.56968900	-0.15289500
C	0.83900000	-2.54301700	-0.76263500
C	-1.26517000	-2.00907000	0.12565600
H	1.88464800	-2.51350100	-1.04818000
C	-1.35115600	-3.30564200	-0.32561600
H	-2.23168100	-3.93362500	-0.28645400
C	0.11982300	1.52107000	0.18550000
C	-1.12568700	1.80699200	0.75941800
C	0.81420300	2.51310900	-0.51878300
C	-1.67783700	3.07486800	0.60346800
H	-1.66858400	1.01426100	1.27189200
C	0.24804200	3.77569800	-0.67373300
H	1.79310200	2.31662500	-0.94251900
C	-0.99719400	4.05667700	-0.11444200
H	-2.65654100	3.28207300	1.02506600
H	0.78384100	4.53881400	-1.22998700
H	-1.43845700	5.04102200	-0.24084200
C	2.55068300	-0.03601500	-0.14332800
C	2.74170700	0.05080200	-1.52935500
C	3.65093200	-0.10946500	0.71120100
C	4.03162500	0.07448000	-2.04985500
H	1.88234700	0.09046600	-2.19670000
C	4.94269000	-0.08055300	0.18430400
H	3.49412400	-0.20517200	1.78225100
C	5.13214900	0.01300300	-1.19218100
H	4.17854400	0.13756200	-3.12370100
H	5.79835700	-0.13765900	0.85011700
H	6.13799500	0.03190500	-1.60111200
N	-2.12802300	-1.15439300	0.70563600
C	-3.33644000	-1.80981900	1.15535100
H	-3.89207300	-2.30924100	0.34111500
H	-3.10784800	-2.57938700	1.91307500

H	-4.00880500	-1.07624500	1.60866700
N	0.96037300	-0.28258200	2.17740000
C	1.17260400	0.90886200	2.99843900
H	0.21995700	1.34977300	3.32102500
H	1.75243900	0.62406500	3.88282700
H	1.73381700	1.66833000	2.44739100
C	0.27490400	-1.36917700	2.88601800
H	0.24652500	-2.27113100	2.27425100
H	0.84135500	-1.58082100	3.79871600
H	-0.75508200	-1.08917400	3.13520600
C	-2.95938700	0.10280100	-1.06908500
S	-4.24049600	0.79285100	-0.42783600
S	-1.96629100	-0.18707800	-2.27669600
C	-0.05610400	-3.73233700	-0.94924100
H	0.40511800	-4.61729100	-0.48268900
H	-0.15132800	-3.97010900	-2.02089300

17NMe$_2$p

Sum of electronic and thermal Free Energies = -2060.432547 a.u.

P	0.69097200	-0.04790100	0.49093200
C	-0.15324200	-1.63246600	0.67502500
C	0.43627400	-2.69322000	1.26334000
C	-1.48274500	-2.05342600	0.15701600
H	1.39978100	-2.68841500	1.75885100
C	-1.67201300	-3.35204700	0.46920100
H	-2.54871400	-3.93953400	0.22551200
C	-0.30154300	1.46438600	0.60713300
C	-1.60257800	1.40907300	1.11952300
C	0.28037700	2.70721100	0.32987500
C	-2.32946800	2.58347200	1.30003900
H	-2.05782300	0.45442200	1.36691400
C	-0.45332700	3.87591400	0.51536300
H	1.30290500	2.77190300	-0.03106700
C	-1.76168800	3.81683600	0.99156500
H	-3.34673800	2.52799000	1.67534900
H	0.00126400	4.83445000	0.28371700
H	-2.33511300	4.72914500	1.12374200
C	2.20096000	-0.02073400	-0.53563100
C	2.37863700	0.86233900	-1.60601700
C	3.20883800	-0.93815000	-0.21910900
C	3.56106400	0.82969500	-2.34168200
H	1.58681500	1.54768500	-1.88984700
C	4.37723600	-0.98174800	-0.97508200
H	3.08658500	-1.60690600	0.62701300

C	4.55879500	-0.09293000	-2.03298000
H	3.69085700	1.51884800	-3.17039200
H	5.14760100	-1.70693400	-0.73071400
H	5.47280300	-0.12273600	-2.61858900
N	-2.42699800	-1.20302100	-0.44307900
C	-3.82938700	-1.40045600	-0.08225700
H	-4.36124700	-1.95918100	-0.86030900
H	-3.86876200	-1.94120600	0.86392400
H	-4.31411800	-0.42683900	0.01504800
N	1.48343900	-0.02698500	2.05286900
C	2.48461100	1.01732900	2.28174800
H	2.01888900	2.00306700	2.44504300
H	3.05374200	0.75844500	3.18157600
H	3.18424100	1.09256800	1.44864100
C	0.59926700	-0.07707300	3.21995000
H	-0.18871900	-0.81988700	3.08996100
H	1.19328100	-0.35822800	4.09695900
H	0.13088100	0.90036100	3.41880700
C	-2.09792700	-0.34938400	-1.47786500
S	-3.26817700	0.54546800	-2.25513500
S	-0.41615000	-0.28124200	-1.91645900
C	-0.46487200	-3.88749100	1.17477200
H	-0.68710700	-4.28299000	2.17616300
H	0.00463700	-4.70784400	0.61311800

17OMe.closed

Sum of electronic and thermal Free Energies = -1206.624342 a.u.

P	0.06119200	-0.22866800	0.37182400
C	1.14893600	-1.70902900	0.45980000
C	1.32836900	-1.78365800	-0.98068300
C	2.25313200	-2.72033400	-1.29662800
H	2.63717600	-3.00754600	-2.26658600
C	-1.74854600	-0.17142900	0.06731500
C	-2.51514200	0.75925800	0.78117000
C	-2.37219200	-1.01058500	-0.85916300
C	-3.88438800	0.86214900	0.55197100
H	-2.02871100	1.39903300	1.51296200
C	-3.74971400	-0.92663400	-1.06374800
H	-1.77212100	-1.72366700	-1.41649100
C	-4.50460300	0.01404700	-0.36654800
H	-4.46886700	1.59834000	1.09610600
H	-4.22970800	-1.59263300	-1.77485900
H	-5.57508600	0.08681300	-0.53647600
C	0.86170100	1.38982600	0.14623600

C	2.03205900	1.68803800	0.84806300
C	0.33798400	2.31638500	-0.75849200
C	2.68132300	2.90181500	0.63334300
H	2.42419000	0.97355000	1.56629700
C	0.97943300	3.53791700	-0.95590000
H	-0.57924900	2.09308100	-1.29883200
C	2.15509500	3.82884800	-0.26569500
H	3.59452900	3.12756200	1.17627100
H	0.56035000	4.26059800	-1.65001200
H	2.65803700	4.77827300	-0.42490000
N	0.44645800	-0.81813400	-1.39101300
C	0.38537300	-0.25865100	-2.71386800
H	0.50932200	-1.05313800	-3.46032200
H	-0.59428900	0.20562500	-2.87801000
H	1.16147300	0.50342300	-2.88659100
H	2.04809300	-2.76759100	2.15601200
C	1.93607400	-2.58965800	1.09186100
O	-0.06715300	0.04928800	2.05609900
C	-0.65926800	-0.94019000	2.86897700
H	-0.33373500	-1.95060400	2.58558100
H	-0.35532700	-0.74825600	3.90120500
H	-1.75548000	-0.90181000	2.80719900
C	2.71455200	-3.33628800	0.01741800
H	2.51773500	-4.41722200	0.08211200
H	3.79474300	-3.21214500	0.18770500

TS17OMe'

Sum of electronic and thermal Free Energies = -1206.610376 a.u.

P	0.10576800	-0.05365500	0.65719500
C	-0.83342600	-1.55821500	0.62987600
C	-1.17347300	-1.97144400	-0.73908000
C	-1.96980000	-3.09498000	-0.62726100
H	-2.38532100	-3.68546900	-1.43326400
C	-0.79230700	1.37215800	0.01669700
C	-0.16880800	2.61956300	0.10273500
C	-2.10363500	1.25932200	-0.45316600
C	-0.85832700	3.76418400	-0.29496400
H	0.85233700	2.69653100	0.47135400
C	-2.78906800	2.40915800	-0.83418900
H	-2.56362100	0.27900800	-0.54514900
C	-2.16768300	3.65728600	-0.75966600
H	-0.37256100	4.73373000	-0.24228300
H	-3.80645600	2.32888300	-1.20444000
H	-2.70556500	4.54848500	-1.06981400

C	1.82207400	-0.08769600	0.09988500
C	2.84013300	-0.16986200	1.05672700
C	2.13070200	0.00700200	-1.26169100
C	4.17143000	-0.16816300	0.64544600
H	2.59431500	-0.23055100	2.11123400
C	3.46487200	0.02474800	-1.65756200
H	1.31870400	0.03225000	-1.98075000
C	4.48337000	-0.06846500	-0.70881100
H	4.96217900	-0.24193500	1.38577900
H	3.70820400	0.09963700	-2.71295100
H	5.52221000	-0.06504600	-1.02632700
N	-0.63569200	-1.16349100	-1.65574700
C	-0.96295100	-1.48755300	-3.01864800
H	-2.05169600	-1.43191800	-3.21419300
H	-0.47026900	-0.78974300	-3.70694600
H	-0.64760300	-2.51073900	-3.29631400
H	-1.21803800	-2.32687000	2.64145400
C	-1.33056700	-2.38608100	1.56351700
O	0.33820700	0.30755600	2.23019700
C	-0.76857600	0.74449900	3.02567500
H	-1.65237400	0.12309000	2.85156500
H	-0.45117400	0.65291700	4.06456600
H	-1.00395300	1.78786800	2.79631500
C	-2.10285800	-3.46232300	0.83280000
H	-3.14035000	-3.48191300	1.20544300
H	-1.67791100	-4.44822700	1.08553300

17OMe.open

Sum of electronic and thermal Free Energies = -1206.614520 a.u.

P	0.16154000	-0.13081000	0.49565300
C	-0.26275900	1.50715400	-0.11535400
C	-1.39300100	1.71885400	-0.91113000
C	0.58712500	2.57051500	0.21863300
C	-1.66098800	3.00533600	-1.37708500
H	-2.06732600	0.89283300	-1.11774900
C	0.30189000	3.85205000	-0.24051800
H	1.47001500	2.39460200	0.83012500
C	-0.82151900	4.06586800	-1.04149100
H	-2.53677400	3.17792800	-1.99476100
H	0.95506600	4.67914500	0.01994000
H	-1.04205400	5.06586100	-1.40395600
C	1.91988900	-0.38334600	0.17964600
C	2.44104000	-0.07063100	-1.08099900
C	2.74133600	-0.93642100	1.16511700

C	3.78402600	-0.31476000	-1.35328400
H	1.80041300	0.36600300	-1.84418500
C	4.08612400	-1.17518800	0.88620700
H	2.32866700	-1.17138800	2.14124000
C	4.60555500	-0.86674500	-0.36966100
H	4.18929700	-0.07125900	-2.33052600
H	4.72676900	-1.60258800	1.65141800
H	5.65361300	-1.05450200	-0.58347700
N	-2.81456800	-0.63224700	0.60953000
C	-4.24451300	-0.80246400	0.64858400
H	-4.71145100	-0.69215200	-0.35103000
H	-4.54270100	-1.80452900	1.01397200
H	-4.69832000	-0.05650800	1.31128600
C	-0.97663900	0.41488900	2.86348900
H	-1.91970700	-0.01100500	2.51232600
H	-0.74697600	0.15670600	3.89669900
H	-0.97213200	1.50110200	2.73386100
C	-2.21314700	-1.52077300	-0.17990600
C	-0.73556700	-1.41946900	-0.31028400
C	-0.22742900	-2.37683600	-1.11153100
H	0.81619800	-2.53123800	-1.36862300
H	-3.59109200	-2.96340000	-1.11856200
C	-2.58591400	-2.58559700	-0.98560100
C	-1.37193200	-3.21548400	-1.61457100
H	-1.36859900	-3.20752300	-2.71758700
H	-1.20327900	-4.26719400	-1.32661200
O	0.11222300	-0.15184500	2.09039000

TS17OMe

Sum of electronic and thermal Free Energies = -2041.010020 a.u.

P	0.94884600	-0.08121800	0.51593700
C	0.30914800	-1.53507900	-0.26281500
C	0.94991100	-2.29030500	-1.17850000
C	-1.03209000	-2.08566300	0.06275200
H	1.94627500	-2.12844200	-1.57849200
C	-1.17606300	-3.21930300	-0.70802600
H	-2.02587700	-3.88921800	-0.70323300
C	0.14595800	1.40809600	-0.06521400
C	0.16346900	2.55339800	0.73952200
C	-0.44146300	1.43237200	-1.33156000
C	-0.43034100	3.72189200	0.27664900
H	0.62650000	2.52404600	1.72298500
C	-1.03300100	2.60791000	-1.78771100
H	-0.46835800	0.53219300	-1.94007700

C	-1.03226100	3.74509500	-0.98311100
H	-0.43749100	4.60938000	0.90160400
H	-1.51922100	2.62190700	-2.75802000
H	-1.51234500	4.65386900	-1.33354500
C	2.70850600	0.01878300	0.14037300
C	3.20234600	0.96388900	-0.76180200
C	3.57373500	-0.90288600	0.74361000
C	4.56437900	0.98604500	-1.06059700
H	2.53071700	1.68113200	-1.22611400
C	4.93160200	-0.87146900	0.44445700
H	3.18322700	-1.63504100	1.44546000
C	5.42562500	0.07156300	-0.45882200
H	4.94989300	1.72041600	-1.76093900
H	5.60453500	-1.58208900	0.91424600
H	6.48608800	0.09279600	-0.69192600
N	-1.78842300	-1.43002000	0.95282100
C	-2.93796000	-2.19729700	1.38338800
H	-3.59317400	-2.50346600	0.54726500
H	-2.62951100	-3.12433700	1.89726300
H	-3.53741500	-1.60224300	2.08104700
O	0.95820100	-0.10096800	2.10696000
C	-0.20224400	0.01484700	2.97237700
H	-0.57477800	-0.98427000	3.18777800
H	0.17173200	0.51767300	3.86570900
H	-0.99857400	0.58084400	2.48585500
C	-3.11365300	0.14782000	-0.24988900
S	-3.27638000	-0.57129100	-1.64736700
S	-3.33203100	1.25547600	0.86660100
C	0.04813600	-3.43501000	-1.55345300
H	0.56470000	-4.38941000	-1.36261400
H	-0.15411400	-3.41474100	-2.63623900

17OMep

Sum of electronic and thermal Free Energies = -2041.064109 a.u.

P	0.72840600	-0.12459100	0.53399800
C	-0.13294300	-1.69763200	0.60821000
C	-1.44993000	-2.00300100	0.00145100
C	-1.74694000	-3.29625900	0.24578600
H	-2.64791900	-3.81375800	-0.06034200
C	-0.32674100	1.33657600	0.75073700
C	0.02353300	2.56178300	0.17531900
C	-1.51725000	1.22063300	1.47366100
C	-0.80101500	3.66795500	0.34861800
H	0.91585100	2.63993600	-0.44008900

C	-2.34916600	2.32972800	1.62656600
H	-1.81266500	0.26467300	1.90160400
C	-1.98833400	3.55419800	1.07265500
H	-0.52848600	4.61519100	-0.10626200
H	-3.28178800	2.22936100	2.17377900
H	-2.63920400	4.41559800	1.18741800
C	2.38480100	0.03990400	-0.21105900
C	3.22522900	1.05509100	0.25627100
C	2.83370500	-0.84728900	-1.19121300
C	4.49822700	1.20438100	-0.28815100
H	2.88934500	1.71707400	1.04902000
C	4.12095800	-0.71230400	-1.70619800
H	2.18024600	-1.63593300	-1.55367700
C	4.94865200	0.31907700	-1.26623100
H	5.14189100	2.00552900	0.06257700
H	4.47080700	-1.40948200	-2.46134800
H	5.94537400	0.43092700	-1.68267200
N	-2.27531900	-1.04600300	-0.61484400
C	-3.71377800	-1.14382300	-0.37506800
H	-3.87223500	-1.76033200	0.51009400
H	-4.11666000	-0.14110600	-0.21630900
H	-4.22683800	-1.57935500	-1.23901800
H	1.30287500	-2.88835300	1.71088700
C	0.35742700	-2.81194300	1.18507300
O	1.42766300	-0.18400900	2.06702000
C	0.68959400	-0.17362600	3.27476800
H	-0.11583500	-0.91937000	3.26364100
H	1.39155100	-0.42387400	4.07332300
H	0.26216900	0.81676300	3.46664700
C	-0.61704400	-3.93797400	0.99584300
H	-0.92643900	-4.35232600	1.96588600
H	-0.17380600	-4.77036400	0.43080900
C	-1.80389500	-0.13996500	-1.53721600
S	-2.82590900	0.87833500	-2.35975700
S	-0.07339800	-0.12401700	-1.82256300